An application of the discontinuous Galerkin method for solving kinetic equations

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6. The nonlinear Boltzmann equation
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Introduction
In recent years, deterministic solvers to the Boltzmann or similar kinetic equations were considered in the literature. These methods provide accurate results which, in general, agree well with those obtained from DSMC simulations, sometimes at a comparable or even less computational time. Here, I wish to show some simulation results (also, in collaboration with Irene Gamba, Chi-Wang Shu and Yingda Chen) to demonstrate the performance of solvers based on the Discontinuous Galerkin (DG) method.
Keywords: kinetic equation, discontinuous Galerkin

- W. H. Reed, Report Los Alamos LA-UR-73-479 (1973)
A. A. Alexeenko, C. Galitzine and A. M. Alekseenko, 40th Thermophysics Conference (2008)
A. M., Kinetic and Related models (2011)
....... and other papers
A kinetic equation

\[ \frac{\partial f}{\partial t} + \eta(v) \cdot \nabla_x f + A(t, x) \cdot \nabla_v f = C(f) + S(t, x, v), \]  

(1)

where,

- \( f = f(t, x, v) \) is the distribution function - the unknown -,
- \( \eta \) is a given vectorial function of the velocity \( v \),
- \( A \) is given or related to another equation, for instance, the Poisson equation,
- \( C(f) \) is the linear or nonlinear collision operator, and
- \( S(t, x, v) \) is the source term.
We denote by \( \Omega_v \in \mathbb{R}^d (d = 1, 2, 3) \) the domain of the velocity. If the set \( \Omega_v \) is not bounded, it is necessary to choose a new reasonable large but bounded subset of \( \Omega_v \) and modify the collision operator \( C \) in order to avoid that particles, having velocities belonging to this new set, after the collision, assume velocities outside this set. We assume that \( \Omega_v \) is bounded, and the distribution function \( f \) vanishes on the boundary of \( \Omega_v \).

The physical domain depends on the problem, strongly. Moreover, in order to solve the kinetic equation, we need to assume initial and boundary conditions.
The DG method allows to find approximate solutions of the kinetic equation by solving a (usually large) set of ordinary differential equations in time. Then, we easily derive an approximation of the distribution function $f$ and we can evaluate its moments.

There are some reasons to introduce an intermediate step.

- the variables $x$ and $v$ have a different physical meaning, and, usually, we are interested in the main moments of $f$ instead of $f$ itself;
- usually, the boundary conditions on $\partial \Omega_v$ do not change.
Therefore, we discretize the kinetic equation with respect only to the velocity variable $\mathbf{v}$ and we obtain a set of equations, where the new unknowns depend only on the time $t$ and the spatial coordinates $\mathbf{x}$.

To this scope, we introduce a partition of the set $\Omega_v$, by means of a finite family of open cells $C_\alpha$, such that

$$C_\alpha \subseteq \Omega_v \quad \forall \alpha, \quad C_\alpha \cap C_\beta = \emptyset \quad \forall \alpha \neq \beta, \quad \bigcup_{\alpha=1}^{N} C_\alpha = \Omega_v.$$  

Remark: No restriction on the partition.
An example of a grid in two-dimensional velocity space.
DG assumption

We choose in each cell $C_\alpha$ a finite dimensional vector space $\mathcal{V}_\alpha$ of function of $v$ defined in $C_\alpha$, and we assume that, in $C_\alpha$, the distribution function $f$ can be approximated by means a linear combination of elements of $\mathcal{V}_\alpha$ with coefficients depending on space and time.

*These coefficients are the new unknowns.*

For instance, if the basis of $\mathcal{V}_\alpha$ is the set $\{1, v, v^2\}$, then

$$f(t, x, v) \approx a_\alpha(t, x) + b_\alpha(t, x) \cdot v + c_\alpha(t, x) v^2 \quad \forall v \in C_\alpha \text{ and } \forall t, x.$$

Remark: We can change vector space from a cell to another.
To make clear the application of DG method, we consider the linear kinetic equation

\[
\frac{\partial f}{\partial t} + \eta(v) \cdot \nabla_x f + A(t, x) \cdot \nabla_v f
\]

\[
= \int_{\Omega_v} \left[ K(v', v) f' - K(v, v') f \right] dv' + S(t, x, v). \tag{2}
\]

Here, \( K(v', v) \) is the kernel of the integral operator and, as usual, \( f' = f(t, x, v') \).
If \( \{ \psi_{\alpha,i}(v) : i = 1, \ldots, n_{\alpha} \} \) is the basis of the vector space \( V_{\alpha} \), then in the cell \( C_{\alpha} \) we have

\[
f(t, x, v) \approx \sum_{i=1}^{n_{\alpha}} f_{\alpha,i}(t, x) \psi_{\alpha,i}(v).
\] (3)

Now, if we multiply both sides of the equation by \( \psi_{\alpha,k}(v) \) and integrate in \( C_{\alpha} \) we obtain the exact equation

\[
\frac{\partial}{\partial t} \int_{C_{\alpha}} f(t, x, v) \psi_{\alpha,k}(v) \, dv + \nabla_x \int_{C_{\alpha}} \eta(v) f(t, x, v) \psi_{\alpha,k}(v) \, dv
\]
\[
+ A(t, x) \cdot \int_{C_{\alpha}} [\nabla_v f(t, x, v)] \psi_{\alpha,k}(v) \, dv = \int_{C_{\alpha}} S(t, x, v) \psi_{\alpha,k}(v) \, dv
\]
\[
+ \int_{C_{\alpha}} \left[ \int_{\Omega_v} [K(v', v) f(t, x, v') - K(v, v') f(t, x, v)] \, dv' \right] \psi_{\alpha,k}(v) \, dv \].
\] (4)
The approximation is introduced using Eq. (3). So, for instance, we have

\[
\frac{\partial}{\partial t} \int_{C_\alpha} f(t, x, v) \psi_{\alpha,k}(v) \, dv \approx \sum_{i=1}^{n_\alpha} \left[ \int_{C_\alpha} \psi_{\alpha,i}(v) \psi_{\alpha,k}(v) \, dv \right] \frac{\partial f_{\alpha,i}(t, x)}{\partial t}
\]

\[
\nabla_x \int_{C_\alpha} \eta(v) f(t, x, v) \psi_{\alpha,k}(v) \, dv \approx \sum_{i=1}^{n_\alpha} \left[ \int_{C_\alpha} \eta(v) \psi_{\alpha,i}(v) \psi_{\alpha,k}(v) \, dv \right] \nabla_x f_{\alpha,i}(t, x)
\]

We note that the coefficients of the partial derivatives in the r.h.s are \textit{numerical constant parameters}.

We show the complete equation in the simplest case: \( n_\alpha = 1 \) and \( \psi_{\alpha,1}(v) = 1 \).
Now, we have

\[
M_{\alpha} \frac{\partial f_{\alpha}}{\partial t} + \left[ \int_{C_\alpha} \eta(v) \, dv \right] \cdot \nabla_x f_{\alpha} + A(t, x) \cdot \left[ \int_{\partial C_\alpha} f(t, x, v) \, n \, d\sigma \right] \\
\approx \sum_{\beta=1}^{N} \left[ \int_{C_\alpha} \int_{C_{\beta}} d\nu \int_{C_{\beta}} d\nu' K(\nu', \nu) \right] f_{\beta} - \left[ \int_{C_\alpha} \int_{\Omega_v} d\nu \int_{\Omega_v} d\nu' K(\nu, \nu') \right] f_{\alpha} \\
+ \int_{C_\alpha} S(t, x, v) \, dv ,
\]

(5)

where \( M_{\alpha} \) is the measure of the cell \( C_\alpha \).

In order to have only the unknowns \( f_{\alpha}(t, x) \) in Eq. (5), we must find, for fixed \( t \) and \( x \), a suitable relationship between the value of the distribution function \( f \) on boundary of the cell \( C_\alpha \) and the new unknowns.

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Hence, we have a set of partial differential equations, which can be solved applying again the DG method or another technique.
The Boltzmann equation for an electron gas in a semiconductor

\[ \frac{\partial f}{\partial t} + \frac{1}{\hbar} \nabla_k \varepsilon \cdot \nabla_x f - \frac{q}{\hbar} \mathbf{E} \cdot \nabla_k f = Q(f). \]

- \( \hbar \) is the Planck constant divided by \( 2\pi \)
- \( \nabla_k \) is the gradient with respect to the wave vector \( \mathbf{k} \)
- \( \nabla_x \) is the gradient with respect to the space coordinates \( \mathbf{x} \)
- \( q \) is the positive electric charge
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The Transport Equation: the electron energy

\[
\frac{\partial f}{\partial t} + \frac{1}{\hbar} \nabla_k \epsilon \cdot \nabla_x f - \frac{q}{\hbar} \mathbf{E} \cdot \nabla_k f = Q(f).
\]

If the Kane model is assumed, then the electron energy is

\[
\epsilon(k) = \frac{1}{1 + \sqrt{1 + 2 \frac{\tilde{\alpha}}{m^*} \frac{\hbar^2}{|k|^2} |k|^2}} \frac{\hbar^2}{m^*} |k|^2.
\]

- \(m^*\) is the effective electron mass
- \(\tilde{\alpha}\) is the nonparabolicity factor
The Boltzmann-Poisson System

\[
\frac{\partial f}{\partial t} + \frac{1}{\hbar} \nabla_k \varepsilon \cdot \nabla_x f - \frac{q}{\hbar} \mathbf{E} \cdot \nabla_k f = Q(f).
\]

The electric field \( \mathbf{E} \) satisfies the Poisson equation

\[
\nabla_x (\varepsilon \nabla_x V) = q \left[ n(t, \mathbf{x}) - N_D(\mathbf{x}) \right], \quad \mathbf{E} = -\nabla_x V
\]
\nabla_x (\epsilon \nabla_x V) = q [n(t, x) - N_D(x)], \quad E = -\nabla_x V

- \textbf{V} is the electric potential
- \( \epsilon(x) \) is the permittivity
- \( n(t, x) = \int_{\mathbb{R}^3} f(t, x, k) \, dk \) is the charge density
- \( N_D(x) \) is the doping.
\[ \nabla_x (\epsilon \nabla_x V) = q [n(t, x) - N_D(x)] , \quad \mathbf{E} = -\nabla_x V \]

- \( V \) is the electric potential
- \( \epsilon(x) \) is the permittivity
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- $V$ is the electric potential
- $\epsilon(x)$ is the permittivity
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- $N_D(x)$ is the doping.
The Boltzmann equation
\[
\frac{\partial f}{\partial t} + \frac{1}{\hbar} \nabla_k \varepsilon \cdot \nabla_x f - \frac{q}{\hbar} \mathbf{E} \cdot \nabla_k f = Q(f).
\]

The collision operator
\[
Q(f)(t, \mathbf{x}, \mathbf{k}) = \int_{\mathbb{R}^3} \left[ S(k', \mathbf{k}) f(t, \mathbf{x}, k') - S(k, k') f(t, \mathbf{x}, \mathbf{k}) \right] dk'.
\]
The Boltzmann-Poisson Problem

\[ \frac{\partial f}{\partial t} + \frac{1}{\hbar} \nabla_k \epsilon \cdot \nabla_x f - \frac{q}{\hbar} E \cdot \nabla_k f = Q(f). \]  \hspace{1cm} (6)

\[ \nabla_x (\epsilon \nabla_x V) = q [n(t, x) - N_D(x)] , \hspace{1cm} E = -\nabla_x V \]  \hspace{1cm} (7)

and initial and boundary conditions.
The one dimensional silicon $n^+ - n - n^+$ 50nm channel diode, where the doping $N_D = 5 \times 10^{18} \text{ cm}^{-3}$ in the $n^+$ and $N_D = 1 \times 10^{15} \text{ cm}^{-3}$ in the $n$ region. We use an unstructured grid: $64 \times 60 \times 20$. 
The diode

Numerical examples

Density of charge (cm$^{-3}$) at $t = 3.0$ ps

DSMC BTE (DG)
mean velocity
(cm s$^{-1}$)
at $t = 3.0$ ps

DSMC
BTE (DG)
Numerical examples

The diode

<table>
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<th>x</th>
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<tr>
<td>0.05</td>
<td>6E+24</td>
</tr>
<tr>
<td>0.1</td>
<td>7.5E+24</td>
</tr>
<tr>
<td>0.15</td>
<td>9E+24</td>
</tr>
<tr>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>0.25</td>
<td></td>
</tr>
</tbody>
</table>

momentum (cm$^{-2}$ s$^{-1}$) at $t = 3.0$ ps

DSMC
BTE (DG)

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DG method & kinetic equations
Numerical examples

The diode

mean energy (eV) at $t = 3.0$ ps

DSMC
BTE (DG)
An example of simulation of a 2D device (3D in velocity).
The double gate MOSFET

Grid: $24 \times 12 \times 24 \times 8 \times 6 = 331776$
Numerical examples

The double gate MOSFET

density of charge (cm$^{-3}$)
Numerical examples

The double gate MOSFET

x-component of the mean velocity (cm s\(^{-1}\))
Numerical examples

The double gate MOSFET

y-component of the mean velocity (cm s$^{-1}$)

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Numerical examples

The double gate MOSFET

energy (eV)

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DG method & kinetic equations
Here, we have a one dimensional silicon $n^+ - n - n^+ 0.4 \mu m$ channel diode, where the doping $N_D = 5 \times 10^{17} \text{ cm}^{-3}$ in the $n^+$ and $N_D = 2 \times 10^{15} \text{ cm}^{-3}$ in the $n$ region.

We use a regular grid: 120 cells in space and $60 \times 24$ for the velocity. Total number of cells = 172800.
Numerical examples

The diodo: stress tests

density of charge (cm$^{-3}$) at $t = 0.5$ ps
velocity (cm s$^{-1}$) at $t = 0.5$ ps
energy (eV) at $t = 0.5$ ps
Positivity.

$$10^{-3} \geq \# f > 10^{-4}, \; 10^{-4} \geq \# f > 10^{-5}, \ldots$$
Numerical examples

The diodo: stress tests

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DG method & kinetic equations
Numerical examples

The diodo: stress tests

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DG method & kinetic equations
The radiative transport equation

\[ \frac{1}{v} \partial_t l(t, \mathbf{x}, \Omega) + \Omega \cdot \nabla_{\mathbf{x}} l(t, \mathbf{x}, \Omega) = -\mu_t(\mathbf{x}) l(t, \mathbf{x}, \Omega) + \mu_s(\mathbf{x}) \int_{S^{n-1}} K(\Omega, \Omega') l(t, \mathbf{x}, \Omega') \, d\Omega' + S(t, \mathbf{x}, \Omega), \quad (8) \]

where \( l \) represents the energy density, or intensity, at each position \( \mathbf{x} \), unit direction \( \Omega \) and time \( t \).

\( v \) is the constant wave speed and \( S \) accounts for any sources within the medium.

The total scattering coefficient \( \mu_t = \mu_s + \mu_a \) is the sum of the scattering coefficient \( \mu_s \) and the absorption coefficient \( \mu_a \), and \( S^{n-1} \) denotes the unit circle in 2D problems \((n = 2)\) and the unit sphere in 3D problems \((n = 3)\).
We consider the 2D domain

\[ D = \left\{ (x, y) \in \mathbb{R}^2 : |x| \leq 1.5 \text{ and } |y| \leq 1.5 \right\}. \]

Here, \( \Omega = (\cos(\theta), \sin(\theta)) \).

The boundary condition is

\[ I(x_b, y_b, \theta) = 0 \quad \text{on} \quad \Gamma_{in} = \{ \partial D \times [0, 2\pi] \text{ s.t. } n(x_b, y_b) \cdot \theta < 0 \}. \]

Moreover,

\[ S(x, y, \theta) = \frac{2}{\pi} e^{-2(x^2 + y^2)}, \]

\[ K(\theta, \theta') = \frac{1}{2\pi} \frac{1 - g^2}{1 + g^2 - 2 \cos(\theta - \theta')} \quad (g = 0.9). \]

Grid: 16x16x19 = 4864.
the intensity distribution in direction $\theta = \pi$. 
The radiative transport equation

2D test problem

the total intensity.
The Boltzmann equation

\[ \frac{\partial f}{\partial t} + \xi \cdot \frac{\partial f}{\partial x} = Q(f, f). \quad (9) \]

The collision operator is

\[ Q(f, f) = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} W(\xi, \xi* | \xi', \xi*) (f' f' - ff*) \, d\xi \, d\xi' \, d\xi*. \]

where the kernel \( W \) is defined by

\[ W(\xi, \xi* | \xi', \xi*) = K(n \cdot V, |V|) \delta(\xi + \xi* - \xi' - \xi*) \delta(|\xi|^2 + |\xi*|^2 - |\xi'|^2 - |\xi*|^2). \]

The function \( K(n \cdot V, |V|) \) is related to the interaction law between colliding particles, with

\[ n = \frac{\xi - \xi'}{|\xi - \xi'|} \quad \text{and} \quad V = \xi - \xi*. \]
We apply the discontinuous Galerkin method to the Boltzmann equation (9) using in every cell the same basis \( \{1, \xi, \xi^2\} \). This guarantees the conservation of mass, momentum and energy for homogeneous solutions.
The nonlinear Boltzmann equation

$f$ versus $|\xi|$ at time $t = 0$. 

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The nonlinear Boltzmann equation

\[ f \text{ versus } |\xi| \text{ (transient)}. \]
The nonlinear Boltzmann equation

$f$ versus $|\xi|$ at time $t = 0.05$. 

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DG method & kinetic equations
\[ \int f \log f \, d\xi \] versus time.
Thank you for your attention
V.V. Aristov,

C. Cercignani,

C. Cercignani,

Valmor F. de Almeida
L. L. Baker and N. G. Hadjiconstantinou, 

Y. Cheng, I. M. Gamba, A. Majorana and C.-W. Shu, 

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*A numerical model of the Boltzmann equation related to the discontinuous Galerkin method*, Kinetic and Related models, **4** (2011), 139–151.