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Los Angeles

A Unified Numerical Model for Pool Boiling Curve with Parallel Computing

A dissertation submitted in partial satisfaction of the requirements for the degree Doctor of Philosophy in Mechanical Engineering

by

Deepak Garg

2017

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ABSTRACT OF THE DISSERTATION

A Unified Numerical Model for Pool Boiling Curve with Parallel Computing

by

Deepak Garg

Doctor of Philosophy in Mechanical Engineering University of California, Los Angeles, 2017 Professor Vijay K. Dhir, Chair

Boiling heat transfer research spans several decades with extensive data accumulation from several experiments. Several mechanistic models and empirical correlations have also been put forth but their applicability is limited to the narrow range of parameters over which they have been developed. For the past few decades several numerical methods have also been developed and gained considerable momentum to study boiling process. The most popular of these numerical methods are volume of fluid method, level set method and front tracking methods, however some other computational methods like Lattice Boltzmann, Moving particle semi-implicit gridless and cellular automata SIMPLER methods have also been developed. In the present study level set method is used to simulate the entire boiling curve in a temperature controlled mode spanning all the three regimes *viz*. nucleate, transition and film boiling with a unified numerical model supplemented with correlations specifying nucleation site density and bubble waiting time. In order to improve the performance of the code parallel computing has also been implemented. Both two-dimensional and three-dimensional simulations have been done for saturated water with different contact angles for a horizontal surface with uniform wall superheat applied to it. Temporal and spatial averaged wall heat flux and wall void fraction computed for a fixed wall superheat case are plotted and analyzed. For a specified contact angle and by incrementing the wall superheat as two independent input parameters, the entire boiling curve along with vapor removal patterns capturing its vital points like the maximum heat flux and minimum heat flux are shown.

The two-dimensional assumption yields opposite trend for the nucleate boiling regime heat flux variation with contact angle but this anomaly was not observed in the three-dimensional simulations which infers that the two-dimensional assumption is an incorrect representation to study the essential physics of the boiling process. The trend of critical heat flux with contact angle was found to be decreasing with increase in contact angle for both two-dimensional and three-dimensional case, with the trend being steeper for the former.

Wall void fraction was found to increase with increase in wall superheat as different regimes of boiling were traversed, and also with increase in contact angle at a given wall superheat. Mushroom type vapor bubbles are seen in the nucleate boiling regime with liquid macrolayer trapped underneath it while long column of sustained vapor is seen at the critical heat flux condition continuously being fed by nucleating cavities at the surface. Upon increasing the wall superheat beyond critical heat flux the negative slope of the boiling curve is captured characterized by the transition boiling regime with intermittent liquid solid contacts seen. Finally, the transition to film boiling is seen with entire surface covered with superheated vapor and wall void fraction reaching unity. Energy partitioning from wall into liquid, interface and microlayer has also been examined for the 3D cases. For the 3D coarse grid case it was found that, as the wall void fraction increases the percent energy going into liquid decreases from about 85% in lower nucleate boiling to 6% in film boiling while the microlayer contribution peaks around CHF to a value of about 45%. The energy partition from the fine grid cases were however inconclusive as they couldn't be run long enough to obtain any meaningful results.

The dissertation of Deepak Garg is approved.

Adrienne Lavine

Laurent Pilon

Tajendra V. Singh

Warren Mori

Vijay K. Dhir, Committee Chair

University of California, Los Angeles

2017

Dedicated to my wife, Neha Doshi Garg

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Nomenclature

А	matrix
Ar	Archimedes Number
C ₂	constant
F_L	fractional area occupied by liquid
g	gravitational acceleration, m/s ²
h	grid height
\overline{h}	average heat transfer coefficient, W/K
h_{fg} , h_{lv}	latent heat of vaporization, W/kg
Н	domain height, m, Heaviside function
Ι	interface
k	thermal conductivity, W/m-k
1	length,m
L	sub-matrix
р	pressure, N/m ²
q	heat flux,W/m ²
t	time, s
Т	temperature, K
'n	mass flux, kg/m ²
n	normal
М	matrix
Ν	number of cavities

Na	nucleation site density, sites/cm ²
Nu	Nusselt number
R_0	radial distance from the cavity center to the microlayer starting point, m
R_1	radial distance from the cavity center to the microlayer end point, m
u,v,w	velocity, m/s
V	volume, m ³
x,y,z	dimensionless length

Greek symbols

Δx	grid spacing in x direction
Δy	grid spacing in y direction
λ_{D}	Taylor's dangerous wavelength,m
τ	pseudo time
ρ	density, kg/m ³
Φ	level set function
δ_{T}	thermal layer thickness, m
δ	microlayer thickness, m
٤	distance, m
δ_0	initial microlayer thickness, m
φ	contact angle, °
β	constant, ratio of sensible heat to latent heat
β_{T}	coefficient of thermal expansion,1/K

α	thermal diffusivity, m ² /s, wall void fraction
σ	surface tension, N-m
μ	dynamic viscosity, Pa-s
Γ	interface
Ω	phase domain
E	element of
к	curvature
Λ	coefficient matrix
l	evaporation coefficient
ΔV_{micro}	Vapor side control volume near micro region

Subscripts

0	initial
atm	atmospheric
b	black
bub	bubble
col	columns
d	dry
e,w,n,s	east, west, north and south
eff	effective
ev	evaporation
f	phase

l,liq	liquid
n	old time step
n+1	new time step
nc	natural convection
0	characteristic
Р	principal cell
р	processor
r	red
sat	saturated
Т	thermal, transpose
int	interface
micro	microlayer
min	minimum
max	maximum
v,vap	vapor
wait	waiting
wall	wall
у	y direction
Х	X direction
zub	zuber
* **	dimensionless, intermediate value

Superscripts

- G ghost cell
- L user specified

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Vita

2006	Bachelors in Marine Engineering, Jadavpur University Kolkata, WB, India
2012	Masters in Mechanical Engineering, Purdue University West Lafayette, IN, USA
2015	Masters in Aerospace Engineering, UCLA Los Angeles, CA, USA

Publications

Deepak Garg, "Controlling Microbial Degradation of Diesel Engine Oil using Magnetic Field", *International Conference on Recent Advances of in Marine Antifouling Technology*, NIOT Chennai, pp. 400-408, November 2006

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1. Introduction

Boiling is a process of turning liquid at its saturation temperature into vapor by applying heat, similar to flashing where liquid is converted to vapor by reducing the pressure. Boiling heat transfer is a widespread phenomenon and has myriad applications ranging from cooking, power generation to industrial process control. Heat transfer by virtue of boiling is the preferred mode in both conventional and nuclear power plants as single phase methods including both natural convection and forced convection renders the technique incapable of meeting cooling requirements. Apart from that, boiling is also used to cool electronic components in power electronics industry and in refrigeration industry as well. Boiling heat transfer has significantly higher heat transfer coefficient than single phase heat transfer. Enhanced understanding of boiling process, in terms of all the dependent parameters and limitations, is essential for optimized technological applications.

An efficient control of the boiling process can be achieved by highly resolved experiments or by high fidelity numerical simulations achievable using high performance computing. Some of the physics behind boiling still remains to be elusive owing to the small length and time scales associated with the boiling process. For the past several decades numerous researchers have studied this process theoretically, experimentally and numerically. Analytical solutions exist only for simple problems like steady-state motion of bubbles and droplets in stokes flow and oscillations of bubbles and droplets. From the mathematical point of view of modeling of boiling, which is one form of multiphase flow, apart from non-linear nature of the governing equation and interacting sub-processes, accurate tracking of the phase boundary is also an elusive task.

Nukiyama (1934) published one of the most phenomenal work in boiling heat transfer by plotting the heat transferred to the boiling water over a large range of wall superheats. Nukiyama's boiling curve has never been disputed but the shape has been the subject of discussion especially with respect to transient or steady-state conditions. A typical boiling curve is shown in Figure 1 showing different boiling regimes obtained in a temperature controlled mode.

Initially, at low wall superheats heat transfer occurs only by natural convection. The wall superheat is higher than the saturation temperature of the liquid but not high enough to activate any nucleation site. Upon increasing the wall superheat the first of the bubbles nucleate at the surface and this point is called the onset of nucleate boiling (ONB). After the onset of boiling isolated bubbles grow and eventually detach the boiling surface without interacting with each other with increase in wall heat flux. Under high heat flux conditions vertical coalescence of the bubbles occurs forming vapor columns and the lateral coalescence of these vapor columns results in the formation of a vapor mass below which a liquid macrolayer is entrapped. The thickness of the macrolayer decreases with time while the vapor mass grows. As the size of the nucleating cavity varies inversely with wall superheat, as the wall superheat is increased more nucleation sites are activated augmenting bubble density. With the bubbles interacting with each other leading to further enhancement of heat flux occurs ultimately reaching up to a point where any further increase in wall superheat results in the decrease of wall heat flux, known as the point of critical heat flux (CHF). This region marked by the negative slope is known as the transition boiling regime and continues upto the point where a stable vapor film between the liquid and the wall is formed known as the film boiling, which corresponds to point c of Figure 1.

Typically an efficient cooling mechanism should operate in the nucleate boiling regime where high heat flux can be removed at moderate wall superheats. Minimization of the wall superheat is one of the optimal points of operation in power generation cycle or cooling device. In some instances like spray cooling and quenching process film boiling is used to achieve desired heat transfer rates. One of the most important aspect of boiling heat transfer is the 3-phase contact line. The local heat flux at the 3-phase contact line reaches a maximum value. It has been reported that during the advancing motion of the contact line there is an increase in the local heat transfer. However, the temporal and spatial resolution of the different measurement techniques like Thermochromic Liquid Crystals, High Speed Infra Red Thermography and Micro heater arrays, etc are still short of unraveling the microscale heat transfer mechanism in the vicinity of the 3-phase contact line.

Numerical simulations to study boiling offers promising avenue and several numerical methods have been developed for simulation of incompressible two phase flows with phase change. The past couple of decades have witnessed widespread implementation of different phase change models into a variety of novel and traditional computational schemes. Numerical modeling have improved considerably in terms of spatial and temporal resolution and capturing the physics across the interface thus increasing the overall accuracy. One classical approach is to employ moving mesh methods so that the interface coincides with the grid points. Although matching conditions at the interface in these methods are easy to implement yet they become very complicated for merging and breaking of interfaces but matching conditions at the interface gets difficult. Lagrangian based methods are not easy to implement for problems involving changes in interface

topology. Surface tension on the moving interface must be considered to account for capillary effects and other curvature related phenomenon. In the presence of interfacial tension, the algorithm should be able to obtain and follow an interface including merging and breaking. To treat surface tension effects the continuum surface force (CSF) model is widely used. The number of methods can be divided into different categories like front tracking (Juric and Tryggvason (1998), volume of fluid (Hirt and Nicolas, (1981)), level set method (Osher and Sethian (1988)), and hybrid methods (McKee *et al*, (2008)). Gibou *et al*.(2007) used level set method to capture the interface evolution using ghost fluid method. Discontinuity nature of material properties like density and viscosity are tracked and implemented using level set function.



Figure 1 A Typical Boiling Curve [Ref: Winterton, Richard, H.S., Thermopedia]

1.1 Nucleate Boiling

Point b in the Figure 1 corresponds to onset of nucleate boiling, and once nucleate boiling is initiated any increase in surface temperature causes an increase in wall heat flux. With an increase in wall superheat more and more sites participate in nucleation thus setting the stage for isolated bubble regime commonly called as partial nucleate boiling. Transient conduction into liquid adjacent to the surface is the most important mechanism for heat removal in this regime. Upon increasing the wall superheat further, the region c-e of the boiling curve is fully developed nucleate boiling where evaporation is the dominant mode of heat transfer. The early models of nucleate boiling were based on bubble growth and enhanced convection transport in the liquid at the vicinity of the bubble. Apart from empirical correlations, some mechanism based correlations were also proposed. One such correlation obtained by accounting the contribution of transient conduction, microlayer evaporation and natural convection and expressed as:

$$q'' = \frac{K^2}{2} \sqrt{\pi \left(k\rho C_p\right)}_l f D_d^2 N_a \Delta T_w + \left(1 - \frac{K^2 N_a \pi D_d^2}{4}\right) \overline{h}_{nc} \Delta T_w + \overline{h}_{ev} \Delta T N_a \frac{\pi}{4} D_d^2$$
(1)

In the above correlation, the constant, K depends on the ratio of the area of influence of a bubble to the cross sectional area of the bubble, Na is the number of nucleate site density, D_d is the bubble diameter and f is the bubble release frequency, the first two terms on the right side were also used by Mikic and Rohsenow (1961) while the last term was suggested by Judd and Hwang (1976) accounting for the microlayer heat transfer. The value of K proposed by them was $\sqrt{1.8}$ with the model predictions matching the data as shown in Figure 2. Rohsenow (1962) proposed one of first nucleate pool boiling correlations given in the following form:

$$q'' = \mu_l h_{lv} \left[\frac{g(\rho_l - \rho_v)}{\sigma} \right]^{1/2} \Pr^{-s/r} \left[\frac{1}{C_{sf}} \right]^{1/r} \left[\frac{C_{pl} \left(T_w - T_{sat} \right)}{h_{lv}} \right]^{1/r}$$
(2)

Gaertner (1965) presented a photographic study of the pool boiling of saturated water at atmospheric pressure. The nucleate boiling region was subdivided into four regions depending on the mode of vapor generation. At fully developed nucleate boiling, large billowing clouds of vapor were formed at the surface. He observed that massive bubbles were attached to the surface by numerous vapor stems and described them as vapor mushrooms. These vapor mushrooms were planted in the thermal layer and nourished at the vapor liquid interface by evaporation. The length and diameter of the vapor stems reported by him was found to be inversely proportional to the square root of the heat flux.

Lida & Kobayasi (1969) studied local void fractions averaged with time on horizontal heating surface in a saturated pool boiling of water at atmospheric pressure. For the minimum heat flux point they recorded wall void fraction of 96% implying that liquid was still in contact with the heating surface. Void fractions varied according to the superheat and heat flux of the surface. The map of void fraction described from the measured values indicates the statistical situation of the vapor bubbles in nucleate boiling.

Chekanov (1977) performed the earliest experiments to investigate the interaction between two artificial nucleation sites. Chekanov postulated that the bubbles effect one another by acoustic actions and hydrodynamic mixing. In addition to this, it was reported that when the ratio of cavity spacing to bubble departure diameter (S/D) was less than three, the formation of a bubble at one nucleation site inhibited the activation of another site. On the contrary, when S/D > 3 the formation



Figure 2 - Nucleate boiling heat transfer model by Judd and Hwang (1976)

of bubble promoted the nucleation of another site. Lastly, if the S/D ratio is very large then there were no interactions between the sites.

Stephan and Abdelsalam (1980) developed a more comprehensive correlation obtained from approximately 5000 data points for nucleate boiling on horizontal surfaces and given as:

$$q'' = 0.023 \left(\frac{k_l \Delta T}{D_d}\right) \left(\frac{q'' D_d}{k_l T_{sat}}\right)^{0.674} \left(\frac{\rho_v}{\rho_l}\right)^{0.297} \left(\frac{h_{lv} D_d^2}{\alpha_l^2}\right)^{0.371} \left(\frac{\rho_l - \rho_v}{\rho_l}\right)^{-1.73} \left(\frac{\rho_l \alpha_l^2}{\sigma D_d}\right)^{0.35}$$
(3)

Cooper (1984) proposed a correlation applicable for saturated pool nucleate boiling employing reduced pressure, molecular weight and surface roughness, which is expressed as:

$$q'' = 55.0 \left[\left\{ \left(\frac{P}{P_c} \right) 0.12 - 0.21 \log_{10}^{R_p} \right\} \left\{ -\log_{10} \left(\frac{P}{P_c} \right) \right\}^{-0.55} M^{-0.5} \Delta T_w \right]^3$$
(4)

The above two correlations are among most widely used to predict nucleate boiling heat flux but still have limited applicability as development of comprehensive models are hindered by inability to predict accurately other factors like nucleation sites, bubble frequency and departure diameter, etc.

Lee and Nydahl (1989) performed numerical calculation of bubble growth in nucleate boiling regime using numerical mapping technique. Simulation was done for water at 1 atm and 8.5 K wall superheat. They reported that microlayer was the dominant mechanism for heat transfer providing as much as 90% of the energy for bubble growth and 87% of the overall heat transfer. They also found from their analysis that microconvection heat transfer effects during bubble growth being non-existent. Liaw and Dhir (1989) performed experiments in a vertical wall using saturated water at atmospheric pressure. The wettability of the surface was controlled by the degree of oxidation of the surface and static contact angle was used as a reference. They inferred that the boiling phenomenon on the heater surface can be subdivided into three regions: the wall dominated region, vapor flow dynamics dominated region, and the intermediate region. They noted that the maximum void fraction occurs at a distance of 1-1.3 mm away from the wall and vapor flow dynamics dominate the region beyond which the maximum void fraction location. The intermediate region is influenced by the wall as well as vapor flow dynamics away from the wall. Their experiments showed that the maximum heat flux values increased as the surface wettability improves. Also, the wall void fraction at which the maximum heat flux condition is limited by vapor outflow dynamics for well wetted surface and evaporation rate near the surface for poorly wetted surface.

Wang and Dhir (1993) conducted experiments of pool boiling of saturated water at 1 atm on three surfaces with contact angles of 18° , 35° and 90° . They determined that the active nucleation site density varies as q^2 , where q is the wall heat flux, and decreases as the surface wettability improves. They found that the spatial distribution and distribution of nearest neighbor distance follows Poisson distribution.

Son *et al.* (1999) performed complete numerical simulation of the hydrodynamics and heat transfer associated with a single bubble using level set method. The computational domain was divided in macro and micro region and hence treated separately with the effect of microlayer being incorporated as the source term in the continuity equation of the macrolayer solution. The

contribution of microlayer to the total heat flux was found to be about 20%. The variation of bubble size and growth with contact angle and wall superheat was also reported.

Basu *et al.* (2002) developed correlations for nucleation site density, independent of flow rate and liquid subcooling but dependent on contact angle. They found that the nucleation site density depends on static contact angle and wall superheat. The effect of velocity, subcooling is implicit in the relation between heat flux and wall superheat and doesn't influence the nucleation site density independently.

Theofanous *et al.* (2002) presented experimental results of nucleate pool boiling conducted using electrically heated, vapor-deposited sub-micron Ti of 140 nm thickness. Heater's surface nanomorphology and chemistry were characterized using atomic force microscopy, scanning electron microscopy and X ray diffraction spectroscopy. From the onset of nucleation to the boiling crisis, dynamic thermal patterns on the heater surface were visualized using high speed, high resolution infra red camera. Experimental data of nucleation and boiling heat transfer at high heat fluxes between aged and fresh heaters are presented. They reported a linear relation between q and ΔT for aged heaters which is in stark contrast that the dependence may be as high as third power. As the bubble base corresponds to dark spots on the thermal pattern, it was argued that active sites are effective heat sinks.

Mukherjee and Dhir (2004) numerically studied lateral bubble merger for different orientations, contact angles and superheats for a horizontal surface. Their code was however based on finite volume approach with SIMPLE method to solve the pressure equation and power law scheme to solve the convective terms in the conservation equations. Their results show that bubble merger significantly increases the wall heat transfer due to formation of vapor bridges with trapping of liquid layer underneath the bubbles and by drawing cooler liquid towards the wall after merging.

Aparajith *et al.* (2006) performed the dynamics and simulation of multiple bubble merger during pool boiling under reduced gravity using PF5060 as the test fluid. Scaling relations for PF5060 with respect to gravity for bubble departure diameter and growth period were reported. The effect of cavity spacing and orientation of cavities on bubble departure diameter, bubble growth period, vapor interfacial structure and heat flux were also investigated.

Li and Dhir (2007) conducted numerical simulations of sliding bubble on a downward facing heater surface. The bubble shape was found to change from spheroids to ellipsoids and finally to a bubble cap. They found that the temperature gradient on the wall behind the bubble is significantly increased by the sliding motion of the bubble leading to enhanced heat transfer on the heater surface.

Sussman *et al.* (2007) presented a coupled level set and volume of fluid method based on sharp interface method for computing two-phase flows of immiscible fluids. Their method can be reduced to a single phase approach in the limiting case of zero gas density and zero gas viscosity. A cell-centered semi-implicit treatment for the viscous terms was developed and hence viscous jump was treated as sharp. Their improved accuracy over conventional continuum approach and ghost fluid method can reliably handle complex interfacial geometries.

Wu *et al.* (2007) coupled the level set method with moving mesh method to simulate subcooled nucleate pool boiling under strong temperature gradient near the surface. Comparison of dimensionless terminal velocities of rising bubbles and growth rate of bubbles for various grid sizes with wall superheat and liquid subcooling was done with improved accuracy due to moving

mesh method.

Son and Dhir (2008) studied numerically nucleate boiling at high heat fluxes on horizontal surfaces with two-dimensional assumption. The effect of contact angle, wall superheat and waiting period on the bubble dynamics and wall heat flux were investigated. The model was used in conjunction with correlations specifying nucleation site density and bubble waiting time. Heat fluxes obtained from the model were within $\pm 25\%$ of Stephan and Abdelsalam (1980) correlation.

Gerardi *et al.* (2010) used synchronized high speed imaging and infrared thermometry to obtain spatial and temporal resolved information on bubble nucleation and heat transfer in pool boiling of water. Measurements were made for bubble departure diameter, frequency, growth, waiting times as well as for microlayer radius and dryout radius. However, they stated that the relative importance of wall/microlayer heat transfer and superheated liquid layer around the bubble depends on fluid, heater surface characteristics like roughness, wettability, etc and heat flux and couldn't draw any definitive conclusion.

Golobic *et al.* (2012) examined the growth of an isolated bubble and coalescence between bubbles of dissimilar sizes during nucleate pool boiling of water on horizontal surface. Transient distributions of wall heat flux were mapped using wall temperature measurements made by high speed IR camera. They observed that following contact between the bubble, complex disturbances to the heat flux in the contact areas of both bubbles were seen. The bubble shape oscillations observed during coalescence were more as the difference in the bubbles sizes increases.

Sato and Niceno (2013) used a conservative two phase flow model and introduced a color function as the volume fraction of liquid inside a control volume. In order to maintain strict mass conservation and accurate interface shape, the CIP-CSL2 scheme was used. The smearing of
the interface was further prevented using an interface sharpening equation. They calculated the mass transfer rate directly from the heat flux at the liquid-vapor interface. A three-dimensional verification case of a growing vapor bubble in a superheated liquid has been simulated for zero gravity conditions.

Sielaff *et al.* (2015) performed experimental and numerical studies on horizontal bubble coalescence under varying pressure conditions. The fluid used was FC72 for pressure values of 500,700 and 900 mbar. At low pressures residual droplet was observed for both experimental and numerical work. The frequency of bubble coalescence showed a strong dependence on pressure. For a given nucleation site density distance, an optimal pressure leading to maximum coalescence probability and frequency was demonstrated. While heat transfer rates between experiments and numerical simulations were in agreement, however the bubble dynamics in terms of its shape after merging of the bubbles differed from the experiments.

Gong and Cheng (2015) used the phase change Lattice Boltzmann method and investigated the effect of wettability on saturated pool boiling heat transfer for the case of constant wall superheat on a substrate of finite thickness. Both hydrophobic and hydrophilic surfaces were considered and they reported that a hydrophobic surface has a higher heat flux than a hydrophilic surface at low superheats. Also, for hydrophobic surface a residual bubble was left in comparison to hydrophilic surface and exhibits lower onset of boiling temperature, higher boiling heat transfer at low superheats and lower critical heat flux comparatively. This model however has a limitation on maximum density ratio of approximately 100 which can be simulated.

1.2 Maximum Heat Flux

Maximum heat flux (CHF) represents the upper limit of fully developed nucleate boiling regime (point e of Figure 1). The early models for prediction of maximum heat flux, also known as "far-field model", were proposed by Kutateladze (1948) and Zuber (1959) which are based on the hydrodynamics of vapor flow. Zuber's hydrodynamic theory assumes that at CHF the vapor escape velocity and vapor flow area fraction reaches their critical values. At the critical vapor velocity the jets in a countercurrent situation become unstable and thus impediment the outflow of vapor. This instability occurs away from the heater surface and is unaffected by the surface conditions. Zuber's expression for CHF is:

$$\dot{q}_{\max,zub} = \frac{\pi}{24} \rho_{\nu} h_{fg} \sqrt[4]{\frac{\sigma g(\rho_l - \rho_{\nu})}{\rho_{\nu}^2}} \left[\left(\frac{\rho_l (16 - \pi)}{\rho_l (16 - \pi) + \rho_{\nu} \pi} \right) \left(\frac{\rho_l + \rho_{\nu}}{\rho_l} \right)^{1/2} \right]$$
(5)

The same theory has been extended by Lienhard & Dhir (1973) to evaluate CHF for pool boiling on finite size heaters. According to this extended hydrodynamic theory, the CHF can be expressed as:

$$\frac{q_{\max}}{\dot{q}_{\max,zub}} = f(l') \tag{6}$$

Where,

$$l' = \frac{l}{\sqrt{g(\rho_l - \rho_v)/\sigma}}$$

An alternative model known as "near-surface model" which was proposed by Haramura and Katto (1983) hypothesizes that vapor stems supporting the mushroom type bubbles is subjected to Helmholtz instability instead. The model also postulates that the macrolayer formed on the surface reduces in thickness while a vapor mass hovers over it. Other factors which influence the CHF are surface contamination, heater thickness and material, system pressure, gravity, mode of heating surface, liquid subcooling and flow velocity (Dhir, 1998).

Ha and No (1998) proposed a dry-spot model for high heat flux nucleate boiling and critical heat flux (CHF) based on Poisson distribution of active nucleation sites. They postulated that a dry-spot is formed when the number of bubbles surrounding one bubble exceeds the critical number thus inhibiting the flow of liquid under the bubble base thus triggering CHF condition. Their model was validated with experimental data of pool boiling including CHF.

Rule and Kim (1999) made detailed local measurements of wall heat flux for saturated pool boiling of FC-72 using an array of 96 heaters in a temperature controlled mode. They obtained the data in nucleate boiling, critical heat flux and transition boiling regimes. The CHF values obtained by them were approximately 33% higher than Zuber's model. They further observed that the inner heaters reach CHF at lower wall superheats than the array averaged heat flux whereas the maximum heat flux for the edge heaters was observed to be more than the CHF of the inner heaters. In the transition boiling regime, heat transfer during liquid contact was observed to decrease with increase in wall superheat, contrary to the previously reported models.

He *et al.* (2001) proposed a numerical simulation model based on macrolayer model where the thickness of the macrolayer is determined along with the growth rate of vapor stem. By using bisection method, the boiling curve of water and FC-72 were obtained. They concluded that evaporation at the interface of vapor stem-liquid is the main part of the total heat flux. With increasing heat flux, the evaporation due to the decay of macrolayer plays a more important role.

Their boiling curve shifted towards left with the increase of surface roughness with the CHF value remaining almost the same.

Kandlikar (2001) developed a theoretical model for CHF prediction in saturated pool boiling. An important factor in this model was the horizontal component of the force due to the evaporation from the liquid vapor interface. This force exceeds the retaining forces due to surface tension and gravity resulting the spreading of the vapor bubble along the heater surface and thus initiating the CHF condition. The proposed model considers the effect of dynamic receding contact angle and subcooling and predicts the experimental data very well for water, refrigerants and cryogenic liquids. The model considered the range of contact angle from 20° to 110° and the predicted CHF value decreases as the contact angle increases.

Theofanous *et al.* (2002) conducted burnout experiments on fresh and aged heaters with CHF's varying from 50% to 140% of the hydrodynamic limit. Based on the high speed, high resolution infrared thermometry, they concluded that CHF cannot be (macro) hydrodynamically limited rather it is controlled by the microhydrodynamics and rupture of an extended liquid microlayer, They remarked that dynamics and stability of the liquid microlayer were likely to be governed by the distance between the neighboring nucleation sites. At high superheats, both reversible and irreversible dry spots were observed by them. Through the reversible dryspots only irreversible dry spots arise. The dynamics of the reversible dry spot is affected by nearby nucleation event while an irreversible dry spot is characterized by the growth velocity rate of millimeters per second just prior to thermal runway.

Zhao *et al.* (2002) proposed a model to predict the nucleate boiling regime including the CHF. Their model gives a dynamic structure of vapor liquid-solid contacts. In their model heat

transfer is mainly attributed to the evaporation of the microlayer formed periodically during the inception of new bubbles. The local evaporation and partial dryout speed of the microlayer increases with increase in wall superheat due to thinning of the microlayer. According to them, the developing process of the isolated dry-areas beneath individual bubbles results in CHF.

Auracher *et al.* (2004) performed experiments for steady state boiling curve in the transition boiling regime with a clean heater surface and didn't observe any hysteresis. They also presented a concept of reaction-diffusion model to predict CHF where instability of the dry spots on the surface is accompanied by a temperature wave. The CHF values obtained by them were higher than those given by the hydrodynamic theory.

Luttich *et al.* (2004) presented a unifying correlation to calculate the heat flux along the entire boiling curve. They supplemented their model by relying on experimental observations to calculate the interfacial geometry close to the boiling surface. Key parameters used in their model were vapor fraction, interfacial velocity, interfacial line (contact line), area densities and their respective fluxes on the boiling surface. They successfully correlated the boiling curve of FC 72 and CHF data for water with interfacial geometry found using optical probe measurements and applying multiphase flow averaging theory.

Das *et al.* (2006) developed an analytical model of heat transfer applicable for pool boiling based on the evaporation of micro and macrolayers during the vapor bubble growth. They ignored the influence of adjacent bubbles on a particular growing bubble which is not true for the case of high heat fluxes. The effect of fluid motion was also ignored. The boiling curve was obtained by considering the bubble dynamics and decreasing thickness of liquid layer along with the increase in the dry spot radius.

Chu and Yu (2009) developed a new comprehensive model for nucleate pool boiling of pure liquid upto CHF. The model proposed by them was expressed in terms of total number, minimum and maximum sizes of active nucleation sites, fractal dimension, wall superheat and properties of fluids. The model was shown to be in good agreement with the experimental data.

Guan *et al.* (2011) proposed a new mechanistic model for predicting CHF in pool boiling system with pentane, hexane and FC-72. They postulated that the film boiling occurs when the vapor momentum flux is sufficiently high to lift the liquid macrolayer from the surface thus inhibiting wetting. Their obtained expression for CHF is of the same form as Zuber's instability model but over predicts the CHF value obtained from Zuber's model for the case of higher pressures at 300-450 kPa.

Buchholz *et al.* (2006) used an array of 36 microthermocouples embedded in a horizontal copper heater. The test fluids used for their study was isopropanol and FC-3284. They observed very localized and rapid temperature drops at the bottom of the bubbles in the nucleate boiling. At low heat flux nucleate boiling the vapor is slightly superheated while the liquid superheat is strong. However, at high wall superheats the vapor becomes even more superheated while the liquid is close to saturation temperature. A liquid rich layer, whose thickness decreases with increasing superheat, above the surface was confirmed by micro optical probe in their experiments. At CHF conditions, dry patches were observed at the surface while at the film boiling surface temperature fluctuations were very weak. At film boiling, the vapor superheat present in the bubble decreases with increasing distance.

1.3 Transition Boiling

Region e-f of the Figure 1 shows the transition boiling regime characterized by reduction in surface heat flux with an increase in wall superheat and can be bypassed if the boiling curve is performed in a heat flux controlled setting. It has traditionally been interpreted as a combination of nucleate and film boiling alternatively and is probably the least understood regime as it is practically of less importance than nucleate boiling along with the fact that its mechanisms are far more complicated. Since transition boiling can be viewed as a combination of liquid and solid contacts, Berenson (1962) expressed the transition boiling heat flux as:

$$q'' = Fq_l' + (1 - F)q_v''$$
⁽⁷⁾

where,

$$F = \exp\left(-2.2\frac{\Delta T}{\Delta T_{CHF}} + 2\right)$$

In the above expression, F is the average ratio of the liquid contact area at any given instance, ΔT_{CHF} is the wall superheat at critical heat flux (CHF), q"_{max}. With the assumption that a unique transition boiling curve exists, another correlation was given by Kalinin *et al.* (1976) as:

$$q'' = q_l' F_l + (1 - F_l) q_v''$$
(8)

Where, q_l and q_v are the heat fluxes associated with liquid and vapor respectively.

Lee *et al.* (1985) did the measurement of the local surface temperature history in transition and film boiling on surfaces at high wall superheats. From their measurements they observed direct liquid solid contacts for both the transition and film boiling regimes. Both the local liquid contact fraction and the average contact duration increased monotonically with decreasing surface superheat. They inferred that the liquid-solid contacts might be the dominant mechanism of energy transport in the transition boiling process.

Ramilson and Lienhard (1987) re-created the Berenson flat plate transition boiling experiment and conducted experiments with several fluids on mirror-polished, roughened and teflon coated surface. They confirmed the prior conclusion that the burn out heat flux suffers a secondary dependence on surface conditions. They also proposed a model to calculate the heat flux at the boundary between pure-film and film transition regime as a function of the advancing contact angle.

Dhir and Liaw (1989) developed a framework for theoretical prediction of boiling curve except in the isolated bubble regime. By assuming the existence of stationary vapor stems at the wall two dimensional steady state conduction equations are solved to determine the temperature distribution and the heat transfer into the thermal layer. By employing experimentally observed void fractions, apart from nucleate and transition boiling heat fluxes, maximum and minimum heat fluxes with their dependence on contact angle are also predicted from their model . Additionally, the model predicted values of vapor stem spacing and diameter to decrease with increase in temperature and contact angle.

Maruyama *et al.* (1992) simulated the transition boiling curve by developing an instantaneous heat flux model. Their heat flux model was based on the combined effect of increase of void fraction and the decay of the macrolayer thickness with time. Spatial pattern of the vapor stems with random positions and sizes was assumed initially. An initial thickness of the macrolayer was taken from Rajvanshi *et al.* (1990) and the time varying model of the macrolayer

thickness at any time could be solved independently of the void fraction.

1.4 Film Boiling

At point f of the boiling curve, due to very high wall superheats a layer of vapor film completely blankets the surface and transport of heat across the vapor film from the wall is achieved by conduction, convection and radiation. Point f demarcates the boundary between transition boiling and film boiling regime and corresponds to the minimum heat flux condition of the boiling curve. It is alternatively referred as the Leidenfrost point.

Berenson (1961) obtained the expression for the heat transfer coefficient during saturated film boiling on horizontal surfaces, given in the form of Nusselt number (Nu) as:

$$Nu = 0.42 \left[\frac{\rho_v \left(\rho_l - \rho_v\right) g h_{fg}}{k_v \mu_v \Delta T} \right]^{1/4} \left[\frac{\sigma}{g \left(\rho_l - \rho_v\right)} \right]^{3/8}$$
(9)

Klimenko (1981) carried out generalized analysis of film boiling on horizontal flat plate and developed correlations for variety of liquids including cryogen.

$$Nu = 3.02 \times 10^{-2} \operatorname{Ar}^{1/3} \operatorname{Pr}^{1/3} f_1(\beta) \quad \text{for } \operatorname{Ar} < 10^8$$

= 1.37 \times 10^{-3} \text{Ar}^{1/2} \text{Pr}^{1/3} f_2(\beta) \quad \text{for } \operatorname{Ar} < 10^8

where,

$$f_{1} = 1 \qquad \text{for } \beta > 0.71 \qquad f_{2} = 1 \qquad \text{for } \beta > 0.50$$
$$= 0.71\beta^{-1/2} \quad \text{for } \beta < 0.50 \qquad = 0.89\beta^{-1/3} \quad \text{for } \beta < 0.71$$
(10)

In the above expression, Ar is the Archimedes number
$$\begin{pmatrix} (2\pi)^3 g l_o^3 \rho_v (\rho_l - \rho_v) / \mu_v^2 \end{pmatrix}$$
 and

 β is the ratio of sensible heat to latent heat.

Juric and Tryggvason (1998) presented front tracking method to simulate liquid vapor phase change using a single field formulation with just one set of conservation equations of mass, momentum and energy. The interface matching conditions are implicitly imposed by the interfacial source terms with the help of delta functions which leads to smeared out profiles for different variables. Two dimensional film boiling simulations were done and overall heat transfer rates and wall temperatures were compared with experimental observations and correlations.

Esmaeeli and Tryggvason (2004) performed direct numerical simulation of film boiling using one set of conservation equations to represent heat transfer, mass transfer, and fluid flow for both the liquid and the vapor phase. The method described by them had also been extended to study multimode film boiling (where evolution of phase boundary leads to formation of bubbles of different sizes and spacings) on horizontal surfaces, explosive boiling and boiling in complex geometries. By imposing periodic boundary conditions at the horizontal boundaries, evolution of liquid/vapor interface and velocity field during film boiling process at Ja = 0.064 was shown.

Tomar *et al.* (2005) presented a coupled level set and volume of fluid approach for modeling incompressible flows with surface tension. Planar simulations of bubble growth in water at near critical pressure and R134a refrigerant was done. The effect of saturation pressure on the bubble formation frequency was also studied. At near critical pressures, for film boiling, there exists a critical superheat beyond which jet-like-columns arise at the nodes while bubble growth and detachment occurs periodically at the anti-nodes. They also did the Fast Fourier Transform (FFT) of the space-averaged Nusselt number and reported two dominant frequency peaks for a superheat of 10 K.

Gibou *et al.* (2006) described a sharp interface capturing method by using a ghost fluid approach to impose the jump conditions at the interface. They applied their algorithm for the simulation of two dimensional film boiling. Their treatment preserves the discontinuous nature of all variables across the interface except for the viscosity, for which a delta formulation mechanism was used for simplicity. Furthermore, viscosity was treated as explicit. The jump conditions in the pressure derivatives were balanced by considering real velocities.

From the above studies it is concluded that although several theoretical, experimental and numerical work has been done yet no study has been focused on a unified approach to numerically predict the entire boiling curve. The importance of nucleation site density along with the contact angle is vital in predicting the heat fluxes at the surface. Several attempts were made to predict the heat flux for a particular regime but they didn't account the combined effect of nucleation site density and the waiting time for a specified contact angle.

1.5 Objective of the Present Study

The objective of the present study is to numerically reproduce the boiling curve in a temperature controlled mode using a unified numerical model supplemented by correlations specifying nucleation site density and bubble waiting time as a function of wall superheat for different contact angles. Steady state boiling curve for all the three regimes *viz*. nucleate, transition and film boiling has been obtained with a unified numerical model by incrementing the wall superheat for a range of static contact angles for both two dimensional and three dimensional cases. Additionally, a 3D parallel framework has also been implemented to enhance the performance of the code with the future intention of optimization and scaling up.

2. Numerical Model

Some of the methods used to study multiphase process numerically are:

- Marker and Cell Method (MAC) : Developed by Harlow and Welch (1965), it was one of the earliest attempts made to compute solution of fluid dynamics problems with free boundaries were made in 1960s. The interface is marked by weightless particles which under the influence of velocity field are convected and can be explicitly used to reconstruct the interface on a fixed mesh.
- 2. Volume of Fluid Method (VOF) : Developed in 1970s the Volume of Fluid Method (VOF) employs a piecewise constant scalar field to track the location of both the phases. Information about the volume fraction of one of the phases in a cell is contained and convected under the influence of velocity field. This implicit approach allows simple handling of topological changes but unlike MAC schemes does not involve any additional consideration while explicit reconstruction of the interface.
- 3. Arbitrary Lagrangian-Eulerian Method (ALE): ALE method is the finite element method in which the computational domain is not fixed a priori. The mesh follows the interface and can precisely track the motion of the interface. It helps to combine the respective advantages of the Lagrangian and Eulerian formulations however its implementation requires the formulation of mesh-update procedure that assigns mesh-node velocities at each time step.
- Level-Set Method (LS) : Introduced at the end of 1980s by Osher and Sethian (1988), the interface is defined as the zero level set of the continuous higher dimensional scalar field. Interface and shapes are tracked by a level set function which is convected in the velocity

field. Similar to the VOF the LS technique reduces the complexity in handling the interface during topological changes like breaking and merging, but in contrast the level set function is globally continuous and hence the solution is less effected by numerical diffusion during the transport process.

5. Lattice Boltzmann Method (LB): LBM for simulating immiscible binary fluids in two dimension were introduced in 1990s by Gunstensen *et al.* (1991). The liquid or vapor state at each lattice point is determined by the thermodynamic relations given by equation of state thus eliminating the need to track the interface explicitly.

2.1 Governing Equations

Direct numerical simulation (DNS) of the two phase flows with application to boiling heat transfer has been performed since 1990s. Following the work of Son *et al.* (1999) and Son and Dhir (2008), the computational domain is divided into macrolayer and microlayer (Figure 3). The microlayer is discussed in Section 2.7 while for the macrolayer, the governing equations for global conservation of mass, momentum and energy for each phase are given as:

$$\nabla .u_{f} = 0$$

$$\rho_{f} \left(\frac{\partial u_{f}}{\partial t} + u_{f} . \nabla u_{f} \right) = -(\nabla p)_{f} + \rho_{f} g + \nabla . \mu_{f} \left(\nabla u + \nabla u^{T} \right)_{f}$$

$$\rho_{f} c_{f} \left(\frac{\partial T_{f}}{\partial t} + u_{f} . \nabla T_{f} \right) = \nabla . k_{f} \left(\nabla T \right)_{f}$$
(11)

The subscript *f* denotes the phase (liquid or vapor). The interface between the different phases is captured using a level set function Φ . The interface, for all times $t \in [0,T]$ is given by

$$\Gamma_f(\mathbf{t}) = \{ \vec{x} : \phi(\vec{x}, \mathbf{t}) = 0 \}$$
(12)



Figure 3 Numerical simulation model with micro region and macro region (Son *et al.* 1999)

The Level-Set Equation (LSE) is typically a smooth (Lipschitz continuous) function defined as:

$$\frac{\partial \phi}{\partial t} + U_{\text{int}} \cdot \nabla \phi = 0 \tag{13}$$

Where U_{int} is defined as:

$$U_{\rm int} = u_f + \frac{\dot{m}\ddot{n}}{\rho_f} \tag{14}$$

 ϕ is defined as the signed distance function such that

.

$$\phi(\vec{x},t) = \begin{cases} <0 \ if \ \vec{x} \in \Omega_{liq} \\ =0 \ if \ \vec{x} \in \Gamma_{int} \\ >0 \ if \ \vec{x} \in \Omega_{vap} \end{cases}$$
(15)

In the above expression, Ω_{tiq} and Ω_{tap} are domains of liquid and vapor phase, and Γ_{int} is the interface between them. The solution of level set function does not satisfy the condition of a distance function, i.e., its gradient becomes very large or very small near the interface for which it is reinitialized to a distance function by a smoother, less distorted function by solving the following equation (Sussman *et al.*, 1994) :

$$\frac{\partial \Phi}{\partial \tau} = S\left(\Phi_{o}\right)\left(1 - \left|\nabla \Phi\right|\right) \tag{16}$$

Where,

$$S\left(\Phi_{o}\right) = \frac{\Phi_{o}}{\sqrt{\Phi_{o} + h^{2}}}$$
(17)

Here h is the grid spacing. Since the grid spacing is not constant throughout the domain, effective grid spacing for level set function is defined as (Son and Dhir, 2007):

$$h = \sqrt{\frac{\left(\frac{\partial\Phi}{\partial x}\right)^{2} \left(\Delta x\right)^{2} + \left(\frac{\partial\Phi}{\partial y}\right)^{2} \left(\Delta y\right)^{2} + \left(\frac{\partial\Phi}{\partial z}\right)^{2} \left(\Delta z\right)^{2}}{\left(\frac{\partial\Phi}{\partial x}\right)^{2} + \left(\frac{\partial\Phi}{\partial y}\right)^{2} + \left(\frac{\partial\Phi}{\partial z}\right)^{2}}$$
(18)

The normal to the interface n and the interface curvature κ are defined as:

$$\vec{n} = \frac{\nabla \Phi}{|\nabla \Phi|}$$

$$\kappa = \nabla \vec{n} = \nabla \cdot \frac{\nabla \Phi}{|\nabla \Phi|} = \frac{\Phi_{xx} \Phi_{y}^{2} - 2\Phi_{x} \Phi_{y} \Phi_{xy} + \Phi_{yy} \Phi_{x}^{2}}{\left(\Phi_{x}^{2} + \Phi_{y}^{2}\right)^{3/2}}$$
(19)

For the treatment of the surface tension acting on the interface, the Continuum Surface Force (CSF) developed by Brackbill *et al.* (1992) is used, where the interfacial tension is transformed into a body force for the cells containing the interface. Other ways to treat surface tension are Continuum Surface Stress (CSS) model and using a variational approach using the Laplace-Beltrami operator on the free surface. The former approach is generally used where variation of surface tension force along the interface is considered.

2.2 Assumptions

- 1. Material properties like density, viscosity, specific heat and thermal conductivity are taken as constant for each phase.
- 2. Both the fluids are newtonian and incompressible.
- 3. Effect of turbulence is negligible.
- 4. Interface is maintained at the saturation temperature.
- 5. Uniform wall superheat is applied to the surface.

2.3 Boundary Conditions

The boundary conditions for the governing equations are defined as:

At the wall (y=0) :

$$u = v = 0 ; w = 0 (For 3D)$$

$$T = T_{wall}$$

$$\frac{\partial \Phi}{\partial y} = -\cos \varphi$$

$$\frac{\partial p}{\partial y} = \rho g$$
(20)

At the planes of symmetry:

At
$$x = 0$$
, L: $\frac{\partial u}{\partial x} = \frac{\partial v}{\partial x} = \frac{\partial w}{\partial x} = \frac{\partial T}{\partial x} = \frac{\partial \Phi}{\partial x} = \frac{\partial p}{\partial x} = 0$
At $z = 0$, L: $\frac{\partial u}{\partial z} = \frac{\partial v}{\partial z} = \frac{\partial w}{\partial z} = \frac{\partial T}{\partial z} = \frac{\partial \Phi}{\partial z} = \frac{\partial p}{\partial z} = 0$ (For 3D) (21)

At the top boundary (y=H):

• •

$$\frac{\partial u}{\partial y} = \frac{\partial v}{\partial y} = \frac{\partial \Phi}{\partial y} = 0 ; \frac{\partial w}{\partial y} = 0 \text{ (For 3D)}$$

$$p = p_{atm}$$

$$T = T_{sat}$$
(22)

The boundary condition of pressure $\left(\frac{\partial p}{\partial y} = \rho g\right)$ at y = 0 is converted into homogeneous

Neumann boundary condition $\frac{\partial p}{\partial y} = 0$ by projecting Equation 34 onto the outer unit normal of the domain boundary (Croce *et al*, 2004).

2.4 Interface Velocity and Jump Conditions

Liquid and vapor phases are separated across an interface through which phase change occurs. A numerical approach to the multiphase flow problems requires tracking/capturing the interface as well as enforcing the appropriate boundary conditions at the tracked/captured interface. Typically δ -function formulation is used to enforce the appropriate boundary conditions across the interface which suffers from the drawback that the δ -function formulation smears out the numerical quantities across the interface (Nguyen *et al., 2001*). Hence, to address the aforementioned shortcomings the discretization of the equations near the interface which is not coincident with the grid points is facilitated using ghost fluid method (GFM) as proposed by Fedkiw *et al.* (1999).

Since mass transfer is occurring at the interface normal velocity is discontinuous across the interface. From conservation of mass across the interface:

$$\rho_l \left[u_{l,n} - u_{\text{int},n} \right] = \rho_v \left[u_{v,n} - u_{\text{int},n} \right]$$
(23)

Where $u_{l,n}, u_{v,n}, u_{int,n}$ are the liquid, vapor and interface velocities normal to the interface obtained by taking the dot product of the velocity vector and normal vector, which gives the following velocity and pressure jump conditions at the interface provided the interface is not a contact discontinuity (Gibou *et al.* (2006)):

$$\dot{m} = \frac{1}{h_{\nu}} \bar{n} \cdot (\mathbf{k}_{1} \nabla \mathbf{T}_{1} - \mathbf{k}_{\nu} \nabla \mathbf{T}_{\nu})$$
(24)

$$u_{l,n} - u_{\nu,n} = \dot{m} \left(\frac{1}{\rho_{\nu}} - \frac{1}{\rho_{l}} \right) = \dot{m}\alpha$$
(25)

$$p_{l} - p_{v} = \sigma \kappa - \alpha \dot{m}^{2} + \bar{n} \left[\mu_{l} \left(\nabla \bar{u} + \nabla \bar{u}^{T} \right)_{l} - \mu_{v} \left(\nabla \bar{u} + \nabla \bar{u}^{T} \right)_{v} \right]$$
(26)

As explained in detail by Nguyen *et al.* (2001), the tangential velocities and stresses are however continuous but are completely uncoupled for the case of contact discontinuity. By using δ -function formulation, smearing of the jump conditions can occur which, for the case of velocity jump conditions, adds a compressible character to the flow field in the near vicinity of the interface as the divergence free conditions are not exactly satisfied. By implementing the above mentioned jump condition, the conservation equations of both the phases are coupled as (Gibou *et al.* (2006), Son and Dhir (2008)) : $\nabla . u = \alpha \dot{mn} . \nabla H + \dot{V}_{micro}$

$$\hat{\rho}\left(\frac{\partial u}{\partial t}+u.\nabla u\right) = -\left(\nabla p + \left(\sigma\kappa - \alpha\dot{m}^{2}\right)\nabla H\right) + \hat{\rho}\left[1 - \beta_{T}\left(T_{f} - T_{sat}\right)\right]g + \nabla.\hat{\mu}\left(\left(\nabla u - \alpha\dot{m}\vec{n}.\nabla H\right) + \left(\nabla u - \alpha\dot{m}\vec{n}.\nabla H\right)^{T}\right)$$

$$\hat{\rho}\hat{c}\left(\frac{\partial T}{\partial t} + u.\nabla T\right) = \nabla.\hat{k}\left(\nabla T\right)$$

where,

$$H = 1 \text{ if } \Phi > 0$$

$$= 0 \text{ if } \Phi \le 0$$

$$u_{l} = u + v_{lv} \dot{mn}(1 - H)$$

$$u_{v} = u - v_{lv} \dot{mn}(H)$$

$$\hat{\rho} = \rho_{v}(1 - F) + \rho_{l}F$$

$$\hat{c} = c_{v}(1 - F) + c_{l}F$$

$$\hat{\mu}^{-1} = \hat{\mu}_{v}^{-1}(1 - F) + \hat{\mu}_{l}^{-1}F$$

$$\hat{k}_{f} = \hat{k}_{l} = k_{l} / F$$

$$F = 1 \text{ if } H(\phi_{A}) = H(\phi_{B}) = 1$$

$$= 0 \text{ if } H(\phi_{A}) = H(\phi_{B}) = 0$$

$$= \frac{\max(\phi_{A}, \phi_{B})}{\max(\phi_{A}, \phi_{B}) - \min(\phi_{A}, \phi_{B})} \text{ otherwise}$$
(27)

In the above equation ϕ_A, ϕ_B are evaluated at the adjacent grid points and \dot{V}_{micro} is obtained from microlayer solution which is explained in Section 2.7.

2.5 Discretization

For discretization of the governing equations spatially, a staggered grid system is used. This method was first used by Harlow and Welch (1965) in their MAC method for free surface flows as a variant of PIC method. Since the pressure gradient is not calculated *a priori* and is computed during the course of the solution it is possible to create a pressure field with checkerboarded pattern which can persist in the final solution. The remedy for such checkerboarding is staggered grid where fluid and interface velocities are defined at cell faces while pressure (and other scalars) at cell centers, as shown in Figure 4. The density at the cell center is defined as:

$$\rho_P = \rho_v + (\rho_l - \rho_v) H(\Phi_P)$$
⁽²⁸⁾

Where

$$H(\Phi_{P}) = 1 \quad if \quad \Phi > 0$$

= 0 $if \quad \Phi \le 0$ (29)

The effective viscosity is calculated from the level set function as

$$\mu = \mu_{l} \quad \text{if } \Phi > 0$$

$$= \mu_{v} \quad \text{if } \Phi \leq 0$$

$$= \frac{\Phi_{\max} \mu_{l}^{-1} - \Phi_{\max} \mu_{v}^{-1}}{\Phi_{\max} - \Phi_{\min}} \quad \text{for all other cases.}$$
where,
$$\Phi_{\max} = \max(\Phi_{i,j-1/2}, \Phi_{i-1,j-1/2})$$

$$\Phi_{\min} = \max(\Phi_{i,j-1/2}, \Phi_{i-1,j-1/2}) \quad (30)$$

For discretization of continuity equation in each phase, ghost fluid methodology is used. As the normal velocity is discontinuous across the interface, care has to taken when applying numerical discretization in the vicinity of the interface. Following GFM a band of ghost cells is populated on either side of the interface that can be used by the fluid velocities on the other side of the interface. The level set function, Φ is defined as the cell center and its offset values at cell faces can be computed with simple averaging. The cell face values can then be used to determine which velocity field corresponds to water or vapor phase.

$$\left(\nabla . u_f\right)_P = \frac{u_{l,e} - u_{l,w}}{\Delta x} + \frac{v_{l,n} - v_{l,s}}{\Delta y}$$
(31)

If the problem is convection dominated then the accuracy of the convective term is essential for the spatial discretization. The principle behind ENO interpolation is in using the smoother approximation where smoothness is measured by the absolute value of the second order divided difference (John and Novo, 2012). For discretization of momentum equation spatially the convection terms are thereby treated by second order ENO scheme while the viscous diffusion terms by second order central difference scheme. Treating the viscosity implicitly is preferred but it's implicit formulation is very difficult (Gibou *et al.*, 2006) hence the semi-implicit treatment of the viscous terms is implemented in which viscosity is explicitly treated and has been shown to be unconditional stable by Li *et al.* (2000). For temporal discretization the convection and source terms are treated by first order explicit scheme and diffusion term by fully implicit scheme.

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Figure 4 Staggered grid arrangement

$$\frac{u_f^{n+1} - u^*}{\Delta t} = -\frac{1}{\rho_f} \left(\nabla p \right)_f + \frac{1}{\rho_f} \left(\nabla . \mu_{eff} \nabla u^{n+1} + S_u^n \right)$$

Where,

$$u^{*} = u_{f}^{n} + \Delta t \left(-u_{f}^{n} \cdot \nabla u_{f}^{n} + \overline{g} \right)$$

$$S_{u} = \nabla \cdot \mu_{eff} \nabla u^{T} - \nabla \cdot \mu_{eff} \left[\left(\alpha \dot{m} n \nabla H \right)^{T} + \left(\alpha \dot{m} n \nabla H \right) \right]$$
(32)

The momentum equation is solved using projection method. The projection method is an efficient way of solving time dependent incompressible Navier-Stokes equations by decoupling velocity with pressure. It consists of three stages, first the intermediate velocity field is computed by solving the momentum equation without the pressure gradient term.

$$\frac{u_f^{**} - u^*}{\Delta t} = \frac{1}{\rho_f} \left(\nabla . \mu_{eff} \nabla u^{**} + \left(\nabla . \mu_{eff} \nabla u^T - \nabla . \mu_{eff} \left[\left(\alpha \dot{m} n \nabla H \right)^T + \left(\alpha \dot{m} n \nabla H \right) \right] \right)^n \right)$$
(33)

$$\frac{u^{n+1}-u^{**}}{\Delta t} = \frac{1}{\tilde{\rho}} \left[\nabla p + \left(\sigma \kappa - \alpha \dot{m}^2 \right) \nabla H^{n+1} \right]$$
(34)

The second stage defines the solution of the following Poisson equation to satisfy the incompressibility condition. For incompressible flows pressure is not a thermodynamic variable and hence cannot be related to equation of state rather it is a Lagrange multiplier which constraints the velocity field to remain divergence free (Gresho and Sani, 1987). Pressure propagates at infinite speed in order to keep the flow incompressible and it is often computationally expensive to compute. The resulting system of linear equations obtained from discretization of the Poisson equation is hence solved using preconditioned conjugate gradient algorithm using Multigrid as the

preconditioner to accelerate convergence.

$$\nabla \cdot \frac{1}{\widetilde{\rho}} \nabla p = \frac{\nabla \cdot u^{**} - \left(\alpha \dot{mn} \cdot \nabla H\right)^{n+1}}{\Delta t} - \nabla \cdot \frac{1}{\widetilde{\rho}} \left(\sigma \kappa - \alpha \dot{m}^2\right) \nabla H^{n+1}$$
(35)

The final stage requires the corrected flow field velocity to be projected to the divergence free field as:

$$u_f^{n+1} = u_n^* - \Delta t \frac{\nabla p^{n+1}}{\widetilde{\rho}}$$
(36)

The spatial discretization of the energy equation is done by implementing the dirichlet boundary condition $T_{int} = T_{sat}$ at the interface (Ishii (1975)). The convection term is discretized using a second order ENO scheme while the diffusion term by fully implicit scheme. The energy equation takes the following form:

$$\frac{T_f^{n+1} - T_f^n}{\Delta t} = -u_f^n \cdot \nabla T_f^n + \frac{1}{\rho_f c_f} \left(\nabla \cdot k \nabla T \right)_f^{n+1}$$
(37)

The diffusion term is discretized as (Son and Dhir, 2008):

$$\left(\frac{\partial}{\partial x}k\frac{\partial T}{\partial x}\right)_{fi} = \frac{1}{\Delta x} \left[\left(k_f \frac{T_{f,i+m} - T_{f,i}}{x_{i+m} - x_i}\right) - \left(k_f \frac{T_{f,i} - T_{f,i-m}}{x_i - x_{i-m}}\right) \right]$$
(38)

which results in:

$$\left(\frac{\partial}{\partial x}k\frac{\partial T}{\partial x}\right)_{fi} = \frac{1}{\Delta x} \left[\left(\tilde{k}_{f,i+1/2}\frac{T_{f,i+m} - T_{f,i}}{x_{i+1} - x_i}\right) - \left(\tilde{k}_{f,i-1/2}\frac{T_{f,i} - T_{f,i-m}}{x_i - x_{i-1}}\right) \right]$$
(39)

Where effective thermal conductivity is defined as,

$$\widetilde{k}_{f,\pm 1/2} = \frac{k_f}{\max\left(\varepsilon, \frac{x_i - x_{i\pm m}}{x_i - x_{i\pm 1}}\right)} \quad \text{if} \quad \Phi_i \Phi_{i\pm 1} \leq 0$$

$$= k_f \quad \text{if} \quad \Phi_i \Phi_{i\pm 1} > 0$$
(40)

Close to the interface, the temperature field needs to be extrapolated in order to define ghost points. Possible ways to extrapolate using constant, linear and quadratic extrapolation are (Gibou *et al.*, 2001):

$$T_{i+1}^{G} = T_{I}$$

$$T_{i+1}^{G} = \frac{T_{I} + (\theta - 1)T_{i}}{\theta}$$

$$T_{i+1}^{G} = \frac{2T_{I} + (2\theta^{2} - 2)T_{i} + (-\theta^{2} + 1)T_{i-1}}{\theta^{2} + \theta}$$
(41)
where,
$$\theta = \frac{X_{I} - X_{i}}{\Delta x} = \frac{|\phi|}{\Delta x}$$

For the present study, the ghost temperature field is populated using constant extrapolation as it effectively moves the interface to the closest grid point while the remaining two extrapolation techniques behave poorly for small θ . As cited in (Gibou *et al.*, 2001) this second order accurate perturbation does not degrade the overall second order accuracy of the solution as long as the desired solution has bounded first derivatives. Temperature gradient is discretized as (Figure 5):

$$\left(\frac{\partial T}{\partial x}\right)_{fi} = \left(\frac{\partial T}{\partial x}\right)_{fi}^{-} \quad \text{if } \Phi_i \Phi_{i-1} \leq 0 \text{ or } |\Phi_{i-1}| < |\Phi_{i+1}|$$

$$= \left(\frac{\partial T}{\partial x}\right)_{fi}^{+} \quad \text{if } \Phi_i \Phi_{i+1} \leq 0 \text{ or } |\Phi_{i-1}| > |\Phi_{i+1}|$$

$$= \frac{1}{2} \left[\left(\frac{\partial T}{\partial x}\right)_{fi}^{+} + \left(\frac{\partial T}{\partial x}\right)_{fi}^{+} \right] \quad \text{if } \Phi_i \Phi_{i-1} \leq 0 \text{ and } \Phi_i \Phi_{i-1} \leq 0$$

Where,

$$\left(\frac{\partial T}{\partial x}\right)_{fi}^{\pm} = \frac{T_{fi} - T_{f,i\pm m}}{x_i - x_{i\pm m}} \quad \text{if} \quad \frac{x_i - x_{i\pm m}}{x_i - x_{i\pm i}} \ge 0.01$$
$$= \frac{T_{f,i\mp m} - T_{f,i\pm m}}{x_{i\mp m} - x_{i\pm m}} \quad \text{otherwise}$$
(42)



Figure 5 Discretization near the interface [Son and Dhir (2008)]

The computed $\partial T_f / \partial n$ is then extrapolated along the characteristics that flow outward from the interface by solving the following Hamilton-Jacobi equation.

$$\frac{\partial}{\partial \tau} \left(\frac{\partial T_f}{\partial n} \right) + sign\left(\Phi \right) \bar{n} \cdot \nabla \left(\frac{\partial T_f}{\partial n} \right) = 0$$
(43)

Rather than converging the above equation to a steady state, an alternative static Hamilton-Jacobi equation of the following form is solved:

$$\nabla \left(\frac{\partial T_f}{\partial n}\right) \cdot \nabla \Phi = 0 \tag{44}$$

The above equation can also be solved using central differencing scheme but upward differencing is employed as information is propagated along the characteristics (Osher and Fedkiw, 2002). The fast marching method (FMM) yields the same result as PDE based extrapolation and can be extended to higher order extrapolation analogous to the PDE based approach. (Aslam 2003, McCaslin *et al.* 2014). Mass flux is then evaluated from the energy balance at the interface by:

$$\dot{m} = \frac{1}{h_{lv}} \bar{n} \cdot \left(k_l \nabla T_l - k_v \nabla T_v\right)$$
(45)

The mass flux evaluated at the interface is then further populated across a narrow band on both sides of the interface to be used in the computation of ghost fluid cells. Level set equations are discretized by using a second-order, essentially nonoscillatory (ENO) scheme described as:

$$U\left(\frac{\partial\Phi}{\partial x}\right)_{i} = \max\left(U_{i}, 0\right)\left(\frac{\partial\Phi}{\partial x}\right)_{i}^{-} + \min\left(U_{i}, 0\right)\left(\frac{\partial\Phi}{\partial x}\right)_{i}^{+}$$
$$\left(\frac{\partial\Phi}{\partial x}\right)_{i}^{2} = \max\left[s\left(\frac{\partial\Phi}{\partial x}\right)_{i}^{-}, -s\left(\frac{\partial\Phi}{\partial x}\right)_{i}^{+}, 0\right]^{2}$$

$$\left(\frac{\partial\Phi}{\partial x}\right)_{i}^{-} = \left(\frac{\Phi_{i}-\Phi_{i-1}}{h}\right) + 0.5h \min \operatorname{mod}\left(\frac{\Phi_{i+1}+\Phi_{i-1}-2\Phi_{i}}{h^{2}}, \frac{\Phi_{i}+\Phi_{i-2}-2\Phi_{i-1}}{h^{2}}\right)$$
$$\left(\frac{\partial\Phi}{\partial x}\right)_{i}^{+} = \left(\frac{\Phi_{i}-\Phi_{i-1}}{h}\right) - 0.5h \min \operatorname{mod}\left(\frac{\Phi_{i+1}+\Phi_{i-1}-2\Phi_{i}}{h^{2}}, \frac{\Phi_{i}+\Phi_{i+2}-2\Phi_{i+1}}{h^{2}}\right)$$
(46)

Where,

$$U_i = \frac{U_{i+1/2} + U_{i-1/2}}{2}, s = sign(S)$$

 $\min \operatorname{mod}(a,b) = \operatorname{sign}(a) \min(|a|,|b|) \quad \text{if } ab > 0$

= 0 *otherwise*

Adaptive time stepping is used where the overall time step is the minimum of incompressible time step and level set time step. A CFL restriction of 0.5 is chosen.

$$\Delta t = \min\left\{\Delta t^{L}, \frac{0.5}{\max(\frac{|u_{\max}|}{\Delta x}, \frac{|v_{\max}|}{\Delta y}, \frac{|w_{\max}|}{\Delta z})}\right\}$$
(47)

2.6 Method of Solution

The set of linear algebraic equations obtained leads to a system with a tridiagonal matrix of coefficients. Direct methods of solving the discretization equations for 2 dimensions (or 3 dimensions) require excessive storage and computation time. Since the set of nominally linear equations must be solved after every iteration the computation cost of direct solution is

unacceptable. Conjugate gradient method being the most prominent iterative method for solving sparse system of linear equations is used. The speed of convergence for the pressure Poisson equation is further enhanced by implementing the block correction procedure (Patankar (1981); Settari and Aziz (1973)). The coefficient matrix A is known and is symmetric positive definite matrix. With knowing the coefficient matrix A, residual vector b, and the scalar Φ , preconditioner M, maximum number of iteration i_{max} , error tolerance ϵ , the linear algebraic equations were solved using preconditioned conjugate gradient algorithm is given in next page. For computation of velocities and temperature field Gauss Siedel, Jacobi or TDMA is used as a preconditioner while Multigrid is used as a preconditioner for Pressure computations. The PCG algorithm is defined in Figure 6:

$$i \leftarrow 0$$

$$r \leftarrow b - A\Phi$$

$$d \leftarrow M^{-1}r$$

$$\delta_{new} \leftarrow r^{T}d$$

$$\delta_{0} \leftarrow \delta_{new}$$

while $i < i_{max}$ and $\delta_{new} > \varepsilon^{2}\delta_{0}$
{

$$q \leftarrow Ad$$

$$\alpha \leftarrow \frac{\delta_{new}}{d^{T}q}$$

$$\Phi \leftarrow \Phi + \alpha d$$

If i is divisible by 50 then

$$r \leftarrow b - A\Phi$$

else

$$r \leftarrow r - \alpha q$$

$$s \leftarrow M^{-1}r$$

$$\delta_{old} \leftarrow \delta_{new}$$

$$\delta_{new} \leftarrow r^{T}s$$

$$\beta \leftarrow \frac{\delta_{new}}{\delta_{old}}$$

$$d \leftarrow s + \beta d$$

$$i \leftarrow i + 1$$

}

Figure 6 PCG Algorithm (Shewchuk, 1994)

2.7 Microlayer

The microscopic region where liquid-vapor interface meets the wall is of tremendous importance in boiling heat transfer also known as microlayer. Its existence under a bubble was first confirmed experimentally by Cooper and Llyod (1969). In this region the adhesion forces between the fluid molecules and the wall molecules are important as the liquid film consists of only few molecular layers thick (of the order of few nanometers) and doesn't evaporate due to adhesion forces. This region is called the adsorbed film. As the radial distance is increased the effect of the adhesion forces is decayed and the macroscopic hydrodynamics governs the interface shape. As the thickness of the liquid film grows the value of the interface curvature gets high leading to high pressure jump across the interface. The local saturation temperature is different than the corresponding pressure in the macroscopic region thus changing the local thermodynamic equilibrium.

Figure 7 shows the microlayer formed under the bubble. Comprehensive analysis of microlayer including disjoining pressure, vapor recoil pressure and interfacial heat transfer resistance has been carried out by Lay and Dhir (1995).



Figure 7 Microlayer under the bubble

According to the lubrication theory the conservation equation for mass, momentum and energy are given as:

$$\frac{\partial \delta}{\partial t} = v_l - \frac{q}{\rho_l h_{fg}} \tag{48}$$

$$\frac{\partial p_l}{\partial r} = \mu_l \frac{\partial^2 u_l}{\partial y^2} \tag{49}$$

$$q = \frac{k_{l} (T_{w} - T_{int})}{\delta} = h_{ev} \left[T_{int} - T_{v} + \frac{(p_{l} - p_{v})T_{v}}{\rho_{l} h_{fg}} \right]$$
(50)

The pressure in the vapor and liquid phase are related as

$$P_{l} = P_{v} - \sigma k - \frac{A}{\delta^{3}} + \frac{q^{2}}{\rho_{v} h_{lv}^{2}}$$

$$\tag{51}$$

The combination of mass, momentum and energy equation gives a fourth order differential equation of the following form:

$$\delta^{""} = f(\delta, \delta', \delta^{"}, \delta^{"})$$
(52)

The above fourth order differential equation can be cast into four first ordinary differential equations written as following:

$$\frac{d\delta}{dr} = \delta'$$

$$\frac{d\delta'}{dr} = \frac{\left(1 + \delta'^2\right)^{3/2}}{\sigma} \left(p_c - \frac{A}{\delta^3}\right)$$

$$\frac{dp_c}{dr} = -\frac{3\mu_l Q}{\rho_l h_{fg} \delta^3}$$

$$\frac{dQ}{dr} = \frac{T_{wall} - T_{sat} \left(1 + \frac{p_c}{\rho_l h_{fg}}\right)}{\frac{\delta}{k_l} + \frac{T_{sat} \sqrt{2\pi R_g T_{sat}} (2 - t)}{h_{fg}^2 \rho_v 2t}$$
(53)

The above ODE is solved in the direction from R_0 to R_1 with the following boundary conditions

at
$$\mathbf{r} = \mathbf{R}_0$$
 $\delta = \delta_o, \delta' = 0, \delta''' = 0$ (54)
at $\mathbf{r} = \mathbf{R}_1$ $\delta'' = 0$
δ_o is the equilibrium microlayer thickness, $\delta'=0$ because the slope of the film is zero and $\delta'''=0$ because of zero mass flow rate. R₀ and R₁ are related further by the following relation:

$$\tan \varphi = \left(\frac{h/2}{R_1 - R_0}\right)$$

(56) With Hamaker;s constant, A, being unknown its values is iterated unless the height of the microlayer at R₁ is same as half of the grid spacing defined by the sixth condition defined as:

$$\delta = h / 2$$

(57)

The solution procedure of microlayer is as follows:

- 1. Obtain the value of R_1 from the macrolayer solution.
- 2. Calculate the value of R_0 from Equation 56.
- 3. Guess a value for Hamaker's constant, A, and solve the fourth order ODE (Equation 53).
- 4. If Equation 57 is satisfied then microlayer solution is accepted else repeat step 3.

Figure 12 and Figure 13 shows the interface profile and heat flux near the contact line obtained from solution of the above mentioned fourth order ODE. It can be seen that local heat fluxes as high as 1.6×10^8 [W/cm²] can exist near the contact line as previously reported by Lay and Dhir (1995). Two-dimensional quasistatic model of microlayer coupling with macrolayer which was first proposed by Son *et al.* (1999) is used as shown earlier in Figure 3 .The microlayer solution, \dot{V}_{micro} , obtained is evaluated by following equation as given by Son and Dhir (2008)

$$\dot{V}_{micro} = \int_{R_0}^{R_1} \frac{k_l \left(T_w - T_{sat}\right) dr}{\rho_v h_{lv} \delta \Delta V_{micro}}$$
(58)

3. Parallelization Framework

3.1 Introduction

Parallel computing has spearheaded research in computational sciences in an unparalleled way. A new era of multi-core computer has emerged which can be utilized by developing parallel applications. Requirement of sheer computational horsepower are increasingly met with tightly knitted integrated cluster systems comprising thousands of processors, petabytes of storage with high bandwidth/low latency of interconnects consuming megawatts of power, all of which are the paraphernalia of a parallel programming model thus abandoning the tradition of sequential algorithms.

For the comprehensive understanding of the multiphase phenomenon, the resolution of fluid-fluid interactions on very small scales is essential. This requires the usage of parallel computers to study the problem more accurately. The problem is solved on structured grid and domain decomposition method has been implemented using a distributed memory paradigm. Standard MPI protocols are used to communicate between the processors. Currently, the main domain is decomposed into three or more sub-domains in z direction in total. The parallel code is executed on UCLA's Hoffman2 cluster which has 12,516 cores with Ethernet and infiniband interconnects.

Numerical solution of PDEs almost always implies a numerical lattice as the description of domain from which whole solution is sought. The two-dimensional domain has been decomposed into horizontal domains spanning along the vertical direction while the three dimensional domain is decomposed into vertically sliced sub-domains. Each block (or sub-domain) is assigned to one processor (Figure 8). Each processor computes for its block and exchanges halo points (ghost points) with the neighboring processors when required. The value of halo points are updated between the iterations. Since, the width of the finite difference stencils employed in the present implementation ranges up to two grid cells, therefore, upto two slices of boundary ghost cells have to be attached at each domain. The boundary ghost values must be sent by the neighboring processors during the communication phase in the time stepping loop. Section 3.2 to section 3.4 explains the parallelization of the two-dimensional code while section 3.5 explains the parallelization of the three dimensional version.



Figure 8 Parallelization by domain decomposition

3.2 Parallelization of Tri-Diagonal Matrix Algorithm (TDMA)

Presently, there are several approaches for parallelization of the Tri-Diagonal Matrix Algorithm (TDMA). Some of these are listed as:

- 1. Partition Method
- 2. PPT Algorithm
- 3. PDD Algorithm
- 4. LU Pipelining Algorithm
- 5. PTH Method and PPD Algorithm

The algorithm developed by Mattor *et al.* (1995) is implemented and described in detail which is analogous to the inhomogeneous linear differential equation and can be generalized to 5-diagonal and higher banded systems. It is conceptually different from parallel factorization in the sense that no manipulations are performed on the original matrix before subdividing it into different processors. The method adopted is based on LU decomposition, which is more efficient than cyclic reduction as multiple systems of equations needs to be solved.

The problem involving N x N linear system is considered on a parallel computer with P processors.

$$\Lambda X = R$$
where,

$$\Lambda = \begin{bmatrix} B_{1} & C_{1} & & \\ A_{2} & B_{2} & C_{2} & & \\ & \ddots & \ddots & \\ & & \ddots & \ddots & \\ & & & C_{N-1} \\ & & & A_{N} & B_{N} \end{bmatrix}$$
(59)

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 & \mathbf{X}_2 & \mathbf{X}_3 \dots \mathbf{X}_N \end{bmatrix}^T$$
$$\mathbf{R} = \begin{bmatrix} \mathbf{R}_1 & \mathbf{R}_2 & \mathbf{R}_3 \dots \mathbf{R}_N \end{bmatrix}^T$$
(60)

The linear system of order N is subdivided into P subsystems of order M (N=PM, for simplicity). Thus, the N x N matrix Λ is divided into P submatrices L_p, each of dimension M x M.

Where, e_p is the p-th column of the M x M identity matrix. Similarly, vectors X and R are subdivided into P components as:

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 & \mathbf{X}_2 & \mathbf{X}_3 \dots \mathbf{X}_P \end{bmatrix}^T$$
$$\mathbf{R} = \begin{bmatrix} \mathbf{R}_1 & \mathbf{R}_2 & \mathbf{R}_3 \dots \mathbf{R}_P \end{bmatrix}^T$$
(62)

The sub-matrix L_p is given as:

$$\mathbf{L}_{p} = \begin{bmatrix} \mathbf{B}_{M(p-1)+1} & \mathbf{C}_{M(p-1)+1} \\ A_{M(p-1)+2} & \mathbf{B}_{M(p-1)+2} & \mathbf{C}_{M(p-1)+2} \\ \vdots & \ddots & \vdots \\ \vdots & \vdots & \vdots \\ \mathbf{C}_{Mp-1} \\ A_{Mp} & \mathbf{B}_{Mp} \end{bmatrix} = \begin{bmatrix} \mathbf{b}_{1} & \mathbf{c}_{1}^{p} \\ \mathbf{a}_{2}^{p} & \mathbf{b}_{2}^{p} & \mathbf{c}_{2}^{p} \\ \vdots & \ddots & \vdots \\ \vdots & \ddots & \vdots \\ \vdots & \vdots & \vdots \\ \mathbf{c}_{M-1} \\ \mathbf{a}_{M}^{p} & \mathbf{b}_{M}^{p} \end{bmatrix}$$
(63)

For each subsystem p, three vectors X_p^{R} , X_p^{UH} and X_p^{LH} are obtained by solving the following system of equations:

$$L_{p}X_{p}^{R} \equiv \mathbf{r}_{p}$$

$$L_{p}X_{p}^{UH} \equiv \begin{bmatrix} -\mathbf{a}_{1}^{p} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} \end{bmatrix}^{T}$$

$$L_{p}X_{p}^{LH} \equiv \begin{bmatrix} \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} & -\mathbf{c}_{M}^{p} \end{bmatrix}^{T}$$
(64)

The subscripts on the X stand for particular solution, upper homogeneous solution and lower homogeneous solution. The general solution of subsystem P is obtained by the following combination:

$$\mathbf{X}_{p} = \mathbf{X}_{p}^{R} + \boldsymbol{\xi}_{p}^{UH} \mathbf{X}_{p}^{UH} + \boldsymbol{\xi}_{p}^{LH} \mathbf{X}_{p}^{LH}$$

$$\tag{65}$$

Where ξ_p^{UH} and ξ_p^{LH} are undetermined coefficients that depend on coupling to the neighboring solutions, and are obtained by solving the following system of equations:

$$\begin{bmatrix} X_{1,M}^{LH} & -1 & & & \\ -1 & X_{2,1}^{UH} & X_{2,1}^{LH} & & & \\ & X_{2,M}^{UH} & X_{2,M}^{LH} & -1 & & \\ & & -1 & X_{3,1}^{UH} & X_{3,1}^{LH} & & \\ & & & X_{2,M}^{UH} & X_{3,1}^{LH} & & \\ & & & & X_{2,M}^{UH} & X_{3,1}^{LH} & & \\ & & & & X_{2,M}^{UH} & X_{3,1}^{LH} & & \\ & & & & X_{2,M}^{UH} & X_{3,1}^{LH} & & \\ & & & & X_{2,M}^{UH} & -1 & \\ & & & & X_{2,M}^{UH} & -1 & \\ & & & & X_{2,M}^{UH} & -1 & \\ & & & & X_{2,M}^{UH} & -1 & \\ & & & & X_{2,M}^{UH} & -1 & \\ & & & & X_{2,M}^{UH} & -1 & \\ & & & & X_{2,M}^{UH} & -1 & \\ & & & & X_{2,M}^{UH} & -1 & \\ & & & & X_{2,M}^{UH} & -1 & \\ & &$$

-

3.2 Parallelization of Multigrid

Multigrid algorithms are fast and efficient means of solving a variety of integral and partial differential equations by accelerating the convergence especially when applied to elliptic and parabolic equations. It requires that the problem is solved on a hierarchy of grids with different mesh sizes. With ever increasing demand for high resolution PDEs the parallelization of Multigrid for getting asymptotic performance is critical. Parallel Multigrid yields efficient schemes as long as there is sufficient computation to be performed by each processor. Nevertheless, on many parallel architecture, communication latencies are high compared to processor speed making coarse grid calculation dominated by communication. There are mostly four broad categories under which Multigrid can be run in parallel (Chow et al. 2006). These are concurrent iterations, multiple coarse corrections, full domain partitioning and block factorizations. For partitioning, the fine grid is usually subdivided ignoring the coarse mesh divisions. For the present problem, in

order to reduce the inter-processor communication during prolongation and restriction operation, the coarse mesh is derived from the fine mesh partition. The LNTDMA smoother used at every level is parallelized at every level using the decomposition in X and Y direction alternatively as shown in Figure 10. For a general linear equation written in the following form (for the two-dimensional case):

$$a_{i,j}\Phi_{i-1,j} + b_{i,j}\Phi_{i,j} + c_{i,j}\Phi_{i+1,j} + e_{i,j+1}\Phi_{i,j+1} + f_{i,j-1}\Phi_{i,j-1} = d_{i,j}$$
(67)

For sweeping in the X direction, the above equation is modified in the following form:

$$a_{i,j}\Phi_{i-1,j} + b_{i,j}\Phi_{i,j} + c_{i,j}\Phi_{i+1,j} = d_{i,j} - e_{i,j}\Phi_{i,j-1} - f_{i,j}\Phi_{i,j+1}$$
(68)

Which can be further cast into two similar equation as:

$$a_{i,j}\Phi_{i-1,j} + b_{i,j}\Phi_{i,j} + c_{i,j}\Phi_{i+1,j} = d'_{i,j}$$

$$e_{i,j}\Phi_{i,j-1} + b_{i,j}\Phi_{i,j} + c_{i,j}\Phi_{i,j+1} = d''_{i,j}$$
(69)

for i=iist until *iiend* do {Local 'i' loop for every processor} for j = 2 step until NJ do

$$m = \frac{a_{i,j}}{b_{i,j-1}}$$

$$b_{i,j} = b_{i,j} - mc_{i,j}$$

$$d'_{i,j} = d'_{i,j} - md'_{i,j-1}$$
end loop (j)
Backward substitution phase

$$\Phi_{i,j} = \frac{d'_{i,j}}{b_{i,j}}$$
for j = NJ-1 stepdown until 1 do

$$\Phi_{i,j} = \frac{d'_{i,j} - c_{i,j}\Phi_{i,j+1}}{b_{i,j}}$$

end loop (j) end loop (i)

for j=jjst until jjend do {Local 'j' loop for every processor} for i = 2 step until NI do

$$m = \frac{a_{i,j}}{e_{i,j-1}}$$

$$e_{i,j} = e_{i,j} - mf_{i,j}$$

$$d_{i,j}^{"} = d_{i,j}^{"} - md_{i,j-1}^{"}$$
end loop (i)
Backward substitution phase

$$\Phi_{i,j} = \frac{d_{i,j}^{"}}{b_{i,j}}$$
for j = NJ-1 stepdown until 1 do

$$\Phi_{i,j} = \frac{d_{i,j}^{"} - c_{i,j}\Phi_{i,j+1}}{b_{i,j}}$$

end loop (i) end loop (i)

15	7	16 8	3
5	13	6 14	1
11	3	12	4
1	9	2 10	D

Figure 9 Red-black ordering of Gauss-Siedel algorithm

For parallelization of Gauss-Siedel algorithm, commonly used red-black ordering (Figure 9) is described next (Zhu, 1994). The coefficient matrix A in

$$A\Phi = B \tag{70}$$

has the following form,

$$A = \begin{bmatrix} D_b & E\\ E^T & D_r \end{bmatrix}$$
(71)

Where, D_b and D_r are diagonal matrices with -4 on the main diagonal while E is a sparse matrix with only 1s as its entries. Applying the Gauss-Siedel iteration to the unknown :

$$\begin{bmatrix} D_b & 0\\ E^T & D_r \end{bmatrix} \begin{bmatrix} \Phi_b\\ \Phi_r \end{bmatrix}^k = \begin{bmatrix} 0 & E\\ 0 & 0 \end{bmatrix} \begin{bmatrix} \Phi_b\\ \Phi_r \end{bmatrix}^{k-1} + \begin{bmatrix} B_b\\ B_r \end{bmatrix}$$
(72)

The above equation can be separated as:

$$D_b \Phi_b^k = E \Phi_r^{k-1} + B_b$$
$$E^T \Phi_r^k + D_r \Phi_r^k = B_r$$
(73)

Also, D_B is a diagonal matrix with -4 on the main diagonal, which yields:

$$\Phi_b^k = -\left[\frac{E\Phi_r^{k-1} + B_b}{4}\right] \tag{74}$$

The above equation means that all components of $\Phi_b^{\ k}$ can be calculated simultaneously following which all the red unknowns can be calculated as:

$$\Phi_r^k = -\left[\frac{B_r - E^T \Phi_b^k}{4}\right] \tag{75}$$

The completed Gauss Siedel relaxation scheme can be given as:

Initialize error = $1e^{6}$

While (error> tolerance)

- 1. Update all the black unknown points.
- 2. Communicate the black unknown points to the neighboring processors.
- 3. Update all the red unknown points.
- 4. Communicate the red unknown points to the neighboring processors.
- 5. Calculate error.

End

The SOR algorithm can also be parallelized in a similar way.



Figure 10 Domain decomposition in vertical and horizontal directions

3.4 Parallel Two Phase Solver

The parallel framework is summarized in the following algorithm:

Initialization

Initialize level set function with the bubble embryo.

Initialize temperature profile throughout the domain with initial thermal boundary layer.

Time Loop

While current time \leq final time:

Time step restriction.

Compute local time step, δt .

Solve for Level set function (Φ).

Exchange neighbor values of level set function.

Compute ghost values of velocity (U,V,W).

Exchange neighbor values of velocity and temperature.

Solve energy equation to compute temperature (T).

Exchange neighbor values of temperature.

Compute mass flux across the interface.

Extrapolate mass flux at the interface to a narrow band using Fast Marching Method (FMM).

Solve momentum equation to compute velocities.

Exchange neighbor values of velocities.

Solve pressure Poisson equation with intermediate U,V,W to compute P.

Exchange neighbor values of P.

Projection of velocity to divergence free space.

Exchange neighbor values of U,V,W.

Call boundary conditions of U,V,W.

Increment $t = t + \delta t$.

3.5 Parallelization of the coefficient matrix for the 3D two phase solver

The parallelization approach described in section 3.2 to 3.4 was further supplemented using hypre library (for parallelization of the three-dimensional code only). Hypre is a software library for high performance preconditioners and solvers for the solution of large, sparse system of linear equations suitable for massively parallel computers. It supports four conceptual interfaces as follows:

- 1. Structured-grid system interface
- 2. Semi-structured grid system interface
- 3. Finite element interface
- 4. Linear-algebraic system interface

Out of the above four interfaces, the Linear-algebraic system interface (IJ interface) was used as it was possible to couple with the existing three-dimensional code to the IJ interface without changing rest of the code, to enable code scaling upto thousands of processors. The problem data is passed into this interface in the distributed form and matrices are assumed to be distributed in the following form:

$$\begin{bmatrix} A_{0} \\ A_{1} \\ A_{2} \\ . \\ . \\ . \\ . \\ A_{p-1} \end{bmatrix}$$
(76)
65

The resulting system of equations can be solved using variety of preconditioners, some of which are explained in the next section.

3.5.1 ParaSails

ParaSails is a parallel implementation of a sparse approximate inverse preconditioner, using *a priori* sparsity patterns and Frobenius norm least-squares minimization. Additionally it uses a post-filtering technique to reduce the cost of applying the preconditioner. Symmetric positive definite (SPD) problems are handled using a factored SPD sparse approximate inverse while non-symmetric problems are handled with an unfactored sparse approximate inverse. More details about the ParaSails preconditioner can be found from Chow, E. (2000).

3.5.2 BoomerAMG

BoomerAMG is a parallel implementation of the algebraic multigrid method which can be used both as a solver as well as a preconditioner. Different parallel coarsening techniques, interpolation and relaxation schemes can be used. Some of the coarsening techniques that can be used are:

- 1. Cleary-Luby-Jones-Plassman (CJLP) coarsening.
- 2. Falgout coarsening, which is a combination of CJLP and RS coarsening algorithm.
- 3. CGC and CGC-E coarsening.
- 4. PMIS and HMIS coarsening.

Similarly, various interpolation techniques like classical, direct, standard, multipass, two stage and Jacobi, etc can also be used.

3.6 Conclusion

The parallelization techniques discussed in the present chapter aren't sufficient to enable the entire code to be executed in parallel and hence speed up gained was limited to approximately 20% . TDMA, GS and Hypre Library were used interchangeably to solve the linear system of equations as no single technique was sufficient for different conditions like grid stretching, coarse grids etc . In future, rest of the code can be undertaken in parallel with implementation of advanced data structures and algorithms.

4. Two Dimensional Boiling Curve Simulation

4.1 Introduction

In carrying out two-dimensional numerical simulations, the properties of saturated water at 1 atm were used. The contact angles considered are 27°, 38°, 54°, 69° and 90°. In actuality, the contact angle varies dynamically between an advancing contact angle and a receding contact angle however, the effect of dynamic contact angle is not considered in the present work. The dimensionless computational domain for the present study is thus chosen to be $0 \le x \le 5$ and $0 \le x \le 5$ $y \le 50$ resolved by grid density of 386 x 386. The width of the computation domain has to be atleast 2.5 cm for simulating the entire boiling curve as the Taylor most dangerous wavelength (λ_D) corresponding to earth normal gravity is approximately 2.5 cm. The height of the domain is chosen to be large enough so that the bubble motion would not get affected by the top boundary of the computational domain. A non uniform grid spacing in the y direction is taken with the node expansion ratio of 1.01, except near the wall $0 \le y \le 0.45$, where the node spacing is uniform as Δy . The node spacing in the x direction is uniform throughout with Δx while the side boundaries at x = 0 and x = 5 are treated as symmetric. The non-dimensional governing equations of mass, momentum and energy are solved for both the liquid and vapor phases. The non-dimensionalized length (l_0) , time (t_0) and velocity (u_0) scales are defined in terms of surface tension (σ), earth normal gravity (g), water density (ρ_l) and vapor density (ρ_v) as:

$$l_o = \sqrt{\frac{\sigma}{g\left(\rho_l - \rho_v\right)}}, \ u_o = \sqrt{\left(gl_o\right)}, \ t_o = \frac{l_o}{u_o}$$
(77)

The values of non-dimensionalized scales defined above are evaluated as $l_0 = 2.5$ mm, $t_0 = 15.97$ ms and $u_0 = 0.16$ m/s. The liquid temperature profile is defined as linear in the natural convection thermal boundary layer and the fluid velocity is set equal to zero. The initial thermal

boundary layer thickness, δ_r , is evaluated from the following turbulent natural convection heat transfer correlation:

$$\delta_T = 7.14 \left(\frac{\mu_l \alpha_l}{\rho_l g \beta_T \Delta T} \right)^{1/3}$$
(78)

Since heat conduction in the solid phase is not computed, in order to simulate realistic surface bubble nucleation frequency and cavity density (*Na*) are obtained from correlations reported in the literature. There are many expressions for bubble waiting time which however require the knowledge of the cavity size and the thermal properties of the heater (Hsu and Graham, 1986, Kocamustafaogullari and Ishii, 1983). Therefore, the correlation proposed by Basu et al. (2005) (Equation 79, 80) is used for computing the waiting period and nucleation site density.

$$t_{wait} = \frac{139.1\Delta T^{-4.1}}{t_o}$$
(79)

$$Na \; (\text{sites/cm}^2) = 0.34 \left[1 - \cos \varphi \right] \Delta T^{2.0} \quad \text{for } \Delta T < 15 \text{ K}$$
$$Na \; (\text{sites/cm}^2) = 3.4 \times 10^{-5} \left[1 - \cos \varphi \right] \Delta T^{5.3} \text{for } \Delta T \ge 15 \text{ K}$$
(80)

To obtain the number of cavities for the two-dimensional case (of length L_x) from the actual experimental correlation, which is for three-dimensional case, the following relation is derived based on square grid arrangement of cavities in three-dimensional case:

$$N = L_X \sqrt{Na} \tag{81}$$

The value of L_x for the two-dimensional case is 1.25 cm. The properties of the water used for the present case are listed in Table 1.

Properties	Value	Units
Thermal conductivity of liquid	0.681	W/m-k
Thermal conductivity of vapor	0.0248	W/m-k
Surface tension	0.0589	N/m
Specific heat capacity of liquid	4212	J/kg-k
Specific heat capacity of vapor	2020	J/kg-k
Density of liquid	958	Kg/m ³
Density of vapor	0.5977	Kg/m ³
Kinematic Viscosity of liquid	$3.0 \ge 10^{-7}$	m^2/s
Kinematic Viscosity of vapor	2.01 x 10 ⁻⁵	m^2/s
Thermal expansion coefficient	7.1 x 10 ⁻⁴	1/k
Latent heat of vaporization	$2.26 \ge 10^6$	J/Kg

Table 1 Property values used for the current study

Contact Angle	ΔT _w [K]	Na (Basu) [Sites/cm ²]	Na (2D Case) [Sites/cm]	t _{wait} * [-]
27	10	4	2	0.69186636
27	15	6	3	0.13123451
27	20	29	7	0.04034588
27	24	76	11	0.0191054
27	28	173	16	0.01015487
27	30	250	20	0.00765288
38	10	7	3	0.69186636
38	15	12	4	0.13123451
38	20	57	9	0.04034588
38	24	149	15	0.0191054
38	28	337	23	0.01015487
38	30	485	28	0.00765288
54	10	14	5	0.69186636
54	15	24	6	0.13123451
54	20	110	13	0.04034588
54	24	289	21	0.0191054
54	28	655	32	0.01015487
54	30	944	38	0.00765288
69	10	22	6	0.69186636
69	15	37	8	0.13123451
69	20	171	16	0.04034588
69	24	450	27	0.0191054
69	28	1019	40	0.01015487
69	30	1469	48	0.00765288
90	10	34	7	0.69186636
90	15	58	10	0.13123451
90	20	267	20	0.04034588
90	24	702	33	0.0191054
90	28	1589	50	0.01015487
90	30	2290	60	0.00765288

Table 2	Waiting	time and	nucleation	site densit	y for (different	contact	angles
					/			

Initially small bubble embryos are placed sequentially along the heater surface with nucleation time interval equal to the waiting time between cavities. The addition of new bubble depends on the waiting period thereafter. Cavities are evenly spaced along the length of the heater with the maximum limit of 100 cavities in order to keep the cavities separated by at least 3-4 grid points. Table 2 shows the number of cavities (rounded off) and the waiting time for different superheat considered for the current work till wall superheat of 30 °C. For the present work dry region at the heater surface during boiling process is considered by accounting the area of the adsorbed film under the bubble, corresponding to the radius R_0 from the cavity centre, as shown in Figure 11 whereas the wall heat flux and the heat flux going into the vapor phase are computed from the following two equations, where q_{mic} is the microlayer contribution to the wall heat flux computed separately near the contact line.

$$q_{wall} = \left(\frac{-k_{liq} \left(\frac{\partial T_f}{\partial y}\right)_{|y=0} A_{liq} - k_{vap} \left(\frac{\partial T_f}{\partial y}\right)_{|y=0} A_{vap} + q_{mic} A_{mic}}{A_{wall}}\right)$$
(82)

$$\vec{q}_{vap}^{"} = \vec{n} \cdot \left(k_l \nabla T_l - k_v \nabla T_v \right) \tag{83}$$

In Equation 82, A_{liq} is the liquid occupied area of the surface, A_{vap} is the dry area below the bubble excluding the microlayer area and A_{mic} is the microlayer area underneath the bubble calculated by multiplying the contact line length by the length of the microlayer. The microlayer profile and heat flux, with respect to distance from R₀, obtained by solving microlayer equations for contact angles 38° and 69° are shown in Figure 12 and Figure 13 respectively.



Figure 11 Dry area under the bubble.



Figure 12 Interface profile and heat flux variation along microlayer (ϕ = 38 ° and ΔT = 12 ° K)



Figure 13 Interface profile and heat flux variation along microlayer (ϕ = 69 ° and Δ T=12 ° K)

4.2 Results and Discussion - Contact Angle 38°

Figure 14 - Figure 19 shows the bubble growth and merger pattern with liquid velocity vectors along with wall heat flux and wall void fraction variation for different superheats for the case of contact angle of 38° only Figure 14 shows the boiling process for wall superheat of 17 °C (Point a in Figure 26). At $t^* = 0.30$ all the cavities have nucleated with the bubbles still attached to the surface pushing the liquid out of the domain shown by upward pointing velocity vectors. As the simulation progresses, the periodical formation of liquid macrolayer formed due to liquid entrapment below lateral merger of the bubbles is observed during the whole period of vapor evolution. At $t^* = 6.00$ bubbles have merged in both the vertical and horizontal directions creating an elongated vapor mass continuously being fed from bubbles nucleating from the surface. It can be seen at $t^* = 8.00$ that the process has transitioned into a quasi-static state in which the same pattern is seen repeating multiple times as time proceeds. Figure 15 shows the temporal variation of wall void fraction and heat fluxes per unit surface area of the heater from the wall and into vapor production. When the heat fluxes are averaged over the entire area, except the early computation time ($t^* \ge 6$), it is found that about 50% of the energy from the wall is utilized in vapor production (including microlayer) while the other half is utilized in superheating the liquid. Since vapor is assumed to be saturated for the present case, energy utilized for superheating of vapor is zero.







Figure 15 Temporal variation of heat fluxes and wall void fraction (Nucleate boiling, $\Delta T = 17$ °C)



Figure 16 shows the boiling process numerically simulated at CHF corresponding to wall superheat of 27.5 °C (Point b in Figure 26). Long vapor columns or jets can be seen evolving at t* = 11.50 which constricts near to the surface. At $t^* = 13.47$ multiple liquid droplets can be seen getting entrained into the vapor column which merge and break among themselves inside the vapor core. This pattern resembling at $t^* = 13.47$ is seen repeating again at $t^* = 14.37$, $t^* = 16.11$ and at t^* = 18.19. However, at $t^* = 16.11$ liquid filament is seen inside the vapor column rather than droplets unlike $t^* = 14.37$ and $t^* = 18.19$. Figure 17 shows the temporal variation of wall void fraction and heat fluxes for this case. Except for the early simulation time, a drop in the wall void fraction at any time instant causes a spike in the wall heat flux. At $t^* = 4.00$ a temporary drop in the wall void fraction to 0.56 causes the instantaneous spatial averaged wall heat flux to rise to 107.34 W/cm^2 showing negative correlation between wall heat flux and wall void fraction. Between $t^* = 4.00$ to $t^* = 11.50$ only minor oscillations in the heat flux is seen as the jet is still rising and wall void fraction is almost constant. After $t^* = 11.50$ as the vapor exits the domain, liquid inflow occurs from the sides. Significant oscillations in the heat fluxes is seen thereafter as the jet breaks near the surface altering the wall void fraction. The temporal averaging is done after $t^* \ge 12$ over the entire area to compute wall heat flux and wall void fraction. Figure 18 shows the boiling process at transition regime corresponding to the wall superheat of 40 °C (Point c in Figure 26). Initially much of the surface area is covered by vapor due to an increase in the active nucleation sites. The average vapor velocity is approximately 0.2 m/s. At $t^* = 6.67$ instability of the vapor column can be seen close to the heater surface which causes it to detach and form an elongated bubble. At $t^* =$ 7.42 vapor slug is seen evolving from the surface and assimilating into the elongated bubble. This process can be seen repeating multiple times henceforth. Temporal variation of wall void fraction

and heat fluxes for the case of transition boiling is plotted in Figure 19. Due to the formation of stationary vapor stems trapping liquid macrolayer between them, no significant oscillation with time in the wall void fraction and thereby wall heat flux is observed (Figure 20). The average value of wall void fraction is computed to be 0.954 for the present case while the value of heat flux from the wall is 38.18 W/cm^2 .

The understanding of the mechanism behind CHF is still unclear. Zuber's (1958) hydrodynamic theory model, later extended by Lienhard and Dhir (1973), does not include the surface effects on maximum heat flux. However, there is substantial evidence that the maximum heat flux is influenced by the degree of wettability of the heater (Costello and Frea (1965), Hasegawa *et al.* (1973), Hahne and Diesselhorst (1978)). Table 3 shows the comparison of the values of critical heat flux, which for the current study is 78.9 W/cm² in comparison to the CHF value of 76.8 W/cm² obtained by Liaw and Dhir (1989), for the same contact angle but for vertical surface. CHF values of 80.3 W/cm² ($\phi = 37^{\circ}$) and 72.75 W/cm² ($\phi = 38^{\circ}$) were obtained experimentally for different surface material by Hahne and Diesselhorst (1978). Figure 27 shows the variation of wall void fraction with superheat, at CHF the value of wall void fraction computed is 0.72, implying that the liquid can access about 25% of the surface and the maximum heat flux, which is lower than the Zuber's model, is due to the limitation on the energy removal mechanism on the liquid occupied region of the surface (Liaw and Dhir (1989)).

Auracher *et al.* (2004) performed experiments for well wetting fluids and fluids with larger contact angle under steady state and transient conditions, and did not observe any hysteresis in the transition region for a clean heater surface. For the present study hysteresis is not considered in the

transition boiling regime, which corresponds to region between wall superheat of 27.5 °C and 110 °C. In the current simulation the value of wall void fraction increases with increase in superheat implying that liquid contact with the surface has decreased. Theoretically using Zuber's value of minimum heat flux (Equation 84), with the value of C_2 taken as 0.09, and Berenson's correlation (Equation 85) for film boiling, the transition to film boiling occurs at a wall superheat of 85.2 °C. However, for the present study since the computed value of wall heat flux at the wall superheat of 130 °C is higher than that of 110 °C it can be stated that 110 °C is the wall superheat corresponding to minimum wall heat flux and wall heat flux starts increasing thereafter.

$$q_{\min}^{"} = C_{2} \rho_{v} h_{fg} \left[\frac{g \sigma \left(\rho_{l} - \rho_{v} \right)}{\left(\rho_{l}^{2} + \rho_{v}^{2} \right)} \right]^{1/4}$$
(84)

$$Nu = 0.42 \left[\frac{\rho_v (\rho_l - \rho_v) g h_{fg}}{k_v \mu_v \Delta T} \right]^{1/4} \left[\frac{\sigma}{g(\rho_l - \rho_v)} \right]^{3/8}$$
(85)

For the case of film boiling, the value of heat flux is computed to be 0.42 W/cm^2 against 2.29 W/cm² given by Berenson's correlation (for film boiling heat transfer coefficient) for a wall superheat of 110 °C while a value of 1.21 W/cm² was obtained by Son and Dhir (1997) at a wall superheat of 100 °C (Table 4).

Contact Angle	Surface	CHF [W/cm ²]	Reference
38 °	Horizontal	78.9 (Numerical)	Present work
38 °	Vertical	76.8 (Experimental)	Liaw and Dhir (1989)
35 °	Vertical	86.27(Experimental)	Wang and Dhir (1993)
37 °	Horizontal (CrNi-Steel)	80.3 (Experimental)	Hahne and Diesselhorst (1978)
38 °	Horizontal (Ta)	72.75 (Experimental)	Hahne and Diesselhorst (1978)
40 °	Horizontal	74.75 (Theoretical)	Kandlikar (2001)
45 °	Horizontal	76.5 (Experimental)	Maracy and Winterton (1988)

Table 3 Comparison of CHF values

Fluid	ΔT (°C)	Berenson's correlation $[W/cm^2]$	Son and Dhir $[W/am^2]$ (1007)	Present work
			[w/cm](1997)	
Water	100	2.14	1.21	
Water	110	2.29		0.42
Water	130	2.60		0.83
Water	158	3.01	2.06	

Table 4 Comparison of heat flux for film boiling



Figure 17 Temporal variation of heat fluxes and wall void fraction (CHF, $\Delta T = 27.5$ °C)




Figure 19 Temporal variation of heat fluxes and wall void fraction (Transition boiling, $\Delta T = 40$ °C)



Figure 20 - Shape of the vapor stem at the surface







Figure 22 Temporal variation of heat fluxes and wall void fraction (Film boiling, $\Delta T = 110$ °C)

At a wall superheat of 110 °C the boiling process is in the regime of film boiling as shown in Figure 21. Only the first cycle of bubble evolution has been shown here. At $t^* = 4.39$ full grown vapor bubbles have evolved and are about to detach from the vapor film formed at the surface while at $t^* = 5.24$ the vapor bubbles have detached completely from the vapor film and start rising upwards. The variation of heat fluxes and wall void fraction is plotted in Figure 22. Since the value of wall void fraction is unity everywhere the value of the computed heat flux from the wall and into the vapor are same.

At a wall superheat of 130 °C (Point d in Figure 26) the boiling process is in the regime of film boiling as shown in Figure 23. Only the first cycle of bubble (which is two-dimensional in shape) evolution has been shown here. At $t^* = 4.81$ thin vapor film is seen at the surface while at $t^* = 44.40$ full grown vapor bubbles have evolved and are about to detach from the vapor film formed at the surface. The second set of bubble is formed at the center at $t^* = 64.13$. The variation of heat fluxes and wall void fraction is plotted in Figure 24 showing the bubble release points also. Since the value of wall void fraction is unity everywhere the value of the computed heat flux from the wall and into the vapor are same. It has to be noted that the initial instability seen at the surface is captured from the numerical model naturally otherwise an initial specification of the vapor film profile has to be user defined in some cases (FLUENT tutorial: Horizontal film boiling, 2005).

Figure 25 shows the fluctuating interface velocity at the middle of the surface. At approximately $t^* = 40$ is close to zero as bubbles are about to be released at the edges of the surface $(x^* = -5 \text{ and } x^* = 5)$. The peaks at $t^* = 50$ and $t^* = 65$ corresponds to the velocity of the departed bubble for the case of $\Delta T = 130$ °C and $\Delta T = 170$ °C. Temporal and spatial averaged wall heat flux

and wall void fraction are plotted versus wall superheat neglecting the variations during early periods of computation ($t^* \le 40$). Figure 26 shows the simulated boiling curve compared against experimental data obtained Gaertner, 1965 (horizontal surface, unspecified contact angle) and Stephan and Abdelsalam correlation (1980) for the nucleate boiling regime and with Berenson's correlation for the film boiling regime.



Figure 23 Boiling process at film boiling ($\Delta T = 130 \text{ °C}$)

 x/l_o



Figure 24 Temporal variation of heat fluxes and wall void fraction (Film boiling, $\Delta T = 130$ °C)



Figure 25 Interface velocity at the centre during the early evolution period $(\phi=38^\circ, \Delta T=130 \ ^\circ C \ \& \ 170 \ ^\circ C)$



Figure 26 Boiling curve for the case of contact angle of 38°



Figure 27 Variation of wall void fraction for contact angle of 38°

4.2 Results and Discussion - Variable Contact Angles ($\phi = 27^{\circ}, 54^{\circ}, 69^{\circ}, 90^{\circ}$)

Figure 29 shows the simulated boiling curves obtained by extending the current numerical model for different contact angles. Even though time dependent conservation equations are being solved, the results are shown only when quasi-static conditions are reached in terms of stabilization of wall heat flux and wall void fraction. The effect of change in contact angle on the boiling curve is clear as the contact angle decreases the boiling curve shifts towards right. Major discrepancy is seen in the trend of the nucleate boiling regimes for the set of simulated boiling curves in the sense that with an increase in contact angle, the nucleate boiling heat flux is lower in comparison to the lesser contact angle case. For eg., at a wall superheat of 18 °C, the nucleate boiling heat flux of 90° is lowest while 27° is highest. Possible explanation for this incorrect trend is that the two-dimensional approximation manifests itself as horizontal vapor cylinders rather than spherical vapor bubbles in reality. For all the contact angles maximum heat flux computed is less than the hydrodynamic theory with the deviation from the hydrodynamic theory yielded values being more as the wettability of the surface is decreased. It is also seen that the superheat at which the maximum heat flux occurs rises as the contact angle is decreased, and thus it can be inferred that the slope of the locus of q_{max} in Figure 29 is around 3 with respect to wall superheat.

The overall heat transfer rate from the surface is the summation of heat removal from both the dry and the wet areas on the surface. In the present analysis, the surface temperature over both the dry and wet areas is held constant which is realizable for thick heaters with high thermal conductivity as for heaters which have poor thermal conductivity and are thin, a significant difference in surface temperature might exist (Dhir (1998)). Hysteresis of the boiling curve is not considered in the present study but as reported by Auracher *et al.* (2004) that single and reproducible boiling curves are obtained provided if precise temperature control system is used in conjunction with a clean heating surface, as even minimal deposits on the surface has the tendency to shift the boiling curve with successive runs. They also stated that the situation is however different for transient modes as the heating and cooling transients yield different boiling curve even for clean surface conditions.

Figure 28 shows the steady state maximum heat flux obtained from the current numerical model. As stated earlier the CHF is seen decreasing with increase in contact angle and the slope of the locus of CHF with variation in contact angle is negative with a magnitude of 1.2 approximately. The numerical value of CHF obtained from the present simulations are in good agreement to the experimental data reported by Hahne and Diesselhorst (1978) done on horizontal cylinders. The data obtained by Liaw and Dhir (1989) is for vertical surface and it can be inferred by virtue of its slope that the effect of contact angle on CHF is weak for the vertical surface as compared to the horizontal surface. For simulations with contact angle of 90° the microlayer contribution is not accounted for with the assumption that there is no microlayer formation. Subsequently, it was found out that the CHF value for a contact angle of 90° is only 8% of that given by Zuber (1959) even when 20% of the surface is covered with liquid. This reinforces the reasoning provided by Liaw and Dhir (1989) that for poorly wetted surface the maximum heat flux conditions are limited by the rate of evaporation near the surface as surface still has access to liquid.

Transition boiling curve is characterized by the negative slope on the boiling curve due to the reduction in wall heat flux on increasing the wall superheat and is inherently unstable. Transition boiling curve also depends on whether it is being approached from nucleate boiling or film boiling side. The effect of surface wettability on hysteresis on the transition boiling curve has been investigated by Liaw and Dhir (1986). Their experiments have shown that the transition boiling heat fluxes during heating mode is higher than that obtained from the cooling mode and the difference in the transition boiling curves obtained from the cooling mode and the heating mode diminishes as the surface wettability reduces. Another study done by Maracy and Winterton (1988) on horizontal surface using water also showed hysteresis at lower contact angles as well with the transition boiling heat flux being higher in the heating mode than in the cooling mode. In the present study the simulations are started from bubble inception rather than using the converged solution of lower wall superheat simulation result as the initial condition.



Figure 28 Comparison of influence of contact angle on CHF

Figure **30** shows the variation of wall void fraction with superheat for different contact angles. Computation of wall void fraction is vital, especially in the transition boiling regime which is unstable by virtue of it being a combination of unstable nucleate boiling and unstable film boiling. Some of the models applicable for the transition boiling models rely on the fraction of liquid contact time on the heater surface. For instance, it has been suggested by Bjornard and Griffith (1977) that the heat flux at any wall superheat is the combination of maximum heat flux (q_{max}) and minimum heat flux (q_{min}) and hence can be given by:

$$q = F_L q_{\text{max}} + (1 - F_L) q_{\text{min}} \tag{86}$$

where, F_L is the fractional area occupied by the liquid and is correlated by:

$$F_{L} = \left[\frac{T_{\min} - T}{T_{\min} - T_{\max}}\right]^{2}$$
(87)

Another way to estimate transition boiling heat flux was proposed by Liaw and Dhir (1986), in which the transition boiling heat transfer coefficients were expressed as the combination of the heat transfer coefficients over wet and dry areas as given below:

$$h = \beta_{h,c} F_l h_l + h_g (1 - \beta_{h,c} F_l)$$
(88)

In the above expression, h_l and h_g are time averaged heat transfer coefficients over the wet and dry areas respectively, F_l is the time averaged fractional area of the heater accessible to the



Figure 29 Comparison of numerically simulated boiling curves for different contact angles



Figure 30 Comparison of numerically computed wall void fraction for different contact angles

liquid, $\beta_{h,c}$ is a parameter depending on heating curve or cooling curve with its value decreasing with increase in contact angle and lies between 0 to 1.

Figure 31 shows the variation of minimum heat flux, q_{min} , as a function of contact angle. It can be seen that the numerically simulated values are lower than those obtained by Liaw and Dhir (1989) for experiments in heating mode on a vertical plate, and are 50-75% less than those given by Berenson's correlation. Overall, in comparison to both experimental and theoretical values very low heat flux is seen in the film boiling region due to vapor fractional area close to unity. The q_{min} values from simulation decreases linearly approximately by a factor of 2 as the contact angle is increased from 27° to 90° since the superheat at which q_{min} occurs is less for the latter with near about same void fraction. This is in agreement to the reasoning provided by Liaw and Dhir (1989) that the incoming liquid spreads quickly on a well wetted surface and hence transition boiling starts earlier with q_{min} being higher.



Figure 31 Variation of minimum heat flux for different contact angles.

4.4 Conclusion

This chapter was focused on attempting to simulate boiling curves for different contact angles under the assumption that boiling process is two-dimensional. The nucleation site density for the two dimensional was obtained by conversion from the correlation values for three dimensional case. The values of q_{max} and q_{min} decreases with increase in contact angle indicating that the trend is consistent with literature. However the trend seen in the nucleate boiling heat flux with contact angle at a particular wall superheat (before CHF) was completely opposite to the trend reported in the literature as the two-dimensional approximation makes a symmetric boundary condition approximation in the third dimension, and hence manifesting an actual spherical vapor bubble to infinitely long cylindrical vapor structures. This incapacitates the two-dimensional model to yield any meaningful physical results and reinforces the statement that three-dimensional simulation are the only way to numerically study the boiling process.

5. Three Dimensional Boiling Curve Simulation

This chapter focuses on carrying out 3D simulations of boiling process. Since 3D simulations require tremendous amount of computational time so both coarse grid results with long run times and fine grid simulations with short run time have been performed. Even though fine grid results are more accurate than coarse grid results *when converged*, the coarse grid results have an excellent property that residuals drop very rapidly as shown in Figure 32. The computational areas for coarse grids and fine grids are taken as dimensionless length and width as $5.5 \times 5.5 (1.89 \text{ cm}^2, 66 \times 98 \times 66)$ and $2 \times 2 (0.258 \text{ cm}^2, 98 \times 194 \times 98)$ respectively. The domain dimensions for coarse grid case has been selected to accommodate Taylor's most dangerous wavelength while for the fine grid cases is smaller as the intention is to investigate the effect of grid size on computational results.

5.1 3D Coarse Grid Simulations, Case I (φ=38°)

Three dimensional numerical simulations on coarse grids were carried out using the properties of saturated water at 1 atm. The contact angle was considered to be static with a value of 38°. In reality, the contact angle varies dynamically between an advancing (maximum) contact angle and a receding (minimum) contact angle depending on the speed of the contact line reviewed earlier by Dusan (1979). Since, the value of non-dimensionalized Taylor's most dangerous wavelength \approx 5, the non-dimensionalized computational domain length and width for the present study is chosen to be $0 \le x \le 5.5$, $0 \le y \le 11$ and $0 \le z \le 5.5$ resolved with a grid density of 66 x 98 x 66.



Figure 32 Residual reduction on different grids (Jacobsen et al. (2013))

Wall superheat, ∆T, (°C)	Cavity density, (Basu <i>et al.,</i> 2005) φ = 38° Na , [Sites/cm ²]	Number of cavities, N $\varphi = 38^{\circ}$ (3D Coarse) Area = 1.89 cm ²	Number of cavities, N $\varphi = 38^{\circ}$ (3D Fine) Area = 0.258 cm ²	Number of cavities, N $\varphi = 69^{\circ}$ (3D Fine) Area = 0.258 cm ²	Waiting time (Milliseconds)
15	12	24	4	9	2.09
18	32	61	8	24	0.64
20	57	107	15	44	0.43
24	149	281	38	116	0.25
28	337	400	87	263	0.18
33.5	871	400	225	680	0.12
40	2230	400	575	900	0.037
60	19124	400	900	900	0.007
100	286661	400	900	900	0.0008
125	935388	400	900	900	0.0003
130	1151512	400	900	900	0.0002

Table 5 Nucleation sites and waiting time used for the 3D simulations



Figure 33 Maximum cavity distribution of 400 for coarse grid cases

Gaertner (1963) and Sultan and Judd (1978) found that active sites are randomly distributed on a heated surface obeying Poisson distribution. Also as pointed out in Shoji (2003), nucleation sites can interact with each other altering the local wall superheat and other parameters that determine the nuclei stability. They also affect the number of active sites causing intermittence in bubble production. However, for the present case small bubble embryos are placed sequentially along the heater surface with atleast 3-4 grid spacing apart and already nucleated at the start of the simulation. The addition of new bubble on a particular cavity occurs after the previous bubble has left with time interval being equal to the waiting time. Table 5 shows the number of cavities and the waiting time obtained from the correlation of Basu et al. (2005) for different superheats considered for the current work. The maximum cavities that can be placed depends on the number of grids and hence the fine grid cases can accommodate more cavities than the coarse grid cases. It has to be noted here that upon successive nucleation the creation of artificial vapor bubble displaces the already present superheated liquid thus altering the mass and energy content of the computational domain and manifests itself as the numerical artifact. Contrary to the two-dimensional case the vapor is not assumed to be saturated and hence energy equation is being solved for both the phases. Figure 34- Figure 37 shows the bubble evolution for different regimes of the boiling curve at a cross section of z = 3.49 mm which is at quarter length of the z extent of the domain. The starting bubble evolution period of 30 ms during which the mushroom shaped bubble is formed is





ignored and only the period for which the heat flux is stabilized demonstrating quasi-static case has been shown for Figure 34. The interface is shown as a dark black line separating the two phases while the temperature fields are shown as colored contours on a normalized scale of 0 (saturated) to 1 (wall superheat). Figure 34 (a), (b), (c) and (d) corresponds to t = 0.0 ms, 13.0 ms, 22.3 ms and 30.2 ms of Figure 38, showing time varying wall heat flux and wall void fraction. The vapor evolution configuration at a wall superheat of 15 °C is shown in Figure 34. Repeated formation of macrolayer, which is millimeter scale liquid layer left attached to the heater surface influencing nucleation and contact line phenomenon, beneath the mushroom bubble is seen. The mushroom bubble is being fed continuously by nucleating bubbles at the surface in addition to the vapor generated from the vapor stems implanted in the thermal layer (superheated liquid layer). From the temperature profile being developed close to the surface it can be seen that the thermal layer inside the vapor is elongating upwards due to the dominant effect of convection transport due to rising vapor while the thermal layer in the liquid side is constricted due to the downward inflow of the liquid from the top. The mushroom bubble formed breaks at a time of approximately 30 ms from the surface at which wall heat flux also drops as there are no formation of vapor stems beneath the bubble.

The area and temporal averaged wall heat flux for wall superheat of 15 °C is 15 [W/cm²] approximately while wall void fraction being 0.15. Upon increasing the wall superheat to 27°C additional nucleation sites gets activated and a sustained vapor column is seen carrying superheated vapor out of the domain from the top. From Figure 39 it can be inferred that the average value of heat flux computed at CHF is about 60 [W/cm²] with wall void fraction value being 0.68. The simulation from CHF onwards are done keeping the nucleation sites to a fixed

value of 400 as any more accumulation of nucleation sites is not possible from computational point of view (Figure 33), as nucleating bubbles occupy 3-4 grid spacing and sites are denoted by point cavities located at discrete grid points. When a sustained superheat vapor column is formed (Figure 35), some of the nucleation sites are eclipsed by the vapor column base and only the sites which are away from the vapor columns nucleate. The bubbles thus generated drift inwards upon departure from the surface towards the vapor column under the action on liquid inflow at the sides. Upon increasing the wall superheat to 30°C the computed wall heat flux drops from its peak value of 60 [W/cm²] to 40 [W/cm²] marking the transition boiling regime as shown in Figure 36. Figure 37 shows the film boiling simulation observed at a wall superheat of 130°C. The entire surface is covered with a vapor film with the value of wall void fraction reaching unity. For the case of film boiling, no temperature gradient in the liquid phase is observed signifying zero liquid superheat. On the contrary, for the vapor phase the trend seen is opposite - for lower nucleate boiling regime the vapor superheat is less and as the wall superheat is increased the vapor gets more superheated. Similar observations were reported by Buchholz et al. (2006) who measured vapor superheat of approximately 2 [K] at lower nucleate boiling and upto 40 [K] vapor superheat for wall superheat of 80 [K].





Figure 37 Bubble evolution at film boiling (Z=3.49 mm, Δ T=130 °C)



Figure 38 Variation of wall heat flux and wall void fraction (ΔT =15 °C)



Figure 39 Variation of wall heat flux and wall void fraction (ΔT=27 °C)



Figure 40 Growing mushroom bubble (top) along with the cavity distribution (bottom) $(\Delta T = 15.0 \text{ K})$



Figure 41 Formation of vapor column (top) and cavity distribution (bottom) ($\Delta T = 27.5 \text{ K}$)

Vertical Height [mm]	Vapor Fraction [-]	Jet Diameter (mm)	Vapor Velocity [m/s]	Vapor Flow Rate [mm ³ /s]
6.87	0.51	11.09	0.92	89172
13.75	0.59	11.92	0.79	89126
20.62	0.45	10.49	1.03	89311
27.15	0.17	6.51	2.66	88645

Table 6 Average vapor velocity, vapor fraction and jet diameter with height at CHF


Figure 42 Vertical velocity variation with lateral distance at different heights at CHF

Figure 42 shows the planar velocity profile at three different height of the sustained vapor column seen during CHF (Figure 41). It can be seen that the centerline vapor velocity inside the vapor column has a maximum value lying in the range of about 6-8 [m/s]. Although liquid is primarily flowing down yet it has upward velocity close to the interface due to the shear forces exhibited by the outgoing vapor at the interface. However, at the vertical distance of 6.75 mm the liquid velocity has only negative values stating that liquid does not experiences significant drag. Table 6 shows the average vapor velocity, vapor fraction and equivalent jet diameter at three different height for the case of CHF.

Figure 43 shows the simulated boiling curve and comparison to the existing correlations. The nucleate boiling regime of the boiling curve is under predicted from Stephan and Abdelsalam (1980) and Rohsenow (1952) correlation with the slope of the simulated boiling curve being approximately 4. It can be seen that the differences between the Stephan and Abdelsalam (1980) correlation values and the simulated values increases from 33% approximately at the low superheat to about 50% at the higher end of nucleate boiling.

Figure 44 shows the variation of wall void fraction with superheat in comparison to the two dimensional numerical simulation performed earlier by Garg and Dhir (2015) plotted on a linear scale for clarity. Since no data for wall void fraction spanning the entire boiling curve is available for horizontal surface, comparison is made with the two-dimensional simulations performed earlier using the same numerical model. For the transition boiling regime the deviation in the values of wall void fraction is very low and it is seen that for a wall superheat of 40°C onwards more than 90% of the area is covered with vapor for both the cases.

In the transition boiling regime some comparison can still be made as experimental data is available. Figure 45 shows the variation of F-factor, fraction of liquid contact, as a function of wall superheat. Experimental values reported by Lee et al. (1985) are considerably different and higher than the numerical values as the F factor calculated by them is rather local liquid contact time fraction, which is the time during which the liquid makes contact with the heater surface at a particular point, rather than the fraction of liquid area on the heater surface. With the assumption that the process is ergodic (Lee et al. 1985), the F factor can be approximated as the ratio of liquid contact area to total area which equals to liquid contact time to total time at any given point. Data points from Ragheb and Cheng (1979) is originally for flow boiling with the assumption that F=1 at q_{max} and F=0 and q_{min} while that from Tong and Young (1974) is simply the ratio of transition boiling heat flux to critical heat flux. In the present study, the F factor is both temporal and spatial averaged and hence can be simply expressed as 1 - α (wall void fraction). As pointed out by Buchholz *et al.* (2006) due to high driving ΔT in the transition boiling, the local evaporation process is very fast and the intermittent liquid solid contacts is expected to be related to high vapor velocity. They reported that these local rewetting and vapor growth at the surface leads to temperature drop rates of upto 30 [K/ms]. In the present simulations intermittent liquid-solid contacts (frequency ~ 100 contacts s⁻¹) are seen during the simulations for the transition boiling as can be inferred from Figure 36 with 4 contacts in a time span of roughly 40 ms. For the present case some liquid solid contacts were seen in the film boiling as well with the computed F factor value being non zero at a wall superheat of 100 °C onwards till 125 °C (F-Factor of 0.0013), also it has been reported that the F factor value has a non zero value into the film boiling regime as well signifying some degree of intermittent liquid solid contacts



Figure 43 Simulated boiling curve



Figure 44 Variation of wall void fraction with superheat



Figure 45 Variation of F factor with superheat in the transition boiling regime



Figure 46 Vapor configuration (top) and cavity distribution (bottom) ($\Delta T = 40.0$ K)



27.5 mm



Figure 47 Bubble release (top) and cavity distribution (bottom) ($\Delta T = 130.0$ K)

5.2 3D Fine Grid Simulations , Case II (φ=38°, φ=69°)

The case described in the present section case was run for finer grid with the intention of resolving the anomaly observed in the trend for nucleate boiling regime for the two-dimensional cases. Simulation were run for two contact angles of 38° and 69° with the quarter domain extents being $0 \le x \le 2$, $0 \le y \le 10$ and $0 \le z \le 2$ (non dimensionalized form) resolved with a grid density of 98 x 194 x 98. The cavity distributions for both the contact angles are shown in Figure 48 and Figure 49 while the simulated boiling processes are shown in Figure 50 - Figure 53. It has to be noted here that the cavity points are marked by circles as shown in Figure 48 and Figure 49 with the cavities in close proximity (but within) to the boundaries marked by semi-circles. The simulated nucleate boiling curves are compared against coarse grid results as shown in Figure 54. Unlike the two-dimensional case the nucleate boiling heat flux is higher for larger contact angles for the three-dimensional finer grid case. The contact angle of 69° has higher nucleate boiling heat flux than 38° case as the nucleation site density is more for the same superheat. However the maximum heat flux for the 38° is more than 69° case with the CHF values being 60.4 [W/cm²] and 54.8 [W/cm²] for 38° and 69° respectively. Figure 55 shows the variation of wall void fraction computed for the fine grid cases in comparison to the coarse grid.





Figure 48 Nucleation sites distribution for contact angle of 38°. (Field of view 5 mm x 5 mm)



Figure 49 Nucleation sites distribution for contact angle of 69°. (Field of view 5 mm x 5 mm)



Figure 50 Boiling process for $\phi = 38^{\circ}$, $\Delta T = 15$ [K] (Field of view 5 mm x 25 mm x 5 mm)



Figure 51 Boiling process for $\phi = 69^{\circ}$, $\Delta T = 15$ [K] (Field of view 5 mm x 25 mm x 5 mm)



Figure 52 Boiling process for $\phi = 38^{\circ}$, $\Delta T = 20$ [K] (Field of view 5 mm x 25 mm x 5 mm)



Figure 53 Boiling process for $\varphi = 69^{\circ}$, $\Delta T = 20$ [K] (Field of view 5 mm x 25 mm x 5 mm)



Figure 54 Comparison of boiling curves for 3D cases



Figure 55 Comparison of wall void fraction for 3D cases



Figure 56 Variation of CHF with contact angle

Figure 56 shows the comparison of computed CHF, which is under predicted for both the contact angles in the present study, against value previously reported by Maracy and Winterton (1988) and Liaw & Dhir (1989). Maracy and Winterton (1988) computed the boiling heat flux using Kudryavtsev two point method which requires two known temperature values as a function of time.

Figure 57 - Figure 59 shows the energy partitioning from the wall into superheating the liquid, interface and microlayer for the three-dimensional cases. The comparison of the energy partitioning has been done with respect to both wall void fraction and wall superheat. The fine grid cases haven't been run long enough because of which the trend seen is inconclusive. A rough estimate for the duration for which fine grid cases should be run is approximately $t^* > 5$. The energy going into superheating the liquid is calculated by subtracting the energy utilized for vapor production from the energy provided by the wall. The coarse grid ($\phi = 38^\circ$) yields a downward trend with wall void fraction for the fraction of energy going into superheating the liquid is caround 85% for the coarse grid case while it is around 50% for the fine grid cases at 15°C. Previously, Dhir (2006) had reported 70% energy from the wall going into superheating the liquid at a wall superheat ($\phi = 54^\circ$, $\Delta T = 8$ °C). Finally, the fraction of energy utilized for superheating the liquid drops to almost zero for a wall superheat of 130°C as all of the wall heat flux goes into vapor.

Figure 58 shows the energy fraction going through the interface (excluding the microlayer) which for the coarse grid case ($\varphi = 38^\circ$) is around 23% at CHF, has a value of 65% for most of the transition boiling regime and ultimately attains a value of 100% at a wall superheat of 130 °C due

to entire surface being covered with vapor film. The energy fraction going into the microlayer is shown in Figure 59 which for the coarse grid ($\varphi = 38^\circ$) peaks at the critical heat flux case with the value of around 45% and finally goes to zero at wall superheat of 130 °C. Experiments done by Stephan et al. (2009) also concluded that 50-60% of the energy fueling bubble growth comes through microlayer. Since, Microlayer contribution increases linearly with superheat and depends on contact line density, for coarse grid case a near about constant value of 25% -30% is observed even as the wall superheat increases from 40 °C to 100 °C as the dry area is increased from 90% to 99% over the same range. Fine grid cases for both the contact angles show approximate value of 40% of the energy being transferred into vapor through the interface for the range of wall superheat considered. For contact angle of 38° about 40% of the energy has been computed for superheating the liquid while the 69° counterpart shows a slightly higher value of 50% for the same range of superheats. Microlayer contribution for both the contact angles has been found to be much lower in comparison to the coarse grid case with an approximate value of 10-20 % with 38° contact angle being approximately 5% more than 69° over the range of wall void fraction plotted as shown in Figure 59.



Figure 57 Energy fraction utilized for superheating of liquid for 3D cases



Figure 58 Energy fraction going into interface for 3D cases



Figure 59 Energy fraction going into microlayer for 3D cases

5.4 Conclusion

This chapter focused on three-dimensional simulation of the entire boiling curve as two-dimensional approximation is inadequate in capturing the essential physics of the process. The trend observed for the nucleate boiling heat flux regime with variation in contact angles is correct as seen in the fine grid case and is different than the two-dimensional studies done earlier. For the 3D coarse grid case at CHF, sustained superheated vapor column is seen with the CHF value computed to be the same with that obtained from fine grid. For fine grid cases the CHF value decreased with increase in contact angle. The average vapor velocity at CHF condition for 3D coarse grid was found to be approximately 1 [m/s] which is only 25% of the theoretical critical Helmholtz vapor velocity. Intermittent liquid-surface contacts are seen for the transition boiling case. Upon increasing the superheat further, the entire surface gets covered with a superheated vapor film thus entering the film boiling regime.

Summary

Both two-dimensional and three-dimensional numerical simulations of the entire boiling curve in a temperature controlled mode have been performed by a unified numerical model under the framework of parallel computing in conjunction with correlations specifying nucleation site density and bubble waiting time as functions of wall superheat and contact angle.

- The two-dimensional assumption renders the numerical model incapable of correctly predicting the trend of nucleate boiling heat flux with variation in contact angles due to the inbuilt manifestation of symmetric boundary conditions along the frontal plane of the domain. The trend of CHF with variation in contact angle is however correct.
- The three-dimensional simulations (coarse grid cases) show the rising mushroom shaped vapor bubbles in the nucleate boiling regime. Sustained vapor column with average vapor velocity of approximately 1 [m/s] is seen for maximum heat flux conditions. The transition boiling shows intermittent liquid surface contacts and upon increasing the superheat eventually the entire surface gets covered with vapor film characterized by film boiling regime. Energy partitioning from wall into liquid shows decreasing trend with superheat.
- Three-dimensional simulations with fine grids captures the correct trend in the nucleate boiling heat flux (till CHF) with contact angle

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Appendix I - Matrix Solvers

Multigrid Algorithm

Considering a linear PDE - Lu(x)=f(x); where, $L = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$ The above equation can be discretized as following:

$$a_{i,j}^{p}\phi_{i,j} = a_{i,j}^{w}\phi_{i-1,j} + a_{i,j}^{e}\phi_{i+1,j} + a_{i,j}^{n}\phi_{i,j+1} + a_{i,j}^{s}\phi_{i,j-1} + b_{i,j}$$

The residual vector is defined as:

$$r_{i,j} = a_{i,j}^{w} \phi_{i-1,j} + a_{i,j}^{e} \phi_{i+1,j} + a_{i,j}^{n} \phi_{i,j+1} + a_{i,j}^{s} \phi_{i,j-1} + b_{i,j} - a_{i,j}^{p} \phi_{i,j}$$

The sum of all the residuals given as below is extended to all the residuals of the block

$$\begin{aligned} R_{I,J} &= \sum r_{i,j} = \sum (b_{i,j} - a_{i,j}^{p}\phi_{i,j}) + a_{i,j}^{w}\phi_{i-1,j} + a_{i,j}^{e}\phi_{i+1,j} + a_{i,j}^{n}\phi_{i,j+1} + a_{i,j}^{s}\phi_{i,j-1} + \\ a_{i+1,j}^{w}\phi_{i,j} + a_{i+1,j}^{e}\phi_{i+2,j} + a_{i+1,j}^{n}\phi_{i+1,j+1} + a_{i+1,j}^{s}\phi_{i+1,j-1} + \\ a_{i,j+1}^{w}\phi_{i-1,j+1} + a_{i,j+1}^{e}\phi_{i+1,j+1} + a_{i,j+1}^{n}\phi_{i,j+2} + a_{i,j+1}^{s}\phi_{i,j} + \\ a_{i+1,j+1}^{w}\phi_{i,j+1} + a_{i+1,j+1}^{e}\phi_{i+2,j+1} + a_{i+1,j+1}^{n}\phi_{i+1,j+2} + a_{i+1,j+1}^{s}\phi_{i+1,j} \end{aligned}$$

An additive correction, Φ , restricted to be constant in each block is used to improve the current value of ϕ .

$$\begin{split} \phi_{i,j} &\leftarrow \phi_{i,j} + \Phi_{i,j} \\ \phi_{i,j} &\leftarrow \phi_{i+1,j} + \Phi_{i,j} \\ \phi_{i,j} &\leftarrow \phi_{i,j+1} + \Phi_{i,j} \\ \phi_{i,j} &\leftarrow \phi_{i+1,j+1} + \Phi_{i,j} \end{split}$$

The intention is to impose the block residual after the correction:

$$R_{I,J}=0$$



Figure 60 Agglomeration of Cells

$$\begin{split} & a_{i,j}^{w} \Big(\phi_{l-l,j} + \Phi_{I-l,J} \Big) + a_{i,j}^{e} \Big(\phi_{l+l,j} + \Phi_{I,J} \Big) + a_{i,j}^{n} \Big(\phi_{l,j+1} + \Phi_{I,J} \Big) + a_{i,j}^{s} \Big(\phi_{l,j-1} + \Phi_{I,J-1} \Big) + b_{l,j} - a_{i,j}^{p} \Big(\phi_{l,j} + \Phi_{I,J} \Big) + a_{i+l,j}^{n} \Big(\phi_{l,j+1} + \Phi_{I,J} \Big) + a_{i+l,j}^{s} \Big(\phi_{l+l,j+1} + \Phi_{I,J} \Big) + a_{i+l,j}^{s} \Big(\phi_{l+l,j-1} + \Phi_{I,J-1} \Big) + b_{i+l,j} \Big) + a_{i+l,j}^{p} \Big(\phi_{l+l,j+1} + \Phi_{I,J} \Big) + a_{i+l,j}^{s} \Big(\phi_{l+l,j+1} + \Phi_{I,J} \Big) + a_{i,j+1}^{s} \Big(\phi_{l+l,j+1} + \Phi_{I,J} \Big) + a_{i,j+1}^{s} \Big(\phi_{l+l,j+1} + \Phi_{I,J} \Big) + a_{i,j+1}^{s} \Big(\phi_{l+1,j+1} + \Phi_{I,J} \Big) + a_{i+l,j+1}^{s} \Big(\phi_{l+1,j+1} + \Phi_{I,J} \Big) = 0 \end{split}$$

The correction equation is thus obtained as follows:

$$\begin{split} A \Phi &= B \\ A_{I,J}^{p} \Phi_{I,J} &= A_{I,J}^{w} \Phi_{I-1,J} + A_{I,J}^{e} \Phi_{I-1,J} + A_{I,J}^{s} \Phi_{I,J-1} + A_{I,J}^{n} \Phi_{I,J+1} + B_{I,J} \end{split}$$

where

$$\begin{split} A_{I,J}^{p} &= \sum a_{i,j}^{p} - \left(a_{i+1,j}^{w} + a_{i+1,j+1}^{w} + a_{i,j}^{e} + a_{i,j+1}^{e} + a_{i,j}^{n} + a_{i+1,j}^{n} + a_{i,j+1}^{s} + a_{i+1,j+1}^{s}\right) \\ A_{I,J}^{w} &= a_{i,j}^{w} + a_{i,j+1}^{w} \\ A_{I,J}^{e} &= a_{i,j}^{e} + a_{i+1,j+1}^{e} \\ A_{I,J}^{n} &= a_{i,j+1}^{n} + a_{i+1,j+1}^{n} \\ B_{I,J} &= \sum r_{i,j} \end{split}$$

Line by Line Tri Diagonal Matrix Algorithm (LNTDMA)

$$a_{i,j}^{p}\phi_{i,j} = a_{i,j}^{w}\phi_{i-1,j} + a_{i,j}^{e}\phi_{i+1,j} + a_{i,j}^{n}\phi_{i,j+1} + a_{i,j}^{s}\phi_{i,j-1} + b_{i,j}$$

The principle to solve the linear algebraic equation using line-by-line method is to solve for the unknown scalars along one line by the TDMA while using the approximate values of neighboring scalars. The above equation can hence be approximated by:

$$A_i \phi_i = B_i \phi_{i+1} + C_i \phi_{i-1} + D_i$$

In the above formulation, A_i, B_i, C_i and D_i are the known coefficients. Suppose the grid points along the considered line are numbered as 1,2,...,M+1 with 1 and M+1 denoting the boundary points and the range 2,...M constituting the internal points for which the solution has to be found out. With the unknown boundary values getting eliminated:

$$C_2 = 0; \ B_M = 0$$

TDMA Algorithm is explained as:

$$P_2 = \frac{B_2}{A_2}; \quad Q_2 = \frac{D_2}{A_2}$$

For i = 3,...,M, the variables P and Q are calculated as:

$$P_i = \frac{B_i}{A_i - C_i P_{i-1}}; \quad Q_i = \frac{D_i + C_i Q_{i-1}}{A_i - C_i P_{i-1}}$$

With $P_M = 0$ and setting $\phi_M = Q_{M..}$ The following expression is used to compute $\phi_{M-1,...} \phi_2$ by back substitution.

$$\phi_i = P_i \phi_{i+1} + Q_i$$

Block Correction Procedure

The speed of convergence can further be enhanced by supplementing it with additive-correction method.

$$a_{i,j}^{p}\phi_{i,j} = a_{i,j}^{w}\phi_{i-1,j} + a_{i,j}^{e}\phi_{i+1,j} + a_{i,j}^{n}\phi_{i,j+1} + a_{i,j}^{s}\phi_{i,j-1} + b_{i,j}$$

The above equation is written for all the internal grid points defined by i = 2,...M and j =

The concept behind block correction is that an unconverged field ϕ^* obtained from

2,...N. If the unknown boundary values have been eliminated then:

$$a^{e}_{\mathrm{M},j} = 0, \; a^{w}_{2,j} = 0, \; \; a^{n}_{i,\mathrm{N}} = 0, \; a^{s}_{i,2} = 0$$

prior iterations is corrected by adding uniform corrections $\overline{\phi}$ along lines of constant i or j. These corrections satisfy the integral conservation over the control volume blocks defined by lines of constant i or j.

$$A_i \overline{\phi_i} = B_i \overline{\phi_{i+1}} + C_i \overline{\phi_{i-1}} + D_i$$

where,

$$A_{i} = \sum \left(a_{i,j}^{P} - a_{i,j-1}^{s} - a_{i,j+1}^{n}\right)$$

$$B_{i} = \sum a_{i,j}^{e}$$

$$C_{i} = \sum a_{i,j}^{w}$$

$$D_{i} = \sum \left(a_{i,j}^{e}\phi_{i+1,j}^{*} + a_{i,j}^{w}\phi_{i-1,j}^{*} + a_{i,j+1}^{n}\phi_{i,j+1}^{*} + a_{i,j-1}^{s}\phi_{i,j-1}^{*} + b_{i,j} - a_{i,j}^{P}\phi_{i,j}^{*}\right)$$

The summation of the above equations are taken for J=2,....N if the LNTDMA is being solved for I=2,....M. Similarly, the procedure can be adopted for block correction on lines of constant J with summation done for I.

Appendix II - Conservation Properties

1. Conservation properties of the numerical model

The present section cross verifies some of the essential conservation properties any numerical technique should possess in order to ensure high fidelity of the numerical results. If there is no vapor in the domain initially and any nucleation occurs then that nucleation event doesn't influence the flow field at all, as the vapor is placed by removing the liquid artificially and hence the mass and energy content of the computational volume gets altered (Figure 61) as an artifact. During nucleation the liquid along with its superheat is removed from the domain as shown in Figure 62. The energy lost by liquid during a simulation time (t) span depends on initial bubble size taken (Vol_{bub}), average superheat of the thermal layer removed ($\Delta \overline{T}$) and total number of nucleation during runtime (N_t). The vapor gets added artificially without consuming any liquid superheat.



Figure 61 Nucleation event



Figure 62 Energy change during nucleation

Under the action of applied wall superheat bubble growth and merger process influences the flow field according to conservation laws. For eg, as the bubble grows, the liquid is pushed out of the domain from the top (Figure 63) in accordance with the principles of mass conservation.



Figure 63 Bubble growth during wall superheated conditions

Estimation related to volume conservation, mass conservation, thermal layer energy conservation and vapor energy conservation are tabulated. For the 2D cases an extruded length of 1 m is assumed for the sake of convenience.

1.1 Mass Conservation

The vapor mass outflow rate from the top of the computational domain gets compensated by the corresponding liquid mass inflow rate to achieve net zero mass flow rate for a constant vapor fraction in the control volume. Net mass imbalance normalized by vapor flow rate out of the control volume during steady state over a computational time step is thereby shown in Table 7. Since the 3D fine grid cases of 38° and 69° contact angle haven`t been run long to observe any vapor escaping the domain, they are not accounted in the present check.

Mass flux conservation error =
$$\left(\frac{\text{Vapor mass flux out} - \text{Liquid mass flux in}}{\text{Vapor mass flux out}}\right) \times 100$$

Mass Conservation ($\phi = 38^{\circ}$) 2D Numerical							
ΔΤ	Time interval	Time	Vapor Mass	Liquid Mass	% Diff Mass		
[K]	Δt [ms]	[ms]	Outflow	Inflow	Conservation		
			[Kg/s]	[Kg/s]			
20	3.32E-03	222.56	1.29E-03	1.30E-03	-0.3		
27.5	7.99E-04	279.2	2.80E-03	2.77E-03	1.32		
Mass Conservation ($\phi = 69^\circ$) 2D Numerical							
ΔΤ	Time interval	Time	Vapor Mass	Liquid Mass	% Diff Mass		
[K]	Δt [ms]	[ms]	Outflow	Inflow	Conservation		
			[Kg/s]	[Kg/s]			
17	3.18E-03	256	5.07E-04	5.00E-04	1.32		
22	1.02E-03	267.2	4.86E-04	4.77E-04	1.9		
Mass Conservation ($\phi = 38^\circ$) 3D Numerical (Coarse)							
ΔΤ	Time interval	Time	Vapor Mass	Liquid Mass	% Diff Mass		
[K]	Δt [ms]	[ms]	Outflow	Inflow	Conservation		
			[Kg/s]	[Kg/s]			
20	1.82E-04	46	7.77E-06	7.79E-06	-0.17		
27	5.70E-04	62	4.50E-05	4.55E-05	-1.2		

Table 7 Mass conservation values

1.2 Volume Conservation

The volume of the computational domain is constant and because of this any vapor bubble that grows during boiling process has to push the liquid out from the top. The difference between the liquid volume flowing out from the domain top, during initial runtime when the vapor hasn't escaped the domain, and the bubble growth volume normalized by the bubble growth volume is shown in Table 8 and is expressed as:

Volume conservation error =
$$\left(1 - \frac{\text{Volume of liquid pushed out}}{\text{Increase in vapor volume}}\right) \times 100$$

Volume conservation ($\phi = 38^\circ$) 2D Numerical									
ΔΤ	Time int.	Time	Vap. volume	Liq. volume	% Diff. volume				
[K]	Δt [ms]	[ms]	increase [m ³]	outflow [m ³]	conservation				
20	3.81E-03	19.20	7.54E-09	7.22E-09	4.3				
27.5	5.40E-04	68.80	3.49E-09	3.38E-09	3.2				
	Volu	me conser	vation ($\phi = 69^\circ$)	2D Numerical					
ΔΤ	AT Time int. Time Van. volume Liq. volume % Diff. volume								
[K]	Δt [ms]	[ms]	increase [m ³]	outflow [m ³]	conservation				
17	1.72E-03	21.3	1.96E-09	2.02E-09	-3.1				
22	2.48E-03	45.1	4.03E-09	3.77E-09	6.42				
	Volume c	onservatio	$\phi = 38^{\circ} 3D$ N	Numerical (Coars	se)				
ΔΤ	Time int.	Time	Vap. volume	Liq. volume	% Diff. volume				
[K]	Δt [ms]	[ms]	increase [m ³]	outflow [m ³]	conservation				
20	4.51E-04	1.6	8.78E-13	9.43E-13	-7.42				
27	2.31E-05	2.4	6.72E-13	6.20E-13	7.65				
EVALUATE: Volume conservation ($\phi = 38^\circ$) 3D Numerical (Fine)									
ΔΤ	Time int.	Time	Vap. volume	Liq. volume	% Diff. volume				
[K]	Δt [ms]	[ms]	increase [m ³]	outflow [m ³]	conservation				
15	2.23E-04	4.8	3.94E-13	3.58E-13	9.1				
20	2.44E-04	9.5	8.78E-13	9.34E-13	-6.4				
EXAMPLE 1 Volume conservation ($\phi = 69^\circ$) 3D Numerical (Fine)									
ΔΤ	Time int.	Time	Vap. volume	Liq. volume	% Diff. volume				
[K]	Δt [ms]	[ms]	increase [m ³]	outflow [m ³]	conservation				
15	9.38E-05	3.2	5.06E-13	4.97E-13	1.75				
20	3.49E-04	15.8	1.00E-12	1.03E-12	-3.72				

Table 8 Volume conservation calculation

1.3 Energy balance at the wall

The energy being provided from the wall goes into dry area (vapor), microlayer and wet area (liquid) as shown in

Figure 64 (sample calculations shown in Table 9). The energy transferred to dry area has been estimated to be less than 1 $[W/cm^2]$



Figure 64 Energy transfer from wall into liquid and vapor

Energy utilized for vapor production = Microlayer heat transfer + Interface heat transfer + Energy

utilized for superheating the vapor

Energy utilized for superheating the liquid = Wall heat flux - Energy utilized for vapor production

Wall heat flux partitioning ($\phi = 38^{\circ}$) 2D Numerical							
<u>А</u> Т [K]	Time [ms]	Time interval [ms]	Wall heat flux [W/cm ²]	Microlayer heat flux [W/cm ²]	Wall to wet area [W/cm2]	Wall to dry area [W/cm2]	Interface heat flux [W/cm ²]
20	90	3.82E-04	41.41	8.65	32.76	0	13.96
27.5	120	5.00E-05	78.92	39.37	39.55	0	9.38
		Wall I	ieat flux partiti	ioning ($\phi = 69^\circ$)	2D Numerica	l	
ΔT [K]	Time [ms]	Time interval [ms]	Wall heat flux [W/cm ²]	Microlayer heat flux [W/cm ²]	Wall to wet area [W/cm2]	Wall to dry area [W/cm2]	Interface heat flux [W/cm ²]
17	192	3.76E-03	19.49	3.8	15.69	0	8.23
22	160	3.58E-03	22.83	4.78	18.05	0	10.01
		Wall heat f	flux partitionin	$g (\phi = 38^{\circ}) 3D N$	umerical (Co	arse)	
ΔТ [K]	Time [ms]	Time interval [ms]	Wall heat flux [W/cm ²]	Microlayer heat flux [W/cm ²]	Wall to wet area [W/cm2]	Wall to dry area [W/cm2]	Interface heat flux [W/cm ²]
20	50	6.64E-04	21.54	1.74	18.8	< 1	1.36
27	60	1.47E-03	60.34	20.57	38.77	< 1	13.99
Wall heat flux partitioning ($\phi = 38^{\circ}$) 3D Numerical (Fine)							
ΔТ [K]	Time [ms]	Time interval [ms]	Wall heat flux [W/cm ²]	Microlayer heat flux [W/cm ²]	Wall to wet area [W/cm2]	Wall to dry area [W/cm2]	Interface heat flux [W/cm ²]
15	15	1.39E-03	12.71	1.17	10.54	< 1	5.5
20	5	4.70E-03	24.31	5.81	17.5	< 1	10.53
		Wall heat	t flux partitioni	$ng (\phi = 69^{\circ}) 3D$	Numerical (F	ine)	
ΔТ [K]	Time [ms]	Time interval [ms]	Wall heat flux [W/cm ²]	Microlayer heat flux [W/cm ²]	Wall to wet area [W/cm2]	Wall to dry area [W/cm2]	Interface heat flux [W/cm ²]
15	10	8.22E-04	16.37	1.87	13.5	< 1	6.7
20	13	7.72E-04	30.59	4.85	24.74	< 1	13.8

Table 9 Wall heat flux partitioning



Figure 65 Energy transfer for the present numerical model

1.4 Thermal layer energy conservation

The thermal layer gets energy from the wall and provides energy to the bubble through the interface. As per the current numerical model during nucleation vapor gets added artificially removing liquid along with thermal layer from its original place (shown in Figure **65**). The energy balance of the thermal layer normalized by time step and heater surface area is documented in Table **10** (time interval is shown in Table **9**) and expressed as:

% Difference in thermal layer energy conservation

$$= \left(1 - \frac{\text{Thermal layer energy rate lost during nucleation per unit wall area}}{\text{Increase in thermal layer energy rate per unit wall area}}\right) \times 100$$

where,

Increase in thermal energy rate per unit wall area

= Wall to wet area energy transfer rate per unit wall area

- Interface energy transfer rate per unit wall area

Thermal layer energy conservation ($\phi = 38^\circ$) 2D Numerical							
ΔT [K]	Time [ms]	Wall to wet area [W/cm2]	Liquid to vapor through interface [W/cm2]	Thermal layer energy lost during nucleation [W/cm2]	Increase in thermal layer energy [W/cm2]	% Diff. in thermal layer energy conservation	
20	90	32.76	13.96	17.89	18.8	4.84	
27.5	120	39.55	9.38	26	30.17	13.82	
		Thermal	layer energy con	servation ($\phi = 69^{\circ}$) 2D Numerical		
ΔT [K]	Time [ms]	Wall to wet area [W/cm2]	Liquid to vapor through interface [W/cm2]	Thermal layer energy lost during nucleation [W/cm2]	Increase in thermal layer energy [W/cm2]	% Diff. in thermal layer energy conservation	
17	192	15.69	8.23	6.2	7.46	16.89	
22	160	18.05	10.01	9.39	8.04	-16.79	
Thermal layer energy conservation ($\phi = 38^{\circ}$) 3D Numerical (Coarse)							
ΔT [K]	Time [ms]	Wall to wet area [W/cm2]	Liquid to vapor through interface [W/cm2]	Thermal layer energy lost during nucleation [W/cm2]	Increase in thermal layer energy [W/cm2]	% Diff. in thermal layer energy conservation	
20	50	18.8	1.36	15.95	17.44	8.54	
27	60	38.77	13.99	27.58	24.78	-11.30	
Thermal layer energy conservation ($\phi = 38^\circ$) 3D Numerical (Fine)							
ΔT [K]	Time [ms]	Wall to wet area [W/cm2]	Liquid to vapor through interface [W/cm2]	Thermal layer energy lost during nucleation [W/cm2]	Increase in thermal layer energy [W/cm2]	% Diff. in thermal layer energy conservation	
15	15	10.54	5.5	5.58	5.04	-10.71	
20	5	17.5	10.53	7.65	6.97	-9.76	
	T	hermal lay	er energy conser	vation (φ = 69°) 3I) Numerical (Fin	le)	
ΔT [K]	Time [ms]	Wall to wet area [W/cm2]	Liquid to vapor through interface [W/cm2]	Thermal layer energy lost during nucleation [W/cm2]	Increase in thermal layer energy [W/cm2]	% Diff. in thermal layer energy conservation	
15	10	13.5	6.7	8	6.8	-17.65	
20	13	24.74	13.8	13.1	10.94	-19.74	

Table 10 Thermal layer energy (normalized by time and area) conservation

1.5 Vapor energy conservation

The vapor is generated at the liquid vapor interface, microlayer and every time a nucleation site gets active a small bubble embryo gets added to the computational domain. Vapor production due to latter becomes significant if the initial bubble embryo size is large and the error gets exacerbated if there are multiple cavities nucleating with high frequency. The vapor energy rate conservation error calculated over a computational time step and normalized by heater surface area is shown in Table **11** (time interval is shown in Table **9**). The vapor volume change in the computational domain is non-zero only for the 3D fine grid cases as vapor didn't escape from the top while for the other case vapor configuration is approximately steady state (constant vapor fraction in the computational domain) for the present calculation.

Vapor energy rate conservation error =
$$\left(\frac{\left(\dot{E}_{vap,out} + \dot{E}_{vap,ch}\right) - \left(\dot{E}_{vap,in} + \dot{E}_{vap,add}\right)}{\dot{E}_{vap,out} + \dot{E}_{vap,ch}}\right) \times 100$$

where,

Energy rate going into vapor per unit wall area (neglecting wall to dry area)

= Microlayer energy rate per unit wall area + Interface energy rate per unit wall area $\dot{E}_{vap,ch} = Vapor energy rate change due to change in vapor volume per unit wall area$ $\dot{E}_{vap,in} = Energy rate going into vapor per unit wall area$ $\dot{E}_{vap,out} = Vapor outflow energy rate per unit area$ $\dot{E}_{vap,add} = Vapor energy rate due to nucleation per unit area$

Vapor energy conservation ($\phi = 38^{\circ}$) 2D Numerical						
ΔT [K]	Time [ms]	Ė _{vap,in} [W/cm ²]	Ė _{vap,add} [W/cm2]	Ė _{vap,ch} [W/cm2]	Ė _{vap,out} [W/cm2]	% Diff. in vapor energy conservation
20	90	22.61	≈ 0	≈ 0	23	1.70
27.5	120	48.75	≈ 0	≈ 0	49.91	2.30
	•	Vapor ene	rgy conserva	tion (φ = 69°) 2D Nume	rical
ΔT [K]	Time [ms]	Ė _{vap,in} [W/cm ²]	Ė _{vap,add} [W/cm2]	Ė _{vap,ch} [W/cm2]	Ė _{vap,out} [W/cm2]	% Diff. in vapor energy conservation
17	192	12.03	≈ 0	≈ 0	12.45	3.37
22	160	14.79	≈ 0	≈ 0	13.44	-10.04
Vapor energy conservation ($\phi = 38^\circ$) 3D Numerical (Coarse)						
ΔT [K]	Time [ms]	Ė _{vap,in} [W/cm ²]	Ė _{vap,add} [W/cm2]	Ė _{vap,ch} [W/cm2]	Ė _{vap,out} [W/cm2]	% Diff. in vapor energy conservation
20	50	3.1	5.05	≈ 0	10.89	25.16
27	60	34.56	18	≈ 0	63.04	16.62
Vapor energy conservation ($\phi = 38^\circ$) 3D Numerical (Fine)						
ΔT [K]	Time [ms]	Ė _{vap,in} [W/cm ²]	Ė _{vap,add} [W/cm2]	Ė _{vap,ch} [W/cm2]	Ė _{vap,out} [W/cm2]	% Diff. in vapor energy conservation
15	15	6.67	≈ 0	7.31	0	8.76
20	5	16.34	≈ 0	15.87	0	-2.96
Vapor energy conservation ($\phi = 69^\circ$) 3D Numerical (Fine)						
ΔT [K]	Time [ms]	Ė _{vap,in} [W/cm ²]	Ė _{vap,add} [W/cm2]	Ė _{vap,ch} [W/cm2]	Ė _{vap,out} [W/cm2]	% Diff. in vapor energy conservation
15	10	8.57	≈ 0	8.74	0	1.95
20	13	18.65	≈ 0	18.16	0	-2.70

Table 11 Vapor energy (normalized by time and area) conservation

Appendix III - 3D Parallel Code

PROGRAM MAIN USE PARAMETERS USE ICHOS USE PROPS USE INDMO USE INDDT USE IGRID USE MUGRD USE IBNDS USE GRID1 USE GRIDB USE GRIDL **USE CHCFL USE IDREF USE UVTBC USE IBUBS USE LVFBC** USE QINTB **USE SPERR USE LEVFN USE ULVLL USE FFSOR USE UVTPB** USE RESLT **USE UVTPP USE CALC1 USE DIMEN USE MPIVAR** IMPLICIT NONE REAL*8 :: AL0,ALPL,BPMAX,BUMAX,BVMAX,BWMAX,RGRAV,RH0,RHOL,RHOV REAL*8 :: CAPL,CAPV,CONDL,CONDV,F0,F1,GRAV,H0,HBOT,HBOT1,HFG,HTOP1,PEL,PMAX,PRL,RAL0,RCV, RCV0,REL,REV REAL*8 :: RMU.RRE.RRHO.RRR.RU0.SURF.TWAIT.U0.UMAX.VMAX.WMAX.VBOT.VTOP.VISL.VISV.X1.XL.Y0.Y 1.YL.ZL INTEGER :: 1.J.K.IACT.IBUB0.IFB.IND.IORDER.IREIN.JI3OUT.JINOUT.JREOUT.JPLOUT.JFLOUT.LTIME.N ************ CALL MULTICORE CALL ALLOT CALL FRAGMENT ! Parallel decomposition ******** PI=ACOS(-1.) CFO=0.5 IINF=1 IOUT=2

ISYM=3 IWAL=4 IWQQ=5	! Constants	
ICONT=1 ICONB=0		
IENO=0 IENOT=1 IORDER=1		
ITIME=0 TIME=0. ICF=1 JCF=1 KCF=1 I2B=1 N2B=2 NBUB(1)=0 NBUB(2)=0 V0H(1)=1. V1H(1)=1. V0H(2)=0. V1H(2)=0. V1H(2)=-1. IREIN=0 ITSOLV=1 JMOVE=0		
QMIC0=0. TINT=0. TWAL=1. DTWS=0. HFGI=0. VBUB=0. TBCW=1. TBCE=1. TBCS=1. TBCN=1. TBCB=1. TBCT=1.		I Road the input file
OPEN(1,FILE='tpi' READ(1,*) READ(1,*) IND,LTI READ(1,*)) ME,NI,NJ,NK,IR,MULT	rteau the input file
READ(1,*) DT0,IU(READ(1,*)	GRD,XL,DL,JMOVE,IENO,IENOT	
READ(1,*) IGRAV, READ(1,*)	IBOIL,IQ_LIQ,IQ_VAP,IBODY,ICO	NT,ICONB
READ(1,*) RCV0,Y READ(1,*) READ(1,*) H0,UIN READ(1,*)	′BUB0,XBND,YBND,ZBND,RBND, 0,QMIC0	ESMAX,EFMAX

READ(1,*) I69, JMONT, JMONIT, JINOUT, JI3OUT, JPLOUT, JREOUT, JFLOUT READ(1,*) READ(1,*) IREF, JREF, KREF READ(1,*) READ(1,*) READ(1,*) IBCW, IBCE, IBCS, IBCN, IBCB, IBCT READ(1,*) READ(1,*) CANGMAX, CANGMIN, CANBMAX, CANBMIN IF(IBOIL.EQ.1) THEN READ(1,*) READ(1,*) RHOL, RHOV, VISL, VISV, CONDL, CONDV READ(1,*) READ(1,*) CAPL,CAPV,SURF,RGRAV,DTWS,BT0,HFG ELSE READ(1,*) READ(1,*) RO1,RO2,VS1,VS2,SFT0,TK1,TK2 ENDIF READ(1,*) READ(1,*) NCAV, TWAIT READ(1,*) READ(1,*) (XCAV(I),I=1,NCAV) READ(1,*) (ZCAV(I),I=1,NCAV) READ(1,*) (TIMEW(I),I=1,NCAV) CLOSE(1) DT=DT0 123=3 IF(NK.LE.3) 123=2 K11=1 KNK=NK IF(I23.EQ.2) THEN NK=3 K11=2 KNK=2 KREF=2 **IBCB=ISYM IBCT=ISYM** FZ1=0. ENDIF IF(IUGRD.EQ.1) THEN XU(2)=0. YV(2)=0. ZW(2)=0. DL=XL/(NI-2) DO 12 I=3,NI XU(I)=XU(I-1)+DL 12 DO 14 J=3,NJ 14 YV(J)=YV(J-1)+DL DO 16 K=3,NK 16 ZW(K)=ZW(K-1)+DL ELSE OPEN(1,FILE='grd') READ(1,*)

DO 22 I=2,NI 22 READ(1,*) XU(I) READ(1,*) DO 24 J=2,NJ 24 READ(1,*) YV(J)IF(I23.EQ.3) THEN READ(1,*) DO 26 K=2,NK 26 READ(1,*) ZW(K) ENDIF CLOSE(1) **ENDIF** IF(I23.EQ.2) ZW(3)=ZW(2)+1. XL=XU(NI) YL=YV(NJ) ZL=ZW(NK) IF (TASKID.EQ.0) THEN **!ONLY MASTER PROCESSOR DISPLAYS THIS.** WRITE(6,'(5X,A,6(1PE12.4))') ' X0, Y0, Z0 =',XU(2),YV(2),ZW(2) WRITE(6,'(5X,A,6(1PE12.4))') ' XL, YL, ZL =',XU(NI),YV(NJ),ZW(NK) ENDIF IF(I69 .EQ. 9) OPEN(9,FILE='mon') IF(IBOIL.EQ.0) GOTO 50 H0=H0*DTWS**(-1./3.) GRAV=9.807 AL0=SQRT(SURF/GRAV/(RHOL-RHOV)) U0=SQRT(GRAV*AL0) REL=U0*AL0/VISL ALPL=CONDL/RHOL/CAPL H0=H0*7.14*(VISL*ALPL/GRAV/BT0)**(1./3.)/AL0 IF (TASKID.EQ.0) THEN WRITE(6,'(A,4(1PE12.4))') ' AL0, U0, H0, RE=',AL0,U0,H0,REL ENDIF RAL0=RGRAV**(-1./2.) RU0=SQRT(RGRAV*RAL0) RH0=RGRAV**(-1./3.)/RAL0 RRE=RAL0*RU0 H0=H0*RH0 REL=REL*RRE IF (TASKID.EQ.0) THEN WRITE(6,'(A,4(1PE12.4))') ' RAL0,RU0,RH0,RRE=',RAL0,RU0,RH0,RRE **ENDIF** RRHO=RHOV/RHOL RMU=RRHO*VISV/VISL REV=REL/RMU SFT0=(RHOL-RHOV)/RHOL PRL=CAPL*VISL*RHOL/CONDL

PEL=REL*PRL HFGI=CAPL*DTWS/HFG RO1=RRHO RO2=1. VS1=REL/RMU VS2=REL TK1=PEL/(CONDV/CONDL) TK2=PEL RC1=RO1*CAPV/CAPL RC2=1. 50 CONTINUE EPS=1.E-5 HEPS=1.E-2 VFG=1./RO1-1./RO2 !-----**!MPI** Functions CALL FRAGMENT CALL GHBUFFER CALL BUFFER ALLOCATE(GHVAR(IIST-2:IIEND+2,JJST-2:JJEND+2,KKST-2:KKEND+2,1:2),STAT=IERR) IF (IERR /=0) PRINT*, 'ERROR IN GHVAR BY', TASKID !-----CALL INIT **!**-----ARO=0.5*(RU(NI)+RU(2))*XL IF(I23.EQ.3) ARO=XL*ZL !----- Contact Angle CANGMAX=CANGMAX*PI/180. CANGMIN=CANGMIN*PI/180. CANBMAX=CANBMAX*PI/180. CANBMIN=CANBMIN*PI/180. COSMIN=COS(CANGMAX) COSMAX=COS(CANGMIN) COBMIN=COS(CANBMAX) COBMAX=COS(CANBMIN) [-----Y0=YBUB0 IF(YBUB0.LT.-10.) Y0=RCV0*COSMIN IF (TASKID.EQ.0) THEN IF(IBOIL.EQ.1) THEN WRITE(6,'(A,4(1PE12.4))') ' DL,YL,RCV0,QMIC0=',DL,YL,RCV0,QMIC0 **ENDIF** ENDIF IF(IBODY.EQ.1) THEN DO 70 K=K11,KNK DO 70 J=1,NJ DO 70 I=1,NI !IF(I23.EQ.3) FZ1=(ZP(K)-ZBND)**2

IF(I23.EQ.3) FZ1=0. S(I,J,K)=SQRT((XP(I)-XBND)**2+(YP(J)-YBND)**2+FZ1)-RBND 70 CALL SUVW_GET IF (TASKID.EQ.0) THEN OPEN(90,FILE='bnd0') DO 72 IFB=-9,2 F0=IFB*XD(2) 72 CALL BNDXY_PLOT(2,F0) CLOSE(90) OPEN(90,FILE='b2xy') CALL BNDXY PLOT(2,0.) CLOSE(90) IF(I23.EQ.3) THEN OPEN(90,FILE='b2zy') CALL BNDZY_PLOT(2,0.) CLOSE(90) **ENDIF** ENDIF ENDIF DO 100 N=1,NCAV FMIN(N)=1.E6 DO 110 K=2,NKM DO 110 I=2,NIM X1=XP(I)-XCAV(N) Y1=YP(2)-Y0 IF(I23.EQ.3) FZ1=(ZP(K)-ZCAV(N))**2 F1=SQRT(X1**2+Y1**2+FZ1) IF(F1 .GT. FMIN(N)) GOTO 110 FMIN(N)=F1 ICAV(N)=I JCAV(N)=2 KCAV(N)=K CONTINUE 110 IF (TASKID.EQ.0) THEN WRITE(6,'(A,I3,3(I4),1PE12.4)') ' Active Cavity: N,I,J,K,DF=',N,ICAV(N),JCAV(N),KCAV(N),FMIN(N) ENDIF 100 CONTINUE DO 115 N=1,NCAV IBCAV(N)=0 IF(TIMEW(N).LE.TWAIT) GOTO 115 NBUB(1)=NBUB(1)+1 IBCAV(N)=NBUB(1) TIMEW(N)=0. 115 CONTINUE IF(IND .EQ. 0) THEN **!**----IACT=0

DO 120 N=1,NCAV IF(IBCAV(N).EQ.0) GOTO 120 IACT=IACT+1 IF(IACT.EQ.1) THEN DO 122 K=K11,KNK DO 122 J=1,NJ DO 122 I=1,NI IBUB(I,J,K,1)=0 F(I,J,K)=1.E6 122 DDF(I,J,K)=DL ENDIF DO 124 K=K11,KNK DO 124 J=1,NJ DO 124 I=1,NI CC(I,J,K) = F(I,J,K)SS(I,J,K)=DDF(I,J,K) IF(I23.EQ.3) FZ1=(ZP(K)-ZCAV(N))**2 IF(I23.EQ.3 .AND. IBODY.EQ.1) FZ1=0. RCV=RCV0 IF(IBODY.EQ.1 .AND. I23.EQ.3) THEN RCV=RCV0+(RCV0-RBND)*0.1*COS(PI*ZP(K)/ZL) ENDIF 124 F(I,J,K)=SQRT((XP(I)-XCAV(N))**2+(YP(J)-Y0)**2+FZ1)-RCV CALL DDF GET DO 126 K=K11,KNK DO 126 J=1,NJ DO 126 I=1,NI IF(CC(I,J,K).LE.SS(I,J,K) .AND. F(I,J,K).LE.DDF(I,J,K)) THEN IF (TASKID.EQ.0) THEN WRITE(I69,*) ' Bubble Merged initially at N,I,K=',N,I,K **ENDIF** STOP ENDIF IF(F(I,J,K).LT.DDF(I,J,K)) IBUB(I,J,K,1)=IBCAV(N) F(I,J,K)=AMIN1(CC(I,J,K),F(I,J,K))126 CONTINUE CALL DDF_GET 120 CONTINUE DO 150 K=K11,KNK DO 150 J=1,NJ DO 150 I=1,NI T(I,J,K)=AMAX1(0.,1.-YP(J)/H0)IF(IGRAV.EQ.0) T(I,J,K)=1. F1=F(I,J,K)/(2.*DDF(I,J,K))F1=AMAX1(0.,AMIN1(1.,F1)) IF(F(I,J,K).GE.0.) T(I,J,K)=F1*(2.-F1)*T(I,J,K) IF(IBODY.EQ.1) THEN RRR=SQRT(XP(I)**2+(YP(J)-Y0)**2)-RBND RCV=RCV0

IF(IBODY.EQ.1 .AND. I23.EQ.3) THEN RCV=RCV0+(RCV0-RBND)*0.1*COS(PI*ZP(K)/ZL) ENDIF T(I,J,K)=AMAX1(0.,1.-RRR/(RCV-RBND)) ENDIF 150 CONTINUE ENDIF IF(IND .NE. 0) CALL RESTF_IN DO 160 K=K11,KNK DO 160 J=1,NJ DO 160 I=1,NI 160 BF(I,J,K)=F(I,J,K)CALL F BC CALL H GET BDEFF=DEFF CALL T_BC CALL U BC CALL V_BC CALL W_BC I2B=2 IF(IND.EQ.0) CALL IBUB INIT CALL IPBUB GET CALL BVOLB GET BUMAX=1.E-10 BVMAX=1.E-10 BWMAX=1.E-10 BPMAX=1.E-10 DO 310 K=K11,KNK DO 310 J=1,NJ DO 310 I=1,NI BUMAX=AMAX1(BUMAX,ABS(U(I,J,K))) BVMAX=AMAX1(BVMAX,ABS(V(I,J,K))) BWMAX=AMAX1(BWMAX,ABS(W(I,J,K))) 310 BPMAX=AMAX1(BPMAX,ABS(P(I,J,K))) CALL INTP GET(HTOP, 2,2,0,2) CALL INTP_GET(HBOT,-2,2,0,2) CALL N GET CALL RK_GET CALL AM_GET CALL FO BC CALL INT2D OUT CALL INT3D OUT DO 320 K=2,NKM DO 320 J=2,NJM DO 320 I=2,NIM 320 BP(I,J,K)=P(I,J,K) WRITE(I69,4021) 1+ITIME, TIME, DT IF(I69 .EQ. 9) CLOSE(9) !-----

ICALL DEBUFFER ICALL DEGHBUFFER IDEALLOCATE(GHVAR,STAT=IERR) IF (IERR /=0) PRINT*,'ERROR IN DEALLOCATE GHVAR BY',TASKID I------

!CALL PLOTF_OUT(JPLOUT)

IF (TASKID.EQ.0) THEN ICALL OFILE_OUT(JFLOUT) IENDIF

DO 500 ITIME=1+ITIME,LTIME

IF (TASKID.EQ.0) THEN print*,'TASKID=',TASKID,'ITIME',ITIME if (ITIME.eq.ITIME/10*10) write(*,*) 'TASKID=',TASKID,'ITIME=',ITIME, F(25,25,25),P(10,50,44),T(5,10,5),V(45,55,35)

!IF (TASKID.EQ.0) THEN IF(I69 .EQ. 9) OPEN(9,FILE='mon',ACCESS='APPEND') ENDIF

IREIN=0 DO 510 N=1,NCAV IF(TIMEW(N) .GT. TWAIT) THEN IREIN=1 TIMEW(N)=0. NBUB(1)=NBUB(1)+1 IBUB0=NBUB(1) IF (TASKID.EQ.0) THEN WRITE(I69,*) 'AddBubble: NBUB(1)=',NBUB(1),ITIME ENDIF

DO 512 K=K11,KNK DO 512 J=1,NJ DO 512 I=1,NI CC(I,J,K)=F(I,J,K) SS(I,J,K)=DDF(I,J,K) IF(I23.EQ.3) FZ1=(ZP(K)-ZCAV(N))**2 512 F(I,J,K)=SQRT((XP(I)-XCAV(N))**2+(YP(J)-Y0)**2+FZ1)-RCV0 CALL DDF_GET

DO 514 K=2,NKM DO 514 J=2,NJM DO 514 I=2,NIM IF(CC(I,J,K).LE.SS(I,J,K) .AND. F(I,J,K).LE.DDF(I,J,K)) THEN IF (TASKID.EQ.0) THEN WRITE(I69,*) ' Additional Bubble Merged ',ITIME ENDIF NBUB(1)=NBUB(1)-1 IBUB0=IBUB(I,J,K,1) **GOTO 515** ENDIF CONTINUE 514 515 CONTINUE DO 516 K=K11,KNK DO 516 J=1,NJ DO 516 I=1,NI IF(F(I,J,K).LE.DDF(I,J,K)) IBUB(I,J,K,1)=IBUB0 F1=F(I,J,K)/(2.*DDF(I,J,K))F1=AMAX1(0.,AMIN1(1.,F1)) IF(F(I,J,K).GE.0.) T(I,J,K)=F1*(2.-F1)*T(I,J,K) F(I,J,K)=AMIN1(CC(I,J,K),F(I,J,K))516 CONTINUE CALL DDF_GET ENDIF 510 CONTINUE IF(IREIN .EQ. 1) THEN IREIN=0 CALL IBUB_GET CALL F_BC CALL H GET CALL T_BC CALL BVOLB_GET CALL N GET CALL RK GET CALL AM GET ENDIF I-----**!CALL FRAGMENT !CALL GHBUFFER !CALL BUFFER** !ALLOCATE(GHVAR(IIST-2:IIEND+2,JJST-2:JJEND+2,KKST-2:KKEND+2,1:2),STAT=IERR) !IF (IERR /=0) PRINT*, 'ERROR IN GHVAR BY', TASKID !-----CALL SOLVE TIME=TIME+DT DO 525 N=1,NCAV TIMEW(N)=TIMEW(N)+DT I=ICAV(N) J=JCAV(N) K=KCAV(N) IF(F(I,J,K) .LT. DDF(I,J,K)/2.) TIMEW(N)=0. 525 CONTINUE UMAX=1.E-10 VMAX=1.E-10 WMAX=1.E-10 PMAX=1.E-10 DO 540 K=K11,KNK

DO 540 J=1,NJ DO 540 I=1,NI UMAX=AMAX1(UMAX,ABS(U(I,J,K))) VMAX=AMAX1(VMAX,ABS(V(I,J,K))) WMAX=AMAX1(WMAX,ABS(W(I,J,K))) 540 PMAX=AMAX1(PMAX,ABS(P(I,J,K))) IF (TASKID.EQ.0) THEN IF(ITIME .EQ. ITIME/JMONT*JMONT) WRITE(I69,4022)& '***TIME,DUVWP = ',TIME,UMAX/BUMAX,VMAX/BVMAX& & & ,WMAX/BWMAX,PMAX/BPMAX ENDIF l-----CALL INTP_GET(HTOP1, 2,2,0,2) CALL INTP GET(HBOT1,-2,2,0,2) VTOP=(HTOP1-HTOP)/DT VBOT=(HBOT1-HBOT)/DT HTOP=HTOP1 HBOT=HBOT1 IF(ITIME/JINOUT*JINOUT .EQ. ITIME.OR.ITIME/JI3OUT*JI3OUT .EQ. ITIME) CALL FO_BC IF(ITIME/JINOUT*JINOUT .EQ. ITIME) CALL INT2D OUT IF(ITIME/JI3OUT*JI3OUT .EQ. ITIME) CALL INT3D OUT IF(ITIME/JREOUT*JREOUT .EQ. ITIME) CALL RESTF_OUT IF(ITIME/JFLOUT*JFLOUT .EQ. ITIME) CALL OFILE OUT(JFLOUT) IF(ITIME/JPLOUT*JPLOUT .EQ. ITIME) CALL PLOTF_OUT(JPLOUT) BUMAX=UMAX BVMAX=VMAX BWMAX=WMAX BPMAX=PMAX IF(I69 .EQ. 9) CLOSE(9) 500 CONTINUE !-----!MPI Functions to deallocate CALL DEBUFFER CALL DEGHBUFFER DEALLOCATE(GHVAR.STAT=IERR) IF (IERR /=0) PRINT*, 'ERROR IN DEALLOCATE GHVAR BY', TASKID 4021 FORMAT(I8,5(1PE12.4)) 4022 FORMAT(A,6(1PE12.4)) 4023 FORMAT(A,3(I4),4(1PE12.4)) CALL MULTIEND END SUBROUTINE SOLVE **USE PARAMETERS**

```
USE ICHOS
USE PROPS
USE INDMO
USE INDDT
USE IGRID
USE GRID1
USE GRIDB
USE CHCFL
USE LEVFN
USE ULVLL
USE FFSOR
USE ROGAM
USE QMSOR
USE RESLT
USE UVTPP
USE CALC1
USE FUNC
USE MPIVAR
IMPLICIT NONE
INTEGER :: I,J,K
REAL (KIND=8) :: CF1,UMAX,VMAX,WMAX
[**********
                                     *****
CF=1.E10
DO 10 K=2,NKM
DO 10 J=2.NJM
DO 10 I=2,NIM
UMAX=AMAX1(ABS(U(I,J,K)),ABS(U(I,J,K)+AMX(I,J,K)/RHOF(FU(I,J,K))))
VMAX=AMAX1(ABS(V(I,J,K)-VBUB),ABS(V(I,J,K)-VBUB+AMY(I,J,K)/RHOF(FV(I,J,K))))
WMAX=AMAX1(ABS(W(I,J,K)),ABS(W(I,J,K)+AMZ(I,J,K)/RHOF(FW(I,J,K))))
CF1=AMAX1(UMAX/XC(I),VMAX/YC(J),WMAX/ZC(K))
CF1=1./(CF1+1.E-10)
IF(CF1 .GT. CF ) GOTO 10
CF=CF1
ICF=I
JCF=J
KCF=K
     CONTINUE
10
DT=AMIN1(DT0,CF*CFO)
IF(DT .LT. 1.E-8) WRITE(I69,*) ' DT IS TOO SMALL'
IF(DT .LT. 1.E-8) STOP
BDEFF=DEFF
DO 110 K=K11,KNK
DO 110 J=1,NJ
DO 110 I=1,NI
110 BF(I,J,K)=F(I,J,K)
DO 120 K=2,NKM
DO 120 J=2,NJM
DO 120 I=2,NIM
120 T(I,J,K)=AMAX1(0.,AMIN1(1.,T(I,J,K)))
CALL T BC
```

CALL UL_GET CALL TL_GET IF(NBUB(1).GE. 1) THEN CALL IPBUB_GET CALL BVOLB_MOD CALL F_GET CALL F_MOD IF(JMOVE.EQ.1) CALL F_JMOVE CALL IBUB_MOD CALL H_GET CALL N_GET CALL RK_GET ENDIF	
CALL T_SOLV CALL AM_GET CALL U_SOLV CALL V_SOLV CALL W_SOLV CALL DP_ADD CALL P_SOLV CALL PROJT	
CALL U_BC CALL V_BC CALL W_BC	
RETURN END	
I HANNE HAM_GET SUBROUTINE AM_GET I HANNE HARAMETERS USE PARAMETERS USE ICHOS USE PROPS USE INDDT USE IGRID USE GRID1 USE GRID	* *

REAL (KIND=8) :: DUR, DVR, DWR ***** DO 100 K=K11.KNK DO 100 J=1.NJ DO 100 I=1,NI AM(I,J,K)=0.AMX(I,J,K)=0.AMY(I,J,K)=0.AMZ(I,J,K)=0.100 VM(I,J,K)=0. IF(IBOIL.EQ.0) RETURN CALL QN GET DO 200 K=K11,KNK DO 200 J=1.NJ DO 200 I=1.NI AM(I,J,K)=HFGI*(QN(I,J,K,2)/TK2-QN(I,J,K,1)/TK1) 200 CONTINUE DO 300 K=K11,KNK DO 300 J=1,NJ DO 300 I=1,NI IF (I.NE.1) AMX(I,J,K)=AM(I ,J,K)*FNX(I ,J,K)*XDW(I)+AM(I-1,J,K)*FNX(I-1,J,K)*XDE(I) IF (J.NE.1) AMY(I,J,K)=AM(I,J ,K)*FNY(I,J ,K)*YDS(J)+AM(I,J-1,K)*FNY(I,J-1,K)*YDN(J) IF(I23.EQ.2) GOTO 300 IF(K.NE.1) AMZ(I,J,K)=AM(I,J,K)*FNZ(I,J,K)*ZDB(K)+AM(I,J,K-1)*FNZ(I,J,K-1)*ZDT(K) 300 CONTINUE DO 310 K=2,NKM DO 310 J=2,NJM DO 310 I=2,NI IF(T_1PH(F(I,J,K),F(I-1,J,K))) GOTO 310 IF(S(I,J,K).GT.0. .AND. S(I-1,J,K).GT.0.) GOTO 312 IF(S(I,J,K).LE.0. .AND. S(I-1,J,K).LE.0.) GOTO 310 IF(S(I,J,K)*S(I,J,K)/(S(I,J,K)-S(I-1,J,K)) .LT.S(I,J,K)*F(I,J,K)/(F(I,J,K)-F(I-1,J,K))) GOTO 310 DUR=AMX(I,J,K)*VFG*RU(I)*YC(J)*ZC(K)*SIGN1(F(I,J,K)-F(I-1,J,K)) 312 IF(T_2PH(FU(I,J,K),F(I ,J,K))) VM(I ,J,K)=VM(I ,J,K)+DUR IF(T 2PH(FU(I,J,K),F(I-1,J,K))) VM(I-1,J,K)=VM(I-1,J,K)+DUR 310 CONTINUE DO 320 K=2,NKM DO 320 J=2.NJ DO 320 I=2,NIM IF(T 1PH(F(I,J,K),F(I,J-1,K))) GOTO 320 IF(S(I,J,K).GT.0. .AND. S(I,J-1,K).GT.0.) GOTO 322 IF(S(I,J,K).LE.0. .AND. S(I,J-1,K).LE.0.) GOTO 320 IF(S(I,J,K)*S(I,J,K)/(S(I,J,K)-S(I,J-1,K)) .LT.S(I,J,K)*F(I,J,K)/(F(I,J,K)-F(I,J-1,K))) GOTO 320 DVR=AMY(I,J,K)*VFG*RP(I)*XC(I)*ZC(K)*SIGN1(F(I,J,K)-F(I,J-1,K)) 322 IF(T 2PH(FV(I,J,K),F(I,J ,K))) VM(I,J ,K)=VM(I,J ,K)+DVR IF(T 2PH(FV(I,J,K),F(I,J-1,K))) VM(I,J-1,K)=VM(I,J-1,K)+DVR 320 CONTINUE IF(I23.EQ.2) GOTO 340

DO 330 K=2,NK DO 330 J=2,NJM DO 330 I=2.NIM IF(T_1PH(F(I,J,K),F(I,J,K-1))) GOTO 330 IF(S(I,J,K).GT.0. .AND. S(I,J,K-1).GT.0.) GOTO 332 IF(S(I,J,K).LE.0. .AND. S(I,J,K-1).LE.0.) GOTO 330 IF(S(I,J,K)*S(I,J,K)/(S(I,J,K)-S(I,J,K-1)) .LT.S(I,J,K)*F(I,J,K)/(F(I,J,K)-F(I,J,K-1))) GOTO 330 332 DWR=AMZ(I,J,K)*VFG*XC(I)*YC(J)*SIGN1(F(I,J,K)-F(I,J,K-1)) $IF(T_2PH(FW(I,J,K),F(I,J,K))) VM(I,J,K) = VM(I,J,K) + DWR$ IF(T_2PH(FW(I,J,K),F(I,J,K-1))) VM(I,J,K-1)=VM(I,J,K-1)+DWR 330 CONTINUE 340 IF(QMIC0.LT.1.E-10 .OR. IQ LIQ.EQ.0) RETURN CALL QM GET RETURN END SUBROUTINE BC_ASSS **USE PARAMETERS USE ICHOS USE INDMO USE IGRID USE IBNDS** USE GRID1 **USE GRIDB** USE GRIDL USE UVTBC **USE LVFBC USE LEVFN USE FFSOR USE ROGAM** USE QMSOR **USE APANS USE AEANS USE F2F00 USE UVTPP** USE CALC1 USE FUNC **USE MPIVAR** IMPLICIT NONE LOGICAL T_2PH,T_1PH REAL (KIND=8) :: DF,HX,HY,HZ,HXE,HXW,HZB,HZT,TTN INTEGER :: I,J,K,NT,II,JJ,KK INTEGER :: ITMP, ITMPE, JTMP, JTMPE, KTMP, KTMPE ENTRY U BC CALL SHRINK IF(IBODY.EQ.0) GOTO 105 DO 100 K=2,NKM DO 100 J=2,NJM DO 100 I=3,NIM

100 IF(SU(I,J,K) .LE. 0.) U(I,J,K)=0.

105 DO 110 K=KKST.KKEND DO 110 J=JJST,JJEND IF(IBCW.NE.IOUT) U(2, J, K)=0. IF(IBCE.NE.IOUT) U(NI,J,K)=0. IF(IBCW.EQ.IINF) U(2,J,K)=UIN0 IF(IBCE.EQ.IINF) U(NI,J,K)=UIN0 110 CONTINUE ITMPE = IIEND IF (PIDX.EQ.PROCSX-1) ITMPE = IIEND+1 DO 120 K=KKST,KKEND DO 120 I=IIST,ITMPE U(I, 1, K)=0.U(I,NJ,K)=0. IF(IBCS.EQ.IOUT .OR. IBCS.EQ.ISYM) U(I, 1,K)=U(I, 2,K) IF(IBCN.EQ.IOUT .OR. IBCN.EQ.ISYM) U(I,NJ,K)=U(I,NJM,K) 120 CONTINUE JTMP=JJST JTMPE=JJEND ITMPE=IIEND IF (PIDX.EQ.PROCSX-1) ITMPE = IIEND+1 IF (PIDY.EQ.0) JTMP=JJST-1 IF (PIDY.EQ.PROCSY-1) JTMPE=JJEND+1 IF(I23.EQ.2) RETURN DO 130 J=JTMP,JTMPE !1,NJ DO 130 I=IIST, ITMPE !2, NI U(I,J, 1)=0. U(I,J,NK)=0. IF(IBCB.EQ.IOUT .OR. IBCB.EQ.ISYM) U(I,J, 1)=U(I,J, 2) IF(IBCT.EQ.IOUT .OR. IBCT.EQ.ISYM) U(I,J,NK)=U(I,J,NKM) 130 CONTINUE CALL FRAGMENT CALL RELOAD IF (TASKID.NE.0) THEN CALL MPI_SEND(U(IIST:IIEND,JJST:JJEND,KKST:KKEND), SPANX*SPANY*SPANZ, MPI_DOUBLE_PRECISION, 0, TASKID, MPI_COMM_WORLD, IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI RECV(U(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT), RSPANZ(NT):RSPANZE(NT)),SIZECC(NT),MPI DOUBLE PRECISION,NT,NT ,MPI COMM WORLD, STATUS, IERR) ENDDO **ENDIF**

CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI BCAST(U(1,1,1),SIZE(U),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR) RETURN ENTRY U BCAS IF(IBODY.EQ.0) RETURN DO 140 K=2,NKM DO 140 J=2,NJM DO 140 I=3,NIM IF(SU(I,J,K) .GT. 0.) GOTO 140 AP(I,J,K)=1. AW(I,J,K)=0. AE(I,J,K)=0. AS(I,J,K)=0. AN(I,J,K)=0. AB(I,J,K)=0. AT(I,J,K)=0. 140 CONTINUE RETURN ENTRY U BCSS DO 150 K=KKST,KKEND DO 150 J=JJST,JJEND DO 150 I=IIST,IIEND !3,NIM 150 IF(SU(I,J,K) .LE. 0.) SS(I,J,K)=0. RETURN ENTRY UC SET DO 160 K=KKST,KKEND DO 160 J=JJST,JJEND DO 160 I=IIST,IIEND 160 IF(SU(I,J,K) .LE. 0.) CC(I,J,K)=0. IF (TASKID.NE.0) THEN CALL MPI_SEND(CC(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ, MPI_DOUBLE_PRECISION,0,8,MPI_COMM_WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI RECV(CC(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT) ,RSPANZ(NT):RSPANZE(NT)),SIZECC(NT),MPI DOUBLE PRECISION,NT,8 ,MPI COMM WORLD,STATUS,IERR) **ENDDO** ENDIF CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI_BCAST(CC(1,1,1),SIZE(CC),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR) RETURN
ENTRY V BC ****** ***** IF(IBODY.EQ.0) GOTO 205 DO 200 K=2,NKM DO 200 J=3,NJM DO 200 I=2,NIM 200 IF(SV(I,J,K) .LE. 0.) V(I,J,K)=0. 205 DO 210 K=2,NKM DO 210 J=3,NJM V(1,J,K)=0. V(NI,J,K)=0. IF(IBCW.EQ.IOUT .OR. IBCW.EQ.ISYM) V(1,J,K)=V(2,J,K) IF(IBCE.EQ.IOUT .OR. IBCE.EQ.ISYM) V(NI,J,K)=V(NIM,J,K) 210 CONTINUE DO 220 K=2.NKM DO 220 I=1,NI IF(IBCS.NE.IOUT) V(I, 2,K)=0. IF(IBCN.NE.IOUT) V(I,NJ,K)=0. IF(IBCS.EQ.IINF) V(I, 2,K)=UIN0 IF(IBCN.EQ.IINF) V(I,NJ,K)=UIN0 IF(IBCN.EQ.IOUT) V(I,NJ,K)=V(I,NJM,K) 220 CONTINUE IF(I23.EQ.2) RETURN DO 230 J=2,NJ DO 230 I=1,NI IF(IBCB.EQ.IOUT .OR. IBCB.EQ.ISYM) V(I,J, 1)=V(I,J, 2) IF(IBCT.EQ.IOUT .OR. IBCT.EQ.ISYM) V(I,J,NK)=V(I,J,NKM) 230 CONTINUE RETURN ENTRY V BCAS DO 240 K=2,NKM DO 240 J=3.NJM DO 240 I=2,NIM IF(SV(I,J,K) .GT. 0.) GOTO 240 AP(I,J,K)=1. AW(I,J,K)=0. AE(I,J,K)=0. AS(I,J,K)=0. AN(I,J,K)=0. AB(I,J,K)=0. AT(I,J,K)=0. 240 CONTINUE RETURN ENTRY V_BCSS

DO 250 K=KKST,KKEND DO 250 J=JJST,JJEND DO 250 I=IIST.IIEND 250 IF(SV(I,J,K) .LE. 0.) SS(I,J,K)=0. RETURN ENTRY VC SET DO 260 K=KKST,KKEND DO 260 J=JJST,JJEND DO 260 I=IIST,IIEND 260 IF(SV(I,J,K) .LE. 0.) CC(I,J,K)=0. IF (TASKID.NE.0) THEN CALL MPI SEND(CC(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ, MPI DOUBLE PRECISION,0,8,MPI COMM WORLD,IERR) ENDIF I IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI RECV(CC(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT), RSPANZ(NT):RSPANZE(NT)),SIZECC(NT),MPI DOUBLE PRECISION,NT,8 ,MPI COMM WORLD,STATUS,IERR) **ENDDO** ENDIF CALL MPI BARRIER(MPI COMM_WORLD, IERR) CALL MPI_BCAST(CC(1,1,1),SIZE(CC),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR) RETURN ENTRY W BC ***** ***** IF(I23.EQ.2) RETURN IF(IBODY.EQ.0) GOTO 305 DO 300 K=3.NKM DO 300 J=2,NJM DO 300 I=2,NIM 300 IF(SW(I,J,K) .LE. 0.) W(I,J,K)=0. 305 DO 310 K=3,NKM DO 310 J=2,NJM W(1,J,K)=0. W(NI,J,K)=0. IF(IBCW.EQ.IOUT .OR. IBCW.EQ.ISYM) W(1,J,K)=V(2,J,K) IF(IBCE.EQ.IOUT .OR. IBCE.EQ.ISYM) W(NI,J,K)=V(NIM,J,K) 310 CONTINUE DO 320 K=3,NKM DO 320 I=1,NI W(I, 1,K)=0. W(I,NJ,K)=0.IF(IBCS.EQ.IOUT .OR. IBCS.EQ.ISYM) W(I, 1,K)=W(I, 2,K)

IF(IBCN.EQ.IOUT .OR. IBCN.EQ.ISYM) W(I,NJ,K)=W(I,NJM,K) 320 CONTINUE DO 330 J=1.NJ DO 330 I=1,NI IF(IBCB.NE.IOUT) W(I,J, 2)=0. IF(IBCT.NE.IOUT) W(I,J,NK)=0. IF(IBCB.EQ.IINF) W(I,J, 2)=UIN0 IF(IBCT.EQ.IINF) W(I,J,NK)=UIN0 CONTINUE 330 RETURN ENTRY W BCAS IF(IBODY.EQ.0) RETURN DO 340 K=3,NKM DO 340 J=2,NJM DO 340 I=2,NIM IF(SW(I,J,K) .GT. 0.) GOTO 340 AP(I,J,K)=1. AW(I,J,K)=0. AE(I,J,K)=0. AS(I,J,K)=0. AN(I,J,K)=0.AB(I,J,K)=0. AT(I,J,K)=0. 340 CONTINUE RETURN ENTRY W BCSS DO 350 K=KKST,KKEND DO 350 J=JJST,JJEND DO 350 I=IIST,IIEND 350 IF(SW(I,J,K) .LE. 0.) SS(I,J,K)=0. RETURN ENTRY WC SET DO 360 K=KKST,KKEND DO 360 J=JJST,JJEND DO 360 I=IIST,IIEND 360 IF(SW(I,J,K) .LE. 0.) CC(I,J,K)=0. IF (TASKID.NE.0) THEN CALL MPI SEND(CC(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ, MPI DOUBLE PRECISION,0,8,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1.26 CALL MPI_RECV(CC(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT), RSPANZ(NT):RSPANZE(NT)),SIZECC(NT),MPI_DOUBLE_PRECISION,NT,8,

MPI COMM WORLD, STATUS, IERR) ENDDO ENDIF CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI_BCAST(CC(1,1,1),SIZE(CC),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR) RETURN ENTRY T BC DO 400 K=2,NKM DO 400 J=2,NJM DO 400 I=2,NIM IF(IQ_VAP.EQ.0 .AND. F(I,J,K).LT.0.) T(I,J,K)=TINT IF(IQ_LIQ.EQ.0 .AND. F(I,J,K).GT.0.) T(I,J,K)=TINT IF(F(I,J,K) .EQ. 0.) T(I,J,K)=TINT IF(S(I,J,K) .LE. 0.) T(I,J,K)=TWAL 400 CONTINUE DO 410 K=2,NKM DO 410 J=2,NJM T(1,J,K)=T(2,J,K)410 T(NI,J,K)=T(NIM,J,K) DO 420 K=2.NKM DO 420 I=1,NI T(I, 1,K)=T(I, 2,K)420 T(I,NJ,K)=T(I,NJM,K)IF(I23.EQ.3) THEN DO 430 J=1,NJ DO 430 I=1,NI T(I,J, 1)=T(I,J, 2)430 T(I,J,NK)=T(I,J,NKM) ENDIF IF(IBCS.EQ.IWAL) THEN DO 422 K=2,NKM DO 422 I=2.NIM HY=1. TTN=T(I,2,K)IF(F(I,1,K).LE.0. .AND. IQ_VAP.EQ.0) HY=0. IF(F(I,1,K).GE.0. .AND. IQ LIQ.EQ.0) HY=0. IF(T 2PH(F(I,1,K),F(I,2,K))) THEN HY=F(I,1,K)/(F(I,1,K)-F(I,2,K))TTN=TINT ENDIF HXW=0.5HXE=0.5 IF(T 2PH(F(I,1,K),F(I-1,1,K))) HXW=XD(I)*F(I,1,K)/(F(I,1,K)-F(I-1,1,K))/XC(I) IF(T_2PH(F(I,1,K),F(I+1,1,K))) HXE=XD(I+1)*F(I,1,K)/(F(I,1,K)-F(I+1,1,K))/XC(I) HX=HXW+HXE HZ=1.

IF(I23.EQ.3) THEN HZB=0.5 HZT=0.5 IF(T_2PH(F(I,1,K),F(I,1,K-1))) HZB=ZD(K)*F(I,1,K)/(F(I,1,K)-F(I,1,K-1))/ZC(K) IF(T 2PH(F(I,1,K),F(I,1,K+1))) HZT=ZD(K+1)*F(I,1,K)/(F(I,1,K)-F(I,1,K+1))/ZC(K) HZ=HZB+HZT ENDIF T(I, 1,K)=TTN+(TBCS-TTN)*HY*HX*HZ 422 CONTINUE **ENDIF** RETURN |******** ****** ENTRY T BCAS DO 440 K=2,NKM DO 440 J=2,NJM DO 440 I=2,NIM IF((IQ_VAP.EQ.0 .AND. F(I,J,K).LT.0.) .OR. (IQ_LIQ.EQ.0 .AND. F(I,J,K).GT.0.) .OR.& & (S(I,J,K).LE.0. .OR. F(I,J,K).EQ.0.)) THEN AP(I,J,K)=1. AW(I,J,K)=0. AE(I,J,K)=0. AS(I,J,K)=0. AN(I,J,K)=0.AB(I,J,K)=0. AT(I,J,K)=0. ENDIF 440 CONTINUE RETURN ********* ENTRY T BCSS ********** DO 450 K=KKST,KKEND DO 450 J=JJST,JJEND DO 450 I=IIST, IIEND 450 IF((IQ VAP.EQ.0 .AND. F(I,J,K).LT.0.).OR.(IQ LIQ.EQ.0 .AND. F(I,J,K).GT.0.).OR.(S(I,J,K).LE.0. .OR. F(I,J,K).EQ.0.)) SS(I,J,K)=0. RETURN ENTRY TC SET DO 460 K= KKST, KKEND DO 460 J= JJST, JJEND DO 460 I= IIST, IIEND IF((IQ VAP.EQ.0 .AND. F(I,J,K).LT.0.) .OR. (IQ LIQ.EQ.0 .AND. F(I,J,K).GT.0.) .OR. 460 (S(I,J,K).LE.0. .OR. F(I,J,K).EQ.0.)) CC(I,J,K)=0. IF (TASKID.NE.0) THEN CALL MPI SEND(CC(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ, MPI DOUBLE PRECISION,0,8,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26

CALL MPI RECV(CC(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT), RSPANZ(NT):RSPANZE(NT)),SIZECC(NT),MPI DOUBLE PRECISION,NT.8. MPI COMM WORLD, STATUS, IERR) ENDDO ENDIF CALL MPI_BARRIER(MPI_COMM_WORLD, IERR) CALL MPI BCAST(CC(1,1,1),SIZE(CC),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR) RETURN ENTRY P BC CALL SHRINK ITMP=IIST JTMP=JJST KTMP=KKST ITMPE=IIEND JTMPE=JJEND KTMPE=KKEND DO 510 K=KKST,KKEND !2,NKM DO 510 J=JJST,JJEND !2,NJM P(1,J,K)=P(2,J,K)P(NI,J,K)=P(NIM,J,K) IF(IBCW.EQ.IOUT) P(1,J,K)=0. IF(IBCE.EQ.IOUT) P(NI,J,K)=0. 510 CONTINUE IF (PIDX.EQ.0) ITMP=1 IF (PIDX.EQ.PROCSX-1) ITMPE=ID DO 520 K=KKST,KKEND DO 520 I=ITMP,ITMPE P(I, 1,K)=P(I, 2,K) P(I,NJ,K)=P(I,NJM,K)IF(IBCS.EQ.IOUT) P(I, 1,K)=0. IF(IBCN.EQ.IOUT) P(I,NJ,K)=0. 520 CONTINUE IF (PIDX.EQ.0) ITMP=1 IF (PIDX.EQ.PROCSX-1) ITMPE=ID IF (PIDY.EQ.0) JTMP=1 IF (PIDY.EQ.PROCSY-1) JTMPE=JD IF(I23.EQ.2) RETURN DO 530 J=JTMP,JTMPE DO 530 I=ITMP,ITMPE P(I,J, 1)=P(I,J, 2)P(I,J,NK)=P(I,J,NKM)IF(IBCB.EQ.IOUT) P(I,J, 1)=0. IF(IBCT.EQ.IOUT) P(I,J,NK)=0. 530 CONTINUE CALL FRAGMENT

CALL RELOAD IF (TASKID.NE.0) THEN CALL MPI SEND(P(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ, MPI DOUBLE PRECISION,0,TASKID,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI RECV(P(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT), RSPANZ(NT):RSPANZE(NT)),SIZECC(NT),MPI DOUBLE PRECISION,NT,NT, MPI_COMM_WORLD,STATUS,IERR) ENDD ENDIF CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI BCAST(P(1,1,1),SIZE(P),MPI DOUBLE PRECISION.0,MPI COMM WORLD.IERR) CALL SHRINK CALL RELOAD RETURN ENTRY F BC IF(IBODY.EQ.1 .AND. ICONB.EQ.0) THEN DO 600 K=2,NKM DO 600 J=2,NJM DO 600 I=2,NIM IF(S(I,J,K).LE.0.) F(I,J,K)=SIGN(F(I,J,K),BF(I,J,K)) 600 CONTINUE **ENDIF** DO 610 K=2.NKM DO 610 J=2,NJM F(1,J,K)=F(2,J,K)F(NI,J,K)=F(NIM,J,K)610 CONTINUE DO 620 K=2.NKM DO 620 I=1,NI F(I, 1,K)=F(I, 2,K) 620 F(I,NJ,K)=F(I,NJM,K) IF(I23.EQ.3) THEN DO 630 J=1.NJ DO 630 I=1,NI F(I,J, 1)=F(I,J, 2)F(I,J,NK)=F(I,J,NKM)630 CONTINUE ENDIF IF(IBCS.GE.IWAL) THEN DO 622 K=2.NKM DO 622 I=2,NIM IF(ICONT.EQ.1) THEN DF=(BF(I,1,K)-F(I,2,K))/YD(2)DF=AMIN1(AMAX1(DF,COSMIN),COSMAX) COSBS(I,K)=DF

F(I,1,K)=F(I,2,K)+DF*YD(2)ELSE F(I,1,K)=F(I,2,K)-XDW(3)*(F(I,3,K)-F(I,2,K)) **ENDIF** IF(ICONT.EQ.0) F(I,1,K)=SIGN(F(I,1,K),BF(I,1,K)) 622 CONTINUE ENDIF RETURN ENTRY IBUB_BC DO 1700 I2B=1,N2B DO 710 K=2,NKM DO 710 J=2,NJM IBUB(1,J,K,I2B)=IBUB(2,J,K,I2B) 710 IBUB(NI,J,K,I2B)=IBUB(NIM,J,K,I2B) DO 720 K=2,NKM DO 720 I=1,NI IBUB(I, 1,K,I2B)=IBUB(I, 2,K,I2B) 720 IBUB(I,NJ,K,I2B)=IBUB(I,NJM,K,I2B) IF(I23.EQ.2) RETURN DO 730 J=1,NJ DO 730 I=1,NI IBUB(I,J, 1,I2B)=IBUB(I,J, 2,I2B) IBUB(I,J,NK,I2B)=IBUB(I,J,NKM,I2B) 730 1700 CONTINUE RETURN ENTRY FO BC DO 900 K=K11,KNK DO 900 J=1,NJ DO 900 I=1,NI 900 FO(I,J,K)=F(I,J,K)DO 910 K=1,NK DO 910 J=1.NJ IF(IBCW.EQ.ISYM) FO(0,J,K)=FO(1,J,K) 910 CONTINUE IF(I23.EQ.2) RETURN DO 920 K=1,NK DO 920 I=0,NI+1 IF(IBCS.EQ.ISYM) FO(I,0,K)=FO(I,1,K) 920 CONTINUE IF(I23.EQ.2) RETURN DO 930 J=0,NJ+1 DO 930 I=0,NI+1 IF(IBCB.EQ.ISYM) FO(I,J,0)=FO(I,J,1) 930 CONTINUE

RETURN END SUBROUTINE BUB SUB **USE PARAMETERS USE ICHOS USE PROPS USE INDMO** USE INDDT **USE IGRID** USE GRID1 **USE GRIDB USE GRIDL USE LEVFN USE FFSOR USE QMSOR** USE RESLT **USE IBSUB USE ICHEK USE UVTPP USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,II,JJ,KK,IND0,IND1,IND2,IND9,N,NBUB1,IBUB0,IBUB1,IBUBS,IFX,IFY,IFZ INTEGER (KIND=4), DIMENSION(100) :: MKBUB, IPBUBS REAL (KIND=8) :: AFP, FFP, V00, V11, BVOLBS, VOLHB ENTRY BUB BRK IF(NBUB(I2B) .EQ. 0) RETURN IF(NBUB(I2B) .EQ. 100) RETURN IF(ITIME .NE. ITIME/10*10) RETURN V00=V0H(I2B) V11=V1H(I2B) DO 10 N=1,NBUB(I2B) MKBUB(N)=0 10 DO 20 K=2.NKM DO 20 J=2,NJM DO 20 I=2,NIM 20 MK(I,J,K)=0I-----100 CONTINUE NCHB=0 DO 110 K=2,NKM DO 110 J=2,NJM DO 110 I=2,NIM IF(MK(I,J,K) .EQ. 1) GOTO 110 IF(IBUB(I,J,K,I2B) .EQ. 0) GOTO 110 NCHB=1 IIB(1)=I JJB(1)=J

KKB(1)=K MK(I,J,K)=1IBUB0=IBUB(I,J,K,I2B) **GOTO 115** 110 CONTINUE IF(NCHB.EQ.0) GOTO 190 115 N=0 120 N=N+1 IF(N .GT. NCHB) GOTO 135 II=IIB(N) JJ=JJB(N) KK=KKB(N) DO 130 K=KK-1,KK+1 DO 130 J=JJ-1,JJ+1 DO 130 I=II-1,II+1 IF(MK(I,J,K) .EQ. 1) GOTO 130 IF(IBUB(I,J,K,I2B) .NE. IBUB0) GOTO 130 MK(I,J,K)=1NCHB=NCHB+1 IIB(NCHB)=I JJB(NCHB)=J KKB(NCHB)=K CONTINUE 130 **GOTO 120** 135 CONTINUE IF(MKBUB(IBUB0).EQ.0) THEN MKBUB(IBUB0)=IBUB0 **GOTO 100** ENDIF IBUB0=MKBUB(IBUB0) WRITE(I69,9000) ' Bubble Area Breaking !!!'& & ,ITIME,IBUB0,IIB(1),JJB(1),KKB(1) 9000 FORMAT(A.I8.I4.3(I4)) NBUB(I2B)=NBUB(I2B)+1 NBUB1=NBUB(I2B) BVOLB(NBUB1.I2B)=0. DO 150 N=1,NCHB IBUB(IIB(N), JJB(N), KKB(N), I2B)=NBUB1 VOLHB=VOL(IIB(N),JJB(N),KKB(N))*HB(IIB(N),JJB(N),KKB(N)) BVOLB(NBUB1,I2B)=BVOLB(NBUB1,I2B)& +(V00-V11*H(IIB(N),JJB(N),KKB(N)))*VOLHB & CONTINUE 150 BVOLB(IBUB0,I2B)=BVOLB(IBUB0,I2B)-BVOLB(NBUB1,I2B) IF(BVOLB(NBUB1,I2B).GT.BVOLB(IBUB0,I2B)) THEN BVOLBS=BVOLB(IBUB0,I2B) BVOLB(IBUB0,I2B)=BVOLB(NBUB1,I2B) BVOLB(NBUB1,I2B)=BVOLBS DO 160 K=2,NKM DO 160 J=2,NJM DO 160 I=2,NIM

IBUBS=IBUB(I,J,K,I2B) IF(IBUBS.EQ.IBUB0) IBUB(I,J,K,I2B)=NBUB1 160 IF(IBUBS.EQ.NBUB1) IBUB(I,J,K,I2B)=IBUB0 ENDIF IPBUB(NBUB1,I2B)=IPBUB(IBUB0,I2B) MKBUB(NBUB1)=NBUB1 WRITE(I69,9001) ' NBUB=',NBUB(I2B),' I2B=',I2B,' NCHB=',NCHB,& & ' IBUB0=',IBUB0& ,' VOLB=',BVOLB(NBUB(I2B),I2B),BVOLB(IBUB0,I2B) & 9001 FORMAT(A,I4,A,I4,A,I5,A,I4,A,1PE12.4,1PE12.4) **GOTO 100** 190 CONTINUE RETURN ENTRY BUB MRG(IND1,IND2) IND0=MIN(IND1,IND2) IND9=MAX(IND1,IND2) BVOLB(IND0,I2B)=BVOLB(IND0,I2B)+BVOLB(IND9,I2B) DO 300 K=2,NKM DO 300 J=2,NJM DO 300 I=2.NIM IF(IBUB(I,J,K,I2B) .EQ. IND9) IBUB(I,J,K,I2B)=IND0 300 IF(IBUB(I,J,K,I2B).GT. IND9) IBUB(I,J,K,I2B)=IBUB(I,J,K,I2B)-1 DO 310 N=IND9,NBUB(I2B)-1 IPBUB(N,I2B)=IPBUB(N+1,I2B) BVOLB(N,I2B)=BVOLB(N+1,I2B) 310 BVOLB(NBUB(I2B),I2B)=0. NBUB(I2B)=NBUB(I2B)-1 RETURN ENTRY IPBUB GET IF(N2B.EQ.1) RETURN DO 400 N=1,NBUB(2) IPBUBS(N)=IPBUB(N,2) 400 IPBUB(N,2)=0 IF(NBUB(2).EQ.1) RETURN J=2 DO 410 K=2,NKM DO 410 I=2,NIM IBUB1=IBUB(I,J,K,2) IF(IBUB1.LE.1) GOTO 410 IPBUB(IBUB1,2)=1 410 CONTINUE DO 420 N=1,NBUB(2)

IF(IPBUBS(N).EQ.IPBUB(N,2)) GOTO 420 WRITE(I69,*) 'Bubble: IPBUB=', IPBUB(N,2), N 420 CONTINUE RETURN ENTRY IFFIX GET DO 500 K=2,NKM DO 500 J=2,NJM DO 500 I=2,NIM 500 IFFIX(I,J,K)=0 DO 510 K=2,NKM DO 510 J=2.NJM DO 510 I=2,NIM FFP=ABS(F(I,J,K))IF(FFP.GE.ABS(F(I-1,J,K))) GOTO 510 IF(FFP.GE.ABS(F(I+1,J,K))) GOTO 510 IF(FFP.GE.ABS(F(I,J-1,K))) GOTO 510 IF(FFP.GE.ABS(F(I,J+1,K))) GOTO 510 IF(I23.EQ.3) THEN IF(FFP.GE.ABS(F(I,J,K-1))) GOTO 510 IF(FFP.GE.ABS(F(I,J,K+1))) GOTO 510 ENDIF IFFIX(I,J,K)=1 510 CONTINUE DO 520 K=2,NKM DO 520 J=2,NJM DO 520 I=2,NIM IF(IFFIX(I,J,K).EQ.1) GOTO 520 IFX=MAX(IFFIX(I-1,J,K),IFFIX(I+1,J,K))IFY=MAX(IFFIX(I,J-1,K),IFFIX(I,J+1,K)) FFP=F(I,J,K) AFP=ABS(FFP) IF(IFX.EQ.1) GOTO 524 IF(FFP*F(I-1,J,K).LT.0..AND.AFP.LT.ABS(F(I-1,J,K))) IFFIX(I,J,K)=1 IF(FFP*F(I+1,J,K).LT.0..AND.AFP.LT.ABS(F(I+1,J,K))) IFFIX(I,J,K)=1 524 IF(IFY.EQ.1) GOTO 526 IF(FFP*F(I,J-1,K).LT.0..AND.AFP.LT.ABS(F(I,J-1,K))) IFFIX(I,J,K)=1 IF(FFP*F(I,J+1,K).LT.0..AND.AFP.LT.ABS(F(I,J+1,K))) IFFIX(I,J,K)=1 IF(I23.EQ.2) GOTO 520 526 IFZ=MAX(IFFIX(I,J,K-1),IFFIX(I,J,K+1)) IF(IFZ.EQ.1) GOTO 520 IF(FFP*F(I,J,K-1).LT.0..AND.AFP.LT.ABS(F(I,J,K-1))) IFFIX(I,J,K)=1 IF(FFP*F(I,J,K+1).LT.0..AND.AFP.LT.ABS(F(I,J,K+1))) IFFIX(I,J,K)=1 520 CONTINUE RETURN END

SUBROUTINE BUBBLES

USE PARAMETERS USE ICHOS USE PROPS USE INDMO USE INDDT USE IGRID USE GRID1 USE GRIDB USE IDREF USE LEVFN USE FFSOR USE QMSOR USE RESLT USE IBSUB **USE ICHEK USE UVTPP USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,II,JJ,KK,N1,N2,I1,I2,N,NN,IND1,IBUB0,IBUB1,IIMAX,NIMAX,NBUB0,NIBUB(100) REAL*8 :: DVOLB(100,2),FLUX,FMIN,ROLIQ,ROVAP,V00,V11,VOLH ENTRY BVOLB GET DO 1000 I2B=1,N2B V00=V0H(I2B) V11=V1H(I2B) DO 100 N=1,NBUB(I2B) 100 BVOLB(N,I2B)=0. DO 110 K=2,NKM DO 110 J=2,NJM DO 110 I=2.NIM N=IBUB(I,J,K,I2B) IF(N.LT.1) GOTO 110 VOLH=(V00-V11*H(I,J,K))*VOL(I,J,K)*HB(I,J,K) BVOLB(N,I2B)=BVOLB(N,I2B)+VOLH 110 CONTINUE 1000 CONTINUE RETURN ENTRY BVOLB_MOD |****** DO 200 I2B=1,N2B DO 200 N=1,NBUB(I2B) 200 DVOLB(N,I2B)=0. IF(IBOIL.EQ.1) THEN

ROLIQ=-RO1/(RO2-RO1)

ROVAP= RO2/(RO2-RO1) DO 202 K=2,NKM DO 202 J=2.NJM DO 202 I=2,NIM I1=IBUB(I,J,K,1)I2=IBUB(I,J,K,2) IF(I1.GE.1) DVOLB(I1,1)=DVOLB(I1,1)+VM(I,J,K) IF(I2.GE.1) DVOLB(I2,2)=DVOLB(I2,2)+VM(I,J,K) 202 CONTINUE DO 204 N=1,NBUB(1) DVOLB(N,1)=DVOLB(N,1)*ROVAP 204 DO 206 N=1,NBUB(2) DVOLB(N,2)=DVOLB(N,2)*ROLIQ 206 ENDIF DO 1200 I2B=1,N2B V00=V0H(I2B) V11=V1H(I2B) DO 210 K=2,NKM DO 210 J=2,NJM N=IBUB(2,J,K,I2B) IF(N.GE.1) THEN FLUX=U(2,J,K)*RU(2)*YC(J)*ZC(K)*(V00-V11*H(1,J,K)) DVOLB(N,I2B)=DVOLB(N,I2B)+FLUX ENDIF N=IBUB(NIM,J,K,I2B) IF(N.GE.1) THEN FLUX=U(NI,J,K)*RU(NI)*YC(J)*ZC(K)*(V00-V11*H(NI,J,K)) DVOLB(N,I2B)=DVOLB(N,I2B)-FLUX ENDIF 210 CONTINUE DO 220 K=2,NKM DO 220 I=2,NIM N=IBUB(I, 2,K,I2B) IF(N.GE.1) THEN FLUX=V(I, 2,K)*RP(I)*XC(I)*ZC(K)*(V00-V11*H(I, 1,K)) DVOLB(N,I2B)=DVOLB(N,I2B)+FLUX ENDIF N=IBUB(I,NJM,K,I2B) IF(N.GE.1) THEN FLUX=V(I,NJ,K)*RP(I)*XC(I)*ZC(K)*(V00-V11*H(I,NJ,K)) DVOLB(N,I2B)=DVOLB(N,I2B)-FLUX ENDIF 220 CONTINUE IF(I23.EQ.2) GOTO 235 DO 230 J=2,NJM DO 230 I=2,NIM N=IBUB(I,J, 2,I2B)IF(N.GE.1) THEN

FLUX=W(I,J, 2)*XC(I)*YC(J)*(V00-V11*H(I,J, 1)) DVOLB(N,I2B)=DVOLB(N,I2B)+FLUX ENDIF N=IBUB(I,J,NKM,I2B) IF(N.GE.1) THEN FLUX=W(I,J,NK)*XC(I)*YC(J)*(V00-V11*H(I,J,NK)) DVOLB(N,I2B)=DVOLB(N,I2B)-FLUX ENDIF 230 CONTINUE 235 CONTINUE DO 240 N=1,NBUB(I2B) 240 BVOLB(N,I2B)=BVOLB(N,I2B)+DVOLB(N,I2B)*DT 1200 CONTINUE RETURN |************* ENTRY IBUB GET DO 1300 I2B=1,N2B V11=V1H(I2B) DO 300 K=2,NKM DO 300 J=2.NJM DO 300 I=2,NIM IF(V11*F(I,J,K) .GT. DDF(I,J,K)) IBUB(I,J,K,I2B)=0 300 IF(HB(I,J,K).LT.1.E-8) IBUB(I,J,K,I2B)=0 !----- F<3*DL & IBUB=0 DO 310 K=2,NKM DO 310 J=2,NJM DO 310 I=2,NIM IF(V11*F(I,J,K) .GT. DDF(I,J,K)) GOTO 310 IF(HB(I,J,K).LT.1.E-8) GOTO 310 IF(IBUB(I,J,K,I2B) .NE. 0) GOTO 310 N=0 312 N=N+1 FMIN=1.E30 DO 314 KK=MAX(2,K-N),MIN(NKM,K+N) DO 314 JJ=MAX(2,J-N),MIN(NJM,J+N) DO 314 II=MAX(2,I-N),MIN(NIM,I+N) IF(IBUB(II,JJ,KK,I2B).EQ.0) GOTO 314 IF(ABS(F(I,J,K)-F(II,JJ,KK)).GT.FMIN) GOTO 314 IBUB(I,J,K,I2B)=IBUB(II,JJ,KK,I2B) FMIN=ABS(F(I,J,K)-F(II,JJ,KK)) 314 CONTINUE IF(IBUB(I,J,K,I2B) .NE. 0) GOTO 310 WRITE(I69,9000) ' Bubble ID=0 for F < FDV ',ITIME,I,J,K IF(N .LE. 5) GOTO 312 F(I,J,K)=V11*2.*DDF(I,J,K) IF(IBUB(I,J,K,I2B) .EQ. 0)& &WRITE(I69,9000) ' Bubble ID=0 for F < FDV while N=',N,I2B 9000 FORMAT(A,I8,4(I4))

310 CONTINUE 1300 CONTINUE CALL IBUB_BC RETURN ENTRY IBUB MOD DO 1400 I2B=1,N2B V11=V1H(I2B) IF(NBUB(I2B).EQ.1) GOTO 435 !----- Check Bubble Merging DO 410 K=2,NKM DO 410 J=2,NJM DO 410 I=2,NIMM N1=IBUB(I ,J,K,I2B) N2=IBUB(I+1,J,K,I2B) IF(N1.LE.0 .OR. N2.LE.0 .OR. N1.EQ.N2) GOTO 410 IF(V11*(F(I,J,K)+F(I+1,J,K)) .GT. & (DDF(I,J,K)+DDF(I+1,J,K))/2) GOTO 410 & WRITE(I69,9001) ' Bubble Area Merging:x !!'& ,ITIME,I2B,N1,N2,I,I+1,J,K & CALL BUB MRG(N1,N2) 410 CONTINUE 9001 FORMAT(A,I8,8(I4)) DO 420 K=2.NKM DO 420 J=2,NJMM DO 420 I=2,NIM N1=IBUB(I,J ,K,I2B) N2=IBUB(I,J+1,K,I2B) IF(N1.LE.0 .OR. N2.LE.0 .OR. N1.EQ.N2) GOTO 420 IF(V11*(F(I,J,K)+F(I,J+1,K)) .GT. & (DDF(I,J,K)+DDF(I,J+1,K))/2) GOTO 420 & WRITE(I69,9001) ' Bubble Area Merging: y !!'& & ,ITIME,I2B,N1,N2,I,J,J+1,K CALL BUB MRG(N1,N2) 420 CONTINUE IF(I23.EQ.2) GOTO 435 DO 430 K=2,NKMM DO 430 J=2,NJM DO 430 I=2,NIM N1=IBUB(I,J,K ,I2B) N2=IBUB(I,J,K+1,I2B)IF(N1.LE.0 .OR. N2.LE.0 .OR. N1.EQ.N2) GOTO 430 IF(V11*(F(I,J,K)+F(I,J,K+1)) .GT. & (DDF(I,J,K)+DDF(I,J,K+1))/2) GOTO 430 & WRITE(I69,9001) ' Bubble Area Merging:z !!'& & ,ITIME,I2B,N1,N2,I,J,K,K+1 CALL BUB_MRG(N1,N2) 430 CONTINUE

I_____ ----- Check Bubble Breaking 435 CALL BUB BRK 1400 CONTINUE !-----DO 1500 I2B=1,N2B NBUB0=NBUB(I2B) DO 500 N=1,NBUB(I2B) 500 NIBUB(N)=0 DO 510 K=2,NKM DO 510 J=2,NJM DO 510 I=2,NIM N=IBUB(I,J,K,I2B) IF(N .LE. 0) GOTO 510 NIBUB(N)=NIBUB(N)+1 510 CONTINUE N=0 520 N=N+1 IF(N .GT. NBUB(I2B)) GOTO 530 IF(NIBUB(N) .GT. 0) GOTO 520 IBUB0=N DO 522 NN=N,NBUB(I2B)-1 NIBUB(NN)=NIBUB(NN+1) 522 BVOLB(NN,I2B)=BVOLB(NN+1,I2B) NIBUB(NBUB(I2B))=0 BVOLB(NBUB(I2B),I2B)=0. DO 524 K=2,NKM DO 524 J=2,NJM DO 524 I=2,NIM 524 IF(IBUB(I,J,K,I2B) .GT. IBUB0) IBUB(I,J,K,I2B)=IBUB(I,J,K,I2B)-1 NBUB(I2B)=NBUB(I2B)-1 N=N-1 **GOTO 520** 530 CONTINUE IF(NBUB(I2B) .NE. NBUB0) WRITE(I69,*) & & 'MIBubble: NBUB(I2B)=',NBUB(I2B),I2B,ITIME 1500 CONTINUE CALL IBUB BC RETURN ENTRY IBUB_INIT ! DO 1600 I2B=1,N2B NBUB(12B)=0 V11=V1H(I2B) DO 590 K=2,NKM DO 590 J=2.NJM DO 590 I=2,NIM MK(I,J,K)=0

IBUB(I,J,K,I2B)=1 IF(V11*F(I,J,K).GT.DDF(I,J,K)) IBUB(I,J,K,I2B)=0 IF(HB(I,J,K).LT.1.E-8) IBUB(I,J,K,I2B)=0 IF(IBUB(I,J,K,I2B).EQ.1) NBUB(I2B)=1 590 CONTINUE IF(NBUB(I2B).EQ.0) GOTO 1600 !---------- Check Multi bubbles 600 CONTINUE NCHB=0 DO 610 K=2,NKM DO 610 J=2,NJM DO 610 I=2,NIM .EQ.1) GOTO 610 IF(MK(I,J,K) IF(IBUB(I,J,K,I2B).EQ.0) GOTO 610 NCHB=1 IIB(1)=I JJB(1)=JKKB(1)=K MK(I,J,K)=1IBUB0=IBUB(I,J,K,I2B) **GOTO 615** 610 CONTINUE IF(NCHB.EQ.0) GOTO 665 615 N=0 620 N=N+1 IF(N.GT. NCHB) GOTO 635 II=IIB(N) JJ=JJB(N) KK=KKB(N) DO 630 K=KK-1,KK+1 DO 630 J=JJ-1,JJ+1 DO 630 I=II-1,II+1 IF(MK(I,J,K) .EQ. 1) GOTO 630 IF(IBUB(I,J,K,I2B) .NE. IBUB0) GOTO 630 MK(I,J,K)=1NCHB=NCHB+1 IIB(NCHB)=I JJB(NCHB)=J KKB(NCHB)=K 630 CONTINUE **GOTO 620** 635 IF(NCHB .LT. 3) THEN DO 640 K=2,NKM DO 640 J=2,NJM DO 640 I=2,NIM 640 IF(IBUB(I,J,K,I2B).EQ.NBUB(I2B)) IBUB(I,J,K,I2B)=NBUB(I2B)-1 NBUB(I2B)=MAX(0,NBUB(I2B)-1) **GOTO 600** ENDIF

WRITE(I69,9002) ' Number of Bubbles=',NBUB(I2B),I2B,NCHB

NIBUB(NBUB(I2B))=NCHB 9002 FORMAT(A,I8,I4,I8,8(I4)) IND1=0 DO 650 K=2,NKM DO 650 J=2,NJM DO 650 I=2,NIM IF(MK(I,J,K) .EQ. 1) GOTO 650 IF(IBUB(I,J,K,I2B) .NE. IBUB0) GOTO 650 IBUB(I,J,K,I2B)=NBUB(I2B)+1 IND1=IND1+1 650 CONTINUE IF(IND1.EQ.0) GOTO 665 NBUB(I2B)=NBUB(I2B)+1 **GOTO 600** 665 CONTINUE IF(NBUB(I2B).LE.1) GOTO 1600 NIMAX=0 DO 670 N=1,NBUB(I2B) IF(NIBUB(N).LT.NIMAX) GOTO 670 NIMAX=NIBUB(N) IIMAX=N 670 CONTINUE IF(IIMAX.EQ.1) GOTO 1600 DO 680 K=2,NKM DO 680 J=2,NJM DO 680 I=2.NIM IBUB1=IBUB(I,J,K,I2B) IF(IBUB1.EQ. 1) IBUB(I,J,K,I2B)=IIMAX IF(IBUB1.EQ.IIMAX) IBUB(I,J,K,I2B)=1 680 CONTINUE 1600 CONTINUE RETURN END SUBROUTINE DDF_GET **USE PARAMETERS USE ICHOS USE IGRID USE GRID1 USE GRIDB USE LEVFN USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K REAL*8 :: FX1,FY1,DX1,DY1,DZ1,DET ********* *****

IF(IUGRD.EQ.1) RETURN

CALL FUVW GET DO 100 K=2.NKM DO 100 J=2,NJM DO 100 I=2,NIM FX1=(FU(I+1,J,K)-FU(I,J,K))/XC(I) FY1=(FV(I,J+1,K)-FV(I,J,K))/YC(J)IF(I23.EQ.3) FZ1=(FW(I,J,K+1)-FW(I,J,K))/ZC(K) DET=AMAX1(SQRT(FX1**2+FY1**2+FZ1**2),1.E-10) FX1=FX1/DET FY1=FY1/DET FZ1=FZ1/DET DX1=FX1*XC(I) DY1=FY1*YC(J) DZ1=FZ1*ZC(K) 100 DDF(I,J,K)=AMAX1(DTF(I,J,K),SQRT(DX1**2+DY1**2+DZ1**2)) DO 110 K=2,NKM DO 110 J=2,NJM DDF(1,J,K)=DDF(2,J,K) 110 DDF(NI,J,K)=DDF(NIM,J,K) DO 120 K=2,NKM DO 120 I=1,NI DDF(I, 1, K) = DDF(I, 2, K)120 DDF(I,NJ,K)=DDF(I,NJM,K) IF(I23.EQ.2) RETURN DO 130 J=1,NJ DO 130 I=1,NI DDF(I,J, 1)=DDF(I,J, 2)130 DDF(I,J,NK)=DDF(I,J,NKM) RETURN END SUBROUTINE DDF GET **USE PARAMETERS USE ICHOS USE IGRID USE GRID1 USE GRIDB USE LEVFN USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K REAL*8 :: FX1,FY1,DX1,DY1,DZ1,DET ******** IF(IUGRD.EQ.1) RETURN CALL FUVW_GET

DO 100 K=2,NKM DO 100 J=2.NJM DO 100 I=2,NIM FX1=(FU(I+1,J,K)-FU(I,J,K))/XC(I) FY1=(FV(I,J+1,K)-FV(I,J,K))/YC(J)IF(I23.EQ.3) FZ1=(FW(I,J,K+1)-FW(I,J,K))/ZC(K) DET=AMAX1(SQRT(FX1**2+FY1**2+FZ1**2),1.E-10) FX1=FX1/DET FY1=FY1/DET FZ1=FZ1/DET DX1=FX1*XC(I) DY1=FY1*YC(J) DZ1=FZ1*ZC(K) 100 DDF(I,J,K)=AMAX1(DTF(I,J,K),SQRT(DX1**2+DY1**2+DZ1**2)) DO 110 K=2,NKM DO 110 J=2,NJM DDF(1,J,K)=DDF(2,,K) 110 DDF(NI,J,K)=DDF(NIM,J,K) DO 120 K=2,NKM DO 120 I=1,NI DDF(I, 1,K)=DDF(I, 2,K)120 DDF(I,NJ,K)=DDF(I,NJM,K) IF(I23.EQ.2) RETURN DO 130 J=1,NJ DO 130 I=1,NI DDF(I,J, 1)=DDF(I,J, 2)130 DDF(I,J,NK)=DDF(I,J,NKM) RETURN END SUBROUTINE F GET **USE PARAMETERS USE ICHOS USE PROPS USE INDMO USE INDDT USE IGRID USE GRID1 USE GRIDB** USE GRIDL **USE LEVFN** USE QMSOR USE FNXYZ **USE APANS USE AEANS**

USE UVTPP USE FUNC **USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K REAL*8 :: UIW, UIE, VIS, VIN, FLUX1, FLUX2, FLUX3=0, WIB, WIT, FLX, FLY, FLZ CALL FXYZ_GET 1-----DO 100 K=2,NKM DO 100 J=2,NJM DO 100 I=2,NIM UIW=U(I , J,K)+AMX(I , J,K)/RHOF(FU(I , J,K))UIE=U(I+1,J,K)+AMX(I+1,J,K)/RHOF(FU(I+1,J,K)) FLX=0.5*(RU(I)*UIW+RU(I+1)*UIE)/RP(I) VIS=V(I,J ,K)+AMY(I,J ,K)/RHOF(FV(I,J ,K)) VIN=V(I,J+1,K)+AMY(I,J+1,K)/RHOF(FV(I,J+1,K)) FLY=0.5*(VIS+VIN)-VBUB FLUX1=AMAX1(FLX,0.)*AW(I,J,K)+AMIN1(FLX,0.)*AE(I,J,K) FLUX2=AMAX1(FLY,0.)*AS(I,J,K)+AMIN1(FLY,0.)*AN(I,J,K) IF(I23.EQ.3) THEN WIB=W(I,J,K)+AMZ(I,J,K)/RHOF(FW(I,J,K)) WIT=W(I,J,K+1)+AMZ(I,J,K+1)/RHOF(FW(I,J,K+1)) FLZ=0.5*(WIB+WIT) FLUX3=AMAX1(FLZ,0.)*AB(I,J,K)+AMIN1(FLZ,0.)*AT(I,J,K) ENDIF F(I,J,K)=F(I,J,K)-DT*(FLUX1+FLUX2+FLUX3) 100 CONTINUE 1----CALL F BC CALL DDF GET CALL IBUB GET RETURN END SUBROUTINE F_JMOVE **USE PARAMETERS USE ICHOS USE PROPS** USE INDMO USE INDDT **USE IGRID USE GRID1 USE GRIDB**

USE GRIDL USE LEVFN USE QMSOR **USE APANS USE AEANS USE UVTPP USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K REAL*8 :: HH, VOLV, VOLH, DVBUB, FLUX, FLY VOLV=0. YBUB=0. DO 10 K=2,NKM DO 10 J=2,NJM DO 10 I=2,NIM HH=0.5+F(I,J,K)/DDF(I,J,K)HH=AMAX1(0.,AMIN1(1.,HH)) VOLH=(1.-HH)*VOL(I,J,K)*HB(I,J,K) VOLV=VOLV+VOLH 10 YBUB=YBUB+VOLH*YP(J) YBUB=YBUB/AMAX1(VOLV,1.E-20) DVBUB=(YBUB-YBUB0)/DT VBUB=VBUB+DVBUB CALL FXYZ GET DO 100 K=2,NKM DO 100 J=2,NJM DO 100 I=2,NIM FLY=-DVBUB FLUX=AMAX1(FLY,0.)*AS(I,J,K)+AMIN1(FLY,0.)*AN(I,J,K) F(I,J,K)=F(I,J,K)-DT*FLUX100 CONTINUE !-----CALL F BC CALL DDF GET CALL IBUB GET RETURN END SUBROUTINE F_MOD **USE PARAMETERS USE ICHOS USE INDMO USE INDDT** USE IGRID **USE GRID1 USE GRIDB USE GRIDL**

USE IDREF USE SPERR USE LEVFN USE RESLT USE APANS **USE AEANS** USE IBSUB **USE CALC1** USE FUNC **USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,ITER,NFBUB(100),SN,N REAL*8 :: HH,FX1,FY1,V00,V11,SFMAX,FDS,FSAV,VOLHB |******** FSAV=F(IREF, JREF, KREF) ITER=-1 10 ITER=ITER+1 !---------- REINIT CALL FXYZ_GET CALL IFFIX_GET DO 1 K=2,NKM DO 1 J=2,NJM DO 1 I=2.NIM 1 CC(I,J,K)=F(I,J,K)/SQRT(F(I,J,K)**2+DTF(I,J,K)**2)DO 100 K=2.NKM DO 100 J=2,NJM DO 100 I=2,NIM IF(HB(I,J,K).GE.1.E-8 .AND. IFFIX(I,J,K).EQ.1) GOTO 100 SN=SIGN1(CC(I,J,K)) FX1=(AMAX1(0.,SN*AW(I,J,K),-SN*AE(I,J,K)))**2 FY1=(AMAX1(0.,SN*AS(I,J,K),-SN*AN(I,J,K)))**2 IF(I23.EQ.3) FZ1=(AMAX1(0.,SN*AB(I,J,K),-SN*AT(I,J,K)))**2 SS(I,J,K)=CC(I,J,K)*(SQRT(FX1+FY1+FZ1)-1.)F(I,J,K)=F(I,J,K)-0.5*DTF(I,J,K)*SS(I,J,K) 100 CONTINUE CALL F_BC SFMAX=0. DO 110 K=2,NKM DO 110 J=2,NJM DO 110 I=2,NIM IF(ABS(F(I,J,K)) .GE. 1.5*DDF(I,J,K)) GOTO 110 SFMAX=AMAX1(SFMAX,ABS(SS(I,J,K))) 110 CONTINUE 1-----IF(IBODY.EQ.1 .AND. ICONB.EQ.1) CALL F IMMERSED CALL IBUB_GET DO 1200 I2B=N2B,1,-1

V00=V0H(I2B) V11=V1H(I2B) DO 230 N=1,NBUB(I2B) NFBUB(N)=0 SURB(N,12B)=0. VOLB(N,I2B)=0. 230 DO 240 K=2,NKM DO 240 J=2,NJM DO 240 I=2,NIM N=IBUB(I,J,K,I2B) IF(N.LT.1) GOTO 240 VOLHB=VOL(I,J,K)*HB(I,J,K) HH=0.5+F(I,J,K)/DDF(I,J,K)HH=AMAX1(0.,AMIN1(1.,HH)) VOLB(N,I2B)=VOLB(N,I2B)+(V00-V11*HH)*VOLHB IF(I2B.EQ.1 .AND. IBUB(I,J,K,2).GE.1) THEN IF(IPBUB(IBUB(I,J,K,2),2).EQ.1) GOTO 240 ENDIF FDS=F(I,J,K)/DDF(I,J,K) IF(ABS(FDS).LT.1.) SURB(N,I2B)=SURB(N,I2B)& +VOLHB*0.5*(1.+COS(PI*FDS))/DDF(I,J,K) & IF(ABS(FDS).LT.1.) NFBUB(N)=NFBUB(N)+1 IF(F(I,J,K).LE.0.) NFBUB(N)=NFBUB(N)+1 240 CONTINUE DO 250 N=1.NBUB(I2B) IF(NFBUB(N).LE.0) SURB(N,I2B)=0. IF(SURB(N,I2B).EQ.0.) GOTO 250 SURB(N,I2B)=-V11*(BVOLB(N,I2B)-VOLB(N,I2B))/SURB(N,I2B) CONTINUE 250 DO 260 K=2,NKM DO 260 J=2,NJM DO 260 I=2.NIM N=IBUB(I,J,K,I2B) IF(N.LT.1) GOTO 260 IF(I2B.EQ.2) THEN IF(IPBUB(IBUB(I,J,K,2),2).EQ.0) GOTO 260 ENDIF IF(I2B.EQ.1 .AND. IBUB(I,J,K,2).GE.1) THEN IF(IPBUB(IBUB(I,J,K,2),2).EQ.1) GOTO 260 ENDIF F(I,J,K)=F(I,J,K)+SIGN(AMIN1(DDF(I,J,K),ABS(SURB(N,I2B)))& & ,SURB(N,I2B)) 260 CONTINUE 1200 CONTINUE CALL F BC CALL IBUB_GET

400 IF(ITER .EQ. ITER /JMONIT*JMONIT .AND.&

ITIME .EQ. ITIME/JMONT *JMONT)& & &WRITE(I69,4000) ' F',ITER,F(IREF,JREF,KREF)& & ,F(IREF,JREF,KREF)-FSAV,SFMAX,SURB(1,1),SURB(1,2) IF(ITER .GE. 10)THEN IF(ITIME .EQ. ITIME/JMONT *JMONT)& &WRITE(I69,4000) ' F', ITER, F(IREF, JREF, KREF)& ,F(IREF, JREF, KREF)-FSAV, SFMAX, SURB(1,1), SURB(1,2) & GOTO 20 ENDIF GOTO 10 20 CONTINUE CALL DDF GET CALL IBUB GET 4000 FORMAT(A,I6,6(1PE12.4)) END SUBROUTINE FUVW_GET **USE PARAMETERS USE IGRID USE GRIDB USE LEVFN USE MPIVAR** IMPLICIT NONE INTEGER :: I.J.K *********** DO 110 K=K11,KNK DO 110 J=1,NJ DO 110 I=2,NI 110 FU(I,J,K)=F(I,J,K)*XDW(I)+F(I-1,J,K)*XDE(I) DO 120 K=K11,KNK DO 120 J=2.NJ DO 120 I=1,NI 120 FV(I,J,K)=F(I,J,K)*YDS(J)+F(I,J-1,K)*YDN(J) IF(I23.EQ.2) RETURN DO 130 K=2,NK DO 130 J=1.NJ DO 130 I=1,NI FW(I,J,K)=F(I,J,K)*ZDB(K)+F(I,J,K-1)*ZDT(K)130 DO 140 K=2,NK DO 140 J=2,NJ DO 140 I=2.NI 140 FC(I,J,K)=(FW(I,J ,K)*XDW(I)+FW(I-1,J ,K)*XDE(I))*YDS(J)& & +(FW(I,J-1,K)*XDW(I)+FW(I-1,J-1,K)*XDE(I))*YDN(J) RETURN END

SUBROUTINE FXYZ GET **USE PARAMETERS** USE IGRID **USE IBNDS USE GRID1 USE GRIDB USE LEVFN USE APANS USE AEANS** USE FUNC **USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K ***** *********** DO 100 K=2,NKM DO 100 J=2,NJM DO 100 I=2,NIM AW(I,J,K)=(F(I,J,K)-F(I-1,J,K))/XD(I)AE(I,J,K)=(F(I+1,J,K)-F(I,J,K))/XD(I+1)AC(I,J,K)=(AE(I,J,K)-AW(I,J,K))/(XD(I)+XD(I+1))AS(I,J,K)=(F(I,J,K)-F(I,J-1,K))/YD(J)AN(I,J,K)=(F(I,J+1,K)-F(I,J,K))/YD(J+1)AP(I,J,K)=(AN(I,J,K)-AS(I,J,K))/(YD(J)+YD(J+1))100 CONTINUE DO 110 K=2,NKM DO 110 J=2,NJM AC(1,J,K)=0. 110 AC(NI,J,K)=0. DO 120 K=2,NKM DO 120 I=2.NIM AP(I, 1,K)=0. 120 AP(I,NJ,K)=0. DO 150 K=2,NKM DO 150 J=2,NJM DO 150 I=2,NIM IF(ABS(F(I,J,K)).GT.7.*DDF(I,J,K)) GOTO 150 AW(I,J,K)=AW(I,J,K)+XD(I)*AMIN2(AC(I,J,K),AC(I-1,J,K)) AE(I,J,K)=AE(I,J,K)-XD(I+1)*AMIN2(AC(I,J,K),AC(I+1,J,K)) $AS(I,J,K)=AS(I,J,K)+YD(J)^*AMIN2(AP(I,J,K),AP(I,J-1,K))$ AN(I,J,K)=AN(I,J,K)-YD(J+1)*AMIN2(AP(I,J,K),AP(I,J+1,K)) 150 CONTINUE !-----IF(I23.EQ.2) RETURN DO 300 K=2,NKM DO 300 J=2,NJM

DO 300 I=2,NIM AB(I,J,K)=(F(I,J,K)-F(I,J,K-1))/ZD(K)AT(I,J,K)=(F(I,J,K+1)-F(I,J,K))/ZD(K+1) $300 \quad AC(I,J,K)=(AT(I,J,K)-AB(I,J,K))/(ZD(K)+ZD(K+1))$ DO 310 J=2,NJM DO 310 I=2,NIM AC(I,J, 1)=0. 310 AC(I,J,NK)=0. DO 350 K=2,NKM DO 350 J=2,NJM DO 350 I=2,NIM IF(ABS(F(I,J,K)).GT.7.*DDF(I,J,K)) GOTO 350 AB(I,J,K)=AB(I,J,K)+ZD(K)*AMIN2(AC(I,J,K),AC(I,J,K-1))AT(I,J,K)=AT(I,J,K)-ZD(K+1)*AMIN2(AC(I,J,K),AC(I,J,K+1))350 CONTINUE RETURN END SUBROUTINE H_GET **USE PARAMETERS USE ICHOS USE PROPS USE INDMO** USE IGRID USE IBNDS USE GRID1 **USE GRIDB USE GRIDL USE QINTB USE LEVFN** USE ROGAM USE RESLT USE FUNC **USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,HP,FAC INTEGER :: ITMP, ITMPE, JTMP, JTMPE, KTMP, KTMPE, NT REAL*8 :: HH,VOLH,R1 CALL FUVW_GET DO 100 K=KKST,KKEND !K11,KNK DO 100 J=JJST,JJEND !1,NJ DO 100 I=IIST,IIEND !1,NI HP=1. IF(F(I,J,K).LE.0.) HP=0. RHOP(I,J,K)=RO1+(RO2-RO1)*HP RCP(I,J,K)=RC1+(RC2-RC1)*HP TKP(I,J,K)=TK1+(TK2-TK1)*HP

HH=0.5+F(I,J,K)/DDF(I,J,K) H(I,J,K)=AMAX1(0.,AMIN1(1.,HH))100 CONTINUE CALL RELOAD IF (TASKID.NE.0) THEN CALL MPI SEND(RHOP(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI DOUBLE PR ECISION,0,TASKID,MPI_COMM_WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI RECV(RHOP(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE (NT)),SIZECC(NT),MPI DOUBLE PRECISION,NT,NT,MPI COMM WORLD,STATUS,IERR) **ENDDO** ENDIF CALL MPI_BARRIER(MPI_COMM_WORLD,IERR) CALL MPI_BCAST(RHOP(1,1,1),SIZE(RHOP),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR) I_____ IF (TASKID.NE.0) THEN CALL MPI_SEND(RCP(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PREC ISION,0,TASKID,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(RCP(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT)),SIZECC(NT),MPI_DOUBLE_PRECISION,NT,NT,MPI_COMM_WORLD,STATUS,IERR) **ENDDO** ENDIF CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI BCAST(RCP(1,1,1),SIZE(RCP),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR) **!**----IF (TASKID.NE.0) THEN CALL MPI SEND(TKP(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI DOUBLE PREC ISION,0,TASKID,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1.26 CALL MPI_RECV(TKP(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(N T)),SIZECC(NT),MPI DOUBLE PRECISION,NT,NT,MPI COMM WORLD,STATUS,IERR) ENDDO ENDIF

CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI BCAST(TKP(1,1,1),SIZE(TKP),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR) !-----IF (TASKID.NE.0) THEN CALL MPI_SEND(H(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECISI ON,0,TASKID,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(H(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT)) ,SIZECC(NT),MPI DOUBLE PRECISION,NT,NT,MPI COMM WORLD,STATUS,IERR) ENDDO ENDIF CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI_BCAST(H(1,1,1),SIZE(H),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR) I____ ITMP=IIST **ITMPE=IIEND** JTMP=JJST JTMPE=JJEND KTMP=KKST KTMPE=KKEND IF (PIDX.EQ.0) ITMP=IIST+1 DO 110 K=KKST,KKEND !K11,KNK DO 110 J=JJST,JJEND !1,NJ DO 110 I=IIST,IIEND !2,NI RHOU(I,J,K)=RHOP(I,J,K)IF(T_1PH(F(I,J,K),F(I-1,J,K))) GOTO 110 RHOU(I,J,K)=(F(I,J,K)*RHOP(I,J,K)-F(I-1,J,K)*RHOP(I-1,J,K))/(F(I,J,K)-F(I-1,J,K)) 110 CONTINUE IF (TASKID.NE.0) THEN CALL MPI SEND(RHOU(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI DOUBLE PR ECISION,0,TASKID,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(RHOU(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE (NT)),SIZECC(NT),MPI DOUBLE PRECISION,NT,NT,MPI COMM WORLD,STATUS,IERR) ENDDO **ENDIF**

CALL MPI_BARRIER(MPI_COMM_WORLD,IERR)

CALL MPI_BCAST(RHOU(1,1,1),SIZE(RHOU),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR)

ITMPE=IIEND JTMP=JJST JTMPE=JJEND KTMP=KKST KTMPE=KKEND IF (PIDY.EQ.0) JTMP=JJST+1 DO 120 K=KKST,KKEND !K11,KNK DO 120 J=JJST,JJEND !2,NJ DO 120 I=IIST,IIEND !1,NI RHOV(I,J,K)=RHOP(I,J,K) IF(T 1PH(F(I,J,K),F(I,J-1,K))) GOTO 120 RHOV(I,J,K)=(F(I,J,K)*RHOP(I,J,K)-F(I,J-1,K)*RHOP(I,J-1,K))/(F(I,J,K)-F(I,J-1,K)) 120 CONTINUE IF (TASKID.NE.0) THEN CALL MPI SEND(RHOV(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI DOUBLE PR ECISION,0,TASKID,MPI COMM WORLD,IERR) **ENDIF** IF (TASKID.EQ.0) THEN DO NT=1.26 CALL MPI RECV(RHOV(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE (NT)),SIZECC(NT),MPI DOUBLE PRECISION,NT,NT,MPI COMM WORLD,STATUS,IERR) **ENDDO** ENDIF CALL MPI BARRIER(MPI COMM WORLD, IERR)

CALL

ITMP=IIST

MPI_BCAST(RHOV(1,1,1),SIZE(RHOV),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR)

ITMP=IIST ITMPE=IIEND JTMP=JJST JTMPE=JJEND KTMP=KKST KTMPE=KKEND IF (PIDZ.EQ.0) KTMP=KKST+1

IF(I23.EQ.2) GOTO 135 DO 130 K=KKST,KKEND !2,NK DO 130 J=JJST,JJEND !1,NJ DO 130 I=IIST,IIEND !1,NI RHOW(I,J,K)=RHOP(I,J,K) IF(T_1PH(F(I,J,K),F(I,J,K-1))) GOTO 130 RHOW(I,J,K)=(F(I,J,K)*RHOP(I,J,K)-F(I,J,K-1)*RHOP(I,J,K-1))/(F(I,J,K)-F(I,J,K-1)) 130 CONTINUE IF (TASKID.NE.0) THEN CALL MPI SEND(RHOW(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI DOUBLE PR ECISION,0,TASKID,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(RHOW(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZ E(NT)),SIZECC(NT),MPI DOUBLE PRECISION,NT,NT,MPI COMM WORLD,STATUS,IERR) ENDDO ENDIF CALL MPI BARRIER(MPI_COMM_WORLD, IERR) CALL MPI_BCAST(RHOW(1,1,1),SIZE(RHOW),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR) !-----135 VOLV=0. DO 200 K=2,NKM DO 200 J=2,NJM DO 200 I=2,NIM VOLH=(1.-H(I,J,K))*VOL(I,J,K)*HB(I,J,K) 200 VOLV=VOLV+VOLH IF(I23.EQ.2) THEN IF(IR.EQ.1) THEN IF(IBCS.EQ.ISYM) DEFF=(24.*VOLV)**(1./3.) IF(IBCS.NE.ISYM) DEFF=(12.*VOLV)**(1./3.) ELSE IF(IBCS.EQ.ISYM) DEFF=(16.*VOLV/PI)**(1./2.) IF(IBCS.NE.ISYM) DEFF=(8.*VOLV/PI)**(1./2.) ENDIF ELSE FAC=1. IF(IBCW.EQ.ISYM) FAC=FAC*2. IF(IBCS.EQ.ISYM) FAC=FAC*2. IF(IBCB.EQ.ISYM) FAC=FAC*2. DEFF=(6.*FAC*VOLV/PI)**(1./3.) ENDIF 1___ R0=0. R1=0. K=2 DO 250 I=2,NIM IF(F(I,2,K)*F(I+1,2,K) .LT. 0.) R0=XP(I)-XD(I+1)*F(I,2,K)/(F(I+1,2,K)-F(I,2,K)) IF(F(I,1,K)*F(I+1,1,K).LT. 0.) R1=XP(I)-XD(I+1)*F(I,1,K)/(F(I+1,1,K)-F(I,1,K)) 250 CONTINUE ANGO=ATAN(YD(2)/AMAX1(EPS,R0-R1))*180./PI RETURN END

SUBROUTINE IN_OUTPUT **USE PARAMETERS USE ICHOS USE PROPS USE INDMO** USE INDDT **USE IGRID USE IBNDS USE GRID1 USE GRIDB USE GRIDL** USE IBUBS USE QINTB **USE SPERR USE LEVFN** USE ULVLL USE QMSOR USE RESLT **USE INTXN USE INTXY USE UVTPP USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,II,JJ,KK,N,JFLOUT,JPLOUT,IB1,IB2,ICH,ICH10,ICH100,ICH1000 INTEGER :: JRE=-1,NOUTIN=-1,NOUTI3=-1 REAL*8 :: T0,S0,P0,F0,U1,V1,W1,WI **CHARACTER*5 FILE** ENTRY INT2D_OUT ***** IF(NBUB(1).GE.1) THEN IF(I23.EQ.3) CALL INTZY PLOT(2) IF(I23.EQ.3) CALL INTXZ PLOT(2) ! CALL INTXY_PLOT(2) ENDIF CALL QW_GET CALL QI GET IF(IBODY.EQ.1) CALL QBND_GET NOUTIN=NOUTIN+1 IF(NOUTIN.EQ.0) THEN OPEN(10,FILE='res1') OPEN(11,FILE='heat') OPEN(12,FILE='volb') OPEN(13,FILE='voll') OPEN(19,FILE='qwww') OPEN(21,FILE='i2xy') OPEN(22,FILE='i2zy') ELSE

OPEN(10,FILE='res1',ACCESS='APPEND') OPEN(11,FILE='heat',ACCESS='APPEND') OPEN(12,FILE='volb',ACCESS='APPEND') OPEN(13,FILE='voll',ACCESS='APPEND') OPEN(19, FILE='gwww', ACCESS='APPEND') OPEN(21,FILE='i2xy',ACCESS='APPEND') OPEN(22, FILE='i2zy', ACCESS='APPEND') ENDIF IF(IGRAV.EQ.0) THEN WI=SQRT(ABS(DEFF**2-BDEFF**2)/DT)/2. WRITE(10,4011) TIME, ITIME, HTOP, R0, WI, DEFF, VBUB ELSE WRITE(10,4011) TIME, ITIME, HTOP, R0, ANGO, DEFF, VBUB ENDIF IF(IBODY.EQ.1) THEN WRITE(11,4011) TIME, ITIME, QWAV, QMAV, QIAV, QIA1, QBND ELSE WRITE(11,4011) TIME, ITIME, QWAV, QMAV, QIAV, QIA1, QWS(NIM, NKM) ENDIF WRITE(12,4001) TIME, ITIME, NBUB(1), (VOLB(N,1), N=1, NBUB(1)) WRITE(13,4001) TIME, ITIME, NBUB(2), (VOLB(N,2), N=1, NBUB(2)) IF(IBCS.EQ.IWAL) THEN WRITE(19,4011) TIME, ITIME, QWAV, QMAV, QIAV WRITE(19,4013) ((QWS(I,K),I=2,NIM),K=2,NKM) ENDIF WRITE(21,4012) TIME, ITIME, NPXY, HTOP, R0, ANGO WRITE(21,4013) ((XZ(I,J),YZ(I,J),J=1,2),I=1,NPXY) WRITE(22,4012) TIME, ITIME, NPZY, HTOP, R0, ANGO WRITE(22,4013) ((ZX(I,J),YX(I,J),J=1,2),I=1,NPZY) RETURN ENTRY INT3D OUT ***** IF(I23.EQ.2) RETURN IF(NBUB(1) .LT. 1) RETURN CALL INT3D PLOT NOUTI3=NOUTI3+1 IF(NOUTI3 .EQ. 0) THEN OPEN(20,FILE='i3dd') ELSE OPEN(20,FILE='i3dd',ACCESS='APPEND') ENDIF WRITE(20,*) NP3D, ITIME DO 300 I=1,NP3D WRITE(20,4006) XI(I,1),YI(I,1),ZI(I,1),XI(I,2),YI(I,2),ZI(I,2) 300 WRITE(20,4006) XI(I,3),YI(I,3),ZI(I,3),XI(I,4),YI(I,4),ZI(I,4) CLOSE(20) 4006 FORMAT(6(1PE12.4))

RETURN

ENTRY RESTF IN l***** OPEN(2,FILE='ccc') READ(2,*) TIME, ITIME, NBUB(1), NBUB(2), DT, (TIMEW(N), N=1, NCAV) READ(2,*)DO 410 K=K11,KNK DO 410 I=1,NI DO 410 J=1,NJ 410 READ(2,*) II,JJ,KK,U(I,J,K),V(I,J,K),P(I,J,K),T(I,J,K) IF(I23.EQ.3) THEN READ(2,*) DO 420 K=K11,KNK DO 420 I=1,NI DO 420 J=1,NJ 420 READ(2,*) II,JJ,KK,W(I,J,K) ENDIF READ(2,*) DO 430 K=K11,KNK DO 430 I=1,NI DO 430 J=1,NJ READ(2,*) II,JJ,KK,IBUB(I,J,K,1),IBUB(I,J,K,2),F(I,J,K) 430 CLOSE(2) CALL DDF GET RETURN ENTRY RESTFOUT ****** JRE=JRE+1 IF(JRE .EQ. JRE/2*2) OPEN(2,FILE='re1') IF(JRE .NE. JRE/2*2) OPEN(2,FILE='re2') WRITE(2,4005) TIME, ITIME, NBUB(1), NBUB(2), DT, (TIMEW(N), N=1, NCAV) WRITE(2,*) ' I, J, K,U(I,J,K),V(I,J,K),P(I,J,K),T(I,J,K) ' DO 500 K=K11.KNK DO 500 I=1,NI DO 500 J=1,NJ T0=T(I,J,K)IF(ABS(T0).LE.1.E-99) T0=0. 500 WRITE(2,4002) I,J,K,U(I,J,K),V(I,J,K),P(I,J,K),T0 IF(I23.EQ.3) THEN WRITE(2,*) ' I, J, K,W(I,J,K)' DO 510 K=K11,KNK DO 510 I=1,NI DO 510 J=1,NJ WRITE(2,4002) I,J,K,W(I,J,K) 510 ENDIF WRITE(2,*) ' I, J, K, IBUB(I, J), F(I, J)' DO 520 K=K11,KNK DO 520 I=1,NI DO 520 J=1,NJ IB1=IBUB(I,J,K,1)

IB2=IBUB(I,J,K,2) 520 WRITE(2,4003) I,J,K,IB1,IB2,F(I,J,K),S(I,J,K),H(I,J,K),HB(I,J,K) CLOSE(2) RETURN

ENTRY OFILE_OUT(JFLOUT) ICH=ITIME/JFLOUT ICH1000=ICH/1000 ICH=ICH-ICH1000*1000 ICH100=ICH/100 ICH=ICH-ICH100*100 ICH10=ICH/10 ICH=ICH-ICH10*10 FILE='o'//CHAR(ICH1000+48)//CHAR(ICH100+48)//CHAR(ICH10+48)& & //CHAR(ICH+48) OPEN(2,FILE=FILE) ! WRITE(2,*) 'TITLE="',TIME,ITIME,DT,'" WRITE(2,4016) TIME, ITIME, DT WRITE(2,*) 'VÁRIABLES= "X", "Y", "Z", "U", "V", "W", "T", "F", "P" WRITE(2,*) 'ZONE F=POINT, T="',ITIME,"',I=',NI, ',J=',NJ, ',K=',NK WRITE(2,4002) NBUB DO K=K11,KNK DO J=1,NJ DO I=1,NI T0=T(I,J,K); S0=S(I,J,K); P0=P(I,J,K); F0=F(I,J,K) U1=U(I,J,K); V1=V(I,J,K); W1=W(I,J,K) IF(I.NE.1 .AND. I.NE.NI) THEN $U1=0.5^{(I)}(U(I,J,K)+U(I+1,J,K))$ END IF IF(J.NE.1 .AND. J.NE.NJ) THEN V1=0.5*(V(I,J,K)+V(I,J+1,K)) END IF IF(K.NE.1 .AND. K.NE.NK) THEN $W1=0.5^{*}(W(I,J,K)+V(I,J,K+1))$ END IF END DO END DO END DO CLOSE(2) RETURN *********** ENTRY PLOTF_OUT(JPLOUT) ICH=ITIME/JPLOUT ICH1000=ICH/1000 ICH=ICH-ICH1000*1000 ICH100=ICH/100
ICH=ICH-ICH100*100 ICH10=ICH/10 ICH=ICH-ICH10*10 FILE='p'//CHAR(ICH1000+48)//CHAR(ICH100+48)//CHAR(ICH10+48)& & //CHAR(ICH+48) OPEN(2,FILE=FILE) K=2 WRITE(2,4005) TIME, ITIME, NBUB(1), NBUB(2), DT, (TIMEW(N), N=1, NCAV) WRITE(2,*) ' I,J,K,U(I,J,K),V(I,J,K),P(I,J,K),T(I,J,K) ' DO 700 I=1,NI DO 700 J=1,NJ T0=T(I,J,K)IF(ABS(T0).LE.1.E-99) T0=0. 700 WRITE(2,4002) I,J,K,U(I,J,K),V(I,J,K),P(I,J,K),T0 WRITE(2,*) ' I,J,K,IBUB(I,J,K),F(I,J,K) ' DO 710 I=1,NI DO 710 J=1,NJ IB1=IBUB(I,J,K,1) IB2=IBUB(I,J,K,2)710 WRITE(2,4003) I,J,K,IB1,IB2,F(I,J,K),S(I,J,K),H(I,J,K),HB(I,J,K) CLOSE(2) RETURN 4001 FORMAT(1PE13.5,18,14,100(1PE12.4)) 4005 FORMAT(1PE13.5, I8, I4, I4, 100(1PE12.4)) 4002 FORMAT(I4,I4,I4,4(1PE17.9)) 4003 FORMAT(I4,I4,I4,I4,I4,1(1PE17.9),3(1PE12.4)) 4011 FORMAT(1PE13.5,18,5(1PE12.4)) 4012 FORMAT(1PE13.5, I8, I6, 3(1PE13.5)) 4013 FORMAT(6(1PE13.5)) 4016 FORMAT(1PE13.5, I8, 1PE13.5) 4018 FORMAT(9(1PE13.5)) ****** END SUBROUTINE INIT USE PARAMETERS USE ICHOS **USE INDMO USE IGRID USE MUGRD USE GRID1 USE GRIDB USE LEVFN USE ULVLL** USE QMSOR **USE FNXYZ** USE APANS USE AEANS **USE F2F00** USE IBSUB

USE UVTPP **USE INDIT USE RELXS** USE X2XOO **USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,L REAL*8 :: DIS1,DIS2,DIS3 CHARACTER*3 CHT COMMON/CHAR1/CHT(6) NIM=NI-1 NJM=NJ-1 NKM=NK-1 NIMM=NIM-1 NJMM=NJM-1 NKMM=NKM-1 MX(1)=NIMMY(1)=NJM MZ(1)=NKM DO 1 L=2,MULT IF((MX(L-1)+1) .NE. (MX(L-1)+1)/2*2) THEN IF (TASKID.EQ.0) WRITE(I69,*) ' CHECK **NI*',L,MX(L-1)+1 STOP **ENDIF** IF((MY(L-1)+1) .NE. (MY(L-1)+1)/2*2) THEN IF (TASKID.EQ.0) WRITE(I69,*) ' CHECK **NJ*',L,MY(L-1)+1 STOP ENDIF IF(I23 .EQ. 3 .AND. (MZ(L-1)+1) .NE. (MZ(L-1)+1)/2*2) THEN IF (TASKID.EQ.0) WRITE(I69,*) 'CHECK **NK*',L,MZ(L-1)+1 STOP **ENDIF** MX(L)=(MX(L-1)+1)/2MY(L) = (MY(L-1)+1)/2MZ(L)=(MZ(L-1)+1)/2IF(I23 .EQ. 2) MZ(L)=NKM 1 CONTINUE CALL MULVL -----INITIALIZE !----DO 10 J=1,5 RELAX(J)=1. 10 BRELX(J)=1. CHT(1)='U' CHT(2)=' V' CHT(3)='W' CHT(4)=' T' CHT(5)=' P' DO 20 I=1,5

20 MIT(I)=100 MIT(5)=200 DO 30 K=1,NK DO 30 J=1,NJ DO 30 I=1,NI W(I,J,K)=0.S(I,J,K)=1.E6 SU(I,J,K)=1.E6 SV(I,J,K)=1.E6 SW(I,J,K)=1.E6 HB(I,J,K)=1. AB(I,J,K)=0. AT(I,J,K)=0. DDF(I,J,K)=DL DDS(I,J,K)=DL DTF(I,J,K)=DL FNZ(I,J,K)=0. AMZ(I,J,K)=0.IFFIX(I,J,K)=0 30 MK(I,J,K)=1DO 40 K=0,NK+1 DO 40 J=0,NJ+1 DO 40 I=0,NI+1 40 FO(I,J,K)=1.E5 !----- GRID DO 100 I=2,NIM 100 XP(I)=0.5*(XU(I+1)+XU(I)) XP(1)=XU(2) XP(NI)=XU(NI) DO 110 I=2,NIM 110 XC(I)=XU(I+1)-XU(I) DO 120 I=2,NI 120 XD(I)=XP(I)-XP(I-1) DO 122 I=2,NIM 122 XDE(I)=0.5*XC(I)/XD(I) XDE(NI)=0. DO 124 I=2,NI 124 XDW(I)=1.-XDE(I) DO 130 I=2,NI RU(I)=1. 130 IF(IR .EQ. 1) RU(I)=ABS(XU(I)) DO 140 I=1,NI RP(I)=1. 140 IF(IR .EQ. 1) RP(I)=ABS(XP(I)) DO 200 J=2,NJM 200 $YP(J)=0.5^{*}(YV(J+1)+YV(J))$ YP(1)=YV(2) YP(NJ)=YV(NJ)

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DO 210 J=2,NJM
210 YC(J)=YV(J+1)-YV(J)
DO 220 J=2,NJ
220 YD(J)=YP(J)-YP(J-1)
DO 222 J=2,NJM
222 YDN(J)=0.5*YC(J)/YD(J)
YDN(NJ)=0.
DO 224 J=2,NJ
224 YDS(J)=1.-YDN(J)
DO 300 K=2,NKM
300 ZP(K)=0.5*(ZW(K+1)+ZW(K))
ZP(1)=ZW(2)
ZP(NK)=ZW(NK)
DO 310 K=2,NKM
310 ZC(K)=ZW(K+1)-ZW(K)
DO 320 K=2,NK
320 ZD(K)=ZP(K)-ZP(K-1)
DO 322 K=2,NKM
322 ZDT(K)=0.5*ZC(K)/ZD(K)
ZDT(NK)=0.
DO 324 K=2,NK
324 ZDB(K)=1.-ZDT(K)
DO 350 K=2,NKM
DO 350 J=2.NJM
DO 350 I=2,NIM
VOL(I,J,K)=RP(I)*XC(I)*YC(J)*ZC(K)
350 CONTINUE
IF(IUGRD.EQ.0) THEN
DO 360 K=2,NKM
DO 360 J=2,NJM
DO 360 I=2.NIM
DIS1=AMAX1(ABS(XD(I)),ABS(XD(I+1)))
DIS2=AMAX1(ABS(YD(J)),ABS(YD(J+1)))
DIS3=AMAX1(ABS(ZD(K)),ABS(ZD(K+1)))
IF(I23.EQ.2) DIS3=1.E10
DTF(I,J,K)=AMIN1(DIS1,DIS2,DIS3)
360
     CONTINUE
ENDIF
DO 510 I=1,NI
XPO(I)=XP(I)
    XDO(I)=XD(I)
510
XPO( 0)=XPO( 1)
XPO(NI+1)=XPO(NI)
XDO( 1)=0.
XDO(NI+1)=0.
DO 520 J=1,NJ
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YPO(J)=YP(J) 520 YDO(J)=YD(J)YPO(0)=YPO(1) YPO(NJ+1)=YPO(NJ) YDO(1)=0. YDO(NJ+1)=0. DO 530 K=1,NK ZPO(K)=ZP(K)530 ZDO(K)=ZD(K) ZPO(0)=ZPO(1) ZPO(NK+1)=ZPO(NK) ZDO(1)=0. ZDO(NK+1)=0. RETURN END SUBROUTINE LNTDMA(N, ITER) **USE PARAMETERS** USE APANS **USE AEANS** USE CALC1 **USE MPIVAR USE IGRID** IMPLICIT NONE INTEGER :: NT,II,JJ,KK,I,J,K INTEGER, INTENT(IN) :: N,ITER REAL(KIND=8) :: BETA,SSS,GAMA(MD) INTEGER :: TCOUNT, MPII, MPJJ, MPKK, ONESLICE, TWOSLICE, THREESLICE CALL MPI_BARRIER(MPI_COMM_WORLD,IERR) CC(:,:,:)=0. CALL RELOAD DO K = KKST-1.KKEND+1 DO J = JJST-1, JJEND+1 DO I = IIST-1, IIEND+1 RCC(I,J,K)=0. ENDDO ENDDO **ENDDO** DO 999 NT=1.2 !2 IF ((N.EQ.4).OR.(N.EQ.1).OR.(N.EQ.2).OR.(N.EQ.3)) THEN CALL FRAGMENT CALL RELOAD ENDIF

CALL NEIGHBOUR IF (N.EQ.4) THEN CALL SHRINK CALL RELOAD ENDIF IF (N.EQ.1) THEN CALL CONTRACT(3,2,2,ID-1,JD-1,KD-1) CALL RELOAD ENDIF IF (N.EQ.2) THEN CALL CONTRACT(2,3,2,ID-1,JD-1,KD-1) CALL RELOAD ENDIF IF (N.EQ.3) THEN CALL CONTRACT(2,2,3,ID-1,JD-1,KD-1) CALL RELOAD ENDIF ***** DO 100 K=KKST,KKEND DO 100 J=JJST,JJEND I=IIST SSS=SS(I,J,K)+AN(I,J,K)*RCC(I,J+1,K)+AS(I,J,K)*RCC(I,J-1,K)+AT(I,J,K)*RCC(I,J,K+1)+AB(I,J,K)*RCC(I,J,K)+AN(I,J,K)*AN(I,J,K)*RCC(I,J,K)+AN(I,J,K)*AN(I,J,K)+AN(I,J,K)*AN(I,J,K)+AN(I,J,K-1) BETA=AP(I,J,K) RCC(I,J,K)=SSS/BETA DO 130 I=IIST+1,IIEND SSS=SS(I,J,K)+AN(I,J,K)*RCC(I,J+1,K)+AS(I,J,K)*RCC(I,J-1,K)+AT(I,J,K)*RCC(I,J,K+1)+AB(I,J,K)*RCC(I,J,K)+AN(I,J,K)+AN(I I.J.K-1) GAMA(I)= -AE(I-1,J,K)/BETA BETA=AP(I,J,K)+AW(I,J,K)*GAMA(I) RCC(I,J,K)=(SSS+AW(I,J,K)*RCC(I-1,J,K))/BETA 130 DO 140 I=IIEND-1,IIST,-1 140 RCC(I,J,K)=RCC(I,J,K)-GAMA(I+1)*RCC(I+1,J,K) 100 CONTINUE 1__ DO 200 K=KKST,KKEND DO 200 I=IIST,IIEND J=JJST SSS=SS(I,J,K)+AE(I,J,K)*RCC(I+1,J,K)+AW(I,J,K)*RCC(I-1,J,K)+AT(I,J,K)*RCC(I,J,K+1)+AB(I,J,K)*RCC (I,J,K-1) BETA=AP(I,J,K) RCC(I,J,K)=SSS/BETA

DO 230 J=JJST+1,JJEND SSS=SS(I,J,K)+AE(I,J,K)*RCC(I+1,J,K)+AW(I,J,K)*RCC(I-1,J,K)+AT(I,J,K)*RCC(I,J,K+1)+AB(I,J,K)*RCC (I,J,K-1) -AN(I,J-1,K)/BETA GAMA(J) =BETA=AP(I,J,K)+AS(I,J,K)*GAMA(J) RCC(I,J,K)=(SSS+AS(I,J,K)*RCC(I,J-1,K))/BETA 230 200 CONTINUE I___ IF(I23.EQ.2) GOTO 999 DO 300 J=JJST,JJEND DO 300 I=IIST,IIEND K=KKST SSS=SS(I,J,K)+AE(I,J,K)*RCC(I+1,J,K)+AW(I,J,K)*RCC(I-1,J,K)+AN(I,J,K)*RCC(I,J+1,K)+AS(I,J,K)*RCC (I,J-1,K) BETA=AP(I,J,K) RCC(I,J,K)=SSS/BETA DO 330 K=KKST,KKEND SSS=SS(I,J,K)+AE(I,J,K)*RCC(I+1,J,K)+AW(I,J,K)*RCC(I-1,J,K)+AN(I,J,K)*RCC(I,J+1,K)+AS(I,J,K)*RCC (I,J-1,K) GAMA(K)= -AT(I,J,K-1)/BETA AP(I,J,K)+AB(I,J,K)*GAMA(K) BETA= 330 RCC(I,J,K)=(SSS+AB(I,J,K)*RCC(I,J,K-1))/BETA DO 340 K=KKEND-1,KKST,-1 RCC(I,J,K)=RCC(I,J,K)-GAMA(K+1)*RCC(I,J,K+1)340 300 CONTINUE I_____ 999 CONTINUE DO K = KKST,KKEND !Every Processor fills up its own computed part. DO J = JJST, JJEND DO I = IIST.IIEND CC(I,J,K) = RCC(I,J,K)ENDDO ENDDO **ENDDO** RETURN END SUBROUTINE M1PRTD(I23,IEND,JEND,KEND) ******* **USE PARAMETERS** USE APANS USE AEANS USE M1WRK **USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,IST=2,JST=2,KST=2

INTEGER, INTENT(IN):: 123, IEND, JEND, KEND **** DO 110 I=IST, IEND BE(I)=0. 110 BW(I)=0. DO 112 K=KST,KEND DO 112 J=JST, JEND DO 112 I=IST, IEND BE(I)=BE(I)+AE(I,J,K)112 BW(I)=BW(I)+AW(I,J,K) DO 114 I=IST, IEND 114 BX(I)=BE(I)+BW(I)DO 116 K=KST,KEND DO 116 I=IST, IEND BX(I)=BX(I)+AS(I,JST,K)+AN(I,JEND,K) 116 DO 118 J=JST, JEND DO 118 I=IST, IEND 118 BX(I)=BX(I)+AB(I,J,KST)+AT(I,J,KEND)!-----DO 120 J=JST.JEND BN(J)=0. 120 BS(J)=0. DO 122 K=KST,KEND DO 122 I=IST, IEND DO 122 J=JST, JEND BN(J)=BN(J)+AN(I,J,K)122 BS(J)=BS(J)+AS(I,J,K) DO 124 J=JST,JEND 124 BY(J)=BN(J)+BS(J)DO 126 K=KST,KEND DO 126 J=JST, JEND 126 BY(J)=BY(J)+AW(IST,J,K)+AE(IEND,J,K) DO 128 I=IST, IEND DO 128 J=JST, JEND 128 BY(J)=BY(J)+AB(I,J,KST)+AT(I,J,KEND) !-----IF(I23.EQ.2) RETURN DO 130 K=KST,KEND BT(K)=0. 130 BB(K)=0. DO 132 J=JST, JEND DO 132 I=IST, IEND DO 132 K=KST,KEND BT(K)=BT(K)+AT(I,J,K)BB(K)=BB(K)+AB(I,J,K)132 DO 134 K=KST,KEND 134 BZ(K)=BT(K)+BB(K)DO 136 J=JST, JEND DO 136 K=KST,KEND BZ(K)=BZ(K)+AW(IST,J,K)+AE(IEND,J,K) 136 DO 138 I=IST, IEND DO 138 K=KST,KEND 138 BZ(K)=BZ(K)+AS(I,JST,K)+AN(I,JEND,K)

RETURN END SUBROUTINE M1VTDMA(I23,IEND,JEND,KEND) ******** **USE PARAMETERS USE CALC1 USE APANS USE AEANS USE M1WRK USE TDWK2 USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,NT,IST=2,JST=2,KST=2 INTEGER, INTENT(IN)::123, IEND, JEND, KEND REAL(KIND=8) :: BETA,SSS ********* DO 30 I=IST, IEND 30 BLC(I)=0. DO 32 I=IST, IEND DO 32 K=KST,KEND DO 32 J=JST, JEND 32 BLC(I)=BLC(I)+SS(I,J,K)-AP(I,J,K)*CC(I,J,K)& & +AE(I,J,K)*CC(I+1,J,K)+AW(I,J,K)*CC(I-1,J,K)& & +AN(I,J,K)*CC(I,J+1,K)+AS(I,J,K)*CC(I,J-1,K)& & +AT(I,J,K)*CC(I,J,K+1)+AB(I,J,K)*CC(I,J,K-1) BX(IST) BETA= BCC(IST)=BLC(IST)/BETA DO 34 I=IST+1,IEND GAMA(I)= -BE(I-1)/BETA BETA= BX(I)+BW(I)*GAMA(I) 34 BCC(I)=(BLC(I)+BW(I)*BCC(I-1))/BETA DO 36 I=IEND-1,IST,-1 BCC(I)=BCC(I)-GAMA(I+1)*BCC(I+1) 36 DO 38 I=IST, IEND DO 38 K=KST.KEND DO 38 J=JST, JEND 38 CC(I,J,K)=CC(I,J,K)+BCC(I)1__ DO 40 J=JST, JEND 40 BLC(J)=0. DO 42 J=JST, JEND DO 42 K=KST,KEND DO 42 I=IST, IEND 42 BLC(J)=BLC(J)+SS(I,J,K)-AP(I,J,K)*CC(I,J,K)& & +AE(I,J,K)*CC(I+1,J,K)+AW(I,J,K)*CC(I-1,J,K)& & +AN(I,J,K)*CC(I,J+1,K)+AS(I,J,K)*CC(I,J-1,K)& & +AT(I,J,K)*CC(I,J,K+1)+AB(I,J,K)*CC(I,J,K-1)

!

BCC(JST)=BLC(JST)/BETA DO 43 J=JST+1,JEND GAMA(J)= -BN(J-1)/BETA BETA= BY(J)+BS(J)*GAMA(J) 43 BCC(J)=(BLC(J)+BS(J)*BCC(J-1))/BETA DO 44 J=JEND-1,JST,-1 44 BCC(J)=BCC(J)-GAMA(J+1)*BCC(J+1) DO 48 J=JST.JEND DO 48 K=KST,KEND DO 48 I=IST, IEND 48 CC(I,J,K)=CC(I,J,K)+BCC(J)I_____ IF(I23.EQ.2) GOTO 59 DO 50 K=KST,KEND 50 BLC(K)=0. DO 52 K=KST,KEND DO 52 J=JST, JEND DO 52 I=IST, IEND 52 BLC(K)=BLC(K)+SS(I,J,K)-AP(I,J,K)*CC(I,J,K)& & +AE(I,J,K)*CC(I+1,J,K)+AW(I,J,K)*CC(I-1,J,K)& & +AN(I,J,K)*CC(I,J+1,K)+AS(I,J,K)*CC(I,J-1,K)& & +AT(I,J,K)*CC(I,J,K+1)+AB(I,J,K)*CC(I,J,K-1) BETA= BZ(KST) BCC(KST)=BLC(KST)/BETA DO 54 K=KST+1,KEND GAMA(K)=-BT(K-1)/BETA BETA= BZ(K)+BB(K)*GAMA(K) 54 BCC(K)=(BLC(K)+BB(K)*BCC(K-1))/BETA DO 56 K=KEND-1,KST,-1 BCC(K)=BCC(K)-GAMA(K+1)*BCC(K+1) 56 DO 58 K=KST,KEND DO 58 J=JST, JEND DO 58 I=IST.IEND 58 CC(I,J,K)=CC(I,J,K)+BCC(K)59 DO 999 NT=1.2 DO 100 K=KST,KEND DO 100 J=JST,JEND I=IST SSS=SS(I,J,K)+AN(I,J,K)*CC(I,J+1,K)+AS(I,J,K)*CC(I,J-1,K)& & +AT(I,J,K)*CC(I,J,K+1)+AB(I,J,K)*CC(I,J,K-1) BETA=AP(I,J,K) CC(I,J,K)=SSS/BETA DO 130 I=IST+1,IEND SSS=SS(I,J,K)+AN(I,J,K)*CC(I,J+1,K)+AS(I,J,K)*CC(I,J-1,K)& & +AT(I,J,K)*CC(I,J,K+1)+AB(I,J,K)*CC(I,J,K-1) GAMA(I)= -AE(I-1,J,K)/BETA

BETA=AP(I,J,K)+AW(I,J,K)*GAMA(I) 130 CC(I,J,K)=(SSS+AW(I,J,K)*CC(I-1,J,K))/BETA DO 140 I=IEND-1,IST,-1 140 CC(I,J,K)=CC(I,J,K)-GAMA(I+1)*CC(I+1,J,K)100 CONTINUE 1-----DO 200 K=KST,KEND DO 200 I=IST,IEND J=JST SSS=SS(I,J,K)+AE(I,J,K)*CC(I+1,J,K)+AW(I,J,K)*CC(I-1,J,K)& & +AT(I,J,K)*CC(I,J,K+1)+AB(I,J,K)*CC(I,J,K-1) BETA=AP(I,J,K) CC(I,J,K)=SSS/BETA DO 230 J=JST+1,JEND SSS=SS(I,J,K)+AE(I,J,K)*CC(I+1,J,K)+AW(I,J,K)*CC(I-1,J,K)& & +AT(I,J,K)*CC(I,J,K+1)+AB(I,J,K)*CC(I,J,K-1) GAMA(J)=-AN(I,J-1,K)/BETA BETA=AP(I,J,K)+AS(I,J,K)*GAMA(J) 230 CC(I,J,K)=(SSS+AS(I,J,K)*CC(I,J-1,K))/BETA DO 240 J=JEND-1,JST,-1 240 CC(I,J,K)=CC(I,J,K)-GAMA(J+1)*CC(I,J+1,K) 200 CONTINUE |-----IF(I23.EQ.2) GOTO 999 DO 300 J=JST.JEND DO 300 I=IST,IEND K=KST SSS=SS(I,J,K)+AE(I,J,K)*CC(I+1,J,K)+AW(I,J,K)*CC(I-1,J,K)& +AN(I,J,K)*CC(I,J+1,K)+AS(I,J,K)*CC(I,J-1,K) & BETA=AP(I,J,K) CC(I,J,K)=SSS/BETA DO 330 K=KST+1.KEND SSS=SS(I,J,K)+AE(I,J,K)*CC(I+1,J,K)+AW(I,J,K)*CC(I-1,J,K)& +AN(I,J,K)*CC(I,J+1,K)+AS(I,J,K)*CC(I,J-1,K) & GAMA(K)= -AT(I,J,K-1)/BETA BETA= AP(I,J,K)+AB(I,J,K)*GAMA(K)330 CC(I,J,K)=(SSS+AB(I,J,K)*CC(I,J,K-1))/BETA DO 340 K=KEND-1,KST,-1 340 CC(I,J,K)=CC(I,J,K)-GAMA(K+1)*CC(I,J,K+1) 300 CONTINUE I_____ 999 CONTINUE RETURN END SUBROUTINE M2PRTD(I23,IEND,JEND,KEND)

USE PARAMETERS USE M2APS USE M2WRK USE MPIVAR IMPLICIT NONE INTEGER :: I,J,K,IST=2,JST=2,KST=2 INTEGER, INTENT(IN):: 123, IEND, JEND, KEND ****** ***** DO 110 I=MXS(2),MXE(2) BE(I)=0. 110 BW(I)=0. DO 112 K=MZS(2),MZE(2) DO 112 J=MYS(2),MYE(2) DO 112 I=MXS(2),MXE(2) BE(I)=BE(I)+AE2(I,J,K)BW(I)=BW(I)+AW2(I,J,K) 112 DO 114 I=MXS(2),MXE(2) 114 BX(I)=BE(I)+BW(I) DO 116 K=MZS(2),MZE(2) DO 116 I=MXS(2),MXE(2) BX(I)=BX(I)+AS2(I,MYS(2),K)+AN2(I,MYE(2),K) 116 DO 118 J=MYS(2),MYE(2) DO 118 I=MXS(2),MXE(2) 118 BX(I)=BX(I)+AB2(I,J,MZS(2))+AT2(I,J,MZE(2)) 1-----DO 120 J=MYS(2),MYE(2) BN(J)=0. 120 BS(J)=0. DO 122 K=MZS(2),MZE(2) DO 122 I=MXS(2),MXE(2) DO 122 J=MYS(2),MYE(2) BN(J)=BN(J)+AN2(I,J,K)122 BS(J)=BS(J)+AS2(I,J,K)DO 124 J=MYS(2),MYE(2) 124 BY(J)=BN(J)+BS(J)DO 126 K=MZS(2),MZE(2) DO 126 J=MYS(2),MYE(2) 126 BY(J)=BY(J)+AW2(MXS(2),J,K)+AE2(MXE(2),J,K)DO 128 I=MXS(2),MXE(2) DO 128 J=MYS(2),MYE(2) BY(J)=BY(J)+AB2(I,J,MZS(2))+AT2(I,J,MZE(2))128 1_____ IF(I23.EQ.2) RETURN DO 130 K=MZS(2),MZE(2) BT(K)=0. 130 BB(K)=0. DO 132 J=MYS(2),MYE(2) DO 132 I=MXS(2),MXE(2) DO 132 K=MZS(2),MZE(2) BT(K)=BT(K)+AT2(I,J,K)132 BB(K)=BB(K)+AB2(I,J,K)DO 134 K=MZS(2),MZE(2)

134 BZ(K)=BT(K)+BB(K)DO 136 J=MYS(2),MYE(2) DO 136 K=MZS(2),MZE(2) 136 BZ(K)=BZ(K)+AW2(MXS(2),J,K)+AE2(MXE(2),J,K)DO 138 I=MXS(2),MXE(2) DO 138 K=MZS(2),MZE(2) 138 BZ(K)=BZ(K)+AS2(I,MYS(2),K)+AN2(I,MYE(2),K)RETURN END SUBROUTINE M2VTDMA(I23,IEND,JEND,KEND) **USE PARAMETERS** USE CALC1, ONLY:CC USE M2APS **USE M2WRK USE TDWK2 USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,IST=2,JST=2,KST=2,NT INTEGER, INTENT(IN):: 123, IEND, JEND, KEND REAL(KIND=8)::BETA,SSS l********** DO 30 I=MXS(2),MXE(2) 30 BLC(I)=0. DO 32 I=MXS(2),MXE(2) DO 32 K=MZS(2),MZE(2) DO 32 J=MYS(2),MYE(2) BLC(I)=BLC(I)+SS2(I,J,K)-AP2(I,J,K)*CC(I,J,K)&32 & +AE2(I,J,K)*CC(I+1,J,K)+AW2(I,J,K)*CC(I-1,J,K)& & +AN2(I,J,K)*CC(I,J+1,K)+AS2(I,J,K)*CC(I,J-1,K)& & +AT2(I,J,K)*CC(I,J,K+1)+AB2(I,J,K)*CC(I,J,K-1) BETA= BX(MXS(2)) BCC(MXS(2))=BLC(MXS(2))/BETA DO 34 I=MXS(2)+1,MXE(2) GAMA(I) =-BE(I-1)/BETA BETA= BX(I)+BW(I)*GAMA(I) 34 BCC(I)=(BLC(I)+BW(I)*BCC(I-1))/BETA DO 36 I=MXE(2)-1,MXS(2),-1 BCC(I)=BCC(I)-GAMA(I+1)*BCC(I+1) 36 DO 38 I=MXS(2),MXE(2) DO 38 K=MZS(2),MZE(2) DO 38 J=MYS(2),MYE(2) 38 CC(I,J,K)=CC(I,J,K)+BCC(I)I_____ DO 40 J=MYS(2),MYE(2) 40 BLC(J)=0. DO 42 J=MYS(2),MYE(2) DO 42 K=MZS(2),MZE(2)

DO 42 I=MXS(2),MXE(2) BLC(J)=BLC(J)+SS2(I,J,K)-AP2(I,J,K)*CC(I,J,K)& 42 & +AE2(I,J,K)*CC(I+1,J,K)+AW2(I,J,K)*CC(I-1,J,K)& & +AN2(I,J,K)*CC(I,J+1,K)+AS2(I,J,K)*CC(I,J-1,K)& & +AT2(I,J,K)*CC(I,J,K+1)+AB2(I,J,K)*CC(I,J,K-1) BETA= BY(MYS(2)) BCC(MYS(2))=BLC(MYS(2))/BETA DO 43 J=MYS(2)+1,MYE(2) GAMA(J)=-BN(J-1)/BETA BETA= BY(J)+BS(J)*GAMA(J) 43 BCC(J)=(BLC(J)+BS(J)*BCC(J-1))/BETA DO 44 J=MYE(2)-1,MYS(2),-1 44 BCC(J)=BCC(J)-GAMA(J+1)*BCC(J+1) DO 48 J=MYS(2),MYE(2) DO 48 K=MZS(2),MZE(2) DO 48 I=MXS(2),MXE(2) 48 CC(I,J,K)=CC(I,J,K)+BCC(J)1---IF(I23.EQ.2) GOTO 59 DO 50 K=MZS(2),MZE(2) 50 BLC(K)=0. DO 52 K=MZS(2),MZE(2) DO 52 J=MYS(2),MYE(2) DO 52 I=MXS(2),MXE(2) BLC(K)=BLC(K)+SS2(I,J,K)-AP2(I,J,K)*CC(I,J,K)& 52 & +AE2(I,J,K)*CC(I+1,J,K)+AW2(I,J,K)*CC(I-1,J,K)& & +AN2(I,J,K)*CC(I,J+1,K)+AS2(I,J,K)*CC(I,J-1,K)& & +AT2(I,J,K)*CC(I,J,K+1)+AB2(I,J,K)*CC(I,J,K-1) BETA= BZ(MZS(2)) BCC(MZS(2))=BLC(MZS(2))/BETA DO 54 K=MZS(2)+1,MZE(2) GAMA(K)= -BT(K-1)/BETA BETA= BZ(K)+BB(K)*GAMA(K) 54 BCC(K)=(BLC(K)+BB(K)*BCC(K-1))/BETA DO 56 K=MZE(2)-1,MZS(2),-1 56 BCC(K)=BCC(K)-GAMA(K+1)*BCC(K+1) DO 58 K=MZS(2),MZE(2) DO 58 J=MYS(2),MYE(2) DO 58 I=MXS(2),MXE(2) 58 CC(I,J,K)=CC(I,J,K)+BCC(K)[********** 59 DO 999 NT=1,2 ****** *********** DO 100 K=MZS(2),MZE(2) DO 100 J=MYS(2),MYE(2) I=MXS(2)SSS=SS2(I,J,K)+AN2(I,J,K)*CC(I,J+1,K)+AS2(I,J,K)*CC(I,J-1,K)& & +AT2(I,J,K)*CC(I,J,K+1)+AB2(I,J,K)*CC(I,J,K-1) BETA=AP2(I,J,K)

CC(I,J,K)=SSS/BETA

DO 130 I=MXS(2)+1,MXE(2) SSS=SS2(I,J,K)+AN2(I,J,K)*CC(I,J+1,K)+AS2(I,J,K)*CC(I,J-1,K)& & +AT2(I,J,K)*CC(I,J,K+1)+AB2(I,J,K)*CC(I,J,K-1) GAMA(I)= -AE2(I-1,J,K)/BETA BETA=AP2(I,J,K)+AW2(I,J,K)*GAMA(I) 130 CC(I,J,K)=(SSS+AW2(I,J,K)*CC(I-1,J,K))/BETA DO 140 I=MXE(2)-1,MXS(2),-1 140 CC(I,J,K)=CC(I,J,K)-GAMA(I+1)*CC(I+1,J,K)100 CONTINUE l-----DO 200 K=MZS(2),MZE(2) DO 200 I=MXS(2),MXE(2) J=MYS(2)SSS=SS2(I,J,K)+AE2(I,J,K)*CC(I+1,J,K)+AW2(I,J,K)*CC(I-1,J,K)& & +AT2(I,J,K)*CC(I,J,K+1)+AB2(I,J,K)*CC(I,J,K-1) BETA=AP2(I,J,K) CC(I,J,K)=SSS/BETA DO 230 J=MYS(2)+1,MYE(2) SSS=SS2(I,J,K)+AE2(I,J,K)*CC(I+1,J,K)+AW2(I,J,K)*CC(I-1,J,K)& +AT2(I,J,K)*CC(I,J,K+1)+AB2(I,J,K)*CC(I,J,K-1) & GAMA(J)=-AN2(I,J-1,K)/BETA BETA=AP2(I,J,K)+AS2(I,J,K)*GAMA(J) 230 CC(I,J,K)=(SSS+AS2(I,J,K)*CC(I,J-1,K))/BETA DO 240 J=MYE(2)-1,MYS(2),-1 240 CC(I,J,K)=CC(I,J,K)-GAMA(J+1)*CC(I,J+1,K) 200 CONTINUE 1_____ IF(I23.EQ.2) GOTO 999 DO 300 J=MYS(2),MYE(2) DO 300 I=MXS(2),MXE(2) K=MZS(2)SSS=SS2(I,J,K)+AE2(I,J,K)*CC(I+1,J,K)+AW2(I,J,K)*CC(I-1,J,K)& +AN2(I,J,K)*CC(I,J+1,K)+AS2(I,J,K)*CC(I,J-1,K) & BETA=AP2(I.J.K) CC(I,J,K)=SSS/BETA DO 330 K=MZS(2)+1,MZE(2) SSS=SS2(I,J,K)+AE2(I,J,K)*CC(I+1,J,K)+AW2(I,J,K)*CC(I-1,J,K)& +AN2(I,J,K)*CC(I,J+1,K)+AS2(I,J,K)*CC(I,J-1,K) & GAMA(K)= -AT2(I,J,K-1)/BETA AP2(I,J,K)+AB2(I,J,K)*GAMA(K) BETA= 330 CC(I,J,K)=(SSS+AB2(I,J,K)*CC(I,J,K-1))/BETA DO 340 K=MZE(2)-1,MZS(2),-1 CC(I,J,K)=CC(I,J,K)-GAMA(K+1)*CC(I,J,K+1) 340 300 CONTINUE 1_____ 999 CONTINUE

IIST=MXS(2) JJST=MYS(2) KKST=MZS(2) IIEND=MXE(2) JJEND=MYE(2) KKEND=MZE(2) CALL RELOAD IF (TASKID.NE.0) THEN CALL MPI_SEND(CC(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECI SION,0,TASKID,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(CC(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(N T)),SIZECC(NT),MPI DOUBLE PRECISION,NT,NT,MPI COMM WORLD,STATUS,IERR) **ENDDO** ENDIF CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI BCAST(CC(1,1,1),SIZE(CC),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR) RETURN END SUBROUTINE M3PRTD(I23,IEND,JEND,KEND) *************** **USE PARAMETERS** USE M3APS **USE M3WRK USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,IST=2,JST=2,KST=2 INTEGER, INTENT(IN):: 123, IEND, JEND, KEND ************************************* ******* DO 110 I=MXS(3),MXE(3) BE(I)=0. 110 BW(I)=0. DO 112 K=MZS(3),MZE(3) DO 112 J=MYS(3),MYE(3) DO 112 I=MXS(3),MXE(3) BE(I)=BE(I)+AE3(I,J,K)112 BW(I)=BW(I)+AW3(I,J,K) DO 114 I=MXS(3),MXE(3) 114 BX(I)=BE(I)+BW(I)DO 116 K=MZS(3),MZE(3) DO 116 I=MXS(3),MXE(3) 116 BX(I)=BX(I)+AS3(I,MYS(3),K)+AN3(I,MYE(3),K)

```
DO 118 J=MYS(3),MYE(3)
DO 118 I=MXS(3),MXE(3)
118 BX(I)=BX(I)+AB3(I,J,MZS(3))+AT3(I,J,MZE(3))
[-----
DO 120 J=MYS(3),MYE(3)
BN(J)=0.
120 BS(J)=0.
DO 122 K=MZS(3),MZE(3)
DO 122 I=MXS(3),MXE(3)
DO 122 J=MYS(3),MYE(3)
BN(J)=BN(J)+AN3(I,J,K)
     BS(J)=BS(J)+AS3(I,J,K)
122
DO 124 J=MYS(3),MYE(3)
124
     BY(J)=BN(J)+BS(J)
DO 126 K=MZS(3),MZE(3)
DO 126 J=MYS(3),MYE(3)
126
     BY(J)=BY(J)+AW3(MXS(3),J,K)+AE3(MXE(3),J,K)
DO 128 I=MXS(3),MXE(3)
DO 128 J=MYS(3),MYE(3)
128
     BY(J)=BY(J)+AB3(I,J,MZS(3))+AT3(I,J,MZE(3))
1___
IF(I23.EQ.2) RETURN
DO 130 K=MZS(3),MZE(3)
BT(K)=0.
130
     BB(K)=0.
DO 132 J=MYS(3),MYE(3)
DO 132 I=MXS(3),MXE(3)
DO 132 K=MZS(3),MZE(3)
BT(K)=BT(K)+AT3(I,J,K)
     BB(K)=BB(K)+AB3(I,J,K)
132
DO 134 K=MZS(3),MZE(3)
     BZ(K)=BT(K)+BB(K)
134
DO 136 J=MYS(3),MYE(3)
DO 136 K=MZS(3),MZE(3)
136
     BZ(K)=BZ(K)+AW3(MXS(3),J,K)+AE3(MXE(3),J,K)
DO 138 I=MXS(3),MXE(3)
DO 138 K=MZS(3),MZE(3)
138
     BZ(K)=BZ(K)+AS3(I,MYS(3),K)+AN3(I,MYE(3),K)
RETURN
END
SUBROUTINE M3VTDMA(I23,IEND,JEND,KEND)
USE PARAMETERS
USE CALC1, ONLY:CC
USE M3APS
USE M3WRK
USE TDWK2
USE MPIVAR
IMPLICIT NONE
INTEGER :: I,J,K,IST=2,JST=2,KST=2,NT
```

INTEGER, INTENT(IN):: 123, IEND, JEND, KEND REAL(KIND=8)::BETA,SSS ************ ****** DO 30 I=MXS(3),MXE(3) 30 BLC(I)=0. DO 32 I=MXS(3),MXE(3) DO 32 K=MZS(3),MZE(3) DO 32 J=MYS(3),MYE(3) 32 BLC(I)=BLC(I)+SS3(I,J,K)-AP3(I,J,K)*CC(I,J,K)& & +AE3(I,J,K)*CC(I+1,J,K)+AW3(I,J,K)*CC(I-1,J,K)& & +AN3(I,J,K)*CC(I,J+1,K)+AS3(I,J,K)*CC(I,J-1,K)& & +AT3(I,J,K)*CC(I,J,K+1)+AB3(I,J,K)*CC(I,J,K-1) BETA= BX(MXS(3)) BCC(MXS(3))=BLC(MXS(3))/BETA DO 34 I=MXS(3)+1,MXE(3) GAMA(I)= -BE(I-1)/BETA BETA= BX(I)+BW(I)*GAMA(I) 34 BCC(I)=(BLC(I)+BW(I)*BCC(I-1))/BETA DO 36 I=MXE(3)-1,MXS(3),-1 BCC(I)=BCC(I)-GAMA(I+1)*BCC(I+1) 36 DO 38 I=MXS(3),MXE(3) DO 38 K=MZS(3),MZE(3) DO 38 J=MYS(3),MYE(3) 38 CC(I,J,K)=CC(I,J,K)+BCC(I)|-----DO 40 J=MYS(3),MYE(3) 40 BLC(J)=0. DO 42 J=MYS(3),MYE(3) DO 42 K=MZS(3),MZE(3) DO 42 I=MXS(3),MXE(3) 42 BLC(J)=BLC(J)+SS3(I,J,K)-AP3(I,J,K)*CC(I,J,K)& & +AE3(I,J,K)*CC(I+1,J,K)+AW3(I,J,K)*CC(I-1,J,K)& & +AN3(I,J,K)*CC(I,J+1,K)+AS3(I,J,K)*CC(I,J-1,K)& & +AT3(I,J,K)*CC(I,J,K+1)+AB3(I,J,K)*CC(I,J,K-1) BETA= BY(MYS(3))BCC(MYS(3))=BLC(MYS(3))/BETA DO 43 J=MYS(3)+1,MYE(3) GAMA(J)=-BN(J-1)/BETA BETA= BY(J)+BS(J)*GAMA(J) BCC(J)=(BLC(J)+BS(J)*BCC(J-1))/BETA 43 DO 44 J=MYE(3)-1,MYS(3),-1 BCC(J)=BCC(J)-GAMA(J+1)*BCC(J+1) 44 DO 48 J=MYS(3),MYE(3) DO 48 K=MZS(3),MZE(3) DO 48 I=MXS(3),MXE(3) 48 CC(I,J,K)=CC(I,J,K)+BCC(J)1__ IF(I23.EQ.2) GOTO 59 DO 50 K=MZS(3),MZE(3)

BLC(K)=0. 50 DO 52 K=MZS(3),MZE(3) DO 52 J=MYS(3),MYE(3) DO 52 I=MXS(3),MXE(3) 52 BLC(K)=BLC(K)+SS3(I,J,K)-AP3(I,J,K)*CC(I,J,K)& & +AE3(I,J,K)*CC(I+1,J,K)+AW3(I,J,K)*CC(I-1,J,K)& & +AN3(I,J,K)*CC(I,J+1,K)+AS3(I,J,K)*CC(I,J-1,K)& & +AT3(I,J,K)*CC(I,J,K+1)+AB3(I,J,K)*CC(I,J,K-1) BETA= BZ(MZS(3)) BCC(MZS(3))=BLC(MZS(3))/BETA DO 54 K=MZS(3)+1,MZE(3) GAMA(K)= -BT(K-1)/BETA BETA= BZ(K)+BB(K)*GAMA(K) 54 BCC(K)=(BLC(K)+BB(K)*BCC(K-1))/BETA DO 56 K=MZE(3)-1,MZS(3),-1 56 BCC(K)=BCC(K)-GAMA(K+1)*BCC(K+1) DO 58 K=MZS(3),MZE(3) DO 58 J=MYS(3),MYE(3) DO 58 I=MXS(3),MXE(3) 58 CC(I,J,K)=CC(I,J,K)+BCC(K)|********* ***** 59 DO 999 NT=1,2 ******** DO 100 K=MZS(3),MZE(3) DO 100 J=MYS(3),MYE(3) I=MXS(3)SSS=SS3(I,J,K)+AN3(I,J,K)*CC(I,J+1,K)+AS3(I,J,K)*CC(I,J-1,K)& +AT3(I,J,K)*CC(I,J,K+1)+AB3(I,J,K)*CC(I,J,K-1) & BETA=AP3(I,J,K) CC(I,J,K)=SSS/BETA DO 130 I=MXS(3)+1,MXE(3) SSS=SS3(I,J,K)+AN3(I,J,K)*CC(I,J+1,K)+AS3(I,J,K)*CC(I,J-1,K)& & +AT3(I,J,K)*CC(I,J,K+1)+AB3(I,J,K)*CC(I,J,K-1) GAMA(I)= -AE3(I-1,J,K)/BETA BETA=AP3(I,J,K)+AW3(I,J,K)*GAMA(I) 130 CC(I,J,K)=(SSS+AW3(I,J,K)*CC(I-1,J,K))/BETA DO 140 I=MXE(3)-1,MXS(3),-1 140 CC(I,J,K)=CC(I,J,K)-GAMA(I+1)*CC(I+1,J,K)100 CONTINUE I_____ DO 200 K=MZS(3),MZE(3) DO 200 I=MXS(3),MXE(3) J=MYS(3)SSS=SS3(I,J,K)+AE3(I,J,K)*CC(I+1,J,K)+AW3(I,J,K)*CC(I-1,J,K)& +AT3(I,J,K)*CC(I,J,K+1)+AB3(I,J,K)*CC(I,J,K-1) & BETA=AP3(I,J,K) CC(I,J,K)=SSS/BETA

DO 230 J=MYS(3)+1,MYE(3)

SSS=SS3(I,J,K)+AE3(I,J,K)*CC(I+1,J,K)+AW3(I,J,K)*CC(I-1,J,K)& & +AT3(I,J,K)*CC(I,J,K+1)+AB3(I,J,K)*CC(I,J,K-1) GAMA(J)=-AN3(I.J-1.K)/BETA BETA=AP3(I,J,K)+AS3(I,J,K)*GAMA(J) 230 CC(I,J,K)=(SSS+AS3(I,J,K)*CC(I,J-1,K))/BETA DO 240 J=MYE(3)-1,MYS(3),-1 240 CC(I,J,K)=CC(I,J,K)-GAMA(J+1)*CC(I,J+1,K) 200 CONTINUE I___ IF(I23.EQ.2) GOTO 999 DO 300 J=MYS(3),MYE(3) DO 300 I=MXS(3),MXE(3) K=MZS(3) SSS=SS3(I,J,K)+AE3(I,J,K)*CC(I+1,J,K)+AW3(I,J,K)*CC(I-1,J,K)& & +AN3(I,J,K)*CC(I,J+1,K)+AS3(I,J,K)*CC(I,J-1,K) BETA=AP3(I,J,K) CC(I,J,K)=SSS/BETA DO 330 K=MZS(3)+1,MZE(3) SSS=SS3(I,J,K)+AE3(I,J,K)*CC(I+1,J,K)+AW3(I,J,K)*CC(I-1,J,K)& +AN3(I,J,K)*CC(I,J+1,K)+AS3(I,J,K)*CC(I,J-1,K) & GAMA(K)= -AT3(I,J,K-1)/BETA BETA= AP3(I,J,K)+AB3(I,J,K)*GAMA(K) 330 CC(I,J,K)=(SSS+AB3(I,J,K)*CC(I,J,K-1))/BETA DO 340 K=MZE(3)-1,MZS(3),-1 CC(I,J,K)=CC(I,J,K)-GAMA(K+1)*CC(I,J,K+1) 340 300 CONTINUE 1___ 999 CONTINUE IIST=MXS(3) JJST=MYS(3) KKST=MZS(3) IIEND=MXE(3) JJEND=MYE(3) KKEND=MZE(3) CALL RELOAD IF (TASKID.NE.0) THEN CALL MPI_SEND(CC(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECI SION,0,TASKID,MPI COMM WORLD,IERR) **ENDIF** IF (TASKID.EQ.0) THEN DO NT=1.26 CALL MPI_RECV(CC(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(N T)),SIZECC(NT),MPI DOUBLE PRECISION,NT,NT,MPI COMM WORLD,STATUS,IERR) ENDDO **ENDIF**

CALL MPI_BARRIER(MPI_COMM_WORLD,IERR) CALL MPI_BCAST(CC(1,1,1),SIZE(CC),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR)

END SUBROUTINE M4PRTD(I23,IEND,JEND,KEND) **USE PARAMETERS USE M4APS USE M4WRK USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,IST=2,JST=2,KST=2 INTEGER, INTENT(IN):: 123, IEND, JEND, KEND ******* ****** DO 110 I=MXS(4),MXE(4) BE(I)=0. 110 BW(I)=0. DO 112 K=MZS(4),MZE(4) DO 112 J=MYS(4),MYE(4) DO 112 I=MXS(4),MXE(4) BE(I)=BE(I)+AE4(I,J,K)112 BW(I)=BW(I)+AW4(I,J,K) DO 114 I=MXS(4),MXE(4) 114 BX(I)=BE(I)+BW(I)DO 116 K=MXS(4),MXE(4) DO 116 I=MXS(4),MXE(4) BX(I)=BX(I)+AS4(I,MYS(4),K)+AN4(I,MYE(4),K) 116 DO 118 J=MYS(4),MYE(4) DO 118 I=MXS(4),MXE(4) 118 BX(I)=BX(I)+AB4(I,J,MZS(4))+AT4(I,J,MZE(4))!-----DO 120 J=MYS(4),MYE(4) BN(J)=0. 120 BS(J)=0. DO 122 K=MZS(4),MZE(4) DO 122 I=MXS(4),MXE(4) DO 122 J=MYS(4),MYE(4) BN(J)=BN(J)+AN4(I,J,K)122 BS(J)=BS(J)+AS4(I,J,K)DO 124 J=MYS(4),MYE(4) BY(J)=BN(J)+BS(J)124 DO 126 K=MZS(4),MZE(4) DO 126 J=MYS(4),MYE(4) BY(J)=BY(J)+AW4(MXS(4),J,K)+AE4(MXE(4),J,K)126 DO 128 I=MXS(4),MXE(4) DO 128 J=MYS(4),MYE(4) 128 BY(J)=BY(J)+AB4(I,J,MZS(4))+AT4(I,J,MZE(4))1__

IF(I23.EQ.2) RETURN

RETURN

```
DO 130 K=MXS(4),MXE(4)
BT(K)=0.
130
     BB(K)=0.
DO 132 J=MYS(4),MYE(4)
DO 132 I=MXS(4),MXE(4)
DO 132 K=MZS(4),MZE(4)
BT(K)=BT(K)+AT4(I,J,K)
132
     BB(K)=BB(K)+AB4(I,J,K)
DO 134 K=MZS(4),MZE(4)
     BZ(K)=BT(K)+BB(K)
134
DO 136 J=MYS(4),MYE(4)
DO 136 K=MZS(4),MZE(4)
     BZ(K)=BZ(K)+AW4(MXS(4),J,K)+AE4(MXE(4),J,K)
136
DO 138 I=MXS(4),MXE(4)
DO 138 K=MZS(4),MZE(4) s
138
     BZ(K)=BZ(K)+AS4(I,MYS(4),K)+AN4(I,MYE(4),K)
!
RETURN
END
SUBROUTINE M4VTDMA(I23,IEND,JEND,KEND)
USE PARAMETERS
USE CALC1, ONLY:CC
USE M4APS
USE M4WRK
USE TDWK2
USE MPIVAR
IMPLICIT NONE
INTEGER :: I,J,K,IST=2,JST=2,KST=2,NT
INTEGER, INTENT(IN):: 123, IEND, JEND, KEND
REAL(KIND=8):: BETA,SSS
DO 30 I=MXS(4),MXE(4)
30
     BLC(I)=0.
DO 32 I=MXS(4),MXE(4)
DO 32 K=MZS(4),MZE(4)
DO 32 J=MYS(4),MYE(4)
32
     BLC(I)=BLC(I)+SS4(I,J,K)-AP4(I,J,K)*CC(I,J,K)&
&
            +AE4(I,J,K)*CC(I+1,J,K)+AW4(I,J,K)*CC(I-1,J,K)&
&
            +AN4(I,J,K)*CC(I,J+1,K)+AS4(I,J,K)*CC(I,J-1,K)&
&
            +AT4(I,J,K)*CC(I,J,K+1)+AB4(I,J,K)*CC(I,J,K-1)
BETA=
         BX(MXS(4))
BCC(MXS(4))=BLC(MXS(4))/BETA
DO 34 I=MXS(4)+1,MXE(4)
GAMA(I)=
            -BE(I-1)/BETA
BETA=
        BX(I)+BW(I)*GAMA(I)
     BCC(I)=(BLC(I)+BW(I)*BCC(I-1))/BETA
34
DO 36 I=MXE(4)-1,MXS(4),-1
36
     BCC(I)=BCC(I)-GAMA(I+1)*BCC(I+1)
```

```
DO 38 I=MXS(4),MXE(4)
DO 38 K=MZS(4),MZE(4)
DO 38 J=MYS(4),MYE(4)
38
      CC(I,J,K)=CC(I,J,K)+BCC(I)
l-----
DO 40 J=MYS(4),MYE(4)
40
     BLC(J)=0.
DO 42 J=MYS(4),MYE(4)
DO 42 K=MZS(4),MZE(4)
DO 42 I=MXS(4),MXE(4)
42
      BLC(J)=BLC(J)+SS4(I,J,K)-AP4(I,J,K)*CC(I,J,K)&
&
              +AE4(I,J,K)*CC(I+1,J,K)+AW4(I,J,K)*CC(I-1,J,K)&
&
              +AN4(I,J,K)*CC(I,J+1,K)+AS4(I,J,K)*CC(I,J-1,K)&
&
              +AT4(I,J,K)*CC(I,J,K+1)+AB4(I,J,K)*CC(I,J,K-1)
BETA=
           BY(MYS(4))
BCC(MYS(4))=BLC(MYS(4))/BETA
DO 43 J=MYS(4)+1,MYE(4)
GAMA(J)=
              -BN(J-1)/BETA
BETA=
          BY(J)+BS(J)*GAMA(J)
      BCC(J)=(BLC(J)+BS(J)*BCC(J-1))/BETA
43
DO 44 J=MYE(4)-1,MYS(4),-1
44
      BCC(J)=BCC(J)-GAMA(J+1)*BCC(J+1)
!
DO 48 J=MYS(4),MYE(4)
DO 48 K=MZS(4),MZE(4)
DO 48 I=MXS(4),MXE(4)
48
      CC(I,J,K)=CC(I,J,K)+BCC(J)
I_____
IF(I23.EQ.2) GOTO 59
DO 50 K=MZS(4),MZE(4)
50
      BLC(K)=0.
DO 52 K=MZS(4),MZE(4)
DO 52 J=MYS(4),MYE(4)
DO 52 I=MXS(4),MXE(4)
      BLC(K)=BLC(K)+SS4(I,J,K)-AP4(I,J,K)*CC(I,J,K)&
52
&
              +AE4(I,J,K)*CC(I+1,J,K)+AW4(I,J,K)*CC(I-1,J,K)&
&
             +AN4(I,J,K)*CC(I,J+1,K)+AS4(I,J,K)*CC(I,J-1,K)&
&
             +AT4(I,J,K)*CC(I,J,K+1)+AB4(I,J,K)*CC(I,J,K-1)
BETA=
           BZ(MZS(4))
BCC(MZS(4))=BLC(MZS(4))/BETA
DO 54 K=MZS(4)+1,MZE(4)
GAMA(K)= -BT(K-1)/BETA
BETA=
          BZ(K)+BB(K)*GAMA(K)
      BCC(K)=(BLC(K)+BB(K)*BCC(K-1))/BETA
54
DO 56 K=MZE(4)-1,MZS(4),-1
56
      BCC(K)=BCC(K)-GAMA(K+1)*BCC(K+1)
DO 58 K=MZS(4),MZE(4)
DO 58 J=MYS(4),MYE(4)
DO 58 I=MXS(4),MXE(4)
58
      CC(I,J,K)=CC(I,J,K)+BCC(K)
```

```
59
     DO 999 NT=1,2
*******
DO 100 K=MZS(4),MZE(4)
DO 100 J=MYS(4), MYE(4)
I=MXS(4)
SSS=SS4(I,J,K)+AN4(I,J,K)*CC(I,J+1,K)+AS4(I,J,K)*CC(I,J-1,K)&
             +AT4(I,J,K)*CC(I,J,K+1)+AB4(I,J,K)*CC(I,J,K-1)
&
BETA=AP4(I,J,K)
CC(I,J,K)=SSS/BETA
DO 130 I=MXS(4)+1,MXE(4)
SSS=SS4(I,J,K)+AN4(I,J,K)*CC(I,J+1,K)+AS4(I,J,K)*CC(I,J-1,K)&
             +AT4(I,J,K)*CC(I,J,K+1)+AB4(I,J,K)*CC(I,J,K-1)
&
GAMA(I)=
              -AE4(I-1,J,K)/BETA
BETA=AP4(I,J,K)+AW4(I,J,K)*GAMA(I)
130
     CC(I,J,K)=(SSS+AW4(I,J,K)*CC(I-1,J,K))/BETA
!
DO 140 I=MXE(4)-1,MXS(4),-1
140
     CC(I,J,K)=CC(I,J,K)-GAMA(I+1)*CC(I+1,J,K)
100
      CONTINUE
DO 200 K=MZS(4),MZE(4)
DO 200 I=MXS(4),MXE(4)
J=MYS(4)
SSS=SS4(I,J,K)+AE4(I,J,K)*CC(I+1,J,K)+AW4(I,J,K)*CC(I-1,J,K)&
             +AT4(I,J,K)*CC(I,J,K+1)+AB4(I,J,K)*CC(I,J,K-1)
&
BETA=AP4(I.J.K)
CC(I,J,K)=SSS/BETA
DO 230 J=MYS(4)+1,MYE(4)
SSS=SS4(I,J,K)+AE4(I,J,K)*CC(I+1,J,K)+AW4(I,J,K)*CC(I-1,J,K)&
&
             +AT4(I,J,K)*CC(I,J,K+1)+AB4(I,J,K)*CC(I,J,K-1)
GAMA(J) =
              -AN4(I,J-1,K)/BETA
BETA=AP4(I,J,K)+AS4(I,J,K)*GAMA(J)
230
     CC(I,J,K)=(SSS+AS4(I,J,K)*CC(I,J-1,K))/BETA
DO 240 J=MYE(4)-1,MYS(4),-1
240
      CC(I,J,K)=CC(I,J,K)-GAMA(J+1)*CC(I,J+1,K)
200
      CONTINUE
1_____
IF(I23.EQ.2) GOTO 999
DO 300 J=MYS(4),MYE(4)
DO 300 I=MXS(4),MXE(4)
K=MZS(4)
SSS=SS4(I,J,K)+AE4(I,J,K)*CC(I+1,J,K)+AW4(I,J,K)*CC(I-1,J,K)&
&
             +AN4(I,J,K)*CC(I,J+1,K)+AS4(I,J,K)*CC(I,J-1,K)
BETA=AP4(I,J,K)
CC(I,J,K)=SSS/BETA
DO 330 K=MZS(4)+1,MZE(4)
SSS=SS4(I,J,K)+AE4(I,J,K)*CC(I+1,J,K)+AW4(I,J,K)*CC(I-1,J,K)&
&
             +AN4(I,J,K)*CC(I,J+1,K)+AS4(I,J,K)*CC(I,J-1,K)
```

GAMA(K)= -AT4(I,J,K-1)/BETA BETA= AP4(I,J,K)+AB4(I,J,K)*GAMA(K) 330 CC(I,J,K)=(SSS+AB4(I,J,K)*CC(I,J,K-1))/BETA DO 340 K=MZE(4)-1,MZS(4),-1 CC(I,J,K)=CC(I,J,K)-GAMA(K+1)*CC(I,J,K+1) 340 300 CONTINUE I_____ 999 CONTINUE IIST=MXS(4) JJST=MYS(4) KKST=MZS(4) IIEND=MXE(4) JJEND=MYE(4) KKEND=MZE(4) CALL RELOAD IF (TASKID.NE.0) THEN CALL MPI_SEND(CC(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECI SION,0,TASKID,MPI_COMM_WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(CC(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(N T)),SIZECC(NT),MPI DOUBLE PRECISION,NT,NT,MPI COMM WORLD,STATUS,IERR) **ENDDO ENDIF** CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI_BCAST(CC(1,1,1),SIZE(CC),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR) RETURN END SUBROUTINE M5PRTD(123, IEND, JEND, KEND) **USE PARAMETERS USE M5APS USE M5WRK USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,IST=2,JST=2,KST=2 INTEGER, INTENT(IN):: 123, IEND, JEND, KEND *********** DO 110 I=MXS(5),MXE(5) BE(I)=0. 110 BW(I)=0. DO 112 K=MZS(5),MZE(5)

DO 112 J=MYS(5),MYE(5) DO 112 I=MXS(5),MXE(5) BE(I)=BE(I)+AE5(I,J,K) 112 BW(I)=BW(I)+AW5(I,J,K)DO 114 I=MXS(5),MXE(5) BX(I)=BE(I)+BW(I)114 DO 116 K=MZS(5),MZE(5) DO 116 I=MXS(5),MXE(5) BX(I)=BX(I)+AS5(I,MYS(5),K)+AN5(I,MYE(5),K) 116 DO 118 J=MYS(5),MYE(5) DO 118 I=MXS(5),MXE(5) BX(I)=BX(I)+AB5(I,J,MZS(5))+AT5(I,J,MZE(5)) 118 I_____ DO 120 J=MYS(5),MYE(5) BN(J)=0. 120 BS(J)=0. DO 122 K=MZS(5),MZE(5) DO 122 I=MXS(5),MXE(5) DO 122 J=MYS(5),MYE(5) BN(J)=BN(J)+AN5(I,J,K) 122 BS(J)=BS(J)+AS5(I,J,K) DO 124 J=MYS(5),MYE(5) 124 BY(J)=BN(J)+BS(J)DO 126 K=MZS(5),MZE(5) DO 126 J=MYS(5),MYE(5) 126 BY(J)=BY(J)+AW5(MXS(5),J,K)+AE5(MXE(5),J,K)DO 128 I=MXS(5),MXE(5) DO 128 J=MYS(5),MYE(5) 128 BY(J)=BY(J)+AB5(I,J,MZS(5))+AT5(I,J,MZE(5))!---IF(I23.EQ.2) RETURN DO 130 K=MZS(5),MZE(5) BT(K)=0. 130 BB(K)=0. DO 132 J=MYS(5),MYE(5) DO 132 I=MXS(5),MXE(5) DO 132 K=MZS(5),MZE(5) BT(K)=BT(K)+AT5(I,J,K)132 BB(K)=BB(K)+AB5(I,J,K)DO 134 K=MZS(5),MZE(5) 134 BZ(K)=BT(K)+BB(K)DO 136 J=MYS(5),MYE(5) DO 136 K=MZS(5),MZE(5) BZ(K)=BZ(K)+AW5(MXS(5),J,K)+AE5(MXE(5),J,K)136 DO 138 I=MXS(5),MXE(5) DO 138 K=MZS(5),MZE(5) 138 BZ(K)=BZ(K)+AS5(I,MYS(5),K)+AN5(I,MYE(5),K) RETURN END

SUBROUTINE M5VTDMA(I23,IEND,JEND,KEND)

USE PARAMETERS USE CALC1.ONLY:CC USE M5APS **USE M5WRK** USE TDWK2 **USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,IST=2,JST=2,KST=2,NT INTEGER, INTENT(IN):: 123, IEND, JEND, KEND REAL(KIND=8):: BETA,SSS ****** ******* DO 30 I=MXS(5),MXE(5) BLC(I)=0. 30 DO 32 I=MXS(5),MXE(5) DO 32 K=MZS(5),MZE(5) DO 32 J=MYS(5),MYE(5) 32 BLC(I)=BLC(I)+SS5(I,J,K)-AP5(I,J,K)*CC(I,J,K)& & +AE5(I,J,K)*CC(I+1,J,K)+AW5(I,J,K)*CC(I-1,J,K)& & +AN5(I,J,K)*CC(I,J+1,K)+AS5(I,J,K)*CC(I,J-1,K)& & +AT5(I,J,K)*CC(I,J,K+1)+AB5(I,J,K)*CC(I,J,K-1) BETA= BX(MXS(5)) BCC(MXS(5))=BLC(MXS(5))/BETA DO 34 I=MXS(5)+1,MXE(5) GAMA(I)= -BE(I-1)/BETA BETA= BX(I)+BW(I)*GAMA(I) 34 BCC(I)=(BLC(I)+BW(I)*BCC(I-1))/BETA DO 36 I=MXE(5)-1,MXS(5),-1 BCC(I)=BCC(I)-GAMA(I+1)*BCC(I+1) 36 DO 38 I=MXS(5),MXE(5) DO 38 K=MZS(5),MZE(5) DO 38 J=MYS(5),MYE(5) 38 CC(I,J,K)=CC(I,J,K)+BCC(I)!-----DO 40 J=MYS(5),MYE(5) 40 BLC(J)=0. DO 42 J=MYS(5),MYE(5) DO 42 K=MZS(5),MZE(5) DO 42 I=MXS(5),MXE(5) 42 BLC(J)=BLC(J)+SS5(I,J,K)-AP5(I,J,K)*CC(I,J,K)& & +AE5(I,J,K)*CC(I+1,J,K)+AW5(I,J,K)*CC(I-1,J,K)& & +AN5(I,J,K)*CC(I,J+1,K)+AS5(I,J,K)*CC(I,J-1,K)& & +AT5(I,J,K)*CC(I,J,K+1)+AB5(I,J,K)*CC(I,J,K-1) BETA= BY(MYS(5)) BCC(MYS(5))=BLC(MYS(5))/BETA DO 43 J=MYS(5)+1,MYE(5) GAMA(J) =-BN(J-1)/BETA BY(J)+BS(J)*GAMA(J) BETA= 43 BCC(J)=(BLC(J)+BS(J)*BCC(J-1))/BETA DO 44 J=MYE(5)-1,MYS(5),-1

44 BCC(J)=BCC(J)-GAMA(J+1)*BCC(J+1)

DO 48 J=MYS(5).MYE(5) DO 48 K=MZS(5),MZE(5) DO 48 I=MXS(5),MXE(5) 48 CC(I,J,K)=CC(I,J,K)+BCC(J)I-----IF(I23.EQ.2) GOTO 59 DO 50 K=MZS(5),MZE(5) 50 BLC(K)=0. DO 52 K=MZS(5),MZE(5) DO 52 J=MYS(5),MYE(5) DO 52 I=MXS(5),MXE(5) 52 BLC(K)=BLC(K)+SS5(I,J,K)-AP5(I,J,K)*CC(I,J,K)& & +AE5(I,J,K)*CC(I+1,J,K)+AW5(I,J,K)*CC(I-1,J,K)& & +AN5(I,J,K)*CC(I,J+1,K)+AS5(I,J,K)*CC(I,J-1,K)& & +AT5(I,J,K)*CC(I,J,K+1)+AB5(I,J,K)*CC(I,J,K-1) BETA= BZ(MZS(5)) BCC(MZS(5))=BLC(MZS(5))/BETA DO 54 K=MZS(5)+1,MZE(5) GAMA(K)=-BT(K-1)/BETA BETA= BZ(K)+BB(K)*GAMA(K) BCC(K)=(BLC(K)+BB(K)*BCC(K-1))/BETA 54 DO 56 K=MZE(5)-1,MZS(5),-1 56 BCC(K)=BCC(K)-GAMA(K+1)*BCC(K+1) DO 58 K=MZS(5),MZE(5) DO 58 J=MYS(5),MYE(5) DO 58 I=MXS(5),MXE(5) CC(I,J,K)=CC(I,J,K)+BCC(K)58 ***** ******* 59 DO 999 NT=1,2 ****** DO 100 K=MZS(5),MZE(5) DO 100 J=MYS(5),MYE(5) I=MXS(5) SSS=SS5(I,J,K)+AN5(I,J,K)*CC(I,J+1,K)+AS5(I,J,K)*CC(I,J-1,K)& & +AT5(I,J,K)*CC(I,J,K+1)+AB5(I,J,K)*CC(I,J,K-1) BETA=AP5(I,J,K) CC(I,J,K)=SSS/BETA DO 130 I=MXS(5)+1,MXE(5) SSS=SS5(I,J,K)+AN5(I,J,K)*CC(I,J+1,K)+AS5(I,J,K)*CC(I,J-1,K)& +AT5(I,J,K)*CC(I,J,K+1)+AB5(I,J,K)*CC(I,J,K-1) & GAMA(I)= -AE5(I-1,J,K)/BETA BETA=AP5(I,J,K)+AW5(I,J,K)*GAMA(I) 130 CC(I,J,K)=(SSS+AW5(I,J,K)*CC(I-1,J,K))/BETA DO 140 I=MXE(5)-1,MXS(5),-1 CC(I,J,K)=CC(I,J,K)-GAMA(I+1)*CC(I+1,J,K) 140 100 CONTINUE |_____

```
DO 200 K=MZS(5),MZE(5)
DO 200 I=MXS(5),MXE(5)
J=MYS(5)
SSS=SS5(I,J,K)+AE5(I,J,K)*CC(I+1,J,K)+AW5(I,J,K)*CC(I-1,J,K)&
              +AT5(I,J,K)*CC(I,J,K+1)+AB5(I,J,K)*CC(I,J,K-1)
&
BETA=AP5(I,J,K)
CC(I,J,K)=SSS/BETA
DO 230 J=MYS(5)+1,MYE(5)
SSS=SS5(I,J,K)+AE5(I,J,K)*CC(I+1,J,K)+AW5(I,J,K)*CC(I-1,J,K)&
&
              +AT5(I,J,K)*CC(I,J,K+1)+AB5(I,J,K)*CC(I,J,K-1)
GAMA(J)=
               -AN5(I,J-1,K)/BETA
BETA=AP5(I,J,K)+AS5(I,J,K)*GAMA(J)
230 CC(I,J,K)=(SSS+AS5(I,J,K)*CC(I,J-1,K))/BETA
DO 240 J=MYE(5)-1,MYS(5),-1
240
     CC(I,J,K)=CC(I,J,K)-GAMA(J+1)*CC(I,J+1,K)
200
      CONTINUE
!-----
IF(I23.EQ.2) GOTO 999
DO 300 J=MYS(5),MYE(5)
DO 300 I=MXS(5),MXE(5)
K=MZS(5)
SSS=SS5(I,J,K)+AE5(I,J,K)*CC(I+1,J,K)+AW5(I,J,K)*CC(I-1,J,K)&
              +AN5(I,J,K)*CC(I,J+1,K)+AS5(I,J,K)*CC(I,J-1,K)
&
BETA=AP5(I,J,K)
CC(I,J,K)=SSS/BETA
DO 330 K=MZS(5)+1,MZE(5)
SSS=SS5(I,J,K)+AE5(I,J,K)*CC(I+1,J,K)+AW5(I,J,K)*CC(I-1,J,K)&
              +AN5(I,J,K)*CC(I,J+1,K)+AS5(I,J,K)*CC(I,J-1,K)
&
GAMA(K)= -AT5(I,J,K-1)/BETA
BETA=
        AP5(I,J,K)+AB5(I,J,K)*GAMA(K)
330 CC(I,J,K)=(SSS+AB5(I,J,K)*CC(I,J,K-1))/BETA
DO 340 K=MZE(5)-1,MZS(5),-1
     CC(I,J,K)=CC(I,J,K)-GAMA(K+1)*CC(I,J,K+1)
340
300
     CONTINUE
I_____
999 CONTINUE
IIST=MXS(5)
JJST=MYS(5)
KKST=MZS(5)
IIEND=MXE(5)
JJEND=MYE(5)
KKEND=MZE(5)
CALL RELOAD
IF (TASKID.NE.0) THEN
CALL
```

MPI_SEND(CC(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECI SION,0,TASKID,MPI_COMM_WORLD,IERR) ENDIF

IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(CC(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(N T)),SIZECC(NT),MPI DOUBLE PRECISION,NT,NT,MPI COMM WORLD,STATUS,IERR) **ENDDO ENDIF** CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI BCAST(CC(1,1,1),SIZE(CC),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR) RETURN END SUBROUTINE M6PRTD(I23,IEND,JEND,KEND) **USE PARAMETERS USE M6APS USE M6WRK USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,IST=2,JST=2,KST=2 INTEGER, INTENT(IN):: 123, IEND, JEND, KEND ***** ******* DO 110 I=MXS(6),MXE(6) BE(I)=0. 110 BW(I)=0. DO 112 K=MZS(6),MZE(6) DO 112 J=MYS(6),MYE(6) DO 112 I=MXS(6),MXE(6) BE(I)=BE(I)+AE6(I,J,K)BW(I)=BW(I)+AW6(I,J,K)112 DO 114 I=MXS(6),MXE(6) 114 BX(I)=BE(I)+BW(I)DO 116 K=MZS(6),MZE(6) DO 116 I=MXS(6),MXE(6) BX(I)=BX(I)+AS6(I,MYS(6),K)+AN6(I,MYE(6),K) 116 DO 118 J=MYS(6),MYE(6) DO 118 I=MXS(6),MXE(6) 118 BX(I)=BX(I)+AB6(I,J,MZS(6))+AT6(I,J,MZE(6)) I-----DO 120 J=MYS(6),MYE(6) BN(J)=0. 120 BS(J)=0. DO 122 K=MZS(6),MZE(6) DO 122 I=MXS(6),MXE(6) DO 122 J=MYS(6),MYE(6) BN(J)=BN(J)+AN6(I,J,K)122 BS(J)=BS(J)+AS6(I,J,K) DO 124 J=MYS(6),MYE(6)

124 BY(J)=BN(J)+BS(J)DO 126 K=MZS(6),MZE(6) DO 126 J=MYS(6),MYE(6) 126 BY(J)=BY(J)+AW6(MXS(6),J,K)+AE6(MXE(6),J,K) DO 128 I=MXS(6),MXE(6) DO 128 J=MYS(6),MYE(6) 128 BY(J)=BY(J)+AB6(I,J,MZS(6))+AT6(I,J,MZE(6))I_____ IF(I23.EQ.2) RETURN DO 130 K=MZS(6),MZE(6) BT(K)=0. 130 BB(K)=0. DO 132 J=MYS(6),MYE(6) DO 132 I=MXS(6),MXE(6) DO 132 K=MZS(6),MZE(6) BT(K)=BT(K)+AT6(I,J,K)132 BB(K)=BB(K)+AB6(I,J,K)DO 134 K=MZS(6),MZE(6) 134 BZ(K)=BT(K)+BB(K) DO 136 J=MYS(6),MYE(6) DO 136 K=MZS(6),MZE(6) BZ(K)=BZ(K)+AW6(MXS(6),J,K)+AE6(MXE(6),J,K) 136 DO 138 I=MXS(6),MXE(6) DO 138 K=MZS(6),MZE(6) 138 BZ(K)=BZ(K)+AS6(I,MYS(6),K)+AN6(I,MYE(6),K) RETURN END SUBROUTINE M6VTDMA(I23,IEND,JEND,KEND) *********** **USE PARAMETERS** USE CALC1, ONLY:CC **USE M6APS USE M6WRK USE TDWK2 USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,IST=2,JST=2,KST=2,NT INTEGER, INTENT(IN):: 123, IEND, JEND, KEND REAL(KIND=8):: BETA,SSS *********** ***** DO 30 I=MXS(6),MXE(6) BLC(I)=0. 30 DO 32 I=MXS(6),MXE(6) DO 32 K=MZS(6),MZE(6) DO 32 J=MYS(6),MYE(6) 32 BLC(I)=BLC(I)+SS6(I,J,K)-AP6(I,J,K)*CC(I,J,K)& & +AE6(I,J,K)*CC(I+1,J,K)+AW6(I,J,K)*CC(I-1,J,K)& & +AN6(I,J,K)*CC(I,J+1,K)+AS6(I,J,K)*CC(I,J-1,K)& & +AT6(I,J,K)*CC(I,J,K+1)+AB6(I,J,K)*CC(I,J,K-1) !

BETA= BX(MXS(6)) BCC(MXS(6))=BLC(MXS(6))/BETA DO 34 I=MXS(6)+1,MXE(6) GAMA(I)= -BE(I-1)/BETA BETA= BX(I)+BW(I)*GAMA(I) BCC(I)=(BLC(I)+BW(I)*BCC(I-1))/BETA 34 DO 36 I=MXE(6)-1,MXS(6),-1 36 BCC(I)=BCC(I)-GAMA(I+1)*BCC(I+1) DO 38 I=MXS(6),MXE(6) DO 38 K=MZS(6),MZE(6) DO 38 J=MYS(6),MYE(6) 38 CC(I,J,K)=CC(I,J,K)+BCC(I)I____ DO 40 J=MYS(6),MYE(6) 40 BLC(J)=0. DO 42 J=MYS(6),MYE(6) DO 42 K=MZS(6),MZE(6) DO 42 I=MXS(6),MXE(6) 42 BLC(J)=BLC(J)+SS6(I,J,K)-AP6(I,J,K)*CC(I,J,K)& & +AE6(I,J,K)*CC(I+1,J,K)+AW6(I,J,K)*CC(I-1,J,K)& & +AN6(I,J,K)*CC(I,J+1,K)+AS6(I,J,K)*CC(I,J-1,K)& & +AT6(I,J,K)*CC(I,J,K+1)+AB6(I,J,K)*CC(I,J,K-1) BETA= BY(MYS(6)) BCC(MYS(6))=BLC(MYS(6))/BETA DO 43 J=MYS(6)+1,MYE(6) GAMA(J) =-BN(J-1)/BETA BETA= BY(J)+BS(J)*GAMA(J) 43 BCC(J)=(BLC(J)+BS(J)*BCC(J-1))/BETA DO 44 J=MYE(6)-1,MYS(6),-1 BCC(J)=BCC(J)-GAMA(J+1)*BCC(J+1) 44 DO 48 J=MYS(6),MYE(6) DO 48 K=MZS(6),MZE(6) DO 48 I=MXS(6).MXE(6) CC(I,J,K)=CC(I,J,K)+BCC(J)48 I_____ IF(I23.EQ.2) GOTO 59 DO 50 K=MZS(6),MZE(6) BLC(K)=0. 50 DO 52 K=MZS(6),MZE(6) DO 52 J=MYS(6),MYE(6) DO 52 I=MXS(6),MXE(6) BLC(K)=BLC(K)+SS6(I,J,K)-AP6(I,J,K)*CC(I,J,K)& 52 & +AE6(I,J,K)*CC(I+1,J,K)+AW6(I,J,K)*CC(I-1,J,K)& & +AN6(I,J,K)*CC(I,J+1,K)+AS6(I,J,K)*CC(I,J-1,K)& & +AT6(I,J,K)*CC(I,J,K+1)+AB6(I,J,K)*CC(I,J,K-1) BZ(MZS(6)) BETA= BCC(MZS(6))=BLC(MZS(6))/BETA DO 54 K=MZS(6)+1,MZE(6) GAMA(K)= -BT(K-1)/BETA

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BETA=
         BZ(K)+BB(K)*GAMA(K)
54
     BCC(K)=(BLC(K)+BB(K)*BCC(K-1))/BETA
DO 56 K=MZE(6)-1.MZS(6).-1
56
     BCC(K)=BCC(K)-GAMA(K+1)*BCC(K+1)
DO 58 K=MZS(6),MZE(6)
DO 58 J=MYS(6),MYE(6)
DO 58 I=MXS(6),MXE(6)
58
   CC(I,J,K)=CC(I,J,K)+BCC(K)
                                *****
*********
59
     DO 999 NT=1,2
                   *****
**************
DO 100 K=MZS(6),MZE(6)
DO 100 J=MYS(6),MYE(6)
I=MXS(6)
SSS=SS6(I,J,K)+AN6(I,J,K)*CC(I,J+1,K)+AS6(I,J,K)*CC(I,J-1,K)&
&
             +AT6(I,J,K)*CC(I,J,K+1)+AB6(I,J,K)*CC(I,J,K-1)
BETA=AP6(I,J,K)
CC(I,J,K)=SSS/BETA
DO 130 I=MXS(6)+1,MXE(6)
SSS=SS6(I,J,K)+AN6(I,J,K)*CC(I,J+1,K)+AS6(I,J,K)*CC(I,J-1,K)&
&
             +AT6(I,J,K)*CC(I,J,K+1)+AB6(I,J,K)*CC(I,J,K-1)
GAMA(I)=
             -AE6(I-1,J,K)/BETA
BETA=AP6(I,J,K)+AW6(I,J,K)*GAMA(I)
130
     CC(I,J,K)=(SSS+AW6(I,J,K)*CC(I-1,J,K))/BETA
DO 140 I=MXE(6)-1,MXS(6),-1
140
     CC(I,J,K)=CC(I,J,K)-GAMA(I+1)*CC(I+1,J,K)
100
     CONTINUE
I_____
DO 200 K=MZS(6),MZE(6)
DO 200 I=MXS(6),MXE(6)
J=MYS(6)
SSS=SS6(I,J,K)+AE6(I,J,K)*CC(I+1,J,K)+AW6(I,J,K)*CC(I-1,J,K)&
&
             +AT6(I,J,K)*CC(I,J,K+1)+AB6(I,J,K)*CC(I,J,K-1)
BETA=AP6(I,J,K)
CC(I,J,K)=SSS/BETA
DO 230 J=MYS(6)+1,MYE(6)
SSS=SS6(I,J,K)+AE6(I,J,K)*CC(I+1,J,K)+AW6(I,J,K)*CC(I-1,J,K)&
&
             +AT6(I,J,K)*CC(I,J,K+1)+AB6(I,J,K)*CC(I,J,K-1)
GAMA(J)=
              -AN6(I,J-1,K)/BETA
BETA=AP6(I,J,K)+AS6(I,J,K)*GAMA(J)
     CC(I,J,K)=(SSS+AS6(I,J,K)*CC(I,J-1,K))/BETA
230
DO 240 J=MYE(6)-1,MYS(6),-1
240 CC(I,J,K)=CC(I,J,K)-GAMA(J+1)*CC(I,J+1,K)
200 CONTINUE
l_____
IF(I23.EQ.2) GOTO 999
DO 300 J=MYS(6),MYE(6)
DO 300 I=MXS(6),MXE(6)
```

K=MZS(6) SSS=SS6(I,J,K)+AE6(I,J,K)*CC(I+1,J,K)+AW6(I,J,K)*CC(I-1,J,K)& & +AN6(I,J,K)*CC(I,J+1,K)+AS6(I,J,K)*CC(I,J-1,K) BETA=AP6(I,J,K) CC(I,J,K)=SSS/BETA DO 330 K=MZS(6)+1,MZE(6) SSS=SS6(I,J,K)+AE6(I,J,K)*CC(I+1,J,K)+AW6(I,J,K)*CC(I-1,J,K)& & +AN6(I,J,K)*CC(I,J+1,K)+AS6(I,J,K)*CC(I,J-1,K) GAMA(K)= -AT6(I,J,K-1)/BETA BETA= AP6(I,J,K)+AB6(I,J,K)*GAMA(K)330 CC(I,J,K)=(SSS+AB6(I,J,K)*CC(I,J,K-1))/BETA DO 340 K=MZE(6)-1,MZS(6),-1 340 CC(I,J,K)=CC(I,J,K)-GAMA(K+1)*CC(I,J,K+1) 300 CONTINUE I_____ 999 CONTINUE IIST=MXS(6) JJST=MYS(6) KKST=MZS(6) IIEND=MXE(6) JJEND=MYE(6) KKEND=MZE(6) CALL RELOAD IF (TASKID.NE.0) THEN CALL MPI_SEND(CC(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECI SION,0,TASKID,MPI_COMM_WORLD,IERR) **ENDIF** IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(CC(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(N T)),SIZECC(NT),MPI DOUBLE PRECISION,NT,NT,MPI COMM WORLD,STATUS,IERR) ENDDO ENDIF CALL MPI_BARRIER(MPI_COMM_WORLD,IERR) CALL MPI_BCAST(CC(1,1,1),SIZE(CC),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR) RETURN END SUBROUTINE MU GEAP **USE PARAMETERS USE IGRID**

USE MUGRD USE APANS USE AEANS USE M2APS USE M3APS **USE M4APS USE M5APS USE M6APS USE MPIVAR** IMPLICIT NONE INTEGER :: L,I,J,K,MZNI,NT ***** ***** MZNI=2 ! L=2 IF(I23 .EQ. 3) MZNI=MZ(L) DO K=MZS(L),MZE(L) DO J=MYS(L),MYE(L) DO I=MXS(L),MXE(L) AW2(I,J,K)=0.5*(AW(2*I-2,2*J-1,2*K-2)+AW(2*I-2,2*J-2,2*K-2)+AW(2*I-2,2*J-1,2*K-1)+AW(2*I-2,2*J-2,2*K-2)+AW(2*I-2,2*J-2,2*K-2)+AW(2*I-2,2*J-2,2*K-2)+AW(2*I-2,2*J-2,2*K-2)+AW(2*I-2,2*J-2,2*K-2)+AW(2*I-2,2*J-2,2*K-2)+AW(2*I-K-1)) AE2(I,J,K)=0.5*(AE(2*I-1,2*J-1,2*K-2)+AE(2*I-1,2*J-2,2*K-2)+AE(2*I-1,2*J-1,2*K-1)+AE(2*I-1,2*J-2,2*K-2)+AE(2*I-1,2*K-2)+AE(2*I-1,2*K-2)+AE(2*I-2,2*K-2)+AE(2*I-1)) AS2(I,J,K)=0.5*(AS(2*I-1,2*J-2,2*K-2)+AS(2*I-2,2*J-2,2*K-2)+AS(2*I-1,2*J-2,2*K-1)+AS(2*I-2,2*J-2,2*K-2)+AS(2*I-2,2*L-2)+AS(2*I-2)+A 1)) AN2(I,J,K)=0.5*(AN(2*I-1,2*J-1,2*K-2)+AN(2*I-2,2*J-1,2*K-2)+AN(2*I-1,2*J-1,2*K-1)+AN(2*I-2,2*J-1,2*K-2)+AN(2*I-2,2*K-2)+AN(2*I-1)) AT2(I,J,K)=0.5*(AT(2*I-1,2*J-2,2*K-1)+AT(2*I-2,2*J-2,2*K-1)+AT(2*I-1,2*J-1,2*K-1)+AT(2*I-2,2*J-1,2*K-1))) AB2(I,J,K)=0.5*(AB(2*I-1,2*J-2,2*K-2)+AB(2*I-2,2*J-2,2*K-2)+AB(2*I-1,2*J-1,2*K-2)+AB(2*I-2,2*J-1,2*K-2)+AB(2*I-2,2*J-1,2*K-2)+AB(2*I-2,2*J-1,2*K-2)+AB(2*I-2,2*J-2,2*K-2)+AB(2*I-2,2*K-2)+A 2)) ENDDO **ENDDO ENDDO** DO K= MZS(L), MZE(L) !2, MZ(L)DO J = MYS(L), MYE(L) !2, MY(L)DO I = MXS(L), MXE(L) !2, MX(L)AP2(I,J,K)=AE2(I,J,K)+AN2(I,J,K)+AT2(I,J,K)+AW2(I,J,K)+AS2(I,J,K)+AB2(I,J,K) **ENDDO ENDDO ENDDO** I IF(MULT .EQ. 2) RETURN 1_ L=3 IF(I23 .EQ. 3) MZNI=MZ(L) DO K=MZS(L),MZE(L) DO J=MYS(L),MYE(L) DO I=MXS(L),MXE(L) AW3(I,J,K)=0.5*(AW2(2*I-2,2*J-1,2*K-2)+AW2(2*I-2,2*J-2,2*K-2)+AW2(2*I-2,2*J-1,2*K-1)+AW2(2*I-2,2* J-2,2*K-1))

AE3(I,J,K)=0.5*(AE2(2*I-1,2*J-1,2*K-2)+AE2(2*I-1,2*J-2,2*K-2)+AE2(2*I-1,2*J-1,2*K-1)+AE2(2*I-1,2*J-2,2*K-2)+AE2(2*I-1,2*J-2,2*K-2)+AE2(2*I-1,2*J-2,2*K-2)+AE2(2*I-1,2*J-2,2*K-2)+AE2(2*I-1,2*J-2,2*K-2)+AE2(2*I-1,2*J-2,2*K-2)+AE2(2*I-1,2*J-2,2*K-2)+AE2(2*I-1,2*J-2,2*K-2)+AE2(2*I-1,2*J-2,2*K-2)+AE2(2*I-1,2*J-2,2*K-2)+AE2(2*I-1,2*J-2,2*K-2)+AE2(2*I-1,2*J-2,2*K-2)+AE2(2*I-1,2*J-2,2*K-2)+AE2(2*I-1,2*J-2,2*K-2)+AE2(2*I-1,2*J-2,2*K-2)+AE2(2*I-1,2*J-2,2*K-2)+AE2(2*I-1,2*J-2,2*K-2)+AE2(2*I-1,2*J-2,2*K-2)+AE2(2*I-1,2*Z-2)+AE2(2*I-1,2*Z 2*K-1)) AS3(I,J,K)=0.5*(AS2(2*I-1,2*J-2,2*K-2)+AS2(2*I-2,2*J-2,2*K-2)+AS2(2*I-1,2*J-2,2*K-1)+AS2(2*I-2,2*J-2,2*K-2)+AS2(2*I-2,2*L-2)+AS2(2*I-2)+AS2 2*K-1)) AN3(I,J,K)=0.5*(AN2(2*I-1,2*J-1,2*K-2)+AN2(2*I-2,2*J-1,2*K-2)+AN2(2*I-1,2*J-1,2*K-1)+AN2(2*I-2,2*J-1 ,2*K-1)) AT3(I,J,K)=0.5*(AT2(2*I-1,2*J-2,2*K-1)+AT2(2*I-2,2*J-2,2*K-1)+AT2(2*I-1,2*J-1,2*K-1)+AT2(2*I-2,2*J-1, 2*K-1)) AB3(I,J,K)=0.5*(AB2(2*I-1,2*J-2,2*K-2)+AB2(2*I-2,2*J-2,2*K-2)+AB2(2*I-1,2*J-1,2*K-2)+AB2(2*I-2,2*J-1, 2*K-2)) ENDDO **ENDDO ENDDO** DO K=MZS(L),MZE(L) DO J=MYS(L),MYE(L) DO I=MXS(L),MXE(L) AP3(I,J,K)=AE3(I,J,K)+AN3(I,J,K)+AT3(I,J,K)+AW3(I,J,K)+AS3(I,J,K)+AB3(I,J,K) **ENDDO ENDDO** ENDDO IF(MULT .EQ. 3) RETURN 1_-L=4IF(I23 .EQ. 3) MZNI=MZ(L) DO K=MZS(L),MZE(L) DO J=MYS(L),MYE(L) DO I=MXS(L),MXE(L) AW4(I,J,K)=0.5*(AW3(2*I-2,2*J-1,2*K-2)+AW3(2*I-2,2*J-2,2*K-2)+AW3(2*I-2,2*J-1,2*K-1)+AW3(2*I-2,2* J-2,2*K-1)) AE4(I,J,K)=0.5*(AE3(2*I-1,2*J-1,2*K-2)+AE3(2*I-1,2*J-2,2*K-2)+AE3(2*I-1,2*J-1,2*K-1)+AE3(2*I-1,2*J-2,2*K-2)+AE3(2*I-1,2*J-2,2*K-2)+AE3(2*I-1,2*J-2,2*K-2)+AE3(2*I-1,2*J-2,2*K-2)+AE3(2*I-1,2*J-2,2*K-2)+AE3(2*I-1,2*J-2,2*K-2)+AE3(2*I-1,2*J-2,2*K-2)+AE3(2*I-1,2*J-2,2*K-2)+AE3(2*I-1,2*J-2,2*K-2)+AE3(2*I-1,2*J-2,2*K-2)+AE3(2*I-1,2*J-2,2*K-2)+AE3(2*I-1,2*J-2,2*K-2)+AE3(2*I-1,2*J-2,2*K-2)+AE3(2*I-1,2*J-2,2*K-2)+AE3(2*I-1,2*J-2,2*K-2)+AE3(2*I-1,2*J-2,2*K-2)+AE3(2*I-1,2*J-2,2*K-2)+AE3(2*I-1,2*J-2,2*K-2)+AE3(2*I-1,2*Z-2)+AE3(2*I-1,2*Z-2)+AE3(2*Z-2) 2*K-1)) AS4(I,J,K)=0.5*(AS3(2*I-1,2*J-2,2*K-2)+AS3(2*I-2,2*J-2,2*K-2)+AS3(2*I-1,2*J-2,2*K-1)+AS3(2*I-2,2*J-2, 2*K-1)) AN4(I,J,K)=0.5*(AN3(2*I-1,2*J-1,2*K-2)+AN3(2*I-2,2*J-1,2*K-2)+AN3(2*I-1,2*J-1,2*K-1)+AN3(2*I-2,2*J-1 ,2*K-1)) AT4(I,J,K)=0.5*(AT3(2*I-1,2*J-2,2*K-1)+AT3(2*I-2,2*J-2,2*K-1)+AT3(2*I-1,2*J-1,2*K-1)+AT3(2*I-2,2*J-1, 2*K-1)) AB4(I,J,K)=0.5*(AB3(2*I-1,2*J-2,2*K-2)+AB3(2*I-2,2*J-2,2*K-2)+AB3(2*I-1,2*J-1,2*K-2)+AB3(2*I-2,2*J-1, 2*K-2)) **ENDDO ENDDO** ENDDO DO K=MZS(L),MZE(L) DO J=MYS(L),MYE(L) DO I=MXS(L),MXE(L) AP4(I,J,K)=AE4(I,J,K)+AN4(I,J,K)+AT4(I,J,K)+AW4(I,J,K)+AS4(I,J,K)+AB4(I,J,K) ENDDO **ENDDO ENDDO** !
IF(MULT .EQ. 4) RETURN

I----

L=5 IF(I23 .EQ. 3) MZNI=MZ(L) DO K=MZS(L),MZE(L) DO J=MYS(L),MYE(L) DO I=MXS(L),MXE(L) AW5(I,J,K)=0.5*(AW4(2*I-2,2*J-1,2*K-2)+AW4(2*I-2,2*J-2,2*K-2)+AW4(2*I-2,2*J-1,2*K-1)+AW4(2*I-2,2* J-2.2*K-1)) AE5(I,J,K)=0.5*(AE4(2*I-1,2*J-1,2*K-2)+AE4(2*I-1,2*J-2,2*K-2)+AE4(2*I-1,2*J-1,2*K-1)+AE4(2*I-1,2*J-2,2*K-2)+AE4(2*I-1,2*J-2,2*K-2)+AE4(2*I-1,2*J-2,2*K-2)+AE4(2*I-1,2*J-2,2*K-2)+AE4(2*I-1,2*J-2,2*K-2)+AE4(2*I-1,2*J-2,2*K-2)+AE4(2*I-1,2*J-2,2*K-2)+AE4(2*I-1,2*J-2,2*K-2)+AE4(2*I-1,2*J-2,2*K-2)+AE4(2*I-1,2*J-2,2*K-2)+AE4(2*I-1,2*J-2,2*K-2)+AE4(2*I-1,2*J-2,2*K-2)+AE4(2*I-1,2*J-2,2*K-2)+AE4(2*I-1,2*J-2,2*K-2)+AE4(2*I-1,2*J-2,2*K-2)+AE4(2*I-1,2*J-2,2*K-2)+AE4(2*I-1,2*J-2,2*K-2)+AE4(2*I-1,2*J-2,2*K-2)+AE4(2*I-1,2*Z-2)+AE4(2*I-1,2*Z 2*K-1)) AS5(I,J,K)=0.5*(AS4(2*I-1,2*J-2,2*K-2)+AS4(2*I-2,2*J-2,2*K-2)+AS4(2*I-1,2*J-2,2*K-1)+AS4(2*I-2,2*J-2,2*K-2)+AS4(2*I-2,2*J-2,2*J-2,2*K-2)+AS4(2*I-2,2*J-2, 2*K-1)) AN5(I,J,K)=0.5*(AN4(2*I-1,2*J-1,2*K-2)+AN4(2*I-2,2*J-1,2*K-2)+AN4(2*I-1,2*J-1,2*K-1)+AN4(2*I-2,2*J-1 ,2*K-1)) AT5(I,J,K)=0.5*(AT4(2*I-1,2*J-2,2*K-1)+AT4(2*I-2,2*J-2,2*K-1)+AT4(2*I-1,2*J-1,2*K-1)+AT4(2*I-2,2*J-1, 2*K-1)) AB5(I,J,K)=0.5*(AB4(2*I-1,2*J-2,2*K-2)+AB4(2*I-2,2*J-2,2*K-2)+AB4(2*I-1,2*J-1,2*K-2)+AB4(2*I-2,2*J-1, 2*K-2)) ENDDO ENDDO **ENDDO** T DO K=MZS(L),MZE(L) DO J=MYS(L),MYE(L) DO I=MXS(L),MXE(L) AP5(I,J,K)=AE5(I,J,K)+AN5(I,J,K)+AT5(I,J,K)+AW5(I,J,K)+AS5(I,J,K)+AB5(I,J,K) ENDDO **ENDDO ENDDO** IF(MULT .EQ. 5) RETURN I___ L=6 IF(I23 .EQ. 3) MZNI=MZ(L) DO K=MZS(L).MZE(L) DO J=MYS(L),MYE(L) DO I=MXS(L),MXE(L) AW6(I,J,K)=0.5*(AW5(2*I-2,2*J-1,2*K-2)+AW5(2*I-2,2*J-2,2*K-2)+AW5(2*I-2,2*J-1,2*K-1)+AW5(2*I-2,2* J-2,2*K-1)) AE6(I,J,K)=0.5*(AE5(2*I-1,2*J-1,2*K-2)+AE5(2*I-1,2*J-2,2*K-2)+AE5(2*I-1,2*J-1,2*K-1)+AE5(2*I-1,2*J-2,2*K-2)+AE5(2*I-1,2*J-2,2*K-2)+AE5(2*I-1,2*J-2,2*K-2)+AE5(2*I-1,2*J-2,2*K-2)+AE5(2*I-1,2*J-2,2*K-2)+AE5(2*I-1,2*J-2,2*K-2)+AE5(2*I-1,2*J-2,2*K-2)+AE5(2*I-1,2*J-2,2*K-2)+AE5(2*I-1,2*J-2,2*K-2)+AE5(2*I-1,2*J-2,2*K-2)+AE5(2*I-1,2*J-2,2*K-2)+AE5(2*I-1,2*J-2,2*K-2)+AE5(2*I-1,2*J-2,2*K-2)+AE5(2*I-1,2*J-2,2*K-2)+AE5(2*I-1,2*J-2,2*K-2)+AE5(2*I-1,2*J-2,2*K-2)+AE5(2*I-1,2*J-2,2*K-2)+AE5(2*I-1,2*J-2,2*K-2)+AE5(2*I-1,2*Z-2)+AE5(2*I-1,2*Z-2,2*K-2)+AE5(2*I-1,2*Z-2,2*K-2)+AE5(2*I-1,2*Z-2,2*K-2)+AE5(2*I-1,2*Z-2,2*K-2)+AE5(2*I-1,2*Z-2,2*K-2)+AE5(2*I-1,2*Z-2)+ 2*K-1)) AS6(I,J,K)=0.5*(AS5(2*I-1,2*J-2,2*K-2)+AS5(2*I-2,2*J-2,2*K-2)+AS5(2*I-1,2*J-2,2*K-1)+AS5(2*I-2,2*J-2, 2*K-1)) AN6(I,J,K)=0.5*(AN5(2*I-1,2*J-1,2*K-2)+AN5(2*I-2,2*J-1,2*K-2)+AN5(2*I-1,2*J-1,2*K-1)+AN5(2*I-2,2*J-1 ,2*K-1)) AT6(I,J,K)=0.5*(AT5(2*I-1.2*J-2.2*K-1)+AT5(2*I-2.2*J-2.2*K-1)+AT5(2*I-1.2*J-1.2*K-1)+AT5(2*I-2.2*J-1, 2*K-1)) AB6(I,J,K)=0.5*(AB5(2*I-1,2*J-2,2*K-2)+AB5(2*I-2,2*J-2,2*K-2)+AB5(2*I-1,2*J-1,2*K-2)+AB5(2*I-2,2*J-1, 2*K-2)) ENDDO **ENDDO** ENDDO

ļ DO K=MZS(L),MZE(L) DO J=MYS(L),MYE(L) DO I=MXS(L),MXE(L) AP6(I,J,K)=AE6(I,J,K)+AN6(I,J,K)+AT6(I,J,K)+AW6(I,J,K)+AS6(I,J,K)+AB6(I,J,K) ENDDO ENDDO **ENDDO** RETURN END SUBROUTINE MU_GESS **USE PARAMETERS USE IGRID USE MUGRD** USE CALC1 **USE M2APS USE M3APS USE M4APS USE M5APS USE M6APS USE MPIVAR** IMPLICIT NONE INTEGER :: L,I,J,K ****** ****** L=2 DO 120 K=2,MZ(L) DO 120 J=2,MY(L) DO 120 I=2,MX(L) 120 SS2(I,J,K)=SS(2*I-1,2*J-1,2*K-1)+SS(2*I-1,2*J-2,2*K-1)& & +SS(2*I-2,2*J-1,2*K-1)+SS(2*I-2,2*J-2,2*K-1)& & +SS(2*I-1,2*J-1,2*K-2)+SS(2*I-1,2*J-2,2*K-2)& & +SS(2*I-2,2*J-1,2*K-2)+SS(2*I-2,2*J-2,2*K-2) IF(MULT .EQ. 2) RETURN ! L=3 DO 130 K=2,MZ(L) DO 130 J=2,MY(L) DO 130 I=2,MX(L) 130 SS3(I,J,K)=SS2(2*I-1,2*J-1,2*K-1)+SS2(2*I-1,2*J-2,2*K-1)& & +SS2(2*I-2,2*J-1,2*K-1)+SS2(2*I-2,2*J-2,2*K-1)& & +SS2(2*I-1,2*J-1,2*K-2)+SS2(2*I-1,2*J-2,2*K-2)& & +SS2(2*I-2,2*J-1,2*K-2)+SS2(2*I-2,2*J-2,2*K-2) IF(MULT .EQ. 3) RETURN ! L=4DO 140 K=2,MZ(L) DO 140 J=2,MY(L)

```
DO 140 I=2,MX(L)
140
     SS4(I,J,K)=SS3(2*I-1,2*J-1,2*K-1)+SS3(2*I-1,2*J-2,2*K-1)&
&
          +SS3(2*I-2,2*J-1,2*K-1)+SS3(2*I-2,2*J-2,2*K-1)&
&
          +SS3(2*I-1,2*J-1,2*K-2)+SS3(2*I-1,2*J-2,2*K-2)&
&
          +SS3(2*I-2,2*J-1,2*K-2)+SS3(2*I-2,2*J-2,2*K-2)
IF(MULT .EQ. 4) RETURN
L=5
DO 150 K=2,MZ(L)
DO 150 J=2,MY(L)
DO 150 I=2,MX(L)
     SS5(I,J,K)=SS4(2*I-1,2*J-1,2*K-1)+SS4(2*I-1,2*J-2,2*K-1)&
150
&
          +SS4(2*I-2,2*J-1,2*K-1)+SS4(2*I-2,2*J-2,2*K-1)&
&
          +SS4(2*I-1,2*J-1,2*K-2)+SS4(2*I-1,2*J-2,2*K-2)&
&
          +SS4(2*I-2,2*J-1,2*K-2)+SS4(2*I-2,2*J-2,2*K-2)
!
IF(MULT .EQ. 5) RETURN
L=6
DO 160 K=2,MZ(L)
DO 160 J=2,MY(L)
DO 160 I=2,MX(L)
     SS6(I,J,K)=SS5(2*I-1,2*J-1,2*K-1)+SS5(2*I-1,2*J-2,2*K-1)&
160
&
          +SS5(2*I-2,2*J-1,2*K-1)+SS5(2*I-2,2*J-2,2*K-1)&
&
          +SS5(2*I-1,2*J-1,2*K-2)+SS5(2*I-1,2*J-2,2*K-2)&
&
          +SS5(2*I-2,2*J-1,2*K-2)+SS5(2*I-2,2*J-2,2*K-2)
RETURN
END
SUBROUTINE MU_PRCC(I23,IEND,JEND,KEND,L)
USE PARAMETERS
USE CALC1
USE MPIVAR
IMPLICIT NONE
INTEGER :: I,J,K,IST=2,JST=2,KST=2,NT
INTEGER, INTENT(IN)::123,IEND,JEND,KEND,L
REAL (KIND=8), DIMENSION(ID, JD, KD):: C
                                     *****
************
DO 10 K=MZS(L),MZE(L)
DO 10 J=MYS(L),MYE(L)
DO 10 I=MXS(L),MXE(L)
10
     C(I,J,K)=CC(I,J,K)
IIST=MXS(L)
JJST=MYS(L)
KKST=MZS(L)
IIEND=MXE(L)
JJEND=MYE(L)
```

KKEND=MZE(L)

CALL RELOAD

IF (TASKID.NE.0) THEN CALL MPI_SEND(C(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECISI ON,0,TASKID,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(C(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT)) ,SIZECC(NT),MPI_DOUBLE_PRECISION,NT,NT,MPI_COMM_WORLD,STATUS,IERR) ENDDO ENDIF CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI_BCAST(C(1,1,1),SIZE(C),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR) 1__ ! DO K=MZS(L),MZE(L) DO J=MYS(L),MYE(L) IF (PIDX.EQ.0) THEN CC(2*IST-3,2*J-1,2*K-1)=0. CC(2*IST-3,2*J-2,2*K-1)=0. CC(2*IST-3,2*J-1,2*K-2)=0. CC(2*IST-3,2*J-2,2*K-2)=0. **ENDIF** IF (PIDX.EQ.PROCSX-1) THEN CC(2*IEND ,2*J-1,2*K-1)=0. CC(2*IEND ,2*J-2,2*K-1)=0. CC(2*IEND ,2*J-1,2*K-2)=0. CC(2*IEND ,2*J-2,2*K-2)=0. ENDIF **ENDDO** ENDDO ! DO K=MZS(L),MZE(L) DO I=MXS(L),MXE(L) IF (PIDY.EQ.0) THEN CC(2*I-1,2*JST-3,2*K-1)=0. CC(2*I-2,2*JST-3,2*K-1)=0. CC(2*I-1,2*JST-3,2*K-2)=0. CC(2*I-2,2*JST-3,2*K-2)=0. ENDIF I IF (PIDY.EQ.PROCSY-1) THEN

CC(2*I-1,2*JEND ,2*K-1)=0. CC(2*I-2,2*JEND,2*K-1)=0. CC(2*I-1,2*JEND ,2*K-2)=0. CC(2*I-2,2*JEND ,2*K-2)=0. ENDIF **ENDDO** ENDDO IF(I23 .EQ. 3) THEN DO J=MYS(L),MYE(L) DO I=MXS(L),MXE(L) IF (PIDZ.EQ.0) THEN CC(2*I-1,2*J-1,2*KST-3)=0. CC(2*I-2,2*J-1,2*KST-3)=0. CC(2*I-1,2*J-2,2*KST-3)=0. CC(2*I-2,2*J-2,2*KST-3)=0. ENDIF IF (PIDZ.EQ.PROCSZ-1) THEN CC(2*I-1,2*J-1,2*KEND)=0. CC(2*I-2,2*J-1,2*KEND)=0. CC(2*I-1,2*J-2,2*KEND)=0. CC(2*I-2,2*J-2,2*KEND)=0. ENDIF **ENDDO** ENDDO ENDIF DO 100 K= KST, KEND DO 100 J= JST, JEND DO 100 I= IST, IEND CC(2*I-1,2*J-1,2*K-1)=C(I,J,K) CC(2*I-2,2*J-1,2*K-1)=C(I,J,K)CC(2*I-1,2*J-2,2*K-1)=C(I,J,K)CC(2*I-2,2*J-2,2*K-1)=C(I,J,K)CC(2*I-1,2*J-1,2*K-2)=C(I,J,K) CC(2*I-2,2*J-1,2*K-2)=C(I,J,K) CC(2*I-1,2*J-2,2*K-2)=C(I,J,K) 100 CC(2*I-2,2*J-2,2*K-2)=C(I,J,K) !-----IIST =MXS(L) JJST =MYS(L)

KKST =MZS(L) IIEND=MXE(L) JJEND=MYE(L) KKEND=MZE(L) CALL RELOAD IF (TASKID.NE.0) THEN CALL MPI_SEND(CC(MXS(L):MXE(L),MYS(L):MYE(L),MZS(L):MZE(L)),SPANX*SPANY*SPANZ,MPI_DOUBL E_PRECISION,0,TASKID,MPI_COMM_WORLD,IERR) ENDIF

IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(CC(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(N T)),SIZECC(NT),MPI_DOUBLE_PRECISION,NT,NT,MPI_COMM_WORLD,STATUS,IERR) ENDDO ENDIF

CALL MPI_BARRIER(MPI_COMM_WORLD,IERR) CALL MPI_BCAST(CC(1,1,1),SIZE(CC),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR) ENDIF !------

RETURN

END

SUBROUTINE N GET **USE PARAMETERS** USE ICHOS **USE PROPS USE IGRID USE GRID1 USE GRIDB USE LEVFN USE FNXYZ USE APANS USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,NT REAL (KIND=8) :: DET,FX1,FY1,FZZ1 ****** *********** CALL FUVW GET

DO 100 K=KKST,KKEND DO 100 J=JJST,JJEND DO 100 I=IIST,IIEND IF(I.EQ.1) THEN FX1=(F(I+1,J,K)-F(I,J,K))/XD(I+1) ELSEIF(I.EQ.NI) THEN FX1=(F(I,J,K)-F(I-1,J,K))/XD(I) ELSE FX1=(FU(I+1,J,K)-FU(I,J,K))/XC(I) ENDIF IF(J.EQ.1) THEN FY1=(F(I,J+1,K)-F(I,J,K))/YD(J+1)ELSEIF(J.EQ.NJ) THEN FY1=(F(I,J,K)-F(I,J-1,K))/YD(J)ELSE FY1=(FV(I,J+1,K)-FV(I,J,K))/YC(J)ENDIF IF(I23.EQ.2) GOTO 105 IF(K.EQ.1) THEN FZZ1=(F(I,J,K+1)-F(I,J,K))/ZD(K+1)ELSEIF(K.EQ.NK) THEN FZZ1=(F(I,J,K)-F(I,J,K-1))/ZD(K)ELSE FZZ1=(FW(I,J,K+1)-FW(I,J,K))/ZC(K)ENDIF 105 DET=AMAX1(SQRT(FX1**2+FY1**2+FZZ1**2),1.E-10) FNX(I,J,K)=FX1/DET FNY(I,J,K)=FY1/DET FNZ(I,J,K)=FZZ1/DET 100 CONTINUE IF (TASKID.NE.0) THEN CALL MPI SEND(FNX(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI DOUBLE PREC ISION,0,TASKID,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1.26 CALL MPI_RECV(FNX(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(N T)),SIZECC(NT),MPI_DOUBLE_PRECISION,NT,NT,MPI_COMM_WORLD,STATUS,IERR) **ENDDO** ENDIF CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI BCAST(FNX(1,1,1),SIZE(FNX),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR) **!**----IF (TASKID.NE.0) THEN CALL MPI SEND(FNY(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI DOUBLE PREC ISION,0,TASKID,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1.26 CALL MPI_RECV(FNY(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(N T)),SIZECC(NT),MPI DOUBLE PRECISION,NT,NT,MPI COMM WORLD,STATUS,IERR) ENDDO ENDIF

CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI BCAST(FNY(1,1,1),SIZE(FNY),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR) !-----IF (TASKID.NE.0) THEN CALL MPI SEND(FNZ(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI DOUBLE PREC ISION,0,TASKID,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(FNZ(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(N T)),SIZECC(NT),MPI_DOUBLE_PRECISION,NT,NT,MPI_COMM_WORLD,STATUS,IERR) ENDDO ENDIF CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI_BCAST(FNZ(1,1,1),SIZE(FNZ),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR) RETURN END SUBROUTINE OTHERS ***** **USE PARAMETERS USE ICHOS USE PROPS USE IGRID USE GRID1** USE GRIDB **USE GRIDL USE QINTB USE LEVFN USE ROGAM** USE QMSOR USE RESLT USE APANS **USE INTXN USE INTXY USE UVTPP USE CALC1 USE MPIVAR** IMPLICIT NONE LOGICAL T_2PH,T_1PH INTEGER :: IS,I,J,K,IND INTEGER, INTENT(IN) :: IND0,I0,J0,K0 REAL (KIND=8) :: POINT REAL (KIND=8), DIMENSION(100) :: QMIC1, QMIC2, FAC ****** ******* ENTRY INTP_GET(POINT,IND0,I0,J0,K0)

POINT=0. IS=1 IF(IND0 .LT. 0) IS=-1 IND=IABS(IND0) IF(IND .EQ. 1) THEN DO 110 I=1,NIM IF(F(I,J0,K0)*F(I+1,J0,K0) .GT. 0.) GOTO 110 POINT=XP(I)-F(I,J0,K0)/(F(I+1,J0,K0)-F(I,J0,K0))*XD(I+1) IF(IS.EQ.1) GOTO 115 CONTINUE 110 CONTINUE 115 ELSEIF(IND .EQ. 2) THEN DO 120 J=1,NJM IF(F(I0,J,K0)*F(I0,J+1,K0) .GT. 0.) GOTO 120 POINT=YP(J)-F(I0,J,K0)/(F(I0,J+1,K0)-F(I0,J,K0))*YD(J+1) IF(IS.EQ.1) GOTO 125 120 CONTINUE 125 CONTINUE ELSE DO 130 K=1,NKM IF(F(I0,J0,K)*F(I0,J0,K+1) .GT. 0.) GOTO 130 POINT=ZP(K)-F(I0,J0,K)/(F(I0,J0,K+1)-F(I0,J0,K))*ZD(K+1) IF(IS.EQ.1) GOTO 135 130 CONTINUE 135 CONTINUE **ENDIF** RETURN END SUBROUTINE OTHERS SUB **USE PARAMETERS** USE ICHOS **USE PROPS USE INDMO USE IGRID USE IBNDS USE GRID1 USE GRIDB USE GRIDL** USE UVTBC **USE LVFBC USE QINTB** USE LEVFN **USE ROGAM** USE QMSOR USE RESLT

USE APANS USE INTXN USE INTXY USE UVTPP USE CALC1 **USE FUNC USE MPIVAR** IMPLICIT NONE INTEGER :: N,I,J,K,IBUB1 REAL (KIND=8) :: AR1,COSB,COTB,DDF1,DXE,DXW,DYN,DYS,QMICT,SINB,FDS,ASUM,AREA,QMIC1(100),QMIC2(100) ,FAC(100) REAL (KIND=8) :: TTE, TTN, TTS, TTW, VFG1 LOGICAL T_FW,T_FE,T_FS,T_FN,T_FB,T_FT LOGICAL T_SW,T_SE,T_SS,T_SN,T_SB,T_ST ENTRY QM_GET QMIC=0. IF(ICONT.NE.1) RETURN VFG1=VFG*HFGI/TK2 DO 100 N=1,NBUB(1) QMIC1(N)=0. 100 QMIC2(N)=0. IF(IBCW.NE.IWAL) GOTO 119 DO 110 K=2.NKM DO 110 J=2.NJM QBW(J,K)=0.QMW(J,K)=0. IF(S(2,J,K).LT.0.) GOTO 110 IBUB1=IBUB(2,J,K,1) IF(IBUB1.LT.1) GOTO 110 COSB=COSBW(J,K) DDF1=DDF(2,J,K) IF(COSB.LE.0.) GOTO 110 SINB=AMAX1(1.E-8, SQRT(1.-COSB**2)) COTB=COSB/SINB QMICT=QMIC0*COTB*TBCW FDS=(F(2,J,K)/SINB+0.5*XD(2)*COTB)/DDF1 IF(ABS(FDS).LT.1.) QBW(J,K)=QMICT*0.5*(1.+COS(PI*FDS))/DDF1 FDS=((F(2,J,K)+DDF1)/SINB+DDF1)/DDF1 IF(ABS(FDS).LT.1.) QMW(J,K)=QMICT*0.5*(1.+COS(PI*FDS))/DDF1 AR1=RU(2)*YC(J)*ZC(K) QMIC1(IBUB1)=QMIC1(IBUB1)+QBW(J,K)*AR1 QMIC2(IBUB1)=QMIC2(IBUB1)+QMW(J,K)*AR1 110 CONTINUE

DO 114 N=1,NBUB(1) QMIC=QMIC+QMIC1(N) FAC(N)=QMIC1(N)/AMAX1(1.E-8,QMIC2(N)) FAC(N)=AMIN1(FAC(N),5.) QMIC1(N)=0. 114 QMIC2(N)=0.

DO 116 K=2,NKM DO 116 J=2,NJM IBUB1=IBUB(2,J,K,1) IF(IBUB1.LT.1) GOTO 116 QMW(J,K)=FAC(IBUB1)*QMW(J,K) VM(2,J,K)=VM(2,J,K)+VFG1*QMW(J,K)*RU(2)*YC(J)*ZC(K) 116 CONTINUE

119 IF(IBCE.NE.IWAL) GOTO 129

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. 129 IF(IBCS.NE.IWAL) GOTO 139 DO 130 K=2,NKM DO 130 I=2,NIM QBS(I,K)=0. QMS(I,K)=0. IF(S(I,2,K).LT.0.) GOTO 130 IBUB1=IBUB(I,2,K,1) IF(IBUB1.LT.1) GOTO 130 COSB=COSBS(I,K) DDF1=DDF(I,2,K) IF(COSB.LE.0.) GOTO 130 SINB=AMAX1(1.E-8, SQRT(1.-COSB**2)) COTB=COSB/SINB QMICT=QMIC0*COTB*TBCS

FDS=(F(I,2,K)/SINB+0.5*YD(2)*COTB)/DDF1 IF(ABS(FDS).LT.1.) QBS(I,K)=QMICT*0.5*(1.+COS(PI*FDS))/DDF1

FDS=((F(I,2,K)+DDF1)/SINB+DDF1)/DDF1 IF(ABS(FDS).LT.1.) QMS(I,K)=QMICT*0.5*(1.+COS(PI*FDS))/DDF1

AR1=RP(I)*XC(I)*ZC(K) QMIC1(IBUB1)=QMIC1(IBUB1)+QBS(I,K)*AR1 QMIC2(IBUB1)=QMIC2(IBUB1)+QMS(I,K)*AR1 130 CONTINUE

DO 134 N=1,NBUB(1) QMIC=QMIC+QMIC1(N) FAC(N)=QMIC1(N)/AMAX1(1.E-8,QMIC2(N)) FAC(N)=AMIN1(FAC(N),5.) QMIC1(N)=0. 134 QMIC2(N)=0.

DO 136 K=2,NKM DO 136 I=2,NIM IBUB1=IBUB(I,2,K,1) IF(IBUB1.LT.1) GOTO 136 QMS(I,K)=FAC(IBUB1)*QMS(I,K) VM(I,2,K)=VM(I,2,K)+VFG1*QMS(I,K)*RP(I)*XC(I)*ZC(K) 136 CONTINUE 139 IF(IBCN.NE.IWAL) GOTO 149 149 IF(IBCB.NE.IWAL) GOTO 159 159 IF(IBCT.NE.IWAL) RETURN RETURN ENTRY QW_GET ASUM=0. QWAV=0. QMAV=0. IF(IBCW.NE.IWAL) GOTO 315 DO 310 K=2,NKM DO 310 J=2,NJM DXE=XD(2) TTE=T(2,J,K) CALL DX_TT(1,2,J,K,DXE,TTE,T_FE,T_SE) QWW(J,K)=TK2/TKP(1,J,K)*(T(1,J,K)-TTE)/DXE+QBW(J,K) AREA=RU(2)*YC(J)*ZC(K) ASUM=ASUM+AREA QMAV=QMAV+QBW(J,K)*AREA 310 QWAV=QWAV+QWW(J,K)*AREA IF(IBCE.NE.IWAL) GOTO 325 315 DO 320 K=2,NKM DO 320 J=2,NJM DXW=XD(NI) TTW=T(NIM,J,K) CALL DX TT(NI,NIM,J,K,DXW,TTW,T FW,T SW) QWE(J,K)=TK2/TKP(NI,J,K)*(T(NI,J,K)-TTW)/DXW+QBE(J,K) AREA=RU(NI)*YC(J)*ZC(K) ASUM=ASUM+AREA QMAV=QMAV+QBE(J,K)*AREA 320 QWAV=QWAV+QWE(J,K)*AREA IF(IBCS.NE.IWAL) GOTO 335 325 DO 330 K=2,NKM DO 330 I=2.NIM DYN=YD(2) TTN=T(I,2,K) CALL DY TT(I,1,2,K,DYN,TTN,T FN,T SN) $QWS(I,K) = TK2/TKP(I,1,K)*(T(I,1,\overline{K})-TT\overline{N})/DYN+QBS(I,K)$ AREA=RP(I)*XC(I)*ZC(K) ASUM=ASUM+AREA QMAV=QMAV+QBS(I,K)*AREA 330 QWAV=QWAV+QWS(I,K)*AREA IF(IBCN.NE.IWAL) GOTO 345 335

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DO 340 K=2,NKM
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DO 340 I=2,NIM DYS=YD(NJ) TTS=T(I,NJM,K) CALL DY_TT(I,NJ,NJM,K,DYS,TTS,T_FS,T_SS) QWN(I,K)=TK2/TKP(I,NJ,K)*(T(I,NJ,K)-TTS)/DYS+QBN(I,K) AREA=RP(I)*XC(I)*ZC(K) ASUM=ASUM+AREA QMAV=QMAV+QBN(I,K)*AREA 340 QWAV=QWAV+QWN(I,K)*AREA IF(IBCB.NE.IWAL) GOTO 355 345 355 IF(IBCT.NE.IWAL) GOTO 365 365 CONTINUE QWAV=QWAV/ARO QMAV=QMAV/ARO RETURN ENTRY QI GET QIAV=0. QIA1=0. IF(ABS(HFGI/TK2).LT.1.E-8) RETURN DO 410 K=2,NKM DO 410 J=2,NJM DO 410 I=2.NI IF(T_1PH(F(I,J,K),F(I-1,J,K))) GOTO 410 QIAV=QIAV+AMX(I,J,K)*RU(I)*YC(J)*ZC(K)*SIGN1(F(I,J,K)-F(I-1,J,K)) 410 CONTINUE DO 420 K=2,NKM DO 420 J=2,NJ DO 420 I=2,NIM IF(T_1PH(F(I,J,K),F(I,J-1,K))) GOTO 420 QIAV=QIAV+AMY(I,J,K)*RP(I)*XC(I)*ZC(K)*SIGN1(F(I,J,K)-F(I,J-1,K)) 420 CONTINUE IF(I23.EQ.2) GOTO 435 DO 430 K=2,NK DO 430 J=2.NJM DO 430 I=2,NIM IF(T 1PH(F(I,J,K),F(I,J,K-1))) GOTO 430 QIAV=QIAV+AMZ(I,J,K)*XC(I)*YC(J)*SIGN1(F(I,J,K)-F(I,J,K-1)) 430 CONTINUE 435 CONTINUE DO 440 K=2,NKM DO 440 J=2.NJM DO 440 I=2,NIM 440 QIA1=QIA1+VM(I,J,K)

QIAV=QIAV*TK2/HFGI+QMIC QIA1=QIA1*TK2/HFGI/VFG QIAV=QIAV/ARO QIA1=QIA1/ARO RETURN END SUBROUTINE P_GEAS **USE PARAMETERS USE ICHOS USE PROPS USE INDDT USE IGRID USE IBNDS** USE GRID1 **USE GRIDB USE GRIDL USE LEVFN** USE ULVLL **USE FFSOR USE ROGAM** USE QMSOR **USE APANS** USE AEANS USE UVTPP USE CALC1 **USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,NT REAL (KIND=8) :: HBW, HBS, HBB, FLUX1, FLUX2, FLUX3 LOGICAL T_2PH,T_1PH LOGICAL T FW, T FE, T FS, T FN, T FB, T FT LOGICAL T_SW,T_SE,T_SS,T_SN,T_SB,T_ST CALL SHRINK CALL RELOAD DO 10 K=2.NKM DO 10 J=2,NJM DO 10 I=2,NIM FLUX1=(RU(I)*U(I,J,K)-RU(I+1)*U(I+1,J,K))*YC(J)*ZC(K) FLUX2=(V(I,J,K)-V(I,J+1,K))*RP(I)*XC(I)*ZC(K) IF(I23.EQ.3) FLUX3=(W(I,J,K)-W(I,J,K+1))*XC(I)*YC(J) PSOR(I,J,K)=(VM(I,J,K)+FLUX1+FLUX2+FLUX3)/DT CONTINUE 10 !-----X-DIRECTION DO 110 K=KKST.KKEND DO 110 J=JJST,JJEND DO 110 I=IIST,IIEND HBW=1. IF(SU(I,J,K).LE.0.) HBW=1.E-8 AE(I,J,K)=HBW*RU(I+1)*YC(J)*ZC(K)/RHOU(I+1,J,K)/XD(I+1)

110 AW(I,J,K)=HBW*RU(I)*YC(J)*ZC(K)/RHOU(I,J,K)/XD(I) !-----Y-DIRECTION DO 120 K=KKST.KKEND DO 120 J=JJST,JJEND DO 120 I=IIST,IIEND HBS=1. IF(SV(I,J,K).LE.0.) HBS=1.E-8 AN(I,J,K)=HBS*RP(I)*XC(I)*ZC(K)/RHOV(I,J+1,K)/YD(J+1) 120 AS(I,J,K)=HBS*RP(I)*XC(I)*ZC(K)/RHOV(I,J,K)/YD(J) -----Y-DIRECTION !-----IF(I23.EQ.2) GOTO 135 DO 130 K=KKST,KKEND DO 130 J=JJST,JJEND DO 130 I=IIST, IIEND HBB=1. IF(SW(I,J,K).LE.0.) HBB=1.E-8 AT(I,J,K)=HBB*XC(I)*YC(J)/RHOW(I,J,K+1)/ZD(K+1) 130 AB(I,J,K)=HBB*XC(I)*YC(J)/RHOW(I,J,K)/ZD(K) 135 CONTINUE -----BC I_____ DO 210 K=KKST,KKEND DO 210 J=JJST,JJEND IF(IBCW.NE.IOUT) AW(2,J,K)=0. IF(IBCE.NE.IOUT) THEN AW(NI,J,K)=0. AE(NIM,J,K)=0.ENDIF 210 CONTINUE DO 220 K=KKST,KKEND DO 220 I=IIST,IIEND IF(IBCS.NE.IOUT) AS(I, 2,K)=0. IF(IBCN.NE.IOUT) THEN AS(I,NJ,K)=0. AN(I,NJM,K)=0.ENDIF 220 CONTINUE DO 230 J=JJST.JJEND DO 230 I=IIST,IIEND IF(IBCB.NE.IOUT) AB(I,J, 2)=0. IF(IBCT.NE.IOUT) THEN AB(I,J,NK)=0. AT(I,J,NKM)=0.ENDIF 230 CONTINUE !-----DO 300 K=KKST,KKEND DO 300 J=JJST,JJEND DO 300 I=IIST,IIEND AP(I,J,K)=AE(I,J,K)+AW(I,J,K)+AN(I,J,K)+AS(I,J,K)+AT(I,J,K)+AB(I,J,K) $300 \quad APC(I,J,K)=AP(I,J,K)$ l_____

IF (TASKID.NE.0) THEN CALL MPI_SEND(AE(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECI SION,0,TASKID,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(AE(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT)),SIZECC(NT),MPI DOUBLE PRECISION,NT,NT,MPI COMM WORLD,STATUS,IERR) ENDDO ENDIF CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI BCAST(AE(1,1,1),SIZE(AE),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR) I_____ IF (TASKID.NE.0) THEN CALL MPI_SEND(AW(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECI SION,0,TASKID,MPI COMM WORLD,IERR) **ENDIF** IF (TASKID.EQ.0) THEN DO NT=1.26 CALL MPI_RECV(AW(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(N T)),SIZECC(NT),MPI DOUBLE PRECISION,NT,NT,MPI COMM WORLD,STATUS,IERR) **ENDDO** ENDIF CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI BCAST(AW(1,1,1),SIZE(AW),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR) I___ IF (TASKID.NE.0) THEN CALL MPI_SEND(AN(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECI SION,0,TASKID,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1.26 CALL MPI_RECV(AN(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT)),SIZECC(NT),MPI DOUBLE PRECISION,NT,NT,MPI COMM WORLD,STATUS,IERR) **ENDDO** ENDIF CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI BCAST(AN(1,1,1),SIZE(AN),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR)

IF (TASKID.NE.0) THEN

I___

CALL MPI_SEND(AS(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECI SION,0,TASKID,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(AS(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT)),SIZECC(NT),MPI_DOUBLE_PRECISION,NT,NT,MPI_COMM_WORLD,STATUS,IERR) ENDDO ENDIF CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI BCAST(AS(1,1,1),SIZE(AS),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR) [-----IF (TASKID.NE.0) THEN CALL MPI SEND(AT(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI DOUBLE PRECI SION,0,TASKID,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(AT(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT)),SIZECC(NT),MPI DOUBLE PRECISION,NT,NT,MPI COMM WORLD,STATUS,IERR) ENDDO ENDIF CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI BCAST(AT(1,1,1),SIZE(AT),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR) I_____ IF (TASKID.NE.0) THEN CALL MPI_SEND(AB(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECI SION,0,TASKID,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(AB(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT)),SIZECC(NT),MPI DOUBLE PRECISION,NT,NT,MPI COMM WORLD,STATUS,IERR) **ENDDO** ENDIF CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI BCAST(AB(1,1,1),SIZE(AB),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR)

IF (TASKID.NE.0) THEN

1------

CALL MPI_SEND(AP(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECI SION,0,TASKID,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(AP(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT)),SIZECC(NT),MPI_DOUBLE_PRECISION,NT,NT,MPI_COMM_WORLD,STATUS,IERR) ENDDO ENDIF CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI_BCAST(AP(1,1,1),SIZE(AP),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR) [-----IF (TASKID.NE.0) THEN CALL MPI SEND(APC(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI DOUBLE PREC ISION,0,TASKID,MPI_COMM_WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI RECV(APC(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT)),SIZECC(NT),MPI DOUBLE PRECISION,NT,NT,MPI COMM WORLD,STATUS,IERR) ENDDO ENDIF CALL MPI_BARRIER(MPI_COMM_WORLD,IERR) CALL MPI BCAST(APC(1,1,1),SIZE(APC),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR) RETURN END SUBROUTINE PCGITER **USE PARAMETERS USE IGRID USE SPERR USE APANS USE UVTPP** USE CALC1 **USE RELXS USE WORK1** USE CGSSS **USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,ICGS=1 INTEGER, INTENT(IN) :: N, ITER REAL (KIND=8) :: BETA0=0., CC_A_FC, FCM, FFM, REL1, RELA, SSM

REAL (KIND=8) :: DUMMY,RCC_A_FC,RFC_A_FC REAL (KIND=8) :: RFCC,RFF,RFC_SS,RFCM,RFFM,RSS,RSSM INTEGER :: NT

ENTRY ITERM1(N,ITER)

CALL RELOAD IF(ICGS.EQ.0) GOTO 290 IF(ITER.EQ.0) BETA0=0. IF(ITER.NE.0) THEN CC A FC=0.

DO K= KKST,KKEND DO J= JJST,JJEND DO I= IIST,IIEND CC_A_FC=CC_A_FC+CC(I,J,K)*A_FC(I,J,K) ENDDO ENDDO ENDDO CALL MPI_ALLREDUCE(CC_A_FC,RCC_A_FC,1,MPI_DOUBLE_PRECISION,MPI_SUM,MPI_COMM_WORL D,IERR) CC_A_FC=RCC_A_FC

BETA0=-CC_A_FC/FC_A_FC ENDIF

RELX2(N)=BETA0

290 FC_SS=0.

DO K=KKST,KKEND DO J=JJST,JJEND DO I=IIST,IIEND

IF (N.EQ.1) FF(I,J,K,N)= U(I,J,K) IF (N.EQ.2) FF(I,J,K,N)= V(I,J,K) IF (N.EQ.3) FF(I,J,K,N)= W(I,J,K) IF (N.EQ.4) FF(I,J,K,N)= T(I,J,K) IF (N.EQ.5) FF(I,J,K,N)= P(I,J,K)

BS(I,J,K)=SS(I,J,K) FCC(I,J,K)=CC(I,J,K)+BETA0*FCC(I,J,K) FF(I,J,K,N)=FF(I,J,K,N)+FCC(I,J,K) FC_SS=FC_SS+FCC(I,J,K)*SS(I,J,K)

IF (N.EQ.1) U(I,J,K)= FF(I,J,K,N) IF (N.EQ.2) V(I,J,K)= FF(I,J,K,N) IF (N.EQ.3) W(I,J,K)= FF(I,J,K,N) IF (N.EQ.4) T(I,J,K)= FF(I,J,K,N) IF (N.EQ.5) P(I,J,K)= FF(I,J,K,N) ENDDO ENDDO ENDDO

CALL

MPI_ALLREDUCE(FC_SS,RFC_SS,1,MPI_DOUBLE_PRECISION,MPI_SUM,MPI_COMM_WORLD,IER R) FC_SS=RFC_SS

IF (TASKID.NE.0) THEN CALL MPI_SEND(BS(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECI SION,0,3,MPI_COMM_WORLD,IERR) ENDIF

IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(BS(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT)),SIZECC(NT),MPI_DOUBLE_PRECISION,NT,3,MPI_COMM_WORLD,STATUS,IERR) ENDDO ENDIF

CALL MPI_BCAST(BS(1,1,1),SIZE(BS),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR) CALL MPI_BARRIER(MPI_COMM_WORLD,IERR)

IF (TASKID.NE.0) THEN CALL MPI_SEND(FCC(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PREC ISION,0,3,MPI_COMM_WORLD,IERR) ENDIF

IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(FCC(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT)),SIZECC(NT),MPI_DOUBLE_PRECISION,NT,3,MPI_COMM_WORLD,STATUS,IERR) ENDDO ENDIF

CALL MPI_BCAST(FCC(1,1,1),SIZE(FCC),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR) CALL MPI_BARRIER(MPI_COMM_WORLD,IERR) ! IF (TASKID.NE.0) THEN IF (N.EQ.1) CALL MPI_SEND(U(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECISI ON,0,1,MPI_COMM_WORLD,IERR) IF (N.EQ.2) CALL MPI_SEND(V(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECISI ON,0,2,MPI_COMM_WORLD,IERR) IF (N.EQ.3) CALL MPI_SEND(W(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECISI ON,0,2,MPI_COMM_WORLD,IERR) IF (N.EQ.3) CALL MPI_SEND(W(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECISI ION,0,3,MPI_COMM_WORLD,IERR) IF (N.EQ.4) CALL MPI_SEND(T(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECISI ON,0,4,MPI COMM WORLD,IERR) IF (N.EQ.5) CALL MPI_SEND(P(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECISI ON,0,5,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26 IF (N.EQ.1) CALL MPI_RECV(U(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT)) SIZECC(NT), MPI DOUBLE PRECISION, NT, 1, MPI COMM WORLD, STATUS, IERR) IF (N.EQ.2) CALL MPI_RECV(V(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT)) ,SIZECC(NT),MPI DOUBLE PRECISION,NT,2,MPI COMM WORLD,STATUS,IERR) IF (N.EQ.3) CALL MPI_RECV(W(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT)),SIZECC(NT),MPI DOUBLE PRECISION,NT,3,MPI COMM WORLD,STATUS,IERR) IF (N.EQ.4) CALL MPI_RECV(T(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT)) ,SIZECC(NT),MPI_DOUBLE_PRECISION,NT,4,MPI_COMM_WORLD,STATUS,IERR) IF (N.EQ.5) CALL MPI_RECV(P(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT)) ,SIZECC(NT),MPI DOUBLE PRECISION,NT,5,MPI COMM WORLD,STATUS,IERR) ENDDO ENDIF CALL MPI BARRIER(MPI COMM WORLD, IERR) IF (N.EQ.1) CALL MPI BCAST(U(1,1,1),SIZE(U),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR) IF (N.EQ.2) CALL MPI_BCAST(V(1,1,1),SIZE(V),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR) IF (N.EQ.3) CALL MPI BCAST(W(1,1,1),SIZE(W),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR) IF (N.EQ.4) CALL MPI BCAST(T(1,1,1),SIZE(T),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR) IF (N.EQ.5) CALL MPI BCAST(P(1,1,1),SIZE(P),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR) RETURN ENTRY ITERM2(N, ITER) ******* FC A FC=0. DO 400 K=KKST,KKEND DO 400 J=JJST,JJEND DO 400 I=IIST.IIEND A FC(I,J,K)=BS(I,J,K)-SS(I,J,K)400 FC A FC=FC A FC+FCC(I,J,K)*A FC(I,J,K)

CALL MPI_ALLREDUCE(FC_A_FC,RFC_A_FC,1,MPI_DOUBLE_PRECISION,MPI_SUM,MPI_COMM_WORL D,IERR) FC_A_FC=RFC_A_FC FC_A_FC=SIGN(AMAX1(ABS(FC_A_FC),1.E-99),FC_A_FC)

RELA=FC_SS/FC_A_FC RELAX(N)=RELA BRELX(N)=RELAX(N)

FFM=0. FCM=0. SSM=0. RELA=RELAX(N) REL1=1.-RELA

DO 430 K=KKST,KKEND DO 430 J=JJST,JJEND DO 430 I=IIST,IIEND

IF (N.EQ.1) FF(I,J,K,N)= U(I,J,K) IF (N.EQ.2) FF(I,J,K,N)= V(I,J,K) IF (N.EQ.3) FF(I,J,K,N)= W(I,J,K) IF (N.EQ.4) FF(I,J,K,N)= T(I,J,K) IF (N.EQ.5) FF(I,J,K,N)= P(I,J,K)

 $\begin{array}{ll} \mathsf{FF}(\mathsf{I},\mathsf{J},\mathsf{K},\mathsf{N})=\mathsf{FF}(\mathsf{I},\mathsf{J},\mathsf{K},\mathsf{N})-\mathsf{REL1*FCC}(\mathsf{I},\mathsf{J},\mathsf{K})\\ \mathsf{SS}(\mathsf{I},\mathsf{J},\mathsf{K}) &= \mathsf{SS}(\mathsf{I},\mathsf{J},\mathsf{K}) &+ \mathsf{REL1*A_FC}(\mathsf{I},\mathsf{J},\mathsf{K})\\ \mathsf{SSM}=\mathsf{AMAX1}(\mathsf{SSM},\mathsf{ABS}(\mathsf{SS}(\mathsf{I},\mathsf{J},\mathsf{K})/\mathsf{AP}(\mathsf{I},\mathsf{J},\mathsf{K})))\\ \mathsf{FFM}=\mathsf{AMAX1}(\mathsf{FFM},\mathsf{ABS}(\mathsf{FF}(\mathsf{I},\mathsf{J},\mathsf{K},\mathsf{N})))\\ \mathsf{FCM}=\mathsf{AMAX1}(\mathsf{FCM},\mathsf{ABS}(\mathsf{FCC}(\mathsf{I},\mathsf{J},\mathsf{K}))) \end{array}$

IF (N.EQ.1) U(I,J,K)= FF(I,J,K,N) IF (N.EQ.2) V(I,J,K)= FF(I,J,K,N) IF (N.EQ.3) W(I,J,K)= FF(I,J,K,N) IF (N.EQ.4) T(I,J,K)= FF(I,J,K,N) IF (N.EQ.5) P(I,J,K)= FF(I,J,K,N)

430 CONTINUE

IF (TASKID.NE.0) THEN CALL MPI_SEND(SS(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECI SION,0,3,MPI_COMM_WORLD,IERR) ENDIF

```
IF (TASKID.EQ.0) THEN
DO NT=1,26
CALL
MPI_RECV(SS(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT
)),SIZECC(NT),MPI_DOUBLE_PRECISION,NT,3,MPI_COMM_WORLD,STATUS,IERR)
ENDDO
ENDIF
```

CALL MPI_BCAST(SS(1,1,1),SIZE(SS),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR) CALL MPI_BARRIER(MPI_COMM_WORLD,IERR) IF (TASKID.NE.0) THEN IF (N.EQ.1) CALL MPI_SEND(U(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECISI ON,0,1,MPI COMM WORLD,IERR) IF (N.EQ.2) CALL MPI_SEND(V(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECISI ON,0,2,MPI COMM WORLD,IERR) IF (N.EQ.3) CALL MPI_SEND(W(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECIS ION,0,3,MPI COMM WORLD,IERR) IF (N.EQ.4) CALL MPI_SEND(T(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECISI ON,0,4,MPI COMM WORLD,IERR) IF (N.EQ.5) CALL MPI_SEND(P(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECISI ON,0,5,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26 IF (N.EQ.1) CALL MPI RECV(U(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT)) ,SIZECC(NT),MPI DOUBLE PRECISION,NT,1,MPI COMM WORLD,STATUS,IERR) IF (N.EQ.2) CALL MPI RECV(V(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT)) ,SIZECC(NT),MPI DOUBLE PRECISION,NT,2,MPI COMM WORLD,STATUS,IERR) IF (N.EQ.3) CALL MPI_RECV(W(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT)),SIZECC(NT),MPI DOUBLE PRECISION,NT,3,MPI COMM WORLD,STATUS,IERR) IF (N.EQ.4) CALL MPI_RECV(T(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT)) ,SIZECC(NT),MPI DOUBLE PRECISION,NT,4,MPI COMM WORLD,STATUS,IERR) IF (N.EQ.5) CALL MPI_RECV(P(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT)) ,SIZECC(NT),MPI DOUBLE PRECISION,NT,5,MPI COMM WORLD,STATUS,IERR) ENDDO ENDIF CALL MPI_BARRIER(MPI_COMM_WORLD, IERR) IF (N.EQ.1) CALL MPI_BCAST(U(1,1,1),SIZE(U),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR) IF (N.EQ.2) CALL MPI BCAST(V(1,1,1),SIZE(V),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR) IF (N.EQ.3) CALL MPI BCAST(W(1,1,1),SIZE(W),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR) IF (N.EQ.4) CALL MPI BCAST(T(1,1,1),SIZE(T),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR) IF (N.EQ.5) CALL MPI BCAST(P(1,1,1),SIZE(P),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR)

CALL

MPI_ALLREDUCE(SSM,RSSM,1,MPI_DOUBLE_PRECISION,MPI_MAX,MPI_COMM_WORLD,IERR)

CALL MPI ALLREDUCE(FFM,RFFM,1,MPI DOUBLE PRECISION,MPI MAX,MPI COMM WORLD,IERR) CALL MPI_ALLREDUCE(FCM,RFCM,1,MPI_DOUBLE_PRECISION,MPI_MAX,MPI_COMM_WORLD,IERR) SSM=RSSM FFM=RFFM FCM=RFCM FFM=AMAX1(1.E-30,FFM) FFMAX(N)=FFM SSMAX(N)=SSM/FFM FCMAX(N)=FCM/FFM RETURN END SUBROUTINE PROJT **USE PARAMETERS USE INDDT USE IGRID USE GRID1** USE GRIDB **USE LEVFN USE ROGAM USE UVTPP USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,NT DO 110 K=2,NKM DO 110 J=2,NJM DO 110 I=2,NI IF(SU(I,J,K).LE.0.) GOTO 110 U(I,J,K)=U(I,J,K)-DT*(P(I,J,K)-P(I-1,J,K))/RHOU(I,J,K)/XD(I) 110 CONTINUE DO 120 K=2,NKM DO 120 J=2,NJ DO 120 I=2.NIM IF(SV(I,J,K).LE.0.) GOTO 120 V(I,J,K)=V(I,J,K)-DT*(P(I,J,K)-P(I,J-1,K))/RHOV(I,J,K)/YD(J) 120 CONTINUE IF(I23.EQ.2) RETURN DO 130 K=2,NK DO 130 J=2,NJM DO 130 I=2,NIM IF(SW(I,J,K).LE.0.) GOTO 130 W(I,J,K)=W(I,J,K)-DT*(P(I,J,K)-P(I,J,K-1))/RHOW(I,J,K)/ZD(K) 130 CONTINUE RETURN END

SUBROUTINE QN_EXT(IPHASE) **USE PARAMETERS USE INDMO USE IGRID USE GRID1 USE GRIDB USE GRIDL USE LEVFN** USE QMSOR **USE FNXYZ USE APANS USE AEANS USE ICHEK USE CALC1 USE IJKMK USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,N,L,INC,NN,II,JJ,KK,III,JJJ,KKK,ITER,NCHB0 INTEGER, INTENT(IN) :: IPHASE REAL (KIND=8) :: FMIN LOGICAL T 2PH,T 1PH ********* DO 1 K=K11,KNK DO 1 J=1,NJ DO 1 I=1,NI AC(I,J,K)=0. SS(I,J,K)=0. IMK(I,J,K)=0 JMK(I,J,K)=0KMK(I,J,K)=01 CONTINUE DO 2 N=1,NCHB I=IIB(N) J=JJB(N) K=KKB(N) IMK(I,J,K)=1 JMK(I,J,K)=1KMK(I,J,K)=1CONTINUE 2 ITER=0 10 ITER=ITER+1 !----- CHECK NCHB0=NCHB DO 100 N=1,NCHB0 I=IIB(N) J=JJB(N) K=KKB(N) IF(MK0(I,J,K).GE.2) GOTO 100

```
DO 110 KK=MAX(K-1,K11),MIN(K+1,KNK)
DO 110 JJ=MAX(J-1,1),MIN(J+1,NJ)
DO 110 II=MAX(I-1,1),MIN(I+1,NI)
IF(KK.EQ.K .AND. JJ.EQ.J .AND. II.EQ.I) GOTO 110
IF(MK0(II,JJ,KK).LE.2) GOTO 110
NCHB=NCHB+1
IIB(NCHB)=II
JJB(NCHB)=JJ
KKB(NCHB)=KK
MK0(II,JJ,KK)=2
110
      CONTINUE
100
      CONTINUE
!
N=0
INC=1
DO 290 L=1,2
IF(L.EQ.2) INC=-1
210 N=N+INC
IF(N.GT.NCHB .OR. N.LT.1) GOTO 290
!
I=IIB(N)
J=JJB(N)
K=KKB(N)
IF(MK0(I,J,K).LE.1) GOTO 210
CALL QN SUB(I,J,K,IPHASE)
GOTO 210
290 CONTINUE
IF(ITER.LT.10) GOTO 10
DO 300 N=1,NCHB
I=IIB(N)
J=JJB(N)
K=KKB(N)
IF(MK0(I,J,K).NE.0) GOTO 300
DO 310 KK=MAX(K-4,K11),MIN(K+4,KNK)
DO 310 JJ=MAX(J-4,1),MIN(J+4,NJ)
DO 310 II=MAX(I-4,1),MIN(I+4,NI)
IF(MK0(II,JJ,KK).LE.1) GOTO 310
9001 FORMAT(A,I6,4(I4),A,3(I2),A,4(I2))
NN=0
312
     NN=NN+1
FMIN=1.E30
DO 314 KKK=MAX(KK-NN,K11),MIN(KK+NN,KNK)
DO 314 JJJ=MAX(JJ-NN,1),MIN(JJ+NN,NJ)
DO 314 III=MAX(II-NN,1),MIN(II+NN,NI)
IF(MK0(III,JJJ,KKK).GT.1) GOTO 314
IF(ABS(F(II,JJ,KKK)-F(III,JJJ,KKK)).GT.FMIN) GOTO 314
QN(II,JJ,KK,IPHASE)=QN(III,JJJ,KKK,IPHASE)
FMIN=ABS(F(II,JJ,KK)-F(III,JJJ,KKK))
MK0(II,JJ,KK)=1
314
     CONTINUE
IF(MK0(II,JJ,KK).LE.1) GOTO 310
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IF(NN.EQ.5) THEN WRITE(I69,*) ' QN_EXT ERR', ITIME, I, J, K, II, JJ, KK STOP ENDIF **GOTO 312** 310 CONTINUE 300 CONTINUE RETURN END SUBROUTINE QN GET **USE PARAMETERS USE ICHOS USE PROPS** USE INDDT **USE IGRID USE GRID1 USE GRIDB USE GRIDL USE LEVFN USE ULVLL** USE ROGAM **USE QMSOR** USE FNXYZ USE APANS USE AEANS USE RESLT **USE ICHEK USE UVTPP** USE CALC1 USE FUNC **USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,L,L0,L9,KM1,KP1,IM1,IP1,JM1,JP1,III,JJJ,KKK REAL (KIND=8) :: DXN,DXS,DXW,DXE,DZB,DZT,DYN,DYS,DXE0,DXW0,DXN0,DXS0,DZB0,DZT0,DYN0,DYS0,DXE1,DX W1,DYN1,DYS1,DZB1,DZT1 REAL (KIND=8) :: HB0,HE0,HN0,HS0,HT0,HW0,TXP,TYP,TTB,TTE,TTN,TTP,TTS,TTW,TXE,TXW,TYN,TYS,TTT,TZB,TZP ,TZT LOGICAL T FW, T FE, T FS, T FN, T FB, T FT, T FP, T NOINTF LOGICAL T SW,T SE,T SS,T SN,T SB,T ST LOGICAL T 3W,T 3E,T 3S,T 3N,T 3B,T 3T LOGICAL T IW,T IE,T IS,T IN,T IB,T IT,T IP - ′ _ ′ -L0=1 L9=2 IF(IQ_VAP.EQ.0) L0=2 IF(IQ_LIQ.EQ.0) L9=1

DO 1000 L=L0,L9 NCHB=0 DO 100 K=K11,KNK DO 100 J=1,NJ DO 100 I=1,NI QN(I,J,K,L)=0. MK0(I,J,K)=3IF(S(I,J,K).LE.0.) GOTO 100 T_FP=(L.EQ.1 .AND. F(I,J,K).GE.0.).OR.(L.EQ.2 .AND. F(I,J,K).LE.0.) IF(IBODY.EQ.0 .AND. T FP) GOTO 100 IM1=MAX(I-1, 1) IP1=MIN(I+1,NI)JM1=MAX(J-1, 1) JP1=MIN(J+1,NJ) $T_FW=T_2PH(F(I,J,K),F(IM1,J,K))$ $T_FE=T_2PH(F(I,J,K),F(IP1,J,K))$ $T_FS=T_2PH(F(I,J,K),F(I,JM1,K))$ $T_FN=T_2PH(F(I,J,K),F(I,JP1,K))$ T NOINTF=.NOT. (T FW .OR. T FE .OR. T FS .OR. T FN) IF(I23.EQ.2 .AND. T_NOINTF) GOTO 100 IF(I23.EQ.3) THEN KM1=MAX(K-1, 1) KP1=MIN(K+1,NK) $T_FB=T_2PH(F(I,J,K),F(I,J,KM1))$ T FT=T 2PH(F(I,J,K),F(I,J,KP1))T_NOINTF=T_NOINTF .AND. (.NOT. (T_FB .OR. T_FT)) IF(T_NOINTF) GOTO 100 ENDIF $T_SW=T_2PH(S(I,J,K),S(IM1,J,K))$ $T_SE=T_2PH(S(I,J,K),S(IP1,J,K))$ T SS=T 2PH(S(I,J,K),S(I,JM1,K)) T SN=T 2PH(S(I,J,K),S(I,JP1,K))T 3W=T FW .AND. T SW T_3E=T_FE .AND. T_SE T 3S=T FS .AND. T SS T 3N=T FN .AND. T SN IF(T 3W) T FW=(F(I,J,K)/(F(I,J,K)-F(IM1,J,K))).LT.(S(I,J,K)/(S(I,J,K)-S(IM1,J,K))) IF(T 3E) T FE=(F(I,J,K)/(F(I,J,K)-F(IP1,J,K))).LT.(S(I,J,K)/(S(I,J,K)-S(IP1,J,K))) IF(T_3S) T_FS=(F(I,J,K)/(F(I,J,K)-F(I,JM1,K))).LT.(S(I,J,K)/(S(I,J,K)-S(I,JM1,K))) IF(T_3N) T_FN=(F(I,J,K)/(F(I,J,K)-F(I,JP1,K))).LT.(S(I,J,K)/(S(I,J,K)-S(I,JP1,K))) IF(T 3W) T SW=.NOT. T FW IF(T 3E) T SE=.NOT. T FE IF(T 3S) T SS=.NOT. T FS IF(T_3N) T_SN=.NOT. T_FN !

T NOINTF=.NOT. (T FW .OR. T FE .OR. T FS .OR. T FN) IF(I23.EQ.2 .AND. T NOINTF) GOTO 100 I____ IF(I23.EQ.3) THEN T SB=T 2PH(S(I,J,K),S(I,J,KM1)) $T_ST=T_2PH(S(I,J,K),S(I,J,KP1))$ T 3B=T FB .AND. T SB T_3T=T_FT .AND. T_ST IF(T_3B) T_FB=(F(I,J,K)/(F(I,J,K)-F(I,J,KM1))).LT.& & (S(I,J,K)/(S(I,J,K)-S(I,J,KM1)))IF(T_3T) T_FT=(F(I,J,K)/(F(I,J,K)-F(I,J,KP1))).LT.& & (S(I,J,K)/(S(I,J,K)-S(I,J,KP1))) IF(T_3B) T_SB=.NOT. T_FB IF(T_3T) T_ST=.NOT. T_FT T NOINTF=T NOINTF .AND. (.NOT. (T FB .OR. T FT)) IF(T NOINTF) GOTO 100 ENDIF !-----T_IW=T_3W .AND. T_FW T_IE=T_3E .AND. T_FE T IS=T 3S .AND. T FS T IN=T 3N .AND. T FN T_IP=.NOT. (T_IW .OR. T_IE .OR. T_IS .OR. T_IN) IF(I23.EQ.2 .AND. T_FP .AND. T_IP) GOTO 100 IF(I23.EQ.3) THEN T IB=T 3B .AND. T FB T IT=T 3T .AND. T FT T IP=T IP .AND. (.NOT. (T_IB .OR. T_IT)) IF(T_FP .AND. T_IP) GOTO 100 ENDIF NCHB=NCHB+1 IIB(NCHB)=I JJB(NCHB)=J KKB(NCHB)=K MKO(I,J,K)=0III=MAX(1,2)JJJ=MAX(J,2) DXW0=XD(III) DXE0=XD(IP1) DYS0=YD(JJJ) DYN0=YD(JP1) DXW=DXW0 DXE=DXE0 DYS=DYS0 DYN=DYN0 $IF(T_FW) HW0=F(I,J,K)/(F(I,J,K)-F(IM1,J,K))$

 $IF(T_FE) HE0=F(I,J,K)/(F(I,J,K)-F(IP1,J,K))$

IF(T_FS) HS0=F(I,J,K)/(F(I,J,K)-F(I,JM1,K)) IF(T_FN) HN0=F(I,J,K)/(F(I,J,K)-F(I,JP1,K))

IF(T_FW) DXW=DXW0*AMAX1(HEPS,HW0) IF(T_FE) DXE=DXE0*AMAX1(HEPS,HE0) IF(T_FS) DYS=DYS0*AMAX1(HEPS,HS0) IF(T_FN) DYN=DYN0*AMAX1(HEPS,HN0)

TXP=0.

TYP=0.

IF(T FP) THEN IF(T IW) DXW1=DXW0*AMAX1(HEPS,S(I,J,K)/(S(I,J,K)-S(IM1,J,K))) IF(T IE) DXE1=DXE0*AMAX1(HEPS,S(I,J,K)/(S(I,J,K)-S(IP1,J,K))) IF(T IS) DYS1=DYS0*AMAX1(HEPS,S(I,J,K)/(S(I,J,K)-S(I,JM1,K))) IF(T IN) DYN1=DYN0*AMAX1(HEPS,S(I,J,K)/(S(I,J,K)-S(I,JP1,K))) IF(T IW) TXW=(TINT-TWAL)/AMAX1(HEPS*DXW0,DXW1-DXW) IF(T IE) TXE=(TWAL-TINT)/AMAX1(HEPS*DXE0,DXE1-DXE) IF(T_IS) TYS=(TINT-TWAL)/AMAX1(HEPS*DYS0,DYS1-DYS) IF(T_IN) TYN=(TWAL-TINT)/AMAX1(HEPS*DYN0,DYN1-DYN) IF(T IW) TXP=TXW IF(T IE) TXP=TXE IF(T IW .AND. T IE) TXP=0.5*(TXW+TXE) IF(T IS) TYP=TYS IF(T IN) TYP=TYN IF(T IS .AND. T IN) TYP=0.5*(TYS+TYN) **GOTO 110** ENDIF

$$\label{eq:interm} \begin{split} & \mathsf{IF}(\mathsf{T_SW}) \ \mathsf{DXW} = \mathsf{DXW0}^*\mathsf{AMAX1}(\mathsf{HEPS},\mathsf{S}(\mathsf{I},\mathsf{J},\mathsf{K})/(\mathsf{S}(\mathsf{I},\mathsf{J},\mathsf{K})-\mathsf{S}(\mathsf{IM1},\mathsf{J},\mathsf{K}))) \\ & \mathsf{IF}(\mathsf{T_SE}) \ \mathsf{DXE} = \mathsf{DXE0}^*\mathsf{AMAX1}(\mathsf{HEPS},\mathsf{S}(\mathsf{I},\mathsf{J},\mathsf{K})/(\mathsf{S}(\mathsf{I},\mathsf{J},\mathsf{K})-\mathsf{S}(\mathsf{IP1},\mathsf{J},\mathsf{K}))) \\ & \mathsf{IF}(\mathsf{T_SS}) \ \mathsf{DYS} = \mathsf{DYS0}^*\mathsf{AMAX1}(\mathsf{HEPS},\mathsf{S}(\mathsf{I},\mathsf{J},\mathsf{K})/(\mathsf{S}(\mathsf{I},\mathsf{J},\mathsf{K})-\mathsf{S}(\mathsf{I},\mathsf{JM1},\mathsf{K}))) \\ & \mathsf{IF}(\mathsf{T_SN}) \ \mathsf{DYN} = \mathsf{DYN0}^*\mathsf{AMAX1}(\mathsf{HEPS},\mathsf{S}(\mathsf{I},\mathsf{J},\mathsf{K})/(\mathsf{S}(\mathsf{I},\mathsf{J},\mathsf{K})-\mathsf{S}(\mathsf{I},\mathsf{JP1},\mathsf{K}))) \end{split}$$

TTP=T(I,J,K) TTW=T(IM1,J,K) TTE=T(IP1,J,K) TTS=T(I,JM1,K) TTN=T(I,JP1,K)

IF(T_FW) TTW=TINT IF(T_FE) TTE=TINT IF(T_FS) TTS=TINT IF(T_FN) TTN=TINT

TXW=(TTP-TTW)/DXW TXE=(TTE-TTP)/DXE TYS=(TTP-TTS)/DYS TYN=(TTN-TTP)/DYN

IF(T_FW .AND. T_FE) THEN TXP=0.5*(TXW+TXE) ELSEIF(T_FW) THEN IF(I.NE.NI .AND. HW0.LT.HEPS)& & TXW=(TTE-TINT)/(DXE+DXW)*(1.-HW0/HEPS)+TXW*HW0/HEPS TXP=TXW ELSEIF(T_FE) THEN IF(I.NE.1 .AND. HE0.LT.HEPS)& TXE=(TINT-TTW)/(DXE+DXW)*(1.-HE0/HEPS)+TXE*HE0/HEPS & TXP=TXE ELSEIF(F(IM1,J,K).EQ.F(IP1,J,K)) THEN TXP=0.5*(TXW+TXE) ELSEIF(ABS(F(IM1,J,K)).LT.ABS(F(IP1,J,K))) THEN TXP=TXW ELSEIF(ABS(F(IM1,J,K)).GT.ABS(F(IP1,J,K))) THEN TXP=TXE ENDIF IF(T FS .AND. T FN) THEN TYP=0.5*(TYS+TYN) ELSEIF(T_FS) THEN IF(J.NE.NJ .AND. HS0.LT.HEPS)& & TYS=(TTN-TINT)/(DYN+DYS)*(1.-HS0/HEPS)+TYS*HS0/HEPS TYP=TYS ELSEIF(T_FN) THEN IF(J.NE.1 .AND. HN0.LT.HEPS)& TYN=(TINT-TTS)/(DYN+DYS)*(1.-HN0/HEPS)+TYN*HN0/HEPS & TYP=TYN ELSEIF(F(I,JM1,K).EQ.F(I,JP1,K)) THEN TYP=0.5*(TYS+TYN) ELSEIF(ABS(F(I,JM1,K)).LT.ABS(F(I,JP1,K))) THEN TYP=TYS ELSEIF(ABS(F(I,JM1,K)).GT.ABS(F(I,JP1,K))) THEN TYP=TYN **ENDIF** 110 QN(I,J,K,L)=TXP*FNX(I,J,K)+TYP*FNY(I,J,K)I_____ IF(I23.EQ.2) GOTO 100 KKK=MAX(K,2) DZB0=ZD(KKK) DZT0=ZD(KP1) DZB=DZB0 DZT=DZT0 IF(T FB) HB0=F(I,J,K)/(F(I,J,K)-F(I,J,KM1))IF(T FT) HT0=F(I,J,K)/(F(I,J,K)-F(I,J,KP1))IF(T FB) DZB=DZB0*AMAX1(HEPS,HB0) IF(T FT) DZT=DZT0*AMAX1(HEPS,HT0) TZP=0. IF(T FP) THEN

IF(T_IB) DZB1=DZB0*AMAX1(HEPS,S(I,J,K)/(S(I,J,K)-S(I,J,KM1)))

IF(T IT) DZT1=DZT0*AMAX1(HEPS,S(I,J,K)/(S(I,J,K)-S(I,J,KP1))) IF(T IB) TZB=(TINT-TWAL)/AMAX1(HEPS*DZB0,DZB1-DZB) IF(T_IT) TZT=(TWAL-TINT)/AMAX1(HEPS*DZT0,DZT1-DZT) IF(T IB) TZP=TZB IF(T IT) TZP=TZT IF(T_IB .AND. T_IT) TZP=0.5*(TZB+TZT) **GOTO 120** ENDIF IF(T_SB) DZB=DZB0*AMAX1(HEPS,S(I,J,K)/(S(I,J,K)-S(I,J,KM1))) IF(T ST) DZT=DZT0*AMAX1(HEPS,S(I,J,K)/(S(I,J,K)-S(I,J,KP1))) TTB=T(I,J,KM1) TTT=T(I,J,KP1) IF(T FB) TTB=TINT IF(T FT) TTT=TINT TZB=(TTP-TTB)/DZB TZT=(TTT-TTP)/DZT IF(T_FB .AND. T_FT) THEN TZP=0.5*(TZB+TZT) ELSEIF(T FB) THEN IF(K.NE.NK .AND. HB0.LT.HEPS)& TZB=(TTT-TINT)/(DZT+DZB)*(1.-HB0/HEPS)+TZB*HB0/HEPS & TZP=TZB ELSEIF(T FT) THEN IF(K.NE.1 .AND. HT0.LT.HEPS)& TZT=(TINT-TTB)/(DZT+DZB)*(1.-HT0/HEPS)+TZT*HT0/HEPS & TZP=TZT ELSEIF(F(I,J,KM1).EQ.F(I,J,KP1)) THEN TZP=0.5*(TZB+TZT) ELSEIF(ABS(F(I,J,KM1)).LT.ABS(F(I,J,KP1))) THEN TZP=TZB ELSEIF(ABS(F(I,J,KM1)).GT.ABS(F(I,J,KP1))) THEN TZP=TZT ENDIF 120 QN(I,J,K,L)=QN(I,J,K,L)+TZP*FNZ(I,J,K)100 CONTINUE CALL QN_EXT(L) 1000 CONTINUE RETURN END SUBROUTINE QN SUB(I,J,K,IPHASE) , :********************************** **USE PARAMETERS USE IGRID USE GRID1**

USE GRIDB USE LEVFN USE QMSOR USE FNXYZ USE APANS USE AEANS **USE ICHEK USE CALC1 USE IJKMK USE MPIVAR** IMPLICIT NONE INTEGER, INTENT(IN) :: I,J,K,IPHASE REAL (KIND=8) :: AX0, AC0, AY0, AZ0, FFX, FFY, FFZ LOGICAL T_2PH,T_1PH ******* ***** IF(IMK(I,J,K).EQ.1) GOTO 100 FFX=F(I,J,K)*FNX(I,J,K) IF((FFX.GE.0. .AND. I.EQ. 1) .OR.& & (FFX.LE.0. .AND. I.EQ.NI)) THEN IMK(I,J,K)=1ELSEIF(FFX.GE.0. .AND. MK0(I-1,J,K).LE.1) THEN AX0=ABS(FNX(I,J,K))/XD(I) AC(I,J,K)=AC(I,J,K)+AX0SS(I,J,K)=SS(I,J,K)+AX0*QN(I-1,J,K,IPHASE) IMK(I,J,K)=1ELSEIF(FFX.LE.0. .AND. MK0(I+1,J,K).LE.1) THEN AX0=ABS(FNX(I,J,K))/XD(I+1)AC(I,J,K)=AC(I,J,K)+AX0SS(I,J,K)=SS(I,J,K)+AX0*QN(I+1,J,K,IPHASE) IMK(I,J,K)=1ELSEIF(FFX.GE.0. .AND. F(I-1,J,K)*FNX(I-1,J,K).LE.0.) THEN IMK(I,J,K)=1ELSEIF(FFX.LE.0. .AND. F(I+1,J,K)*FNX(I+1,J,K).GE.0.) THEN IMK(I,J,K)=1**ENDIF** IF(JMK(I,J,K).EQ.1) GOTO 200 100 FFY=F(I,J,K)*FNY(I,J,K) IF((FFY.GE.0. .AND. J.EQ. 1) .OR.& & (FFY.LE.0. .AND. J.EQ.NJ)) THEN JMK(I,J,K)=1ELSEIF(FFY.GE.0. .AND. MK0(I,J-1,K).LE.1) THEN AY0=ABS(FNY(I,J,K))/YD(J) AC(I,J,K)=AC(I,J,K)+AY0SS(I,J,K)=SS(I,J,K)+AY0*QN(I,J-1,K,IPHASE) JMK(I,J,K)=1ELSEIF(FFY.LE.0. .AND. MK0(I,J+1,K).LE.1) THEN AY0=ABS(FNY(I,J,K))/YD(J+1) AC(I,J,K)=AC(I,J,K)+AY0SS(I,J,K)=SS(I,J,K)+AY0*QN(I,J+1,K,IPHASE)JMK(I,J,K)=1ELSEIF(FFY.GE.0. .AND. F(I,J-1,K)*FNY(I,J-1,K).LE.0.) THEN JMK(I,J,K)=1

ELSEIF(FFY.LE.0. .AND. F(I,J+1,K)*FNY(I,J+1,K).GE.0.) THEN JMK(I,J,K)=1ENDIF 200 IF(I23.EQ.2 .OR. KMK(I,J,K).EQ.1) GOTO 300 FFZ=F(I,J,K)*FNZ(I,J,K) IF((FFZ.GE.0. .AND. K.EQ. 1) .OR.& & (FFZ.LE.0. .AND. K.EQ.NK)) THEN KMK(I,J,K)=1ELSEIF(FFZ.GE.0. .AND. MK0(I,J,K-1).LE.1) THEN AZ0=ABS(FNZ(I,J,K))/ZD(K) AC(I,J,K)=AC(I,J,K)+AZ0SS(I,J,K)=SS(I,J,K)+AZ0*QN(I,J,K-1,IPHASE) KMK(I,J,K)=1ELSEIF(FFZ.LE.0. .AND. MK0(I,J,K+1).LE.1) THEN AZ0=ABS(FNZ(I,J,K))/ZD(K+1) AC(I,J,K)=AC(I,J,K)+AZ0SS(I,J,K)=SS(I,J,K)+AZ0*QN(I,J,K+1,IPHASE) KMK(I,J,K)=1ELSEIF(FFZ.GE.0. .AND. F(I,J,K-1)*FNZ(I,J,K-1).LE.0.) THEN KMK(I,J,K)=1ELSEIF(FFZ.LE.0. .AND. F(I,J,K+1)*FNZ(I,J,K+1).GE.0.) THEN KMK(I,J,K)=1ENDIF 300 IF(IMK(I,J,K).EQ.0 .OR. JMK(I,J,K).EQ.0) RETURN IF(I23.EQ.3 .AND. KMK(I,J,K).EQ.0) RETURN AC0=AMAX1(AC(I,J,K),1.E-30)QN(I,J,K,IPHASE)=SS(I,J,K)/AC0 MK0(I,J,K)=1 I RETURN END SUBROUTINE RK_GET **USE PARAMETERS** USE ICHOS **USE PROPS USE IGRID USE GRID1 USE GRIDB USE GRIDL USE LEVFN USE APANS USE AEANS USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K REAL (KIND=8) :: FYN, FYS, FBT, FZB, FZT, FXW, FXE, CNXE, CNXW, CNYN, CNYS, FX1, FY1, DET ****** ******* DO 100 K=K11,KNK

DO 100 J=1,NJ DO 100 I=1,NI IF(I.NE. 1) AW(I,J,K)=(F(I,J,K)-F(I-1,J,K))/XD(I) IF(J.NE. 1) AS(I,J,K)=(F(I,J,K)-F(I,J-1,K))/YD(J)IF(I23.EQ.2) GOTO 100 IF(K .NE. 1) AB(I,J,K)=(F(I,J,K)-F(I,J,K-1))/ZD(K) 100 CONTINUE DO 110 K=2.NKM DO 110 J=2,NJM DO 110 I=2,NI FYS=AS(I,J ,K)*XDW(I)+AS(I-1,J ,K)*XDE(I) FYN=AS(I,J+1,K)*XDW(I)+AS(I-1,J+1,K)*XDE(I) FY1=0.25*(FYS+FYN)**2 IF(I23.EQ.2) GOTO 115 FZB=AB(I,J,K)*XDW(I)+AB(I-1,J,K)*XDE(I)FZT=AB(I,J,K+1)*XDW(I)+AB(I-1,J,K+1)*XDE(I) FZ1=0.25*(FZB+FZT)**2 115 DET=AMAX1(SQRT(AW(I,J,K)**2+FY1+FZ1),1.E-10) AE(I,J,K)=AW(I,J,K)/DET 110 CONTINUE DO 120 K=2,NKM DO 120 J=2,NJ DO 120 I=2.NIM FXW=AW(I ,J,K)*YDS(J)+AW(I ,J-1,K)*YDN(J) FXE=AW(I+1,J,K)*YDS(J)+AW(I+1,J-1,K)*YDN(J) FX1=0.25*(FXW+FXE)**2 IF(I23.EQ.2) GOTO 125 FZB=AB(I,J,K)*YDS(J)+AB(I,J-1,K)*YDN(J) FZT=AB(I,J,K+1)*YDS(J)+AB(I,J-1,K+1)*YDN(J) FZ1=0.25*(FZB+FZT)**2 125 DET=AMAX1(SQRT(FX1+AS(I,J,K)**2+FZ1),1.E-10) AN(I,J,K)=AS(I,J,K)/DET 120 CONTINUE IF(I23.EQ.2) GOTO 135 DO 130 K=2,NK DO 130 J=2.NJM DO 130 I=2,NIM FXW=AW(I, J, K)*ZDB(K)+AW(I, J, K-1)*ZDT(K)FXE=AW(I+1,J,K)*ZDB(K)+AW(I+1,J,K-1)*ZDT(K) FX1=0.25*(FXW+FXE)**2 FYS=AS(I,J ,K)*ZDB(K)+AS(I,J ,K-1)*ZDT(K) FYN=AS(I,J+1,K)*ZDB(K)+AS(I,J+1,K-1)*ZDT(K) FY1=0.25*(FYS+FYN)**2 DET=AMAX1(SQRT(FX1+FY1+AB(I,J,K)**2),1.E-10) AT(I,J,K)=AB(I,J,K)/DET130 CONTINUE DO 150 K=2,NKM 135

DO 150 J=2,NJM DO 150 I=2,NIM

CNXE=RU(I+1)*AE(I+1,J,K) CNXW=RU(I)*AE(I ,J,K) CNYN=RP(I)*AN(I,J+1,K) CNYS=RP(I)*AN(I,J,K) RK(I,J,K)=((CNXE-CNXW)/XC(I)+(CNYN-CNYS)/YC(J))/RP(I) IF(I23.EQ.2) GOTO 150 RK(I,J,K)=RK(I,J,K)+(AT(I,J,K+1)-AT(I,J,K))/ZC(K)150 CONTINUE RETURN END SUBROUTINE SOLVE **USE PARAMETERS USE ICHOS USE PROPS USE INDMO USE INDDT USE IGRID** USE GRID1 **USE GRIDB USE CHCFL USE LEVFN USE ULVLL USE FFSOR** USE ROGAM USE QMSOR USE RESLT **USE UVTPP USE CALC1** USE FUNC **USE MPIVAR** IMPLICIT NONE INTEGER :: I.J.K REAL (KIND=8) :: CF1,UMAX,VMAX,WMAX !***** CF=1.E10 DO 10 K=2,NKM DO 10 J=2,NJM DO 10 I=2.NIM UMAX=AMAX1(ABS(U(I,J,K)),ABS(U(I,J,K)+AMX(I,J,K)/RHOF(FU(I,J,K)))) VMAX=AMAX1(ABS(V(I,J,K)-VBUB),ABS(V(I,J,K)-VBUB+AMY(I,J,K)/RHOF(FV(I,J,K)))) WMAX=AMAX1(ABS(W(I,J,K)),ABS(W(I,J,K)+AMZ(I,J,K)/RHOF(FW(I,J,K)))) CF1=AMAX1(UMAX/XC(I),VMAX/YC(J),WMAX/ZC(K)) CF1=1./(CF1+1.E-10) IF(CF1 .GT. CF) GOTO 10 CF=CF1 ICF=I JCF=J KCF=K 10 CONTINUE
ļ DT=AMIN1(DT0,CF*CFO) IF(DT .LT. 1.E-8) WRITE(I69,*) ' DT IS TOO SMALL' IF(DT .LT. 1.E-8) STOP BDEFF=DEFF DO 110 K=K11,KNK DO 110 J=1,NJ DO 110 I=1,NI 110 BF(I,J,K)=F(I,J,K) DO 120 K=2,NKM DO 120 J=2,NJM DO 120 I=2,NIM 120 T(I,J,K)=AMAX1(0.,AMIN1(1.,T(I,J,K))) CALL T_BC CALL UL_GET CALL TL_GET IF(NBUB(1) .GE. 1) THEN CALL IPBUB_GET CALL BVOLB MOD CALL F_GET CALL F_MOD IF(JMOVE.EQ.1) CALL F_JMOVE CALL IBUB MOD CALL H_GET CALL N_GET CALL RK_GET ENDIF CALL T_SOLV CALL AM_GET CALL U SOLV CALL V_SOLV CALL W_SOLV CALL DP_ADD CALL P_SOLV CALL PROJT CALL U BC CALL V BC CALL W_BC RETURN END SUBROUTINE T_GEAS **USE PARAMETERS USE ICHOS USE PROPS USE INDDT** USE IGRID **USE IBNDS USE GRID1 USE GRIDB USE GRIDL USE LEVFN USE ULVLL USE FFSOR USE ROGAM USE QMSOR** USE APANS USE AEANS **USE UVTPP** USE CALC1 **USE FUNC USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,L,NT REAL (KIND=8) :: DXN, DXS, DXW, DXE, DZB, DZT, DYN, DYS REAL (KIND=8) :: HB0,HE0,HN0,HS0,HT0,HW0,TX,TY,TXP,TYP,TTB,TTE,TTN,TTP,TTS,TTW,TXE,TXW,TYN,TYS,TTT,T ZB,TZP,TZT REAL (KIND=8) :: TTNN,TTSS,TTEE,TTBB,TYYN,TYYS,TYYP,TYNN,TYSS,TXXP,TXXW,TXXE,TXWW,TXEE,TTWW,TTT T,TZZP,TZZB,TZTT,TZBB,TZZT REAL (KIND=8) :: DZTT, DZC, DZBB, DYSS, DYNN, DYC, DXWW, DXC, DXEE REAL (KIND=8) :: TKM,HZT,HZB,HXE,HXW,HX,HZ,HY,FLUX,FLX,FLY,FLZ=0.,TZ=0. LOGICAL T_FW,T_FE,T_FS,T_FN,T_FB,T_FT,T_2D,T_3D LOGICAL T SW,T SE,T SS,T SN,T SB,T ST LOGICAL T_FWW,T_FEE,T_FSS,T_FNN,T_FBB,T_FTT LOGICAL T SWW,T SEE,T SSS,T SNN,T SBB,T STT T 2D=I23.EQ.2 T 3D=.NOT. T 2D DO 10 K=KKST,KKEND DO 10 J=JJST,JJEND DO 10 I=IIST,IIEND 10 TSOR(I,J,K)=0. I_____ DO 100 K=KKST,KKEND DO 100 J=JJST,JJEND DO 100 I=IIST,IIEND IF(S(I,J,K).LE.0. .OR. F(I,J,K).EQ.0.) GOTO 100 IF(IQ VAP.EQ.0 .AND. F(I,J,K).LT.0.) GOTO 100 IF(IQ_LIQ.EQ.0 .AND. F(I,J,K).GT.0.) GOTO 100 L=1 IF(F(I,J,K).GT.0.) L=2

1----

FLX=0.5*(RU(I)*UL(I,J,K,L)+RU(I+1)*UL(I+1,J,K,L)) FLY=0.5*RP(I)*(VL(I,J,K,L)+VL(I,J+1,K,L))-RP(I)*VBUB IF(T_3D) FLZ=0.5*(WL(I,J,K,L)+WL(I,J,K+1,L)) !------DXW=XD(I) DXE=XD(I+1)

DYS=YD(J) DYN=YD(J+1)

TTP=TL(I ,J,K,L) TTW=TL(I-1,J,K,L) TTE=TL(I+1,J,K,L) TTS=TL(I,J-1,K,L) TTN=TL(I,J+1,K,L)

CALL DX_TT(I,I-1,J,K,DXW,TTW,T_FW,T_SW) CALL DX_TT(I,I+1,J,K,DXE,TTE,T_FE,T_SE) CALL DY_TT(I,J,J-1,K,DYS,TTS,T_FS,T_SS) CALL DY_TT(I,J,J+1,K,DYN,TTN,T_FN,T_SN)

DXC=0.5*(DXW+DXE) DYC=0.5*(DYS+DYN)

TKM=1./TKP(I,J,K) AW(I,J,K)=TKM*RU(I)/DXW/DXC AE(I,J,K)=TKM*RU(I+1)/DXE/DXC AS(I,J,K)=TKM*RP(I)/DYS/DYC AN(I,J,K)=TKM*RP(I)/DYN/DYC AB(I,J,K)=0. AT(I,J,K)=0.

!-----

IF(T_2D) GOTO 110

DZB=ZD(K) DZT=ZD(K+1) TTB=TL(I,J,K-1,L) TTT=TL(I,J,K+1,L)

CALL DZ_TT(I,J,K,K-1,DZB,TTB,T_FB,T_SB) CALL DZ_TT(I,J,K,K+1,DZT,TTT,T_FT,T_ST)

DZC=0.5*(DZB+DZT) AB(I,J,K)=TKM/DZB/DZC AT(I,J,K)=TKM/DZT/DZC

!-----

110 AP(I,J,K)=AE(I,J,K)+AW(I,J,K)+AN(I,J,K)+AS(I,J,K)+AB(I,J,K)+AT(I,J,K)

IF(T_FW .OR. T_SW) TSOR(I,J,K)=TSOR(I,J,K)+AW(I,J,K)*TTW IF(T_FW .OR. T_SW) AW(I,J,K)=0.

IF(T_FE .OR. T_SE) TSOR(I,J,K)=TSOR(I,J,K)+AE(I,J,K)*TTE IF(T_FE .OR. T_SE) AE(I,J,K)=0. $\label{eq:interm} \begin{array}{l} \mathsf{IF}(\mathsf{T}_{\mathsf{F}}\mathsf{S} \ .\mathsf{OR}. \ \mathsf{T}_{\mathsf{S}}\mathsf{S}) \ \mathsf{TSOR}(\mathsf{I},\mathsf{J},\mathsf{K}) \texttt{=} \mathsf{TSOR}(\mathsf{I},\mathsf{J},\mathsf{K}) \texttt{+} \mathsf{AS}(\mathsf{I},\mathsf{J},\mathsf{K}) \texttt{*} \mathsf{TTS} \\ \mathsf{IF}(\mathsf{T}_{\mathsf{F}}\mathsf{S} \ .\mathsf{OR}. \ \mathsf{T}_{\mathsf{S}}\mathsf{S}) \ \mathsf{AS}(\mathsf{I},\mathsf{J},\mathsf{K}) \texttt{=} \mathsf{0}. \end{array}$

 $\label{eq:interm} \begin{array}{l} \mathsf{IF}(\mathsf{T}_{\mathsf{F}}\mathsf{N} \ .\mathsf{OR}. \ \mathsf{T}_{\mathsf{S}}\mathsf{N}) \ \mathsf{TSOR}(\mathsf{I},\mathsf{J},\mathsf{K}) = \mathsf{TSOR}(\mathsf{I},\mathsf{J},\mathsf{K}) + \mathsf{AN}(\mathsf{I},\mathsf{J},\mathsf{K}) * \mathsf{TTN} \\ \mathsf{IF}(\mathsf{T}_{\mathsf{F}}\mathsf{N} \ .\mathsf{OR}. \ \mathsf{T}_{\mathsf{S}}\mathsf{N}) \ \mathsf{AN}(\mathsf{I},\mathsf{J},\mathsf{K}) = 0. \end{array}$

IF(T_2D) GOTO 120 IF(T_FB .OR. T_SB) TSOR(I,J,K)=TSOR(I,J,K)+AB(I,J,K)*TTB IF(T_FB .OR. T_SB) AB(I,J,K)=0.

IF(T_FT .OR. T_ST) TSOR(I,J,K)=TSOR(I,J,K)+AT(I,J,K)*TTT IF(T_FT .OR. T_ST) AT(I,J,K)=0. 120 CONTINUE !----- Convection

TXW=(TTP-TTW)/DXW TXE=(TTE-TTP)/DXE TYS=(TTP-TTS)/DYS TYN=(TTN-TTP)/DYN

IF(FLX.GE.0.) TX=TXW IF(FLX.LT.0.) TX=TXE IF(FLY.GE.0.) TY=TYS IF(FLY.LT.0.) TY=TYN

TXXP=(TXE-TXW)/(DXE+DXW) TYYP=(TYN-TYS)/(DYN+DYS)

IF(T_2D) GOTO 130 TZB=(TTP-TTB)/DZB TZT=(TTT-TTP)/DZT

IF(FLZ.GE.0.) TZ=TZB IF(FLZ.LT.0.) TZ=TZT

TZZP=(TZT-TZB)/(DZT+DZB) 130 CONTINUE !-----IF(FLX.GE.0.) THEN IF(I.EQ.2 .OR. T_FW .OR. T_SW) THEN TX=TX+DXE*TXXP ELSE DXWW=XD(I-1) TTWW=TL(I-2,J,K,L) CALL DX TT(I-1,I-2,J,K,DXWW,TTWW,T FWW,T SWW) TXWW=(TTW-TTWW)/DXWW TXXW=(TXW-TXWW)/(DXW+DXWW) TX=TX+DXE*AMIN2(TXXP,IENOT*TXXW) **ENDIF** ELSE IF(I.EQ.NIM .OR. T FE .OR. T SE) THEN TX=TX-DXW*TXXP ELSE DXEE=XD(I+2)

TTEE=TL(I+2,J,K,L) CALL DX TT(I+1,I+2,J,K,DXEE,TTEE,T FEE,T SEE) TXEE=(TTEE-TTE)/DXEE TXXE=(TXEE-TXE)/(DXEE+DXE) TX=TX-DXW*AMIN2(TXXP,IENOT*TXXE) ENDIF ENDIF I_____ IF(FLY.GE.0.) THEN IF(J.EQ.2 .OR. T_FS .OR. T_SS) THEN TY=TY+DYN*TYYP ELSE DYSS=YD(J-1) TTSS=TL(I,J-2,K,L) CALL DY TT(I,J-1,J-2,K,DYSS,TTSS,T FSS,T SSS) TYSS=(TTS-TTSS)/DYSS TYYS=(TYS-TYSS)/(DYS+DYSS) TY=TY+DYN*AMIN2(TYYP,IENOT*TYYS) ENDIF ELSE IF(J.EQ.NJM .OR. T_FN .OR. T_SN) THEN TY=TY-DYS*TYYP ELSE DYNN=YD(J+2) TTNN=TL(I,J+2,K,L) CALL DY TT(I,J+1,J+2,K,DYNN,TTNN,T FNN,T SNN) TYNN=(TTNN-TTN)/DYNN TYYN=(TYNN-TYN)/(DYNN+DYN) TY=TY-DYS*AMIN2(TYYP,IENOT*TYYN) **ENDIF ENDIF** IF(T_2D) GOTO 150 1___ IF(FLZ.GE.0.) THEN IF(K.EQ.2 .OR. T FB .OR. T SB) THEN TZ=TZ+DZT*TZZP ELSE DZBB=ZD(K-1) TTBB=TL(I,J,K-2,L) CALL DZ_TT(I,J,K-1,K-2,DZBB,TTBB,T_FBB,T_SBB) TZBB=(TTB-TTBB)/DZBB TZZB=(TZB-TZBB)/(DZB+DZBB) TZ=TZ+DZT*AMIN2(TZZP,IENOT*TZZB) **ENDIF** ELSE IF(K.EQ.NKM .OR. T_FT .OR. T_ST) THEN TZ=TZ-DZB*TZZP ELSE DZTT=ZD(K+2) TTTT=TL(I,J,K+2,L) CALL DZ_TT(I,J,K+1,K+2,DZTT,TTTT,T_FTT,T_STT) TZTT=(TTTT-TTT)/DZTT

TZZT=(TZTT-TZT)/(DZTT+DZT) TZ=TZ-DZB*AMIN2(TZZP,IENOT*TZZT) ENDIF ENDIF !-----150 FLUX=FLX*TX+FLY*TY+FLZ*TZ TSOR(I,J,K)=TSOR(I,J,K)+RCP(I,J,K)*(RP(I)*TL(I,J,K,L)/DT-FLUX) 100 CONTINUE -----BC I_____ IF(IBCW.NE.IWAL) THEN DO 210 K=KKST,KKEND DO 210 J=JJST,JJEND AP(2,J,K) = AP(2,J,K) - AW(2,J,K)210 AW(2,J,K)=0. ENDIF ! IF(IBCE.NE.IWAL) THEN DO 220 K=KKST,KKEND DO 220 J=JJST,JJEND AP(NIM,J,K)=AP(NIM,J,K)-AE(NIM,J,K)220 AE(NIM,J,K)=0. ENDIF IF(IBCS.NE.IWAL) THEN DO 230 K=KKST,KKEND DO 230 I=IIST,IIEND AP(1,2,K)=AP(1,2,K)-AS(1,2,K) 230 AS(I,2,K)=0. ENDIF IF(IBCN.NE.IWAL) THEN DO 240 K=KKST,KKEND DO 240 I=IIST, IIEND AP(I,NJM,K)=AP(I,NJM,K)-AN(I,NJM,K) 240 AN(I,NJM,K)=0. ENDIF IF(T 2D) GOTO 290 IF(IBCB.NE.IWAL) THEN DO 250 J=JJST,JJEND DO 250 I=IIST, IIEND AP(I,J,2) = AP(I,J,2) - AB(I,J,2)250 AB(I,J,2)=0. ENDIF IF(IBCN.NE.IWAL) THEN DO 260 J=JJST,JJEND DO 260 I=IIST.IIEND AP(I,J,NKM)=AP(I,J,NKM)-AT(I,J,NKM) 260 AT(I,J,NKM)=0. ENDIF I_____

290 DO 300 K=KKST,KKEND

DO 300 J=JJST,JJEND DO 300 I=IIST,IIEND AP(I,J,K)=AP(I,J,K)+RCP(I,J,K)*RP(I)/DT $300 \quad APC(I,J,K)=AP(I,J,K)$!-----BCC IF(IBCS.EQ.IWAL) THEN DO 430 K=KKST,KKEND DO 430 I=IIST, IIEND HY=1. IF(F(I,1,K).LE.0. .AND. IQ_VAP.EQ.0) HY=0. IF(F(I,1,K).GE.0. .AND. IQ LIQ.EQ.0) HY=0. IF(T 2PH(F(I,1,K),F(I,2,K))) HY=F(I,1,K)/(F(I,1,K)-F(I,2,K))HXW=0.5 HXE=0.5 IF(T_2PH(F(I,1,K),F(I-1,1,K))) HXW=XD(I)*F(I,1,K)/(F(I,1,K)-F(I-1,1,K))/XC(I) IF(T 2PH(F(I,1,K),F(I+1,1,K))) HXE=XD(I+1)*F(I,1,K)/(F(I,1,K)-F(I+1,1,K))/XC(I) HX=HXW+HXE HZ=1. IF(I23.EQ.3) THEN HZB=0.5 HZT=0.5 IF(T_2PH(F(I,1,K),F(I,1,K-1))) HZB=ZD(K)*F(I,1,K)/(F(I,1,K)-F(I,1,K-1))/ZC(K) IF(T 2PH(F(I,1,K),F(I,1,K+1))) HZT=ZD(K+1)*F(I,1,K)/(F(I,1,K)-F(I,1,K+1))/ZC(K) HZ=HZB+HZT ENDIF AP(I, 2,K)=AP(I, 2,K)-AS(I, 2,K)*(1.-HY*HX*HZ) 430 CONTINUE ENDIF IF (TASKID.NE.0) THEN CALL MPI SEND(TSOR(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI DOUBLE PRE CISION,0,TASKID,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(TSOR(RSPANX(NT);RSPANXE(NT),RSPANY(NT);RSPANYE(NT),RSPANZ(NT);RSPANZE (NT)),SIZECC(NT),MPI_DOUBLE_PRECISION,NT,NT,MPI_COMM_WORLD,STATUS,IERR) ENDDO ENDIF CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI BCAST(TSOR(1,1,1),SIZE(TSOR),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR) RETURN END SUBROUTINE T_GEAS_SUB

USE PARAMETERS USE PROPS USE IGRID USE GRID1 USE LEVFN USE FUNC **USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K REAL (KIND=8) :: TTW, TTS, TTB REAL (KIND=8), INTENT(INOUT) :: DXW, DYS, DZB INTEGER, INTENT(IN) :: 11,12,J1,J2,K1,K2,IY,IZ,JX,JZ,KX,KY LOGICAL T FW,T FS,T FB,T SW,T SS,T SB ******** ********* ENTRY DX_TT(I1,I2,JX,KX,DXW,TTW,T_FW,T_SW) ******* J=JX K=KX $T_FW=T_2PH(F(I1,J,K),F(I2,J,K))$ T_SW=T_2PH(S(I1,J,K),S(I2,J,K)) IF(T_FW .AND. T_SW) THEN T_FW=(F(I1,J,K)/(F(I1,J,K)-F(I2,J,K))).LT.& (S(I1,J,K)/(S(I1,J,K)-S(I2,J,K))) & T SW=.NOT. T_FW ENDIF IF(T FW) THEN DXW=DXW*AMAX1(HEPS,F(I1,J,K)/(F(I1,J,K)-F(I2,J,K))) TTW=TINT ENDIF IF(T SW) THEN DXW=DXW*AMAX1(HEPS,S(I1,J,K)/(S(I1,J,K)-S(I2,J,K))) TTW=TWAL **ENDIF** RETURN ENTRY DY TT(IY, J1, J2, KY, DYS, TTS, T FS, T SS) I=IY K=KY T FS=T_2PH(F(I,J1,K),F(I,J2,K)) T SS=T 2PH(S(I,J1,K),S(I,J2,K)) IF(T_FS .AND. T_SS) THEN T_FS=(F(I,J1,K)/(F(I,J1,K)-F(I,J2,K))).LT.& (S(I,J1,K)/(S(I,J1,K)-S(I,J2,K)))& T SS=.NOT. T FS **ENDIF** IF(T FS) THEN DYS=DYS*AMAX1(HEPS,F(I,J1,K)/(F(I,J1,K)-F(I,J2,K))) TTS=TINT ENDIF IF(T_SS) THEN DYS=DYS*AMAX1(HEPS,S(I,J1,K)/(S(I,J1,K)-S(I,J2,K))) TTS=TWAL

ENDIF RETURN |******** ENTRY DZ_TT(IZ,JZ,K1,K2,DZB,TTB,T_FB,T_SB) I=IZ J=JZ $T_FB=T_2PH(F(I,J,K1),F(I,J,K2))$ T_SB=T_2PH(S(I,J,K1),S(I,J,K2)) IF(T_FB.AND. T_SB) THEN $T_FB=(F(I,J,K1)/(F(I,J,K1)-F(I,J,K2))).LT.\&$ & (S(I,J,K1)/(S(I,J,K1)-S(I,J,K2))) T_SB=.NOT. T_FB ENDIF IF(T_FB) THEN DZB=DZB*AMAX1(HEPS,F(I,J,K1)/(F(I,J,K1)-F(I,J,K2))) TTB=TINT **ENDIF** IF(T_SB) THEN DZB=DZB*AMAX1(HEPS,S(I,J,K1)/(S(I,J,K1)-S(I,J,K2))) TTB=TWAL ENDIF RETURN END SUBROUTINE TL GET **USE PARAMETERS USE ICHOS USE PROPS USE IGRID USE GRID1 USE LEVFN USE ULVLL USE UVTPP USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,NT INTEGER :: ITMP, ITMPE, JTMP, JTMPE, KTMP, KTMPE ********

DO 110 K=KKST,KKEND DO 110 J=JJST,JJEND DO 110 I=IIST,IIEND TL(I,J,K,1)=T(I,J,K) TL(I,J,K,2)=T(I,J,K) 110 CONTINUE

IF(IBOIL.EQ.1) THEN DO 120 K=KKST,KKEND DO 120 J=JJST,JJEND DO 120 I=IIST,IIEND IF(S(I,J,K).LE.0.) GOTO 120 IF(F(I,J,K).LE.0.) TL(I,J,K,2)=TINT IF(F(I,J,K).GT.0.) TL(I,J,K,1)=TINT 120 CONTINUE ENDIF

!-----

RCCG(IIST:IIEND,JJST:JJEND,KKST:KKEND,1:2)= TL(IIST:IIEND,JJST:JJEND,KKST:KKEND,1:2) CALL GHNEIGHBOUR

ITMP=IIST-2 ITMPE=IIEND+2 JTMP=JJST-2 JTMPE=JJEND+2 KTMP=KKST-2 KTMPE=KKEND+2 IF (PIDX.EQ.0) ITMP=IIST IF (PIDX.EQ.PROCSX-1) ITMPE=IIEND IF (PIDY.EQ.0) JTMP=JJST IF (PIDY.EQ.PROCSY-1) JTMPE=JJEND IF (PIDZ.EQ.0) KTMP=KKST IF (PIDZ.EQ.PROCSZ-1) KTMPE=KKEND TL(ITMP:ITMPE,JTMPE,KTMPE,KTMPE,1:2)=RCCG(ITMP:ITMPE,JTMPE,KTMPE,KTMPE,1: 2)

CALL RELOAD IF (TASKID.NE.0) THEN CALL MPI_SEND(TL(IIST:IIEND,JJST:JJEND,KKST:KKEND,1:2),SPANX*SPANY*SPANZ*2,MPI_DOUBLE_P RECISION,0,TASKID,MPI COMM WORLD,IERR) **ENDIF**

IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(TL(RSPANX(NT):RSPANXE(NT).RSPANY(NT):RSPANYE(NT).RSPANZ(NT):RSPANZE(NT),1:2),SIZECC(NT)*2,MPI DOUBLE PRECISION,NT,NT,MPI COMM WORLD,STATUS,IERR) ENDDO ENDIF

CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI_BCAST(TL(1,1,1,1),SIZE(TL),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR) 1-----

RETURN END

SUBROUTINE U GEAS

USE PARAMETERS USE ICHOS

USE PROPS USE INDDT USE IGRID USE IBNDS USE GRID1 **USE GRIDB USE GRIDL USE LEVFN** USE ULVLL **USE FFSOR USE ROGAM** USE QMSOR **USE APANS** USE AEANS **USE UVTPP** USE CALC1 USE FUNC **USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,L,NT INTEGER :: ITMP, ITMPE, JTMP, JTMPE, KTMP, KTMPE REAL (KIND=8) :: DXE,DXW,DYN,DYS,DZB,DZT,DIFB,DIFE,DIFN,DIFS,DIFT,DIFW,DUDX,DUIM,DVDY,DXEE,DXWW,DY NN, DYSS, DZBB, DZTT REAL (KIND=8) :: RPU,UXE,UYN,UYS,UXW,UZB,UZT,UXEE,UXWW,UXXE,UXXP,UXXW,UYNN,UYSS,UYYN,UYYP,UYY S,UZBB,UZTT,UZZB,UZZP,UZZT REAL (KIND=8) :: FLUX,FLX,FLY,FLZ,UX,UY,UZ REAL (KIND=8) :: VISB, VISE, VISM, VISN, VISS, VIST, VISW LOGICAL T_FW,T_FE,T_FS,T_FN,T_FB,T_FT,T_2D,T_3D LOGICAL T_SW,T_SE,T_SS,T_SN,T_SB,T_ST *********** T 2D=I23.EQ.2 T 3D=.NOT. T 2D IF (PIDX.EQ.0) THEN IIST = 3ELSE IF (PIDX.EQ.PROCSX-1) THEN IIEND = ID-1ENDIF IF (PIDY.EQ.0) THEN JJST = 2ELSE IF (PIDY.EQ.PROCSY-1) THEN JJEND = JD-1**ENDIF** IF (PIDZ.EQ.0) THEN KKST = 2 ELSE IF (PIDZ.EQ.PROCSZ-1) THEN KKEND = KD-1 ENDIF DO 10 K=KKST,KKEND DO 10 J=JJST,JJEND

DO 10 I=IIST,IIEND USOR(I,J,K)=0. 10 SS(I,J,K)=0. 1-----DO 100 K=KKST,KKEND DO 100 J=JJST,JJEND DO 100 I=IIST,IIEND IF(SU(I,J,K).LE.0.) GOTO 100 L=1 IF(FU(I,J,K).GT.0.) L=2 I-----FLX=0.25*(RU(I)*UL(I,J,K,L)+RU(I+1)*UL(I+1,J,K,L)+RU(I)*UL(I,J,K,L)+RU(I-1)*UL(I-1,J,K,L)) FLY=0.25*(RP(I)*(VL(I ,J+1,K,L)+VL(I,J,K,L))+RP(I-1)*(VL(I-1,J+1,K,L)+VL(I-1,J,K,L)))-RU(I)*VBUB IF(T 3D) FLZ=0.25*(WL(I,J,K+1,L)+WL(I,J,K,L)+WL(I-1,J,K+1,L)+WL(I-1,J,K,L)) I_____ VISW=1./VISMF(FU(I,J,K),FU(I-1,J,K),FV(I-1,J,K),FV(I-1,J+1,K),FW(I-1,J,K),FW(I-1,J,K+1)) VISE=1./VISMF(FU(I,J,K),FU(I+1,J,K),FV(I ,J,K),FV(I ,J+1,K),FW(I ,J,K),FW(I ,J,K+1)) VISS=1./VISMF(FU(I,J,K),FU(I,J-1,K),FV(I,J,K),FV(I-1,J,K),FC(I,J,K),FC(I,J,K+1)) VISN=1./VISMF(FU(I,J,K),FU(I,J+1,K),FV(I,J+1,K),FV(I-1,J+1,K),FC(I,J+1,K),FC(I,J+1,K+1)) IF(T_3D) THEN VISB=1./VISMF(FU(I,J,K),FU(I,J,K-1),FW(I,J,K),FW(I-1,J,K),FC(I,J,K),FC(I,J+1,K)) VIST=1./VISMF(FU(I,J,K),FU(I,J,K+1),FW(I,J,K+1),FW(I-1,J,K+1),FC(I,J,K+1),FC(I,J+1,K+1)) ENDIF |-----DXW=XC(I-1)*FAC_EPS(SU(I,J,K),SU(I-1,J,K)) DXE=XC(I)*FAC_EPS(SU(I,J,K),SU(I+1,J,K)) DYS=YD(J) *FAC EPS(SU(I,J,K),SU(I,J-1,K))DYN=YD(J+1)*FAC EPS(SU(I,J,K),SU(I,J+1,K))IF(T 3D) THEN DZB=ZD(K)*FAC EPS(SU(I,J,K),SU(I,J,K-1)) DZT=ZD(K+1)*FAC EPS(SU(I,J,K),SU(I,J,K+1)) ENDIF !----- Digonal Diffusion AW(I,J,K)=VISW*RP(I-1)/DXW/XD(I) AE(I,J,K)=VISE*RP(I)/DXE/XD(I) AS(I,J,K)=VISS*RU(I)/DYS/YC(J) AN(I,J,K)=VISN*RU(I)/DYN/YC(J) IF(T 3D) THEN AB(I.J.K)=VISB/DZB/ZC(K) AT(I,J,K)=VIST/DZT/ZC(K) ENDIF ----- OFF-Digonal Diffusion 1___ !----- [mr(du/dx)]e-w/dx DIFW=VISW*RP(I-1)*(UL(I,J,K,L)-UL(I-1,J,K,L))/XC(I-1) DIFE=VISE*RP(I)*(UL(I+1,J,K,L)-UL(I,J,K,L))/XC(I)USOR(I,J,K)=USOR(I,J,K)+(DIFE-DIFW)/XD(I) !----- [mr(dv/dx)]n-s/dv RPU=0.5*(RP(I)+RP(I-1)) DIFS=VISS*(VL(I,J,K,L)-VL(I-1,J,K,L))/XD(I) DIFN=VISN*(VL(I,J+1,K,L)-VL(I-1,J+1,K,L))/XD(I) USOR(I,J,K)=USOR(I,J,K)+RPU*(DIFN-DIFS)/YC(J) !------ [m(du/dx)+m(dv/dy)]

IF(IR.EQ.1) THEN

DUDX=0.5*(VISW*(UL(I,J,K,L)-UL(I-1,J,K,L))+VISE*(UL(I+1,J,K,L)-UL(I,J,K,L)))/XD(I) DVDY=0.5*(VISW*(VL(I-1,J+1,K,L)-VL(I-1,J,K,L))+VISE*(VL(I,J+1,K,L)-VL(I,J,K,L)))/YC(J) USOR(I,J,K)=USOR(I,J,K)+DUDX+DVDY ENDIF !----- [m(dw/dx)]t-b/dz IF(T 3D) THEN DIFB=VISB*(WL(I,J,K ,L)-WL(I-1,J,K ,L))/XD(I) DIFT=VIST*(WL(I,J,K+1,L)-WL(I-1,J,K+1,L))/XD(I) USOR(I,J,K)=USOR(I,J,K)+(DIFT-DIFB)/ZC(K) ENDIF ----- Convection I-----UXW=(UL(I,J,K,L)-UL(I-1,J,K,L))/DXW UXE=(UL(I+1,J,K,L)-UL(I,J,K,L))/DXE UYS=(UL(I,J,K,L)-UL(I,J-1,K,L))/DYS UYN=(UL(I,J+1,K,L)-UL(I,J,K,L))/DYN IF(FLX.GE.0.) UX=UXW IF(FLX.LT.0.) UX=UXE IF(FLY.GE.0.) UY=UYS IF(FLY.LT.0.) UY=UYN IF(T 3D) THEN UZB=(UL(I,J,K,L)-UL(I,J,K-1,L))/DZBUZT=(UL(I,J,K+1,L)-UL(I,J,K,L))/DZT IF(FLZ.GE.0.) UZ=UZB IF(FLZ.LT.0.) UZ=UZT ENDIF IF(IENO.EQ.0) GOTO 150 !-----UXXP=(UXE-UXW)/(DXE+DXW) UYYP=(UYN-UYS)/(DYN+DYS) IF(T_3D) UZZP=(UZT-UZB)/(DZT+DZB) 1-----IF(FLX.GE.0.) THEN IF(I.EQ.3 .OR. T 2PH(SU(I,J,K),SU(I-1,J,K))) THEN UX=UX+DXE*UXXP ELSE DXWW=XC(I-2)*FAC EPS(SU(I-1,J,K),SU(I-2,J,K)) UXWW=(UL(I-1,J,K,L)-UL(I-2,J,K,L))/DXWW UXXW=(UXW-UXWW)/(DXW+DXWW) UX=UX+DXE*AMIN2(UXXP,UXXW) ENDIF ELSE IF(I.EQ.NIM .OR. T 2PH(SU(I,J,K),SU(I+1,J,K))) THEN UX=UX-DXW*UXXP ELSE DXEE=XC(I+1)*FAC EPS(SU(I+1,J,K),SU(I+2,J,K)) UXEE=(UL(I+2,J,K,L)-UL(I+1,J,K,L))/DXEE UXXE=(UXEE-UXE)/(DXEE+DXE) UX=UX-DXW*AMIN2(UXXP,UXXE) ENDIF ENDIF

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IF(FLY.GE.0.) THEN IF(J.EQ.2 .OR. T 2PH(SU(I,J,K),SU(I,J-1,K))) THEN UY=UY+DYN*UYYP ELSE DYSS=YD(J-1)*FAC EPS(SU(I,J-1,K),SU(I,J-2,K)) UYSS=(UL(I,J-1,K,L)-UL(I,J-2,K,L))/DYSS UYYS=(UYS-UYSS)/(DYS+DYSS) UY=UY+DYN*AMIN2(UYYP,UYYS) ENDIF ELSE IF(J.EQ.NJM .OR. T 2PH(SU(I,J,K),SU(I,J+1,K))) THEN UY=UY-DYS*UYYP ELSE DYNN=YD(J+2)*FAC EPS(SU(I,J+1,K),SU(I,J+2,K)) UYNN=(UL(I,J+2,K,L)-UL(I,J+1,K,L))/DYNN UYYN=(UYNN-UYN)/(DYNN+DYN) UY=UY-DYS*AMIN2(UYYP,UYYN) ENDIF ENDIF I_____ IF(T_2D) GOTO 150 IF(FLZ.GE.0.) THEN IF(K.EQ.2 .OR. T 2PH(SU(I,J,K),SU(I,J,K-1))) THEN UZ=UZ+DZT*UZZP ELSE DZBB=ZD(K-1)*FAC EPS(SU(I,J,K-1),SU(I,J,K-2)) UZBB=(UL(I,J,K-1,L)-UL(I,J,K-2,L))/DZBB UZZB=(UZB-UZBB)/(DZB+DZBB) UZ=UZ+DZT*AMIN2(UZZP,UZZB) ENDIF ELSE IF(K.EQ.NKM .OR. T_2PH(SU(I,J,K),SU(I,J,K+1))) THEN UZ=UZ-DZB*UZZP ELSE DZTT=ZD(K+2)*FAC EPS(SU(I,J,K+1),SU(I,J,K+2)) UZTT=(UL(I,J,K+2,L)-UL(I,J,K+1,L))/DZTT UZZT=(UZTT-UZT)/(DZTT+DZT) UZ=UZ-DZB*AMIN2(UZZP,UZZT) ENDIF ENDIF I-----150 FLUX=FLX*UX+FLY*UY+FLZ*UZ USOR(I,J,K)=USOR(I,J,K)+RHOU(I,J,K)*(RU(I)*UL(I,J,K,L)/DT-FLUX) 100 CONTINUE !-----BC DO 210 K=KKST,KKEND DO 210 I=IIST.IIEND IF(IBCS.EQ.IOUT .OR. IBCS.EQ.ISYM) AS(I, 2,K)=0. IF(IBCN.EQ.IOUT .OR. IBCN.EQ.ISYM) AN(I,NJM,K)=0.

210 CONTINUE

IF(T_2D) GOTO 225

DO 220 J=JJST,JJEND DO 220 I=IIST,IIEND IF(IBCB.EQ.IOUT .OR. IBCB.EQ.ISYM) AB(I,J, 2)=0. IF(IBCT.EQ.IOUT .OR. IBCT.EQ.ISYM) AT(I,J,NKM)=0. 220 CONTINUE 1___ 225 IF(IBOIL.EQ.0) GOTO 390 DO 300 K=KKST,KKEND DO 300 J=JJST,JJEND DO 300 I=IIST,IIEND IF(T 2PH(FU(I,J,K),FU(I-1,J,K))) THEN DUIM=(FU(I,J,K)*AMX(I-1,J,K)-FU(I-1,J,K)*AMX(I,J,K))/ABS(FU(I,J,K)-FU(I-1,J,K))*VFG SS(I,J,K)=SS(I,J,K)+AW(I,J,K)*DUIM ENDIF IF(T 2PH(FU(I,J,K),FU(I+1,J,K))) THEN DUIM=(FU(I,J,K)*AMX(I+1,J,K)-FU(I+1,J,K)*AMX(I,J,K))/ABS(FU(I,J,K)-FU(I+1,J,K))*VFG SS(I,J,K)=SS(I,J,K)+AE(I,J,K)*DUIM ENDIF IF(T_2PH(FU(I,J,K),FU(I,J-1,K))) THEN DUIM=(FU(I,J,K)*AMX(I,J-1,K)-FU(I,J-1,K)*AMX(I,J,K))/ABS(FU(I,J,K)-FU(I,J-1,K))*VFG SS(I,J,K)=SS(I,J,K)+AS(I,J,K)*DUIM ENDIF IF(T 2PH(FU(I,J,K),FU(I,J+1,K))) THEN DUIM=(FU(I,J,K)*AMX(I,J+1,K)-FU(I,J+1,K)*AMX(I,J,K))/ABS(FU(I,J,K)-FU(I,J+1,K))*VFG SS(I,J,K)=SS(I,J,K)+AN(I,J,K)*DUIMENDIF IF(T_2D) GOTO 300 IF(T 2PH(FU(I,J,K),FU(I,J,K-1))) THEN DUIM=(FU(I,J,K)*AMX(I,J,K-1)-FU(I,J,K-1)*AMX(I,J,K))/ABS(FU(I,J,K)-FU(I,J,K-1))*VFG SS(I,J,K)=SS(I,J,K)+AB(I,J,K)*DUIM ENDIF IF(T 2PH(FU(I,J,K),FU(I,J,K+1))) THEN DUIM=(FU(I,J,K)*AMX(I,J,K+1)-FU(I,J,K+1)*AMX(I,J,K))/ABS(FU(I,J,K)-FU(I,J,K+1))*VFG SS(I,J,K)=SS(I,J,K)+AT(I,J,K)*DUIMENDIF 300 CONTINUE 390 CONTINUE DO 400 K=KKST,KKEND DO 400 J=JJST.JJEND DO 400 I=IIST,IIEND USOR(I,J,K)=USOR(I,J,K)+SS(I,J,K)VISM=1./VISF(FU(I.J.K)) AP(I,J,K)=RHOU(I,J,K)*RU(I)/DT+IR*VISM/RU(I)+AE(I,J,K)+AW(I,J,K)+AN(I,J,K)+AS(I,J,K)+AT(I,J,K)+AB (I,J,K)400 APC(I,J,K)=AP(I,J,K)

IF (TASKID.NE.0) THEN

CALL MPI SEND(USOR(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ.MPI DOUBLE PR ECISION,0,TASKID,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(USOR(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE (NT)),SIZECC(NT),MPI_DOUBLE_PRECISION,NT,NT,MPI_COMM_WORLD,STATUS,IERR) ENDDO ENDIF CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI BCAST(USOR(1,1,1),SIZE(USOR),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR) RETURN END SUBROUTINE UL GET ****** **USE PARAMETERS USE ICHOS USE PROPS USE IGRID USE LEVFN USE ULVLL** USE QMSOR **USE UVTPP USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,NT INTEGER :: ITMP, JTMP, KTMP, ITMPE, JTMPE, KTMPE ************* DO 110 K=KKST,KKEND DO 110 J=JJST,JJEND DO 110 I=IIST.IIEND UL(I,J,K,1)=U(I,J,K)VL(I,J,K,1)=V(I,J,K)WL(I,J,K,1)=W(I,J,K)UL(I,J,K,2)=U(I,J,K)VL(I,J,K,2)=V(I,J,K)WL(I,J,K,2)=W(I,J,K)110 CONTINUE IF(IBOIL.EQ.1) THEN DO 120 K=KKST,KKEND DO 120 J=JJST,JJEND DO 120 I=IIST,IIEND IF(FU(I,J,K).LE.0.) UL(I,J,K,2)=U(I,J,K)+AMX(I,J,K)*VFG IF(FU(I,J,K).GT.0.) UL(I,J,K,1)=U(I,J,K)-AMX(I,J,K)*VFG

IF(FV(I,J,K).LE.0.) VL(I,J,K,2)=V(I,J,K)+AMY(I,J,K)*VFG IF(FV(I,J,K).GT.0.) VL(I,J,K,1)=V(I,J,K)-AMY(I,J,K)*VFG IF(I23.EQ.2) GOTO 120 IF(FW(I,J,K).LE.0.) WL(I,J,K,2)=W(I,J,K)+AMZ(I,J,K)*VFG IF(FW(I,J,K).GT.0.) WL(I,J,K,1)=W(I,J,K)-AMZ(I,J,K)*VFG 120 CONTINUE ENDIF !------RCCG(IIST:IIEND,JJST:JJEND,KKST:KKEND,1:2)= UL(IIST:IIEND,JJST:JJEND,KKST:KKEND,1:2) CALL GHNEIGHBOUR

ITMP=IIST-2 ITMPE=IIEND+2 JTMP=JJST-2 JTMPE=JJEND+2 KTMP=KKST-2 KTMP=KKEND+2 IF (PIDX.EQ.0) ITMP=IIST IF (PIDX.EQ.PROCSX-1) ITMPE=IIEND IF (PIDY.EQ.PROCSX-1) JTMPE=JJEND IF (PIDY.EQ.PROCSY-1) JTMPE=JJEND IF (PIDZ.EQ.0) KTMP=KKST IF (PIDZ.EQ.PROCSZ-1) KTMPE=KKEND UL(ITMP:ITMPE,JTMP:JTMPE,KTMPE,1:2)=RCCG(ITMP:ITMPE,JTMPE,KTMP:KTMPE,1: 2)

CALL RELOAD IF (TASKID.NE.0) THEN CALL MPI_SEND(UL(IIST:IIEND,JJST:JJEND,KKST:KKEND,1:2),SPANX*SPANY*SPANZ*2,MPI_DOUBLE_P RECISION,0,TASKID,MPI_COMM_WORLD,IERR) ENDIF

IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(UL(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT),1:2),SIZECC(NT)*2,MPI_DOUBLE_PRECISION,NT,NT,MPI_COMM_WORLD,STATUS,IERR) ENDDO ENDIF

CALL MPI_BARRIER(MPI_COMM_WORLD,IERR) CALL MPI_BCAST(UL(1,1,1,1),SIZE(UL),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR)

!-----

RCCG(IIST:IIEND,JJST:JJEND,KKST:KKEND,1:2)= VL(IIST:IIEND,JJST:JJEND,KKST:KKEND,1:2) CALL GHNEIGHBOUR

ITMP=IIST-2 ITMPE=IIEND+2 JTMP=JJST-2 JTMPE=JJEND+2 KTMP=KKST-2 KTMPE=KKEND+2 IF (PIDX.EQ.0) ITMP=IIST IF (PIDX.EQ.PROCSX-1) ITMPE=IIEND IF (PIDY.EQ.0) JTMP=JJST IF (PIDY.EQ.PROCSY-1) JTMPE=JJEND IF (PIDZ.EQ.0) KTMP=KKST IF (PIDZ.EQ.PROCSZ-1) KTMPE=KKEND VL(ITMP:ITMPE,JTMPE,KTMPE,KTMPE,1:2)=RCCG(ITMP:ITMPE,JTMPE,KTMPE,KTMPE,1: 2) CALL RELOAD IF (TASKID.NE.0) THEN CALL MPI_SEND(VL(IIST:IIEND,JJST:JJEND,KKST:KKEND,1:2),SPANX*SPANY*SPANZ*2,MPI_DOUBLE_P RECISION,0,TASKID,MPI COMM WORLD,IERR) ENDIF IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(VL(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT),1:2),SIZECC(NT)*2,MPI DOUBLE PRECISION,NT,NT,MPI COMM WORLD,STATUS,IERR) ENDDO ENDIF CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI BCAST(VL(1,1,1,1),SIZE(VL),MPI DOUBLE PRECISION,0,MPI COMM WORLD,IERR) !----RCCG(IIST:IIEND,JJST:JJEND,KKST:KKEND,1:2)= WL(IIST:IIEND,JJST:JJEND,KKST:KKEND,1:2) CALL GHNEIGHBOUR ITMP=IIST-2 ITMPE=IIEND+2 JTMP=JJST-2 JTMPE=JJEND+2 KTMP=KKST-2 KTMPE=KKEND+2 IF (PIDX.EQ.0) ITMP=IIST IF (PIDX.EQ.PROCSX-1) ITMPE=IIEND IF (PIDY.EQ.0) JTMP=JJST IF (PIDY.EQ.PROCSY-1) JTMPE=JJEND IF (PIDZ.EQ.0) KTMP=KKST IF (PIDZ.EQ.PROCSZ-1) KTMPE=KKEND WL(ITMP:ITMPE,JTMPE,KTMPE,KTMPE,1:2)=RCCG(ITMP:ITMPE,JTMPE,KTMPE,KTMPE,1: 2) CALL RELOAD

IF (TASKID.NE.0) THEN CALL MPI_SEND(WL(IIST:IIEND,JJST:JJEND,KKST:KKEND,1:2),SPANX*SPANY*SPANZ*2,MPI_DOUBLE_P RECISION,0,TASKID,MPI_COMM_WORLD,IERR) ENDIF

IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(WL(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(N T),1:2),SIZECC(NT)*2,MPI DOUBLE PRECISION,NT,NT,MPI COMM WORLD,STATUS,IERR) ENDDO **ENDIF** CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI_BCAST(WL(1,1,1,1),SIZE(WL),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR) RETURN END SUBROUTINE UVPT SOLVE **USE PARAMETERS USE ICHOS USE INDMO USE INDDT USE IGRID** USE MUGRD **USE GRID1** USE GRIDB USE IDREF **USE SPERR USE LEVFN** USE ULVLL **USE FFSOR USE ROGAM** USE QMSOR **USE APANS** USE AEANS **USE UVTPP** USE CALC1 USE INDIT USE RELXS **USE CHAR1** USE MISC **USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,N,ITER,MPII,MPJJ,MPKK INTEGER :: ITMP,ITMPE,JTMP,JTMPE,KTMP,KTMPE,oldsize(3),newsize(3),starts(3),arr) INTEGER :: NT, TCOUNT, DISPL(27) ENTRY U SOLV CALL CONTRACT(3,2,2,ID-1,JD-1,KD-1) CALL RELOAD !-----

N=1

CALL U_BC

CALL CONTRACT(3,2,2,ID-1,JD-1,KD-1) CALL RELOAD

CALL U_GEAS CALL U_BCAS

CALL FRAGMENT CALL RELOAD RCC(IIST:IIEND,JJST:JJEND,KKST:KKEND)=U(IIST:IIEND,JJST:JJEND,KKST:KKEND) CALL NEIGHBOUR U(IIST-1:IIEND+1,JJST-1:JJEND+1,KKST-1:KKEND+1)=RCC(IIST-1:IIEND+1,JJST-1:JJEND+1,KKST-1: KKEND+1)

CALL CONTRACT(3,2,2,ID-1,JD-1,KD-1) CALL RELOAD

DO 110 K=KKST,KKEND DO 110 J=JJST,JJEND DO 110 I=IIST,IIEND 110 SS(I,J,K)=USOR(I,J,K)-APC(I,J,K)*U(I,J,K)+AE(I,J,K)*U(I+1,J,K)+AW(I,J,K)*U(I-1,J,K)+AN(I,J,K)*U(I,J+1, K)+AS(I,J,K)*U(I,J-1,K)+AT(I,J,K)*U(I,J,K+1)+AB(I,J,K)*U(I,J,K-1) CALL U_BCSS

IT(N)=-1 100 IT(N)=IT(N)+1 ITER=IT(N)

if (taskid.eq.0) then IF(ITER .EQ. ITER /JMONIT*JMONIT .AND.ITIME .EQ. ITIME/JMONT *JMONT) WRITE(I69, 9004) CHT(N),ITER,U(IREF,JREF,KREF),SSMAX(N),FCMAX(N),RELAX(N),RELX2(N) endif

IF(ITER .GE. 1 .AND. SSMAX(N) .LE. ESMAX.AND. FCMAX(N) .LE. EFMAX) THEN

if (taskid.eq.0) then IF(ITIME .EQ. ITIME/JMONT*JMONT) WRITE(I69, 9004) CHT(N),ITER,U(IREF,JREF,KREF),SSMAX(N),FCMAX(N),RELAX(N),RELX2(N) endif

CALL U_BC

RETURN ENDIF

IF(ITER .GE. MIT(N)) THEN

if (taskid.eq.0) then WRITE(I69,*) ' ITERATION EXCEEDED FOR',CHT(N),ITIME endif STOP ENDIF CALL LNTDMA(N, ITER) CALL UC SET CALL ITERM1(N, ITER) CALL U_BC CALL FRAGMENT CALL RELOAD RCC(IIST:IIEND,JJST:JJEND,KKST:KKEND)=U(IIST:IIEND,JJST:JJEND,KKST:KKEND) CALL NEIGHBOUR U(IIST-1:IIEND+1,JJST-1:JJEND+1,KKST-1:KKEND+1)=RCC(IIST-1:IIEND+1,JJST-1:JJEND+1,KKST-1: KKEND+1) CALL CONTRACT(3,2,2,ID-1,JD-1,KD-1) CALL RELOAD DO 120 K=KKST,KKEND DO 120 J=JJST,JJEND DO 120 I=IIST,IIEND 120 SS(I,J,K)=USOR(I,J,K)-APC(I,J,K)*U(I,J,K)+AE(I,J,K)*U(I+1,J,K)+AW(I,J,K)*U(I-1,J,K)+AN(I,J,K)*U(I,J+1, K)+AS(I,J,K)*U(I,J-1,K)+AT(I,J,K)*U(I,J,K+1)+AB(I,J,K)*U(I,J,K-1) CALL U BCSS CALL ITERM2(N,ITER) **GOTO 100** ****** ENTRY V SOLV CALL CONTRACT(2,3,2,ID-1,JD-1,KD-1) CALL RELOAD !-----N=2 CALL V_BC CALL V_GEAS CALL V_BCAS CALL FRAGMENT CALL RELOAD RCC(IIST:IIEND,JJST:JJEND,KKST:KKEND)=V(IIST:IIEND,JJST:JJEND,KKST:KKEND) CALL NEIGHBOUR V(IIST-1:IIEND+1,JJST-1:JJEND+1,KKST-1:KKEND+1)=RCC(IIST-1:IIEND+1,JJST-1:JJEND+1,KKST-1: KKEND+1) CALL CONTRACT(2,3,2,ID-1,JD-1,KD-1)

CALL CONTRACT (2,3,2,1D-1,3D-1,KD-CALL RELOAD DO 210 K=KKST,KKEND DO 210 J=JJST,JJEND DO 210 I=IIST.IIEND 210 SS(I,J,K)=VSOR(I,J,K)-APC(I,J,K)*V(I,J,K)+AE(I,J,K)*V(I+1,J,K)+AW(I,J,K)*V(I-1,J,K)+AN(I,J,K)*V(I,J+1, K)+AS(I,J,K)*V(I,J-1,K)+AT(I,J,K)*V(I,J,K+1)+AB(I,J,K)*V(I,J,K-1) CALL V BCSS IT(N)=-1 200 IT(N)=IT(N)+1 ITER=IT(N) IF(ITER.EQ.ITER/JMONIT*JMONIT.AND.ITIME.EQ.ITIME/JMONT*JMONT) WRITE(I69, 9004) CHT(N),ITER,V(IREF,JREF,KREF),SSMAX(N),FCMAX(N),RELAX(N),RELX2(N) IF(ITER .GE. 1 .AND. SSMAX(N) .LE. ESMAX .AND. FCMAX(N) .LE. EFMAX) THEN IF(ITIME .EQ. ITIME/JMONT*JMONT) WRITE(I69, 9004) CHT(N),ITER,V(IREF,JREF,KREF),SSMAX(N),FCMAX(N),RELAX(N),RELX2(N) CALL V_BC RETURN **ENDIF** IF(ITER .GE. MIT(N)) THEN WRITE(I69,*) ' ITERATION EXCEEDED FOR',CHT(N),ITIME STOP **ENDIF** CALL LNTDMA(N, ITER) CALL VC SET CALL ITERM1(N,ITER) CALL V_BC CALL FRAGMENT CALL RELOAD RCC(IIST:IIEND,JJST:JJEND,KKST:KKEND)=V(IIST:IIEND,JJST:JJEND,KKST:KKEND) CALL NEIGHBOUR V(IIST-1:IIEND+1,JJST-1:JJEND+1,KKST-1:KKEND+1)=RCC(IIST-1:IIEND+1,JJST-1:JJEND+1,KKST-1: KKEND+1) CALL CONTRACT(2,3,2,ID-1,JD-1,KD-1) CALL RELOAD DO 220 K=KKST.KKEND DO 220 J=JJST,JJEND DO 220 I=IIST,IIEND 220 SS(I,J,K)=VSOR(I,J,K)-APC(I,J,K)*V(I,J,K)+AE(I,J,K)*V(I+1,J,K)+AW(I,J,K)*V(I-1,J,K)& +AN(I,J,K)*V(I,J+1,K)+AS(I,J,K)*V(I,J-1,K)+AT(I,J,K)*V(I,J,K+1)+AB(I,J,K)*V(I,J,K-1) & CALL V BCSS CALL ITERM2(N, ITER)

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GOTO 200 ***** ENTRY W SOLV CALL CONTRACT(2,2,3,ID-1,JD-1,KD-1) CALL RELOAD |_____ IF(I23.EQ.2) RETURN N=3 CALL W BC CALL W_GEAS CALL W BCAS CALL FRAGMENT CALL RELOAD RCC(IIST:IIEND,JJST:JJEND,KKST:KKEND)=W(IIST:IIEND,JJST:JJEND,KKST:KKEND) CALL NEIGHBOUR W(IIST-1:IIEND+1,JJST-1:JJEND+1,KKST-1:KKEND+1)=RCC(IIST-1:IIEND+1,JJST-1:JJEND+1,KKST-1 :KKEND+1) CALL CONTRACT(2,2,3,ID-1,JD-1,KD-1) CALL RELOAD DO 310 K=KKST,KKEND DO 310 J=JJST,JJEND DO 310 I=IIST, IIEND 310 SS(I,J,K)=WSOR(I,J,K)-APC(I,J,K)*W(I,J,K)+AE(I,J,K)*W(I+1,J,K)+AW(I,J,K)*W(I-1,J,K)+AN(I,J,K)*W(I,J,K) +1,K)+AS(I,J,K)*W(I,J-1,K)+AT(I,J,K)*W(I,J,K+1)+AB(I,J,K)*W(I,J,K-1) CALL W_BCSS IT(N)=-1 300 IT(N)=IT(N)+1 ITER=IT(N) IF(ITER .EQ. ITER /JMONIT*JMONIT .AND.& ITIME .EQ. ITIME/JMONT *JMONT)& & &WRITE(I69, 9004) CHT(N), ITER, W(IREF, JREF, KREF), SSMAX(N)& ,FCMAX(N),RELAX(N),RELX2(N) & IF(ITER .GE. 1 .AND. SSMAX(N) .LE. ESMAX& .AND. FCMAX(N) .LE. EFMAX) THEN & IF(ITIME .EQ. ITIME/JMONT*JMONT)& &WRITE(I69, 9004) CHT(N), ITER, W(IREF, JREF, KREF), SSMAX(N)& & ,FCMAX(N),RELAX(N),RELX2(N) CALL W BC RETURN ENDIF IF(ITER .GE. MIT(N)) THEN WRITE(I69,*) ' ITERATION EXCEEDED FOR', CHT(N), ITIME STOP

ENDIF

CALL LNTDMA(N,ITER) CALL WC_SET CALL ITERM1(N,ITER)

CALL W_BC

CALL FRAGMENT CALL RELOAD RCC(IIST:IIEND,JJST:JJEND,KKST:KKEND)=W(IIST:IIEND,JJST:JJEND,KKST:KKEND) CALL NEIGHBOUR W(IIST-1:IIEND+1,JJST-1:JJEND+1,KKST-1:KKEND+1)=RCC(IIST-1:IIEND+1,JJST-1:JJEND+1,KKST-1 :KKEND+1)

CALL CONTRACT(2,2,3,ID-1,JD-1,KD-1) CALL RELOAD

DO 320 K=KKST,KKEND DO 320 J=JJST,JJEND DO 320 I=IIST,IIEND 320 SS(I,J,K)=WSOR(I,J,K)-APC(I,J,K)*W(I,J,K)+AE(I,J,K)*W(I+1,J,K)+AW(I,J,K)*W(I-1,J,K)+AN(I,J,K)*W(I,J +1,K)+AS(I,J,K)*W(I,J-1,K)+AT(I,J,K)*W(I,J,K+1)+AB(I,J,K)*W(I,J,K-1)

CALL W_BCSS CALL ITERM2(N,ITER)

GOTO 300

CALL SHRINK CALL RELOAD

IF(IBOIL.EQ.0) RETURN N=4

CALL T_BC CALL T_GEAS CALL T_BCAS

CALL FRAGMENT CALL RELOAD RCC(IIST:IIEND,JJST:JJEND,KKST:KKEND)=T(IIST:IIEND,JJST:JJEND,KKST:KKEND) CALL NEIGHBOUR T(IIST-1:IIEND+1,JJST-1:JJEND+1,KKST-1:KKEND+1)=RCC(IIST-1:IIEND+1,JJST-1:JJEND+1,KKST-1: KKEND+1) CALL SHRINK CALL RELOAD

DO 410 K=KKST,KKEND

DO 410 J=JJST,JJEND DO 410 I=IIST,IIEND 410 SS(I,J,K)=TSOR(I,J,K)-APC(I,J,K)*T(I,J,K)+AE(I,J,K)*T(I+1,J,K)+AW(I,J,K)*T(I-1,J,K)+AN(I,J,K)*T(I,J+1,K))+AS(I,J,K)*T(I,J-1,K)+AT(I,J,K)*T(I,J,K+1)+AB(I,J,K)*T(I,J,K-1)

CALL T_BCSS

!-----

CALL

MPI_TYPE_CREATE_SUBARRAY(3,OLDSIZE,NEWSIZE,STARTS,MPI_ORDER_FORTRAN,MPI_DOU BLE_PRECISION,ARR,IERR) CALL MPI_TYPE_COMMIT(ARR,IERR)

DO NT=0,26 DISPL(1)=0 IF (NT.GT.0) DISPL(NT+1)= DISPL(NT)+1 SIZECC(NT)=1 ENDDO

CALL

MPI_ALLGATHERV(rcc,SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECISION,SS(1,1,1),SIZECC,DISPL, ARR,MPI_COMM_WORLD,IERR)

!-----

IF (TASKID.NE.0) THEN

CALL

MPI_SEND(SS(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRECI SION,0,TASKID,MPI_COMM_WORLD,IERR) ENDIF

IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(SS(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE(NT)),SIZECC(NT),MPI_DOUBLE_PRECISION,NT,NT,MPI_COMM_WORLD,STATUS,IERR) ENDDO ENDIF

CALL MPI_BARRIER(MPI_COMM_WORLD,IERR) CALL MPI_BCAST(SS(1,1,1),SIZE(SS),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR)

IT(N)=-1 400 IT(N)=IT(N)+1 ITER=IT(N)

if (taskid.eq.0) then IF (ITER .EQ. ITER /JMONIT*JMONIT .AND.ITIME .EQ. ITIME/JMONT *JMONT) WRITE(I69, 9004) CHT(N),ITER,T(IREF,JREF,KREF),SSMAX(N),FCMAX(N),RELAX(N),RELX2(N) endif

IF (ITER .GE. 1 .AND. SSMAX(N) .LE. ESMAX.AND. FCMAX(N) .LE. EFMAX) THEN if (taskid.eq.0) then

IF (ITIME .EQ. ITIME/JMONT*JMONT) WRITE(I69, 9004) CHT(N), ITER, T(IREF, JREF, KREF), SSMAX(N), FCMAX(N), RELAX(N), RELX2(N) endif CALL T BC RETURN ENDIF IF(ITER .GE. MIT(N)) THEN if (taskid.eq.0) then WRITE(I69,*) ' ITERATION EXCEEDED FOR',CHT(N),ITIME endif STOP ENDIF CALL LNTDMA(N, ITER) CALL TC SET CALL ITERM1(N,ITER) CALL T_BC CALL FRAGMENT CALL RELOAD RCC(IIST:IIEND,JJST:JJEND,KKST:KKEND)=T(IIST:IIEND,JJST:JJEND,KKST:KKEND) CALL NEIGHBOUR T(IIST-1:IIEND+1,JJST-1:JJEND+1,KKST-1:KKEND+1)=RCC(IIST-1:IIEND+1,JJST-1:JJEND+1,KKST-1: KKEND+1) CALL SHRINK CALL RELOAD DO 420 K= KKST, KKEND DO 420 J= JJST, JJEND DO 420 I= IIST, IIEND 420 SS(I,J,K)=TSOR(I,J,K)-APC(I,J,K)*T(I,J,K)+AE(I,J,K)*T(I+1,J,K)+AW(I,J,K)*T(I-1,J,K)+AN(I,J,K)*T(I,J+1,K))+AS(I,J,K)*T(I,J-1,K)+AT(I,J,K)*T(I,J,K+1)+AB(I,J,K)*T(I,J,K-1) CALL T BCSS CALL ITERM2(N, ITER) **GOTO 400** ENTRY P SOLV ******** CALL SHRINK CALL RELOAD I____ _____ N=5

DO 510 K=K11,KNK DO 510 J=1,NJ DO 510 I=1.NI SS(I,J,K)=0. AW(I,J,K)=0.AS(I,J,K)=0.AB(I,J,K)=0. AC(I,J,K)=0.510 AP(I,J,K)=0. CALL P BC CALL P GEAS CALL MU GEAP CALL M1PRTD(I23,MX(1),MY(1),MZ(1)) IF(MULT .GE. 2) CALL M2PRTD(I23,MX(2),MY(2),MZ(2)) IF(MULT .GE. 3) CALL M3PRTD(I23,MX(3),MY(3),MZ(3)) IF(MULT .GE. 4) CALL M4PRTD(I23,MX(4),MY(4),MZ(4)) IF(MULT .GE. 5) CALL M5PRTD(I23,MX(5),MY(5),MZ(5)) IF(MULT .GE. 6) CALL M6PRTD(I23,MX(6),MY(6),MZ(6)) DO 530 K=2,NKM DO 530 J=2,NJM DO 530 I=2,NIM 530 SS(I,J,K)=PSOR(I,J,K)-APC(I,J,K)*P(I,J,K)+AE(I,J,K)*P(I+1,J,K)+AW(I,J,K)*P(I-1,J,K)+AN(I,J,K)*P(I,J+1, K)+AS(I,J,K)*P(I,J-1,K)+AT(I,J,K)*P(I,J,K+1)+AB(I,J,K)*P(I,J,K-1)

!-----SUM=0. DO 540 K=2,NKM DO 540 J=2,NJM DO 540 I=2,NIM 540 SUM=SUM+SS(I,J,K) IF(ITIME .EQ. ITIME/JMONT*JMONT) WRITE(I69,9003) ' ***SUM=',SUM

IT(N)=-1 500 IT(N)=IT(N)+1

ITER=IT(N)

IF(ITER.EQ.ITER/JMONIT*JMONIT.AND.ITIME.EQ.ITIME/JMONT*JMONT) WRITE(I69, 9004) CHT(N),ITER,P(IREF,JREF,KREF),SSMAX(N),FCMAX(N),RELAX(N),RELX2(N)

IF(ITER.GE.1.AND.SSMAX(N).LE.ESMAX.AND. FCMAX(N) .LE. EFMAX) THEN

IF(ITIME .EQ. ITIME/JMONT*JMONT) WRITE(I69, 9004) CHT(N),ITER,P(IREF,JREF,KREF),SSMAX(N),FCMAX(N),RELAX(N),RELX2(N)

CALL P_BC RETURN ENDIF IF(ITER .GE. MIT(N)) THEN WRITE(I69,*) ' ITERATION EXCEEDED FOR', CHT(N), ITIME ! STOP CALL P BC RETURN ENDIF CALL MU_GESS DO 550 K=1,NK DO 550 J=1,NJ DO 550 I=1,NI 550 CC(I,J,K)=0. IF(MULT .GE. 6) CALL M6VTDMA(I23,MX(6),MY(6),MZ(6)) IF(MULT .GE. 6) CALL MU PRCC(I23,MX(6),MY(6),MZ(6),6) IF(MULT .GE. 5) CALL M5VTDMA(I23,MX(5),MY(5),MZ(5)) IF(MULT .GE. 5) CALL MU_PRCC(I23,MX(5),MY(5),MZ(5),5) IF(MULT .GE. 4) CALL M4VTDMA(I23,MX(4),MY(4),MZ(4)) IF(MULT .GE. 4) CALL MU_PRCC(I23,MX(4),MY(4),MZ(4),4) IF(MULT .GE. 3) CALL M3VTDMA(I23,MX(3),MY(3),MZ(3)) IF(MULT .GE. 3) CALL MU_PRCC(I23,MX(3),MY(3),MZ(3),3) IF(MULT .GE. 2) CALL M2VTDMA(I23,MX(2),MY(2),MZ(2)) IF(MULT .GE. 2) CALL MU PRCC(I23,MX(2),MY(2),MZ(2),2) CALL M1VTDMA(I23,MX(1),MY(1),MZ(1)) CALL SHRINK CALL RELOAD CALL ITERM1(N, ITER) CALL P BC DO 560 K=2,NKM DO 560 J=2,NJM DO 560 I=2,NIM SS(I,J,K)=PSOR(I,J,K)-APC(I,J,K)*P(I,J,K)+AE(I,J,K)*P(I+1,J,K)+AW(I,J,K)*P(I-1,J,K)& 560 & +AN(I,J,K)*P(I,J+1,K)+AS(I,J,K)*P(I,J-1,K)+AT(I,J,K)*P(I,J,K+1)+AB(I,J,K)*P(I,J,K-1) CALL ITERM2(N, ITER) **GOTO 500** 9003 FORMAT(A,5(1PE12.4)) 9004 FORMAT(A,I5,6(1PE12.4)) 9005 FORMAT(I3,I3,6(1PE12.4)) END SUBROUTINE V GEAS **USE PARAMETERS USE ICHOS USE PROPS**

USE INDDT USE IGRID USE IBNDS USE GRID1 USE GRIDB **USE GRIDL USE LEVFN USE ULVLL USE FFSOR USE ROGAM USE QMSOR USE APANS USE AEANS USE UVTPP** USE CALC1 USE FUNC **USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,L,NT REAL (KIND=8) :: DXE,DXW,DYN,DYS,DZB,DZT,DIFB,DIFE,DIFN,DIFS,DIFT,DIFW,DVIM,DVDY,DXEE,DXWW,DYNN,DY SS, DZBB, DZTT REAL (KIND=8) :: RPU,VXE,VYN,VYS,VXW,VZB,VZT,VXEE,VXWW,VXXE,VXXP,VXXW,VYNN,VYSS,VYYN,VYYP,VYYS, VZBB,VZTT,VZZB,VZZP,VZZT REAL (KIND=8) :: FLUX,FLX,FLY,FLZ,VX,VY,VZ,FBDY,TMV REAL (KIND=8) :: VISB, VISE, VISM, VISN, VISS, VIST, VISW LOGICAL T_FW,T_FE,T_FS,T_FN,T_FB,T_FT,T_2D,T_3D LOGICAL T_SW,T_SE,T_SS,T_SN,T_SB,T_ST T_2D=I23.EQ.2 T 3D=.NOT. T 2D DO 10 K=KKST,KKEND DO 10 J=JJST,JJEND DO 10 I=IIST.IIEND TMV=T(I,J,K)*YDS(J)+T(I,J-1,K)*YDN(J)FBDY=IGRAV*(-1.+BT0*DTWS*TMV) IF(FV(I,J,K).LE.0.) FBDY=IGRAV*(-1.) VSOR(I,J,K)=RP(I)*RHOV(I,J,K)*FBDY 10 SS(I,J,K)=0. 1__ DO 100 K=KKST,KKEND DO 100 J=JJST,JJEND DO 100 I=IIST,IIEND IF(SV(I,J,K).LE.0.) GOTO 100 L=1 IF(FV(I,J,K).GT.0.) L=2 I___ FLX=0.25*(RU(I+1)*(UL(I+1,J,K,L)+UL(I+1,J-1,K,L))+RU(I)*(UL(I ,J,K,L)+UL(I ,J-1,K,L))) FLY=0.25*RP(I)*(VL(I,J+1,K,L)+2.*VL(I,J,K,L)+VL(I,J-1,K,L))-RP(I)*VBUB IF(T_3D) FLZ=0.25*(WL(I,J,K+1,L)+WL(I,J-1,K+1,L)+WL(I,J,K ,L)+WL(I,J-1,K ,L))

I_____

VISW=1./VISMF(FV(I,J,K),FV(I-1,J,K),FU(I ,J,K),FU(I ,J-1,K),FC(I ,J,K),FC(I ,J,K+1)) VISE=1./VISMF(FV(I,J,K),FV(I+1,J,K),FU(I+1,J,K),FU(I+1,J-1,K),FC(I+1,J,K),FC(I+1,J,K+1)) VISS=1./VISMF(FV(I,J,K),FV(I,J-1,K),FU(I,J-1,K),FU(I+1,J-1,K),FW(I,J-1,K),FW(I,J-1,K+1)) VISN=1./VISMF(FV(I,J,K),FV(I,J+1,K),FU(I,J ,K),FU(I+1,J ,K),FW(I,J ,K),FW(I,J ,K+1)) IF(T 3D) THEN VISB=1./VISMF(FV(I,J,K),FV(I,J,K-1),FW(I,J,K),FW(I,J-1,K),FC(I,J,K),FC(I+1,J,K)) VIST=1./VISMF(FV(I,J,K),FV(I,J,K+1),FW(I,J,K+1),FW(I,J-1,K+1),FC(I,J,K+1),FC(I+1,J,K+1)) ENDIF I____ DXW=XD(I)*FAC_EPS(SV(I,J,K),SV(I-1,J,K)) DXE=XD(I+1)*FAC EPS(SV(I,J,K),SV(I+1,J,K)) DYS=YC(J-1)*FAC EPS(SV(I,J,K),SV(I,J-1,K)) DYN=YC(J)*FAC EPS(SV(I,J,K),SV(I,J+1,K)) IF(T 3D) THEN DZB=ZD(K)*FAC_EPS(SV(I,J,K),SV(I,J,K-1)) DZT=ZD(K+1)*FAC EPS(SV(I,J,K),SV(I,J,K+1)) ENDIF !----- Digonal Diffusion AW(I,J,K)=VISW*RU(I)/DXW/XC(I) AE(I,J,K)=VISE*RU(I+1)/DXE/XC(I) AS(I,J,K)=VISS*RP(I)/DYS/YD(J) AN(I,J,K)=VISN*RP(I)/DYN/YD(J) IF(T 3D) THEN AB(I,J,K)=VISB/DZB/ZC(K) AT(I,J,K)=VIST/DZT/ZC(K) ENDIF !----- Off-Digonal Diffusion . !----- [mr(du/dy)]e-w/dx DIFW=VISW*RU(I)*(UL(I,J,K,L)-UL(I,J-1,K,L))/YD(J) DIFE=VISE*RU(I+1)*(UL(I+1,J,K,L)-UL(I+1,J-1,K,L))/YD(J) VSOR(I,J,K)=VSOR(I,J,K)+(DIFE-DIFW)/XC(I) !----- [mr(dv/dy)]n-s/dy DIFS=VISS*RP(I)*(VL(I,J ,K,L)-VL(I,J-1,K,L))/YC(J-1) DIFN=VISN*RP(I)*(VL(I,J+1,K,L)-VL(I,J ,K,L))/YC(J)VSOR(I,J,K)=VSOR(I,J,K)+(DIFN-DIFS)/YD(J) !----- [m(dw/dy)]t-b/dz IF(T 3D) THEN DIFB=VISB*(WL(I,J,K ,L)-WL(I,J-1,K ,L))/YD(J) DIFT=VIST*(WL(I,J,K+1,L)-WL(I,J-1,K+1,L))/YD(J) VSOR(I,J,K)=VSOR(I,J,K)+(DIFT-DIFB)/ZC(K) ENDIF 1__ ----- Convection VXW=(VL(I,J,K,L)-VL(I-1,J,K,L))/DXW VXE=(VL(I+1,J,K,L)-VL(I,J,K,L))/DXE VYS=(VL(I,J,K,L)-VL(I,J-1,K,L))/DYS VYN=(VL(I,J+1,K,L)-VL(I,J,K,L))/DYN IF(FLX.GE.0.) VX=VXW IF(FLX.LT.0.) VX=VXE IF(FLY.GE.0.) VY=VYS IF(FLY.LT.0.) VY=VYN 1___

IF(T_3D) THEN

VZB=(VL(I,J,K,L)-VL(I,J,K-1,L))/DZB VZT=(VL(I,J,K+1,L)-VL(I,J,K,L))/DZT IF(FLZ.GE.0.) VZ=VZB IF(FLZ.LT.0.) VZ=VZT ENDIF IF(IENO.EQ.0) GOTO 150 I____ VXXP=(VXE-VXW)/(DXE+DXW) VYYP=(VYN-VYS)/(DYN+DYS) IF(T 3D) VZZP=(VZT-VZB)/(DZT+DZB) !----- X DIRECTION IF(FLX.GE.0.) THEN IF(I.EQ.2 .OR. T 2PH(SV(I,J,K),SV(I-1,J,K))) THEN VX=VX+DXE*VXXP ELSE DXWW=XD(I-1)*FAC EPS(SV(I-1,J,K),SV(I-2,J,K)) VXWW=(VL(I-1,J,K,L)-VL(I-2,J,K,L))/DXWW VXXW=(VXW-VXWW)/(DXW+DXWW) VX=VX+DXE*AMIN2(VXXP,VXXW) **ENDIF** ELSE IF(I.EQ.NIM .OR. T 2PH(SV(I,J,K),SV(I+1,J,K))) THEN VX=VX-DXW*VXXP ELSE DXEE=XD(I+2)*FAC EPS(SV(I+1,J,K),SV(I+2,J,K)) VXEE=(VL(I+2,J,K,L)-VL(I+1,J,K,L))/DXEE VXXE=(VXEE-VXE)/(DXEE+DXE) VX=VX-DXW*AMIN2(VXXP,VXXE) **ENDIF** ENDIF 1_____ IF(FLY.GE.0.) THEN IF(J.EQ.3 .OR. T_2PH(SV(I,J,K),SV(I,J-1,K))) THEN VY=VY+DYN*VYYP ELSE DYSS=YC(J-2)*FAC EPS(SV(I,J-1,K),SV(I,J-2,K)) VYSS=(VL(I,J-1,K,L)-VL(I,J-2,K,L))/DYSS VYYS=(VYS-VYSS)/(DYS+DYSS) VY=VY+DYN*AMIN2(VYYP,VYYS) ENDIF ELSE IF(J.EQ.NJM .OR. T_2PH(SV(I,J,K),SV(I,J+1,K))) THEN VY=VY-DYS*VYYP ELSE DYNN=YC(J+1)*FAC EPS(SV(I,J+1,K),SV(I,J+2,K)) VYNN=(VL(I,J+2,K,L)-VL(I,J+1,K,L))/DYNN VYYN=(VYNN-VYN)/(DYNN+DYN) VY=VY-DYS*AMIN2(VYYP,VYYN) ENDIF ENDIF I____

IF(T_2D) GOTO 150

IF(FLZ.GE.0.) THEN IF(K.EQ.2 .OR. T 2PH(SV(I,J,K),SV(I,J,K-1))) THEN VZ=VZ+DZT*VZZP ELSE DZBB=ZD(K-1)*FAC EPS(SV(I,J,K-1),SV(I,J,K-2)) VZBB=(VL(I,J,K-1,L)-VL(I,J,K-2,L))/DZBB VZZB=(VZB-VZBB)/(DZB+DZBB) VZ=VZ+DZT*AMIN2(VZZP,VZZB) ENDIF ELSE IF(K.EQ.NKM .OR. T_2PH(SV(I,J,K),SV(I,J,K+1))) THEN VZ=VZ-DZB*VZZP ELSE DZTT=ZD(K+2)*FAC_EPS(SV(I,J,K+1),SV(I,J,K+2)) VZTT=(VL(I,J,K+2,L)-VL(I,J,K+1,L))/DZTT VZZT=(VZTT-VZT)/(DZTT+DZT) VZ=VZ-DZB*AMIN2(VZZP,VZZT) ENDIF ENDIF !-----150 FLUX=FLX*VX+FLY*VY+FLZ*VZ VSOR(I,J,K)=VSOR(I,J,K)+RHOV(I,J,K)*(RP(I)*VL(I,J,K,L)/DT-FLUX) 100 CONTINUE !----------BC DO 210 K=KKST,KKEND DO 210 J=JJST,JJEND IF(IBCW.EQ.IOUT .OR. IBCW.EQ.ISYM) AW(2,J,K)=0. IF(IBCE.EQ.IOUT .OR. IBCE.EQ.ISYM) AE(NIM,J,K)=0. 210 CONTINUE IF(T_2D) GOTO 225 DO 220 J=JJST,JJEND DO 220 I=IIST,IIEND IF(IBCB.EQ.IOUT .OR. IBCB.EQ.ISYM) AB(I,J, 2)=0. IF(IBCT.EQ.IOUT .OR. IBCT.EQ.ISYM) AT(I,J,NKM)=0. 220 CONTINUE |_____ 225 IF(IBOIL.EQ.0) GOTO 390 DO 300 K=KKST.KKEND DO 300 J=JJST,JJEND DO 300 I=IIST,IIEND IF(T_2PH(FV(I,J,K),FV(I-1,J,K))) THEN DVIM=(FV(I,J,K)*AMY(I-1,J,K)-FV(I-1,J,K)*AMY(I,J,K))& /ABS(FV(I,J,K)-FV(I-1,J,K))*VFG & SS(I,J,K)=SS(I,J,K)+AW(I,J,K)*DVIM ENDIF IF(T 2PH(FV(I,J,K),FV(I+1,J,K))) THEN DVIM=(FV(I,J,K)*AMY(I+1,J,K)-FV(I+1,J,K)*AMY(I,J,K))& & /ABS(FV(I,J,K)-FV(I+1,J,K))*VFG SS(I,J,K)=SS(I,J,K)+AE(I,J,K)*DVIM ENDIF

IF(T_2PH(FV(I,J,K),FV(I,J-1,K))) THEN DVIM=(FV(I,J,K)*AMY(I,J-1,K)-FV(I,J-1,K)*AMY(I,J,K))& & /ABS(FV(I,J,K)-FV(I,J-1,K))*VFG SS(I,J,K)=SS(I,J,K)+AS(I,J,K)*DVIM ENDIF

IF(T_2PH(FV(I,J,K),FV(I,J+1,K))) THEN DVIM=(FV(I,J,K)*AMY(I,J+1,K)-FV(I,J+1,K)*AMY(I,J,K))& & /ABS(FV(I,J,K)-FV(I,J+1,K))*VFG SS(I,J,K)=SS(I,J,K)+AN(I,J,K)*DVIM ENDIF

IF(T_2D) GOTO 300 IF(T_2PH(FV(I,J,K),FV(I,J,K-1))) THEN DVIM=(FV(I,J,K)*AMY(I,J,K-1)-FV(I,J,K-1)*AMY(I,J,K))& & /ABS(FV(I,J,K)-FV(I,J,K-1))*VFG SS(I,J,K)=SS(I,J,K)+AB(I,J,K)*DVIM ENDIF

IF(T_2PH(FV(I,J,K),FV(I,J,K+1))) THEN DVIM=(FV(I,J,K)*AMY(I,J,K+1)-FV(I,J,K+1)*AMY(I,J,K))& & /ABS(FV(I,J,K)-FV(I,J,K+1))*VFG SS(I,J,K)=SS(I,J,K)+AT(I,J,K)*DVIM ENDIF

300 CONTINUE

390 CONTINUE DO 400 K=KKST,KKEND DO 400 J=JJST,JJEND DO 400 I=IIST,IIEND VSOR(I,J,K)=VSOR(I,J,K)+SS(I,J,K) AP(I,J,K)=RHOV(I,J,K)*RP(I)/DT+AE(I,J,K)+AW(I,J,K)+AN(I,J,K)+AS(I,J,K)+AT(I,J,K)+AB(I,J,K) 400 APC(I,J,K)=AP(I,J,K)

IF (TASKID.NE.0) THEN CALL MPI_SEND(VSOR(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI_DOUBLE_PRE CISION,0,TASKID,MPI_COMM_WORLD,IERR) ENDIF

IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(VSOR(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZE (NT)),SIZECC(NT),MPI_DOUBLE_PRECISION,NT,NT,MPI_COMM_WORLD,STATUS,IERR) ENDDO ENDIF

CALL MPI_BARRIER(MPI_COMM_WORLD,IERR) CALL MPI_BCAST(VSOR(1,1,1),SIZE(VSOR),MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,IERR) RETURN END

SUBROUTINE W GEAS ******* **USE PARAMETERS USE ICHOS USE PROPS** USE INDDT **USE IGRID USE IBNDS USE GRID1 USE GRIDB** USE GRIDL USE LEVFN USE ULVLL **USE FFSOR USE ROGAM** USE QMSOR **USE FNXYZ USE APANS** USE AEANS **USE UVTPP** USE CALC1 **USE FUNC USE MPIVAR** IMPLICIT NONE INTEGER :: I,J,K,L,NT REAL (KIND=8) :: DXW,DXE,DYN,DYS,DZT,DZB,DYSS,DYNN,DZTT,DZBB,DXWW,DXEE,DWIM,DIFW,DIFT,DIFS,DIFN, DIFE, DIFB REAL (KIND=8) :: WX,WY,WZ,WXW,WXE,WZT,WZB,WYN,WYS,WXXW,WXXP,WXXE,WXEE,WXWW,WYNN,WYYS,WY YP,WYYN,WYSS,WZBB,WZZT,WZZP,WZZB,WZTT REAL (KIND=8) :: VIST, VISB, VISE, VISW, VISN, VISS, FLX, FLZ, FLY, FLUX LOGICAL T_FW,T_FE,T_FS,T_FN,T_FB,T_FT,T_2D,T_3D LOGICAL T SW,T SE,T SS,T SN,T SB,T ST DO 10 K=KKST,KKEND DO 10 J=JJST,JJEND DO 10 I=IIST,IIEND WSOR(I,J,K)=0. 10 SS(I,J,K)=0. 1___ DO 100 K=KKST,KKEND DO 100 J=JJST,JJEND DO 100 I=IIST,IIEND IF(SW(I,J,K).LE.0.) GOTO 100 L=1 IF(FW(I,J,K).GT.0.) L=2 <u>|</u>_.

FLX=0.25*(UL(I+1,J,K,L)+UL(I+1,J,K-1,L)&

+UL(I ,J,K,L)+UL(I ,J,K-1,L))FLY=0.25*(VL(I,J+1,K,L)+VL(I,J+1,K-1,L)& & +VL(I,J ,K,L)+VL(I,J ,K-1,L))-VBUB FLZ=0.25*(WL(I,J,K+1,L)+2.*WL(I,J,K,L)+WL(I,J,K-1,L)) [-----VISW=1./VISMF(FW(I,J,K),FW(I-1,J,K),FU(I ,J,K),FU(I ,J,K-1)& ,FC(I ,J,K),FC(I ,J+1,K)) & VISE=1./VISMF(FW(I,J,K),FW(I+1,J,K),FU(I+1,J,K),FU(I+1,J,K-1)& ,FC(I+1,J,K),FC(I+1,J+1,K)) ጲ VISS=1./VISMF(FW(I,J,K),FW(I,J-1,K),FV(I,J ,K),FV(I,J ,K-1)& ,FC(I,J ,K),FC(I+1,J ,K)) & VISN=1./VISMF(FW(I,J,K),FW(I,J+1,K),FV(I,J+1,K),FV(I,J+1,K-1)& ,FC(I,J+1,K),FC(I+1,J+1,K)) & VISB=1./VISMF(FW(I,J,K),FW(I,J,K-1),FU(I,J,K-1),FU(I+1,J,K-1)& & ,FV(I,J,K-1),FV(I,J+1,K-1)) VIST=1./VISMF(FW(I,J,K),FW(I,J,K+1),FU(I,J,K),FU(I+1,J,K))& & ,FV(I,J,K),FV(I,J+1,K)) 1__ DXW=XD(I)*FAC EPS(SW(I,J,K),SW(I-1,J,K)) DXE=XD(I+1)*FAC_EPS(SW(I,J,K),SW(I+1,J,K)) DYS=YD(J)*FAC_EPS(SW(I,J,K),SW(I,J-1,K)) DYN=YD(J+1)*FAC EPS(SW(I,J,K),SW(I,J+1,K))DZB=ZC(K-1)*FAC_EPS(SW(I,J,K),SW(I,J,K-1)) DZT=ZC(K)*FAC EPS(SW(I,J,K),SW(I,J,K+1)) !----- Digonal Diffusion AW(I,J,K)=VISW/DXW/XC(I) AE(I,J,K)=VISE/DXE/XC(I) AS(I,J,K)=VISS/DYS/YC(J) AN(I,J,K)=VISN/DYN/YC(J) AB(I,J,K)=VISB/DZB/ZD(K) AT(I,J,K)=VIST/DZT/ZD(K) !----- Off-Digonal Diffusion ----- [m(du/dz)]e-w/dx DIFW=VISW*(UL(I ,J,K,L)-UL(I ,J,K-1,L))/ZD(K) DIFE=VISE*(UL(I+1,J,K,L)-UL(I+1,J,K-1,L))/ZD(K) WSOR(I,J,K)=WSOR(I,J,K)+(DIFE-DIFW)/XC(I) !----- [m(dv/dz)]n-s/dy DIFS=VISS*(VL(I,J ,K,L)-VL(I,J ,K-1,L))/ZD(K) DIFN=VISN*(VL(I,J+1,K,L)-VL(I,J+1,K-1,L))/ZD(K) WSOR(I,J,K)=WSOR(I,J,K)+(DIFN-DIFS)/YC(J) !----- [m(dw/dz)]t-b/dz DIFB=VISB*(WL(I,J,K ,L)-WL(I,J,K-1,L))/ZC(K-1) DIFT=VIST*(WL(I,J,K+1,L)-WL(I,J,K ,L))/ZC(K) WSOR(I,J,K)=WSOR(I,J,K)+(DIFT-DIFB)/ZD(K) -- Convection WXW=(WL(I,J,K,L)-WL(I-1,J,K,L))/DXW WXE=(WL(I+1,J,K,L)-WL(I,J,K,L))/DXE WYS=(WL(I,J,K,L)-WL(I,J-1,K,L))/DYS WYN=(WL(I,J+1,K,L)-WL(I,J,K,L))/DYN WZB=(WL(I,J,K,L)-WL(I,J,K-1,L))/DZBWZT=(WL(I,J,K+1,L)-WL(I,J,K,L))/DZT

IF(FLX.GE.0.) WX=WXW

IF(FLX.LT.0.) WX=WXE IF(FLY.GE.0.) WY=WYS IF(FLY.LT.0.) WY=WYN IF(FLZ.GE.0.) WZ=WZB IF(FLZ.LT.0.) WZ=WZT IF(IENO.EQ.0) GOTO 150 I---WXXP=(WXE-WXW)/(DXE+DXW) WYYP=(WYN-WYS)/(DYN+DYS) WZZP=(WZT-WZB)/(DZT+DZB) !----- X DIRECTION IF(FLX.GE.0.) THEN IF(I.EQ.2 .OR. T 2PH(SW(I,J,K),SW(I-1,J,K))) THEN WX=WX+DXE*WXXP ELSE DXWW=XD(I-1)*FAC EPS(SW(I-1,J,K),SW(I-2,J,K))WXWW=(WL(I-1,J,K,L)-WL(I-2,J,K,L))/DXWW WXXW=(WXW-WXWW)/(DXW+DXWW) WX=WX+DXE*AMIN2(WXXP,WXXW) ENDIF ELSE IF(I.EQ.NIM .OR. T_2PH(SW(I,J,K),SW(I+1,J,K))) THEN WX=WX-DXW*WXXP ELSE DXEE=XD(I+2)*FAC EPS(SW(I+1,J,K),SW(I+2,J,K)) WXEE=(WL(I+2,J,K,L)-WL(I+1,J,K,L))/DXEE WXXE=(WXEE-WXE)/(DXEE+DXE) WX=WX-DXW*AMIN2(WXXP,WXXE) ENDIF ENDIF 1-----IF(FLY.GE.0.) THEN IF(J.EQ.2 .OR. T_2PH(SW(I,J,K),SW(I,J-1,K))) THEN WY=WY+DYN*WYYP ELSE DYSS=YD(J-1)*FAC EPS(SW(I,J-1,K),SW(I,J-2,K)) WYSS=(WL(I,J-1,K,L)-WL(I,J-2,K,L))/DYSS WYYS=(WYS-WYSS)/(DYS+DYSS) WY=WY+DYN*AMIN2(WYYP,WYYS) ENDIF ELSE IF(J.EQ.NJM .OR. T_2PH(SW(I,J,K),SW(I,J+1,K))) THEN WY=WY-DYS*WYYP ELSE DYNN=YD(J+2)*FAC EPS(SW(I,J+1,K),SW(I,J+2,K)) WYNN=(WL(I,J+2,K,L)-WL(I,J+1,K,L))/DYNN WYYN=(WYNN-WYN)/(DYNN+DYN) WY=WY-DYS*AMIN2(WYYP,WYYN) ENDIF ENDIF I___

IF(FLZ.GE.0.) THEN IF(K.EQ.3 .OR. T_2PH(SW(I,J,K),SW(I,J,K-1))) THEN
WZ=WZ+DZT*WZZP ELSE DZBB=ZC(K-2)*FAC_EPS(SW(I,J,K-1),SW(I,J,K-2)) WZBB=(WL(I,J,K-1,L)-WL(I,J,K-2,L))/DZBB WZZB=(WZB-WZBB)/(DZB+DZBB) WZ=WZ+DZT*AMIN2(WZZP,WZZB) ENDIF ELSE IF(K.EQ.NKM .OR. T_2PH(SW(I,J,K),SW(I,J,K+1))) THEN WZ=WZ-DZB*WZZP ELSE DZTT=ZC(K+1)*FAC EPS(SW(I,J,K+1),SW(I,J,K+2)) WZTT=(WL(I,J,K+2,L)-WL(I,J,K+1,L))/DZTT WZZT=(WZTT-WZT)/(DZTT+DZT) WZ=WZ-DZB*AMIN2(WZZP,WZZT) ENDIF ENDIF I____ 150 FLUX=FLX*WX+FLY*WY+FLZ*WZ WSOR(I,J,K)=WSOR(I,J,K)+RHOW(I,J,K)*(WL(I,J,K,L)/DT-FLUX) 100 CONTINUE -----BC [-----DO 210 K=KKST,KKEND DO 210 J=JJST,JJEND IF(IBCW.EQ.IOUT .OR. IBCW.EQ.ISYM) AW(2,J,K)=0. IF(IBCE.EQ.IOUT .OR. IBCE.EQ.ISYM) AE(NIM,J,K)=0. 210 CONTINUE DO 220 K=KKST,KKEND DO 220 I=IIST,IIEND IF(IBCS.EQ.IOUT .OR. IBCS.EQ.ISYM) AS(I, 2,K)=0. IF(IBCN.EQ.IOUT .OR. IBCN.EQ.ISYM) AN(I,NJM,K)=0. 220 CONTINUE IF(IBOIL.EQ.0) GOTO 390 DO 300 K=KKST.KKEND DO 300 J=JJST,JJEND DO 300 I=IIST,IIEND IF(T 2PH(FW(I,J,K),FW(I-1,J,K))) THEN DWIM=(FW(I,J,K)*AMZ(I-1,J,K)-FW(I-1,J,K)*AMZ(I,J,K))& /ABS(FW(I,J,K)-FW(I-1,J,K))*VFG & SS(I,J,K)=SS(I,J,K)+AW(I,J,K)*DWIM ENDIF IF(T 2PH(FW(I,J,K),FW(I+1,J,K))) THEN DWIM=(FW(I,J,K)*AMZ(I+1,J,K)-FW(I+1,J,K)*AMZ(I,J,K))& & /ABS(FW(I,J,K)-FW(I+1,J,K))*VFG SS(I,J,K)=SS(I,J,K)+AE(I,J,K)*DWIMENDIF IF(T 2PH(FW(I,J,K),FW(I,J-1,K))) THEN

DWIM=(FW(I,J,K)*AMZ(I,J-1,K)-FW(I,J-1,K)*AMZ(I,J,K))& & /ABS(FW(I,J,K)-FW(I,J-1,K))*VFG SS(I,J,K)=SS(I,J,K)+AS(I,J,K)*DWIM ENDIF IF(T 2PH(FW(I,J,K),FW(I,J+1,K))) THEN DWIM=(FW(I,J,K)*AMZ(I,J+1,K)-FW(I,J+1,K)*AMZ(I,J,K))& /ABS(FW(I,J,K)-FW(I,J+1,K))*VFG & SS(I,J,K)=SS(I,J,K)+AN(I,J,K)*DWIM ENDIF IF(T_2PH(FW(I,J,K),FW(I,J,K-1))) THEN DWIM=(FW(I,J,K)*AMZ(I,J,K-1)-FW(I,J,K-1)*AMZ(I,J,K))& /ABS(FW(I,J,K)-FW(I,J,K-1))*VFG & SS(I,J,K)=SS(I,J,K)+AB(I,J,K)*DWIMENDIF IF(T 2PH(FW(I,J,K),FW(I,J,K+1))) THEN DWIM=(FW(I,J,K)*AMZ(I,J,K+1)-FW(I,J,K+1)*AMZ(I,J,K))& & /ABS(FW(I,J,K)-FW(I,J,K+1))*VFG SS(I,J,K)=SS(I,J,K)+AT(I,J,K)*DWIM ENDIF 300 CONTINUE I____ 390 CONTINUE DO 400 K=KKST,KKEND DO 400 J=JJST.JJEND DO 400 I=IIST,IIEND WSOR(I,J,K)=WSOR(I,J,K)+SS(I,J,K)AP(I,J,K)=RHOW(I,J,K)/DT+AE(I,J,K)+AW(I,J,K)+AN(I,J,K)+AS(I,J,K)+AT(I,J,K)+AB(I,J,K) APC(I,J,K)=AP(I,J,K)400 IF (TASKID.NE.0) THEN CALL MPI SEND(WSOR(IIST:IIEND,JJST:JJEND,KKST:KKEND),SPANX*SPANY*SPANZ,MPI DOUBLE PR ECISION,0,TASKID,MPI_COMM_WORLD,IERR) **ENDIF** IF (TASKID.EQ.0) THEN DO NT=1,26 CALL MPI_RECV(WSOR(RSPANX(NT):RSPANXE(NT),RSPANY(NT):RSPANYE(NT),RSPANZ(NT):RSPANZ E(NT)),SIZECC(NT),MPI DOUBLE PRECISION,NT,NT,MPI COMM WORLD,STATUS,IERR) **ENDDO ENDIF** CALL MPI BARRIER(MPI COMM WORLD, IERR) CALL MPI BCAST(WSOR(1,1,1),SIZE(WSOR),MPI DOUBLE PRECISION.0,MPI COMM WORLD,IERR)

RETURN END