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

G. Vereshchagin, A. Aksenov. Relativistic Kinetic Theory. CUP, 2017 C. Cercignani and G.M. Kremer. The Relativistic Boltzmann Equation. Birkhauser, 2012 G. Dimarco and L. Pareschi. Acta Numerica, 23(2014)369 C. Mouhot and L. Pareschi. Mathematics of Computation, 75(2006)1833 R. Yano. Journal of Computational Physics, 330(2017)1010 J. Hu, Q. Li, and L. Pareschi. Journal of Scientific Computing, 62(2015)555 J. Hu and L. Ying. Commun. Math. Sci., 10(2012)989 A.L. Garcia and W. Wagner. Phys. Rev. E 68(2003)056703

$$
J(\vec{p}_1) + H(\vec{p}_2) \leftrightarrow H(\vec{p}_3) + IV(\vec{p}_4)
$$
\n
$$
\dot{f}_I(\vec{p}_1) = \int d^3 \vec{p}_2 d^3 \vec{p}_3 d^3 \vec{p}_4
$$
\n
$$
\times \left[W_{(34|12)} f_{III}(\vec{p}_3) f_{IV}(\vec{p}_4) \left(1 \pm \frac{f_I(\vec{p}_1)}{2h^{-3}} \right) \left(1 \pm \frac{f_{II}(\vec{p}_2)}{2h^{-3}} \right) \right]
$$
\n
$$
- W_{(12|34)} f_I(\vec{p}_1) f_{II}(\vec{p}_2) \left(1 \pm \frac{f_{III}(\vec{p}_3)}{2h^{-3}} \right) \left(1 \pm \frac{f_{IV}(\vec{p}_4)}{2h^{-3}} \right)
$$
\n
$$
\dot{f}_H(\vec{p}_2) = \int d^3 \vec{p}_1 d^3 \vec{p}_3 d^3 \vec{p}_4
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\times \left[W_{(34|12)} f_{III}(\vec{p}_3) f_{IV}(\vec{p}_4) \left(1 \pm \frac{f_I(\vec{p}_1)}{2h^{-3}} \right) \left(1 \pm \frac{f_{II}(\vec{p}_2)}{2h^{-3}} \right) \right]
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- W_{(12|34)} f_I(\vec{p}_1) f_{II}(\vec{p}_2) \left(1 \pm \frac{f_{III}(\vec{p}_3)}{2h^{-3}} \right) \left(1 \pm \frac{f_{IV}(\vec{p}_4)}{2h^{-3}} \right)
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$$
\vdots
$$
\n*E.A. Lehling. Physical Review, 45(1934)917*

E.A. Uehling. Physical Review, 46(1934)917 E.A. Uehling and G.E. Uhlenbeck. Physical Review, 43(1933)552

Discretization of U-U Equations

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

Discretization of U-U Equations
\nIntroducing cells in phase spaces
$$
\vec{p}_i \in \Omega_i^{\alpha}
$$
 we get unification of the RHS
\n
$$
\left\{ \int d^3 \vec{p}_1 \ \dot{f}_1(\vec{p}_1), \int d^3 \vec{p}_2 \ \dot{f}_n(\vec{p}_2), \int d^3 \vec{p}_3 \ \dot{f}_m(\vec{p}_3), \int d^3 \vec{p}_4 \ \dot{f}_m(\vec{p}_4) \right\} =
$$
\n
$$
\int d^3 \vec{p}_1 d^3 \vec{p}_2 d^3 \vec{p}_3 d^3 \vec{p}_4
$$
\n
$$
\times \left[W_{(34|12)} f_{III}(\vec{p}_3) f_{IV}(\vec{p}_4) \left(1 \pm \frac{f_I(\vec{p}_1)}{2h^{-3}} \right) \left(1 \pm \frac{f_{III}(\vec{p}_2)}{2h^{-3}} \right) - W_{(12|34)} f_I(\vec{p}_1) f_{II}(\vec{p}_2) \left(1 \pm \frac{f_{III}(\vec{p}_3)}{2h^{-3}} \right) \left(1 \pm \frac{f_{IV}(\vec{p}_4)}{2h^{-3}} \right) \right]
$$
\nbesides the difference in the integration limits –
\nthat also vanishes in the individual differential terms of integration sums

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Reaction-oriented approach

= use the sums of differential terms

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$\Delta^3 \vec{p}_1 \Delta^3 \vec{p}_2 \Delta^3 \vec{p}_3 \Delta^3 \vec{p}_4 \times \left[W_{(34 12)} f_{III}(\vec{p}_3) f_{IV}(\vec{p}_4) \left(1 \pm \frac{f_I(\vec{p}_1)}{2h^{-3}} \right) \left(1 \pm \frac{f_{II}(\vec{p}_2)}{2h^{-3}} \right) \right]$ \n
- $W_{(12 34)} f_I(\vec{p}_1) f_{II}(\vec{p}_2) \left(1 \pm \frac{f_{III}(\vec{p}_3)}{2h^{-3}} \right) \left[1 \pm \frac{f_{IV}(\vec{p}_4)}{2h^{-3}} \right]$ \n
for all 4+ collision integral estimations – avoid recalculations
$W_{(12 34)} = \frac{\hbar^2 c^6}{(2\pi)^2} \frac{ M ^2}{16\varepsilon_1 \varepsilon_2 \varepsilon_3 \varepsilon_4} \delta(\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \varepsilon_4) \delta^3(\vec{p}_1 + \vec{p}_2 - \vec{p}_3 - \vec{p}_4)$ \n
MA. Prakapenia, I.A. Sittsou, G.V. Vereshchagin. DOI 10.1016/j.jcp.2018.07.010 Journal of Computational Physics, 373(2018) 533, arXiv:1801.02408

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

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

of energy-momentum, they should be represented by special treatment
As distribution function in every phase space cell is prescribed to be W's include δ -functions related to the conservation laws

a constant, naive scheme of put violates energy and momentum conservatio n

Particle splitting techn
W's include δ -functions related to the conservation laws
of energy-momentum, they should be represented by special tre
As distribution function in every phase space cell is prescribed
a const We can join the problems to solve them $-\delta$ -functions can be represented by an interpolation scheme, **Particle splitting techn**
W's include δ -functions related to the conservation laws
of energy-momentum, they should be represented by special tre.
As distribution function in every phase space cell is prescribed a
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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 example

In the case of syn momentum conservation law are satisfied automatically

Spherical symmetry nullifies all 3 average momentum components = only energy conservation should be treated $\mathbf{Example} \text{pponents} \Rightarrow$ $\textbf{exp}(e) \Rightarrow$
 $\varepsilon_{k+1} > \varepsilon \geq \varepsilon_k$ $\mathsf{ample}\Bigg\vert_{\mathcal{E}\geq \mathcal{E}_k}$

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

s vation should b e tre 1 1 1 1 for () () f or 0 for all oth er *k k k k k i k k k i D* + + + + − −− − → = [−]

Collision integrals in spherical symmetry

 $\{\varepsilon,\mu=\cos\theta,\phi\},\ d^3\vec{p}=c^{-2}p\varepsilon$ metry
 $d\phi$
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 \downarrow and ϕ ₄

defined

eous **Collision integrals in spherical sy**

Usual approach: $\vec{p} \rightarrow \{ \varepsilon, \mu = \cos \theta, \phi \}$, $d^3 \vec{p} = c^{-2} p \varepsilon d \varepsilon$

and exclude all parameters of the particle *III* and energy

parametrizing integrals by directional angles of 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 i **integrals in spherical symmetr**
 $\vec{p} \rightarrow \{ \varepsilon, \mu = \cos \theta, \phi \}, d^3 \vec{p} = c^{-2} p \varepsilon \, d \varepsilon \, d \mu \, d \phi$

arameters of the particle *III* and energy of *IV*,

egrals by directional angles of particle *IV* μ_4 and ϕ_4

su **herical symmetry**
 *I*³ $\vec{p} = c^{-2} p \epsilon \, d \epsilon \, d \mu \, d \phi$
 III and energy of *IV*,

les of particle *IV* μ_4 and ϕ_4

parameters are not defined

ome of them extraneous

m for particles *III* and *IV*
 $\vec{p}_t = \vec{p$ grals in spherical symmetry
 $\varepsilon, \mu = \cos \theta, \phi\}$, $d^3 \vec{p} = c^{-2} p \varepsilon \, d \varepsilon \, d \mu \, d \phi$

rs of the particle *III* and energy of *IV*,

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roach: excluded parameters are μ a φ ntegrals in spherical symmetry

→ { $\varepsilon, \mu = \cos \theta, \phi$ }, $d^3 \vec{p} = c^{-2} p \varepsilon d \varepsilon d \mu d \phi$

unneters of the particle III and energy of IV,

rals by directional angles of particle IV μ_4 and ϕ_4

all approach: excluded p **Solutify the Solution State 1**
 A all parameters of the particle *I*
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the usual approach: excluded p

4 and ϕ_4 – two roots for ε_4 , son

th: change of coordinate system

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 $\rightarrow \{ \varepsilon, \mu \}$

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 ϕ_4 – two reads *III* III $d\mu d\phi$
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oach: $\bar{p} \rightarrow \{e, \mu = \cos \theta, \phi\}$, $d^3 \bar{p} = c^2 p e d e d \mu d \phi$

e all parameters of the particle *III* and energy of *IV*,

ing integrals by directional angles of particle *IV* μ_4 and of *IV*,
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{ $\epsilon, \mu = \cos \theta, \phi$ }, $d^3 \vec{p} = c^{-2} p \epsilon \, d \epsilon \, d \mu \, d \phi$

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³, $d^3 \vec{p} = c^{-2} p \epsilon \, d \epsilon \, d \mu \, d$

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<u>um $$ *p p p* erical symmetry
 $\dot{\rho} = c^{-2} p \varepsilon \, d \varepsilon \, d \mu \, d \phi$

and energy of *IV*,

of particle *IV* μ_4 and ϕ_4

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for particles *III* and *IV*
 $= \vec{p}_3 - \vec{p}_4$ and use

article

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

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

> *M.A. Prokopenya, I.A. Siutsou, G.V. Vereshchagin. In preparation*

Our approach to integration

Our approach to integration
\n
$$
\delta(\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \varepsilon_4)\delta^3(\vec{p}_1 + \vec{p}_2 - \vec{p}_3 - \vec{p}_4) =
$$
\n
$$
\frac{\delta(\varepsilon_3 - \varepsilon_3^*)\delta(\mu_3 - \mu_3^*)\delta(\phi_3 - \phi_3^*)\delta(\mu_4 - \mu_4^*)}{p_3 p_4 p_t}
$$
\n
$$
\varepsilon_4 \text{ and } \phi_4 \text{ define other parameters in unique way, kinematics gives simply defined limits of integration: all } \phi_4 \text{ for } \varepsilon_4 \in (A - B, A + B)
$$
\n
$$
A = \frac{\varepsilon}{2} \left(1 - \frac{m_4^2 - m_3^2}{P \cdot P}\right), \qquad B = \frac{cp_t}{2} \sqrt{\left(1 - \frac{(m_4 - m_3)^2}{P \cdot P}\right) \left(1 - \frac{(m_4 + m_3)^2}{P \cdot P}\right)}
$$

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

Our approach to integration

\n
$$
\delta(\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \varepsilon_4) \delta^3(\vec{p}_1 + \vec{p}_2 - \vec{p}_3 - \vec{p}_4) =
$$
\n
$$
\frac{\delta(\varepsilon_3 - \varepsilon_3^*) \delta(\mu_3 - \mu_3^*) \delta(\phi_3 - \phi_3^*) \delta(\mu_4 - \mu_4^*)}{p_3 p_4 p_t}
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$$
\n
$$
P \cdot P = \varepsilon^2 / c^4 - p_t^2 / c^2
$$
\nBad for CM case — produce 0/0, but of measure 0 (as usual approach) as follows:

\n*MA. Prokopenya, I.A. Sittsou, G.V. Vereshchagin. In preparation*

Bad for CM case – produce $0/0$, but of measure 0 (as usual approach) *M.A. Prokopenya, I.A. Siutsou, G.V. Vereshchagin. In preparation*

Structure of collision coefficients

For U-U equation collision integrals depend on
all the particles in reaction \Rightarrow store all the particle \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 a cross-check of the scheme accuracy 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 U-U equa

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are taken as min of coefs in cells for splitting (otherwise densities can overcome FD limit)

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Computational complexity

 $(3N_{\varepsilon})^3$ 2p-in N_{ε} ⁴ 3p \Rightarrow ~10⁹ reactions for N_{ε} = 60 energy cells

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

Limit of angle integration $-$ is given by the total number of cases

needs to be sampled: sphe Even in spheri
 $(3N_{\varepsilon})^4$ 3p \Rightarrow

Limit of angle

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Finally $(3N_{\varepsilon})^4$

for $N - N -$ **Computational comple:**

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

Limit of angle integration $-$ is given by the total number of cases

nee needs to be sampled: spherical symmetry use kills 3 angles, Limit of angle integration $-$ is given by the total number of cases **Computatio**

ically symmetric case $- (3N_c)^3$
 $\sim 10^9$ reactions for $N_s = 60$ energence

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impled: spherical symmetry use kompled: spherical symmetry of QED

tions even more by particle for some reactions even more by particle quantum indistinguishability **Computatior**

Even in spherically symmetric case $-(3N_c)^3 2$ **r**
 $(3N_c)^4 3p \Rightarrow -10^9$ reactions for $N_c = 60$ energ

Limit of angle integration – is given by the total

needs to be sampled: spherical symmetry use kill

amoun amount of work halved by *P*-symmetry of QED and reduced **Computational complexity**

pherically symmetric case $- (3N_s)^3$ 2p-interactions and
 $\Rightarrow -10^9$ reactions for $N_c = 60$ energy cells

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Exactions and

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case $- (3N_s)^3$ 2p-interaction

s for $N_s = 60$ energy cells

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symmetry of QED and reduced

by particle quantum indistingu

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

Limit of angle integration – is given by the total number of cases

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ds to be sampled: spherical symmetry use kind out of **Computational complexity**

a spherically symmetric case $-(3N_s)^3$ 2p-interactions and
 $3p \Rightarrow -10^9$ reactions for $N_s = 60$ energy cells

of angle integration – is given by the total number of cases

o be sampled: spherical

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

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

Tests of the code in 2p interactions 1∇ **ode in 2p**
 $1-P_{calc}/P_{th}$
angular grid nodes (a₁ $n \leftarrow \frac{1}{n}$ The code in 2p in
 $Q = \frac{1}{n} \sum_{n} |1 - P_{calc} / P_{th}|$

Ped number of angular grid nodes (a_{max} = the code in 2p interactions
= $\frac{1}{n} \sum_{n} |1 - P_{calc} / P_{th}|$
umber of angular grid nodes (a_{max} = 40, k_{max} = 2j_{max}).

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 $O(j_{max}^n)$.

$\mathrm{Process}/j_{max}$	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 $(280X, 280, 7990, 7970, 7950, 7870 XY)$ $- 0.75 \div 2.0$ 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 $0.4 \div 1.4$ 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?