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A New Treatment of Boltzmann-like Collision Integrals in Nuclear Kinetic Equations*,†

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We present a new method to solve the collision-integrals in BUU-type simulations of heavy-ion reactions and compare it to the two currently used full- and parallel-ensemble schemes.

1. INTRODUCTION

To date one of the most challenging questions in nuclear physics is the investigation of the properties of "nuclear matter" characterized in an equilibrium state by its equation of state (EOS). Only little is known about the EOS of nuclear matter and, therefore, various sophisticated experiments have been devoted to the study of hot, dense nuclei. These investigations started in the advent of the 70s with the experiments by the streamer chamber and plastic-ball groups at the Bevalac using beam energies up to 2.1 GeV/u for nuclei as heavy as ^{40}Ca [1], and they are extended today to violent reactions ranging up to 200 GeV/u at CERN.

To disentangle the manifold experimental signals and point out sensitive observables which may provide information about densities, pressures, temperatures, in-medium modification of cross sections, etc., accurate calculations, incorporating the complete dynamical evolution from the highly non-equilibrium initial to the final possibly equilibrized state are neccesary. Unfortunately, at present the full quantum-mechanical many-body problem is not solvable. It is, however, possible to derive semi-classical transport equations that should provide good approximations to the exact solutions.

These transport equations resemble the form of a classical Boltzmann equation, extended by potential terms and Pauli-blocking factors in the collision integral. Several groups have based their studies of heavy-ion reactions on this kind of kinetic equation, referring to it with different names: Boltzmann–Uehling–Uhlenbeck [2–4], Vlasov–Uehling–Uhlenbeck [5, 6], Landau–Vlasov [7], etc.

The main ingredients of this equation are the self-consistent mean field common to all nucleons and the residual NN-interaction which is modeled by the collision integral. In the standard algorithms used so far [2] the calculation of this collision term requires most of the total computing time. In this work we present a new powerful and fast method to solve the collision integral in Boltzmann-like kinetic equations in the nuclear physics context.

In Section 2 we introduce our version of the kinetic equation, the relativistic Boltzmann–Uehling–Uhlenbeck (RBUU) equation. In Section 3 we explain the numerical methods to solve this equation, especially the different possibilities to tackle the collision integral. In Section 4 we compare these various methods and demonstrate the superiority of our new scheme.

2. THEORETICAL BACKGROUND

The description of a heavy-ion collision in principle requires the solution of a coupled set of nonlinear equations of motion for quantum-mechanical field operators of nucleons and mesons. These equations can be written down in a model field-theory, but to date there is no way to solve them exactly. Therefore, one has to apply suitable approximations that lead to a transport equation for the nucleon phase-space density [4, 8–11]. In this approximation the meson-exchange interaction between the nucleons reduces to a mean-field potential. This potential has to be evaluated selfconsistently in accordance with the actual nucleon distribution. In its nonrelativistic form the resulting transport equation is given by [4]

$$\left(\frac{\partial}{\partial t}+\frac{\mathbf{p}_1}{m}\frac{\partial}{\partial \mathbf{r}}-\frac{\partial U(\mathbf{r};t)}{\partial \mathbf{r}}\frac{\partial}{\partial \mathbf{p}_1}\right) f(\mathbf{r},\mathbf{p}_1;t)=I_{\text{coll}},$$

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$$I_{\text{coll}} = \frac{4}{(2\pi)^3} \int d^3p_2 d^3p_3 \, d\Omega \, |v_{12}| \, \frac{d\sigma}{d\Omega}$$
$$\times \delta^{(3)}(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_3 - \mathbf{p}_4)$$
$$\times (f(\mathbf{r}, \mathbf{p}_3; t) f(\mathbf{r}, \mathbf{p}_4; t)(1 - f(\mathbf{r}, \mathbf{p}_1; t))$$
$$\times (1 - f(\mathbf{r}, \mathbf{p}_2; t))$$
$$- f(\mathbf{r}, \mathbf{p}_1; t) f(\mathbf{r}, \mathbf{p}_2; t)(1 - f(\mathbf{r}, \mathbf{p}_3; t))$$
$$\times (1 - f(\mathbf{r}, \mathbf{p}_4; t))), \tag{1}$$

where $f(\mathbf{r}, \mathbf{p}, t)$ is the one-body phase-space density. In its covariant form it reads [3]

$$(\Pi^\mu \partial_\mu^x + (g_V \Pi_\nu F^{\mu\nu} + m^*(\partial_x^\mu m^*)\, \partial_\mu^\Pi)) f(x, \Pi) = I_{\text{coll}},$$
$$I_{\text{coll}} = \frac{2}{(2\pi)^3} \int \frac{d^3\Pi_1}{\Pi_1^0} \frac{d^3\Pi'}{\Pi'^0} \frac{d^3\Pi_1'}{\Pi_1'^0} (\Pi + \Pi_1)^2 \frac{d\sigma}{d\Omega}$$
$$\times \delta^{(4)}(\Pi + \Pi_1 - \Pi' - \Pi_1')$$
$$\times (f(x, \Pi') f(x, \Pi_1')(1 - f(x, \Pi))$$
$$\times (1 - f(x, \Pi_1))$$
$$- f(x, \Pi) f(x, \Pi_1)(1 - f(x, \Pi'))$$
$$\times (1 - f(x, \Pi_1'))), \tag{2}$$

with the field-strength tensor $F_{\mu\nu} = \partial_\mu \omega_\nu(x) - \partial_\nu \omega_\mu(x)$, the effective mass $m^* = m - g_S \sigma(x)$ and the kinetic momentum $\Pi_\mu := p_\mu - g_V \omega_\mu(x)$. Here $f(x, \Pi)$ is the Lorentz-scalar phase-space distribution function. Possible parametrizations of the mean-field potentials $U(\mathbf{r}; t)$, the vector field $\omega(x)$, and the scalar field $\sigma(x)$ can be found, e.g., in [4]. The major difference to the collision-integral known from classical kinetic theory are the Pauli-blocking factors $1 - f(x, \Pi)$, which account for the fermionic nature of the nucleons and prevent scattering of particles into already occupied regions of phase-space. Note that the collision-term is local in r-space.

The extension of this transport-equation to incorporate different particle species or the creation of mesons is straightforward and can be found in, e.g., [12]. We base our following discussion on the RBUU-equation (2), but the algorithm given below can be readily adapted to the non-relativistic description, too.

Possible in-medium corrections of the N-N cross section $d\sigma/d\Omega$, as suggested in [4, 10, 13], are not important for the numerical schemes we will present in this work. We, therefore, use the parametrization of the free cross section $d\sigma/d\Omega$ as given by Cugnon [14], which nevertheless reproduces the experimental rapidity distributions dN/dY in simulations of heavy-ion reactions [15, 16], and include the inelastic channels

$$\begin{aligned} &N + N \to N + \Delta; \qquad &&N + \Delta \to N + N; \\ &N + \Delta \to N + \Delta; \qquad &&\Delta + \Delta \to \Delta + \Delta, \end{aligned} \tag{3}$$

where the Δ's are propagated in the same mean-field as the nucleons.

3. NUMERICAL METHODS

The usual way to solve Eq. (2) is via the test particle method [17]. Here the Lorentz-scalar phase-space distribution function $f(x, \Pi)$ is approximated by a sum of delta functions,

$$f(\mathbf{r}, \mathbf{\Pi}; t) \sim \frac{1}{N} \sum_{i=1}^{NA} \delta^{(3)}(\mathbf{r} - \mathbf{r}_i(t))\, \delta^{(3)}(\mathbf{\Pi} - \mathbf{\Pi}_i(t)) \tag{4}$$

centered at positions $\mathbf{r}_i$ and momenta $\mathbf{\Pi}_i$. In the following we will denote each of these phase-space points as a test particle. One should keep in mind, however, that these "particles" do not represent actual nucleons, but are just a simple tool for approximating a smooth distribution $f(x, \Pi)$. Following this interpretation, A in (4) denotes the number of (physical) nucleons, whereas N stands for the number of (unphysical) test particles per nucleon. These test particles move according to classical equations of motion:

$$\frac{\partial \mathbf{r}_i}{\partial t} = \frac{\mathbf{\Pi}_i}{\Pi_i^0}, \tag{5}$$

$$\frac{\partial \Pi_i^k}{\partial t} = g_V \frac{\Pi_i^\mu}{\Pi_i^0} F_\mu^k(\mathbf{r}_i) + \frac{1}{\Pi_i^0} m^*(\mathbf{r}_i)\, \partial_x^k(m^*(\mathbf{r}_i)),$$
$$k = 1, 2, 3. \tag{6}$$

The first term of Eq. (6) clearly resembles a Lorentz-force proportional to the "particle" velocity $\mathbf{\Pi}_i/\Pi_i^0$.

The Vlasov part of Eq. (2) can now be readily solved: Dividing the time interval of interest into sufficiently small steps, first the mean-field potentials σ and ω have to be determined selfconsistently. Then the test particles are propagated according to Eqs. (5), (6), leading to new source-terms for the fields. Since in Eqs. (5), (6) the derivatives of the fields have to be computed, the densities have to be determined quite accurately. This, in turn, calls for a large number of test particles to reduce the statistical fluctuations.

The straightforward, and until now generally used, way to tackle the collision integral is to let, in a third step, each test particle interact with all the others with a reduced cross

section σ/N. Sticking to a geometrical picture, test particles with a distance less than $\sqrt{\sigma(s)/(N\pi)}$ experience a collision (s being the invariant mass of the NN pair). In the limit $N \to \infty$, one regains the locality in configuration space inherent in I_{coll}, where the distribution functions $f(x, \Pi)$ have to be taken at the same space-time point.

The numerical expense is obvious, too: At each time-step $(A \cdot N) \cdot (A \cdot N - 1)/2$ comparisons have to be made. We, therefore, expect the computing time to increase like $\mathcal{O}((A \cdot N)^2)$. This time can be somewhat reduced by an intelligent sorting of the test particles. Since the interaction range decreases like $\sqrt{1/N}$, it is possible to break the configuration space into small volumes and consider only collisions among particles in the same volume-element and in the small boundary region between two adjacent boxes. This would lead to a scaling like $\mathcal{O}(A \cdot N^2)$. This computation scheme, where all test particles can mutually interact, is called the "full-ensemble" method.

In contrast, the "parallel-ensemble" method allows only collisions among particles belonging to the same ensemble which consists of A test particles; we therefore encounter the situation of N independent cascade runs, coupled, however, via the common mean-field potential [2]. The computational effort is of the order $\mathcal{O}(A^2 \cdot N)$. Since typically $A \approx 200$, $N \approx 500$, the parallel-ensemble method is numerically faster than the full-ensemble method.

Unfortunately, the interaction range in the parallel-ensemble method will be $\sqrt{\sigma/\pi}$, regardless of the number of test particles. Therefore one cannot expect that the solutions converge in the limit $N \to \infty$, $dt \to 0$, to the exact solutions of Eq. (2), since the locality of the collision term is evidently not attained. Nevertheless, it was found by Welke *et al.* [18], that the results of full-ensemble and parallel-ensemble calculations yield comparable results for heavy-ion reactions.

We now propose a new method to solve I_{coll}, already successfully applied in other fields of physics [19], which scales as $\mathcal{O}(A \cdot N)$ and can be shown to converge to the exact solution of the Boltzmann equation. We call this scheme in the following the "local-ensemble" method.

We start with the following assumption: Let the phase-space density $f(x, \Pi)$ be a slowly varying function (on an appropriately small chosen scale) of the four-vector x. This assumption has already been made by discretizing the Vlasov-equation in time and computing the fields only on discrete space-time grid-points. At each time-step we can therefore approximate $f(\mathbf{r}, \Pi)$ by

$$\tilde{f}(\mathbf{r}, \Pi) := \sum_i \delta_i f_i(\Pi), \qquad \begin{cases} \delta_i = 1 & \text{if } \mathbf{r} \in \text{volume-element } i \\ \delta_i = 0, & \text{otherwise.} \end{cases} \tag{7}$$

At each grid point, one thus has to solve a space-independent Boltzmann equation. The probability for one pair of test particles to undergo a collision during the time intervall Δt in the volume element $\Delta^3 x$ is then given by

$$W = \frac{\sigma(s, m_1, m_2)}{N} v_{\text{rel}} \frac{\Delta t}{\Delta^3 x}. \tag{8}$$

Here σ denotes the (total) cross section, s is the invariant mass of the baryon pair, and v_{rel} is the relative velocity of the scattering particles 1 and 2. The latter is given by

$$v_{\text{rel}} = \frac{\lambda^{1/2}(s, m_1^2, m_2^2)}{2\Pi_1^0 \Pi_2^0} \tag{9}$$

with $\lambda(x, y, z) = (x - y - z)^2 - 4yz$.

Out of the $n(n-1)/2$ possible pairs (n being the number of test particles in the cell $\Delta^3 x$) we choose at random $[n/2]$ collision pairs. We therefore have to replace the probability W by W',

$$W' := W \frac{n(n-1)/2}{[n/2]} \tag{10}$$

in order to obtain the correct total transition rate in the cell. In the limit $\Delta^3 x \to 0$, $\Delta t \to 0$, $N \to \infty$, the solutions obtained by this method will converge to the exact solutions of the Boltzmann equation [20, 21]. Furthermore, this prescription is evidently covariant. Since we are dealing with transition rates and do not employ the geometrical interpretation of the full-ensemble or the parallel-ensemble methods described above, no problems connected with the time-ordering of the collision processes occur.

4. RESULTS

We now compare the results of calculations using the three different alogorithms for the treatment of the collision

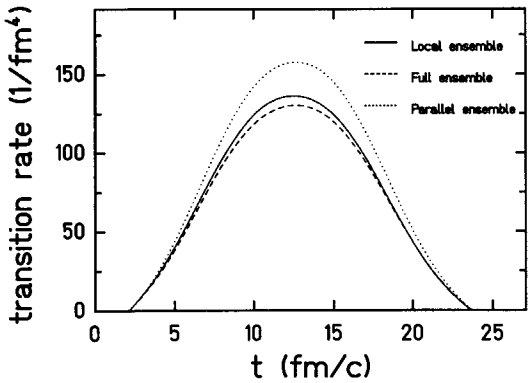

FIG. 1. Transition rate in the central-overlap region for the reaction $^{93}\text{Nb} + ^{93}\text{Nb}$ at 1 GeV/u: solid, local-; dashed, full-; dotted, parallel-ensemble algorithm.

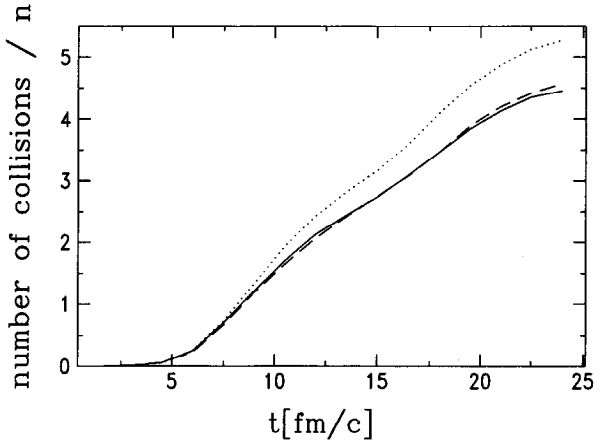

FIG. 2. Average number of collisions per particle in the central-overlap region for the reaction $^{93}Nb + ^{93}Nb$ at 1 GeV/u: solid, local-; dashed, full-; dotted, parallel-ensemble algorithm.

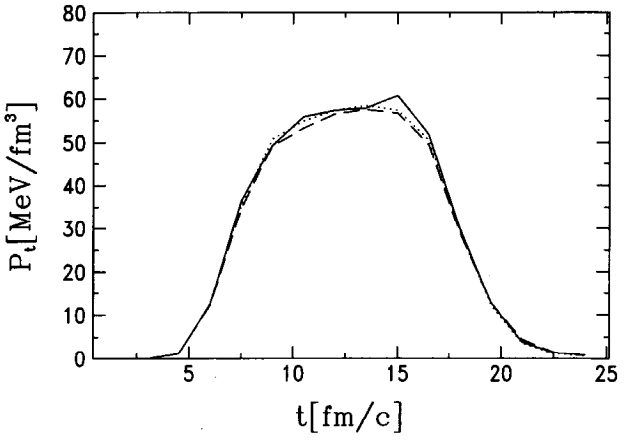

FIG. 4. Transverse pressure in the central overlap-region for the reaction $^{93}Nb + ^{93}Nb$ at 1 GeV/u: solid, local-; dashed, full-; dotted, parallel-ensemble algorithm.

term discussed above. We chose the system $^{93}Nb + ^{93}Nb$ at 1 GeV/u, impact parameter $b = 2.3$ fm, with 1000 test particles per nucleon as a typical example for the kind of reactions currently investigated.

The first quantity of interest is the number of collisions during one time-step in a central volume element of the overlap region of the two nuclei, divided by the time-step size, i.e., the transition rate (cf. Fig. 1). As can be seen, full ensemble and local ensemble methods give about the same results, whereas the collision numbers are somewhat larger for the parallel ensemble method. In Fig. 2 we present the average number of collisions per particle as a function of time. Again, the parallel ensemble method gives by about 15–20% larger numbers than the other two methods.

Whether the established differences in the collision history are important can only be judged by comparing the physical observables of the system. Even if there are only small deviations in the collision numbers, the resulting changes in the dynamical evolution of the system may be quite large, since distinct regions in phase-space are tested. Therefore we investigated the density (Fig. 3) and the transverse pressure (Fig. 4) in the central overlap region (see [22, 23] for details). Since the transverse pressure P_t is dynamically created during the reaction, one might expect it to be sensitive to the collision prescription employed. This, however, turns out to be not the case as can be seen in Fig. 4. The results of all three algorithms agree perfectly for the density as well as for the transverse pressure, proving that the parallel ensemble and local ensemble algorithms yield good approximations to the "exact" solution.

The quantities just discussed are not directly experimentally observable. We, therefore, want to close our comparisons with two quantities that have proven to be quite important and are easily accessible in experiment: The "stopping power" (i.e., the dN/dY distribution which gives the number of particles per unit rapidity bin) [24] and the

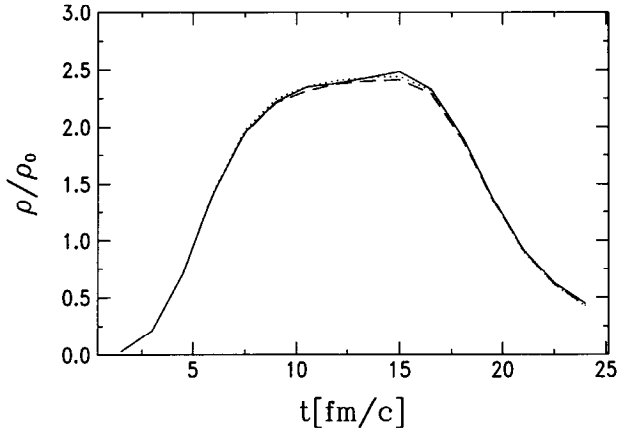

FIG. 3. Density in the central-overlap region for the reaction $^{93}Nb + ^{93}Nb$ at 1 GeV/u: solid, local-; dashed, full-; dotted, parallel-ensemble algorithm.

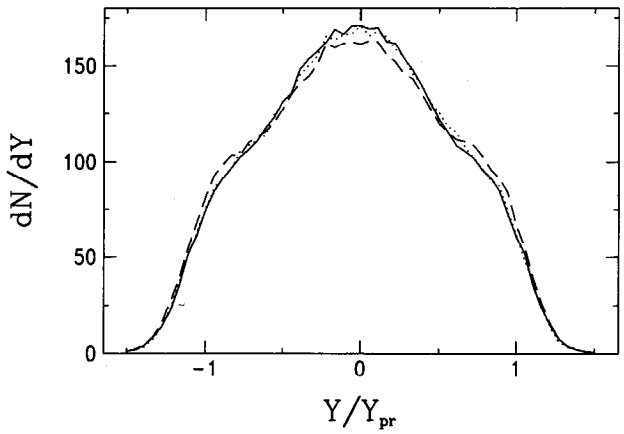

FIG. 5. Stopping power (dN/dY) for the reaction $^{93}Nb + ^{93}Nb$ at 1 GeV/u: solid, local-; dashed, full-; dotted, parallel-ensemble algorithm.

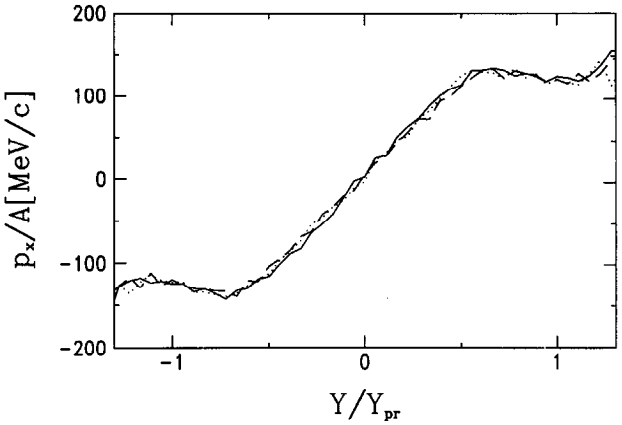

FIG. 6. Transverse flow for the reaction $^{93}Nb + ^{93}Nb$ at 1 GeV/u: solid, local-; dashed, full-; dotted, parallel-ensemble algorithm.

transverse flow (i.e., p_x/A, the transverse momentum per nucleon) [25]. The first is commonly used to gain information about possible modifications of the N-N cross section, whereas the latter is believed to test the influence of the mean field. Again, all three methods yield the same results (cf. Fig. 5 and Fig. 6), assuring that the overall dynamical evolution is the same for all three cases.

The most striking differences among the three methods can be found in the amount of computing time needed. To demonstrate this more clearly, we performed pure cascade calculations without Pauli-blocking. In Fig. 7 we show the amount of computing time needed for one time-step for the two different systems $^{40}Ca + ^{40}Ca$ and $^{93}Nb + ^{93}Nb$ as a function of N (i.e., the number of test particles/A). The linear dependence on N for the parallel and local ensemble methods can be seen quite clearly, whereas the amount of computing time increases quadratically for the full ensemble method. For moderate test-particle numbers, however, the parallel and full ensemble methods need about the same amount of time. Nevertheless, neither approach can compete with the local ensemble method, which is (for 2500 test

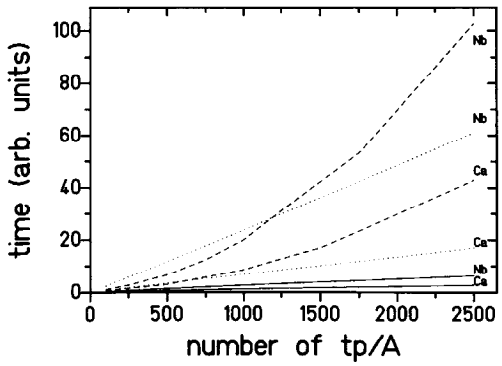

FIG. 7. Computing time as a function of the number of test particles/A for Nb + Nb and Ca + Ca: solid, local-; dashed, full-; dotted, parallel-ensemble algorithm.

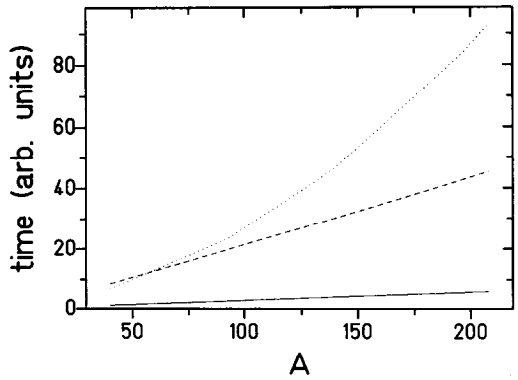

FIG. 8. Computing time as a function of the projectile mass: solid, local-; dashed, full-; dotted, parallel-ensemble algorithm.

particles/A) a factor of 10 (compared to the full ensemble) or six (compared to the parallel ensemble) times faster, respectively.

The dependence on the projectile mass (we investigated only symmetric systems) is shown in Fig. 8 for 1000 test particles/A. We find our initial statement confirmed: The time needed by local and full ensemble increases linearly, whereas for the parallel ensemble it increases quadratically. Since future experiments will definitely aim at high mass numbers, this again demonstrates the superiority of the local ensemble method.

5. SUMMARY

We have presented in this work a new method—called the local ensemble method—to solve the collision integrals in BUU-type simulations of heavy-ion reactions. All three methods we compared—the parallel ensemble, the full ensemble, and the local ensemble—delivered the same results for all the physical observables investigated. The local ensemble method, however, has the following advantages compared to its predecessors:

- Its solutions will converge (in the limit $N \to \infty$, $\Delta^3 x \to 0$, $\Delta t \to 0$) to the exact solutions of the Boltzmann equation. In contrast, the solutions of the parallel ensemble method can only be approximations to the exact solutions, since it clearly violates the locality of the collision integral.
- The local ensemble method is fully covariant and does not exhibit any problems of time-ordering.
- Whereas the full and parallel ensemble methods show a computing time behaviour like $\mathcal{O}(A \cdot N^2)$ and $\mathcal{O}(A^2 \cdot N)$, respectively, the time needed by the local ensemble method increases only linearly (i.e., like $\mathcal{O}(A \cdot N)$). As we have shown, the savings in computing time may be tremendous. Factors of 5–10 can be easily reached. Furthermore, since each cell in configuration space can be treated completely independently from all the others, modern computing

techniques like massive parallelization and vectorization can be quite easily adopted, improving the situation even more.

We hope that the local ensemble method will lead to a "quantum leap" in the theoretical investigations of heavy-ion reactions. It is quite simple to implement and possible extensions are straightforward (e.g., introduction of other particle species, creation of mesons).

REFERENCES

1. H. H. Gutbrod, A. M. Poskanzer, and H. G. Ritter, *Rep. Prog. Phys.* **52**, 1267 (1989).
2. G. Bertsch and S. das Gupta, *Phys. Rep.* **160**, 189 (1988).
3. B. Blättel, V. Koch, W. Cassing, and U. Mosel, *Phys. Rev. C* **38**, 1767 (1988).
4. W. Cassing and U. Mosel, *Prog. Part. Nucl. Phys.* **25**, 235 (1990).
5. H. Kruse, B. Jacak, and H. Stöcker, *Phys. Rev. Lett.* **54**, 289 (1985).
6. C. M. Ko, *Nucl. Phys. A* **495**, 321c (1989).
7. C. Grégoire, B. Remaud, F. Sebille, L. Vinet, and Y. Raffray, *Nucl. Phys. A* **465**, 317 (1987).
8. W. Cassing and S. J. Wang, *Z. Phys. A* **337**, 1 (1990).
9. B. Schürmann, W. Zwermann, and R. Malfliet, *Phys. Rep.* **147**, 1 (1987).
10. W. Botermans and R. Malfliet, *Phys. Lett. B* **215**, 617 (1988).
11. W. Botermans and R. Malfliet, *Phys. Rep.* **198**, 115 (1990).
12. S. de Groot, W. van Leeuwen, and C. van Weert, *Relativistic Kinetic Theory* (North Holland, Amsterdam, 1980).
13. G. F. Bertsch, G. E. Brown, V. Koch, and B.-A. Li, *Nucl. Phys. A* **490**, 745 (1988).
14. J. Cugnon, T. Mizutani, and J. Vandermeulen, *Nucl. Phys. A* **352**, 505 (1981).
15. L. Neise, M. Berenguer, C. Hartnack, G. Peilert, H. Stöcker, and W. Greiner, *Nucl. Phys. A* **519**, 375c (1990).
16. V. Koch, B. Blättel, W. Cassing, and U. Mosel, *Nucl. Phys. A* **532**, 715 (1991).
17. C.-Y. Wong, *Phys. Rev. C* **25**, 1460 (1982).
18. G. M. Welke, R. Malfliet, C. Gregoire, M. Prakash, and E. Suraud, *Phys. Rev. C* **40**, 2611 (1989).
19. F. Gropengiesser, H. Neunzert, and J. Struckmeier, in *Venice 1989: The State of Art in Appl. and Industrial Math*, (edited by R. Spigler, Kluwer Academic, Boston, 1990).
20. H. Babovsky, *Eur. J. Mech. B* **8**, 41 (1989).
21. H. Bavovsky and R. Illner, *SIAM J. Numer. Anal.* **26**, 45 (1989).
22. A. Lang, B. Blättel, V. Koch, K. Weber, W. Cassing, and U. Mosel, *Phys. Lett. B* **245**, 147 (1990).
23. A. Lang, B. Blättel, W. Cassing, V. Koch, U. Mosel, and K. Weber, *Z. Phys. A* **340**, 287 (1991).
24. H. H. Gutbrod, K. H. Kampert, B. W. Kolb, A. M. Poskanzer, H. G. Ritter, and H. R. Schmidt, *Z. Phys. A* **337**, 57 (1990).
25. K.-H. Kampert, *J. Phys. G* **15**, 691 (1989).