Kinetic simulation of heat transport in collision plasmas:

stochastic & deterministic approaches

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OBJECTIVE & MOTIVATION

- **- high temperature and density gradients**
- **- the electron heat transport, heat flux**
- ***- spatial-temporal scales (temperature inhomogeneity less or equal to …..electron mean free path lengths) - →***
- ***- non-applicability of the classical transport theory***

- **- *kinetic description* - →**
- **- analytical approach - (!?)**
- **-numerical simulation →**
- **- laboratory and space plasmas**
- **-stochastic & deterministic approaches**

OUTLINE

Preliminaries / Parameters / Equations

DSMC method for LFP equation – (3V + 1D)

Asymptotic-preserving scheme -- (1D +2V)

Illustrative results

Parameters (normalization)

- Collision frequency $\nu = n\sigma v,\quad \nu_{ei} = \dfrac{4\sqrt{\pi}Z^2 e^4 n_e L_{ei}}{3m_e^{1/2}T_e^{3/2}} = t_{ei}^{-1}$
- Mean free path $\lambda_e = v_e t_{ee}$
- Thermal velocity $v_{th} = \sqrt{\dfrac{3T}{m}}$
- Scale hierarchy:

$$r_D << \lambda_{ei} << L \qquad \omega_{pe} >> \nu_{ei} >> t^{-1}$$

Spatial temporal scaling

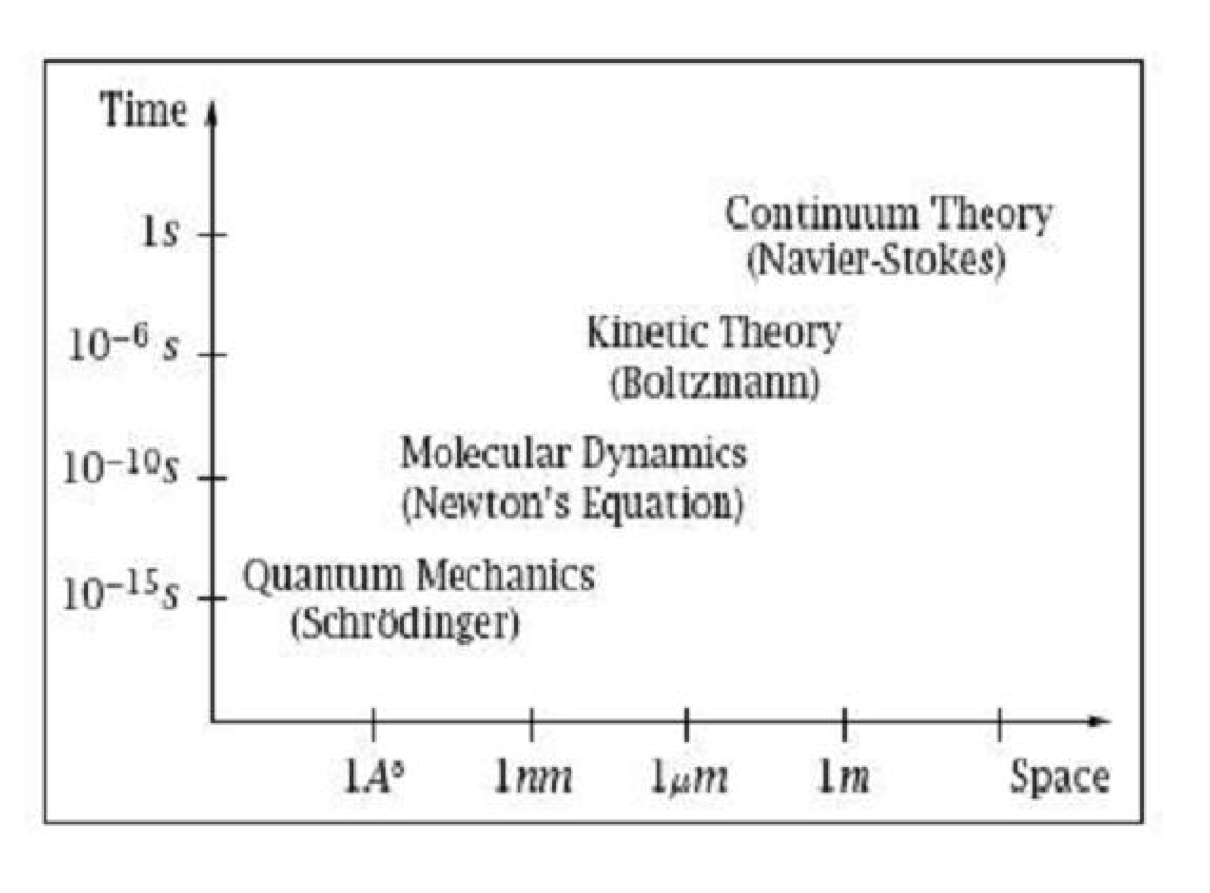


Figure: from E & Engquist, AMS Notice

$Kn = \lambda / L -$

Knudsen number

(*unified description*)

$\lambda / L: \quad << 1 \quad - MHD,$

$\lambda / L: \quad >> 1 \quad - Vlasov\ eq.,$

$\lambda / L: \quad \sim 1 \quad - LFP\ eq.$

Kinetic description of plasmas

Kinetic description of plasmas

$f_\alpha(\mathbf{v},\mathbf{r},\mathrm{t})$ - **distribution function**

$$\int_{\mathbf{R}_3} f_\alpha(\mathbf{v},\mathbf{r},\mathrm{t})\,\mathrm{d}^3\mathbf{v} = n_\alpha(\mathbf{r},\mathrm{t})$$

Kinetic equation:

$$D_\alpha f_\alpha = \left\{\frac{\partial}{\partial t} + \mathbf{v}\frac{\partial}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m}\frac{\partial}{\partial \mathbf{v}}\right\} f_\alpha$$

$$D_\alpha f_\alpha = \sum_\beta Q_{\alpha\beta}[f_\alpha, f_\beta]$$

Boltzmann collision integral

$$Q_{\alpha\beta}(f_\alpha, f_\beta) = \int_{\mathbb{R}^3\times\mathbf{S}^2} \mathrm{d}\mathbf{w}\,\mathrm{d}\mathbf{n}\; g_{\alpha\beta}(\mathrm{u},\mu)\left\{f_\alpha(\mathbf{v}')f_\beta(\mathbf{w}') - f_\alpha(\mathbf{v})f_\beta(\mathbf{w})\right\}$$

$$g_{\alpha\beta}(\mathrm{u},\mu) = \mathrm{u}\cdot\sigma_{\alpha\beta}(\mathrm{u},\mu)$$

$$\mathbf{v}' = \mathbf{U} + \frac{m_{\alpha\beta}}{m_\alpha}\mathrm{u}\,\mathbf{n}, \qquad \mathbf{U} = \frac{m_\alpha\mathbf{v} + m_\beta\mathbf{w}}{m_\alpha + m_\beta}$$

$$\mathrm{u} = |\mathbf{v}-\mathbf{w}|, \qquad \mu = \frac{\mathbf{u}\cdot\mathbf{n}}{\mathrm{u}}$$

$$\mathbf{w}' = \mathbf{U} - \frac{m_{\alpha\beta}}{m_\beta}\mathrm{u}\,\mathbf{n}, \qquad m_{\alpha\beta} = \frac{m_\alpha m_\beta}{m_\alpha + m_\beta}$$

Conservation laws / invariants

- Density, momentum, energy (one sort)

$$\propto \qquad \int dv\, f = n, \quad \int dv\, v\, f = \langle v, \rangle \quad \int dv\, v^2\, f = \langle \varepsilon \rangle$$

$$\int_{\mathbb{R}^3} Q(f, f)\, \varphi(v)\, dv = 0 \quad \text{if} \quad \varphi(v) = 1,\ v,\ |v|^2$$

$$f_{Maxw} = \frac{n_e T_e^{3/2}}{(2\pi m_e)^{3/2}} \exp\left[-\frac{m_e \mathrm{v}^2}{2T_e}\right], \qquad \frac{m_e}{2}\langle \varepsilon_e \rangle = \frac{3}{2} n_e T_e$$

Landau-Fokker-Planck integral –

Landau (1936), Rosenbluth et al (1957)

Grazing collisions :

$$u\sigma(u,\mu)\equiv 0 \quad if \quad -1\le \mu=\cos\theta\le 1-\delta^2,\ 0<\delta<<1$$

$$C_{\alpha\beta}^{(L)}(f_\alpha,f_\beta)=\frac{m_{\alpha\beta}^2}{2m_\alpha^2}\frac{\partial}{\partial \mathrm{v}_i}\int \mathrm{d}^3\mathbf{w}\,\mathrm{u}\,\sigma_{\alpha\beta}^{(tr)}(\mathrm{u})\mathrm{R}_{ij}(\mathbf{u})\left\{\frac{\partial}{\partial \mathrm{v}_j}-\frac{m_\alpha}{m_\beta}\frac{\partial}{\partial \mathrm{w}_j}\right\}f_\alpha(\mathbf{v})f_\beta(\mathbf{w})$$

$$R_{ij}(u)=u^2\delta_{ij}-u_i\,u_j,$$

$$\sigma^{(tr)}(\mathrm{u})=\frac{1}{2}\int d\mu\,d\varphi\,\sigma(u,\mu)\,(1-\mu)\ \text{– transport cross section}$$

$$U\sim\frac{1}{r^\beta},\ \ \beta=1;$$

$$\sigma_R^{(tr)}(\mathrm{u})=4\pi\left(\frac{e_\alpha e_\beta}{m_{\alpha\beta}\mathrm{u}^2}\right)^2 L_{\alpha\beta}\ \text{– for Rutherford cross-section}$$

$$g^{(tr)}(u)=u\,\sigma_{\alpha\beta}^{(tr)}(\mathrm{u})=4\pi\left(\frac{e_\alpha e_\beta}{m_{\alpha\beta}}\right)^2 L_{\alpha\beta}\ \frac{1}{u^3}$$

КИНЕТИЧЕСКОЕ ОПИСАНИЕ ПЛАЗМЫ И ЧИСЛЕННОЕ РЕШЕНИЕ

Кинетическое уравнение:

$$\left\{ \frac{\partial}{\partial t} + \mathbf{v}\frac{\partial}{\partial \mathbf{r}} + \frac{\mathbf{F}_\alpha}{m_\alpha}\frac{\partial}{\partial \mathbf{v}} \right\} f_\alpha = \sum_\beta C_{\alpha\beta}[f_\alpha, f_\beta]$$

Интеграл столкновений Ландау (Фоккера-Планка):

$$C_{\alpha\beta}[f_\alpha, f_\beta] = \frac{m_{\alpha\beta}^2}{2m_\alpha^2}\frac{\partial}{\partial \mathrm{v}_i}\int d^3\mathbf{w}\, \mathrm{u}\, \sigma_{\alpha\beta}^{(tr)}(\mathrm{u}) \mathrm{R}_{ij}(\mathbf{u}) \left\{ \frac{\partial}{\partial \mathrm{v}_j} - \frac{m_\alpha}{m_\beta}\frac{\partial}{\partial \mathrm{w}_j} \right\} f_\alpha(\mathbf{v}) f_\beta(\mathbf{w})$$

$$\mathrm{u} = |\mathbf{v} - \mathbf{w}| \qquad \mathrm{R}_{ij}(\mathbf{u}) = \mathrm{u}^2\delta_{ij} - \mathrm{u}_i \cdot \mathrm{u}_j \qquad \sigma_{\alpha\beta}^{(tr)}(\mathrm{u}) = \frac{4\pi q_\alpha^2 q_\beta^2 \Lambda_{\alpha\beta}}{m_{\alpha\beta}^2 \mathrm{u}^4} \qquad \mathbf{F}_\alpha = q_\alpha\left(\mathbf{E} + \frac{1}{c}\mathbf{v}\times\mathbf{B}\right)$$

Численное решение:

Расщепление по физическим процессам

Уравнение Власова

$$\frac{\partial f_\alpha}{\partial t} + v_x\frac{\partial f_\alpha}{\partial x} + \frac{q_\alpha E_x}{m_\alpha}\frac{\partial f_\alpha}{\partial v_x} = 0$$

Метод частица в ячейке (PIC)

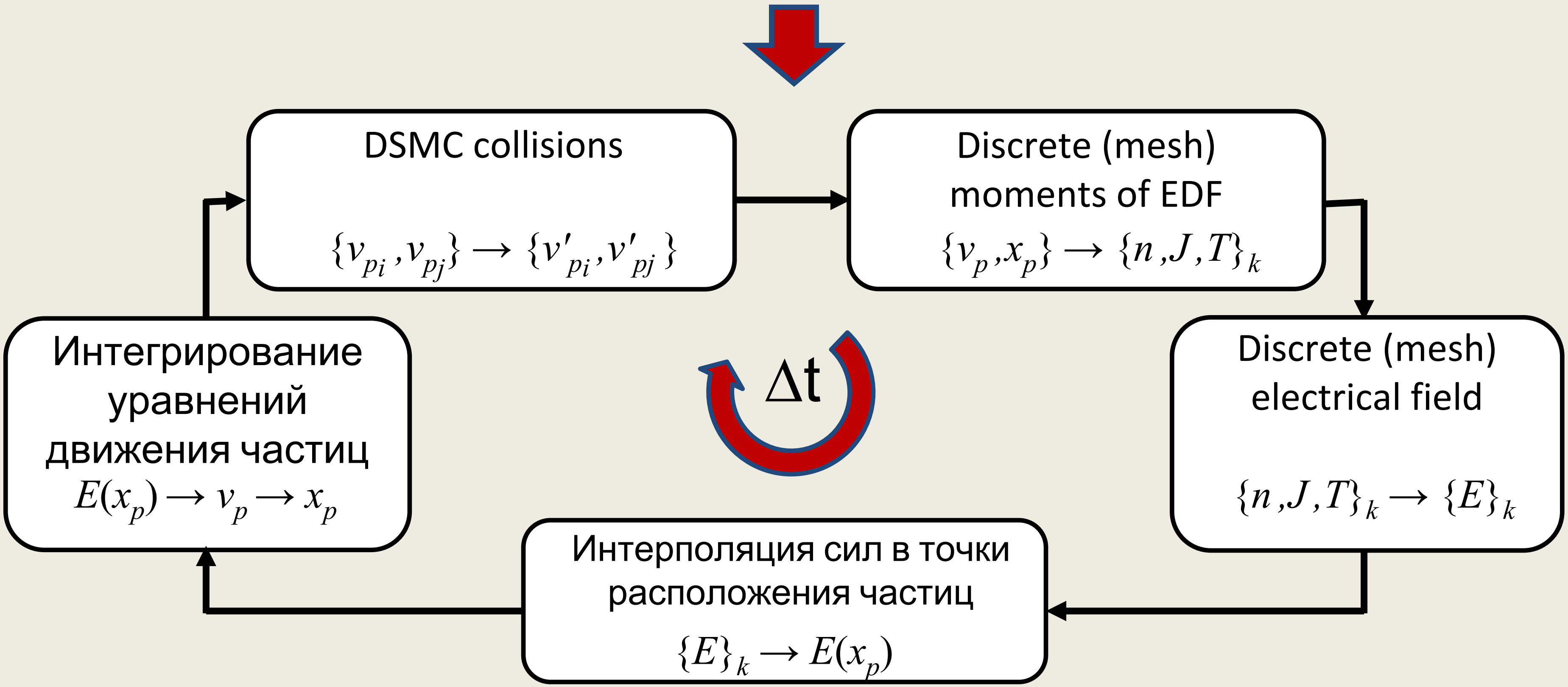
Уравнение Ландау

$$\frac{\partial f_\alpha}{\partial t} = \sum_\beta C_{\alpha\beta}[f_\alpha, f_\beta]$$

Метод прямого дискретного моделирования

Algorithm (electrostatic case)

$$\frac{\partial f}{\partial t}+v_x\frac{\partial f}{\partial x}+\frac{q}{m}E_x\frac{\partial f}{\partial v_x}=C\left(f,f\right)$$



A general approach to Monte Carlo methods for Coulomb collisions

A general approach to Monte Carlo methods for Coulomb collisions

Taylor expansion of Boltzmann integral with respect to small $\mathbf{v}-\mathbf{v}'$ *and* $\mathbf{w}-\mathbf{w}$ (μ~1) A formal series:

$$Q_{\alpha\beta}(f_\alpha, f_\beta) = \sum_{k=1}^{\infty} Q_{\alpha\beta}^{(k)}(f_\alpha, f_\beta)$$

The first term is the Landau integral

$$Q_{\alpha\beta}^{(1)}(f_\alpha, f_\beta) = Q_{\alpha\beta}^{(L)}(f_\alpha, f_\beta)$$

<u>The rest terms (k≥2):</u>

$$Q_{\alpha\beta}^{(k)}(f_\alpha, f_\beta) = \int_{\mathbf{R}_3} d\mathbf{w} g_{\alpha\beta}^{(k)}(\mathrm{u}) A_{\alpha\beta}^{(k)}(\mathbf{v}, \mathbf{w}),$$

$$g_{\alpha\beta}^{(k)}(\mathrm{u}) = 2\pi \int_{-1}^{1} d\mu \, g_{\alpha\beta}(\mathrm{u}, \mu)(1-\mu)^k .$$

<u>The condition of applicability of the approximation of LFP equation:</u>

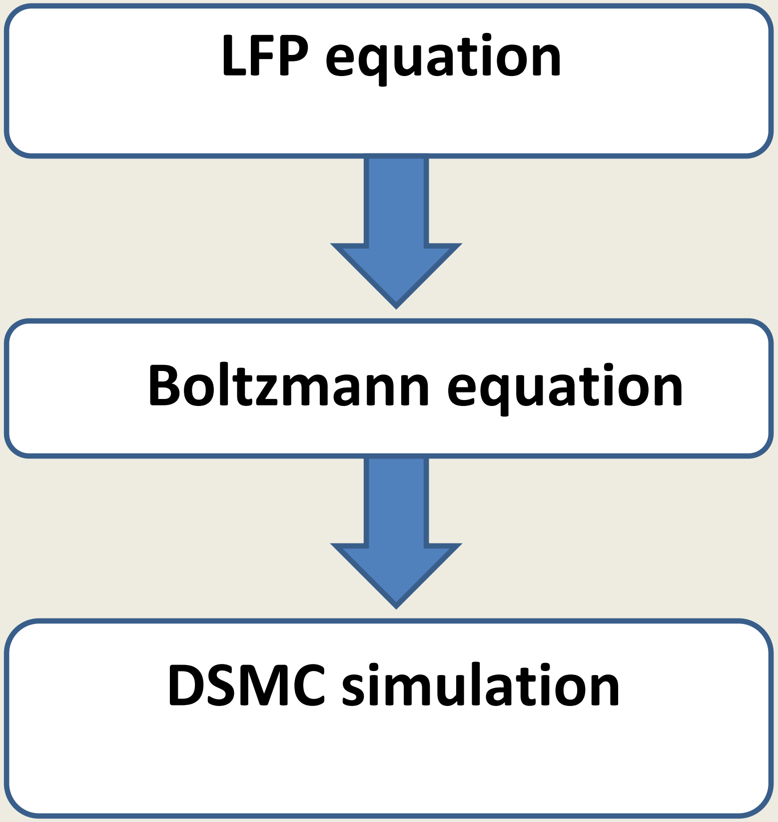
$$\lim_{\varepsilon \to 0} 2\pi \int_{-1}^{1} d\mu g_{\alpha\beta}(\mathrm{u}, \mu, \varepsilon)(1-\mu) = g_{\alpha\beta}^{(tr)}(\mathrm{u}),$$

$$\lim_{\varepsilon \to 0} 2\pi \int_{-1}^{1} d\mu g_{\alpha\beta}(\mathrm{u}, \mu, \varepsilon)(1-\mu)^{\mathrm{k}} = 0.$$

$$g_{\alpha\beta}(u, \mu, \varepsilon) = \frac{1}{2\pi\varepsilon} \delta\left[1 - \mu - \varepsilon a_{\alpha\beta}(u)\right]$$

$$a_{\alpha\beta}(u) = \begin{cases} g_{\alpha\beta}^{(tr)}(u), \; \text{for } 0 < \varepsilon g_{\alpha\beta}^{(tr)} \le 2 \\ 2/\varepsilon, \; \text{otherwise} \end{cases}$$

LFP equation and DSMC simulation



model cross section:

$$g_{\alpha\beta}(\mathrm{u},\mu,\varepsilon) = \frac{1}{2\pi\varepsilon}\delta\left[(1-\mu) - \varepsilon a_{\alpha\beta}(\mathrm{u})\right]$$

$$a_{\alpha\beta}(u) = \begin{cases} g_{\alpha\beta}^{(tr)}(u), \text{ for } & 0 < \varepsilon g_{\alpha\beta}^{(tr)} \le 2 \\ 2/\varepsilon, & \text{otherwise} \end{cases}$$

<u>Important consequences:</u>

$$\mu = \cos\theta = 1 - Min\left\{\frac{a\varepsilon}{\mathrm{u}^3}, 2\right\},\ \ a = const$$

$$g_{\alpha\beta}^{tot}(u,\varepsilon) = 2\pi\int_{-1}^{1} d\mu\, g_{\alpha\beta}\left(u,\mu,\varepsilon\right) = \varepsilon^{-1} = const$$

<u>The collision frequency of particles of any kind is constant</u> – “quasi Maxwellian”

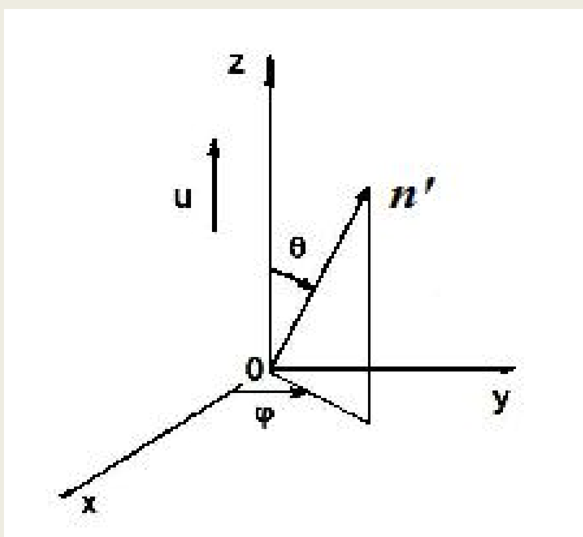
algorithm

$$V_N(t)=\{v_1(t),v_2(t),...,v_N(t)\}\in R_{3N} \rightarrow \left(\sum_{1\le i\le j\le n} p_{ij}=1,\right) \rightarrow \left\{v_i^{(\alpha)}, v_j^{(\beta)}\right\} \rightarrow$$

$$v'_i = \frac{1}{m_\alpha+m_\beta}(m_\alpha v_i + m_\beta v_j + m_\beta u n'), \quad v'_j = \frac{1}{m_\alpha+m_\beta}(m_\alpha v_i + m_\beta v_j - m_\alpha u n'); \rightarrow$$

$$\mu=\cos\theta = 1 - Min\left\{\frac{a\varepsilon}{u^3}, 2\right\}, \ a=const; \quad n'=\frac{u'}{|u|}, \quad \varphi=2\pi r, \ r\in[0,1); \rightarrow$$

$\tau_N - \varepsilon/N;$ $t=t+\tau_N;$ *after N steps:* $V_N=V_N(t+\Delta t)$



All conservation laws

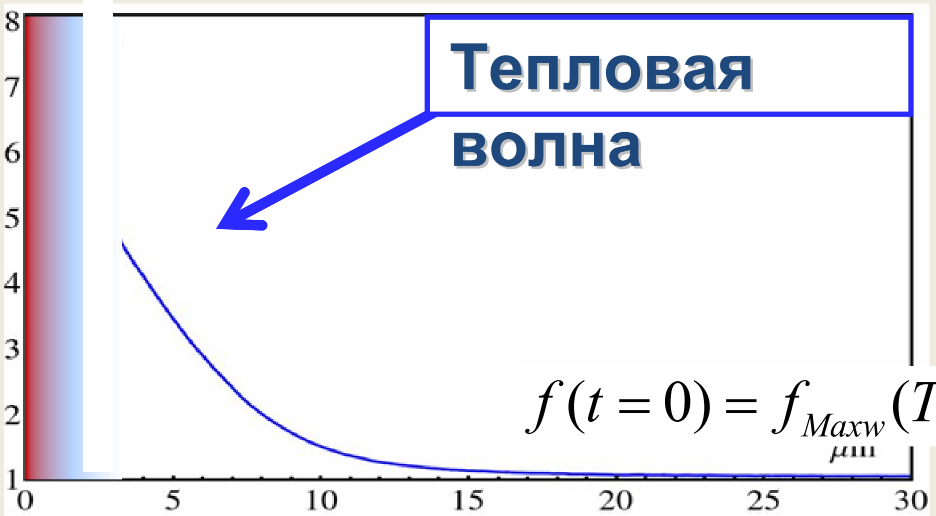
N operations

ЗАДАЧА О РАСПРОСТРАНЕНИИ ТЕПЛОВОЙ ВОЛНЫ

Горячая стенка:

$$T\big|_{x=0} = T_1\eta(t)$$

$$0 < \eta(t) \le 1$$



Хвосты функции распределения?

Многомасштабный характер задачи:

дебаевская длина : $\lambda_D = 3\times10^{-4}\,\mu m,\quad \omega_p^{-1} = 1.7\times10^{-4}\,ps;$

длина свободного пробега при $T_0 = 20\,eV$: $\lambda_{ei}(T_0) = 2.6\times10^{-3}\,\mu m,\quad \tau_{ei}(T_0) = 1.4\times10^{-3}\,ps;$

длина свободного пробега при $T_1 = 200\,eV$: $\lambda_{ei}(T_1) = 0.1\,\mu m,\quad \tau_{ei}(T_1) = 0.02\,ps;$

размеры задачи: $\tau_{расч} = 10\,ps\ [10^4\tau_{ei}(T_0)],\ L_{\min} \ge 50\,\mu m\ [2\times10^4\lambda_{ei}(T_0)]$

для параметров : $T_0 = 20\,eV,\ n_0 = 10^{22}\,cm^{-3},\ Z_i = 2.$

Advantage of DSMC

Multidimensional simulation – (1D…+3V)

3 conservation laws for collision operator

Speedy

Disadvantage of DSMC

Time limits /numerical noise, spurious heating/

Distribution function-?

If 1D+2V kinetic equation →

finite-difference scheme

Monte Carlo methods for LE Key references (predecessors):

- 1 **Takizuka and Abe** (1977);
- 2 **Nanbu** (1997);

The methods of TA and N are based on *heuristic* (physical) arguments.
In particular, Nanbu (1997) does not use any kinetic equation;
sophisticated cross-section

A general approach to Monte Carlo methods for Coulomb collisions

Bobylev and Potapenko, *J. Comp. Phys.,* 2013

Карпов, Потапенко, Физика плазмы, 2015

Бобылев, Потапенко, Карпов, Матем. Модел., 2012

Potapenko,.Bobylev, Mossberg, Transp. Theory Stat. Phys. 2008

Electron distribution function : $f(t, \mathbf{x}, \mathbf{v})$, fixed ions

$$\underbrace{\frac{\partial f}{\partial t} + \mathbf{v}.\nabla_{\mathbf{x}} f}_{\text{advection term}} + \underbrace{\frac{q}{m}(\mathbf{E} + \mathbf{v} \times \mathbf{B}).\nabla_{\mathbf{v}} f}_{\text{force term}} = \underbrace{C_{e,e}(f, f) + C_{e,i}(f)}_{\text{collisional terms}},$$

Maxwell equations

$$\frac{\partial \mathbf{E}}{\partial t} = -\,\mathbf{j} \qquad (Ampere) \qquad n_{e,i}(\mathbf{x}, t) = \int_{\mathbb{R}^3} f_{e,i}(\mathbf{x}, \mathbf{v}, t)\, d\mathbf{v},$$

$$\nabla_{\mathbf{x}}.\mathbf{E} = e\,(n_i - n_e) \qquad (Gauss) \qquad \mathbf{j} = q \int_{\mathbb{R}^3} f(\mathbf{x}, \mathbf{v}, t)\, \mathbf{v}\, d\mathbf{v}.$$

Parameters for the collisional processes analysis :

- the mean free path : λ_{ei},
- the thermal velocity : $v_{th} = \sqrt{\frac{k_B T}{m_e}}$,
- the electron-ion collision frequency : $\nu_{ei} = \frac{v_{th}}{\lambda_{e,i}}$.

$$\alpha = \frac{\lambda_{De}}{\lambda_{ei}}$$

Scaling used for collisional processes

$$\tilde{t} = \nu_{e,i} t, \qquad \tilde{x} = x / \lambda_{e,i}, \qquad \tilde{v} = v / v_{th}.$$

Dimensionless Fokker-Planck-Landau -Maxwell system

$$\frac{\partial f}{\partial t} + \mathbf{v}.\nabla_{\mathbf{x}} f - \nabla_{\mathbf{v}}.(\ \mathbf{E}\ f) = C_{e,e}(f,f) + C_{e,i}(f),$$

$$\frac{\partial \mathbf{E}}{\partial t} = -\frac{\mathbf{j}}{\alpha^2}, \qquad \nabla_{\mathbf{x}}.\mathbf{E} = \frac{1}{\alpha^2}(1-n),$$

Simplified case

Electrostatic case 1D2V : [x, v=|v|, cos(v^E)]

$$\begin{cases} \dfrac{\partial f}{\partial t} + v_x \partial_x f - E \partial_{v_x} f = C_{e,e}(f,f) + C_{e,i}(f), \\ \dfrac{\partial E}{\partial t} = -\dfrac{j}{\alpha^2}, \end{cases}$$

with Maxwell-Poisson satisfied at the initial time.

Remark Quasi-neutral regime : $\alpha = \dfrac{\lambda_{De}}{\lambda_{ei}} \to 0$

$$\begin{cases} \dfrac{\partial f}{\partial t} + v_x \partial_x f - E \partial_{v_x} f = C_{e,e}(f,f) + C_{e,i}(f), \\ j = 0, \end{cases}$$

with $n = 1$ at the initial time.

Reformulated system

$$\begin{cases} \dfrac{\partial f}{\partial t} + \partial_x(vf) - \partial_v(Ef) = C_{e,e}(f,f) + C_{e,i}(f), \\ -\alpha^2 \dfrac{\partial^2 E}{\partial t^2} + E \displaystyle\int_{\mathbb{R}} v \partial_v f dv = \partial_x\left(\int_{\mathbb{R}} v^2 f\right) dv - \int_{\mathbb{R}} C_{e,i} v dv, \end{cases}$$

with Maxwell-Poisson satisfied at the initial time.

Limit system when $\alpha \to 0$

$$\begin{cases} \dfrac{\partial f}{\partial t} + \partial_x(vf) - \partial_v(Ef) = C_{e,e}(f,f) + C_{e,i}(f), \\ E = \dfrac{\partial_x(\int_{\mathbb{R}} v^2 f dv) - \int_{\mathbb{R}} C_{e,i} v dv}{\int_{\mathbb{R}} v \partial_v(f) dv}, \end{cases}$$

with $n = 1$ and $j = 0$ at the initial time.

Numerical schemes

Discrete model / Problem of the classical scheme

Classical scheme for the Maxwell-Ampere electrostatic equation

$$\frac{E^{n+1} - E^n}{\Delta t} = -\frac{j^n}{\alpha^2}.$$

If $\lambda_{ei} >> \lambda_{De}$, quasi-neutrality : $\alpha \to 0$

$$j^n \Longrightarrow 0$$

$$E^{n+1} = \ ?$$

Stability condition for the classical scheme : $\Delta t \approx \alpha^2$

Discrete model *explicit scheme*

Electrostatic case with one dimension for space ($x \in \mathbb{R}$) and one for velocity ($v \in \mathbb{R}$) *(to shorten descrition)*

$$\frac{f^{n+1} - f^n}{\Delta t} + \nabla_x(v f^n) - \partial_v(E^{n+1} f^n) = C_{e,e}(f^n, f^n) + C_{e,i}(f^n).$$

Electric current : $\quad j^n = -\int_v f^n v \, dv,$

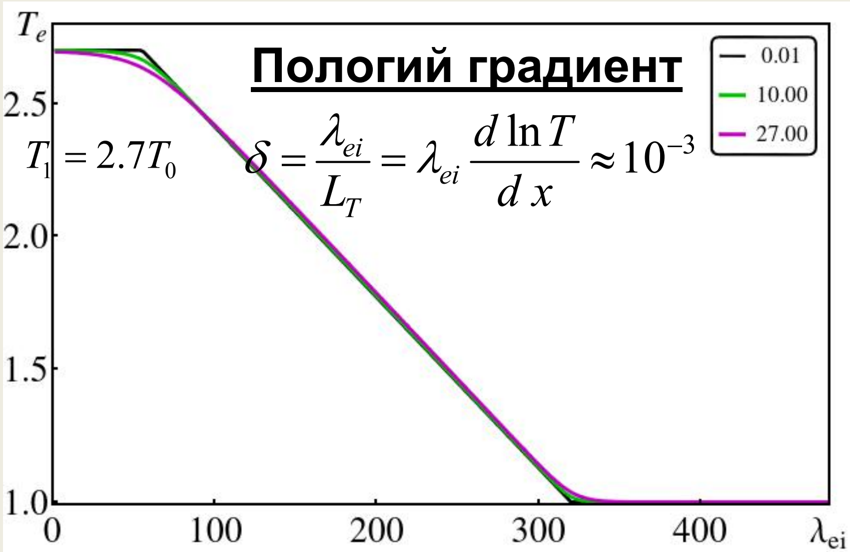
$$\begin{cases} \dfrac{j^{n+1} - j^n}{\Delta t} = \beta_1(f^n) E^{n+1} + \beta_2(f^n), \\ \dfrac{E^{n+1} - E^n}{\Delta t} = -\dfrac{j^{n+1}}{\alpha^2}. \end{cases}$$

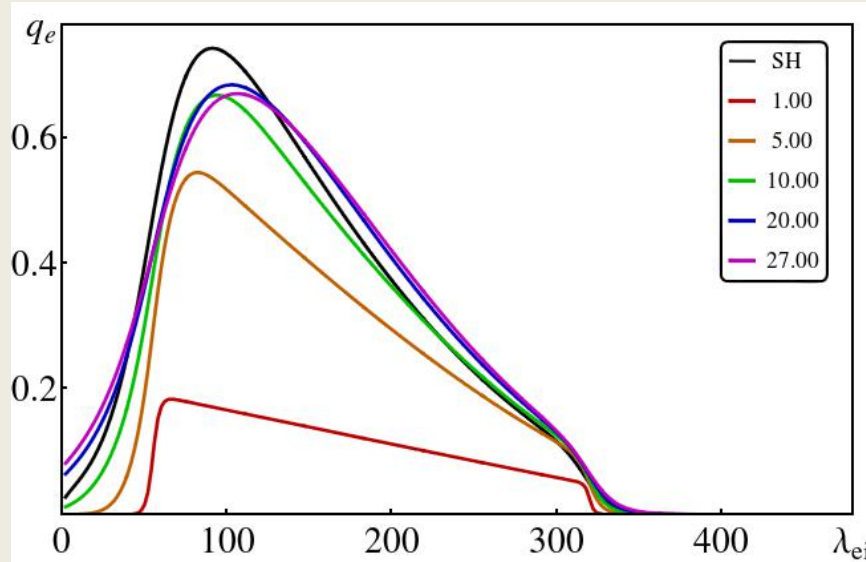
$$E^{n+1} = \frac{-\dfrac{\alpha^2 E^n}{\Delta t^2} + \beta_2(f^n) + \dfrac{j^n}{\Delta t}}{-\dfrac{\alpha^2}{\Delta t^2} - \beta_1(f^n)}.$$

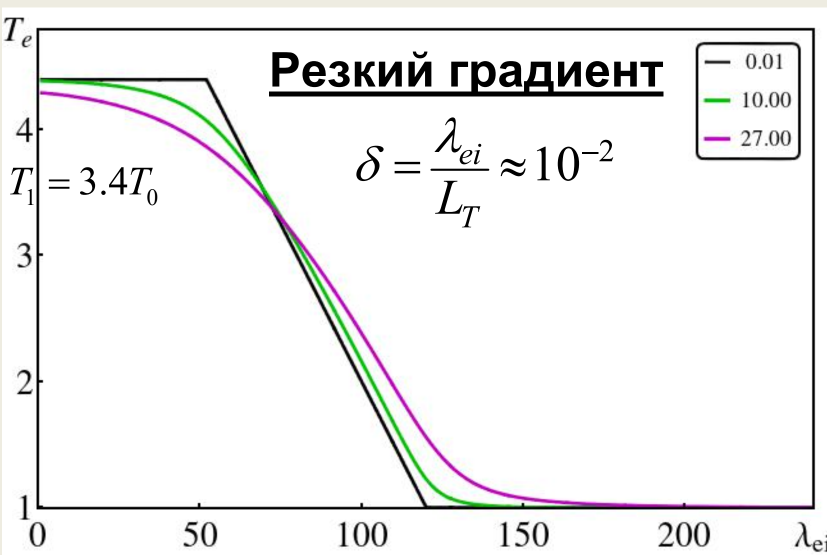
If $\alpha \to 0$ we can obtain E^{n+1}, Δt is not constrained by α.

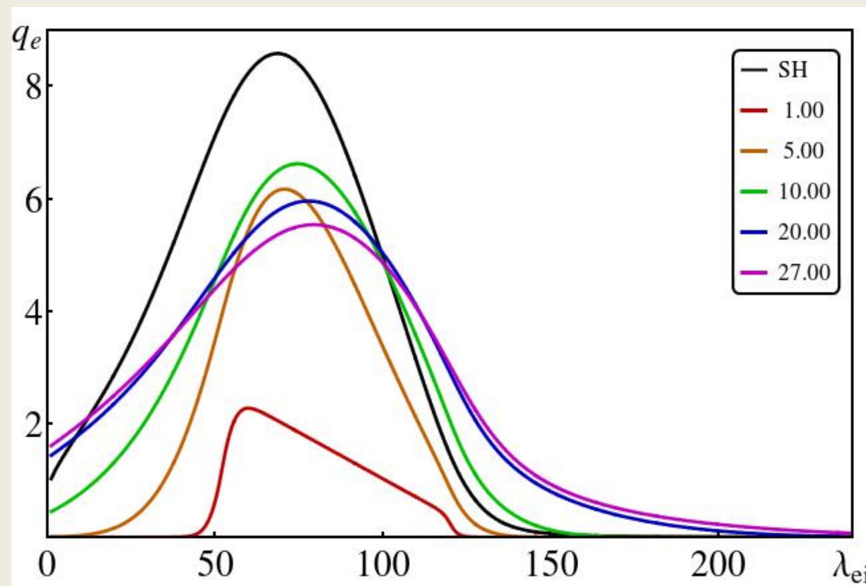
РЕЛАКСАЦИЯ НАЧАЛЬНОГО ПРОФИЛЯ ТЕМПЕРАТУРЫ

ЭВОЛЮЦИЯ ПРОФИЛЯ ТЕПЛОВОГО ПОТОКА СО ВРЕМЕНЕМ





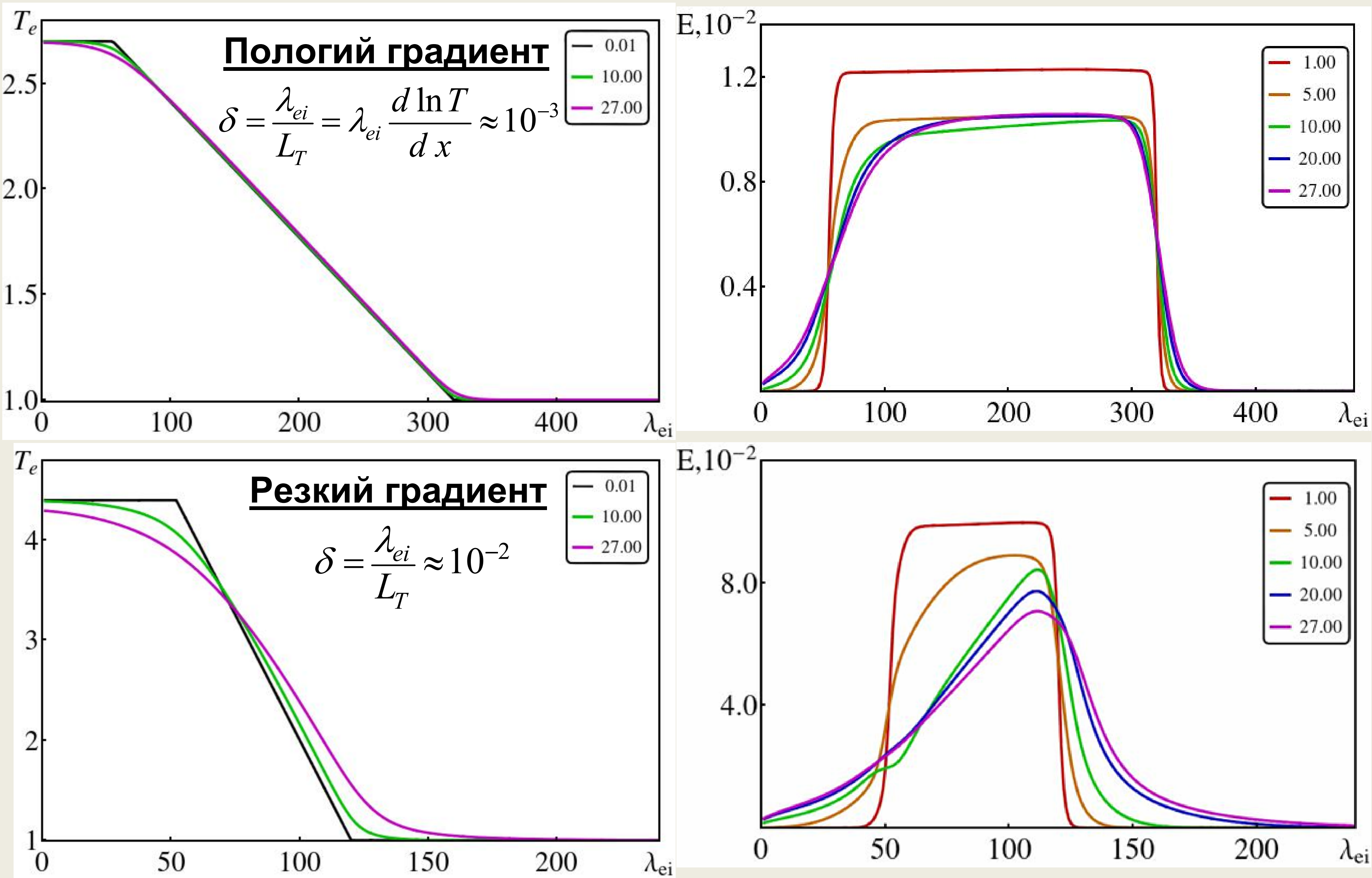




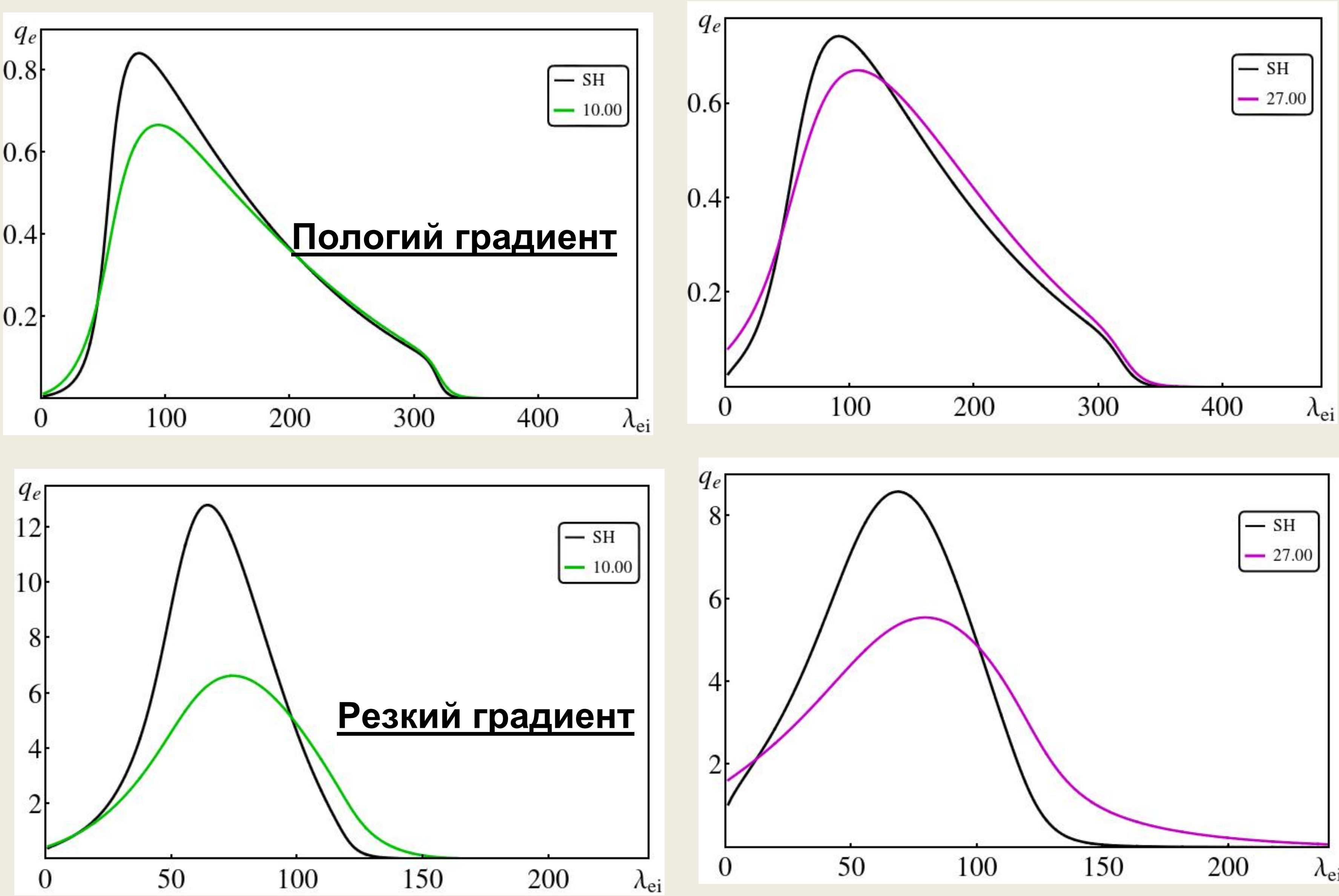
$$T_0 = 270\,eV,\, n_e = 5\cdot 10^{22}\,cm^{-3},\, Z = 4,\; m_i/m_e = 10^4$$

РЕЛАКСАЦИЯ НАЧАЛЬНОГО ПРОФИЛЯ ТЕМПЕРАТУРЫ

ПРОФИЛИ АМБИПОЛЯРНОГО ЭЛЕКТРИЧЕСКОГО ПОЛЯ



ЭВОЛЮЦИЯ ПРОФИЛЯ ТЕПЛОВОГО ПОТОКА СО ВРЕМЕНЕМ



T. Asahina, H. Nagatomo, A. Sunahara,T. Johzaki, M. Hata, K. Mima,and Y. Sentoku

Asymptotic-Preserving Schemes

F. Filbet and S.Jin J. Comp. Phys. 2010
P. Degond, et al   J. Comput. Phys. 2010

S. Guisset, S. Brull, B. Dubroca, E. d'Humieres, S. Karpov, I. Potapenko
Commun. in Comp. Phys. *2016*
Collision LFP operator: Potapenko,.Bobylev, Mossberg, Transp. Theory Stat. Phys. 2008

Nonlinear LFP collision integral is treated with completely conservative difference schemes

Self consistent electrical field is computed from the electronutrality condition at each time step.

Finite-difference explicit scheme → more accurate but time consuming

2 (exact) conservation laws for LFP operator. Constraints at v~0

СПАСИБО

ЗА ВНИМАНИЕ!..