Title

Topical center for terascale simulation of the plasma physics of intense ion beams for inertial fusion energy

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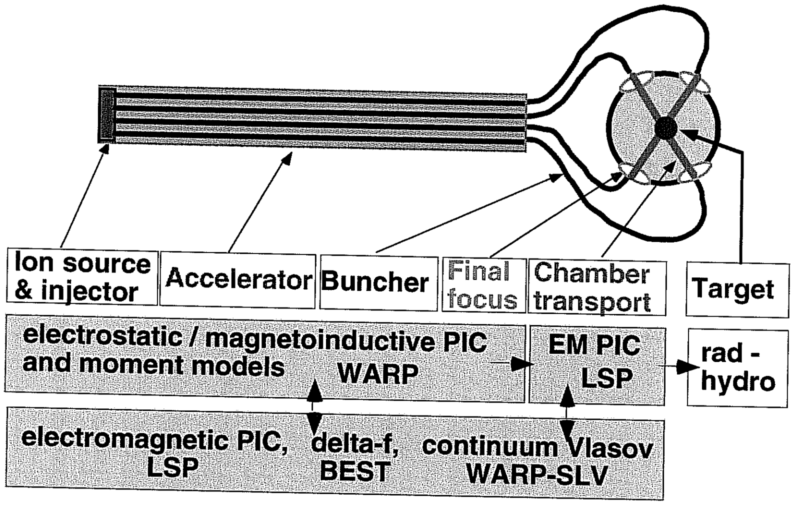
Scientific Discovery through Advanced Computing: Advanced Computational Research in Fusion Science
Announcement LAB 01-10 and Program Notice 01-10

Topical Center for Terascale Simulation of the Plasma Physics of Intense Ion Beams for Inertial Fusion Energy*



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*This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore and Lawrence Berkeley National Laboratories under Contract Numbers W-7405-Eng-48 and DE-AC03-76SF00098, by the Princeton Plasma Physics Laboratory under Contract Number DE-AC02-76CH03073, by the University of Maryland under Contract Number DE-FG02-92ER54178, and by the Naval Research Laboratory under Contract Number DE-AI02-94ER54232.

Scientific Discovery through Advanced Computing: Advanced Computational Research in Fusion Science
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Cover Letter: Collaboration of DOE National Laboratories with Private Sector

Topical Center for Terascale Simulation of the Plasma Physics of Intense Ion Beams for Inertial Fusion Energy

Principal Investigators: Alex Friedman, *LLNL and LBNL*
Ronald C. Davidson, *PPPL*
Dale R. Welch, *Mission Research Corporation*
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Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL), and the Princeton Plasma Physics Laboratory (PPPL) propose to enter into a collaboration with Mission Research Corporation (MRC), Albuquerque, NM, and the University of Maryland (U. Md.). The goal of this collaboration is to establish and develop a topical Center for Terascale Simulation of the Plasma Physics of Intense Ion Beams for Inertial Fusion Energy, that will be funded through the Scientific Discovery through Advanced Computing (SciDAC) initiative, and to carry out advanced simulation research under the umbrella of this center.

LBNL, LLNL, and PPPL have already entered into a Heavy Ion Fusion Virtual National Laboratory (VNL) agreement to jointly pursue the goals of the Heavy Ion Fusion research program, through agreement of the Laboratory directors and the concurrence of the Office of Fusion Energy Sciences. Thus, collaboration of the three laboratories in this initiative is a natural extension of the existing VNL. However, key expertise and talent in the required research areas exists outside of the laboratory system, in particular at MRC and at U. Md., but also at the Naval Research Laboratory, from which a senior investigator will participate on an unfunded basis. A number of other senior investigators at the other participating institutions will also lend their time and expertise on such a basis, to coordinate their own research efforts with those of the Center, to advise students, and in a general collaborative role.

In addition, this Proposal requests funds from the Office of Advanced Scientific Computing Research (OASCR) to support the activities of a computer scientist at LBNL who will support the effort, particularly in the area of advanced solution methods for partial differential equations.

It is the intent of the proposal team to coordinate the work of the Center with proposed advanced computing research to be carried out under the auspices of the Office of High Energy and Nuclear Physics.

The Center will be managed by the team of Principal Investigators, which includes National Laboratory employees and a private industry employee. In general, we expect to manage by consensus among the Principal Investigators, with input from the other Senior Investigators. Day-to-day coordination will be provided by Alex Friedman, an LLNL employee who plays a management role for both LLNL and LBNL staff. Frequent video-teleconferences and periodic workshops will ensure a well-coordinated effort.

LLNL, LBNL, and PPPL will contribute their expertise in intense-beam simulation and theory to the effort, and will offer experimental data for code benchmarking. The University of Maryland will contribute their expertise in comparison of simulations with experiments, and the senior investigators there will supervise a graduate student. MRC will contribute their expertise in simulating beam interactions with plasma, and will make a well-developed computer code available to the collaboration as a key basis of the capability to be developed.

This tightly coupled multi-organization effort will offer capabilities far exceeding those that could be brought to bear by any one organization. Intense-beam physics for Inertial Fusion Energy will advance far more rapidly than otherwise would be possible.

Scientific Discovery through Advanced Computing: Advanced Computational Research in Fusion Science
Announcement LAB 01-10 and Program Notice 01-10

Topical Center for Terascale Simulation of the Plasma Physics of Intense Ion Beams for Inertial Fusion Energy*

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Date:

Requested funding ($k)

OFES:	**FY01: $700**	**FY02: $1000**	**FY03: $1050**	**Total: $2750**
OASCR:	**160**	**170**	**180**	**510**
TOTAL:	**$860**	**$1170**	**$1230**	**$3260**

Use of human subjects in proposed project: No **Use of vertebrate animals in proposed project: No**

72%

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Abstract

Topical Center for Terascale Simulation of the Plasma Physics of Intense Ion Beams for Inertial Fusion Energy*

Principal Investigators:	Alex Friedman, *LLNL and LBNL* Ronald C. Davidson, *PPPL* Dale R. Welch, *Mission Research Corporation*
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We propose to establish a topical Center to develop new terascale intense beam simulation capabilities and apply them to further the basic understanding of the physics of heavy ion beams for Inertial Fusion Energy. The knowledge so gained will also be relevant to a range of emerging beam applications in other fields. Our vision is a "source-to-target" simulation capability: a description of the underlying physics in this complex system that is both *integrated* and *detailed*, and is well benchmarked against experiments. The research described in this proposal will represent the key step in realizing this vision; the "hypothesis to be tested" is that the understanding of intense beams can be advanced rapidly via large-scale simulations.

Beams are nonneutral plasmas, and we will employ methods developed in the plasma fusion, accelerator, and computational science communities. We will improve existing tools to run optimally on the new platform; develop new algorithms and entirely new methods (*e.g.*, for larger timesteps, multiple beams, multispecies effects, magnetoinductive particle simulation, and continuum Vlasov phase-fluid simulation of beams); consolidate novel methods from three beam-plasma simulation codes into a single tool; exploit emerging computational paradigms, including scripting methods for code control; validate the new capabilities; employ them on important physics problems; and make them available to others. Significantly, the detailed beam description will be self-consistently carried from source to target along a "main sequence" employing two large codes, with "sideways" linkages into subsidiary simulations that explore key issues in detail, using models within those codes and one additional physics code.

Narrative

Background and Significance

The Heavy Ion Fusion approach to Fusion Energy

The Heavy Ion Fusion (HIF) program's principal mission is to develop the body of knowledge needed for Inertial Fusion Energy (IFE) to realize its promise. Heavy ion beam-driven IFE is the "principal alternate" approach to fusion energy; it has a number of favorable attributes and is very different from magnetic confinement.[1,2] In Heavy Ion Fusion, intense beams of heavy ions (with masses in the range 100-200 AMU) will be accelerated to multi-GeV kinetic energies (several megaJoules total), temporally compressed to durations of ~ 10 ns, and focused onto a series of small (few-mm) targets, each containing a spherical capsule of fusion fuel. The capsules are compressed and heated to a point where fusion ignition and a propagating "burn" occur. The energy so produced is captured and used to heat a working fluid, and electricity is produced using conventional steam turbine generators. Heavy ion drivers are attractive for this purpose because of their efficiency and because the final focusing onto the target is achieved by magnetic lenses which can be made robust to the effects of the target explosions, which must repeat at rates of order five Hz. This system is depicted schematically in Figure 1. While such a system is many years from fruition, ongoing experiments in the U.S. (under OFES support) are developing the novel and challenging intense-beam physics needed for its realization.

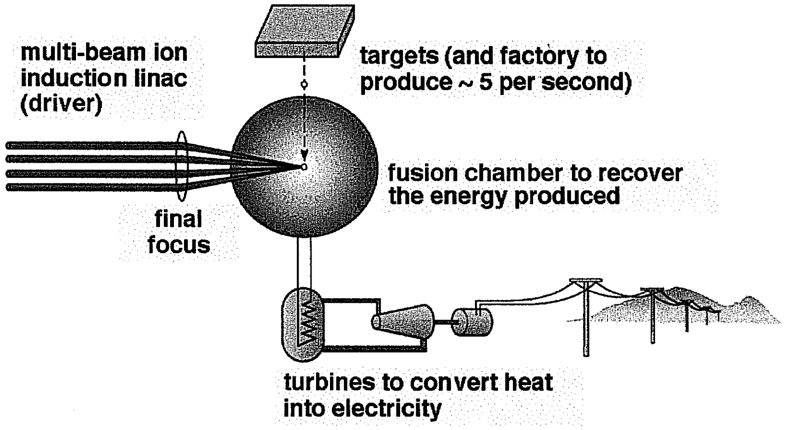


Figure 1. Schematic depiction of a heavy ion fusion system for electric power production.

In the U.S. approach to Heavy Ion Fusion, multiple ion beams are accelerated in parallel through a sequence of ferromagnetic toroids ("cores") in an induction linear accelerator ("linac"). Effectively, the beams act as the secondary winding of a transformer. Induction linacs are attractive because they naturally drive high currents. In addition, they are "asynchronous" devices (that is, the particles are not accelerated by an oscillating field of fixed frequency), so that the current can be amplified as the beams progress down the beamline. A schematic of such a system is shown in Figure 2. Here, an "electric focus accelerator" is one in which the transverse beam confinement is effected by means of electric quadrupole lenses, while a "magnetic focus accelerator" (which comprises most of the machine) uses magnetic quadrupoles. In contrast, the European and Japanese approaches to Heavy Ion Fusion emphasize more conventional radio-frequency linacs, and must achieve current amplification through the use of multiple storage rings. The beam requirements on target are similar in the two approaches.

The intense ion beams that will drive Heavy Ion Fusion targets are *nonneutral plasmas* both in the driver and in the highly-ionized chamber environment, and exhibit collective, nonlinear dynamics which must be understood using the kinetic models of plasma physics. Advanced methods of plasma simulation are well suited to this application. This beam physics is both rich and subtle: a wide range in spatial and temporal scales is involved (see figure 3), and effects associated with both instabilities and non-ideal processes must be understood in order to optimize physics performance.

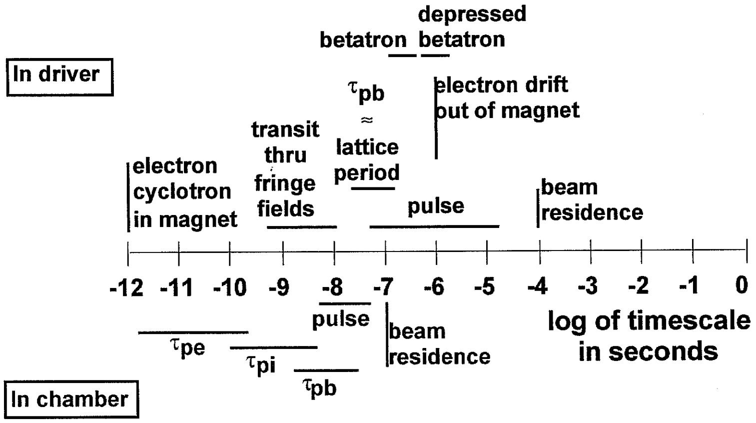


Figure 3. Timescales in a Heavy Ion Fusion driver and fusion chamber. Spatial scale lengths range from electron gyroradii in the magnets ~ 0.01 mm, to the beam Debye length ~ 1 mm, to the beam radius ~ 1 cm, to the machine length ~ km's.

chamber. This means that interactions between phenomena in different segments of the accelerator, and phenomena which happen slowly over long time scales, have not been adequately modeled (examples appear below). With terascale facilities, the full problem can be simulated, and qualitatively new behavior may emerge.

Many of the calculations mentioned above have been done only in 2–D due to computational facility limitations. Terascale computations are also needed to extend the computations to 3–D and add realistic boundary conditions.

Finally, there are parts of the physics model — multi-beam phenomena, and magnetoinductive effects, for instance — which cannot be included (except by way of very approximate models) in present-day calculations due to computational limitations. In sum, the complexity of the physics, plus the spatial and time resolution required, make terascale computing a necessity if the physics of the full HIF system, including connecting the accelerated beams to complex plasma phenomena in the chamber, is to be understood.

Physics problems requiring greater understanding

We now summarize some of the key physics problems where the need for improved understanding is greatest. These fall into two general areas: (1) *the interaction of intense ion beams with background populations*, including: the physics of beam propagation through the plasma environment in the fusion chamber (the largest part of our effort will go into this area); and multi-species effects, especially beam interactions with "stray" electrons in the accelerator and transport lines; and (2) *non-ideal dynamical effects in intense beams*, especially the generation of an outlying population of "halo" particles and the dilution of the beam phase space as a result of the accumulation of distortions over long times.

Interaction of intense ion beams with background populations

Beam interactions with fusion chamber environment: 3-D simulations of the propagation of the cluster of beams through the final focusing optics, and onward through the fusion chamber's environment of gas and plasma, are required in order to provide a realistically complete model of the target illumination. The beam and background plasma dynamics include: multibeam effects; return current formation and dynamics (multi-species instabilities); imperfect charge neutralization; beam stripping; emittance growth; and photo-ionization of the beam ions and background gas.[12] Of these effects, many of the uncertainties and computational challenges are associated with multiple-beam interactions near the target, and these will be one important focus of the research efforts. A key uncertainty is the extent of the length must be resolved) and the system size requires that at the very least a hundred cells transversely, and thousands longitudinally, be used.

Need for improved computational methods

The simulation tools that have been developed for Heavy Ion Fusion have been effective in addressing the problems to which they have been applied, but they have not been fully optimized for the emerging supercomputing environment of thousands of processors and multi-level memory access. Single-processor performance may perhaps be further optimized by rearranging data structures and making algorithmic changes to increase cache effectiveness and decrease memory accesses. Optimal methods of solving partial differential equations that minimize off-node communication and are appropriate to the very large problem sizes that arise in multi-beam simulations have yet to be implemented.

In addition, certain important physics is missing from the codes, much of it expected to be relevant to the next series of experiments in the program. For example, the High Current Experiment getting underway at LBNL will employ driver-scale line charge densities ~ 0.25 μC/m as well as magnetic quadrupoles. The latter, in contrast with the electric quadrupoles that have heretofore been used in the program, do not naturally "sweep" stray electrons out of the system. Also the large space-charge potential changes the electron dynamics, so that electron trapping in the beam path becomes an issue. The presence of an electron component opens the door to a class of instabilities. Therefore, beam halo generation, the interactions of halo particles with walls, gas ionization, electron trapping, and instabilities all need to be understood, requiring model improvements.

Therefore, in the proposed research program, considerable effort will be devoted to improvement of computational tools so that they run optimally on the new platform and those expected to follow it. This includes development of new algorithms and of entire new methods (e.g., for larger timesteps, and for continuum Vlasov phase-fluid simulation); consolidation of novel methods from three beam-plasma simulation codes into a single tool optimized for multi-species calculations; validation of the new capabilities; and employment of them on important beam physics problems. We now describe the rationale for another key element of the proposed work, the linkage of this merged tool and other tools into an integrated capability.

Need for an *integrated* source-to-target simulation capability

The capability to carry out *integrated* simulations is becoming increasingly important.[25] While considerable progress can (and indeed has) been made by simulating the "pieces" separately, such an approach is limited in the fidelity it can achieve. A simulation of a part of the system using an idealized incoming beam can yield at best an approximate simulated beam at downstream observing stations. In some cases, the simulated beam can differ greatly from its real counterpart. Accurate simulation of *real-world* (not idealized) beams is essential if experimental results are to be compared one-to-one with simulations. Similarly, high fidelity is essential to the development and exploration of concepts for a full-scale fusion driver.

The limitations of partial-machine simulations come about because of a number of considerations. In the first place, injected beams are imperfect. Indeed, accurate simulation of the beams through the particle sources, injectors, and matching sections, including such practical effects as misalignments and voltage ripple, are very challenging, requiring a thorough characterization of the real system. Such "front-end" simulations are important in their own right, but they are essential to ensure that one is simulating the "most realistic" beam downstream.

Second, collisionless beams such as those needed for Heavy Ion Fusion have a "long memory." The dominant relaxation mechanism is phase mixing of the various waves supported by the beam. This mechanism is often slow, and it typically does not lead all the way to thermal equilibrium. Thus, the beams in both the driver and the fusion chamber are not in, and are often not near, equilibrium, although the assumption that they are is often useful for design and analysis purposes. In fact, no exact nonsingular equilibria are known for systems which employ quadrupole-lens confinement, and none may in fact exist except for approximate periodically focused equilibria at sufficiently small transverse betatron frequency distribution introduces uncertainties. With improved codes on terascale facilities, we will be able to address the full problem with a very strong likelihood of success.

Another view of the benefits to be obtained from this research is shown in Table 1, below.

	Present day	**End of proposal period**
Driver beam physics	2-D simulations of present-day & next-generation experiments; 3-D of sections of driver; run linking.	Integrated 3-D simulations of driver from source to chamber; multibeam effects.
Chamber propagation physics	Single-beam studies using axisymmetric electromagnetic particle codes.	Studies in 3-D; linkage from driver simulation; multibeam effects; collective instabilities; effects of inhomogeneities.
Halo and instabilities in driver	Studies using idealized initial conditions.	Linkage of end-to-end run data into halo and instability calculations to ensure fidelity.

Table 1. Benefits to be obtained from the work of the proposed Center

Relevance to the research needs identified by the Office of Science

Simulations of intense beams have already had a major impact on Inertial Fusion Energy research. In a real sense, simulations have established the potential of Heavy Ion Fusion drivers. By showing that instabilities predicted in early approximate analytical studies in fact saturated at low levels, simulations motivated, and were confirmed by, subsequent experiments. Simulations have predicted and reproduced observations on a number of laboratory-scale experiments.

Thus, we can confidently predict that the terascale simulations enabled by the proposed Center will advance the mission of the Office of Fusion Energy Sciences, and that of the Office of Science in general, by furthering the understanding of key scientific issues in beam and plasma physics, and improving the effectiveness of future Inertial Fusion Energy facilities. This research will impact the program direction by introducing new capabilities, ideas, and talent. Fusion research will benefit from earlier and more complete studies of 3-D, multi-beam, inhomogeneity, and instability effects in the various possible modes of chamber propagation, and of 3-D single- and multi-beam physics in the driver. The full and quantitative understanding that will be enabled by this Center will decrease the risks and enhance the benefits of all future heavy-ion Inertial Fusion Energy experimental efforts.

The scientific themes of this work have broad relevance; they include the nonlinear dynamics of Liouvillean flows, collective interactions in self-consistent fields, and a wide range of spatial and temporal scales. The computational physics will also offer potential spin-off benefits, since it includes themes such as rapid solution of partial and ordinary differential equations, dynamic load balancing, particle and continuum phase-fluid methods, code linkage, interactive and script-driven code steering,[26] and the visualization of a time-dependent 6-D phase space.

Other accelerator applications will also benefit, and the proposed topical Center will make coordination with research funded by other programs in the Office of Science one of its explicit goals. Because Heavy Ion Fusion beams are near the limit of complete space-charge dominance, there is the potential to impact other areas where space charge effects are of increasing importance. Thus the front end of a possible muon collider and the interaction region of, *e.g.*, the B-factory may obtain benefit from the physics learned by, the computer codes made available by or co-developed with, or the numerical methods invented by, the proposed Center.

The SciDAC White Paper recommends coordinating beam studies between the Office of Fusion Energy Sciences and the Office of High Energy and Nuclear Physics. As described elsewhere in this

Method	Code	Applicability	Geometry, field representation, comments
Follow particles (plasma particle-in-cell method)			
	WARP	**driver**	3-D (or r,z or x,y) ES+, detailed models of applied fields; cut-cell boundary avoids "Lego-land" effect.
	LSP	**chamber & driver**	3-D or (r,z) implicit (or explicit) EM or ES, hybrid (kinetic/fluid), rich physics models.
	BPIC	chamber	3-D or (r,z) EM, dynamic grid, improved outgoing-wave boundary conditions.
	BIC	chamber	(r,z) EM, tapered nearly-orthogonal grid.
Follow particles and perturbation to distribution function (δ*f*)			
	BEST	**chamber & driver**	3-D EM, Darwin, or ES, offers reduced noise, multi-species dynamics.
Evolve distribution function (*f*) on a multi-dimensional grid			
	WARP-SLV	**driver**	2-D (x,y,p_x,p_y) ES Semi-Lagrangian Vlasov solver (a package in the WARP code).
Evolve moments of *f* (transverse "envelopes" on slices which are coupled in z via a fluid model)			
	WARP-CIRCE	driver	3-D ES, analytic approximation to E_z.
	WARP-HERMES	driver	3-D ES, uses (r,z) field-solver for E_z.

Table 2. Methods (representations of the phase space) of codes for HIF beams, codes in current use, and domains of applicability. The proposed Center will focus its attention on the packages in boldface type. Here ES means electrostatic, ES+ adds models for inductive and magnetic effects, EM means electromagnetic, and Darwin means magneto-inductive. We will merge key algorithms from BIC and BPIC into LSP, and will link WARP, LSP, and BEST, as described below.

The codes in current use for HIF studies are listed in Table 2, which characterizes the codes by their general methods (representations of the phase space) and by their regimes of applicability. WARP (not an acronym; the name derives from the "warped" coordinate system used to describe bent beamlines) and LSP (Large Scale Plasmas) are fairly large and complex codes offering many options; they are, more accurately, code frameworks, and are well-positioned to move quickly to the new hardware platform. BEST (Beam Equilibrium, Stability, and Transport) is a smaller (*i.e.*, with far fewer lines of source) physics code that serves as an innovative test-bed for new simulation methods, in addition to being a very useful tool in its own right. BPIC (Beam Particle-In-Cell, a modern explicit code with significant innovations) and BIC (Beam-In-Chamber, an older tool still in regular use) are electromagnetic codes used for chamber propagation simulations. Our plan is to improve, couple, and employ WARP and LSP as our "main-sequence" tools, and BEST as a key detailed physics simulation tool. As described later in this proposal, the physics and numerical methods developed in BPIC and BIC will be merged into LSP.

WARP [7,10,26,30,33,34,35,36,37] has been developed over the course of a decade by Heavy Ion Fusion researchers at LLNL and LBNL, with elements contributed by researchers at NRL and the University of Maryland. It offers 3-D, axisymmetric, and "transverse-slice" 2-1/2D (x,y,p_x,p_y,p_z) geometries, and is used extensively throughout the Heavy Ion Fusion program for studies of beams in the accelerator, pulse-compression line, and final focusing system. WARP runs on a variety of platforms, Moment based models CIRCE [38] and HERMES (neither is an acronym), useful for rapid scoping and synthesis, are also implemented within the WARP framework. In these models, the beam is divided into slices. Each slice contains a fixed amount of charge, and can compress or expand longitudinally. The transverse boundary of each slice obeys its own "envelope" (second moment) equations. While in CIRCE the arrival times of the slice boundaries at a given position along the beamline are calculated, in HERMES the positions of all slice boundaries are followed as functions of time. The latter approach allows direct calculation of the longitudinal electric space-charge field, using either an (r,z) Poisson solver or semi-analytically using a Bessel series expansion. One key role of these tools is as a "spotting scope" for the synthesis of final focusing and pulse compression systems.

LSP [12,39] offers (*r*,*z*) and 3-D geometries, implicit or explicit EM or ES PIC and fluid models, a multi-block mesh which allows simulation of non-rectangular (*e.g.*, L-shaped) regions, and domain decomposition designed for multilevel memory access. Its implicit hybrid model enables simulation of dense-plasma scenarios. LSP has extensive gas and surface interaction physics models; it already offers secondary emission, kinetic neutrals, ionization, scatter and neutral recycling, and has achieved good scaling using up to 256 processors on problems of intermediate size. LSP is written in C using elements of an object-oriented style. It has been benchmarked against the recent Scaled Final Focus Experiment at LBNL for beam charge neutralization. A predecessor code, IPROP, successfully modeled self-pinched transport experiments on the Gamble II proton accelerator at NRL.[40] It has already been used to model the DARHT–II injector.[41] Since LSP is terascale-ready and embodies physics models that facilitate the study of all chamber transport modes under consideration in the Heavy Ion Fusion program, it will be employed in these studies to treat, for the first time, pulse-shaped beams, multibeam effects, inhomogeneous background plasmas, and other important effects.

LSP uses a 3-D implementation of the direct-implicit particle-in-cell algorithm with its electro- and magneto-static and its electromagnetic field solvers. The benefits of this treatment are that the usual limitations on time step, namely the need to resolve the cyclotron and plasma frequencies, are greatly relaxed. Also, the "finite-grid" (aliasing) Debye length instability, responsible for numerically heating (in explicit algorithms) a plasma until the Debye length is roughly the cell size, is nearly eliminated in useful regimes, including regimes with nominal "explicit" time steps. To enhance the range of application of the implicit algorithm, LSP has two key numerical enhancements over the standard direct-implicit scheme. First, LSP has a hybrid operation in which electron particles are treated with either fluid or kinetic equations. Populations of each type may co-exist or pass back and forth between the two descriptions while conserving momentum. In addition, LSP uses a variable damping scheme [29] to reduce the effect of spurious high-frequency fields on particle orbits, and to damp under-resolved field modes. Additionally, LSP models particle interactions using Monte Carlo techniques, including beam stripping, particle impact and photon ionization and gas breakdown models have been added. These features facilitate use over a wide range of plasma densities, time scales, and spatial scales.

The LSP code is particularly suited to the simulation of beam-plasma interactions. Using the implicit algorithm, the energy conservation for a simple simulation of a plasma in a drift tube remains excellent for a wide range of time steps and for a numerical cell size much greater than the Debye length. An explicit algorithm with a standard particle push shows the usual finite-grid instability when the cell size is greater than the Debye length—a typical example with cell size to Debye length ratio of 80 exhibited numerically-driven energy error exceeding 200% after 130 plasma periods. The same problem, using the implicit algorithm with purely kinetic particles and small "explicit" steps, maintains energy error less than 0.5%. The implicit fluid-electron algorithm permits the same degree of energy conservation but for an order of magnitude greater time step. Thus, the LSP hybrid model offers the potential of highly accurate simulations with a wide range of plasma conditions.

BEST [18,19,20,21,22,23,24] offers nonlinear-perturbative ("δf") simulation in 3-D polar geometry and has been parallelized using a combination of MPI and OpenMP and two-dimensional domain decomposition suitable for a supercomputer equipped with both shared and distributed memory. The code has been designed to elucidate mode structures by minimizing discrete-particle noise, to employ a new Darwin (magnetoinductive) model algorithm, and, to compensate for the mass ratio (about 250,000) of the heavy ions to the electrons, to use a newly-developed adiabatic pushing and deposition algorithm.

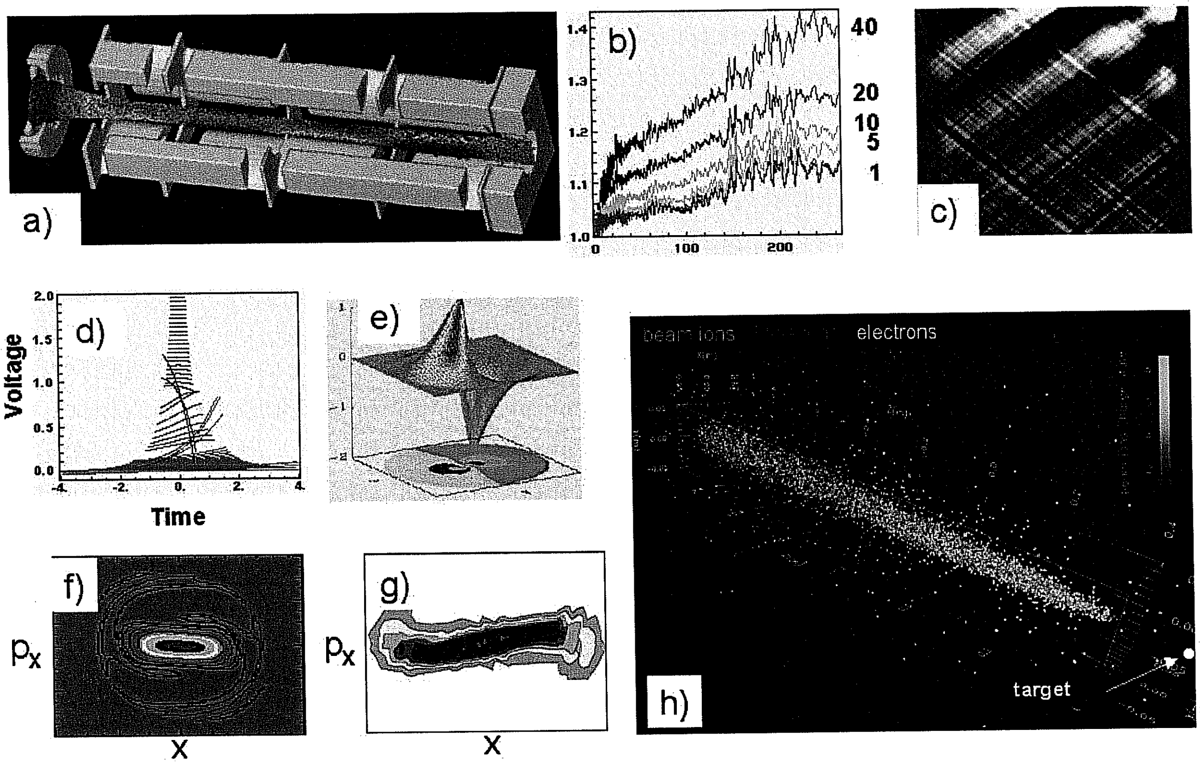


Figure 4. Representative output from Heavy Ion Fusion beam simulations: (a) WARP3d simulation of space-charge-limited emission off a curved surface, and acceleration in a 3-D structure, including subgrid-scale placement of conductor boundaries (cut-cell method); (b) WARPxy study of beam emittance versus time in an imperfectly-aligned beamline, for five different intervals between applications of steering; (c) WARP3d study of longitudinal waves on beam, driven unstable by the impedances of the accelerating structures. Here, each horizontal row represents a time history of the line charge density (denoted by color) at a particular "observing station"—the vertical offset of the row corresponds to the observing station's location; (d) accelerating waveforms for a possible future experimental accelerator, for use in WARP simulations; (e) BEST simulation of unstable electron-ion two-stream dipole mode in a beamline; (f) semi-Lagrangian Vlasov simulation of beam halo generation due to anharmonic focusing fields, using prototype model in WARP-SLV; (g) distorted beam phase space in final focusing, as simulated using WARPxy; (h) BPIC simulation of beam transit through fusion chamber environment and onto the target.

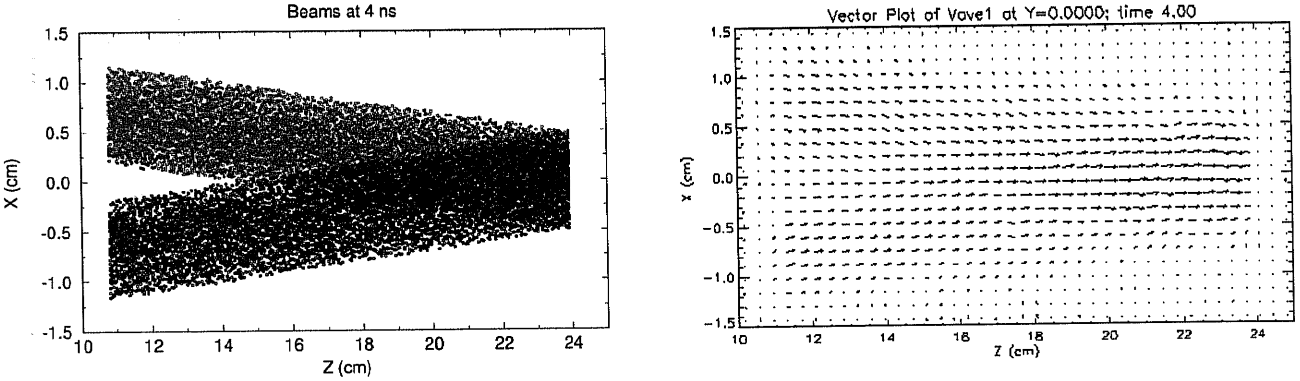
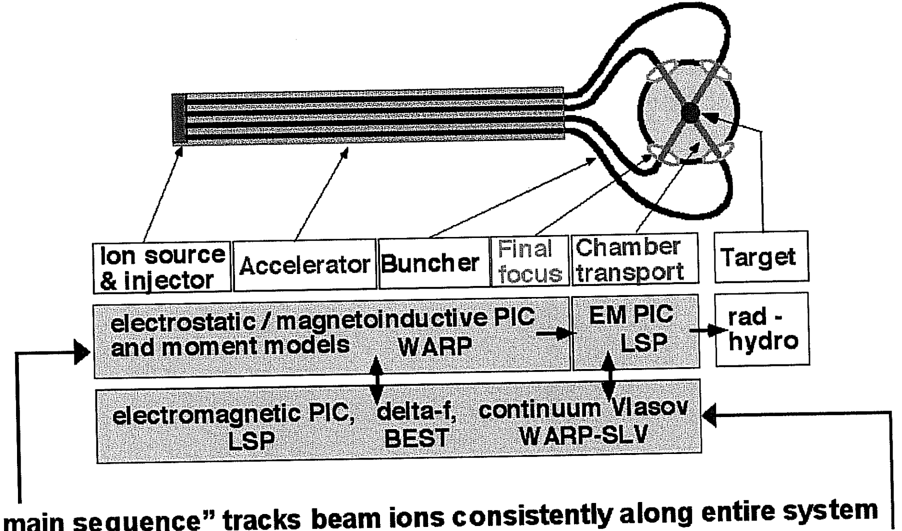


Figure 5. A 3-D LSP simulation of the coalescence of two beams near the fusion target is shown on the left. The plasma electron velocity vectors are shown on the right. The plasma motion effectively neutralizes the beam charge and much of the beam current, for the parameters simulated.

the beam. For this to be accurate, it is necessary to understand beam halo quantitatively, and for this the marker-following capabilities of BEST and/or the Vlasov solver in WARP are employed in coupled side calculations. BEST is also used to study collective beam instabilities in detail, using parameters transferred from WARP and LSP.



"main sequence" tracks beam ions consistently along entire system

instabilities, halo, electrons, ... are studied via coupled detailed models

Figure 8. Depiction of source-to-target simulation strategy (see text)

The major developments to be carried out in the proposed research include: (i) optimization of codes for efficiency on emerging computer architectures; (ii) development of new and improved numerical algorithms (*e.g.*, for larger timesteps and Vlasov solution); and (iii) development of improved physics models (*e.g.*, for multibeam, converging beam, self-magnetic, atomic physics, and module impedance effects) that will be made practical by the terascale capability. The codes will be linked via self-describing data files (*e.g.*, NetCDF and/or HDF), and via scripting tools (especially Python) or workspace tools should run-time intercommunication prove important. The "data glut" associated with saving information from the many processors will be addressed by incorporating optimized parallel input/output capabilities. The challenges of visualizing a time-dependent 6-D phase space will be addressed through the use of volume and isosurface rendering, coupled with projection and range selection along the non-visualized coordinate directions. Animation will also be further developed and employed. The simulations will entail self-consistent field descriptions requiring interprocessor communication, but will employ optimized domain decomposition and dynamic load balancing so as to be scalable on terascale architectures. The majority of the proposed simulations are between one and two orders of magnitude beyond current practice; in the terascale environment we anticipate typical run times of order a day.

We will develop and employ the simulation tools to address the two key areas requiring coupled terascale simulations based on advanced methods: (1) the interaction of intense ion beams with background populations, including: the physics of beam propagation through the plasma environment in the fusion chamber (the largest element of the proposed effort); and multi-species effects, especially collective beam interactions with "stray" electrons in the accelerator and transport lines; and (2) non-ideal dynamical effects in intense beams, especially the generation of an outlying population of "halo" particles. The simulation of beam halos will be a key point of collaboration with colleagues supported by High Energy and Nuclear Physics (HENP) funding for advanced computing.

Improvements to tools for interaction of intense beams with background populations

Beginning with existing tools, we will further develop and employ electromagnetic Particle-In-Cell (PIC) methods and related nonlinear perturbative methods to study beam propagation through the fusion chamber environment. We will generalize the LSP implicit hybrid electromagnetic PIC code. We will "mismatch" oscillations at transition points in a Heavy Ion Fusion driver (*e.g.*, a transition from electrostatic to magnetic beam confinement). Even matched (in an RMS sense) non-ideal beams can produce halo particles, through, *e.g.*, collective-mode excitations,[23] and an understanding of halo production and control will also be developed for such beams. Such an understanding is critical to the Heavy Ion Fusion effort, since the beam halo size sets the requirement for space available outside the beam core. It is also critical to a wide variety of other accelerator applications, though the details differ for high energy and nuclear physics applications.

We will develop novel methods of solving the continuum Vlasov equation on 4-D and 5-D grids in phase space (ultimately 6-D grids should become practical), and will apply them in critical problem areas. The Vlasov approach is especially well-suited to problems of halo formation since, in contrast with PIC simulations, low-density regions of phase space are represented as well as high-density regions. We anticipate valuable informal collaboration with French, German, and Japanese experts in Vlasov methods.

We will also develop and apply a "particle Vlasov" approach, using elements of PIC and nonlinear "delta-f" methods, to these problems. We will compare the continuum and particle Vlasov results with each other, and with results from large-scale PIC simulations using tools developed in HENP community. Since the means by which fine-grained information is ultimately discarded differs greatly among these methods, considerable scientific knowledge will be gained.

The other major class of non-ideal dynamical effects is associated with beam propagation over long distances. In Years Two and Three, we will generalize WARP to include a true multi-beam description (using simplified moment models for all but one beam), and will apply this technique to the study of non-ideal effects such as resistive instabilities, inductive field couplings, and time-dependent multi-beam interactions. This will be a key element of an effective source-to-target beam simulation capability.

Integrated capability

From the considerations presented earlier, it is evident that that an integrated simulation capability is ultimately essential. However, we are fortunate in that, for the most part, information flows with the beams downstream along the system. Thus, we believe that in general one-way coupling of particle and field data from the driver simulation code (WARP) to the chamber simulation code (LSP) at chamber entrance will suffice. This implies that the linkage can be effected through self-describing data files (NetCDF or HDF). The linkage into the target simulation code can similarly be done via data files; in this case, the target output radiation spectrum influences the chamber environment and can photo-ionize the incoming beams to higher charge states. To account for this, the time-dependent output spectrum from the target code run can be saved and used to improve later chamber code runs. A tight loop is not necessary, since the target can be driven with "perfect" beams as a first approximation, and then if it fails to work with the simulated driving beams we will know that the beams need be improved, the target design modified, or both.

The "main sequence" calculations will be carried out using optimized algorithms on a state-of-the-art supercomputer. Nonetheless, coupled "local" simulations must be an important element of an integrated simulation capability if the results are to carry with them the highest possible confidence. Such subsidiary simulations will be used to examine important local processes in detail. For such local simulations we can use tools that are difficult or too costly to employ over the entire system The beam parameters from the main sequence must be transferred into these detailed simulations, to ensure that the latter are "solving the correct physics problems." This can be done by transferring particle data in some cases, and detailed multi-dimensional moment data in others, as appropriate.

For example, formation of a beam "halo" (tenuous outlying ion population) is primarily of concern at special locations where the beamline changes character, so that beam "mismatch" (oscillations in cross-section due to imperfect radius and/or convergence/divergence angles for the new section) is likely to be induced. Thus, we will employ "local" models to validate the mainstream calculation and to give quantitative predictions of the extent and density of the halo. One such model is based on the nonlinear-perturbative (δf) method as embodied in BEST. Here, we can concentrate the particles (markers which carry distribution function information) in those phase-space regions which advect into the halo region. In number of particles, and that a driver will be approximately 5 to 10 times longer than the beamlines in the simulations done to date, on the order of 100 million particles or more will be needed in order to avoid excessive spurious heating.

The time step size is set primarily by the requirement that the "fringe fields" of the applied focusing elements be resolved, leading to a requirement of ~ 100 steps per lattice period. A driver-scale accelerator will have on the order of 1000 lattice periods, requiring a total of 100,000 time steps. Given that the electrostatic field solve time for a mesh of 128×128×4096 on 256 processors of NERSC's T3E is 1.4 seconds, and the particle advance time for 100 M particles is 7.5 seconds per step, the total time required of a driver simulation would then be approximately 250 hours. Scaling by the peak flop rate, 900 Mflops times 256 processors for the T3E and 5 Tflops for the machine we assume, leads to an estimate of 11.5 hours on the 5 Tflops machine. Linear scaling is justified for the overall time since the particle advance time, which scales linearly to large numbers of processors, will dominate over the field solve time, which may scale less than linearly since it is a global operation. Including additional physics such as a magnetostatic or Darwin field solver, non-ideal applied fields, and multiple beam effects might be expected to very roughly double the computation time, giving a "wall clock" time of order a day.

	Cray T3E-900				IBM SP2			
Numbers of processors	32	64	128	256	32	64	128	256
32M particles, 128x128x4096 grid	20.2	10.3	5.4	2.8	9.6	5.0	3.0	2.1
Particles only	10.9	5.6	2.8	1.4	4.6	2.4	1.2	0.7
Field solve only	9.3	4.7	2.6	1.4	4.7	2.5	1.7	1.2

Table 3. Timings for ion beam particle simulations using WARP3d code. Times are in seconds, for one step. The FFT Poisson solver, one of several available options, was used. The timings for the particles does not include diagnostic calculations. Including the diagnostics, the time to advance 100 M particles for one step is estimated to be roughly 7.5 seconds on 256 processors on the T3E.

Fusion chamber propagation main sequence

Based on previous 2-D and 3-D simulations with LSP on NERSC's current T3E, we estimate a time of two days on a 5 Teraflops system to carry out a full 3-D chamber simulation with 16 interacting ion beams. This simulation will include detailed physics of the beam-plasma and target interactions. The mesh size will be of order 200×200×600 and the number of particles is typically 360 million (~15 per cell). In the transverse plane, the mesh must resolve the gradients across each beam. The longitudinal cell scale-length can be somewhat greater than that of the transverse scale but no more than the radius of the beam. The number of time steps is determined by the requirement that a particle not skip more than a single cell. An approximate estimate is 10000 steps to transport the beams over three meters, assuming a factor of three reduction due to the use of dynamic regridding. Given 5 Teraflops and similar assumptions of scalability to those described above for the driver simulation, we estimate that 48 hours of wall-clock time will be needed for such a run. Expected improvements in the field solver are likely to improve the speed and permit the simulation of even more beams.

Research timetable

Year One

Tool development

We will implement into LSP the methodology for advective correction of vector potential errors due to dynamic mesh refinement that was originally developed in BPIC. The appropriate boundary conditions for a simulation in the laboratory frame will be developed. We will test the method for stability and effectiveness in removing a pre-defined error for both explicit and implicit operation.

We will implement the newly-developed Darwin model that advances canonical momenta, and determine the importance of magnetic and inductive effects in high intensity beams, using BEST as a testbed.

We will develop a generalized dynamic mesh refinement capability for LSP. This will involve developing optimal techniques for modification of the LSP mesh, including interpolation of field quantities to refined grid coordinates. We will then determine the extent to which the mesh can be dynamically altered while preserving the integrity of the electromagnetic field solution. In initial work, the grid adaptation will be pre-programmed.

We will improve BEST as needed for halo studies that will use a "particle-Vlasov" approach that concentrates the simulation particles in those phase-space regions which advect into the halo region.

We will also optimize WARP-SLV for studies of beam halo formation, to achieve improved parallelism and single-processor performance. We will consider implementing a distribution of axial momenta, in a paraxial approximation whereby those momenta are conserved; this approximation effectively reduces the 5-D problem to a set of coupled 4-D problems, but yields a code capable of studying chromatic effects.

We will improve WARP3d's capability to follow beams over long distances in the driver. To this end, we will finalize studies of, and implement, the most promising code developments identified in Year One, especially those aimed at allowing larger timesteps. We will choose and implement a faster field solver, evaluating options from the Chombo Adaptive Mesh Refinement package [52] as well as a stand-alone parallel multigrid method.

We will begin the implementation of a multi-beam driver model in WARP3d that models the effects of non-identical beams.

We will develop an improved multi-dimensional domain decomposition on the IBM SP2 platform based on a hybrid parallel scheme (OpenMP and MPI), using BEST as a testbed.

We will develop seamless (automated) links between codes. These will include linkage of WARP data to LSP for a fully-integrated main-sequence simulation, and linkage from both WARP and LSP to BEST, for detailed physics simulations.

Physics studies: Interaction of intense beams with background populations

We will distill and incorporate into WARP runs an additional time-dependent charge source using knowledge from electron-timescale simulations carried out during Year One. The code development needed is expected to be minor, and we will concentrate on obtaining new physics understanding.

We will investigate two-stream and filamentation instabilities and other multi-species effects in heavy ion fusion drivers and target chamber, using BEST.

Physics studies: Non-ideal dynamical effects in intense beams

We will perform locally-integrated simulations of drift compression and final focusing, including pulse tailoring in the driver to initiate the compression, using WARP3d and WARP-HERMES.

We will exploit and compare the various approaches to beam halo simulation that have been developed during Years One and Two on realistic problems associated with transitions in the beamline structure, and will compare them with PIC simulations that will be carried out under the high energy and nuclear physics research program with which we are coordinating.

Year Three

Tool development

If necessary, we will implement the capability to intermittently run the electron-scale calculations simultaneously with WARP. The decision will be made based on what is learned during Year One and Year Two. This capability will be developed using either a "workspace" tool or the development of a unified executable code.

We will implement a Darwin model in LSP and/or WARP, based on what is learned from our experience using BEST as a testbed, and our assessment of needs (it may suffice to use approximate semi-analytic models of multi-beam magnetic and inductive effects in WARP, for example).

collaboration of the three laboratories in this initiative is a natural extension of the existing VNL. However, key expertise and talent in the required research areas exists outside of the laboratory system, in particular at MRC and at U. Md., but also at the Naval Research Laboratory, from which a senior investigator will participate on an unfunded basis. A number of other Senior Investigators at all participating institutions will also lend their time and expertise on such an unfunded basis, to coordinate their own research efforts with those of the Center, to advise students, and in a general collaborative role.

LLNL, LBNL, and PPPL will contribute their expertise in intense-beam simulation and theory to the effort, and will offer experimental data for code benchmarking. U. Md. and NRL will contribute their expertise in comparison of simulations with experiments (the Maryland experiments are well suited for code benchmarking), and the senior investigators there will supervise a graduate student. MRC will contribute its expertise in simulations of beam interactions with plasma, and will make a well-developed computer code available to the collaboration as a key basis of the capability to be developed.

Partnerships with HENP and OASCR supported researchers

This work will capitalize on coordinated work in the high-energy and nuclear physics community and the Computer Science community, some of which is existing, and some of which is to be proposed for SciDAC funding. In Year One, the principal collaboration with high-energy and nuclear physics researchers will address beam halo code development and initial applications. We also intend to coordinate the proposed studies of electron effects in ion accelerators with high-energy and nuclear physics research. Indeed, the electron-proton instability in proton storage rings is an area where significant contributions to understanding have already been made by members of this research team.

It is our intent to carry out research on beam halos in collaboration with HENP-funded staff, who are proposing an initiative in advanced accelerator simulation, with this area as an important element. Much of the expertise in this area resides in the fusion community; thus the proposed fusion effort in halo physics and Vlasov methods will be capable of standing on its own, but will be considerably augmented if the HENP effort is funded. We anticipate that computational tools will be developed collaboratively and will become important shared resources. Coordination will be accomplished by regular meetings between the leaders and appropriate other members of the fusion and high-energy and nuclear physics SciDAC research teams.

In addition, this Proposal requests funds from the Office of Advanced Scientific Computing Research (OASCR) to support the activities of a computer scientist at LBNL (Peter McCorquodale) who will support the effort, particularly in the area of advanced solution methods for partial differential equations. He is already involved in supporting heavy ion fusion research under the support of internal LBNL funds of finite duration, as described later in this section.

With the support of LBNL Laboratory-Directed Research and Development funding, some members of this research team are collaborating with the NERSC computational science group in the integration of Adaptive Mesh Refinement (AMR) techniques with the Heavy Ion Fusion PIC simulation code WARP. That group initially developed the AMR method for application to combustion and fluid flow studies. We anticipate that the method will be useful in simulation studies of heavy ion beams in several contexts: mesh refinement around the beam in a PIC code; around internal conducting structures to capture subtle but important field details; and around key phase-space structures in a continuum Vlasov calculation in 4–D, 5-D, and ultimately 6-D, where straightforward methods would require a very large mesh.

The NERSC Applied Numerical Algorithms Group (headed by Phil Colella) is proposing that a multi-laboratory Center for computational solutions of partial differential equations (PDE's) be funded by SciDAC. Such a Center could be of great value to the fusion simulation community. We will work closely with that Center so that the state-of-the-art in rapid solution methods for the PDE's which must be solved in beam simulation codes will be significantly advanced. Should that Center be funded, it is our expectation that it would supply the funding for the computer scientist mentioned earlier in this section.

For example, LSP's implicit EM field solver uses an iterative "alternating-direction implicit" method. This scheme is suboptimal, so we will explore both multigrid and conjugate-gradient methods. There are currently available routines (e.g. SNL's Aztec package) that are already optimized for multi-processing.

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Budget and Budget Explanation

BUDGET SUMMARY

OFES support (post-docs denoted "p"; students denoted "s")	Year 1		Year 2		Year 3	
	Staff	$k	Staff	$k	Staff	$k
LLNL	.5	133	.5+1p	228	.5+1p	237
LBNL	.25+1p+1s	202	.4+1p+1s	247	.4+1p+1s	263
University of Maryland	1s	45	1s	50	1s	55
PPPL	1+.5p	220	1+1p+1s	350	1+1p+1s	365
Mission Research Corp.	.5	100	.6	125	.6	130
TOTAL	2.25+1.5p+2s	700	2.5+3p+3s	1000	2.5+3p+3s	1050

OASCR support	Year 1		Year 2		Year 3	
	Staff	$k	Staff	$k	Staff	$k
LBNL	1.0	160	1.0	170	1.0	180

(Budget pages and explanations from participating institutions appear on the following pages)

Other Support of Investigators

Biographical Sketches

Curriculum Vitae for Ronald H. Cohen

PRESENT POSITION

Physicist (since 8/74) and Theory/Computations Program/Group Leader (since 1988)
Magnetic Fusion Energy Program, Lawrence Livermore National Laboratory

PERSONAL

Birth date: 8/2/46 Citizenship: U.S.

EDUCATION

9/68-1/73,	Massachusetts Institute of Technology, Ph.D. (Physics), awarded 6/73
9/64-6/68,	Massachusetts Institute of Technology, S.B. (Physics), awarded 6/68

PREVIOUS RESEARCH EXPERIENCE

Research Associate, Princeton University Plasma Physics Laboratory, 1/73-8/74
Research and Teaching Assistant, Massachusetts Institute of Technology, 9/64-8/68
Staff member, MIT Lincoln Laboratory, summer 1971
Staff member, MIT Haystack Observatory, summer 1969
Staff member, Stanford Linear Accelerator Center, summer 1968
Staff member, Xerox Research Laboratories, summers 1966, 1967

HONORS

American Physical Society Fellow
National Science Foundation Fellow Designate, 1968
Honorary Woodrow Wilson Foundation Fellow
Co-PI of team that won 1999 Gordon Bell Award for computations performance

GENERAL RESEARCH INTERESTS

Fusion Plasmas, Nonlinear Dynamics and Chaos, Astrophysical and Space Plasmas; Turbulence; Fluid Dynamics

SELECTED PUBLICATIONS

R.H. Cohen, W.P. Dannevik, A. Dimits, D.E. Eliasn, A.A. Mirin, Y.K. Zhou, D.H. Porter and P. Woodward, "Three-Dimensional Simulation of a Richtmyer-Meshkov Instability with a Two-Scale Initial Perturbation", to be submitted to Physics of Fluids.

R.H. Cohen, R.H. Cohen, X.Q. Xu, and M. J. Schaffer, "X-Point heating, potentials, and temperature asymmetries in edge plasmas," accepted by Contributions to Plasma Physics (2000).

D.D. Ryutov and R.H. Cohen, "Particle Trajectories in a Sheath in a Strongly Tilted Magnetic Field," Physics of Plasmas, **5**, March 1998.

R.H. Cohen, W.P. Dannevik, A.M. Dimits, D.E. Eliason, A.A. Mirin, O. Schilling, D.H. Porter and P. Woodward, "Three-Dimensional High-Resolution Simulations of Richtmyer-Meshkov Mixing and Shock-Turbulence Interaction," Proceedings of Sixth Int'l. Workshop on the Physics of Compressible Turbulent Mixing, Marseille, France (1997)

R.H. Cohen and T.D. Rognlien, "Induced Magnetic-Field Effects in Inductively Coupled Plasmas," Phys. Plasmas, vol 3, 1839 (1996).

Cohen, R.H., Mirror Theory Applied to Toroidal Systems, in "Physics of Mirrors, Reversed Field Pinches and Compact Tori", Proceeding of Course and Workshop held at Varenna, Italy, Sept 1-11, 1987 (Editrice Compositori, Societa Italiana di Fisica, Bologna, Italy, 1988) V. II, p. 945.

Cohen, B.I. and Cohen, R.H., "An Electromagnetic Trapped-Particle Sideband Instability," Phys. Fluids **31**, 3444 (1988).

Cohen, R.H., Nevins, W.M. and Berk, H.L., "Tandem-Mirror Trapped-Particle Modes at Arbitrary Collisionality," Phys. Fluids **29**, 5 (1986).

Cohen, R.H., Hizanidis, K., Molvig, K. and Bernstein, I.B., "Lagrangian Formulation of Transport Theory: Like Particle Collisional Transport and Variational Principle," Phys. Fluids **27**, 2 (1984).

Cohen, R.H., Bernstein, I.B., Dorning, J.J., and Rowlands, G., "Particle and Energy Exchange Between Untrapped and Electrostatically Confined Populations in Magnetic Mirrors," Nuclear Fusion **20**, 11 (1980).

Cohen, R.H., Rowlands, G., and Foote, J.H., "Nonadiabaticity in Mirror Machines," Phys. Fluids **21**, 14 (1978).

Curriculum Vitae for Ronald C. Davidson

Ronald C. Davidson has been Professor of Astrophysical Sciences at Princeton University since 1991, and was Director of the Princeton Plasma Physics Laboratory from 1991-1996. He received the B.Sc. degree from McMaster University in 1963, and the Ph.D. degree from Princeton University in 1966. He was Assistant Research Physicist at the University of California at Berkeley from 1966-1968, an Assistant Professor of Physics at the University of Maryland from 1968-1971, an Alfred P. Sloan Foundation Fellow from 1970-1972, an Associate Professor of Physics from 1971-1973, a Professor of Physics at the University of Maryland from 1973-1978, and Professor of Physics at the Massachusetts Institute of Technology from 1978-1991. Dr. Davidson has made numerous fundamental theoretical contributions to several areas of pure and applied plasma physics, including nonneutral plasmas, nonlinear effects and anomalous transport, kinetic equilibrium and stability properties, intense charged particle beams, advanced accelerator concepts, and coherent radiation generation by relativistic electron beams. He is the author of more than two hundred and fifty journal articles and books, including three advanced research monographs: "Methods in Nonlinear Plasma Theory" (Academic Press, New York, 1972), "Theory of Nonneutral Plasmas" (W.A. Benjamin, Reading, Massachusetts, 1974, reissued in Addison-Wesley Advanced Book Classics Series, 1989), and "Physics of Nonneutral Plasmas" (Addison-Wesley, Reading, Massachusetts, 1990). During 1976-1978 he served as Assistant Director for Applied Plasma Physics, Office of Fusion Energy, Department of Energy. Dr. Davidson also served as Director of the MIT Plasma Fusion Center from 1978-1988, as the first Chairman of the DOE Magnetic Fusion Advisory Committee (MFAC) from 1982-1986, as chairman of the American Physical Society Plasma Physics Division during 1983-1984, and has participated in numerous national and international committees on plasma physics and fusion research. Dr. Davidson is a Fellow of the American Physical Society, a Fellow of the American Association for the Advancement of Science, and a member of Sigma Xi. He is also a recipient of the Department of Energy Distinguished Associate Award and the Fusion Power Associates Leadership Award, both in 1986, and recipient of The Kaul Foundation's Award for Excellence in 1993.

Curriculum Vitae for David P. Grote

Present Position:

Staff Scientist
Heavy Ion Fusion Virtual National Laboratory (LBNL, LLNL, and PPPL)
Lawrence Livermore National Laboratory
University of California

Education:

Ph.D.	Applied Science	University of California, Davis, 1994
M.S.	Applied Science	University of California, Davis, 1989
B.S.	Physics	University of Dayton, 1987

Professional Interests:

Simulations of accelerator beams; physics relevant to inertial fusion driven by heavy ion beams; computational physics; massively parallel and object oriented programming.

Professional Experience:

Y Division/ICF Program, LLNL as a career employee, from March 2000 to the present. Plays a lead role in the development, maintenance, and application of the WARP simulation code.

X Division/ICF Program, LLNL as a term employee, from March 1997 to March 2000.

X Division/ICF Program, LLNL as a post-doctorate, from March 1994 to March 1997.

ICF Program, LLNL as a graduate student/employee of University of California, Davis, from September 1987 to March 1994. Ph.D. Thesis work carried out under Dr. Alex Friedman.

Awards, and Professional Affiliations:

Hertz Fellowship, UC Davis/LLNL
Sigma Pi Sigma, American Physical Society

Selected Publications:

"New Developments in WARP3d: Progress Toward End-to-End Simulation," David P. Grote, A. Friedman, I. Haber, W. Fawley, J. L. Vay, *Nuclear Inst. and Methods in Physics Research, A*, 415, Nos 1, 2, p 428, 1998

"Three-Dimensional Simulations of High-Current Beams in Induction Accelerators with WARP3d," D. P. Grote, A. Friedman, I. Haber, S. Yu, *Fusion Engineering and Design*, 32-33 (1996) 193-200.

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Curriculum Vitae for Rami Alfred Kishek

EDUCATION

Ph.D.	Nuclear Engineering	*University of Michigan, Ann Arbor, MI*	1997
M. S. E.	Nuclear Engineering	*University of Michigan, Ann Arbor, MI*	1995
B. S. E.	Electrical Engineering	*University of Michigan, Ann Arbor, MI*	1993

EMPLOYMENT SUMMARY

Institute for Plasma Research, University of Maryland, College Park, MD
Charged Particle Beams Laboratory

Instructor for Undergraduate course on scientific computation	*starting Jan. 2001*
Assistant Research Scientist.	*Apr. 1999-Present*
Assistant Project Manager, UMD Electron Ring (UMER).	*Feb. 1999-Present*
Research Associate.	*May 1997-Jun. 1999*

FM Technologies, Fairfax, VA

Staff Scientist.	*Summer of 1996*

University of Michigan, Ann Arbor, MI

Graduate Student Teaching Assistant.	*Jan. 1996- May 1996*
Graduate Student Research Assistant.	*Sep. 1993 - Apr. 1997*

SELECTED PUBLICATIONS

Design and field measurements of printed-circuit quadrupoles and dipoles, W. W. Zhang, S. Bernal, H. Li, T. Godlove, R. A. Kishek, P. G. O'Shea, M. Reiser, V. Yun, and M. Venturini, *PRST-AB,* 3, 122401 (2000).

Energy Transfer in non-Equilibrium Space-Charge-Dominated Beams, R. A. Kishek, P. G. O'Shea, and M. Reiser, Phys. Rev. Lett., 85 (21), 4514 (2000).

Observation and Simulation of Radial Density Oscillations in Space-Charge Dominated Electron Beams, S. Bernal, R. A. Kishek, M. Reiser, and I. Haber, Phys. Rev. Lett., 82, 4002 (1999).

Recent Progress in the Simulations of Heavy Ion Beams, I. Haber, A. Friedman, D. P. Grote, S. M. Lund, and R. A. Kishek, *Phys. Plasmas,* 6, 2254 (1999).

Multipactor Discharge on Metals and Dielectrics: Historical Review and Recent Theories, R. A. Kishek, Y. Y. Lau, L. K. Ang, A. Valfells, and R. M. Gilgenbach, *Phys. Plasmas,* 5 (5), 2120 (1998).

Power Deposited on a Dielectric by Multipactor, L. K. Ang, Y. Y. Lau, R. A. Kishek, and R. M. Gilgenbach, *IEEE Trans. On Plasma Science*, 26 (3), 290 (1998).

Multipactor Discharge on a Dielectric, R. A. Kishek and Y. Y. Lau, *Phys. Rev. Lett.,* 80 (1), 193 (1998).

A Novel Phase Focusing Mechanism in Multipactor Discharge, R. A. Kishek and Y. Y. Lau, *Physics of Plasmas (Letters)*, 3, 5 (1996).

Interaction of Multipactor Discharge and rf Circuit, R. Kishek and Y. Y. Lau, *Phys. Rev. Lett.*, 75, 1218 (1995).

Curriculum Vitae for Patrick Gerard O'Shea

EDUCATION

Ph.D. (Physics) University of Maryland, College Park, 1986.

M.S. (Physics) University of Maryland, College Park, 1982.

B.Sc. (Experimental Physics) National University of Ireland, University College Cork, 1979.

RECENT EMPLOYMENT SUMMARY

Current Appointments:

University of Maryland:
Acting Director, Institute for Plasma Research (2000-)
Associate Professor, Dept. of Electrical and Computer Engineering, (1998-)
Duke University, Adjunct Associate Professor of Physics (1999-)

Previous Appointments:

Los Alamos National Laboratory (1986 - 1999):
Project Leader APEX Free-Electron Laser Facility (1990 - 1994).
Deputy Project Leader APEX Free-Electron Laser Facility (Jan. - Dec. 1990).
Chief Accelerator Physicist, Beam Experiments Aboard Rocket Project (1986-1989)
Leave of absence at Duke University, Assistant Professor of Physics (1994-1998)

PUBLICATIONS

Over eighty publications in particle beam and free-electron laser technology and applications

Selected recent publications:

Gamma-Ray Production in a Storage Ring Free-Electron Laser, V. N. Litvinenko, B. Burnham, M. Emamian, N. Hower, J. M. J. Madey, P. Morcombe, P. G. O'Shea, S. H. Park, R. Sachtschale, K. D. Straub, G. Swift, P. Wang, Y. Wu , R. S. Canon, C. R. Howell, N. R. Roberson, E. C. Schreiber, M. Spraker, W. Tornow, H. R. Weller , I. V. Pinayev, N. G. Gavrilov, M. G. Fedotov, G. N. Kulipanov, G. Y. Kurkin, S. F. Mikhailov, V. M. Popik, A. N. Skrinsky, and N. A. Vinokurov, B. E. Norum , A. Lumpkin and B. Yang, *Physical Review Letters*. **78**, 4569 (1997)

Reversible and Irreversible Emittance Growth in Charged Particle Beams, P. G. O'Shea, Phys. Rev. E, **57**, 1081 (1998)

The Effect of a Matched Electron Beam on High-Gain Free-Electron Laser Amplifier Performance H.P. Freund and P.G. O'Shea, *Physical Review Letters*., **80**, 520 (1998)

Production of Radioisotopes via Direct Electron Activation, K.J. Weeks and P.G. O'Shea, *Medical Physics* **25**, 488 (1998)

RF Photoinjector Using a LaB$_6$ Cathode and a Nitrogen Drive-Laser, P.G O'Shea, J.A. Lancaster and C.R Jones, *Applied. Physics. Letters*., 73, 411 (1998)

A Non-Destructive Electron Beam Diagnostic for a SASE FEL using Coherent Off-Axis Undulator Radiation, C. Neuman, M. Ponds, G. Barnett, J. Madey, P. G. O'Shea, Nucl. Instr. Meth A429, 287 (1999)

Coherent Off-Axis Radiation from Short Electron Bunches, C.P. Neuman, W.S. Graves, and P.G. O'Shea, *Physical Review ST-AB*, 3 030701 (2000)

Two-Color Operation in High-Gain Free-Electron Lasers, H.P. Freund and P.G. O'Shea, *Physical Review Letters* , 84 2861 (2000)

Energy Transfer in Nonequilribium Space-Charge-Dominated Beams, **R.A. Kishek, P.G. O'Shea, M. Reiser, *Physical Review Letters*. 85, 4514 (2000)**

Design and Field Measurements of Printed-Circuit Quadrupoles and Dipoles, WW. Zhang, H. Li, S. Bernal, T. Godlove, R.A Kishek, P.G. O'Shea, M. Reiser, M. Venturini, V. Yun Phys. Rev. ST Accel. Beams 3, 122401 (2000)

Curriculum Vitae for David V. Rose

B.A. (Physics) Temple University, 1986
M.S. (Applied Physics) Johns Hopkins University, 1990
Ph.D. (Computational Sciences and Informatics) George Mason University, 1997

Dr. Rose joined Mission Research Corporation's Particle Beam Applications group in September 1999. His present research includes high-power charged-particle-beam transport, high-power diode physics, radiographic source development, and plasma physics code development.

From 1987 until August 1999, he was a senior scientist with Jaycor in McLean, Virginia. During this period he was a full-time consultant to the Naval Research Laboratory's Plasma Physics Division, in Washington, DC. He was responsible for theoretical modeling and experimental data analysis in support of ongoing experiments in pulsed power systems, plasma opening switches, intense charged particle beam generation and transport, intense radiation sources, and magnetically insulated transmission lines.

In addition, Dr. Rose is a part-time instructor in the Department of Mathematics and Statistics at the University of New Mexico and he has worked as a part-time Assistant Professor for George Mason University, Northern Virginia Community College, and Dickinson College teaching graduate and undergraduate level courses in mathematics, physics, and computational science.

Publications and papers by Dr. Rose include:

D. V. Rose, D. R. Welch, B. V. Oliver, R. E. Clark, W. M. Sharp, and A. Friedman, "*Ballistic-neutralized chamber transport of intense heavy ion beams*," to appear in Nucl. Instrum. Meth. Phys. Res. A (2001).

D. V. Rose, P. F. Ottinger, D. R. Welch, B. V. Oliver, and C. L. Olson, "*Numerical simulations of self-pinched transport of intense ion beams in low-pressure gases*," Phys. Plasmas **6**, 4094 (1999).

D. V. Rose and J. U. Guillory, "*Numerical simulation of limiting currents for transport of intense relativistic electron beams in conducting waveguides*," J. Appl. Phys. **78**, 5787 (1995).

D. V. Rose, P. F. Ottinger, and C. L. Olson, "*Transport efficiency studies for light-ion inertial-confinement-fusion systems using ballistic transport with solenoidal lens focusing*," IEEE Trans. Plasma Sci. **23**, 163 (1995).

D. V. Rose and M. R. Kuzma, "*Nonequilibrium periodic reorientation induced by magnetic field in lyotropic nematic liquid crystals*," Mol. Cryst. Liq. Cryst. Lett. **4**, 39 (1986).

Curriculum Vitae for Jean-Luc Vay

BS	(Physics) University of Poitiers, France, 1991
MS	(Physics) University of Paris-Denis Diderot, France, 1993
Ph.D.	(Physics) University of Paris-Orsay, France, 1996

During his Ph.D. studies, Jean-Luc Vay developed the first 3-D Particle-In-Cell code (BPIC) applied to the study of the propagation of a beam through a Heavy Ion Fusion reactor. New numerical techniques that he developed during the Ph.D. rendered it possible on the computers available at the time. BPIC is being used at Lawrence Berkeley National Laboratory and at Stanford Linear Accelerator Center for plasma lens studies.

During his post-doctorate from Nov. 1996 to Nov. 1998, at Lawrence Berkeley National Laboratory in the Heavy Ion Fusion group, he continued on the same subject to develop new numerical techniques in order to further reduce the computational needs. He developed a new discretization scheme of Maxwell equations which allows a natural implementation of the mesh refinement technique and a new efficient "outgoing wave" boundary condition. Both have led to recent publications in the *Journal of Computational Physics*. The latter was implemented during a two month effort collaboration in France in the code EMI2D from Ecole Polytechnique (Palaiseau, France) used for laser-plasma interaction modeling for the fast-ignitor scheme.

From Nov. 1998 to Sep. 2000, together with Dr. W. Fawley, he developed a "slice" XY accelerator code which is being applied to the study of beam emittance growth for the second axis of DARHT (Dual Axis Radiographic Hydrodynamics Test).

In Dec. 2000, he joined the Heavy Ion Fusion group at LBNL as a carrier physicist.

Selected Publications

" An Extended FDTD scheme for the Wave Equation: Application to Multiscale Electromagnetic Simulation ", J.-L. Vay, *Journal of Computational Physics* (to be published)

" A New Absorbing Layer Boundary Condition for the Wave Equation ", J.-L. Vay, *Journal of Computational Physics*, Vol. 165, No. 2, pp. 511-521, December 2000

" Intense Ion Beam Propagation in a Reactor Sized Chamber ", *Nucl. Instr. & Meth. A.*, as part of *Proc. Int. Sympos. on Heavy Ion Inertial Fusion*, San Diego, CA, March 2000 (to be published)

" Charge compensated ion beam propagation in a reactor sized chamber " J-L. Vay and C. Deutsch, *Physics of Plasmas*, VOL. 5, N. 4, April 1998

" A 3D electromagnetic PIC-MCC code to simulate heavy ion beam propagation in the reaction chamber " J.-L. Vay and C. Deutsch, *J. of Fusion Engineering and Design*, 32-33, pp. 467-476, 1996

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Curriculum Vitae for Simon S. Yu

PRESENT POSITION:

Senior Staff Scientist
Lawrence Berkeley National Laboratory
Berkeley, CA. 94720
(510) 486-5477

Fellow, American Physical Society

EMPLOYMENT HISTORY:

1992 – present	-Physicist, Lawrence Berkeley National Laboratory
1984 – 1992	-Physicist, Program Leader for Theory, LLNL
1983 –1984	-Physicist, Stanford Linear Accelerator Center, Accelerator Theory (Klystron Physics)
1977 – 1983	-Physicist, LLNL
1973 – 1977	-Postdoctoral Research High Energy Physics and Atomic Theory, University of Pittsburgh
1970 – 1973	-Postdoctoral Research, High Energy Physics and Atomic Physics, University of Washington

PROJECT PRINCIPAL INVESTIGATOR:

DARHT II Injector
RTA, -Two Beam Accelerator Project, LBNL/LLNL
Channel Transport for HIF
2 MV HIF Injector LBNL
Heavy Ion Recirculator Project LLNL
Relativistic Klystron, LLNL/SLAC/LBNL

SELECTED PUBLICATIONS AND OTHER PAPERS:

- "Filamentation of a Heavy-Ion Beam in a Reactor Vessel," with E.P. Lee, H.L. Buchanan, F.W. Chambers, M.N. Rosenbluth, Phys. Of Fluids 23, (1980), 2095.
- "Phase-space Distortion of a Heavy Ion Beam Propagating Through a Vacuum Reactor Vessel," with E.P. Lee and W.A. Barletta, Nuclear Fusion 21, 961 (1981).
- "2-1/2-D Particle-in-Cell Simulation of High Power Klystrons," with A. Drobot, P.Wilson, Proceedings of Particle Accelerator Conference, Vancouver, B.C. (1985).
- "Relativistic Klystron Two-Beam Accelerator," with A.M. Sessler, Physical Review Letters, Vol. 58, No. 23, pp.2439-2442 (1987)
- "A Plasma-Based Adiabatic Focuser," with P. Chen and K. Oide, Stanford Linear Accelerator Center, A.M. Sessler, LBL, Physical Review Letters, UCRL-102053, (1989).
- "Relativistic Klystron Simulations Using RKTW2D," with R.D. Ryne, 1990 Linear Accelerator Conference, Albuquerque, NM, UCRL-JC-103798 (1990).
- "Transverse Instabilities in a Relativistic Klystron Two-Beam Accelerator," with G.A. Westenskow and T.L. Houck. Proceedings of the 16th International LINAC Conference, Ottawa, Ontario, Canada, August 24-28, 1992, UCRL-JC-110195.
- "Recirculating Induction Accelerators as Drivers for Heavy Ion Fusion," with J.J. Barnard, et al, Phys. Fluids. B, 1993.
- " A Driver-Scale Injector for Heavy-Ion Fusion," with F. Deadrick, S. Eylon, A. Faltens, D. Grote, E. Henestroza, R. Hipple, C. Peters, L. Reginato, J. Stoker, and D. Vanacek, LBL and LLNL, May 16, 1994, HIFAN Note 629, LBL-35641a.
- "Relativistic-Klystron Two-Beam Accelerator as a Power Source for a 1 TeV Next Linear collider – A Systems Study," with F. Deadrick, N. Goffney, E. Henestroza, Westenskow, August 1994, LBL-36232.
- "Ion Sources for Heavy Ion Fusion," S. Yu et al. Proceedings of the 6th International Conference on Ion Sources," Whistler, BC, Canada, Review of Scientific Instruments Vol 67, No. 3, Part II (1996)
- "Three-dimensional Simulations of High-Current Beams with WARP3D", with D. Grote et al., Proceedings of the International Symposium on Heavy Ion Fusion, Fusion Engineering and Design (1996)
- "Heavy Ion Fusion 2 MV Injector", S. Yu et al., Proceedings of the 1995 Particle Accelerator Conference, p.1178 (1996)

Description of Facilities and Resources

The research described in this proposal will make use of computational facilities at the National Energy Research Supercomputer Center, Lawrence Berkeley National Laboratory. In addition, workstations, networks, and other computational facilities at the individual sites will be employed; all are suitable to the needs of this research program.

In addition, the sites participating in this distributed topical Center are linked by video-teleconference facilities, which is already being used for interactions on various topics in Heavy Ion Fusion research.

Experimental facilities at four of the partnering institutions will play a key role in the code validation process, by making data available for code benchmarking, and by working closely with the team members to make sure that the experimental configuration is accurately represented in the code inputs. The Heavy Ion Fusion program has a long history of partnerships between simulators and experimenters, and the Center will build on this. Ultimately, the success of the proposed simulation capability will be measured by its ability to predict experimental behaviors with confidence.

The Lawrence Berkeley National Laboratory has fielded a number of scaled experiments, and these have offered simulators an opportunity to develop and hone their tools by applying them to beam transport, plasma lens formation, beam pinch-mode propagation, and beam injection. For example, the LSP code was able to reproduce the improvement in focal spot size obtained in the Final Focus Scaled Experiment when neutralizing electrons were introduced using a hot filament. Also, WARP was used to understand pulse compression in the Multiple Beam Experiment–4 apparatus. The greatest emphasis in the near future will be on a High Current Experiment, which will transport a beam of full driver-like line charge density. In addition, a high-current focusing and chamber transport experiment is planned for the near future, and high-current injector experiments will continue.

The University of Maryland Electron Ring (UMER) experiment is designed to explore, on a scaled basis, the physics of space charge dominated beams. Because of the use of electrons and a ring geometry, this apparatus will allow, for the first time, the detailed experimental investigation of long timescale beam dynamics of such a beam. A significant feature of UMER is the extent to which computer simulation, using WARP, has been employed from the outset in the design. Also significant are the extensive diagnostics planned in the deployment of the ring, such as a large number of beam position monitors, phosphor screens emittance scanners (slit-slit and pepper pot), and a longitudinal energy diagnostic. These diagnostics will be deployed around the ring as it assembled and have been designed with the explicit purpose of comparing the data they collect with parallel simulation of the beam dynamics.

At the Princeton Plasma Physics Laboratory, experiments are getting underway to develop a "Paul Trap" beam simulator.[54] The plan is to confine a stationary plasma with time-varying fields that closely model the alternating-gradient fields of a real accelerator or beamline as they are experienced by the moving beam. Such a configuration can be well-diagnosed and will lend insight into the kinetic behaviors of beams in relevant regimes.

At Lawrence Livermore National Laboratory, a high-voltage test stand is being assembled, with the goal of developing a novel plasma ion source / multi-beamlet injector concept that will merge a large number of mm-scale beams into a high-current elliptical beam, while using as little cross-sectional area and length as possible. The basic principle behind this concept is being explored using WARP simulations.

Appendix I

Letters from investigators stating agreement to participate in, or collaborate with, the project

- Robert D. Ryne, Principal Investigator for coordinated High Energy and Nuclear Physics SciDAC proposal "Advanced Computing for 21st Century Accelerator Science and Technology"
- Phillip Colella, Senior Investigator
- David P. Grote, Senior Investigator
- Irving Haber, Senior Investigator
- Rami A. Kishek, Senior Investigator
- Patrick G. O'Shea, Senior Investigator
- William M. Sharp, Senior Investigator
- Simon S. Yu, Senior Investigator
- Ronald H. Cohen, Senior Investigator

Appendix II

Selected Publications and Manuscripts relevant to this Proposal

1. I. Haber, A. Friedman, D. P. Grote, S. M. Lund, and R. A. Kishek, "Recent progress in the simulation of heavy ion beams," *Phys. Plasmas* **6** No. 2, 2254 (1999). [Reference 10 in main text]

2. D. R. Welch, D. V. Rose, B. V. Oliver and R. E. Clark, "Simulation Techniques for Heavy Ion Fusion Chamber Transport", *Proc. Int. Sympos. on Heavy-Ion Inertial Fusion*, San Diego, March 13-17, 2000; in press, *Nucl. Instr. and Meth. A* (2001). [Reference 12 in main text]

3. H. Qin, R. C. Davidson, and W. W. Lee, "Three-dimensional multispecies nonlinear perturbative particle simulation of collective processes in intense particle beams," *Physics Review Special Topics - Accelerators and Beams* **3**, 084401 (2000). [Reference 18 in main text]

4. D. P. Grote, A. Friedman, and I. Haber, "New Methods in WARP," *Proc. International Computational Accelerator Physics Conference*, Sept. 14-18, 1998, Monterey CA*, AIP Conference Proc.* (1998). [Reference 26 in main text]

5. A. Friedman, D. P. Grote, E. P. Lee, and E. Sonnendrucker, "Beam simulations for IRE and driver—status and strategy," *Proc. Int. Sympos. on Heavy-Ion Inertial Fusion*, San Diego, March 13-17, 2000; in press, *Nucl. Instr. and Meth. Phys. Res. A* (2001). [Reference 25 in main text]

Curriculum Vitae for Dale R. Welch

B. S. (Nuclear Engineering) Northwestern University, 1980
M. S. (Nuclear Engineering) University of Illinois, 1982
Ph.D. (Nuclear Engineering) University of Illinois, 1985

Dr. Welch joined the Particle Beam Applications Group of Mission Research Corporation in the fall of 1985. His main interest has been the physics of beam generation and plasma evolution in pulsed-power machines and beam transport in the atmosphere and fusion reactor chambers. He has been involved with analytic modeling and, using the 3-D hybrid codes IPROP and LSP, computational studies of these phenomena. This work has focused on the development of novel dense-plasma numerical algorithms for electromagnetic particle-in-cell simulations. This research had led to several discoveries including mechanisms for electron-beam tracking, ion disruption of the focal spot of intense electron beams and ion-beam self-pinched transport in low-density gases.

Before joining MRC, Dr. Welch was involved in inertial confinement fusion research at the University of Illinois. This work centered on the modeling of laser-fusion implosions, diagnostics and simulation codes. He developed implosion models for the study of shock-compression dynamics in laser-fusion experiments that were utilized in the time-dependent diagnosis of fuel density-radius product and temperature.

Publications by Dr. Welch include:

"Simulation Techniques of Heavy Ion Fusion Chamber Transport," with D. V. Rose, B. V. Oliver and R. E. Clark, *Nucl. Inst. and Meth. in Phys. Res., A* , to be published 2001.

"Self-Pinched Transport of an Intense Proton Beam," with P. F. Ottinger, F. C. Young, S. J. Stephanakis, D. V. Rose, J. M. Neri, B. V. Weber, M. C. Myers, D. D. Hinshelwood, D. Mosher and C. L. Olson, *Physics of Plasmas*, 7, 346-358, January 2000.

"Effects of Target-Emitted Ion on the Focal Spot of an Intense Electron Beam," with T. P. Hughes, *Laser and Particle Beams*, **16**, 285-294, September 1998.

"Gas Breakdown Effects in the Generation and Transport of Light Ion Beams for Fusion," *Physics of Plasmas*, **3**, 2113-2121, May 1996.

"Self-Pinched Transport for Ion-Driven ICF," *Fusion Engineering and Design*, 32-33, 477-483 (1996).

"Simulation of Charged-Particle Beam Transport in a Gas Using a Hybrid Particle-Fluid Plasma Model," *Physics of Plasmas*, **1**, 764-773, March 1994.

"Diffuse Plasma Effects on the Ion-Hose Instability," with T. P. Hughes, *Phys. Fluids B*, Vol. 5, No. 2, pp. 339–343, February 1993.

"Electron-Beam Guiding by a Reduced-Density Channel," *Phys. Rev. Lett.* 65, 17 December 1990, p. 3128, with F. M. Bieniosek and B. B. Godfrey.

Curriculum Vitae for William M. Sharp

Education

BS (Physics) Harvey Mudd College, 1968

MS (Applied Science) University of California Davis/Livermore, 1969

Ph.D. (Applied Science) University of California Davis/Livermore, 1976

Present Position

Dr. Sharp joined the LLNL Heavy-Ion Fusion Group in 1992. His work has included development of a fluid/envelope code CIRCE to model transport of space-charge-dominated beams in induction accelerators, the modeling of the longitudinal space-charge field in ion beams, and the calculation of acceleration and longitudinal-control fields for circular induction accelerators. His research is presently focused on transport of heavy-ion beams in a fusion chamber. Dr. Sharp has been associated with the Virtual National Laboratory for Heavy-Ion Fusion since it was formed in 1998, and his principal workplace is LBNL.

Previous Positions

From 1978 until 1982, Dr. Sharp worked for SAIC in McLean, Virginia, and was assigned to work at the Naval Research Laboratory on electron-beam transport in air. This work was continued when he joined the electron-beam group at LLNL in 1982. Between 1986 and 1992, his principal work was developing and applying simulation codes to model free-electron lasers.

Selected Publications

W. M. Sharp, D. A. Callahan-Miller, and A. B. Langdon, "Improved Modeling of Chamber Transport for Heavy-Ion Fusion," to be published in *Nucl. Instr. Meth. Physics Res.*

W. M. Sharp and D. P. Grote, "Acceleration Schedules for a Recirculating Heavy-Ion Accelerator" in Proc. 1999 Particle Accelerator Conference, New York, 27 March-2 April 1999, p. 1833.

W. M. Sharp and D. P. Grote, "Modeling Acceleration Schedules for a Recirculating Heavy-Ion Accelerator" LLNL Internal Report (1999).

W. M. Sharp, D. P. Grote, M. A. Hernandez, and G. W. Kamin, " Steering Algorithms for a Small Recirculating Heavy-Ion Accelerator," *Nucl. Instr. Meth. Physics Res.* **A415**, 320 (1998).

W. M. Sharp, A. Friedman, and D. P. Grote, "Effects of Longitudinal Space Charge in Beams for Heavy-Ion Fusion," *Fusion Eng Design* **32-33**, 201 (1996).

Curriculum Vitae for Hong Qin

Staff Research Physicist, Plasma Physics Laboratory, Princeton University
Tel: (609) 243-3310, Fax: (609) 243-2662
Email: hongqin@pppl.gov

Education:

- Ph.D., Astrophysical Science, 1998, Princeton University
- M. S., Space Physics, 1993, Beijing University
- B. S., Space Physics, 1990, Beijing University

Research and Work Experience:

- Staff Research Physicist,
  Plasma Physics Laboratory, Princeton University, 2000 –
  Developing numerical and analytical methods for nonlinear beam dynamics with applications to heavy ion fusion drivers and high intensity accelerators.

- Associate Research Physicist,
  Plasma Physics Laboratory, Princeton University, 1998 – 2000
  Developing numerical and analytical methods for nonlinear beam dynamics with applications to heavy ion fusion drivers and high intensity accelerators.

- Visiting Scholar
  Wolfram Research, 1997
  Developing a symbolic computer algebra package for applications in plasma physics.

Expertise and Skills:

- Physics:
  plasma physics, beam physics, and computational physics
- Mathematics:
  differential equations and differential geometry
- Computing:
  numerical methods for differential equations, computer algebra, parallel computing, and particle simulations

Publications:

More than 20 publications in refereed journals.

Curriculum Vitae for W. Wei-li Lee

Dr. W. W. Lee received his B.S. from National Taiwan University, his M.S. from Duke University, and his Ph.D. from Northwestern University. From 1970-1974, he worked as an accelerator physicist at Fermi National Accelerator Laboratory. Since then, he has been a member of the Theory Department at Princeton Plasma Physics Laboratory. Dr. Lee's primary interest is particle simulation of plasmas, and he is the inventor of gyrokinetic particle simulation. He is a Fellow of American Physical Society and a Distinguished Laboratory Fellow at PPPL.

Curriculum Vitae for Irving Haber

Research Physicist
Beam Physics Branch
Plasma Physics Division
Naval Research Laboratory

BEE	Cooper Union, 1961
MS	Polytechnic Institute of Brooklyn, 1965
Ph.D.	Polytechnic Institute of Brooklyn, 1969

During his tenure at the Naval Research Laboratory from 1969 until the present, Dr. Haber has contributed broadly to research in experimental and theoretical plasma physics, charged particle beam physics, and electromagnetics, as well as the development of numerical techniques to facilitate that research. His primary area of current interest is the use of particle-in-cell simulations to investigate the nonlinear dynamics of collisionless beams and plasmas. He has pioneered the use of these techniques to investigate the fundamental properties of non-neutral plasmas, such as are found in intense charged particle beams, and the nonlinear evolution of plasma instabilities.

As accelerator luminosities are increased, a fully nonlinear description of the beam dynamics becomes increasingly important to successful design of these accelerators. At the same time, it becomes increasingly difficult to analytically describe the beam evolution, so that numerical techniques become an increasingly important tool. Dr. Haber has been a pioneer in the use of particle-in-cell plasma simulation techniques to describe the collective nonlinear dynamics which are characteristic of space-charge-dominated beams. These techniques have been successful in predicting aspects of the nonlinear beam dynamics, such as the saturation of collective space-charge instabilities, not amenable to analytic description. These predictions were later verified by experiment. The simulations have also succeeded in reproducing, in fine detail, experimentally measured characteristics of the nonlinear beam dynamics.

Starting in 1969 Dr. Haber was centrally involved in developing and deploying the numerical techniques used in some of the fundamental studies of the nonlinear plasma dynamics associated with collisionless shocks and instabilities in the ionosphere and in fusion devices. In order to conduct the pertinent computer experiments he has also developed methods for the efficient exploitation of modern computer architectures. Dr. Haber has also taught graduate courses in Plasma Physics and Numerical Analysis at George Washington University.

Before joining NRL, Dr. Haber did graduate theoretical and experimental research in plasma and relativistic beam interactions, and electromagnetics. He has also worked as an engineer in the design of microwave devices such as low noise parametric amplifiers.

Curriculum Vitae for Alex Friedman

PRESENT POSITION:
Simulations and Theory Group Leader
Heavy Ion Fusion Virtual National Laboratory (LBNL, LLNL, and PPPL)
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BIOGRAPHICAL INFORMATION:
Alex Friedman carried out his undergraduate and graduate studies at Cornell University. He received his Ph.D. in Applied Physics (with a minor in Computer Science), under the thesis supervision of Prof. Ravindra Sudan. During 1979 and 1980 he did post-doctoral research in computational plasma physics with Prof. Charles (Ned) Birdsall's group at the University of California, Berkeley. He then joined the scientific staff of LLNL, where he has carried out research in laser fusion, magnetic fusion energy, and heavy-ion beam driven inertial fusion energy. From 1992 to 1998 he served as LLNL's Heavy Ion Fusion Project Leader. Since 1998 he has been the Simulations and Theory Group Leader of the Heavy Ion Fusion Virtual National Laboratory, a joint enterprise of LBNL (his principal workplace since early 1999), LLNL, and PPPL.

SCHOLARSHIPS AND HONORS:
Fellow, American Physical Society, 1997
LLNL Physics Department Distinguished Achievement Award, 1992
Cornell Graduate Fellowship, September 1973-June 1975
National Merit Scholarship, awarded 1969
Southern Bell Telephone "Star" Scholarship, awarded 1969
Member, Sigma Xi (scientific honorary society)
Member, Tau Beta Pi (engineering honorary society)

PROFESSIONAL AFFILIATION:
American Physical Society, Divisions of Plasma Physics, Physics of Beams, Computational Physics

RESEARCH INTERESTS:
Heavy Ion Fusion; computational plasma physics and particle-beam physics; computational dynamics; and numerical analysis.

RECENT PUBLICATIONS:

A. Friedman, D. P. Grote, E. P. Lee, and E. Sonnendrucker, "Beam simulations for IRE and driver — status and strategy," submitted to *Nucl. Instr. & Meth. A.*, as part of *Proc. Int. Sympos. on Heavy Ion Inertial Fusion*, San Diego, CA, March 2000.

D. V. Rose, D. R. Welch, B. V. Oliver, W. M. Sharp, and A. Friedman, "Ballistic-Neutralized Chamber Transport of Intense Heavy Ion Beams," submitted to *Nucl. Instr. & Meth. A.*

D. P. Grote, A. Friedman, G. Craig, I. Haber, and W. M. Sharp, "Progress Toward Source-to-Target Simulations," submitted to *Nucl. Instr. & Meth. A.*

E. Sonnendrucker, A. Friedman, J. J. Barnard, D. P. Grote, and S. M. Lund, "Simulation of heavy ion beams with a semi-Lagrangian Vlasov solver," submitted to *Nucl. Instr. & Meth. A.*

I. Haber, A. Friedman, D. P. Grote, S. M. Lund, and R. A. Kishek, "Recent Progress in the Simulations of Heavy Ion Beams," *Phys. Plasmas* **6** (1999).

Curriculum Vitae for Phillip Colella

Dr. Colella received his A.B. (1974), M.A. (1976) and Ph.D. (1979) degrees from the University of California at Berkeley, all in applied mathematics. Dr. Colella has served as a staff scientist at both the Lawrence Berkeley National Laboratory and the Lawrence Livermore National Laboratory. From 1989 to 1995, Dr. Colella was a Professor in the Mechanical Engineering Department at the University of California at Berkeley. He is currently a Senior Mathematician and Group Leader for the Applied Numerical Algorithms Group in the Computing Sciences Directorate at the Lawrence Berkeley National Laboratory. He is a leader in the development of numerical methods for partial differential equations, with contributions in the areas of higher-order Godunov methods, projection methods for incompressible flow, adaptive mesh refinement, fast adaptive particle methods, volume-of-fluid methods for irregular boundaries, and programming language and library design for parallel scientific computing. He has also applied numerical methods in a variety of scientific and engineering fields, including shock dynamics, low-Mach number and incompressible flows, combustion, porous media flows, and astrophysical flows. He has authored or co-authored more than 100 research papers, and has supervised 16 Ph.D. students and 8 postdoctoral researchers.

Selected Publications:

M. J. Berger and P. Colella, "Local adaptive mesh refinement for shock hydrodynamics", J. Comput. Phys. 82(1):64-84 (1989).

A. Zachary, A. Malagoli and P. Colella, "A higher-order Godunov method for multidimensional ideal magnetohydrodynamics", SIAM J. Sci. Stat. Comput. 15(2):263-284 (1994).

A. S. Almgren, T. Buttke and P. Colella, "A fast adaptive vortex method in three dimensions", J. Comput. Phys. 113(2):177-200 (1994).

K. Yelick, L. Semenzato, G. Pike, C. Miyamoto, B. Liblit, A. Krishnamurthy, P. Hilfinger, S. Graham, D. Gay, P. Colella and A. Aiken, "Titanium: a high-performance Java dialect", Concurrency: Practice and Experience, 10:825-836 (1998).

A. S. Almgren, J. B. Bell, P. Colella, L. H. Howell and M. J. Welcome, "A conservative adaptive projection method for the variable density incompressible Navier-Stokes equations", J. Comput. Phys. 142(1):1-46 (1998).

H. Johansen and P. Colella, "A Cartesian grid embedded boundary method for Poisson's equation on irregular domains", J. Comput. Phys. 147(1):60-85 (1998).

P. Colella, M. Dorr and D. Wake, "Numerical solution of plasma fluid equations using locally refined grids", J. Comput. Phys. 152(2):550-583 (1999).

G. Balls and P. Colella, "A finite difference domain decomposition method for solving Poisson's equation using local corrections", Lawrence Berkeley National Laboratory report LBNL-45035, January, 2000, submitted to J. Comput. Phys.

19. W. W. Lee, Q. Qian, and R. C. Davidson, "Stability and Transport Properties of an Intense Ion Beam Propagating Through an Alternating-Gradient Focusing Lattice," *Physics Letters* **A230**, 347 (1997).
20. Q. Qian, W. W. Lee, and R. C. Davidson, "Nonlinear δf Simulation Studies of Intense Ion Beam Propagation Through an Alternating-Gradient Quadrupole Focusing Field," *Phys. Plasmas* **4**, 1915 (1997).
21. H Qin, R. C. Davidson and W. W. Lee, "3D Nonlinear Perturbative Particle Simulations of Two-Stream Collective Processes in Intense Particle Beams," *Physics Letters* **A272**, 389 (2000).
22. H. Qin, R. C. Davidson, and W. W. Lee, "3D Multispecies Nonlinear Perturbative Particle Simulations of Collective Instabilities in Intense Particle Beams," *AIP Conference Proceedings* **496**, 295 (1999).
23. S. Strasburg and R. C. Davidson, "Production of Halo Particles by Excitation of Collective Modes in High-Intensity Charged Particle Beams," *Physical Review* **E61**, 5753 (2000).
24. P. Stoltz, R. C. Davidson, and W. W. Lee, "Nonlinear δf Simulation Studies of High-Intensity Ion Beam Propagation in a Periodic Focusing Field," *Phys. Plasmas* **6**, 298 (1999).
25. A. Friedman, D. P. Grote, E. P. Lee, and E. Sonnendrucker, "Beam simulations for IRE and driver—status and strategy," *Proc. Int. Sympos. on Heavy-Ion Inertial Fusion*, San Diego, March 13-17, 2000; in press, *Nucl. Instr. and Meth. Phys. Res. A* (2001). [included in Appendix]
26. D. P. Grote, A. Friedman, and I. Haber, "New Methods in WARP," *Proc. International Computational Accelerator Physics Conference*, Sept. 14-18, 1998, Monterey CA, *AIP Conference Proc.* (1998). [included in Appendix]
27. A. Friedman, A. B. Langdon, and B. I. Cohen, "A Direct Method for Implicit Particle-in-Cell Simulation," *Comments on Plasma Physics and Controlled Fusion* **6**, 225 (1981).
28. J.-L. Vay, "An Extended FDTD scheme for the Wave Equation: Application to Multiscale Electromagnetic Simulation," *Journal of Computational Physics* (to be published).
29. A. Friedman, "A Second Order Implicit Particle Mover with Adjustable Damping," *J. Comput. Phys.* **90**, 292 (1990).
30. D. P. Grote, A. Friedman, I. Haber, "Methods used in WARP3d, a Three-Dimensional PIC/Accelerator Code," *Proceedings of the 1996 Comput. Accel. Phys. Conf.*, AIP Conference Proceedings **391**, p. 51.
31. R. C. Davidson, H. Qin, P. H. Stoltz, and T.-S. Wang, "Kinetic Description of Electron-Proton Instability in High-Intensity Proton Linacs and Storage Rings Based on the Vlasov-Maxwell Equations," *Physical Review Special Topics on Accelerators and Beams* **2**, 054401 (1999).
32. R. C. Davidson and H. Qin, "Effects of Axial Momentum Spread on the Electron-Ion Two-stream Instability in High-Intensity Ion Beams," *Physics Letters* **A270**, 177 (2000).
33. R. A. Kishek, S. Bernal, M. Reiser, M. Venturini, J. G. Wang, I. Haber, and T. Godlove, "Beam Dynamics Simulations of the University of Maryland Electron-Ring Project," *Nuclear Instruments and Method*, **A415**, 417-421 (1998).
34. A. Friedman, D. P. Grote, and I. Haber, "Three-dimensional particle simulation of heavy-ion fusion beams," *Phys. Fluids* **B 4**, 2203 (1992).
35. R. A. Kishek, S. Bernal, Y. Li, M. Reiser, M. Venturini, I. Haber, and T. F. Godlove, "Simulations of collective Effects in the Space-Charge Dominated beam of the University of Maryland Electron Ring," *Proc. 1999 APS/IEEE Part. Accel. Conf.*, New York City, 1758 (1999). http://ftp.pac99.bnl.gov/Procs/MAIN/PROCS.HTM
36. R. A. Kishek, J. J. Barnard, and D. P. Grote, "Effects of Quadrupole Rotations on the Transport of Space-Charge-Dominated Beams: Theory and Simulations Comparing Linacs with Circular Machines," *Proc. 1999 APS/IEEE Part. Accel. Conf.*, New York City, 1761 (1999). http://ftp.pac99.bnl.gov/Procs/MAIN/PROCS.HTM

Finally, we intend to work with the NERSC and PPPL visualization groups to develop tools that will facilitate our developing an understanding of these complex Liouvillean flows in phase spaces.

This research will be closely coordinated with the Magnetic Fusion Energy elements of the fusion advanced computing activity, through the Plasma Science Advanced scientific Computation Institute (PSACI) and informal interactions.

Physics studies: Interaction of intense beams with background populations

We will apply LSP for studies of multi-beam propagation through the fusion chamber, in both neutralized-ballistic and self-pinch regimes.

Physics studies: Non-ideal dynamical effects in intense beams

We will apply the WARP3d multi-beam model to the study of non-ideal effects such as resistive instabilities, inductive field couplings, and time-dependent multi-beam interactions.

We will study the interaction between beam particles and collective excitations, including halo particle production and chaotic particle motion inside the beam, using both BEST and WARP-SLV.

Physics studies: Integrated beam physics

We will conduct initial source-to-target Heavy Ion Fusion beam simulation runs to exploit the new capabilities developed. This represents a key milestone, and must correspond to a real-world capability that can be exploited again and again.

Throughout the Three Years

We will exercise every opportunity to validate the new tools against ongoing experiments in the U.S., Europe, and Japan.

We will develop and exploit visualization and code-steering capabilities, to facilitate physics insight and understanding of these 3–D time-dependent systems, and ultimately to aid in the design of experiments.

We will "productize" our codes to the maximum degree possible for tools that are themselves the objects of research, and make them available to other researchers as possible and appropriate.

We will export the new capabilities to other programs in the DOE and elsewhere as possible and appropriate, "advertising" them at scientific and computational meetings and within our own laboratories and universities. Usage by others may require support, for which they would be asked to offer funding.

Consortium Arrangements

The goal of this collaboration is to establish and develop a topical Center for Terascale Simulation of the Plasma Physics of Intense Ion Beams for Inertial Fusion Energy, that will be funded through the Scientific Discovery through Advanced Computing initiative, and to carry out advanced simulation research under the umbrella of this center.

Management of the Center

Overall management will be the responsibility of the Principal Investigators, who will seek to achieve consensus on all issues at the strategic level. Day-to-day coordination will be the responsibility of Alex Friedman, an LLNL employee who plays a management role for both LLNL and LBNL staff. In general, goal-oriented multi-institution teams will work on well-posed physics problems (*e.g.* electrons in the driver, instabilities, multibeam effects in driver and chamber), and on well-posed code development tasks. All the institutions partnering in the proposed Center already participate in frequent video-teleconferences and periodic workshops on various aspects of Heavy Ion Fusion research, and these mechanisms will be employed to ensure a closely coordinated effort. In addition, in-person collaborations of varying duration will be employed when appropriate. This tightly coupled multi-organization effort will offer capabilities far exceeding those that could be brought to bear by any one organization. Intense-beam physics for Inertial Fusion Energy will advance far more rapidly than otherwise would be possible.

Expertise and roles of participating institutions

LBNL, LLNL, and PPPL have already entered into a Heavy Ion Fusion Virtual National Laboratory (VNL) agreement to jointly pursue the goals of the Heavy Ion Fusion research program, through agreement of the Laboratory directors and the concurrence of the Office of Fusion Energy Sciences. Thus, We will develop the first two-dimensional Vlasov-Poisson solver for beams in quadrupole-focusing channels, building on the existing WARP-SLV package for beams in uniform-focusing channels. This work will be done in close coordination with colleagues funded for high energy and nuclear physics research.

We will implement an initial set of linkages between simulation tools, allowing exploration of the issues associated with carrying a consistent beam description across varying physics models. For example, in linking from an electrostatic model to an electromagnetic model, we will take pains to ensure that the time-dependent electrostatic field is saved and restored along with the particle data at the linkage plane. However, the electromagnetic radiation field will initially be zero. We need to identify any adverse effects from this inconsistency, which might be reduced by linking from a Darwin model.

We will implement and assess large-scale parallel I/O for particle and field diagnostics, to address the "data-glut" issue, using BEST as a testbed.

We will assess options for a faster field-solving algorithm in LSP, replacing the Alternating-Direction Implicit scheme currently in use. Implementation will begin late in Year One. Some possibilities include the Aztec package [51], the Chombo package for mesh-refined simulations [52], and parallel multigrid and conjugate-gradient methods in the ACTS toolkit [53] and elsewhere.

We will explore methodologies, and identify the most promising, for a multi-beam chamber-propagation simulation capability in LSP, using analysis and test calculations. There are several possibilities that must be assessed. These include static or dynamic refinement of the transverse and longitudinal mesh as the beams compress. We will explore the benefits of an evolving Cartesian grid. We will also explore the option of "4π" simulation of the chamber using a spherical coordinate system that would require less rezoning. In either system, the grid must be able to make appropriate use of available symmetry and adapt to fine-zoned beam regions with sparse zoning in between.

We will explore methodologies, and identify the most promising, for a multi-beam driver simulation capability in WARP, using analysis and test calculations. The model must include coupling to accelerating module impedances, and will employ simplified moment models for all but one beam.

We will study, develop, and assess techniques offering larger timesteps and enhanced accuracy in simulations, examining, *e.g.*, force-averaging and high-order methods, using WARP as a testbed. Implementation will be carried out in Year Two.

Physics studies: Interaction of intense beams with background populations

We will carry out electron-timescale simulations of beams in the driver, using beam and field parameters obtained from WARP simulations, to examine electron trapping in the beam potential (using WARP and/or LSP), and to examine electron-driven instabilities (using BEST and LSP).

Physics studies: Non-ideal dynamical effects in intense beams

We will study the linear and nonlinear dynamics of pressure anisotropy modes at high beam intensity, using BEST with a beam distribution consistent with those obtained in WARP studies.

Year Two

Tool development

We will implement detailed cross sections for stray beam ion interaction with walls into LSP, for studies of electron effects in the driver and beamlines; this will include modeling of realistic contaminants (H_2O, CO) liberated from the surface.

We will develop an adiabatic electron "pusher" model (involving revised particle advance and source deposition) for fast-moving particles, using BEST as a testbed.

We will assess and implement the optimal new numerical method for electromagnetic field solution in LSP, based on work done during Year One.

addition, halo formation is rapid, so that the beam need only be followed over a relatively short distance over which its "core" does not change greatly; this implies that perturbative methods can be used efficiently. Another such model is the continuum-Vlasov model, which evolves the distribution function information on the nodes of a multi-dimensional grid. In such a model, the low-density parts of phase space are tracked as accurately as the high-density parts, so that even tenuous regions with density five orders-of-magnitude below the peak can be well understood. At this point, we do not yet understand the relative virtues of these two advanced approaches to the halo problem, so it is essential to explore both. Comparison of the two methods will be very useful. In addition, traditional PIC can be used to simulate halo production. This has been done with great effect in the high energy and nuclear physics program, and we intend to carry out our halo research effort in close collaboration with researchers funded by that program, as described elsewhere in this proposal.

Other important local simulations will employ LSP to examine electron and neutral gas emission from walls (when stray ions strike the walls), and subsequent electron trapping in the beam potential. In addition, we will use BEST to look at two-stream and other instabilities enabled by the electrons. Such simulations must operate on the electron time scales. These time scales are separated from the full beam residence time by too many orders-of-magnitude for the electrons to be included directly in the main sequence calculations. Furthermore, it is believed that electrons in the beamline must be kept to minimal numbers if beam quality is to be preserved. Thus, coupled side calculations will be carried out. Suitably time-averaged electron densities will then be introduced as a charge (and perhaps beam temperature, due to instability) source into the main sequence simulations, so as to quantify the perturbing effects on the beam as it travels long distances. At present, we expect that the necessary coupling can be done by means of self-describing data files but, if necessary, a tighter coupling between codes will be employed. The possibilities here include the linkage of sub-codes within a common "executable" via a controlling Python interpreter level, and the use of "workspace" tools (e.g., PAWS [50]) to link two running codes.

This approach offers important advantages. Both WARP and LSP are large, mature code frameworks, and the merger of capability from one into the other so as to make a single code would involve much work with little practical gain. In addition, BEST is a smaller (fewer lines) physics-oriented code, and is amenable to "experimental" development. It is easily modified, and makes an ideal testbed platform for new algorithms (such as the recently-developed magneto-inductive Darwin algorithm that advances a canonical, rather than mechanical, momentum) as well as an excellent vehicle for use and improvement by graduate students. Our intent is to transfer the most successful methods identified using BEST into one or both of the two large codes. Other developments, *e.g.*, the Vlasov model, will be done in the large codes directly.

Estimates of computer resource needs

Source-to-fusion chamber main sequence

Based on timings of WARP3d on NERSC's current T3E and SP machines (Table 3), we estimate a run time of the order of one day on a 5 Teraflops system for a source-to-fusion chamber simulation using a moderately high level of resolution and including the major physics. A mesh of size 128×128×4096 is required to resolve the gradients in the transverse fields at the edge of the beam (which have a scale length of order the transverse Debye length), and in the longitudinal field (which has a scale length of order the pipe radius). For a 20 meter long beam and a pipe radius of 3 cm, 4096 cells along z are required to produce a small enough grid cell size, 0.5 cm. The number of simulation particles required is mainly determined by the amount of numerical heating from collisions that can be tolerated. When an insufficient number of simulation "superparticles" is used, each carries a very large charge. Despite the beneficial effects of the grid in smoothing the interparticle force at small impact parameters, an enhanced "numerical" collision rate exists and leads to a spurious growth in the effective phase space volume. In the simulation of a driver-scale accelerator, the rate of the numerical heating from collisions that can be tolerated is much lower than in the shorter simulations which have been done to date, because of the beams' longer residence time. Considering that the rate of heating falls off with the square root of the implement a new method, developed and tested in the BPIC chamber propagation code, for "advecting away" the field errors associated with the evolving cell boundaries, and also BPIC's improved outgoing-wave boundary condition that will allow us to keep the computational box to a minimal size. We will explore the options for multibeam simulation, which include one or more of: spherical coordinates; "tapered" coordinates which are Cartesian in each constant-z plane but for which the cell sizes Δx, Δy, and Δz diminish with z; mesh refinement around the individual beam paths (either static or dynamic); and the ability to slowly adapt the mesh to follow the focusing beams to the target. We will implement the most promising of these options. See Figure 9 for a rendering of the mesh refinement concept. Goals include reduced particle communication across processors, and the possibility of using much larger timesteps until the beams near the target.

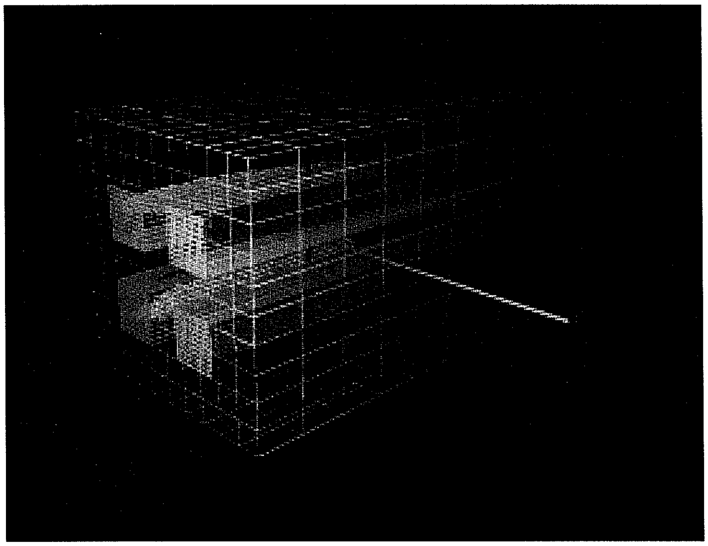

Figure 9. Depiction of a simulation of multiple beams moving through the fusion chamber with mesh refinement around each beam.

For the study of collective instabilities in the fusion chamber, it is appropriate to compare the "main sequence" results with detailed simulations using alternative methods; thus, we will use both LSP and the nonlinear perturbative ("δf") code BEST. Agreement between these tools will be an important confirmation that the results are reliable.

We will also adapt and employ multiple tools as appropriate to study multi-species effects in the ion accelerator, such as electron generation and trapping in the beam, and two-stream instabilities. These include LSP, BEST, and WARP. LSP already offers secondary emission, kinetic neutrals, ionization, scatter and neutral recycling. Required generalizations to LSP include detailed cross sections for beam interaction with surfaces and modeling of realistic contaminants (H_2O, CO) liberated from the surface. Electron scales in the driver will not be resolved in full end-to-end simulations in the near future, so it is essential that coupled disparate-timescale simulations capturing the electron dynamics will be carried out. Early in Year Two, the results of electron-timescale simulations conducted during Year One will be distilled and incorporated into WARP as an additional time-dependent charge source. Depending upon what is learned, we may intermittently run the electron-scale calculations simultaneously with WARP to achieve the greatest fidelity. Such a coupling could be effected by either "workspace" methods or creation of a single executable program combining the required capabilities and run under the control of Python.

Improvements to tools for non-ideal dynamical effects in intense beams

The study of beam halo generation is especially challenging, involving as it does a very wide range of beam densities. We are especially interested in developing a quantitative understanding of the extent and number of resonantly-driven particles excited by self-consistent collective oscillations or so-called

The importance of benchmarking codes is illustrated by an experiment at the University of Maryland studying the effect of an aperture on a space-charge-dominated electron beam. The aperture acts as an initiator for wave-like phenomena (rings) that propagate toward the center of the beam. In figure 6, the top row of images was generated on a phosphor screen at a sequence of observing stations. The lower row is from a WARPxy simulation (the scaling of the images differs slightly). The simulation uses a "semi-Gaussian" initiation of the beam phase space (the initial distribution is uniform as a function of position within an ellipse, and Gaussian as a function of velocity), and results in excellent agreement between the experiment and WARP. If, however, a "Kapchinskij-Vladimirskij" initial distribution [6] (a 3-D shell in the 4-D transverse phase space, with all particles initiated at the same total transverse energy) is used, the rings are not seen in the simulation at all. These waves have been shown to be important in equipartitioning in intense beams.[9,37,49] This comparison employs one of WARP's simulated experimental diagnostics. Such diagnostics will be further developed through the proposed Center.

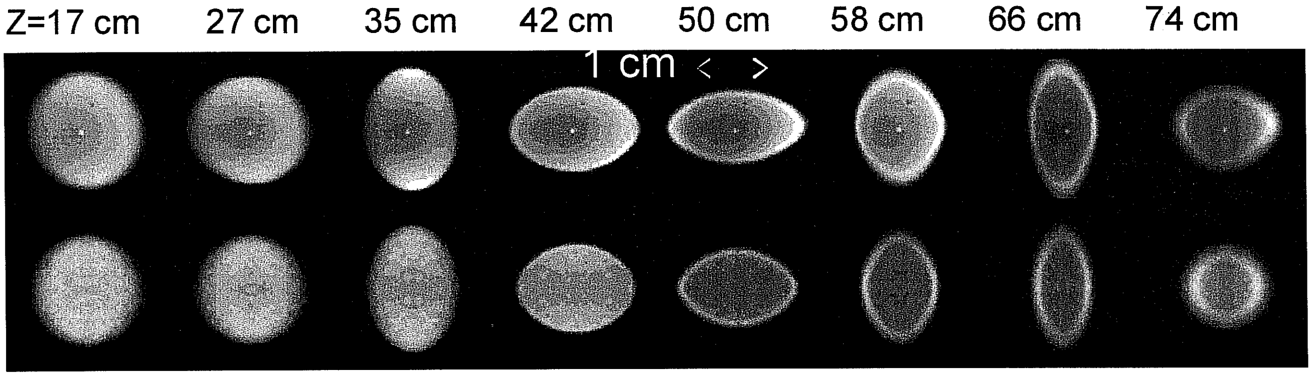

Figure 6. Experimental (top) and simulated images (bottom) at eight stations on an electron beamline (with scaled parameters resembling those of a heavy ion fusion beam) at the University of Maryland.

Figure 7 shows the effect of an improved outgoing-wave boundary condition for solutions of the full Maxwell equations on a cartesian mesh; this capability [13] was originally implemented in the BPIC code and will be added to LSP as part of the Center's code development effort.

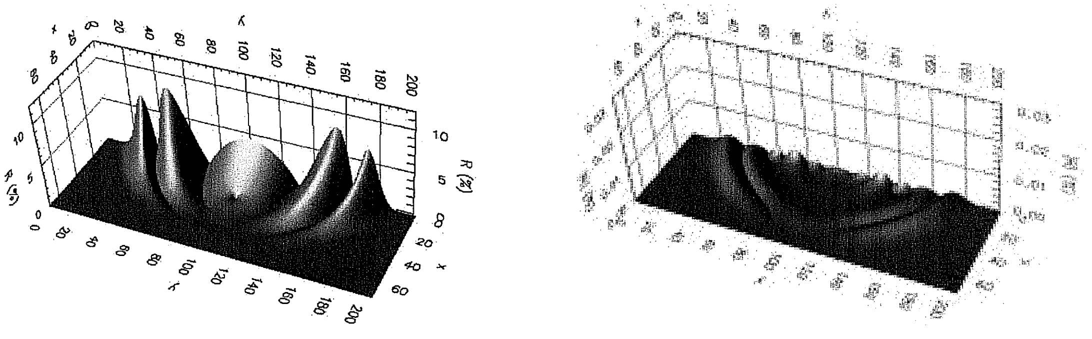

Figure 7. Comparison of conventional (Enquist and Majda) wave-absorbing boundary condition (left) with new "hybrid" prescription (right); the figures show the reflected pulse in a 2-D EM calculation. Minimization of wave reflections from the sides of the computational "box" makes an important contribution to accuracy and also to efficiency, since the computational box can be made smaller.

Research Design and Methods

A concept for source-to-target simulation is shown in Figure 8. In this scenario, the beam is simulated from the source through the final focusing optic using WARP3d, and the particle and field data are then transferred into LSP where the simulation is carried through to the fusion target. At that point, the particle data is used to generate "ray" information for the ion beam source in the target simulation code. Meanwhile, LSP is used to study electron effects in the driver, especially electron sources and trapping in

The geometry is cylindrical with a perfect conducting wall. The applied-field can have arbitrary 3-D structure. The Poisson solver uses (r, θ, z) coordinates, while the pusher uses (x, y, z) coordinates near the axis. If one wants reduced noise by using delta-f algorithm, the applied-field has to be one that permits an equilibrium solution of the Vlasov-Maxwell equation.

As a physics code in simplified geometries, BEST focuses on the key physics with reduced noise and novel algorithms. It provides an important bridge between theoretical understandings and numerical simulations. It is especially suitable for studying the physics of possible detrimental instabilities, such as the two-stream instability and the pressure anisotropy instability. Mode structures, growth rates, damping mechanisms, and other detailed properties of these instabilities discovered by BEST provide valuable information on how to prevent them. In addition, BEST can be used to study the interaction of beam particles and stable or unstable collective excitations, such as the formation and halo particles and chaotic particle motion inside the beam. BEST has been used for long runs, up to ~ 4 x 10^{11} particle-timesteps, using up to 1000 processor-hours on the NERSC IBM SP-2.

Good scaling in BEST has been obtained using up to 512 processors, using a design similar to that of the GTC code for turbulence studies in tokamaks [42]. It is written in Fortran 95. BEST has been used for studying the two-stream instability observed in the Proton Storage Ring at LANL. Initial results [18] compare well with theory.[31,43] Equilibrium and stability properties for a beam in a periodic focusing field have also been studied extensively.[24]

Other codes from which models will be drawn: The BPIC chamber-propagation code [45,46] offers an explicit 3-D or (r,z) electromagnetic PIC model, and uses a time-evolving Cartesian mesh and novel methods for "advecting away" the field errors associated with the evolving cell boundaries.[45] It also uses an advanced "outgoing wave" boundary condition at the edges of the computational grid.[13] It is written in Fortran 95. The BICrz chamber-propagation code [47,48] has been used for Heavy Ion Fusion studies for almost a decade. It employs a time-independent axisymmetric mesh that tapers down toward the target so as to better resolve the converging beam. In the immediate vicinity of the target, the BIC mesh smoothly stops tapering and becomes a conventional cylindrical-coordinate grid. The mesh is nearly orthogonal, and special care was taken with the differencing of the electromagnetic field equation so that accuracy is preserved. BIC is written in a structured superset of Fortran 77 with an interactive interface based on the Basis scripting language. It runs well on vector computers but has not been parallelized.

Representative simulations

Existing codes are used for a wide variety of simulations, as illustrated in Figure 4. We do not attempt to describe the relevant physics in any detail, but indicate here the range of ongoing activities. More information can be found in the references.

LSP in fully-hybrid mode has recently been used to model the interaction of two 0.5-cm beams in a chamber environment near the target. The two 4-kA, 4-GeV Pb^{+5} beams are injected into a $5x10^{13}$ cm^{-3} density plasma (10 times the beam charge density) and followed through the focus. The plasma electrons are initialized in the fluid component, but a significant fraction make the transition into the kinetic component as the beam passes. The plasma ions are mobile. The simulation shows that the plasma electrons respond to the beam so as to nearly negate beam charge and current over the 50-cm length. No discernable deviation from ballistic propagation was observed. Plots of the beams and the kinetic electron velocity vectors in the principal plane as the beams approach focus are shown in Figure 5. The kinetic velocity abruptly changes from just below one-tenth of the beam velocity to below one-fifth of the beam velocity where the two beams overlap, maintaining 99% charge and greater than 80% current neutralization. This simulation demonstrates that a background plasma can nearly negate the beam self fields, essential for the neutralized-ballistic transport of high-perveance beams. The run used 120 CPUs for about 25 hours each on the NERSC Cray T3E. It employed about 25 million particle-in-cell particles, 5000 timesteps of 0.002 ns each, a minimum cell size of 0.05 cm and about two million cells overall.

including parallel machines, including NERSC's Cray T3E-900 and IBM SP, where message passing is implemented via the MPI package. Good scaling has been obtained using up to 256 processors on problems of intermediate size. The problems to be tackled under this initiative will require a more detailed applied field description (more work per particle), and so scalability to thousands of processors should be attainable.

WARP is organized around a set of "physics packages" which contain executable routines and data, and is written in a superset of Fortran that offers features such as dynamic memory allocation and a run-time database that is accessible by all code routines or by the user interactively. It runs under the control of the Python scripting language.[26] This gives the user control over how the simulation proceeds, facilitating, for example, the use of iterative methods for steady problems, as well as fully time-dependent simulations. In practice, most of the "code steering" is conducted by means of user-written scripts. The user's input file is, in effect, a computer program written in the Python language, with Python's native capabilities extended by the high- and low-level capabilities of the WARP internals. Interactive steering is used for special purposes such as run development, debugging, and use of quick-running packages such as an envelope solver and the moment models CIRCE and HERMES described below. WARP also includes a prototype web interface so that, through a browser, the user can query the code, or ask it to generate certain plots, etc., even when the code is running in batch mode.

The code's accelerator description allows "lattice" elements with arbitrary fields, including focusing, accelerating and bending fields, with error terms, offsets, rotations, and fringe fields. A general set of finite-length elements can be specified, including quadrupoles, dipoles, accelerating gaps, and elements with arbitrary multipolar content. The fields of the elements can be specified at several levels of detail, from fields which are axially uniform and hard-edged and where "residence corrections" are used in the particle mover so that the particles receive the correct impulse from each element, to fields that are expressed as axially dependent multipole components, to fields expressed on three-dimensional grids. Another set of elements in the 3-D and (x,y) "slice" models specifies the locations and curvatures of bends. These are not physical elements but are the appropriate coordinate transformations needed to follow the beam around the bends. The self-consistent field is assumed electrostatic, with simple semi-analytic corrections to handle multi-beam inductive effects. Poisson's equation is solved on a Cartesian mesh that moves with the beam, either steadily, or as a "treadmill" so that zone boundaries do not vary from step to step. When bends are used, the field solution is altered to include the curvature of the "warped" coordinates. Electrostatic elements can be described from first principles by inclusion of conductor geometry as boundary conditions in the solution of the self-fields at subgrid-scale resolution, using a "cut-cell" method in 3-D.

WARP has been validated against a number of small experiments in the HIF program.[4,7,37] The field description is at present electrostatic. This is reasonable for low-energy beams, which have been the code's principal application since present-day space-charge-dominated beam experiments operate at low energy. Even in a driver, the beams will never reach speeds greater than about 25% of the speed of light, and self-magnetic field effects in a single beam are generally smaller than electric effects by a ratio of $(v/c)^2$. However, the electric influences of one beam on the others are largely shielded by intervening conductors (except in the accelerating gaps), while the magnetic and inductive influences are not shielded. For the latter part of a driver, where $v/c \sim 0.1$ and ~ 100 beams are accelerated in tandem, a magnetoinductive (Darwin) description (or at least a model incorporating the largest magnetic and inductive effects in a multi-beam system) is needed for a driver. A first, very simple, semi-analytic model has been developed [25], but a full model is needed, as described later in this proposal.

A prototype continuum Vlasov-Poisson package, SLV (Semi-Lagrangian Vlasov), has been implemented in the WARP code and is currently running on simple axisymmetric beam physics problems.[16] Quadrupole focusing represents a challenge. The issue is the rapid variation in the distribution function "slope" in (x,p_x) space in such a system, which leads to a large number of "empty" phase-space cells and a rapid variation of f in each cell. We plan to address this by using a different set of shifted coordinates on every timestep, so that the range of velocities at each position is centered on the mean beam velocity at that position, but this must be tested.

proposal, this team will coordinate its efforts with those of researchers funded by High Energy and Nuclear Physics, and in some areas (*e.g.*, beam halo) the groups will partner in a collaboration.

Relationships with other scientific disciplines

The proposed capability involves nonlinear dynamics, self-consistent fields, large-scale parallel computations, massive data handling, interactive and script-driven code steering, and visualization of a time-dependent multidimensional phase space. These aspects appear in many emerging applications of terascale computing, and considerable cross-fertilization with other areas can be anticipated.

Some of the numerical methods developed by the Heavy Ion Fusion simulators who will participate in this project have had, or can be expected to have, significant impact in a wide range of fields. These include methods for implicit particle-in-cell simulation [27,14]; for outgoing-wave boundary conditions and mesh refinement in electromagnetic calculations [13,28]; for damping of electromagnetic waves in such systems [29]; for Darwin simulation [16,17]; and for Poisson solution with subgrid-scale resolution of boundary surfaces using "cut-cell methods" [30].

Other accelerator applications are moving toward higher beam intensities, and the knowledge gained via this research into very strong space-charge regimes will be relevant to a wide variety of applications. Particle-In-Cell codes are being used to look at beam-beam effects near the interaction point in, *e.g.*, the B-Factory at SLAC, and a basic understanding of collective instabilities is of increasing importance. Furthermore, there is much in common between the physics of beam propagation through a Heavy Ion Fusion chamber and that of beam focusing via plasma lenses, as employed in high energy and nuclear physics (HENP) research (*e.g.*, at SLAC) and in high-energy-density physics studies (at GSI Darmstadt). We anticipate long-term benefits to such efforts as the Spallation Neutron Source, the Very Large Hadron Collider, the Next Linear Collider, an Accelerator for Transmutation of Waste, the Muon Collider, and for application to Boron Neutron Capture Therapy. Members of this research team have served as principal investigators on HENP-funded projects, and have contributed to the understanding of important issues such as electron-proton instabilities in proton storage rings.[31,32]

The Vlasov methods to be developed are of timely interest for gyrokinetic modeling of Magnetic Fusion Energy plasmas, and we anticipate useful information exchanges with researchers in that area. Other areas of common interest include particle advance and field solution in a terascale environment, and advanced visualization, where we have much in common with the gyrokinetic community.

Preliminary Studies

The proposed Center will pursue two general aims: it will develop better tools than those currently available; and it will exercise the improved tools on problems of significance, and encourage their use by others (in Heavy Ion Fusion and other fields) to conduct research into intense particle beams. Thus, we summarize here past research by the proposers that has culminated in tools which are already sophisticated in a number of ways, and present examples of physics studies that have been carried out using existing tools.

Key computational tools

The Heavy Ion Fusion program has developed tools to explore the key physics areas, primarily (but not exclusively) using particle-in-cell (PIC) methods. Plans involve adaptation of exiting codes to run optimally on computers that use a hybrid of shared and distributed memory, tight coupling between those tools, production of new and improved numerical algorithms, e.g., averaging techniques that allow larger time-steps, and development of improved physics models. Some of this work already relies heavily on modern scripting techniques for code steering, and advanced data visualization is playing an increasing role. In all areas, benchmarking with analytical theory, experiments, and among different codes will be essential. The codes to be employed are well positioned to move quickly to a terascale platform.

(the frequency at which the beam ions execute quasi-harmonic oscillations within the beam profile). Therefore, approximate or exact but singular equilibria are used when an equilibrium is needed for analysis. With integrated simulations we can eliminate these difficulties.

Third, simulations must accurately model slow emittance growth (phase space dilution) which occurs over long distances. Increases in the normalized emittance (projected phase space volume) by factors of a few have a major effect on the ultimate focusability of the beams, but such an increase corresponds to a very small, subtle change over a single "lattice period" (the fundamental repetition length of the structure).

Fourth, the target needs to be driven by a "shaped" pulse, which has a long, low-intensity "foot" followed by an intense, ~10 ns main pulse. However, not all pulse shapes are attainable, and the driver simulations through final focus, the chamber-transport simulations, and the target simulations must therefore be consistent. Pulses of different shapes will interact differently with the chamber environment. To some degree the need for pulse shaping can be reduced by employing separate "foot" and "main" beam bundles, each with their own final transport lines, but the key technical issue of pulse shaping still remains. The sensitivity of target designs to the exact details of the incoming beam bundles varies from design to design. In some cases, the capability of transferring simulated ion beam data (positions and velocities versus time at a plane just upstream of the target) at the end of the chamber propagation simulation into the input quantities needed by the target physics simulations will be very important.

Finally, the ultimate size of the achievable focal spots on the target has a strong influence on the target "gain" (ratio of energy produced to energy in the beams), and this spot size depends on both the transverse and longitudinal velocity spreads of the beam. The beam must be longitudinally compressed, requiring a velocity gradient along the beam. This can lead to transverse "mismatch" oscillations at the beam ends and emittance growth. Particle motions along the transverse and longitudinal coordinate axes are coupled by collective effects as well as by some components of the applied fields. When an energy transfer between the degrees of freedom occurs in an upstream section of the system, that transfer strongly influences the character of the beam in all downstream sections, and must be accounted for.

Significance

We propose to develop new terascale simulation capabilities, and apply them to further the basic understanding of key scientific issues in the physics of intense beams for Heavy Ion Fusion. The knowledge so gained will also be relevant to a range of emerging beam applications outside of Inertial Fusion Energy. Our vision is a "source-to-target" beam simulation capability: a description of the underlying physics in this complex system that is both *integrated* and *detailed*. The research to be carried out by the topical Center described herein will represent the key step in realizing this vision.

The physics of the intense ion beams needed for Inertial Fusion Energy is challenging, due to the wide range in spatial and temporal scales involved, and the collective and nonlinear nature of the system. The 3-D chamber calculations proposed here will, for the first time, offer a realistic model of the chamber environment, with which various modes of chamber propagation can be explored. We will employ multiple models, and we will compare, *e.g.,* implicit EM, explicit EM, and Darwin methods. In the accelerator and transport lines, the beam dynamics is a Liouvillean flow, and complex distortions in phase space must be accurately followed. Not only stability, but also heating of the beam distribution must be explored since the final focus of the beam onto the target imposes strict limits on beam phase space volume. The qualitatively improved tools to be developed in this research program will lead to a much deeper physical understanding of these processes, and a much-needed ability to optimize system design. This research will thus play a major role in this promising approach to the long-sought goal of economical and clean fusion energy.

The above-mentioned effects have been simulated approximately and only for isolated segments of the system. It has, to date, been impossible to model the complete system self-consistently, so that the beam distribution function is carried through an end-to-end simulation of the accelerator, into the fusion chamber, and through to the target. Initialization of a beam at mid-system with an idealized particle beam return current path, which determines the point at which beams "talk" to each other. Another important focus of the research efforts in the fusion chamber will be on collective instabilities, such as the resistive hose, filamentation and two-stream modes.

In the chamber, as in the driver, it is appropriate to employ multiple simulation approaches, and we will use particle-in-cell (PIC), hybrid PIC-fluid, and nonlinear perturbative ("δf") methods. The chamber calculations must allow exploration of various propagation modes, e.g. "neutralized-ballistic," "assisted-pinch," etc. The challenges include the need for complex physics models, "outgoing-wave" boundary conditions,[13] an implicit hybrid model for the dense-plasma propagation modes,[12] and of order 10^7-10^8 simulation particles. For clear identification of the physical effects that matter the most, it is also essential to employ multiple simulation models, so as to compare and optimize, *e.g.*, implicit electromagnetic (EM) methods [14] (which can stably under-resolve fast time scales not essential to the physics) with explicit EM methods and with magneto-inductive ("Darwin") methods [16,17] that eliminate light waves from the description.

<u>Multi-species effects in the driver</u>: Collective beam interactions with "stray" electrons in the accelerator and transport lines, including electron generation and trapping within the beam, must be understood quantitatively. This area is computationally challenging because of the ratio between the fast time scale for electron motion and the slow time scales for the ion dynamics and for electron build-up within the beam (the mass ratio is of order 250,000); the need to efficiently gather/scatter and communicate multi-species information for ionization and surface-physics processes; and the need for efficient dynamic load balancing and perhaps an adaptive mesh.

Non-ideal dynamical effects in intense beams

<u>Beam halo generation</u>: In modern particle accelerators, the confining fields are dominated by an "alternating-gradient" transverse quadrupole field configuration produced by a sequence of electric or magnetic lenses. Thus, the confining fields are non-steady in the beam frame, thereby complicating the analysis. Oscillations of the beam "core" can parametrically pump particles into an outlying, or "halo," population. For focusability and also to avoid the adverse effects of ions impinging on walls, the production of beam halo particles must be kept to a minimum. Here, particle-in-cell methods have been used, but emerging continuum-Vlasov [15,16] and nonlinear-perturbative methods [18,19,20,21,22,23,24] may offer advantages.

<u>Long-term evolution of space-charge-dominated beams</u>: In the driver, the array of beams is accelerated by inductive electric fields, and is confined by applied "focusing" fields. The beams dynamics are space-charge-dominated, and the beam dynamics is collisionless and Liouvillean, *i.e.*, the phase space density remains constant along particle orbits. As a result, "emittance growth" (dilution of the phase space) takes place through complicated distortions driven by collective processes, imperfect applied fields, image fields from nearby conductors and inter-beam forces. Such dilution must be kept to a minimum, because of the necessity to focus the beams ultimately onto a small (few mm) focal spot on the fusion target. Simulations must capture the influence of small effects which act over long distances. In addition, collective beam modes, and interactions with the external environment that can drive resistive-wall instabilities, must be understood and minimized. Other challenges include the need to accurately simulate time-dependent space-charge-limited emission from curved surfaces. This area is computationally challenging because of the need for an efficient but detailed description of the applied fields, and the needs for good statistics and mesh resolution. Many simulation particles (10-100 million) are needed to keep fluctuations to an acceptably low level. When an insufficient number of simulation "superparticles" is used, each carries a large charge, and, despite the beneficial effects of the grid in smoothing the interparticle force at small impact parameters, an enhanced "numerical" collision rate leads to a spurious growth in the effective phase space volume. The timesteps used for the computation of particle orbits in the driver must be small relative to the residence time of the beams, because variations in the applied focusing and accelerating fields must be resolved. Thus, a driver simulation will require at least 100,000 steps. The major disparity between the necessary grid resolution (generally, the Debye

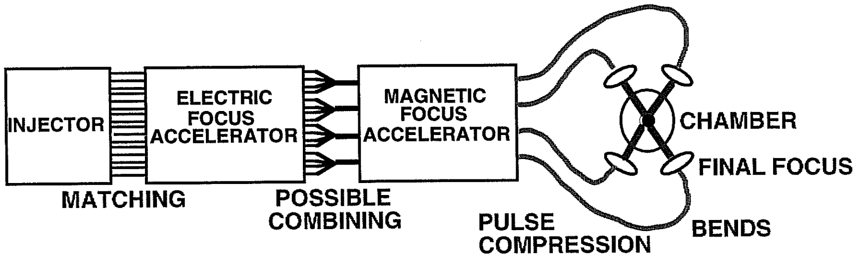

Figure 2. A Heavy Ion Fusion system, showing principal elements.

State of existing knowledge

The induction linac approach to Inertial Fusion Energy, in common with certain other existing and emerging accelerator applications, requires the confinement, acceleration, and precise control of "space-charge-dominated" beams. In such beams, the dominant force balance is between the applied focusing (confining) fields and the space-charge forces, with relatively small contributions by pressure gradient forces. This situation is in contrast with many traditional accelerator applications, where thermal pressure effects play a major role in the force balance, and the beams are "emittance-dominated." Through experiments, analytic theory, and computer simulations, much has been learned about the behavior of space-charge-dominated beams—but much remains to be understood.[3] Some of the missing knowledge is particular to the Inertial Fusion Energy application, and some of it is in the nature of fundamental beam physics with the potential for broader application. In addition, significant gaps exist in our knowledge of the most effective ways to simulate such beams, and we expect to make progress in numerical methods, some of which can be expected to have application beyond the fields of accelerator and plasma physics.

Progress in the study of the key physics problems in Heavy Ion Fusion beams has been made possible by particle-in-cell (PIC) codes running on state-of-the-art platforms. Such codes have established their essential place in Heavy Ion Fusion by uncovering phenomena previously unknown, and thus motivating future experiments. Particle simulations revealed mechanisms for emittance growth in accelerator bends [4] and for coherently oscillating beams in anharmonic transport channels [5] before these effects were seen in experiment. In the early days of the field, PIC simulations were used to show that the rapidly growing instabilities predicted by analytical theory stabilized at low levels [6]. This discovery established feasibility for the Heavy Ion Fusion concept and both motivated and was confirmed by subsequent experiments. Simulations are also irreplaceable in the design of intense beam injectors where the beams are first accelerated on exiting the source. Heavy Ion Fusion injectors are at the state of the art, and 3–D simulations have been the only way to understand injector beam dynamics since the focusing potentials are a significant fraction of the beam energy.[4] Finally, simulations have succeeded in reproducing experimental observations in detail and in explaining other novel physics observed uniquely in space charge dominated beams.[7,8,9,10,11]

There are significant gaps in these calculations, however, which cannot be treated with present-day computational facilities. The size of the system compared to the resolution needed, and the wide disparity of timescales — the long length of the accelerator as compared to the resolution needed for magnet fringe fields, the large ratio of the width of the beam to the Debye length, the large ratio of ion timescales to electron timescales — has meant that calculations of the above-mentioned effects are compute-intensive and have been done in general only for isolated segments of the system. In the fusion chamber, our understanding of the beams' interactions with neutral gas, ambient plasma and target radiation is very incomplete, and only now is a concerted experimental and theoretical effort getting underway, though scaled experiments have been done. The complex multi-dimensional process of beam charge and current neutralization in such an environment demands modeling that includes detailed atomic, surface and dense plasma physics. Thus far, these processes have only been modeled piecemeal.

It has heretofore been impossible to model the complete system self-consistently, so that the beam distribution function is carried through an end-to-end simulation of the accelerator and into the fusion