Title
Early Recognition of Clusters in Molecular Dynamics

Authors
Dorso, C.
Randrup, Jorgen

Publication Date
1992-11-06

LBL-33120
UC-413
Preprint

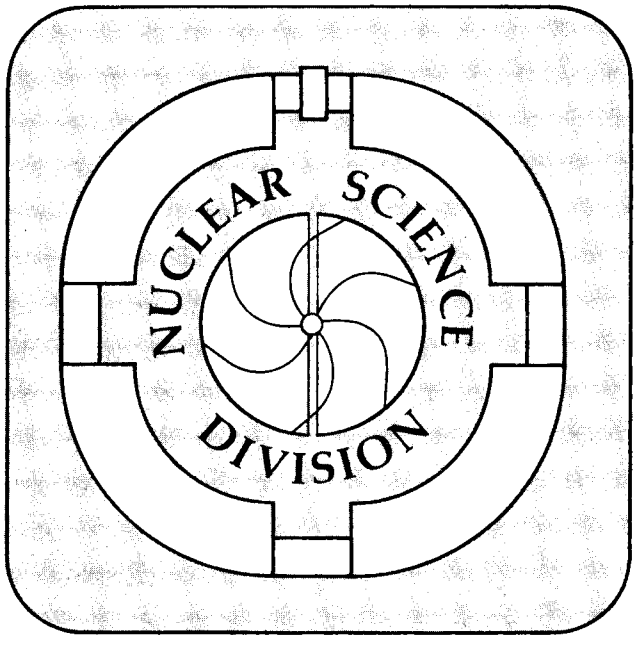
Lawrence Berkeley Laboratory
UNIVERSITY OF CALIFORNIA

Submitted to Physical Letters B

Early Recognition of Clusters in Molecular Dynamics

C. Dorso and J. Randrup

November 1992



Prepared for the U.S. Department of Energy under Contract Number DE-AC03-76SF00098

DISCLAIMER

Physics Letters B LBL-33120

Early Recognition of Clusters in Molecular Dynamics *

C. Dorso[1] *and J. Randrup*

Nuclear Science Division, Lawrence Berkeley Laboratory
University of California, Berkeley, California 94720

November 6, 1992

Abstract:

We propose a novel method for recognizing bound clusters in molecular dynamics simulations of nuclear collisions. Demanding that each particle in a given cluster is bound with respect to that cluster, we employ a Metropolis procedure (akin to simulated annealing) to maximize the cluster binding.

[1] Departemento de Física, Faculdad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Argentina.

*This work was supported in part by the Director, Office of Energy Research, Office of High Energy and Nuclear Physics, Division of High Energy Physics, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

1 Introduction

The exploration of nuclear collisions at intermediate energies relies strongly on microscopic simulations. The most employed methods are the nuclear Boltzmann equation (variously referred to as BUU, VUU, Landua-Vlasov), in which the reduced one-body phase-space density is followed in time, and molecular dynamics (such as QMD, FMD, and AMD) in which the trajectories of all the individual nucleons are followed for an ensemble of independent events. While these models have enjoyed a great deal of success in accounting for the early dynamics of heavy-ion reactions, their applications to the later stages have been more limited, either because of inherent limitations with respect to fragment production (as in mean field BUU-type descriptions) or because of practical problems in identifying the fragments efficiently. It is towards this latter aspect that the present paper is directed.

In molecular dynamics, the individual nucleons typically experience pairwise interactions consisting of a finite-range attraction and a short-range repulsion. Therefore, towards the end of a nuclear collision the nucleons tend to emerge as either free or as part of bound clusters. Once these reaction products have separated sufficiently in space, it is farily straightforward to determine the cluster structure of the system, i.e. the particle number and velocity of each product. In practice, however, the additional running time required to reach this stage limits the practical utility of the model. It is therefore of interest to devise methods for recognizing the clusters as early as possible. The method proposed below makes it possible to discern the final cluster structure already before a spatial separation has occurred, contrary to most standard methods. That this is indeed possible is also interesting from a physical point of view, since it may help to elucidate the mechanism of fragment production.

2 Recognition method

Most often, the cluster structure is determined on the basis of the relative positions of the particles: if two particles are separated by less than a certain clusterization range r_c then they belong to the same cluster. The decomposition of the ensuing graph then yields to the cluster structure of the system. Although this method is relatively simple and fast, it is fairly useless until the clusters are sufficiently well separated. For example, two distinct fragments with a distance of less than r_c will be regarded as a single cluster.

We have therfore explored alternative methods and have found the one described here particularly useful. This cluster analysis is based on the following definiton of a cluster:

> A group of particles C is said to form a cluster if (and only if) each of them is bound with respect to the others, i.e. iff the single-particle energy $\epsilon_i^C \equiv T_i^C + \sum_j' V_{ij}$ is negative for all particles i in the cluster.

Here $T_i^C = p_i^2/2m_i$ is the kinetic energy of the particle in the *CM* frame of the cluster C and V_{ij} is the total interaction potential between the two particles i and j in the

cluster. (The prime on the summation symbol serves to remind of the fact that the term with $j = i$ is absent.) Clearly, this definition makes sense in situations where the clusters are well separated from one another, but it has the advange that it can be employed quite generally, i.e. also when the system is dense and the different clusters partially overlap in space.

Our task is to decompose the total system into disjoint clusters which all satisfy the above criterion. Of course, that criterion may not produce a unique cluster decomposition of the system (especially when the system is dense), and we therefore generally seek to identify that cluster decomposition which maximizes the sum of the individual cluster binding energies. (This quantity does not consider the interaction energy between clusters, nor their kinetic energy, and so it is generally different from the total binding energy in the system.)

The above described task can be solved by a straightforward analysis of all the possible groupings of the particles into different cluster constellations. Thisprocedure will yield the exact solution to the problem, but it is prohibitively slow, unless the total number of particles is uninterestingly small.

We have therefore developed an alternative method which is incomparably faster, but not exact. It is based on a statistical optimization procedure, using the binding as the cost function. The idea is to use a Metropolis procedure to sample the set of cluster decompositions employing a gradually decreasing temperature parameter so that the distribution concentrates around an optimal clusterization.

The "cost" associated with a given cluster decomposition $\mathcal{C} = \{C_1 C_2 \cdots\}$ is thus taken as the corresponding clusterization energy,

$$E_{\mathcal{C}} \equiv \sum_n E_{C_n} \ , \tag{1}$$

i.e. as the sum of the energies of the individual clusters C_n, each one obtained by evaluating the total energy of that cluster in its own *CM* frame and disregarding its interactions with the rest of the system. The canonical probability corresponding to the particular cluster partition $\mathcal{C}$ is then given by

$$P(\mathcal{C}) = \mathrm{e}^{-E_{\mathcal{C}}/\tau} \ , \tag{2}$$

where τ is a prescribed "temperature" parameter.

Starting from an arbitrary cluster decomposition $\mathcal{C}$, a random neighboring decomposition $\mathcal{C}'$ is generated by tranferring one of the particles from its initial cluster C_i to another cluster C_j (including the possibility of liberating it). The associated change in the clusteriaztion energy is then given by

$$\Delta E(\mathcal{C} \to \mathcal{C}') \equiv E_{\mathcal{C}'} - E_{\mathcal{C}} = E_{C_i'} + E_{C_j'} - E_{C_i} - E_{C_j} \ , \tag{3}$$

where C_i' denotes the remainder of the donor cluster and C_j' denotes the resultant receptor cluster (*i.e.* after C_j has been augmented by the transferred particle). On this basis a random walk in the set of cluster decompositions is made. Invoking the standard Metropolis prescription [3], the new decomposition C' is accepted with the probability $P(\mathcal{C}')/P(\mathcal{C})$ (with the understanding that $\mathcal{C}'$ is always accepted if $P(\mathcal{C}') >$

$P(\mathcal{C})$). This procedure samples the canonical distribution of decompostions associated with the particular value chosen for τ. By gradually decreasing this parameter one obtains an ever narrowing distribution which will finally converge on a single optimal decomposition.

In order to speed up the random walk, any cluster decomposition may be considered, without regard for whether its constituent clusters are actually bound. Therefore, the walk may pass through decompositions whose "clusters" fail to meet the criterion stated at the beginning of this section. At the end, after the procedure has converged on an optimal clusterization, it is then checked whether the individual energies ϵ_i are all negative. This has always turned out to be the case and the resultant decomposition therefore consists of real clusters in the sense of the definition above.

Of course, as is typical of such Metropolis sampling, there is no guarantee that this locally optimal decomposition is also the globally optimal one. The importance of this inherent uncertainty can be estimated by repeating the procedure several times and comparing the outcomes.

The efficiency of the procedure can be greatly improved when it is possible to select the initial cluster decomposition so that it already resembles the final result. For sufficiently dilute configurations, such as are typical of the disassembly stage of a nuclear collision, this can be achieved relatively easily by first making a standard cluster decomposition on the basis of the particle positions, using a clusterization range equal to the truncation distance r_c of the nuclear interaction potential $V^N(r)$ (see eq. (6)). This improvement is motivated by the observation that in order for ϵ_i to be negative, at least one of the potential energies V_{ij} must also be negative, and hence i must lie within the interaction range of that particle j. For earlier, more compact configurations it is advantageous to employ the previously determined cluster decomposition as the starting decomposition for the analysis at the subsequent time.

In precise terms, we start by making a standard spatial cluster analysis using the truncation distance $r_c = 6$ fm (see below) as the clusterization range. This results in a number of clusters that are spatially so far apart that they can be analyzed separately. The procedure described below is therefore carried out for each one of these distinct groups of particles. Using each of these macroclusters as an initial clusterization $\mathcal{C}$, we then perform a Metropolis random walk as described above. The initial temperature is taken as $\tau_0 \approx 2.3$ MeV, and it is subsequently decreased by a constant factor, $\tau_{n+1} = 0.85\tau_n$. For each value of the temperature a total of $70A$ Metropolis steps are taken, where A is the total number of particles under consideration. The process is halted when no changes in clusterization occurs during $20A$ consequtive steps.

3 Ilustrative results

In order to discuss the model we make illustrative applications based on a simple molecular dynamics model developed earlier (see ref. [2]). In this model the total Hamiltonian is given by

$$H = \sum_i \frac{p_i^2}{2m_i} + \sum_{i<j} \left[V^P(r_{ij}, p_{ij}) + V^N(r_{ij}) + V^C(r_{ij}) \right] \ , \qquad (4)$$

i.e. the free kinetic energy plus three types of two-body interaction:

1. *Pauli potential.* In order to imitate the momentum distribution of nucleons, we employ the Pauli potential developed in ref. [1],

$$V^P(r,p) = V_0^P \, \mathrm{e}^{-r^2/2q_0^2 - p^2/2p_0^2} \, \delta_{\sigma\sigma'}\delta_{\tau\tau'} \ , \tag{5}$$

   which acts only between particles having the same spin and isospin projections. The parameter values are $V_0^P = 27.33$ MeV, $q_0 = 2.0$ fm, and $p_0 = 6.03\ 10^{-22}$s MeV/fm. This potential serves to endow the nucleons with momenta resembling those of a Fermi-Dirac gas.

2. *Nuclear potential.* For the nuclear part we use a Lennart-Jones type potential,

$$V^N(r) = V_0 \left((\frac{r_1}{r})^{p_1} - (\frac{r_2}{r})^{p_2} \right) [1 + \mathrm{e}^{\beta(r-d)}]^{-1} \ \theta(r - r_c) \ , \tag{6}$$

   with $r_1 = r_2 = 1.87$ fm, $p_1 = 4.6$, $p_2 = 2.8$, $d = 4$ fm, and $\beta = 2$ fm^{-1}, and truncated at the distance $r_c = 6$ fm. This potential, in conjunction with the Pauli potential, leads to a reasonable reproduction of the thermostatic properties of nuclear matter (in particular, nuclear matter saturates at a density of $\rho = 0.17$ fm^{-3} with a binding of ≈ 16 MeV per nucleon, and the compressibility modulus is $K = 350$ MeV). Moreover, it yields reasonable sizes and bindings of not-too-heavy nuclei, as shown in ref. [2].

3. *Coulomb potential.* Finally, the protons interact with the standard point-like Coulomb repulsion, $V^C(r) = e^2/r$.

The above Hamiltonian completely characterizes the dynamical model. In order to enable the reader to gain an impression of the degree to which this simple model mimics nuclear properties, we show in fig. 1 the calculated results for 1) the kinetic energy of a gas of nucleons that interact only via the Pauli potential, 2) the binding energy of nuclear matter as a function of the density, and 3) the binding energy of finite nuclei as a function of their mass number. It is seen that a a sufficiently realistic overall reproduction of the nuclear features is obtained to render the model useful for testing the proposed analysis method.

We shall typically consider central collisions of two calcium nuclei which have been prepared to be in (or near) their ground states. These can be prepared by employing a Metropolis procedure with a gently decreasing temperature parameter. Once the initial state has been specified, the dynamical evolution of the system is obtained by solving the coupled Hamiltonian equations, $\dot{\boldsymbol{p}}_i = \partial H/\partial \boldsymbol{r}_i$ and $\dot{\boldsymbol{r}}_i = -\partial H/\partial \boldsymbol{p}_i$.

We illustrate the cluster recognition method by considering the collision of two calcium nuclei at the bomberding energy of 40 MeV per nucleon. In fig. 2 is shown the nucleon number of the largest cluster, A_{max} (top) and the multiplicity of clusters containing more than two nucleons (bottom). These results have been obtained by averaging over a sample of 106 individual collision events. For reference is shown the result of a standard spatial cluster analysis, using a cluster range of $r_c = 6$ fm (dotted curve). For both methods, the results of the cluster decomposition are shown

as a function of time. It is seen that both methods converge on the same results when sufficient time has elapsed, as would be expected since the clusters are then well separated in space. At earlier times the standard analysis tend to yield fewer clusters, because of the partial overlap of the different clusters. However, the method proposed here exhibits a much weaker time dependence, after the initial steep increase in the multiplicity values. This remarkable fact suggests that the method is able to discern the ultimate cluster structure of the system very early on, before a clear spatial separation has taken place. This is a very useful feature, since calculations aimed at calculating fragment production probabilities may then be considerably reduced in time. Moreover, the result is of physical interest as well, since it demonstrates that the "decision" about the fragment formation is made relatively early on in the process.

The above features are also brought out in fig. 3 which shows the mean multiplicity of fragments in selected size ranges as a function of time for central collisions of the calcium nuclei at bombarding energies of 40 and 60 MeV per nucleon. The results obtained with the present recognition method are indicated by the solid curves, while the dashed curves show those resulting from a standard spatial analysis using the range $r_c = 6$ fm.

Finally, fig. 4 depicts the corresponding multiplicity distributions at three different times in the course of the evolution. It is evident that the results obtained with the present method very quickly approach the final distribution, whereas the spatial analysis displays a significant time dependence: early on, when the system is well connected in position space, the system has one large cluster containing most of the nucleons; as the expansion moves the clusters apart the results converge towards the former ones.

Similar calculations have also been made for larger systems, and at other energies, and the present results are typical.

4 Discussion

In the present note we have described a novel method for recognizing clusters in microscopic dynamical simulations of nuclear collisions. The identification of clusters is based on the requirement that each member of a given cluster be bound with respect to that cluster. Using the sum of the cluster binding energies as a cost function, a Metropolis sampling is then employed to determine an optimal cluster decomposition.

We have demonstrated that this method is very powerful in its ability to identify the approximate cluster structure already during the early stage when all clusters have considerable spatial overlap. The method is therefore of great practical utility in calculations of fragment production in heavy-ion reactions. Furthermore, the associated analysis demonstrates that the cluster structure is determined relatively early on in the process, at times when there is still considerable spatial overlap between the different preclusters. This feature has a bearing on our understanding of the fragment formation mechanism.

It is also important to comment on the fact that the proposed recognition method is not exact. This feature implies that in each particular event it cannot be guaranteed

that the cluster decomposition arrived at is the absolutely most favored. However, it should be recalled that numerical simulations of fragment formation are statistical in nature, usually involving large samples of events calculated events. Therefore, what matters is the *distribution* of cluster decompositions and the statistical recognition method is likely to be much better for this purpose. It should also be noted that the specific cluster criterion adopted is by no means unique, and although all reasonable criteria will yield the same result when the clusters have separated sufficiently, they will generally differ at the early dense stage. Consequently, with the mathematical problem being somewhat fuzzy, the need for exact methods of solution therefore appears less compelling.

We finally wish to draw attention to the fact that similar problems are encountered in other areas of physics, for example in the explosion of suddenly heated liquid drops. Indeed, our method can be regarded as a specific adaptation of the general concept of simulated annealing [4], which has already found application in a variety of areas, including mathematics, economics, and condensed matter physics [5].

This work was supported in part by the Director, Office of Energy Research, Office of High Energy and Nuclear Physics, Division of High Energy Physics, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098. One of us (COD) acknowleges partial support from CONICET and Fundacion Antorchas in Argentina.

References

[1] C. Dorso, S. Duarte, and J. Randrup, Phys. Lett. 188B (1987) 287

[2] C. Dorso and J. Randrup, Phys. Lett. 215B (1988) 611

[3] N. Metropolis, A.W. Rosenblut, M.N. Rosenblut, A.H. Teller, and E. Teller, J. Chem. Phys. 21 (1953) 1087

[4] S. Kirkpatrick, J. Stat. Phys. 34 (1984) 975

[5] *Simulated Annealing: Theory and Applications*, P.J.M. van Laarhoven and E.H.L. Aarts, D. Reidel Publishing Company, Boston (1987)

Figure 1:
The kinetic energy of a gas of nucleons that interact only via the Pauli potential (top), the binding energy of nuclear matter as a function of the density (middle), and the binding energy of finite nuclei as a function of their mass number (bottom), as calculated with the employed molecular dynamics model.

Figure 2:
Based on 106 head-on collisions of Ca with Ca at 40 MeV per nucleon, the figure shows the average particle number of the largest fragment $A_{\mathbf{max}}$ (top) and the average multiplicity of clusters containing more than two particles (bottom), both as functions of the time elapsed since the first contact was made. The full curve connects the results of the simulated annealing analysis, whereas the dots indicate the results of a spacial analysis using a cluster range of $r_c = 6$ fm.

Figure 3:
The average multiplicity binned according to the number of particles A, for central collisions of two calcium nuclei. Top: the same 106 events as used in fig. 1. Bottom: 40 events corresponding to a bombarding energy of 60 meV per nucleon.

Figure 4:
The multiplicity distribution at three different points in time, for the same event set as in fig. 2, using either simulated annealing (solid histogram) or spatial analysis (dots).

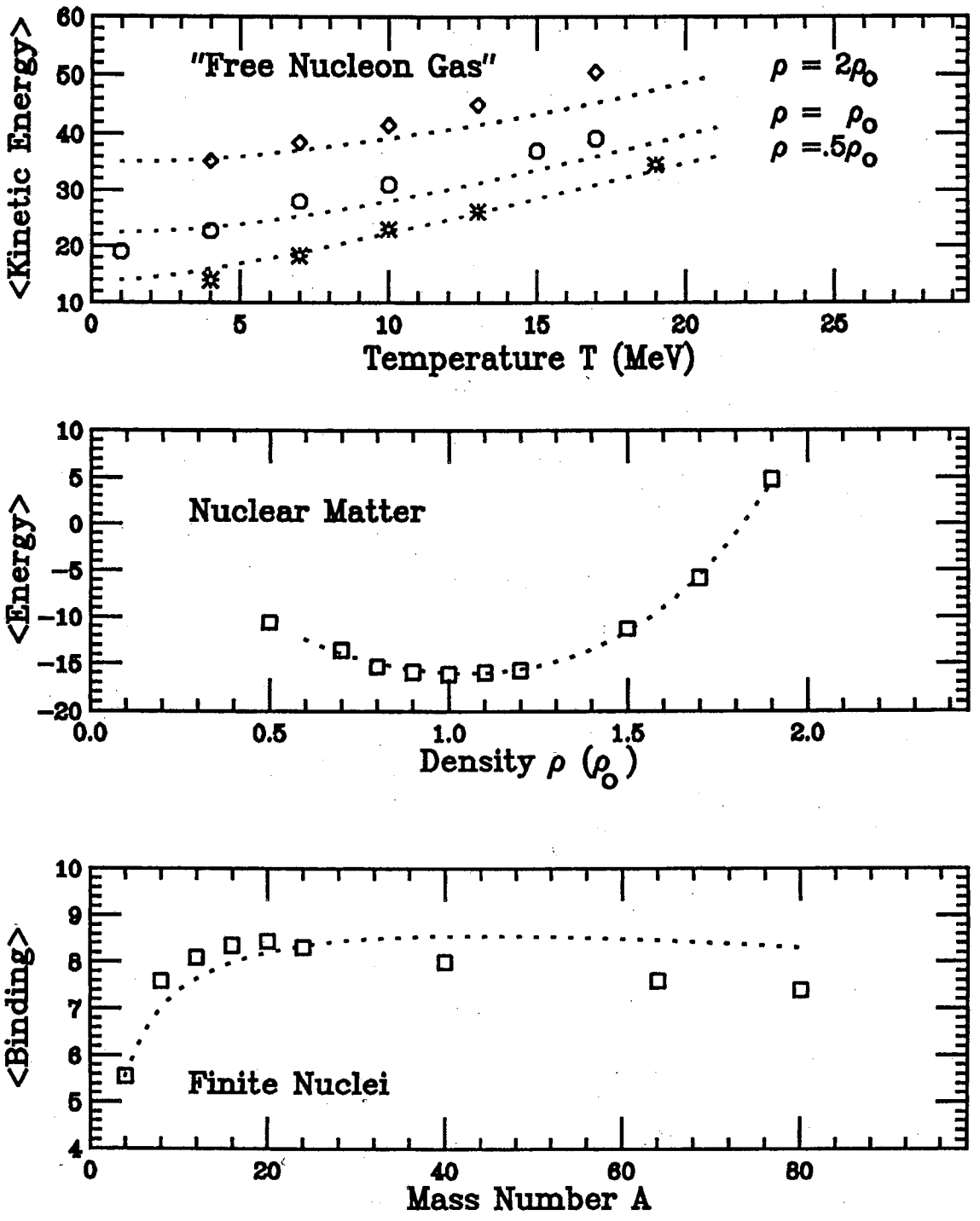

"Free Nucleon Gas"
ρ = 2ρ0
ρ = ρ0
ρ =.5ρ0
<Kinetic Energy>
Temperature T (MeV)
Nuclear Matter
<Energy>
Density ρ (ρ0)
Finite Nuclei
<Binding>
Mass Number A

Figure 1

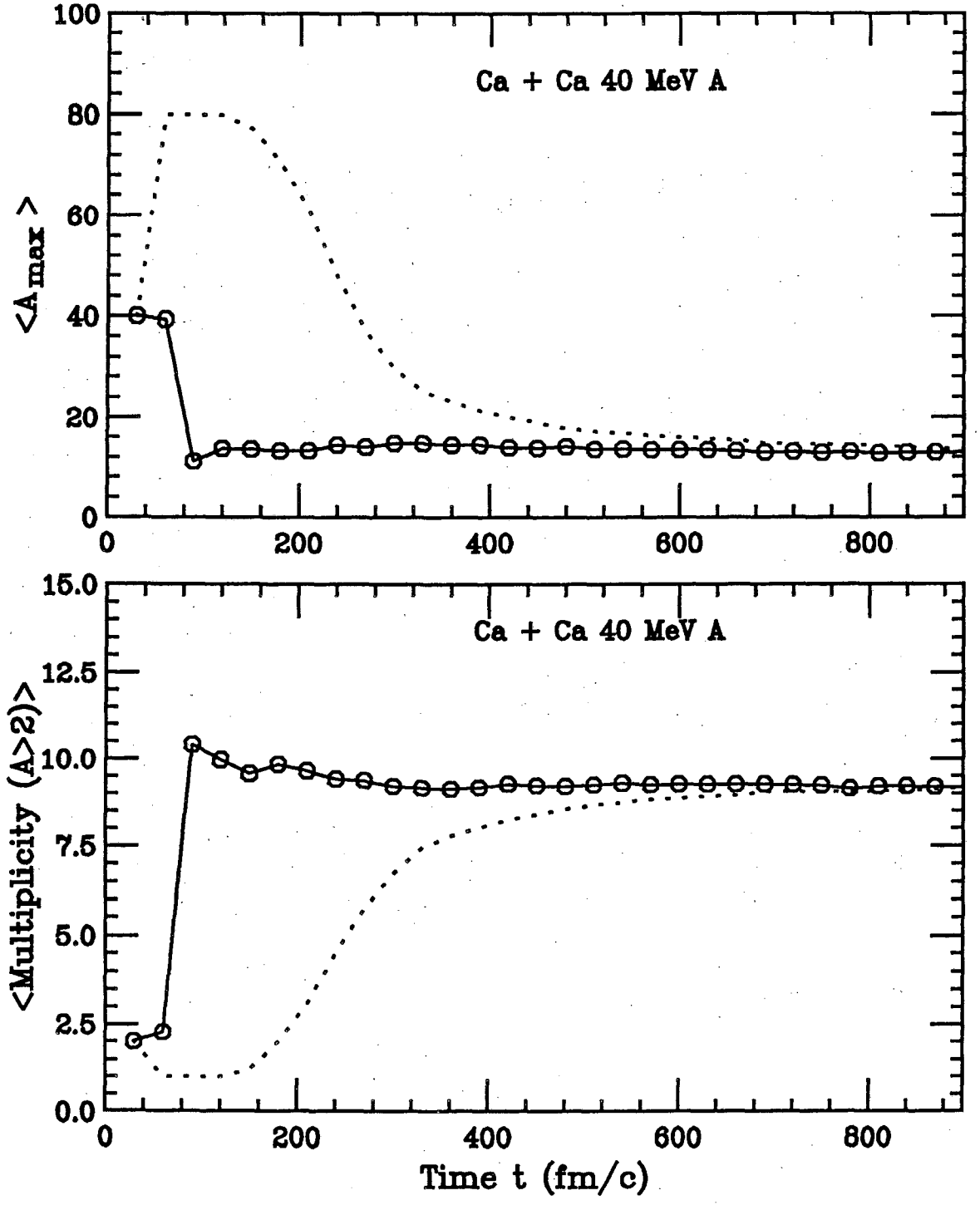

Ca + Ca 40 MeV A
<A max >
100
80
60
40
20
0
0
200
400
600
800
Ca + Ca 40 MeV A
<Multiplicity (A>2)>
15.0
12.5
10.0
7.5
5.0
2.5
0.0
0
200
400
600
800
Time t (fm/c)

Figure 2

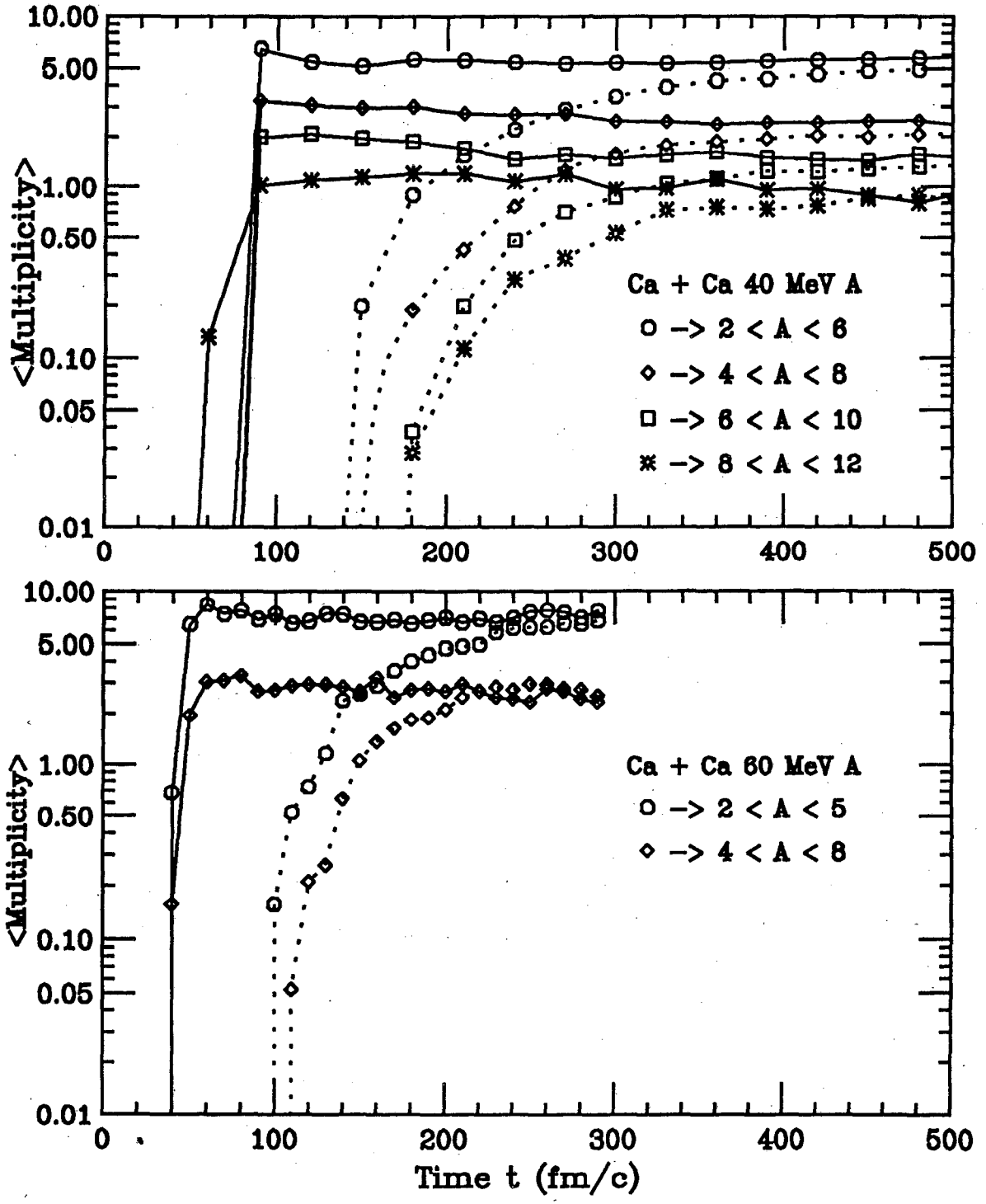

10.00
5.00
1.00
0.50
0.10
0.05
0.01
<Multiplicity>
Ca + Ca 40 MeV A
o -> 2 < A < 6
◇ -> 4 < A < 8
□ -> 6 < A < 10
* -> 8 < A < 12
0
100
200
300
400
500
Ca + Ca 60 MeV A
o -> 2 < A < 5
◇ -> 4 < A < 8
Time t (fm/c)

Figure 3

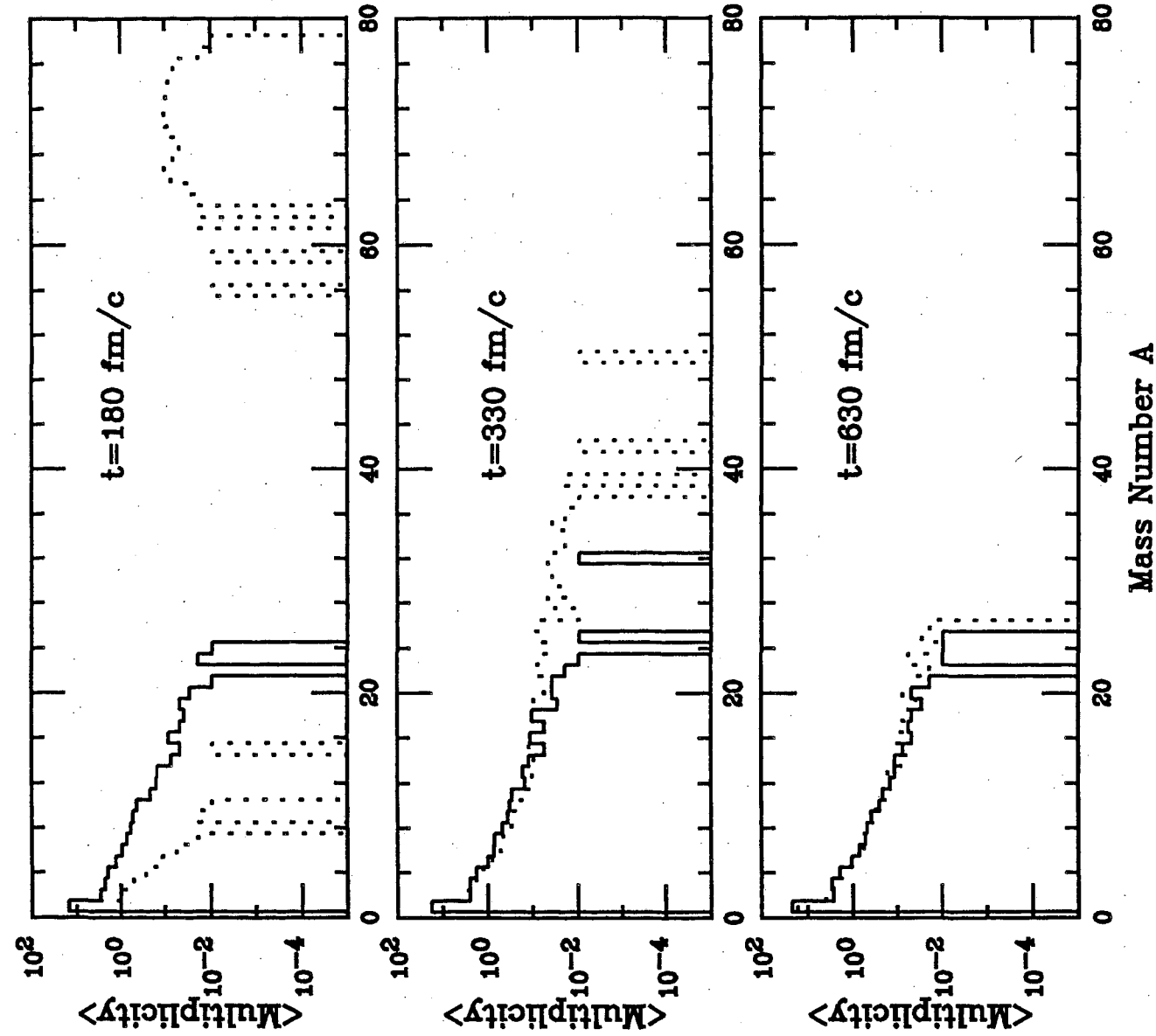

Ca + Ca 40 MeV A
t=180 fm/c
t=330 fm/c
t=630 fm/c
<Multiplicity>
Mass Number A

Figure 4

LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
TECHNICAL INFORMATION DEPARTMENT
BERKELEY, CALIFORNIA 94720