Fast Numerical Scheme with GPGPU Usage for Uehling-Ulenbeck Equation Treatment

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Actual Problems of Microworld Physics
Azjory, 2018 August 16

Introduction — problems

- Numerical treatment of relativistic particles in Boltzmann (or Uehling-Ulenbeck) equations represent a problem as spectral methods does not work due to non-Abelian nature of Lorentz group of boosts

- Mildly relativistic case needs exact QED matrix elements as limiting expressions are not working there

- There is no general solution to take into account BE and FD corrections for the reaction rates, especially difficult this problem is for MC methods

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Uehling-Ulenbeck Equations

$$I(\vec{p}_1) + II(\vec{p}_2) \leftrightarrow III(\vec{p}_3) + IV(\vec{p}_4)$$

$$\dot{f}_I(\vec{p}_1) = \int d^3\vec{p}_2 d^3\vec{p}_3 d^3\vec{p}_4$$

$$\times \left[W_{(34|12)} f_{III}(\vec{p}_3) f_{IV}(\vec{p}_4) \left(1 \pm \frac{f_I(\vec{p}_1)}{2h^{-3}}\right)\left(1 \pm \frac{f_{II}(\vec{p}_2)}{2h^{-3}}\right) \right.$$

$$\left. - W_{(12|34)} f_I(\vec{p}_1) f_{II}(\vec{p}_2) \left(1 \pm \frac{f_{III}(\vec{p}_3)}{2h^{-3}}\right)\left(1 \pm \frac{f_{IV}(\vec{p}_4)}{2h^{-3}}\right) \right],$$

$$\dot{f}_{II}(\vec{p}_2) = \int d^3\vec{p}_1 d^3\vec{p}_3 d^3\vec{p}_4$$

$$\times \left[W_{(34|12)} f_{III}(\vec{p}_3) f_{IV}(\vec{p}_4) \left(1 \pm \frac{f_I(\vec{p}_1)}{2h^{-3}}\right)\left(1 \pm \frac{f_{II}(\vec{p}_2)}{2h^{-3}}\right) \right.$$

$$\left. - W_{(12|34)} f_I(\vec{p}_1) f_{II}(\vec{p}_2) \left(1 \pm \frac{f_{III}(\vec{p}_3)}{2h^{-3}}\right)\left(1 \pm \frac{f_{IV}(\vec{p}_4)}{2h^{-3}}\right) \right],$$

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Discretization of U-U Equations

Introducing cells in phase spaces $\vec{p}_i \in \Omega_i^{\alpha}$ we get unification of the RHS

$$\left\{\int d^3\vec{p}_1\ \dot{f}_I(\vec{p}_1), \int d^3\vec{p}_2\ \dot{f}_{II}(\vec{p}_2), \int d^3\vec{p}_3\ \dot{f}_{III}(\vec{p}_3), \int d^3\vec{p}_4\ \dot{f}_{IV}(\vec{p}_4)\right\} =$$

$$\int d^3\vec{p}_1 d^3\vec{p}_2 d^3\vec{p}_3 d^3\vec{p}_4$$

$$\times\left[W_{(34|12)} f_{III}(\vec{p}_3) f_{IV}(\vec{p}_4)\left(1 \pm \frac{f_I(\vec{p}_1)}{2h^{-3}}\right)\left(1 \pm \frac{f_{II}(\vec{p}_2)}{2h^{-3}}\right)\right.$$

$$\left. - W_{(12|34)} f_I(\vec{p}_1) f_{II}(\vec{p}_2)\left(1 \pm \frac{f_{III}(\vec{p}_3)}{2h^{-3}}\right)\left(1 \pm \frac{f_{IV}(\vec{p}_4)}{2h^{-3}}\right)\right]$$

besides the difference in the integration limits –

that also vanishes in the individual differential terms of integration sums

Reaction-oriented approach

= use the sums of differential terms

$$\Delta^3\vec{p}_1\Delta^3\vec{p}_2\Delta^3\vec{p}_3\Delta^3\vec{p}_4 \times \Big[W_{(34|12)} f_{III}(\vec{p}_3) f_{IV}(\vec{p}_4) \Big(1 \pm \frac{f_I(\vec{p}_1)}{2h^{-3}} \Big) \Big(1 \pm \frac{f_{II}(\vec{p}_2)}{2h^{-3}} \Big)$$

$$- W_{(12|34)} f_I(\vec{p}_1) f_{II}(\vec{p}_2) \Big(1 \pm \frac{f_{III}(\vec{p}_3)}{2h^{-3}} \Big) \Big(1 \pm \frac{f_{IV}(\vec{p}_4)}{2h^{-3}} \Big) \Big]$$

for all 4+ collision integral estimations – avoid recalculations

$$W_{(12|34)} = \frac{\hbar^2 c^6}{(2\pi)^2} \frac{|M|^2}{16\varepsilon_1\varepsilon_2\varepsilon_3\varepsilon_4} \delta(\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \varepsilon_4) \delta^3(\vec{p}_1 + \vec{p}_2 - \vec{p}_3 - \vec{p}_4)$$

M.A. Prakapenia, I.A. Siutsou, G.V. Vereshchagin. DOI 10.1016/j.jcp.2018.07.010
Journal of Computational Physics, 373(2018) 533, arXiv:1801.02408

Particle splitting technique

W's include δ-functions related to the conservation laws of energy-momentum, they should be represented by special treatment

As distribution function in every phase space cell is prescribed to be a constant, naive scheme of putting final particles into the cells where they just fall violates energy and momentum conservation

We can join the problems to solve them –
δ-functions can be represented by an interpolation scheme, effectively splitting final particles into several adjacent cells so that conservation laws are satisfied (proposed by A. Aksenov)

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Particle splitting example

In the case of symmetries some components of momentum conservation law are satisfied automatically

Spherical symmetry nullifies all 3 average momentum components $\Rightarrow$ only energy conservation should be treated

For the grid of central energies of cells $\{\varepsilon_i\}$ we get with $\varepsilon_{k+1} > \varepsilon \geq \varepsilon_k$

$$\delta(\varepsilon - \varepsilon^*) \quad \rightarrow \quad D(\varepsilon_i) = \begin{cases} \dfrac{\varepsilon_{k+1} - \varepsilon}{\varepsilon_{k+1} - \varepsilon_k} & \text{for } \varepsilon_k \\ \dfrac{\varepsilon - \varepsilon_k}{\varepsilon_{k+1} - \varepsilon_k} & \text{for } \varepsilon_{k+1} \\ 0 \text{ for all other } \{\varepsilon_i\} \end{cases}$$

Collision integrals in spherical symmetry

Usual approach: $\vec{p} \rightarrow \{\varepsilon, \mu = \cos\theta, \phi\}$, $d^3\vec{p} = c^{-2} p\varepsilon \, d\varepsilon \, d\mu \, d\phi$
and exclude all parameters of the particle III and energy of IV,
parametrizing integrals by directional angles of particle IV μ_4 and ϕ_4

Problem of the usual approach: excluded parameters are not defined uniqely by μ_4 and ϕ_4 – two roots for ε_4, some of them extraneous

Our approach: change of coordinate system for particles III and IV to align z-axis with their total momentum $\vec{p}_t = \vec{p}_3 - \vec{p}_4$ and use as parameters energy and azimuth angle of particle IV ε_4 and ϕ_4

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In preparation

Our approach to integration

$$\delta(\varepsilon_1+\varepsilon_2-\varepsilon_3-\varepsilon_4)\delta^3(\vec{p}_1+\vec{p}_2-\vec{p}_3-\vec{p}_4)=$$
$$\frac{\delta(\varepsilon_3-\varepsilon_3^*)\delta(\mu_3-\mu_3^*)\delta(\phi_3-\phi_3^*)\delta(\mu_4-\mu_4^*)}{p_3 p_4 p_t}$$

ε_4 and ϕ_4 define other parameters in unique way, kinematics gives simply defined limits of integration: all ϕ_4 for $\varepsilon_4 \in (A-B, A+B)$

$$A=\frac{\varepsilon}{2}\left(1-\frac{m_4^2-m_3^2}{P\cdot P}\right), \qquad B=\frac{cp_t}{2}\sqrt{\left(1-\frac{(m_4-m_3)^2}{P\cdot P}\right)\left(1-\frac{(m_4+m_3)^2}{P\cdot P}\right)},$$

$$P\cdot P=\varepsilon^2/c^4-p_t^2/c^2$$

Bad for CM case – produce $0/0$, but of measure 0 (as usual approach)

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Structure of collision coefficients

For U-U equation collision integrals depend on all the particles in reaction $\Rightarrow$ store all the particles

It is enough to split 2 of the final particles (and only final, initial particle spliting leads to negative densities) $\Rightarrow$ it destroys symmetry of direct and inverse reaction and thus gives a cross-check of the scheme accuracy

BE and FD quantum corrections coefficients for splitted particles are taken as min of coefs in cells for splitting (otherwise densities can overcome FD limit)

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Computational complexity

Even in spherically symmetric case – $(3N_\varepsilon)^3$ 2p-interactions and $(3N_\varepsilon)^4$ 3p $\Rightarrow$ $\sim 10^9$ reactions for $N_\varepsilon = 60$ energy cells

Limit of angle integration – is given by the total number of cases needs to be sampled: spherical symmetry use kills 3 angles, amount of work halved by *P*-symmetry of QED and reduced for some reactions even more by particle quantum indistinguishability

Finally $(3N_\varepsilon)^4 \times N_\mu^2 \times N_\phi^2 / 2 \sim 10^9 N_a^4$ $\sim 10^{15}$ vector sets sampled

for $N_a = N_\mu = N_\phi / 2 = 32$ $\Rightarrow$ CPU time needed $\sim 10^9$ s, GPU $\sim 10^{6\div 7}$ s

Double precision is essential for $|M|^2$ calculations

Tests of the code in 2p interactions

$$Q = \frac{1}{n}\sum_{n}\left|1 - P_{calc}/P_{th}\right|$$

Table 2: Values of Q for selected number of angular grid nodes ($a_{max} = 40, k_{max} = 2j_{max}$).

Process/j_{max}	16	32	64	128
CS	0.0855	0.0403	0.0207	0.0145
PA	0.0231	0.00693	0.00313	0.00138
PC	0.146	0.0657	0.0303	0.0116

Table 3: CPU time (in seconds) of each reaction initial angular integration for selected number of angular grid nodes ($a_{max} = 40, k_{max} = 2j_{max}$), and its exponent of computational cost $O(j_{max}^n)$.

Process/j_{max}	16	32	64	128	n
CS	2.215	14.48	113.2	590.1	2.7
PA	2.106	14.73	100.2	543.1	2.7
PC	0.531	3.619	28.82	223.2	2.9
MS	2.418	16.87	130.5	1030	2.9
BS	3.354	22.74	178.6	1113	2.8

GPGPU calculations

Feature list needed

- 64−bit atomic operations (doubles reduction)
- Large number of computing units
- Reasonable price

Best choice for the tight budget:

- AMD Graphic Core Next (GCN) architecture of Tahiti family

(280X, 280, 7990, 7970, 7950, 7870 XT) — 0.75÷2.0 TFLOPS of FP64

Careful error-handling is implemented to overcome known problems

Alternatives:

- Nvidia GeForce Titan series — only Titan (1.5), Titan Black (1.8), Titan Z (2.7) and Titan V (6.1 TFLOPS) — overpriced, hard to find
- AMD GCN of later families — Hawaii, Fiji, Polaris, Vega — 0.4÷1.4 TFLOPS of FP64 — overpriced for the same performance
- Some professional cards, like AMD W9100, W8100, S9150, S10000, Nvidia Tesla K40, K20, V100, Quadro GP100, etc. — 1.2÷7.4 TFLOPS of FP64 — overpriced for the same performance — best for lavish budget

Conclusions

- We constructed and successfully adopted fast numerical scheme for treatment of binary and triple interactions in relativistic plasma in Uehling-Ulenbeck equations

- The scheme implementation in C/C++ will be made available under a free license after some improvements of current realization (several OpenCL devices handling, automatic error correction)

Thank you for your attention

Questions?