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Energy Conservation Property of MW-CRF Deterministic Particle Method

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To the memory of Prof. Joachim Wick and Dr. Claudio Barone.

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Abstract—A deterministic particle method for kinetic equation in several dimensions was presented by Motta and Wick some years ago. In the present paper, we formulate the method in general coordinates and apply this formulation to an elastic collision kernel. We show that the method preserves exactly the energy conservation property of the elastic kernel. © 2003 Elsevier Science Ltd. All rights reserved.

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1. INTRODUCTION

Numerical methods for the solution of the Boltzmann equation are under continuous investigation [1,2]. The MW-CRF method is a deterministic particle method for conservation laws, which are given as kinetic equations including collisions, presented by Motta and Wick some years ago [3]. In the present short communication we show that, in the case of an elastic collision kernel, energy conservation is exactly preserved by the MW-CRF method. The idea of the method is to write the equation in divergence form (CRF stands for *collision redefined as flux*) and formally to transform the problem in a collisionless one. This can be done by introducing a flux equivalent for the inhomogeneity and by computing, at each time step, the *collision induced force term* for the *collisionless* problem. Then one take advantage of the long experience in solving Vlasov equation with particle methods [4–7]. For this reason in MW-CRF method particles can move in the velocity space but their weight is kept constant. This has some advantage [8] with respect to other well established approaches where particle are kept fixed in the velocity space and the evolution is reflected in changing their weights in time [9–11].

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In [3], the method was numerically tested with model equations. The method was also applied to the classical test case of a semiconductor $N^+N^-N^+$ structure to show that it can be implemented on parallel machine [12]. Comparison with other particle methods was presented in [8]. Recently, a formulation of the method more convenient for computational purpose and a sketch of the MW-CRF algorithm has been presented in [13].

In order to show the energy conservation property it is sufficient to compute the relevant quantities of the method for the elastic model kernel. This is better achieved if one takes advantage of the symmetries of the problem. In a 3D velocity space, energy conservation better appears in spherical coordinates. For this reason, in the next section, the method is presented in a form suitable for coordinate transformations.

2. THE MW-CRF METHOD IN GENERAL COORDINATES

In this section, we briefly present the MW-CRF method. Presentation is slightly different from previous papers, but we find this form easier to introduce coordinate transformations.

Kinetic equation splits usually in the transport and the collision part. The transport part can be written easily in divergence form.

$$\left(\frac{\partial}{\partial t} f\right)_{\text{trans}} = -\operatorname{div}_{\text{space}}(fv) - \operatorname{div}_{\text{momentum}}(fK).$$

Here we are interested in writing the collision part also in this form. Hence, we consider the equation

$$f_t = Q(f), \tag{1}$$

where $\Omega \subset \mathbf{R}^3$, $f : [0, \infty) \times \Omega \to \mathbf{R}$ and

$$\int_\Omega Q(f)\, d\xi = 0. \tag{2}$$

The initial condition $f_0 : \Omega \to \mathbf{R}$ should be a given nonnegative function with

$$\int_{\Omega_\xi} f_0(\xi)\, d\xi = 1. \tag{3}$$

We search for a vector field ψ such that

$$\operatorname{div} \psi = -Q(f), \tag{4}$$

$$\psi(t, \xi) = 0, \qquad \xi \in \partial\Omega. \tag{5}$$

This means the collision $Q(f)$ is expressed as a flux ψ and there is no flux across the boundary of Ω, which guarantees that the conservation property (2) is satisfied. The associated *force-field* g is given according to

$$\int_B gf\, d\xi = \int_B \psi\, d\xi, \tag{6}$$

for all Borel sets $B \subset \Omega$.

Hence, instead of (1), we consider

$$f_t + \operatorname{div}_\xi(fg) = 0. \tag{7}$$

We remark that the full equation reads now as

$$f_t + \operatorname{div}_x(fv) + \operatorname{div}_\xi(f(K + g)) = 0.$$

Let T be a regular coordinate transformation and $|T|$ denotes its Jacobian. Then we find

$$Q(f) = Q((f \circ T)|T|).$$

Since T is time independent we get

$$\partial_t f \circ T = \partial_t (f \circ T) = Q((f \circ T)|T|) \circ T.$$

But $f \circ T$ must be multiplied by $|T|$ to be a density function.

Calling $\tilde{f} = (f \circ T)|T|$ and $\tilde{Q}(\tilde{f}) = (Q((f \circ T)|T|) \circ T)|T|$ we find

$$\partial_t \tilde{f} = \tilde{Q}\left(\tilde{f}\right). \tag{8}$$

Suppose in the chosen coordinate system Ω can be represented as a Cartesian product of three intervals

$$\Omega = [\alpha_1, \beta_1] \times [\alpha_2, \beta_2] \times [\alpha_3, \beta_3].$$

We introduce the set

$$I^i_{[\alpha_i,\gamma_i]} = \{\xi \in \Omega : \alpha_i \leq \xi_i \leq \gamma_i\}, \tag{9}$$

for $i = 1, 2, 3$. Let $\partial I^i_{[\alpha_i,\gamma_i]}$ its boundary and $\Gamma(\gamma_i) \subset \partial I^i_{[\alpha_i,\gamma_i]}$ the set defined by

$$\Gamma(\gamma_i) = \{\xi \in \Omega; \xi_i = \gamma_i\}. \tag{10}$$

The properties shown in [13] still hold as follows.

PROPERTY 1. The surface $\Gamma(\gamma_i)$ is the only part of $\partial I^i_{[\alpha_i,\gamma_i]}$ which does not belong to $\partial\Omega$, i.e.,

$$\Gamma(\gamma_i) \cup \left(\partial I^i_{[\alpha_i,\gamma_i]} \cap \partial\Omega\right) = \partial I^i_{[\alpha_i,\gamma_i]}.$$

PROPERTY 2. The surface $\Gamma(\gamma_i)$ has the outward normal along the axis ξ_i and versus along increasing ξ_i

$$\mathbf{n}_{\Gamma(\gamma_i)} \cdot \hat{\boldsymbol{\xi}}_i = 1.$$

Using (3) and the Gaussian theorem we find

$$-\int_{I^i_{[\alpha_i,\gamma_i]}} \tilde{Q}\left(\tilde{f}\right) d\xi = \int_{I^i_{[\alpha_i,\gamma_i]}} \operatorname{div} \psi \, d\xi = \int_{\Gamma(\gamma_i)} \psi_i \, dS_i, \tag{11}$$

where dS_i is the appropriate surface element. This holds for all $\gamma_i \in [\alpha_i, \beta_i]$. Now we choose $I^i_{[\alpha_i,\gamma_i]}$ as Borel sets in (6). Together with (11), for the r.h.s. we obtain

$$\Psi_i(\gamma_i) = \int_{I^i_{[\alpha_i,\gamma_i]}} \psi_i(t, \xi) \, d\xi = -\int_{I^i_{[\alpha_i,\gamma_i]}} \left(\int_{\alpha_i}^{\xi_i} \tilde{Q}\left(\tilde{f}\right) d\xi_i'\right) d\xi. \tag{12}$$

Hence, we have

$$\int_{\Gamma(\gamma_i)} \tilde{f} g_i \, d\xi = \Psi_i(\gamma_i). \tag{13}$$

This generalises the result obtained in [3].

3. ENERGY CONSERVATION PROPERTY

We turn now to show the energy conservation property of the numerical method. In order to achieve this result we use a model kernel for elastic collisions

$$Q(f) = \int_\Omega S(k',k)\, f(k')\, dk' - f(k) \int_\Omega S(k,k')\, dk', \tag{14}$$

where $S(k,k')$ represents the collision probability per unit time which, for elastic collisions is

$$S(k,k') = A\delta\left(\mathbf{k}'^2 - \mathbf{k}^2\right), \tag{15}$$

where A is a constant terms.

In semiconductor physics (14) represents the probability per unit time of an electron transition from a state k into an empty state k' induced by the lattice imperfections, when Pauli exclusion principle is neglected; and (15) is the elastic limit of the optical nonpolar interaction in the parabolic approximation. Here it is convenient to use the general formulation described in Section 2 using spherical coordinates and to apply the standard MW-CRF algorithm [13].

1. The density function f_0 will be approximated by a discrete measure

$$f_0(\xi) = \frac{1}{N} \sum_{j=1}^{N} \delta\left(\boldsymbol{\xi} - \boldsymbol{\xi}_j^0\right).$$

2. The *i-component* of the collision induced force $\mathbf{g_i}$ is computed using (12) into (13), which then leads to a linear system of order N

$$\mathcal{A}\mathbf{g_i} = \mathbf{\Psi_i}, \tag{16}$$

where $\mathcal{A}$ is a diagonal dominant matrix; $\mathbf{g}_\mathbf{i}^j$ $(j = 1, N)$ is the i-component of the *collision induced force* on the *j-particle* and $\mathbf{\Psi}_\mathbf{i}^j$ $(j = 1, N)$ is the r.h.s. vector of the linear system [13].

3. The approximation points $\boldsymbol{\xi}^j$ are propagated, from the initial condition $\boldsymbol{\xi}^j(0)$, according to

$$\dot{\boldsymbol{\xi}}^j = \mathbf{g}\left(\boldsymbol{\xi}^j\right), \tag{17}$$

using an explicit first-order scheme.

4. Cycle to Step 2 up to t_{final}.

Let (ξ_1, ξ_2, ξ_3), (k_1, k_2, k_3), respectively, the Cartesian and the spherical coordinates, $\Omega_k = [\alpha_1, \beta_1] \times [0, \pi] \times [0, 2\pi]$, and denote by T the coordinate transformation from $\{\xi\} \to \{k\}$ and by $|T| = k_1^2 \sin k_2$ its Jacobian.

The collision term (14) can be expressed as the difference between a gain term G and a lost term L. Then in the new coordinate system we have

$$\tilde{Q}\left(\tilde{f}(k_1,k_2,k_3)\right) = \tilde{G}(k_1,k_2,k_3) - \tilde{L}(k_1,k_2,k_3),$$

where $\tilde{G}$ and $\tilde{L}$ are given by

$$\tilde{G}(k_1,k_2,k_3) = \int_{\Omega_\mu} S(\mu_1,\mu_2,\mu_3,k_1,k_2,k_3)\tilde{f}(\mu_1,\mu_2,\mu_3)k_1^2 \sin k_2\, d\mu,$$
$$\tilde{L}(k_1,k_2,k_3) = \tilde{f}(k_1,k_2,k_3)\tilde{C}(k_1,k_2,k_3),$$

with

$$\tilde{C}(k_1,k_2,k_3) = \int_{\Omega_\mu} S(k_1,k_2,k_3,\mu_1,\mu_2,\mu_3)\mu_1^2 \sin\mu_2\, d\mu,$$

where $\mu = (\mu_1, \mu_2, \mu_3)$. Then $\Psi_i(\gamma_i)$ can be written in the form

$$\Psi_i(\gamma_i) = -\Psi_{\tilde{G},i}(\gamma_i) + \Psi_{\tilde{L},i}(\gamma_i).$$

To evaluate the $\Psi_i(\gamma_i)$ for $i = 1, 2, 3$ we can proceed as in [3,13].

Here we are interested in computing only the first component Ψ_1 as energy is given by the radial component.

After some algebra, taking care of δ-function properties and with an appropriate use of the Heaviside function $H(.)$, one gets for the *Gain term*

$$\tilde{G}(\mathbf{k}) = \frac{1}{N} \sum_{j=1}^{N} S(k_j, k) k_1^2 \sin k_2 \tag{18}$$

and

$$\begin{aligned}
\Psi_{\tilde{G},1}(\gamma_1) &= \int_0^{2\pi} \int_0^{\pi} \int_{\alpha_1}^{\gamma_1} \int_{\alpha_1}^{\beta_1} \frac{1}{N} \sum_{j=1}^{N} S\left(\mathbf{k}_j, k_1', k_2, k_3\right) k_1'^2 \, dk_1' \, dk_1 \, dk_2 \, dk_3 \\
&= \frac{2\pi A}{N} \sum_{j=1}^{N} \int_{\alpha_1}^{\gamma_1} k_1^j H\left[\left(k_1 - k_1^j\right)\left(k_1^j - \alpha_1\right)\right] \\
&= \frac{2\pi A}{N} \sum_{j=1}^{N} k_1^j \left(\gamma_1 - k_1^j\right) H\left[\left(\gamma_1 - k_1^j\right)\left(k_1^j - \alpha_1\right)\right].
\end{aligned} \tag{19}$$

We now consider the *Loss* term. One has

$$\begin{aligned}
\tilde{C}(\mathbf{k}) &= \int_{\Omega_\mu} A\delta\left(\mu_1^2 - k_1^2\right) \mu_1^2 \sin \mu_2 \, d\mu_1 \, d\mu_2 \, d\mu_3 \\
&= 4\pi A \int_{\alpha_1}^{\beta_1} \mu_1^2 \delta\left(\mu_1^2 - k_1^2\right) \, d\mu_1 \\
&= 2\pi A k_1 H[(\beta_1 - k_1)(k_1 - \alpha_1)]
\end{aligned}$$

and

$$\begin{aligned}
\Psi_{\tilde{L},1}(\gamma_1) &= \int_{I^1_{[\alpha_1,\gamma_1]}} \left(\int_{\alpha_1}^{k_1} \tilde{f}(\mathbf{k}) \tilde{C}(\mathbf{k}) \, dk_1' \, d\mathbf{k} \right) \\
&= \frac{2\pi A}{N} \sum_{j=1}^{N} \int_{\alpha_1}^{\gamma_1} k_1^j H\left[\left(k_1 - k_1^j\right)\left(k_1^j - \alpha_1\right)\right].
\end{aligned} \tag{20}$$

Comparing (20) with (19) one has

$$\Psi_1 = -\Psi_{\tilde{G},1} + \Psi_{\tilde{L},1} = 0.$$

Collision *induced* forces are computed throughout (16). The r.h.s. term for the first component is identically zero,

$$\mathcal{A}\mathbf{g}_1 = 0.$$

As the matrix $\mathcal{A}$ is not singular then ${\mathbf{g}_1}^j = 0, \forall j = 1, N$. Equation (17) then shows that the radial component, k_1^j, of the particles does not change with time. In spherical coordinates this means that the energy of particles does not change with time. This shows that the energy conservation property of the elastic collision kernel is exactly preserved by the MW-CRF method.

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