An application of the discontinuous Galerkin method for solving kinetic equations

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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

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A kinetic equation

$$\frac{\partial f}{\partial t} + \eta(\mathbf{v}) \cdot \nabla_{\mathbf{x}} f + \mathbf{A}(t, \mathbf{x}) \cdot \nabla_{\mathbf{v}} f = C(f) + S(t, \mathbf{x}, \mathbf{v}) \,, \tag{1}$$

where,

- $f = f(t, \mathbf{x}, \mathbf{v})$ is the distribution function - the unknown -,
- η is a given vectorial function of the velocity $\mathbf{v}$,
- $\mathbf{A}$ is given or related to another equation, for instance, the Poisson equation,
- $C(f)$ is the linear or nonlinear collision operator, and
- $S(t, \mathbf{x}, \mathbf{v})$ is the source term.

We denote by $\Omega_{\mathbf{v}} \in \mathbb{R}^d$ $(d = 1, 2, 3)$ the domain of the velocity.
If the set $\Omega_{\mathbf{v}}$ is not bounded, it is necessary to choose a new reasonable large but bounded subset of $\Omega_{\mathbf{v}}$ 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 $\Omega_{\mathbf{v}}$ is bounded, and the distribution function f vanishes on the boundary of $\Omega_{\mathbf{v}}$.

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.

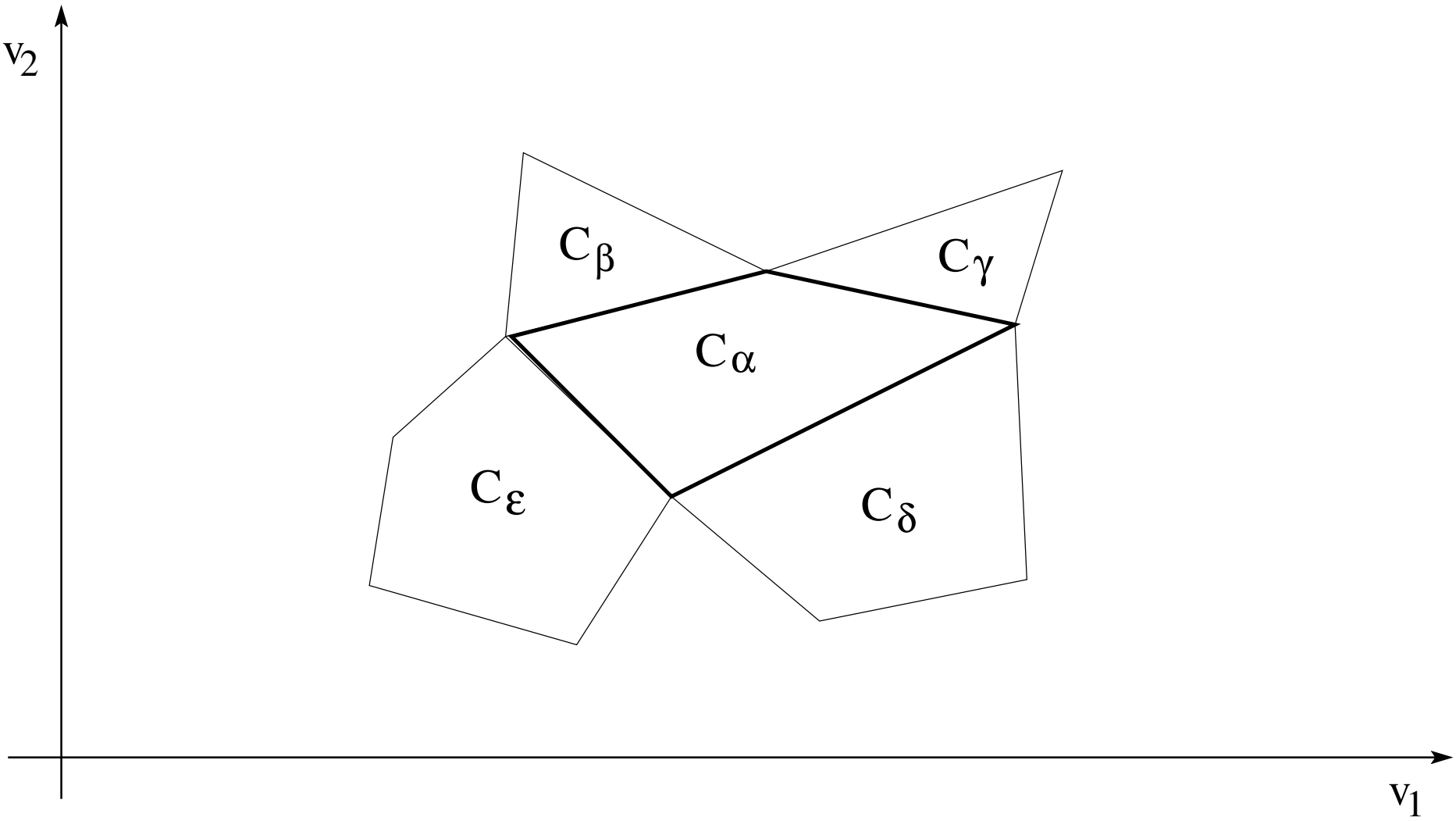
- the variables $\mathbf{x}$ and $\mathbf{v}$ have a different physical meaning, and, usually, we are interested in the main moments of f instead of f itself;
- usually, the boundary conditions on $\partial\Omega_{\mathbf{v}}$ do not change.

Therefore, we discretize the kinetic equation with respect only to the velocity variable **v** and we obtain a set of equations, where the new unknowns depend only on the time t and the spatial coordinates **x**.

To this scope, we introduce a partition of the set $\Omega_{\mathbf{v}}$, by means of a finite family of open cells C_α, such that

$$C_\alpha \subseteq \Omega_{\mathbf{v}} \quad \forall \alpha\,, \qquad C_\alpha \cap C_\beta = \emptyset \quad \forall \alpha \neq \beta\,, \qquad \bigcup_{\alpha=1}^{N} \overline{C_\alpha} = \Omega_{\mathbf{v}}\,.$$

Remark: No restriction on the partition.



An example of a grid in two-dimensional velocity space.

DG assumption

We choose in each cell C_α
a finite dimensional vector space $\mathcal{V}_\alpha$ of function of $\mathbf{v}$ defined in C_α,
and we assume that, in C_α,
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 $\{1, \mathbf{v}, \mathbf{v}^2\}$, then

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

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

$$\frac{\partial f}{\partial t} + \eta(\mathbf{v}) \cdot \nabla_{\mathbf{x}} f + \mathbf{A}(t, \mathbf{x}) \cdot \nabla_{\mathbf{v}} f = \int_{\Omega_{\mathbf{v}}} \left[K(\mathbf{v}', \mathbf{v})\, f' - K(\mathbf{v}, \mathbf{v}')\, f \right] d\mathbf{v}' + S(t, \mathbf{x}, \mathbf{v})\,. \tag{2}$$

Here, $K(\mathbf{v}', \mathbf{v})$ is the kernel of the integral operator and, as usual, $f' = f(t, \mathbf{x}, \mathbf{v}')$.

If $\{\psi_{\alpha,i}(\mathbf{v}) : i = 1, .., n_\alpha\}$ is the basis of the vector space $\mathcal{V}_\alpha$, then in the cell C_α we have

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

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

$$\frac{\partial}{\partial t}\int_{C_\alpha} f(t, \mathbf{x}, \mathbf{v})\, \psi_{\alpha,k}(\mathbf{v})\, d\mathbf{v} + \nabla_{\mathbf{x}} \int_{C_\alpha} \eta(\mathbf{v})\, f(t, \mathbf{x}, \mathbf{v})\, \psi_{\alpha,k}(\mathbf{v})\, d\mathbf{v}$$

$$+ \mathbf{A}(t, \mathbf{x}) \cdot \int_{C_\alpha} [\nabla_{\mathbf{v}} f(t, \mathbf{x}, \mathbf{v})]\, \psi_{\alpha,k}(\mathbf{v})\, d\mathbf{v} = \int_{C_\alpha} S(t, \mathbf{x}, \mathbf{v})\, \psi_{\alpha,k}(\mathbf{v})\, d\mathbf{v}$$

$$+ \int_{C_\alpha} \left[\int_{\Omega_{\mathbf{v}}} \left[K(\mathbf{v}', \mathbf{v})\, f(t, \mathbf{x}, \mathbf{v}') - K(\mathbf{v}, \mathbf{v}')\, f(t, \mathbf{x}, \mathbf{v}) \right] d\mathbf{v}' \right] \psi_{\alpha,k}(\mathbf{v})\, d\mathbf{v}\,. \tag{4}$$

The approximation is introduced using Eq, (3). So, for instance, we have

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

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

We note that the coefficients of the partial derivatives in the r.h.s are *numerical constant parameters.*

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

Now, we have

$$
\begin{aligned}
& M_\alpha \frac{\partial f_\alpha}{\partial t} + \left[\int_{C_\alpha} \eta(\mathbf{v})\, d\mathbf{v} \right] \cdot \nabla_{\mathbf{x}} f_\alpha + \mathbf{A}(t,\mathbf{x}) \cdot \left[\int_{\partial C_\alpha} f(t,\mathbf{x},\mathbf{v})\, \mathbf{n}\, d\sigma \right] \\
& \approx \sum_{\beta=1}^{N} \left[\int_{C_\alpha} d\mathbf{v} \int_{C_\beta} d\mathbf{v}'\, K(\mathbf{v}',\mathbf{v}) \right] f_\beta - \left[\int_{C_\alpha} d\mathbf{v} \int_{\Omega_{\mathbf{v}}} d\mathbf{v}' K(\mathbf{v},\mathbf{v}') \right] f_\alpha \\
& + \int_{C_\alpha} S(t,\mathbf{x},\mathbf{v})\, d\mathbf{v}\,, \qquad (5)
\end{aligned}
$$

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

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

$$\frac{\partial f}{\partial t} + \frac{1}{\hbar}\nabla_{\mathbf{k}}\varepsilon \cdot \nabla_{\mathbf{x}} f - \frac{q}{\hbar}\mathbf{E} \cdot \nabla_{\mathbf{k}} f = Q(f).$$

- $\hbar$ is the Planck constant divided by 2π
- $\nabla_{\mathbf{k}}$ is the gradient with respect to the wave vector $\mathbf{k}$
- $\nabla_{\mathbf{x}}$ is the gradient with respect to the space coordinates $\mathbf{x}$
- q is the positive electric charge

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

$$\varepsilon(\mathbf{k}) = \frac{1}{1 + \sqrt{1 + 2\,\frac{\tilde{\alpha}}{m^*}\hbar^2\,|\mathbf{k}|^2}}\,\frac{\hbar^2}{m^*}\,|\mathbf{k}|^2 \quad .$$

- m^* is the effective electron mass
- $\tilde{\alpha}$ is the nonparabolicity factor

$$\frac{\partial f}{\partial t} + \frac{1}{\hbar}\nabla_{\mathbf{k}}\varepsilon \cdot \nabla_{\mathbf{x}} f - \frac{q}{\hbar}\mathbf{E} \cdot \nabla_{\mathbf{k}} f = Q(f).$$

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

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

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- V is the electric potential
- $\epsilon(\mathbf{x})$ is the permittivity
- $n(t,\mathbf{x}) = \int_{\mathbb{R}^3} f(t,\mathbf{x},\mathbf{k})\, d\mathbf{k}$ is the charge density
- $N_D(\mathbf{x})$ is the doping.

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The Boltzmann equation

$$\frac{\partial f}{\partial t} + \frac{1}{\hbar}\nabla_{\mathbf{k}}\varepsilon \cdot \nabla_{\mathbf{x}} f - \frac{q}{\hbar}\mathbf{E} \cdot \nabla_{\mathbf{k}} f = Q(f).$$

The collision operator

$$Q(f)(t,\mathbf{x},\mathbf{k}) = \int_{\mathbb{R}^3} \left[S(\mathbf{k}',\mathbf{k}) f(t,\mathbf{x},\mathbf{k}') - S(\mathbf{k},\mathbf{k}') f(t,\mathbf{x},\mathbf{k}) \right] d\mathbf{k}' .$$

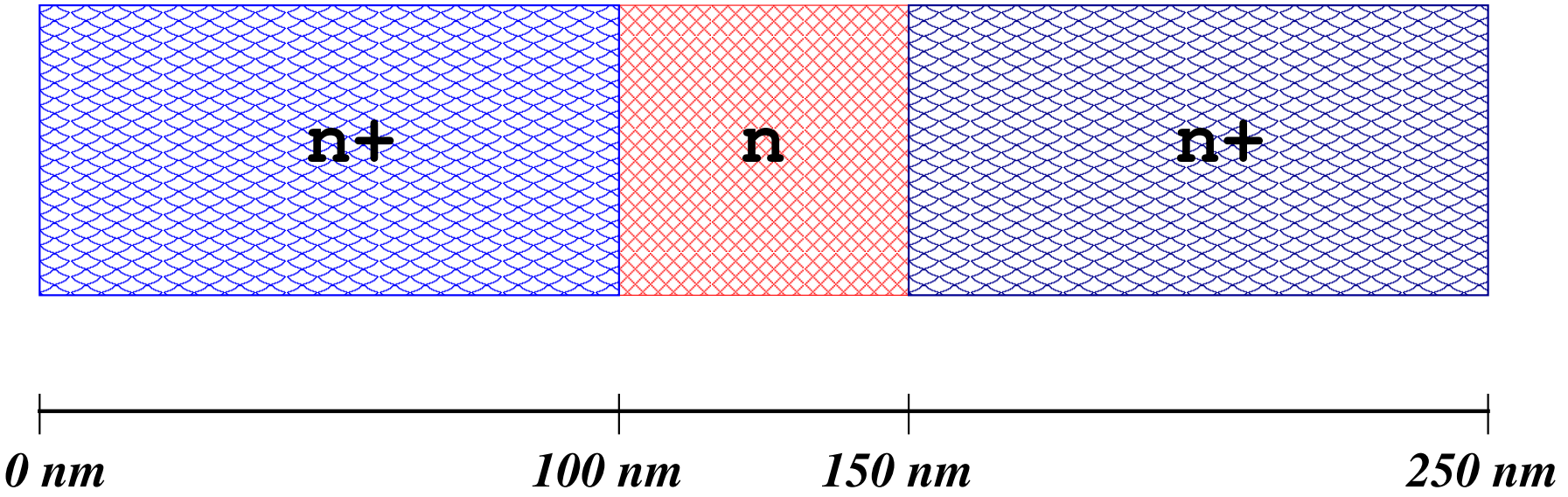
The Boltzmann-Poisson Problem

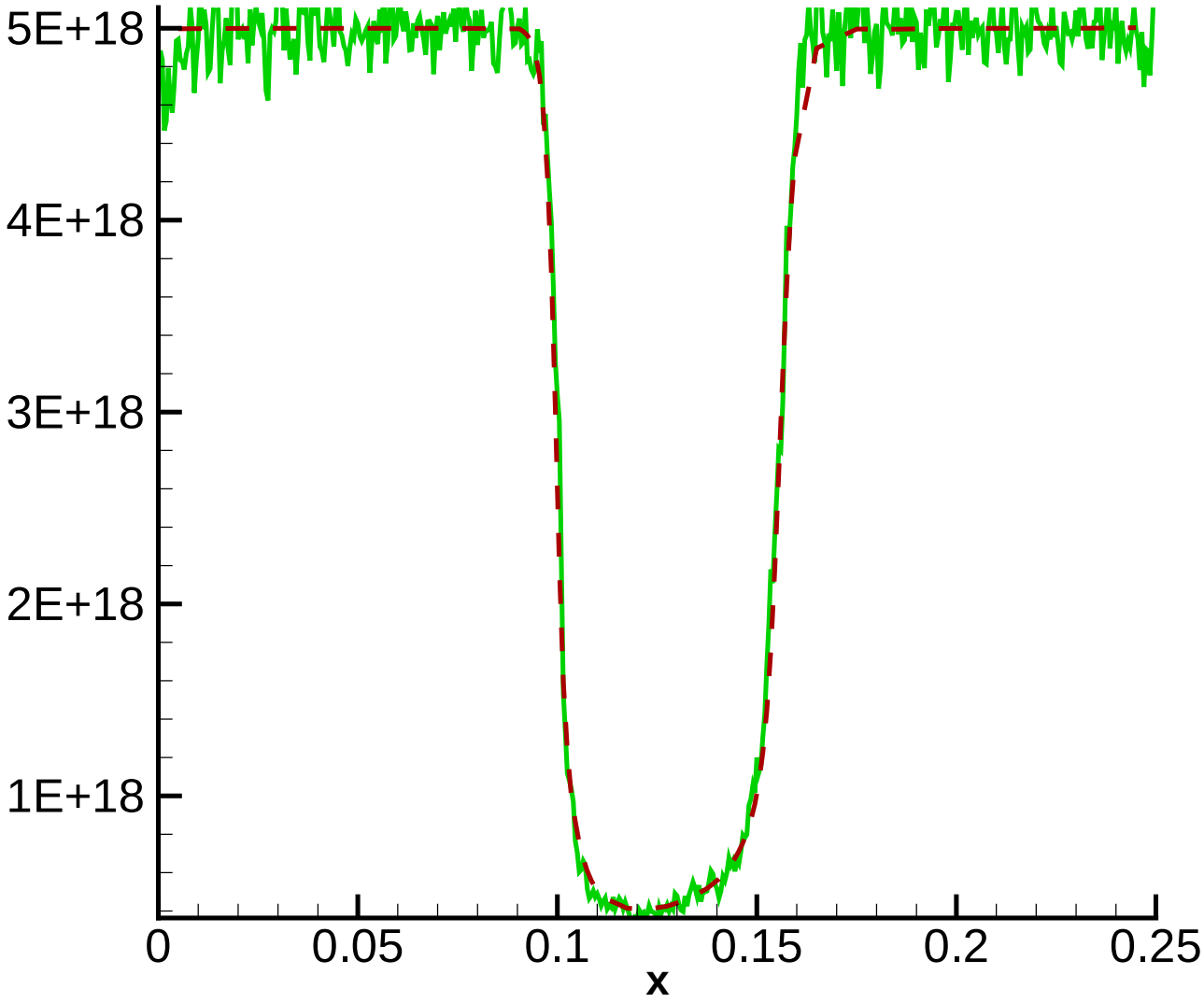
$$\frac{\partial f}{\partial t} + \frac{1}{\hbar}\nabla_{\mathbf{k}}\varepsilon \cdot \nabla_{\mathbf{x}} f - \frac{q}{\hbar}\mathbf{E} \cdot \nabla_{\mathbf{k}} f = Q(f). \tag{6}$$

$$\nabla_{\mathbf{x}}(\epsilon \nabla_{\mathbf{x}} V) = q\left[n(t,\mathbf{x}) - N_D(\mathbf{x})\right], \quad \mathbf{E} = -\nabla_{\mathbf{x}} V \tag{7}$$

and initial and boundary conditions.

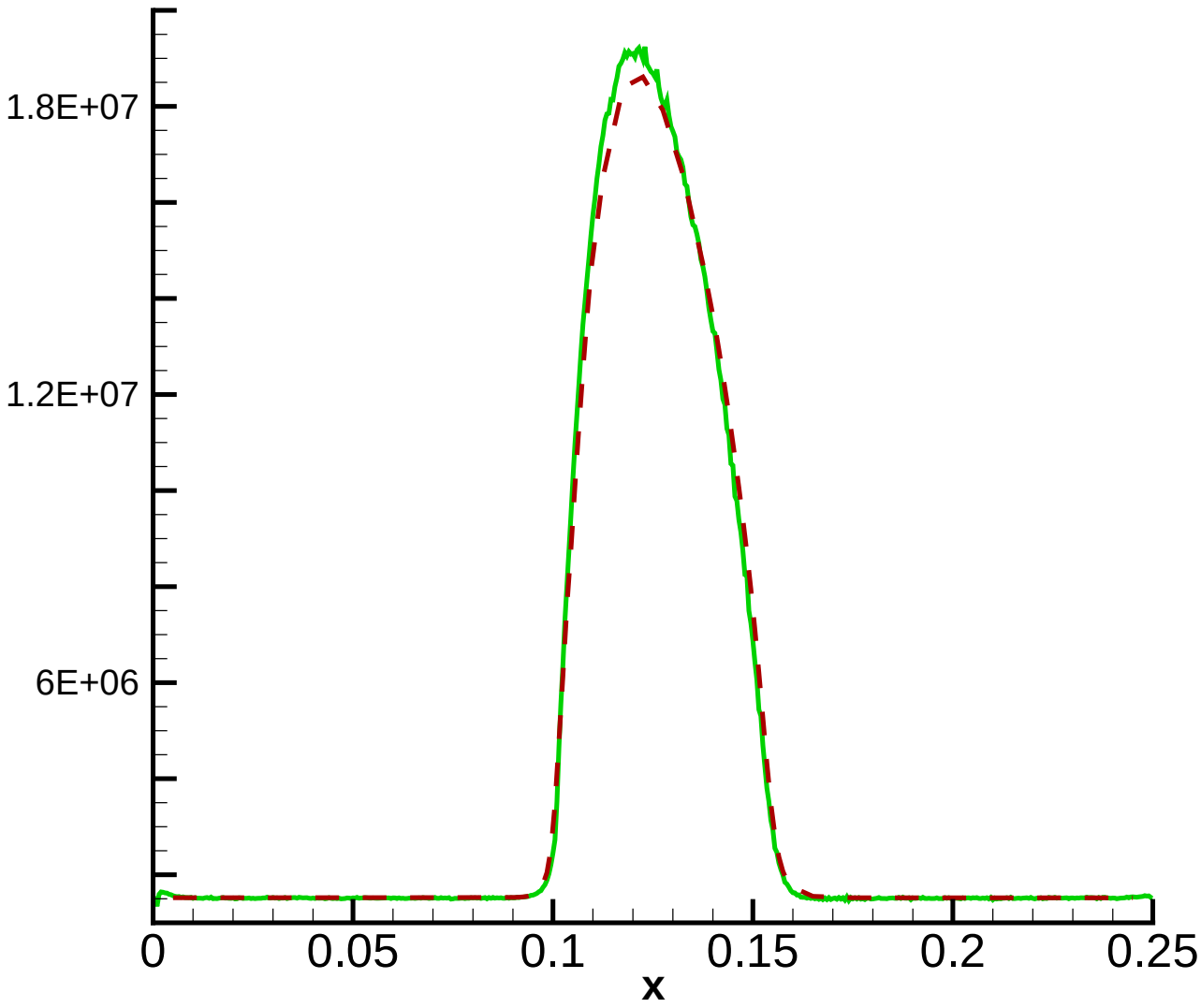
The one dimensional silicon $n^+ - n - n^+$ 50nm channel diode, where the doping $N_D = 5 \times 10^{18}$ cm^{-3} in the n$^+$ and $N_D = 1 \times 10^{15}$ cm^{-3} in the n region. We use an unstructured grid: $64 \times 60 \times 20$.





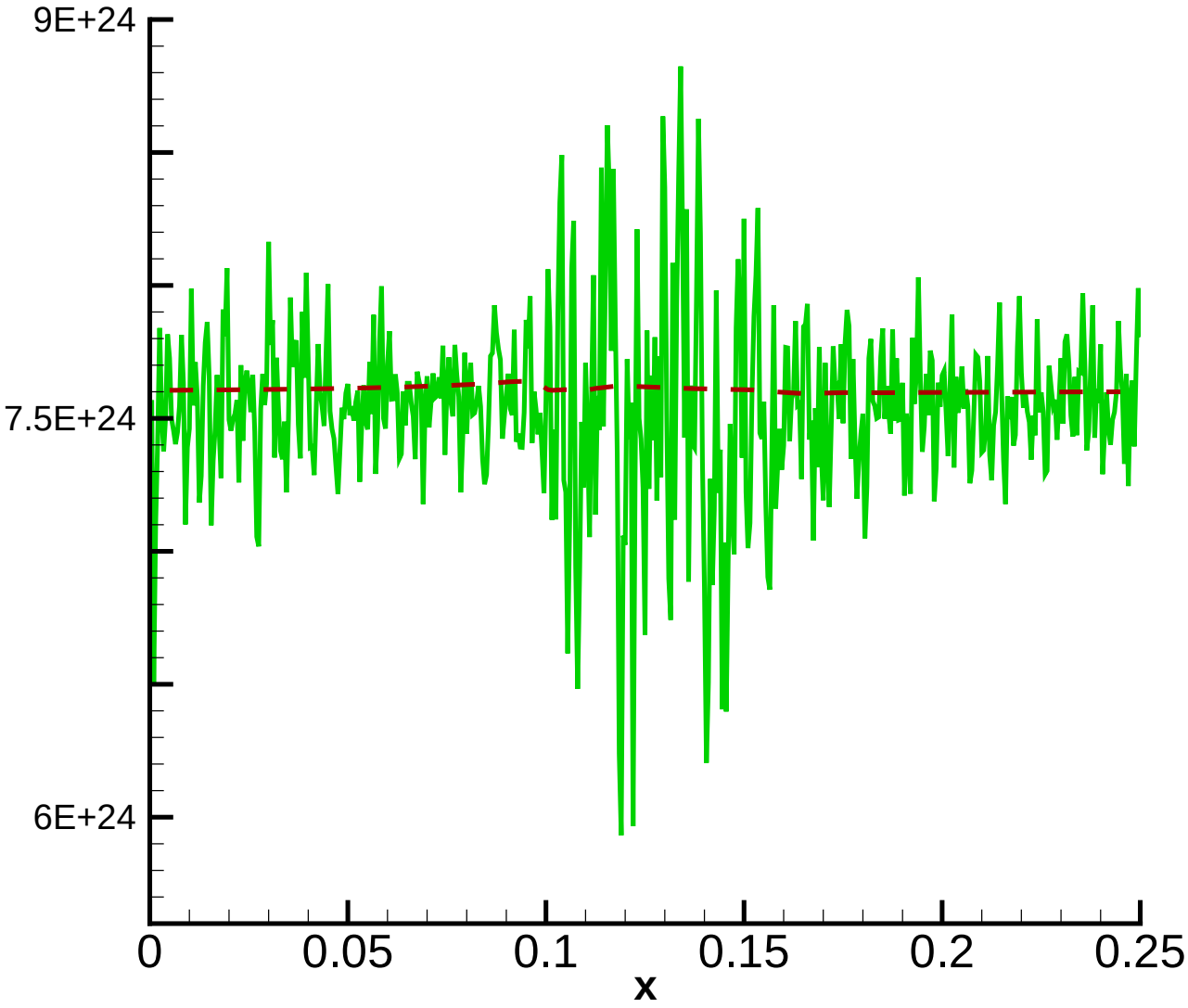
density
of charge
(cm^{-3})
at $t = 3.0$ ps

DSMC
BTE (DG)



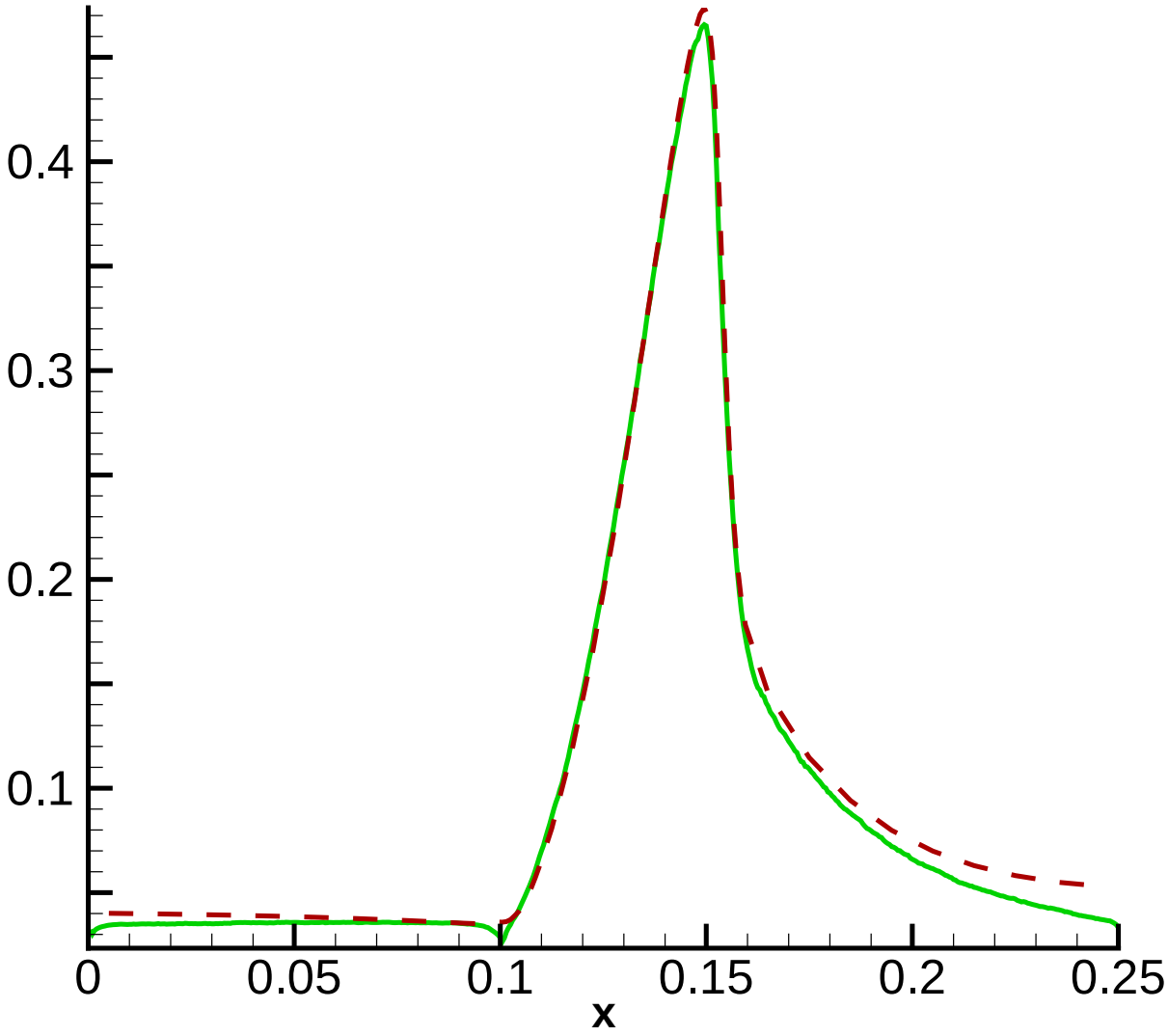
mean velocity
(cm s^{-1})
at $t = 3.0$ ps

DSMC
BTE (DG)



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

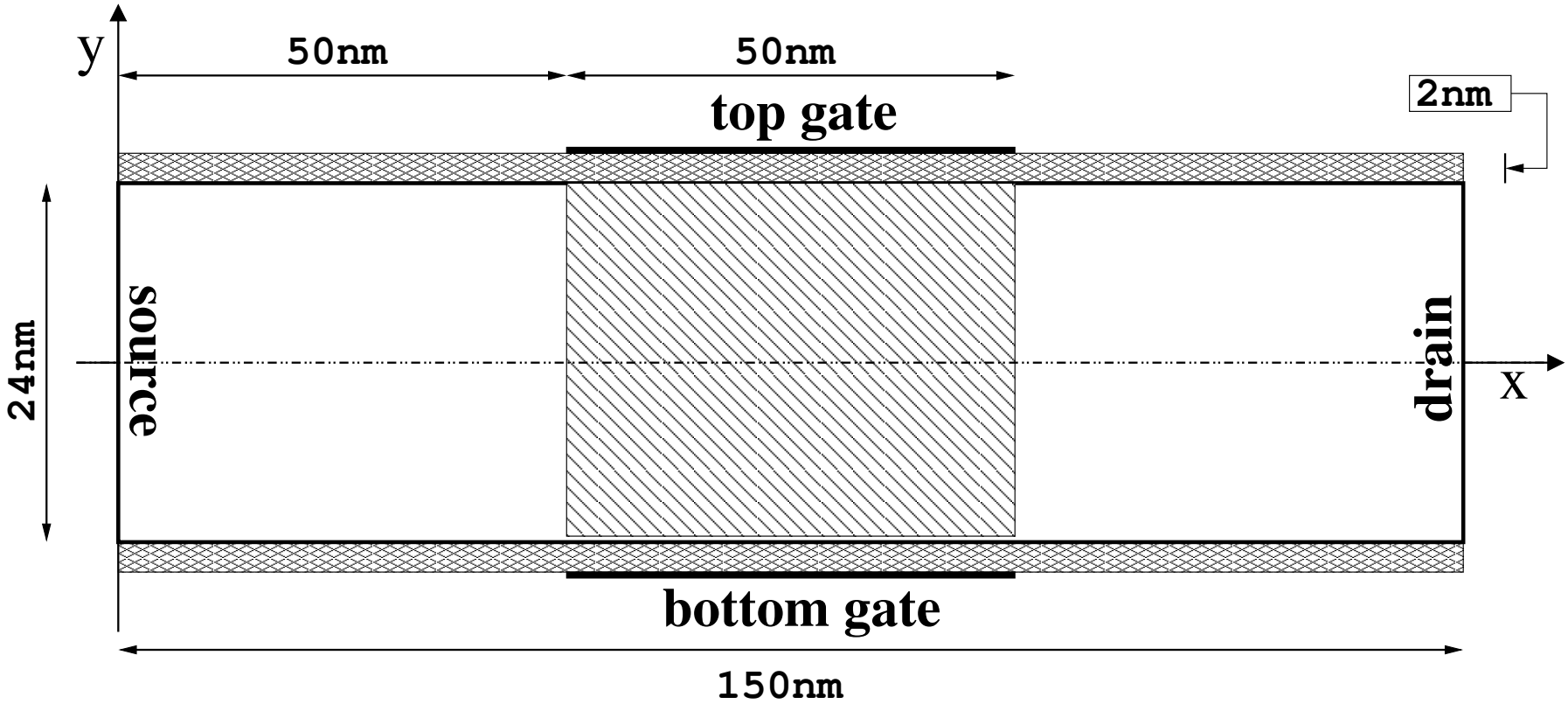
DSMC
BTE (DG)



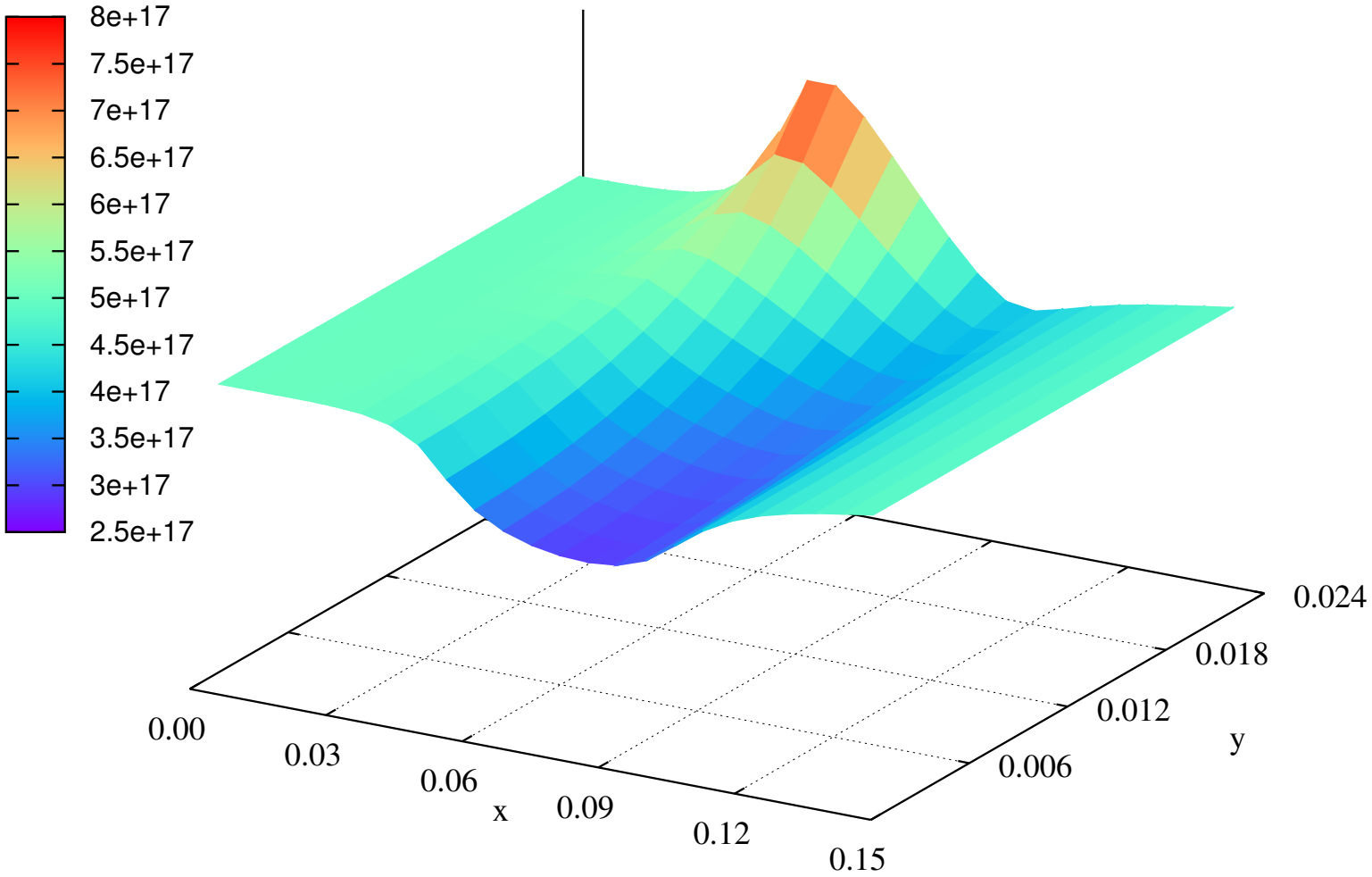
mean energy
(eV)
at $t = 3.0$ ps

DSMC
BTE (DG)

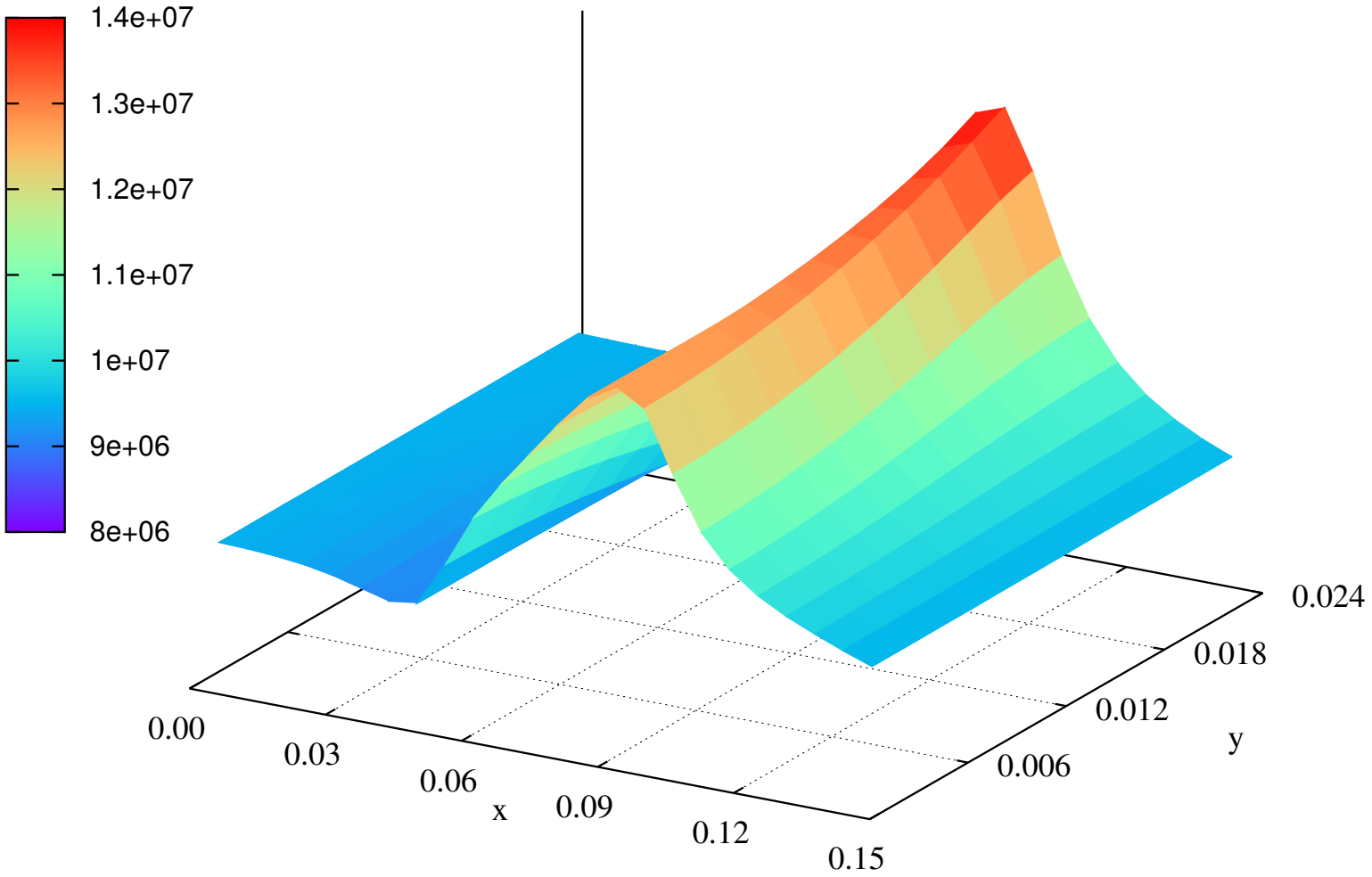
An example of simulation of a $2D$ device ($3D$ in velocity).
The double gate MOSFET



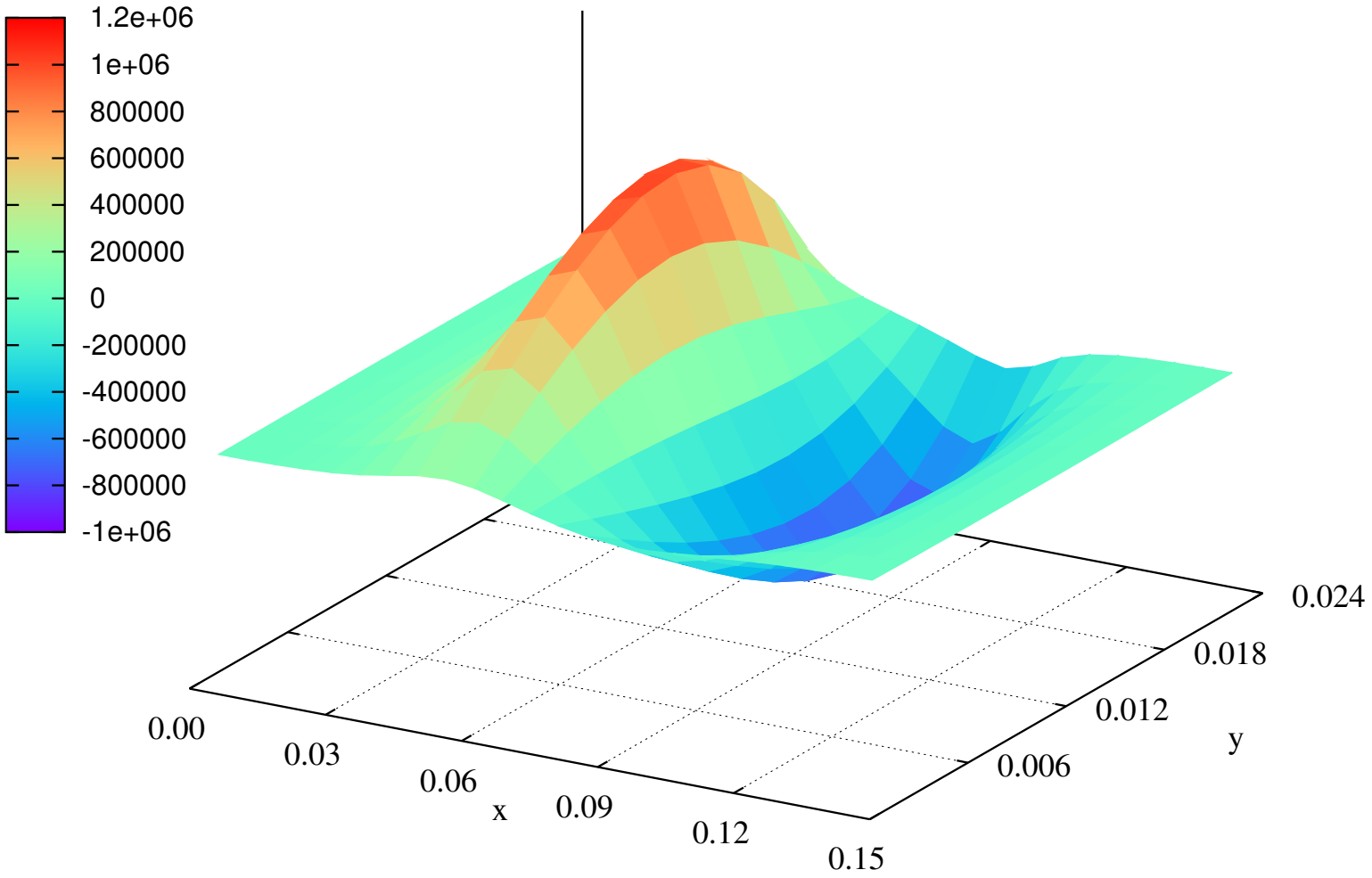
Grid: 24x12x24x8x6 = 331776



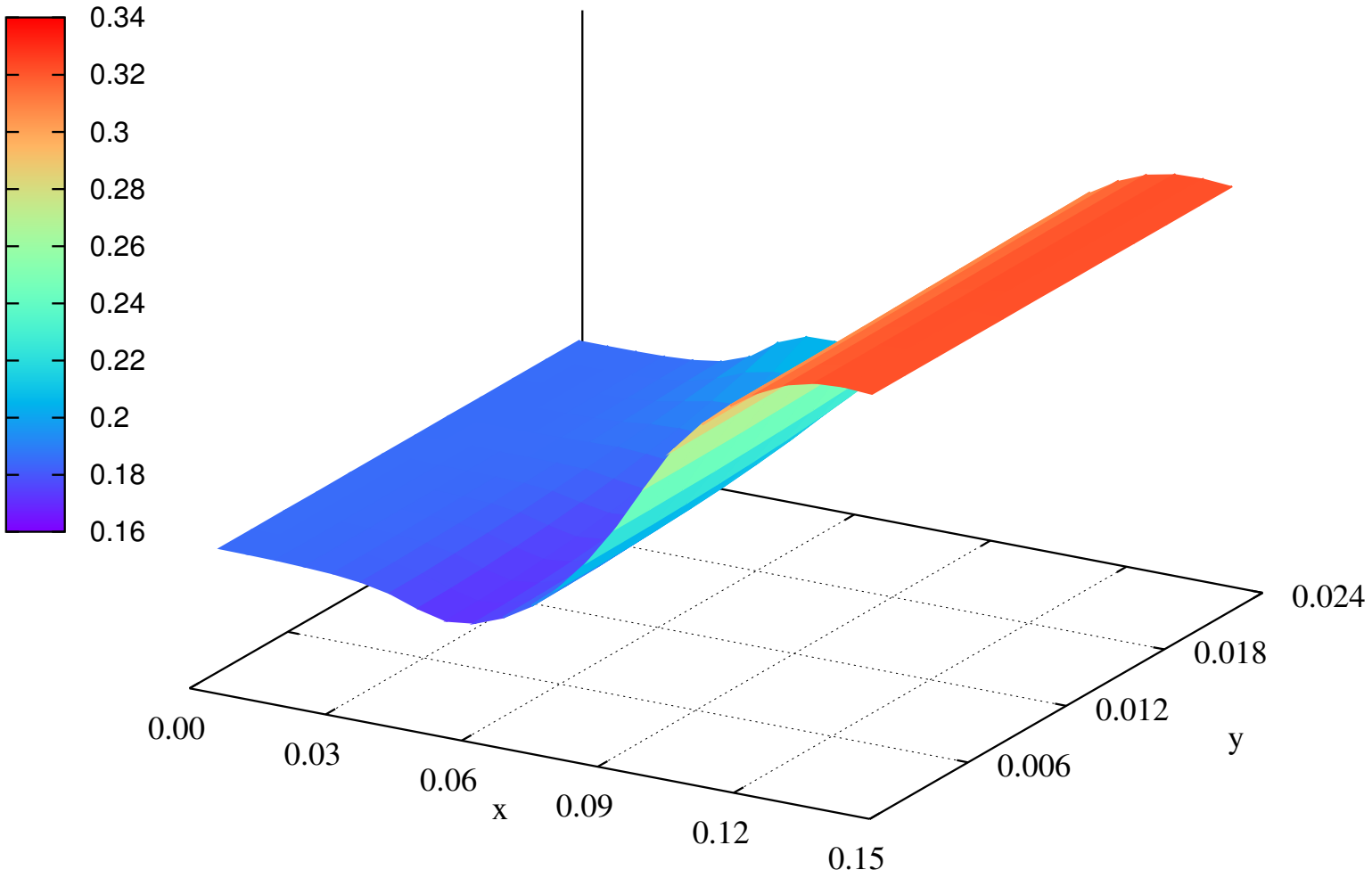
density of charge (cm^{-3})



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

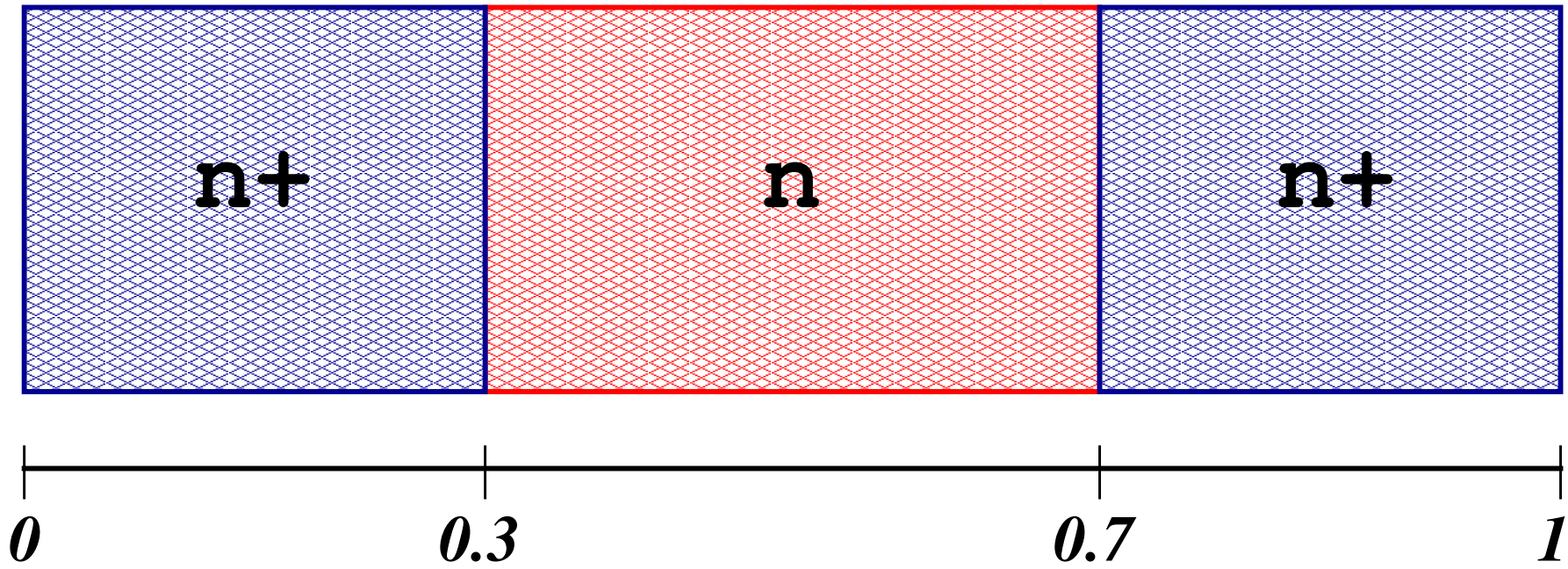


y-component of the mean velocity (cm s^{-1})

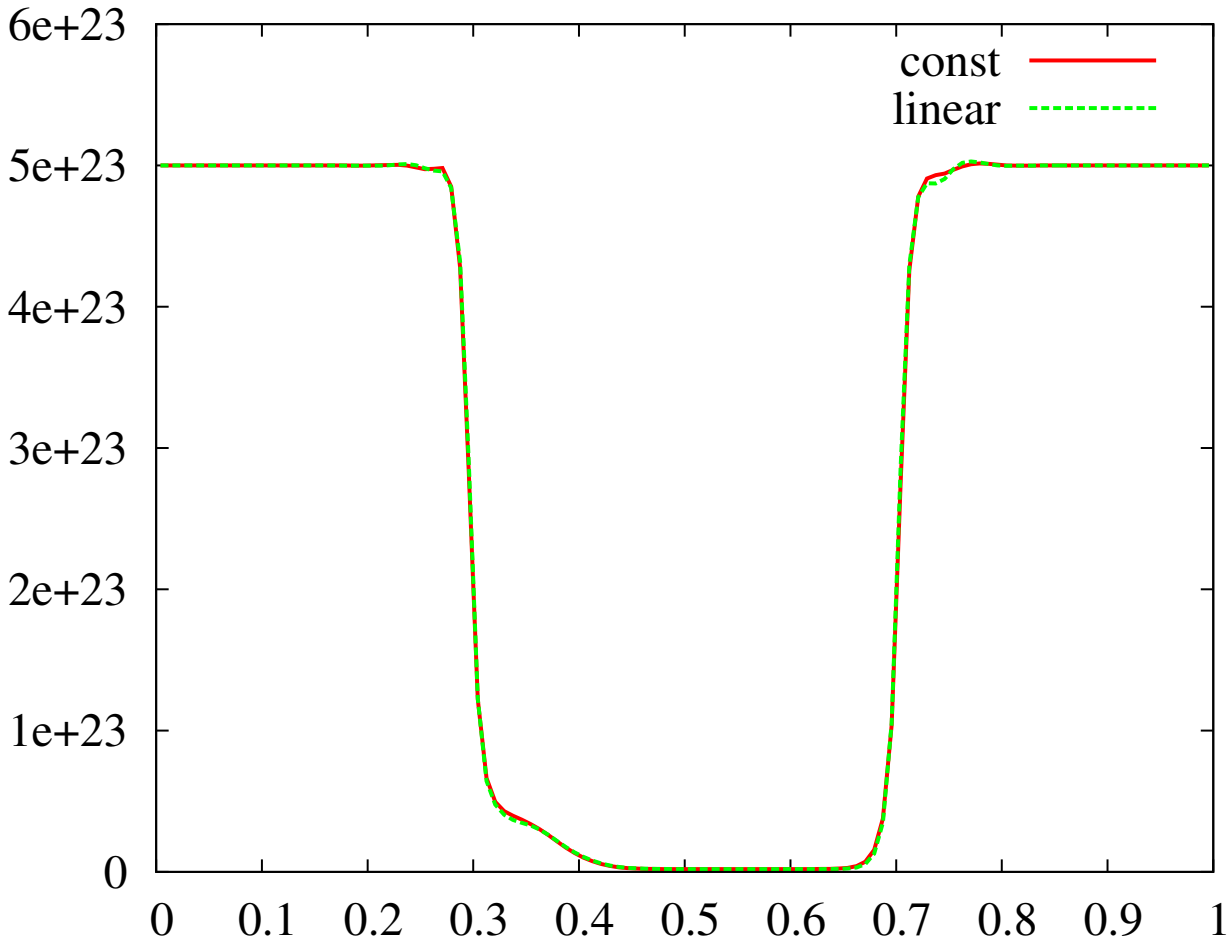

0.34
0.32
0.3
0.28
0.26
0.24
0.22
0.2
0.18
0.16
0.00
0.03
0.06
0.09
0.12
0.15
x
0.006
0.012
0.018
0.024
y

energy (eV)

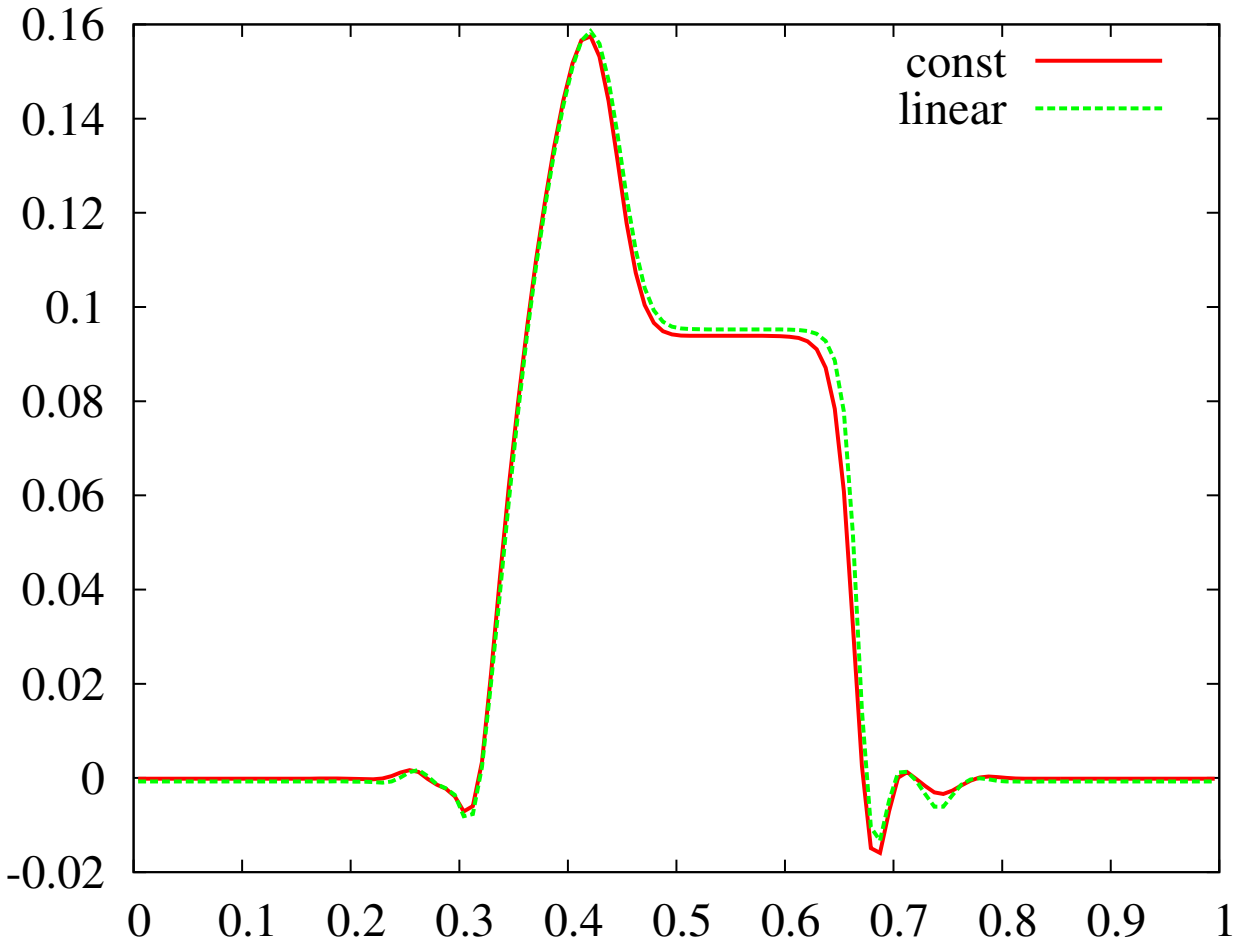
Here, we have a one dimensional silicon $n^+ - n - n^+$ 0.4 μm channel diode, where the doping $N_D = 5 \times 10^{17}$ cm^{-3} in the n$^+$ and $N_D = 2 \times 10^{15}$ cm^{-3} in the n region.



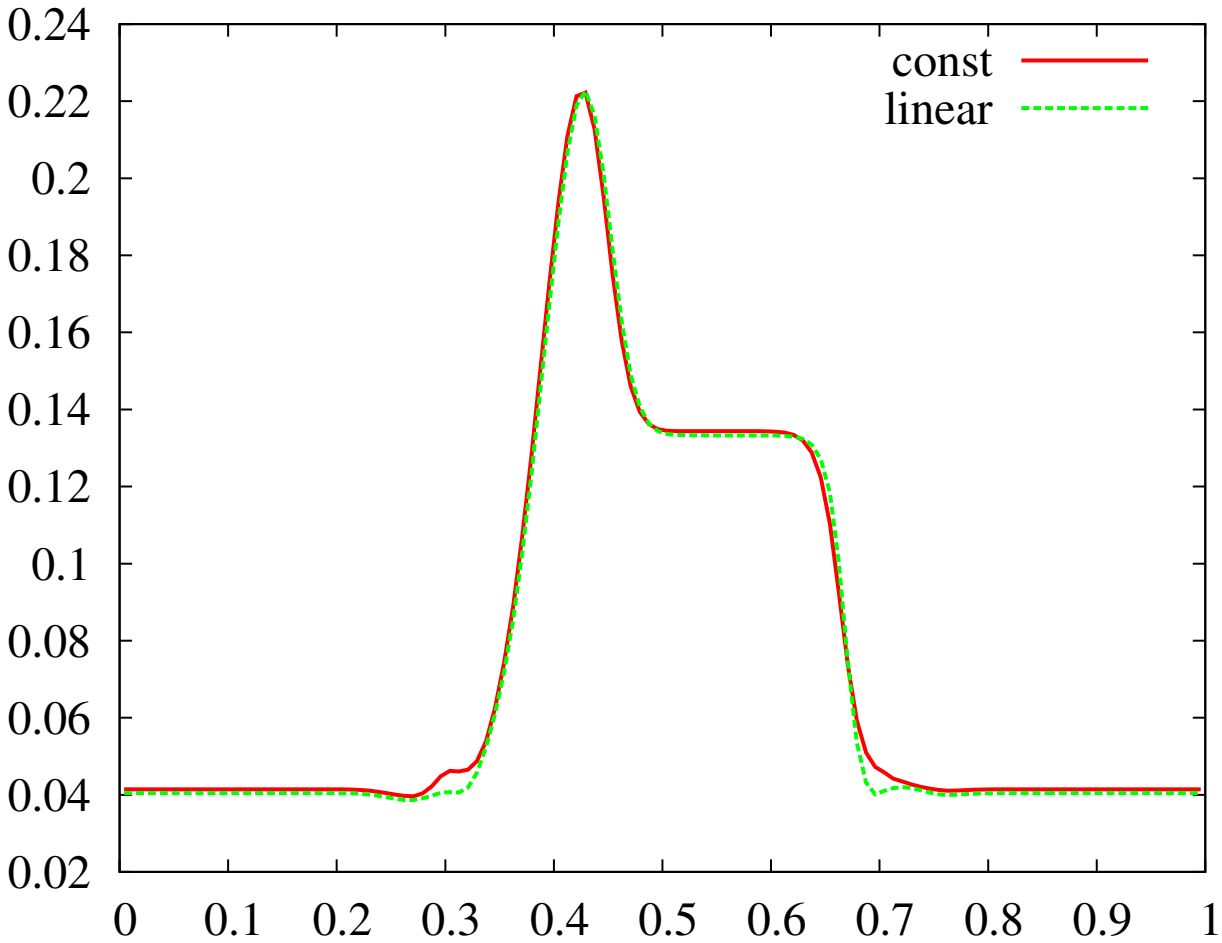
We use a regular grid: 120 cells in space and 60 $\times$ 24 for the velocity. Total number of cells = 172800.



density of charge (cm^{-3}) at $t = 0.5$ ps

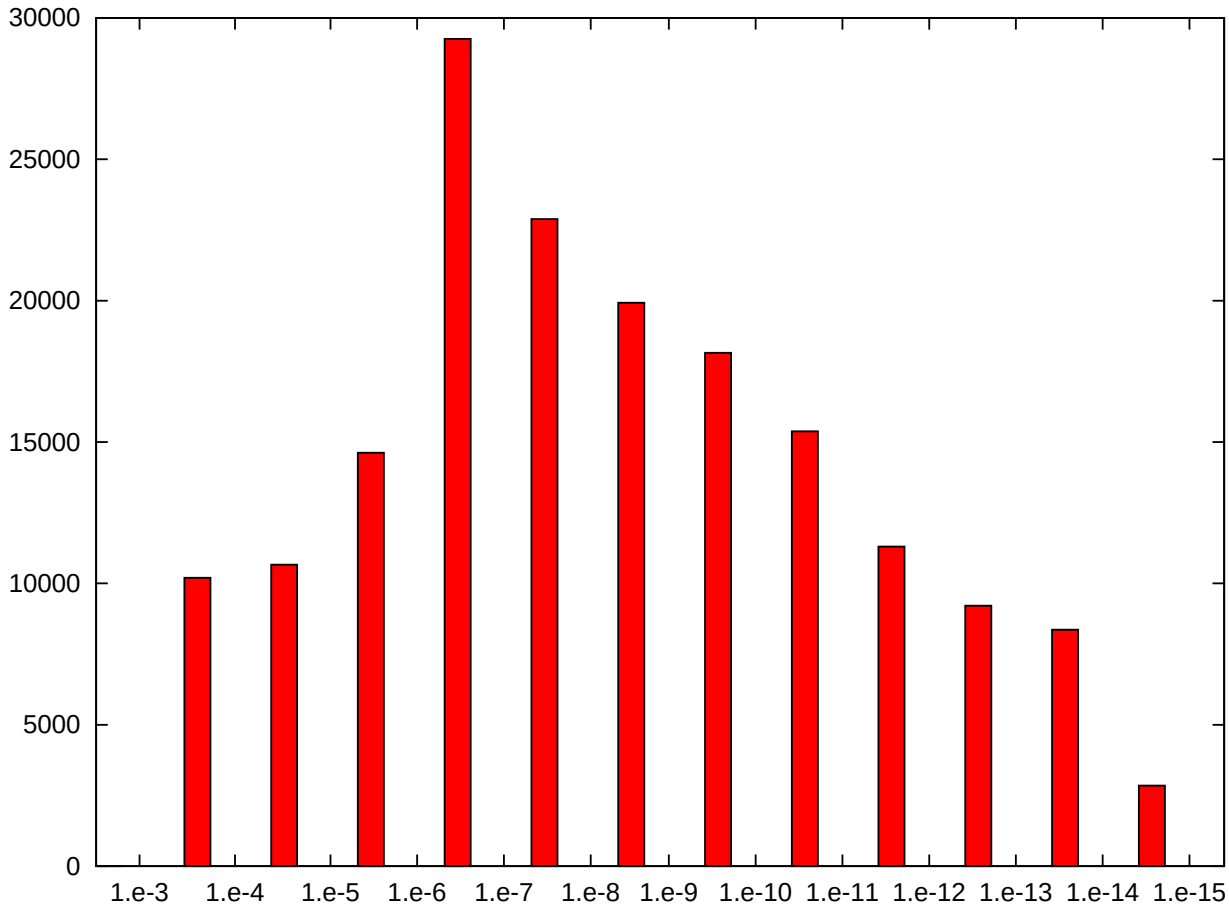


velocity (cm s^{-1}) at $t = 0.5$ ps

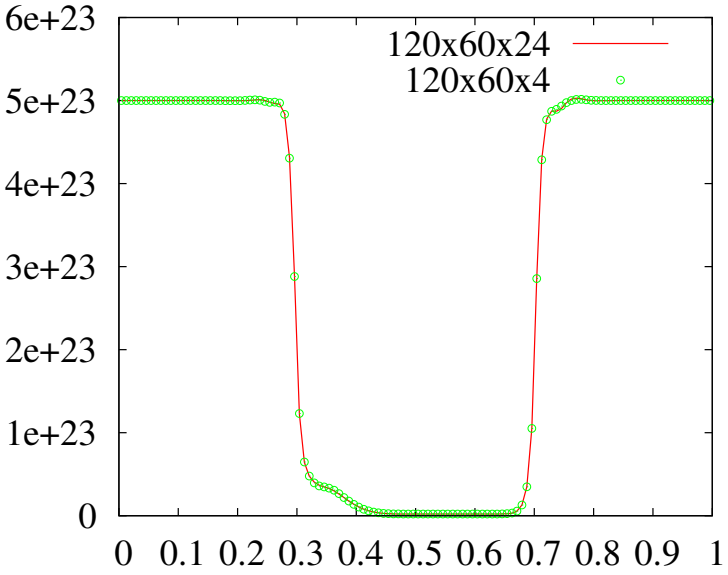


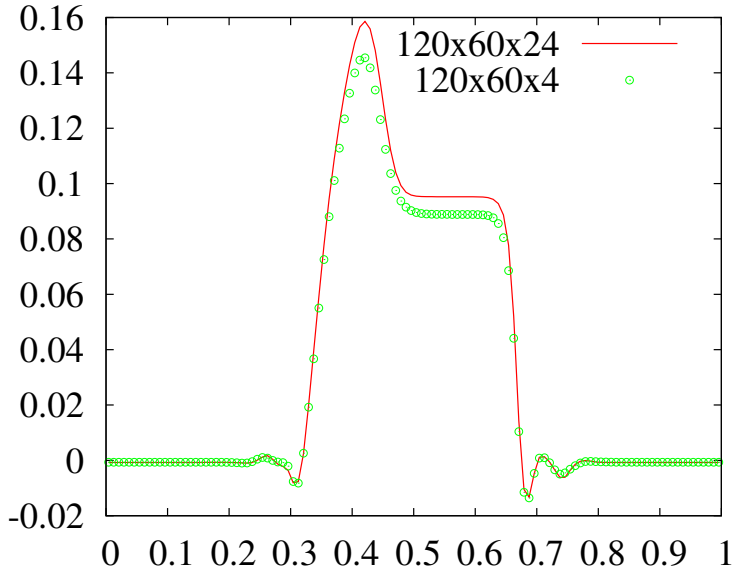
energy (eV) at $t = 0.5$ ps

Positivity.



$10^{-3} \geq \#f > 10^{-4}$, $10^{-4} \geq \#f > 10^{-5}$, ...


120x60x24
120x60x4
6e+23
5e+23
4e+23
3e+23
2e+23
1e+23
0
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1


120x60x24
120x60x4
0.16
0.14
0.12
0.1
0.08
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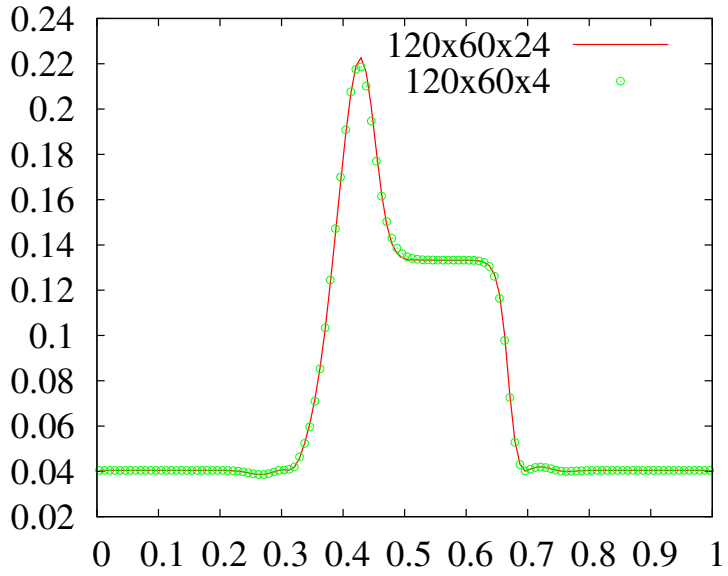
0.04
0.02
0
-0.02
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1


120x60x24
120x60x4
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0.2
0.18
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0.14
0.12
0.1
0.08
0.06
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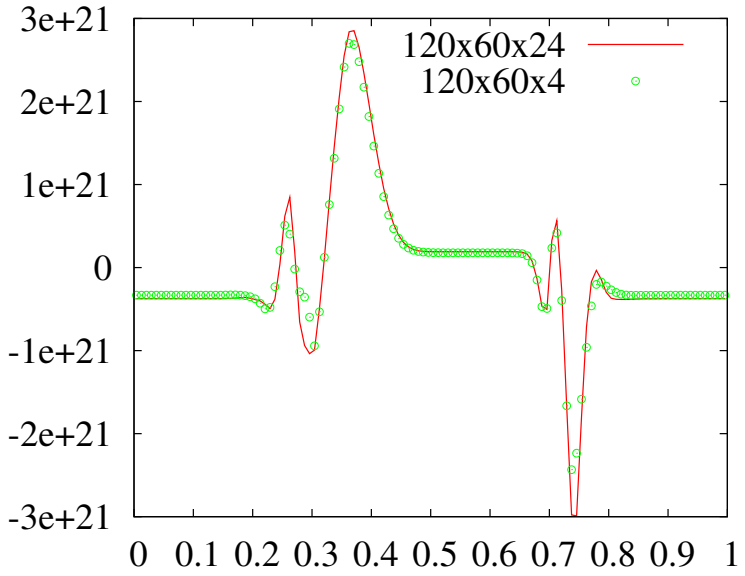
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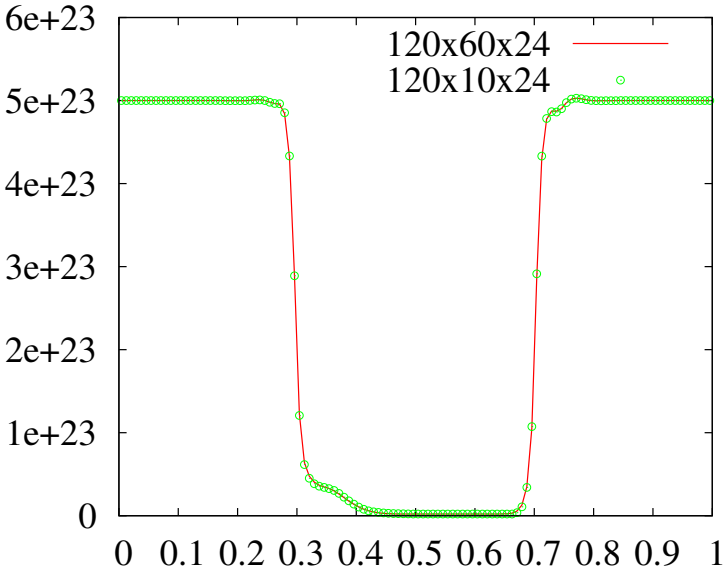
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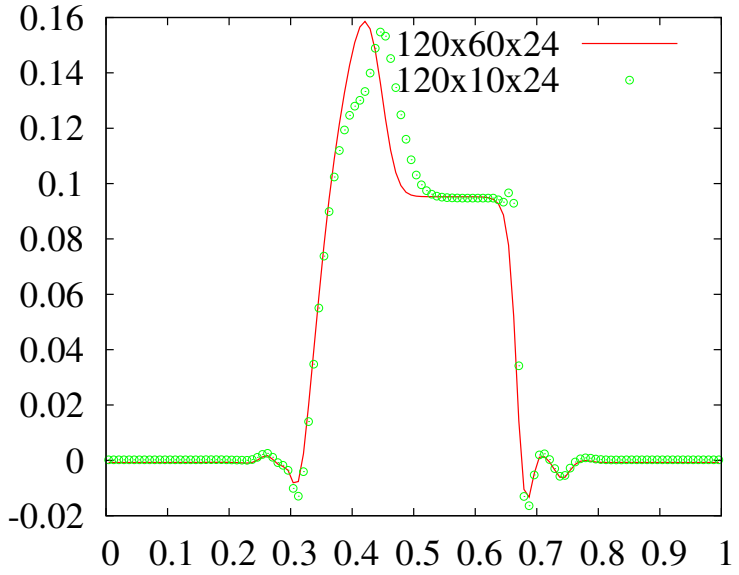
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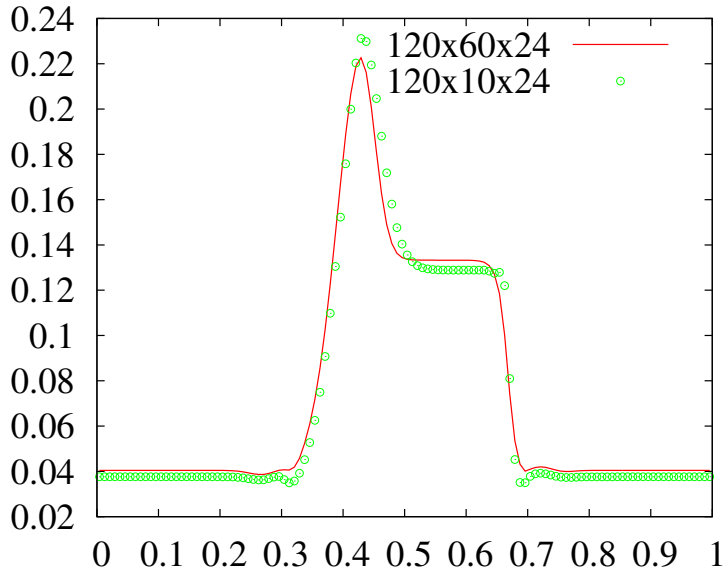
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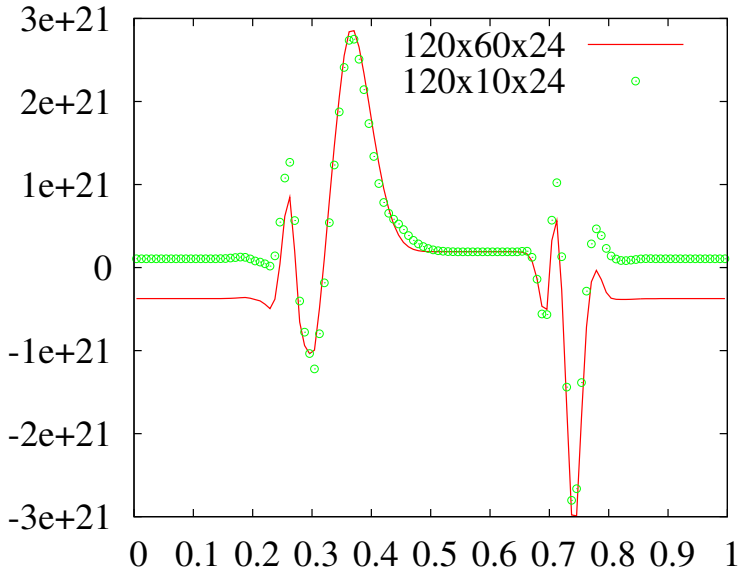
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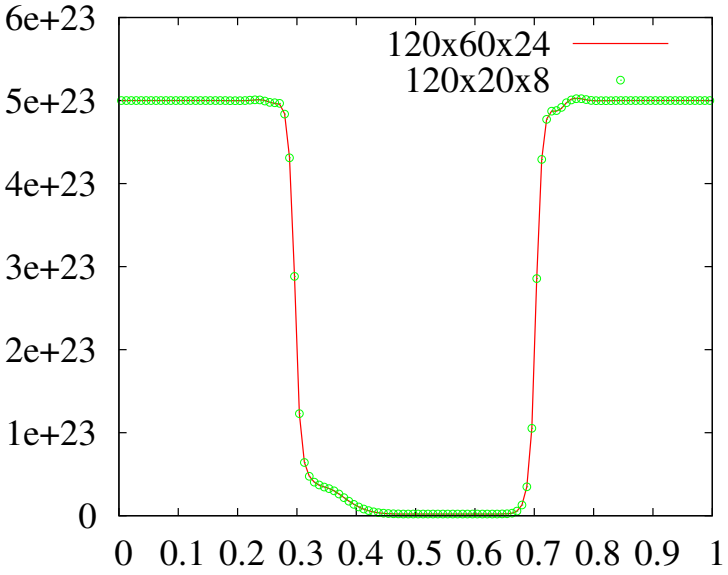
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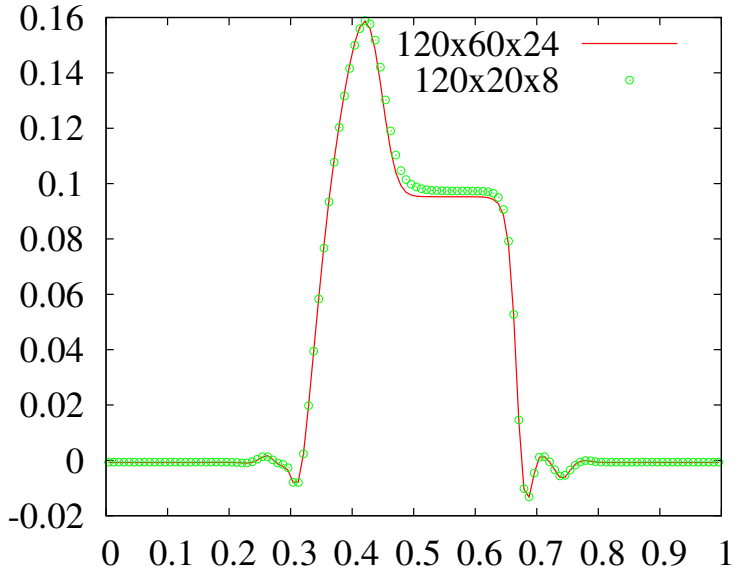
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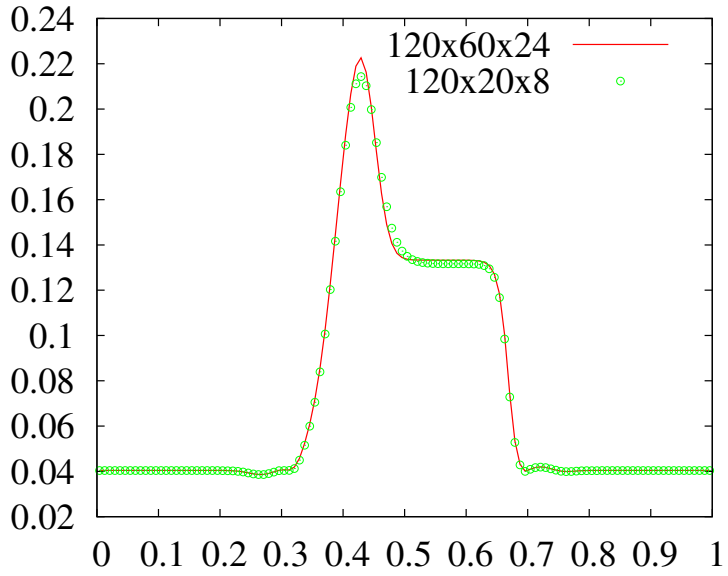
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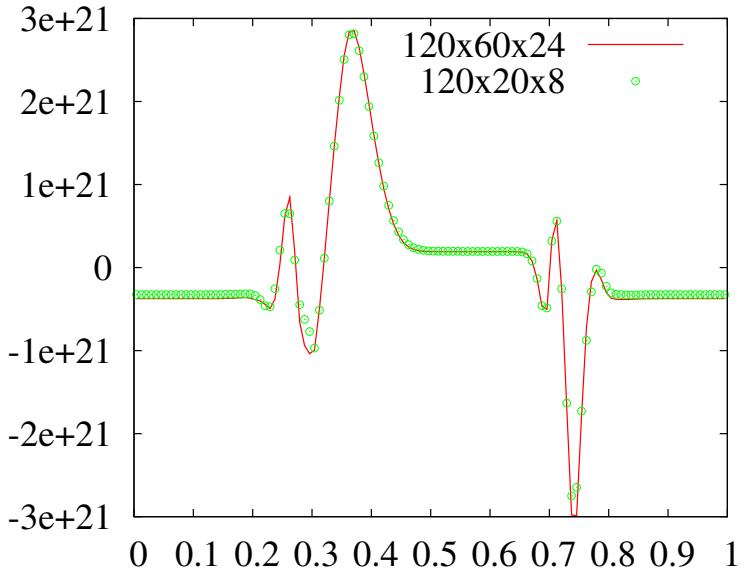
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The radiative transport equation

$$\frac{1}{v}\,\partial_t I(t,\mathbf{x},\Omega) + \Omega\cdot\nabla_{\mathbf{x}} I(t,\mathbf{x},\Omega) = -\mu_t(\mathbf{x})\, I(t,\mathbf{x},\Omega) + \mu_s(\mathbf{x}) \int_{\mathbb{S}^{n-1}} K(\Omega,\Omega')\, I(t,\mathbf{x},\Omega')\, d\Omega' + S(t,\mathbf{x},\Omega)\,, \qquad (8)$$

where I represents the energy density, or intensity, at each position $\mathbf{x}$, unit direction Ω 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 μ_s and the absorption coefficient μ_a, and $\mathbb{S}^{n-1}$ 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, $\boldsymbol{\Omega} = (\cos(\theta), \sin(\theta))$.
The boundary condition is

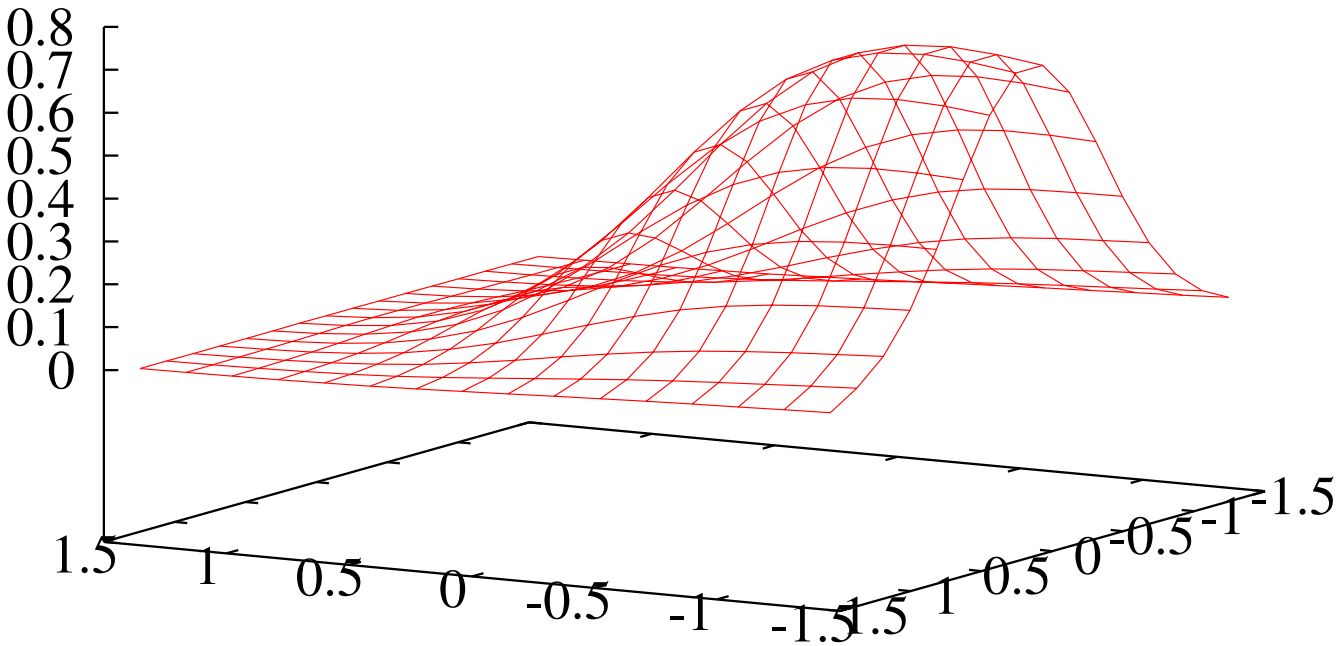
$$I(x_b, y_b, \theta) = 0 \quad \text{on } \Gamma_{in} = \{\partial D \times [0, 2\pi] \text{ s.t. } \mathbf{n}(x_b, y_b) \cdot \boldsymbol{\theta} < 0\}.$$

Moreover,

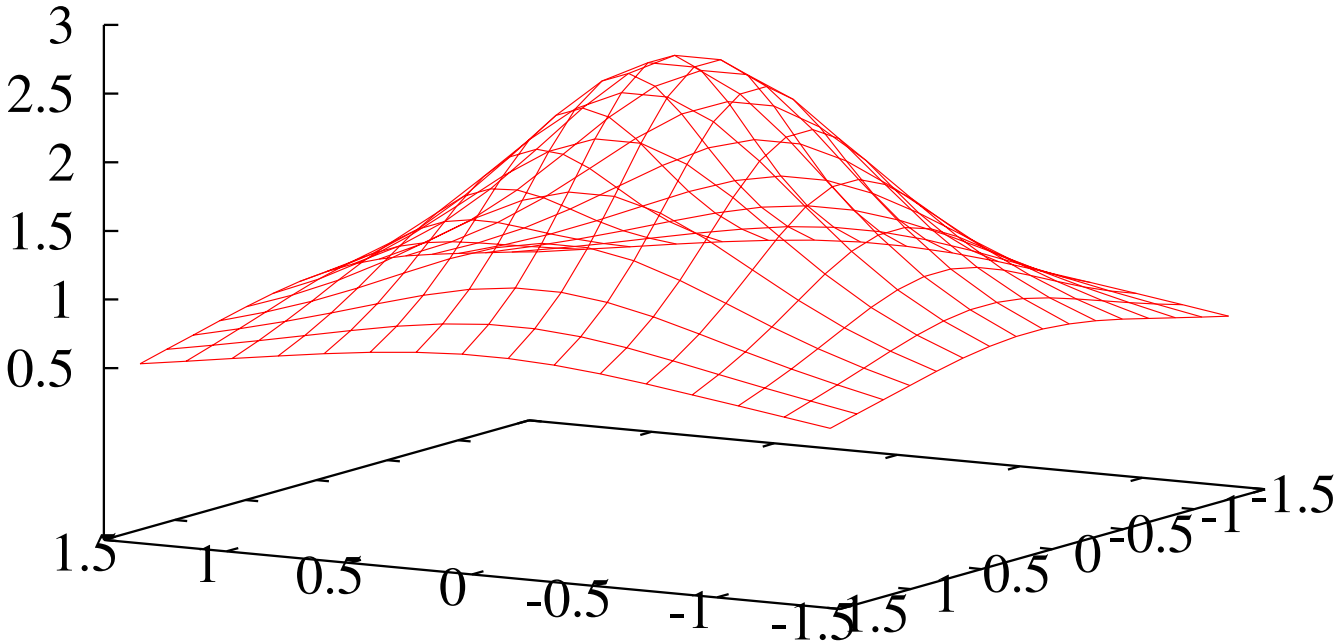
$$S(x, y, \theta) = \frac{2}{\pi} \mathrm{e}^{-2(x^2+y^2)},$$

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

Grid: 16x16x19 = 4864.



the intensity distribution in direction $\theta = \pi$.



the total intensity.

The Boltzmann equation

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{x}} = Q(f, f)\,. \tag{9}$$

The collision operator is

$$Q(f,f) = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} W(\boldsymbol{\xi}, \boldsymbol{\xi}_* | \boldsymbol{\xi}', \boldsymbol{\xi}_*') \left(f' f_*' - f f_*\right) d\boldsymbol{\xi}_*\, d\boldsymbol{\xi}'\, d\boldsymbol{\xi}_*'\,,$$

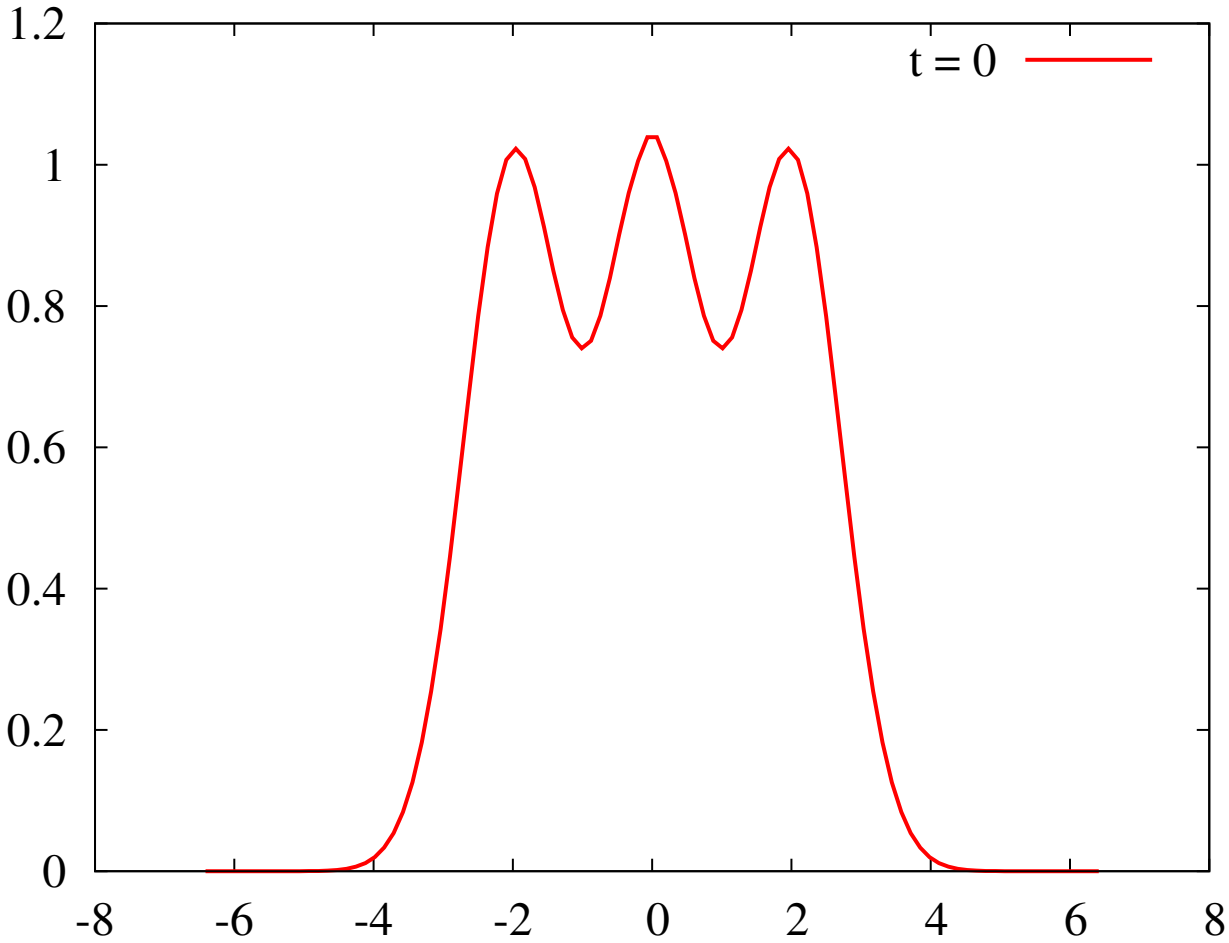
where the kernel W is defined by

$$W(\boldsymbol{\xi}, \boldsymbol{\xi}_* | \boldsymbol{\xi}', \boldsymbol{\xi}_*') = K(\mathbf{n}\cdot\mathbf{V}, |\mathbf{V}|)\, \delta(\boldsymbol{\xi}+\boldsymbol{\xi}_*-\boldsymbol{\xi}'-\boldsymbol{\xi}_*')\, \delta(|\boldsymbol{\xi}|^2+|\boldsymbol{\xi}_*|^2-|\boldsymbol{\xi}'|^2-|\boldsymbol{\xi}_*'|^2)\,.$$

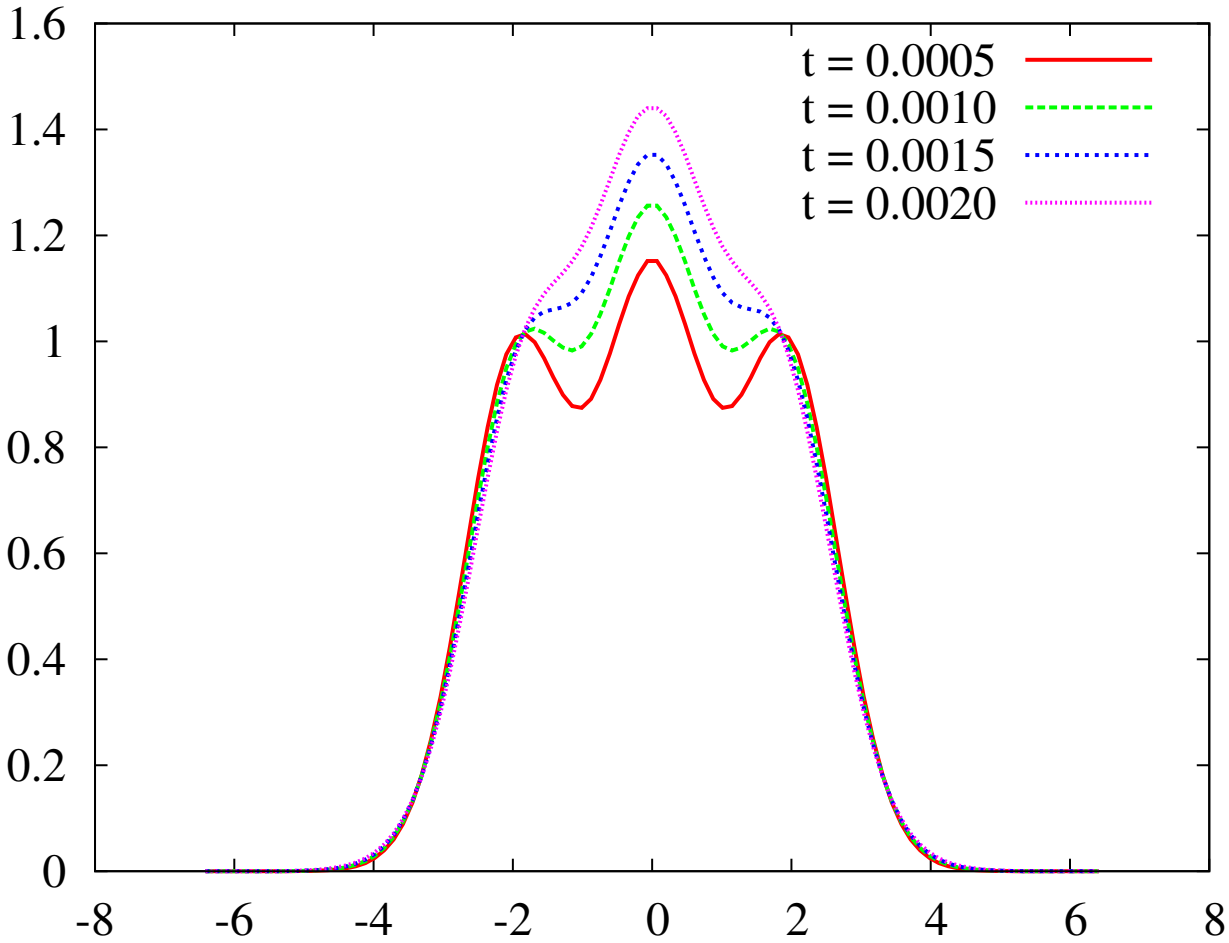
The function $K(\mathbf{n}\cdot\mathbf{V}, |\mathbf{V}|)$ is related to the interaction law between colliding particles, with

$$\mathbf{n} = \frac{\boldsymbol{\xi} - \boldsymbol{\xi}'}{|\boldsymbol{\xi} - \boldsymbol{\xi}'|} \quad \text{and} \quad \mathbf{V} = \boldsymbol{\xi} - \boldsymbol{\xi}_*\,.$$

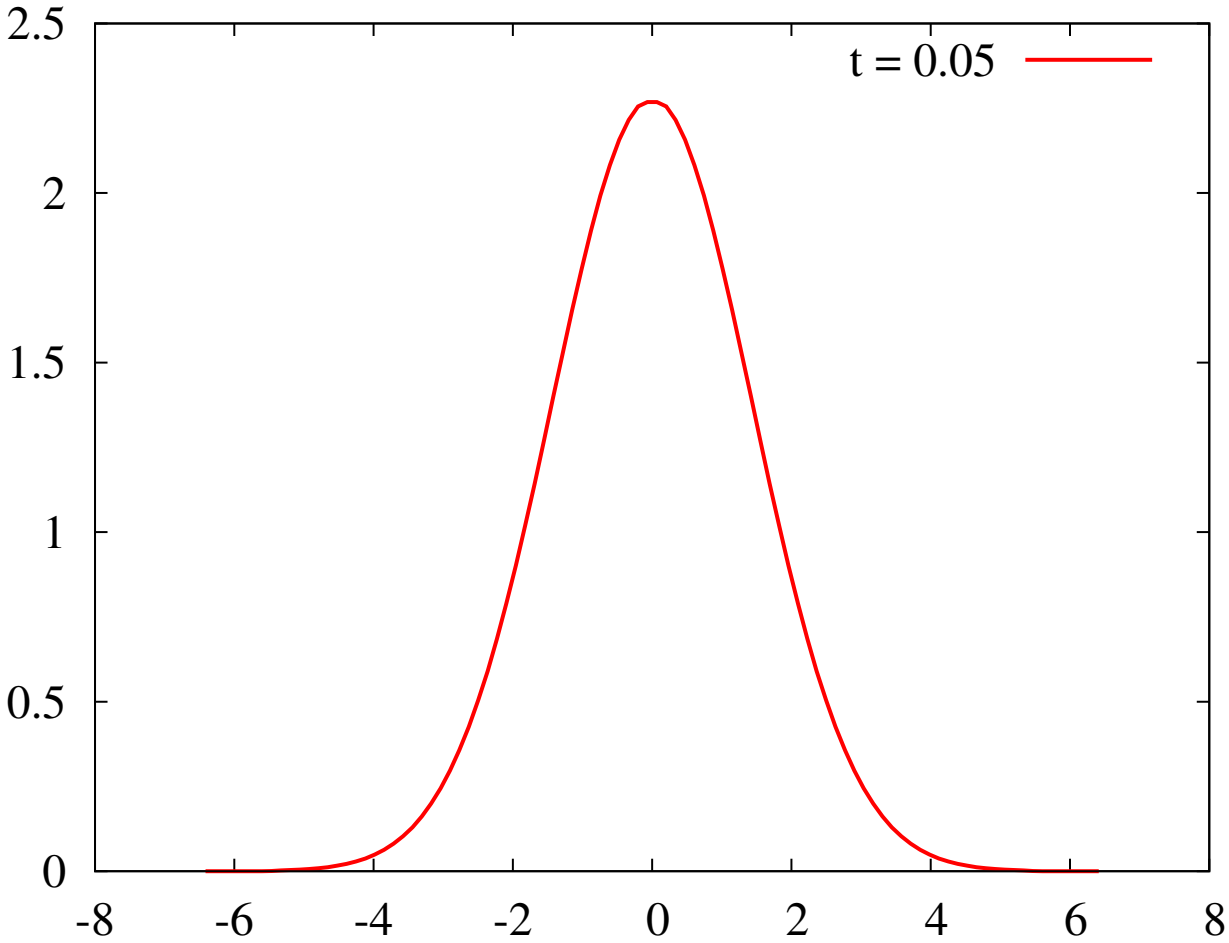
We apply the discontinuous Galerkin method to the Boltzmann equation (9) using in every cell the same basis $\{1, \xi, \xi^2\}$.
This guarantees the conservation of mass, momentum and energy for homogeneous solutions.



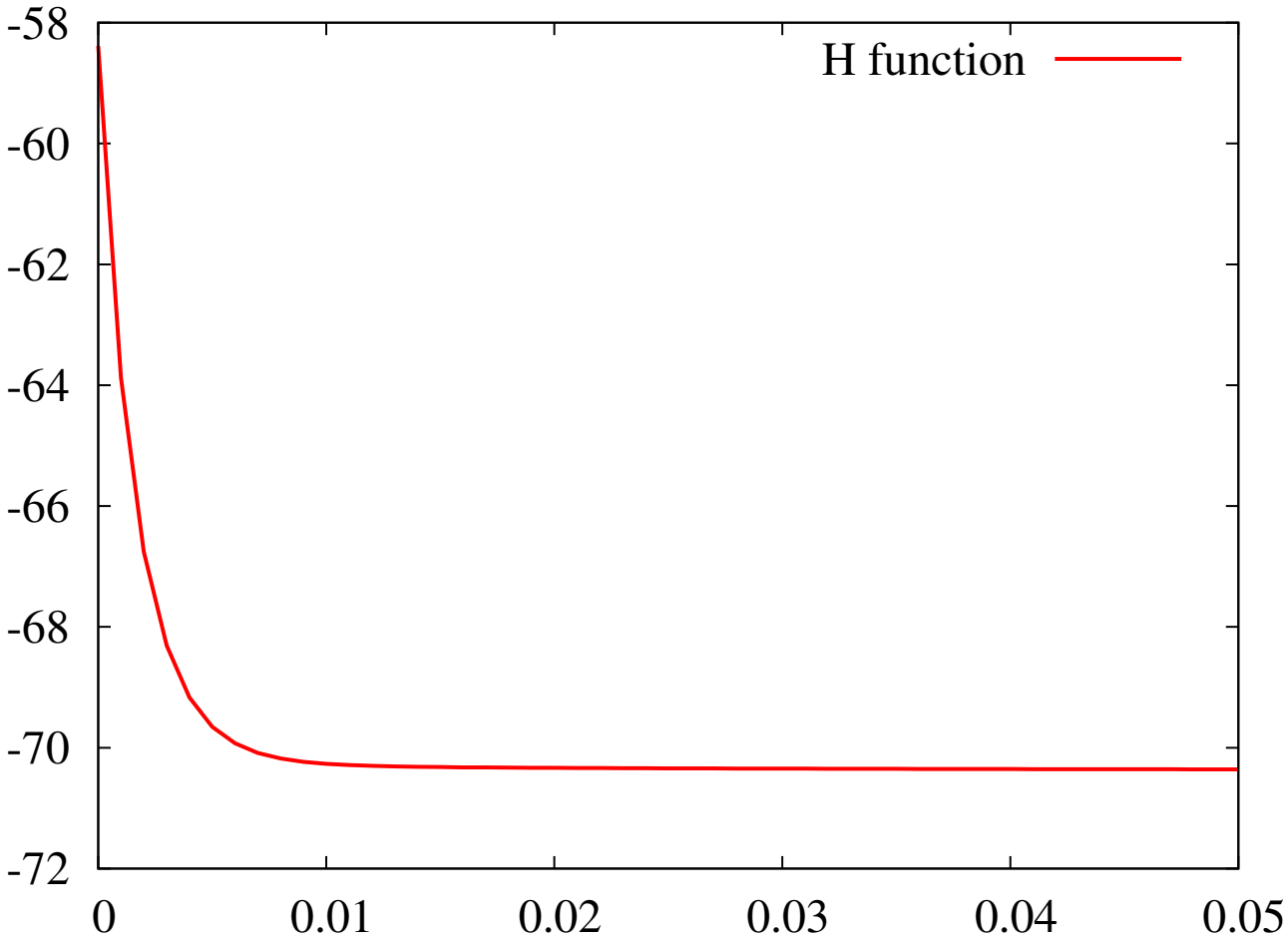
f versus $|\xi|$ at time $t = 0$.



f versus $|\xi|$ (transient).



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



$\int f \log f \, d\xi$ versus time.

Thank you for your attention

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