ЕВРОПЕЙСКИ СЪЮЗ
ЕВРОПЕЙСКИ ФОНД ЗА РЕГИОНАЛНО РАЗВИТИЕ

ИКТ
ЦЕНТЪР ЗА ВЪРХОВИ ПОСТИЖЕНИЯ ПО ИНФОРМАТИКА И ИНФОРМАЦИОННИ И КОМУНИКАЦИОННИ ТЕХНОЛОГИИ

ОПЕРАТИВНА ПРОГРАМА
НАУКА И ОБРАЗОВАНИЕ ЗА ИНТЕЛИГЕНТЕН РАСТЕЖ

Нови алгоритми на метод Монте Карло за пряка симулация на газови течения

Стефан Стефанов
Институт по механика

- Outline:

Introduction

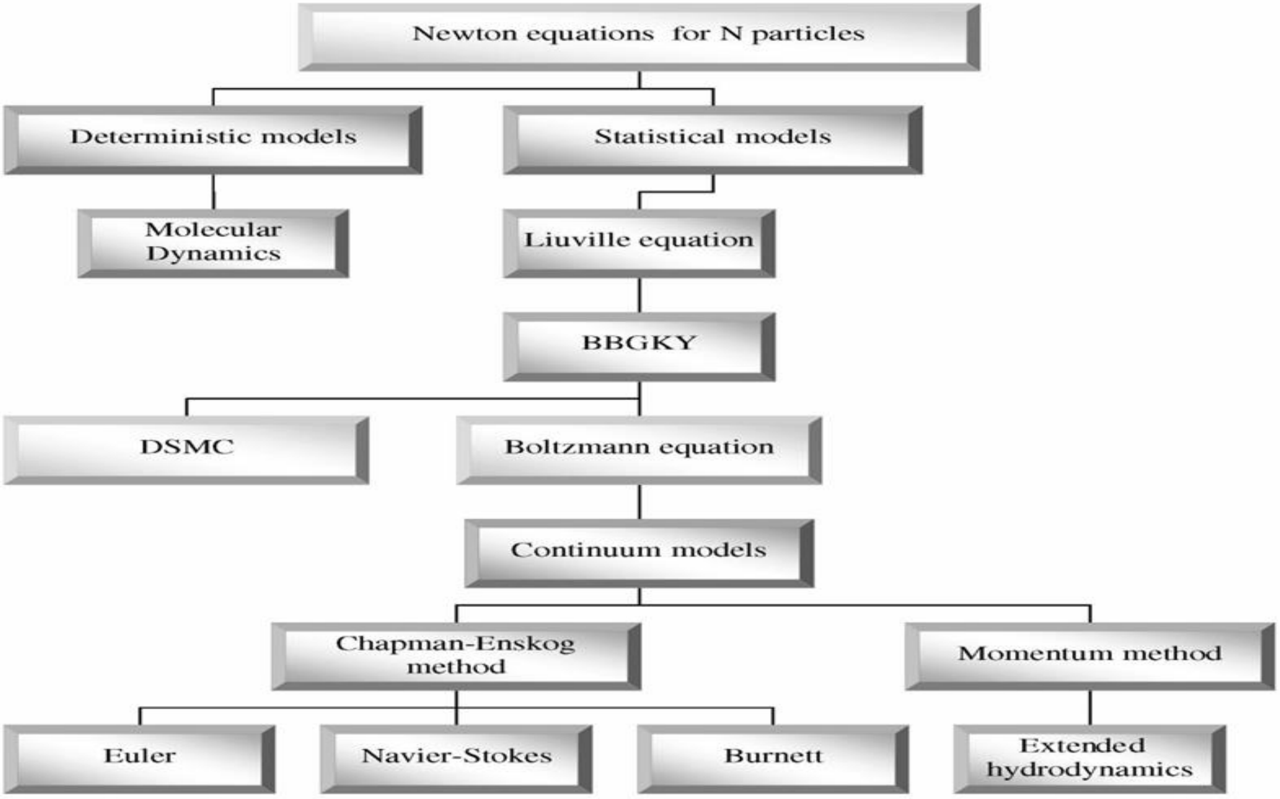
A novel non-homogeneous N-particle equation

Operator approach and new algorithms

Examples of simulations

Conclusions

Hierarchy of gas dynamics description



More details of the following statements are given in the paper

- S.K. Stefanov, *On the basic concepts of the direct simulation Monte Carlo method*, Phys. Fluids, 31 (2019) 067104

the Liouville equation can be rewritten in the form

$$\frac{\partial F_N(t,\mathbb{R},\mathbb{C})}{\partial t} = -\sum_{i=1}^{N} \mathbf{c}_i \frac{\partial F_N(t,\mathbb{R},\mathbb{C})}{\partial \mathbf{r}_i} + \sum_{1\le i<j\le N} \left\{ \int d\boldsymbol{\omega} \Phi_{i,j}(g_{i,j},\theta)\left[F_N(t,\mathbb{R}'_{i,j},\mathbb{C}'_{i,j}) - F_N(t,\mathbb{R},\mathbb{C}) \right] \right\}$$

$$\frac{\partial \tilde{F}_N(t,\mathbb{C})}{\partial t} = \frac{1}{V} \sum_{1\le i<j\le N} \left\{ \int g_{i,j} \left[\tilde{F}_N(t,\mathbb{C}'_{i,j}) - \tilde{F}_N(t,\mathbb{C}) \right] d\sigma_{i,j} \right\}$$

Kac master equation

- A novel non-homogenous and local N-particle equation

$$\frac{\partial \bar{F}_N(t,\mathbf{r},\mathbb{C})}{\partial t}+\sum_{i=1}^{N}\mathbf{c}_i\frac{\partial \bar{F}_N(t,\mathbf{r},\mathbb{C})}{\partial \mathbf{r}}=\sum_{1\le i<j\le N}\left\{\int g_{i,j}\left[\bar{F}_N(t,\mathbf{r},\mathbb{C}'_{i,j})-\bar{F}_N(t,\mathbf{r},\mathbb{C})\right]d\sigma_{i,j}\right\}$$

The new limit

$$\Delta t\to 0,\Delta r^{(l)}\to 0\left(V^{(l)}\to 0,\, M\to\infty\right),\ N=\sum_{l=1}^{M}N^{(l)}\text{- bounded}$$

is essentially different from

$$\Delta t\to 0,\ \Delta r^{(l)}\to 0, N^{(l)}\to\infty,\sigma_{i,j}\to 0,\ N^{(l)}\sigma_{i,j}^2\ -$$

the Boltzmann-Grad limit

Necessary condition $\left(g_{i,j}\sigma_{i,j}\Delta t/V^{(l)}\right)\le 1,\quad \sigma_{i,j}=\int d\sigma_{i,j}$

The new equation is the governing equation of the DSMC

The splitting scheme of DSMC

$$t < \tau \le t + \Delta t,\ l = 1, M$$

$$\left| \begin{array}{l} \tilde{F}^{*}_{N^{(l)}}\left(t+0, \mathbf{r}^{(l)}, \mathbb{C}^{(l)}\right) = \tilde{F}_{N^{(l)}}\left(t, \mathbf{r}, \mathbb{C}^{(l)}\right), \quad \mathbf{r} \in D^{(l)} \subset R^{3} \\ \dfrac{\partial \tilde{F}^{*}_{N^{(l)}}\left(t, \mathbf{r}^{(l)}, \mathbb{C}^{(l)}\right)}{\partial t} = \dfrac{1}{V^{(l)}} \sum_{1 \le i < j \le N^{(l)}} \left\{ \int g_{i,j} \left[\tilde{F}^{*}_{N^{(l)}}\left(t, \mathbf{r}^{(l)}, \mathbb{C}'^{(l)}_{i,j}\right) - \tilde{F}^{*}_{N^{(l)}}\left(t, \mathbf{r}^{(l)}, \mathbb{C}^{(l)}\right) \right] d\sigma_{i,j} \right\} \end{array} \right.$$

$$\left| \begin{array}{l} \tilde{F}^{**}_{N^{(l)}}\left(t+0, \mathbf{r}^{(l)}, \mathbb{C}^{(l)}\right) = \tilde{F}^{*}_{N^{(l)}}\left(t+\Delta t, \mathbf{r}^{(l)}, \mathbb{C}^{(l)}\right), \\ \dfrac{\partial \tilde{F}^{**}_{N^{(l)}}\left(t, \mathbf{r}^{(l)}, \mathbb{C}^{(l)}\right)}{\partial t} = -\sum_{i=1}^{N^{(l)}} \mathbf{c}_i \dfrac{\partial \tilde{F}^{**}_{N^{(l)}}\left(t, \mathbf{r}^{(l)}, \mathbb{C}^{(l)}\right)}{\partial \mathbf{r}} \end{array} \right. \quad \mathbf{r} \in D^{(l)}$$

$$\left| \begin{array}{l} F_{N}\left(t+\Delta t, \mathbf{r}, \mathbb{C}\right) = \sum_{l=1}^{M} \tilde{F}^{**}_{N^{(l)}}\left(t+\Delta t, \mathbf{r}^{(l)}, \mathbb{C}^{(l)}\right) \\ \tilde{F}_{N^{(l)}}\left(t+\Delta t, \mathbf{r}^{(l)}, \mathbb{C}^{(l)}\right) = \int_{D^{(l)}} F_{N}\left(t+\Delta t, \mathbf{r}, \mathbb{C}\right) d\mathbf{r}, \quad \mathbf{r} \in D \subset R^{3} \end{array} \right.$$

General transition operator

$$\frac{\partial \tilde{F}^*_{N^{(l)}}\left(t,\mathbf{r}^{(l)},\mathbb{C}^{(l)}\right)}{\partial t} = \Omega \tilde{F}^*_{N^{(l)}}\left(t,\mathbf{r}^{(l)},\mathbb{C}^{(l)}\right)$$, where

$$\Omega \tilde{F}^*_{N^{(l)}}\left(t,\mathbf{r}^{(l)},\mathbb{C}^{(l)}\right) = \frac{1}{V^{(l)}} \sum_{1\le i<j\le N^{(l)}} \left\{\int g_{i,j}\left[\tilde{F}^*_{N^{(l)}}\left(t,\mathbf{r}^{(l)},\mathbb{C}'^{(l)}_{i,j}\right) - \tilde{F}^*_{N^{(l)}}\left(t,\mathbf{r}^{(l)},\mathbb{C}^{(l)}\right)\right] d\sigma_{i,j}\right\}$$

$$\tilde{F}^*_{N^{(l)}}\left(t+\Delta t,\mathbf{r}^{(l)},\mathbb{C}^{(l)}\right) = \sum_{k=0}^{\infty} \frac{\Omega^k \tilde{F}^*_{N^{(l)}}\left(t,\mathbf{r}^{(l)},\mathbb{C}^{(l)}\right)}{k!} (\nu \Delta t)^k$$

$$\tilde{F}^*_{N^{(l)}}\left(t+\Delta t,\mathbf{r}^{(l)},\mathbb{C}^{(l)}\right) = G(\Delta t)\,\tilde{F}^*_{N^{(l)}}\left(t,\mathbf{r}^{(l)},\mathbb{C}^{(l)}\right)$$

$$\mathrm{G}(\Delta t) = \sum_{k=0}^{\infty} \frac{\Omega^k}{k!} (\nu \Delta t)^k = \exp\left[\Delta t \nu \left(\mathrm{T} - \mathrm{I}\right)\right]$$

Yanitskiy general transition operator

$$\mathrm{I}\psi = \psi, \quad \mathrm{T}_{i,j}\psi = \frac{1}{\sigma_{i,j}} \int_{4\pi} \psi\left(\mathbf{c}_i,\mathbf{c}_j\right)\sigma\left(g_{i,j},\theta\right) d\theta\, d\varepsilon,$$

$$\mathrm{T}\psi = \sum_{1\le i<j\le N^{(l)}} \omega_{i,j}\,\mathrm{T}_{i,j}\,\psi. \quad \nu = \sum_{1\le i<j\le N^{(l)}} \omega_{i,j} \quad \omega_{i,j} = \frac{\sigma_{i,j} g_{i,j}}{V^{(l)}}$$

- The general operator final form used for generating of DSMC collision schemes is given by

$$\mathrm{G}(\Delta t) = \exp\left[\Delta t \sum_{1 \le i < j \le N^{(l)}} \omega_{ij} \left(\mathrm{T}_{ij} - \mathrm{I}\right)\right]$$

No Time Counter (NTC) (Graeme Bird, 1986)

$$\nu_{\max} = \frac{N^{(l)}\left(N^{(l)} - 1\right)}{2} \frac{(\sigma g)_{\max}}{V^{(l)}} = \frac{N^{(l)}\left(N^{(l)} - 1\right)}{2} \omega_{\max}$$

$$\mathrm{G}_{\max}(\Delta t) = \mathrm{G}(\Delta t)$$

A new collision operator

$$\mathrm{T}_{\max,i,j} = \left(1 - \frac{\omega_{i,j}}{\omega_{\max}}\right)\mathrm{I} + \frac{\omega_{i,j}}{\omega_{\max}}\mathrm{T}_{i,j}$$

It describes exactly the acceptance-rejection procedure

$$w_{i,j} = \frac{\omega_{i,j}}{\omega_{\max}} = \frac{\sigma_{i,j} g_{i,j}}{(\sigma g)_{\max}}$$ - collision probability

$$N_{sel} = \lfloor \Delta t \nu_{\max} \rfloor, \quad \mathrm{frac}(\Delta t \nu_{\max}) = \Delta t \nu_{\max} - \lfloor \Delta t \nu_{\max} \rfloor$$

$$N_{sel} = O\left[\left(N^{(l)}\right)\right]$$

- An alternative approximation approach to the general transition operator is developed by Yanitskiy and used by Stefanov, Roohi and collaborators to derive a group of Bernoulli-trials schemes.
- Bernoulli-trials (BT) scheme (Yanitskiy, 1975)

$$\mathrm{G}\left(\Delta t\right)=\prod_{i=1}^{N^{(l)}-1}\prod_{j=i+1}^{N^{(l)}}\exp\left[\Delta t\omega_{i,j}\left(\mathrm{T}_{i,j}-\mathrm{I}\right)\right]$$

$$\mathrm{G}_{BT}\left(\Delta t\right)=\prod_{i=1}^{N^{(l)}-1}\prod_{j=i+1}^{N^{(l)}}\left[\left(1-\Delta t\omega_{i,j}\right)\mathrm{I}+\Delta t\omega_{i,j}\mathrm{T}_{i,j}\right] \qquad N_{sel}=O\left[\left(N^{(l)}\right)^{2}\right]$$

$w_{i,j}=\Delta t\omega_{i,j},\ w_{i,j}\le 1$ - collision probability

Simplified Bernoulli-trials (SBT) scheme (Stefanov, 2011)

$$\mathrm{G}_{SBT}(\Delta t) = \prod_{i=1}^{N^{(l)}-1} \left\{ \left[1 - \sum_{j=1}^{N^{(l)}} \frac{1}{k} \left(k\omega_{i,j} \Delta t \right) \right] \mathrm{I} + \sum_{j=1}^{N^{(l)}} \frac{1}{k} \left(k\omega_{i,j} \Delta t \right) \mathrm{T}_{i,j} \right\} \qquad k = N^{(l)} - i$$

$$N_{sel} = N^{(l)} - 1 \qquad O\left[\left(N^{(l)} \right) \right]$$

Generalized Bernoulli-trials (GBT) scheme (Roohi, Stefanov et. al., 2018)

$$\mathrm{G}_{GBT}(\Delta t) = \prod_{i=1}^{N_{sel}} \left\{ \left[1 - \sum_{j=1}^{N^{(l)}} \frac{1}{k'k} \left(k'k\omega_{i,j} \Delta t \right) \right] \mathrm{I} + \sum_{j=1}^{N^{(l)}} \frac{1}{k'k} \left(k'k\omega_{i,j} \Delta t \right) \mathrm{T}_{i,j} \right\}$$

$$k'k = \frac{N^{(l)} \left(N^{(l)} - 1 \right)}{N_{sel} \left(2N^{(l)} - N_{sel} - 1 \right)} \left(N^{(l)} - i \right)$$

$$1 \le N_{sel} \le N^{(l)} - 1 \qquad O\left[\left(N^{(l)} \right) \right]$$

$$k'k\omega_{i,j} \Delta t \le 1$$

No-time-counter NTC applied to a cell (l)	**Generalized Bernoulli-trials with $N_{sel} = N^{(l)} - 1$ (SBT) applied to a cell (l)**
Compute $A_{sel} = \frac{N^{(l)}\left(N^{(l)}-1\right)}{2} \frac{F_{num}(\sigma g)_{\max}}{V^{(l)}} \Delta t + \Delta A'_{sel}$ $N_{sel} = \lfloor A_{sel} \rfloor$ $\Delta A'_{sel} = A_{sel} - N_{sel}$	Compute $N_{sel} = N^{(l)} - 1$
1. Select a pair (i, j) at random from $N^{(l)}$ particles	1. Select first particle in order from the list $i = 1, \ldots, N_{sel}$; Select second particle (j) at random from $\left(N^{(l)} - i\right)$ particles after i_{th} particle in the list $j \in \left\{i+1, \ldots, N^{(l)}\right\}$
2. Accept collision of (i, j) with probability $w_{i,j} = \frac{\sigma_{i,j} g_{i,j}}{(\sigma g)_{\max}}$ and change $(\mathbf{c}_i, \mathbf{c}_j)$ to post-collision $(\mathbf{c}'_i, \mathbf{c}'_j)$	2. Accept collision (i, j) with probability $w_{i,j} = k'k \frac{F_{num}\sigma_{i,j} g_{i,j}}{V^{(l)}} \Delta t$ and change $(\mathbf{c}_i, \mathbf{c}_j)$ to post-collision $(\mathbf{c}'_i, \mathbf{c}'_j)$
Repeat 1and 2 for N_{sel} collision pairs	Repeat 1and 2 for N_{sel} collision pairs

Operator approach applied to the splitting scheme and hybrid transient adaptive operator

$$\mathrm{S}_{B+G}^{\Delta t} = \prod_{n=1}^{K} \mathrm{S}_{B+G}^{\Delta t/K} \approx \prod_{n=1}^{K} \mathrm{IB}\left(\Delta t / K\right)\left(\sum_{l=1}^{M} \mathrm{G}_{GBT-TAS}^{(l)}(N_{sel})\right)$$

$$\mathrm{G}_{GBT-TAS}^{(l)}(N_{sel}) = \left| \begin{array}{l} \sum_{l_s=1}^{\eta(l)^d} \mathrm{G}_{GBT}^{l_s}\left(N_{sel}, \Delta t^* = \tau\,\eta_{\max}/\eta(l), \Delta r / \eta(l)\right)\mathrm{I}^{(\eta(l))}, \quad t_s(l) \le n\tau \\ \mathbf{I}, \quad t_s(l) > n\tau \end{array} \right.$$

Hybrid Transient adaptive TAS algorithm

DSMChybridTAS

- **Numerical examples:**
- **Homogeneous BKW solution to the unsteady Boltzmann equation**
- Shoja-Sani, A., E. Roohi, and S. Stefanov, Homogeneous relaxation and shock wave problems: Assessment of the simplified and generalized Bernoulli trial collision schemes. Physics of Fluids, 2021. 33(3). https://doi.org/10.1063/5.0039071

$$f(v,0)=F(v,\beta_0)=\left(\frac{m(1+\beta_0)}{2\pi kT}\right)^{3/2}\left(1+\beta_0\left[\frac{m(1+\beta_0)}{2kT}v^2-\frac{3}{2}\right]\right)\exp\left(-\frac{m(1+\beta_0)}{2kT}v^2\right)$$

$$f(v,t)=F(v,\beta(t)) \qquad \beta(t)=\frac{\beta_0\exp(-\lambda_B t)}{1+\beta_0\left[1+\exp(-\lambda_B t)\right]} \qquad \left(0\le\beta_0\le 2/3\right)$$

$$\lambda_B=\frac{\pi n}{2}\frac{2kT}{3\pi\mu}=\frac{P}{3\mu} \qquad \mu=\frac{2}{3\pi}\left(\frac{m}{2\kappa}\right)^{1/2}\frac{kT}{A_2(5)}$$

$$< c_x^4 >= 3\left(\frac{kT}{m}\right)^2\frac{(1+2\beta(t))}{(1+\beta(t))^2}$$

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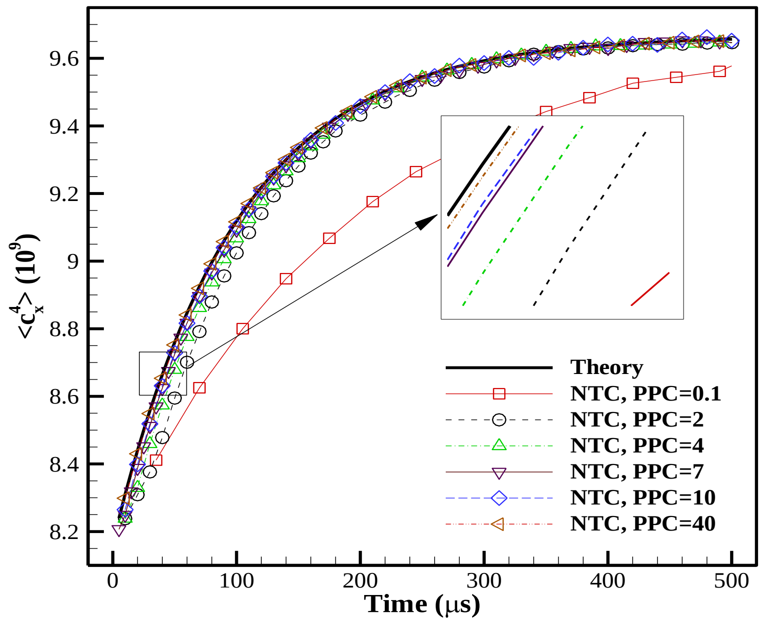
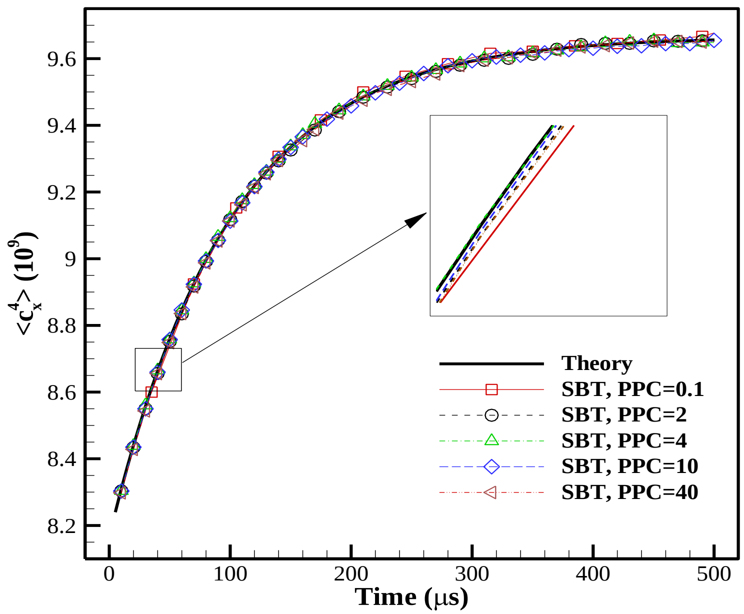
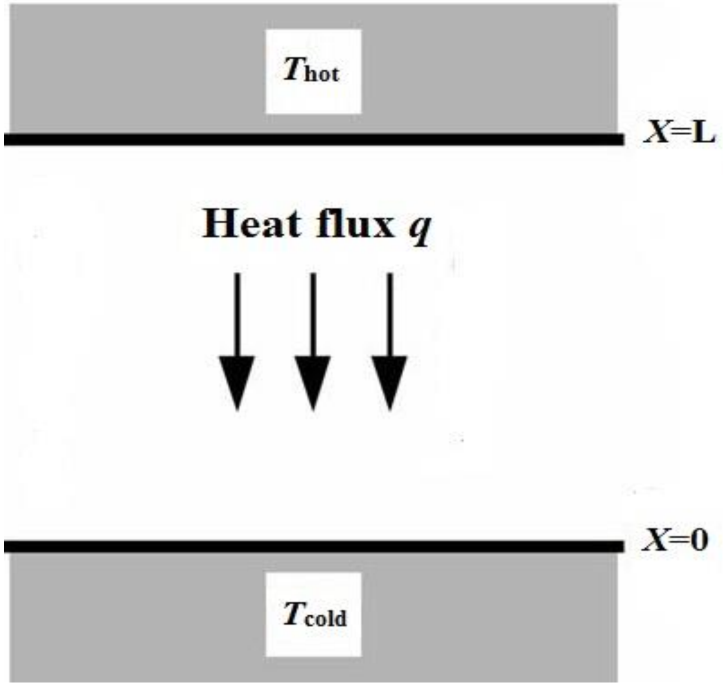




Pure heat conduction of a rarefied gas confined between two walls with different temperatures

S.K. Stefanov, On the basic concepts of the direct simulation Monte Carlo method, Phys. Fluids. 31 (2019) 067104

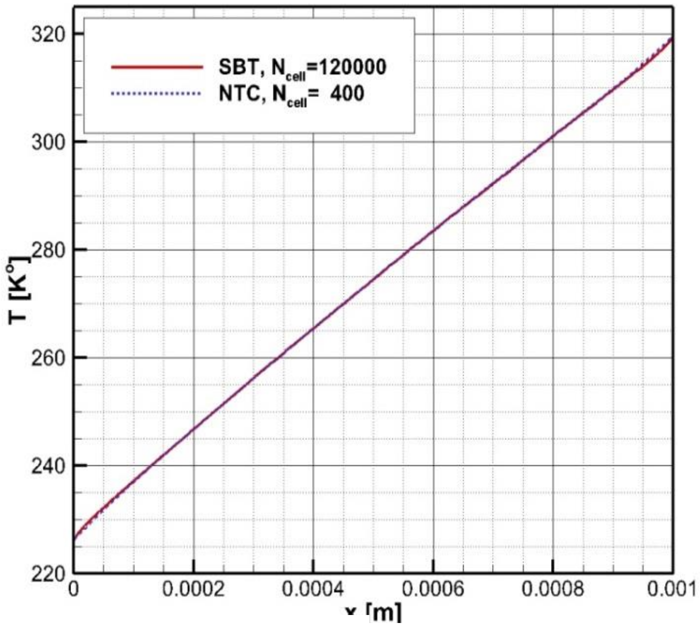


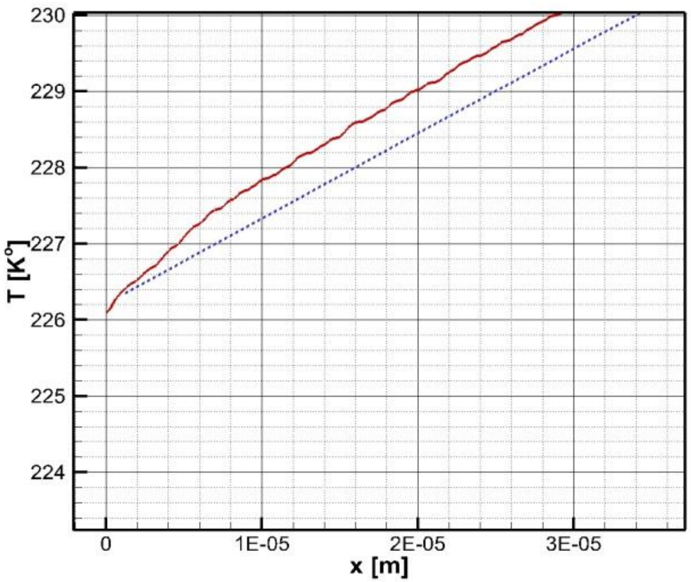
- Heat flux (computed at walls) with constant number of cells between walls and various total number of simulators in domain (a test with respect to the Boltzmann-Grad limit with various of simulators per cell)

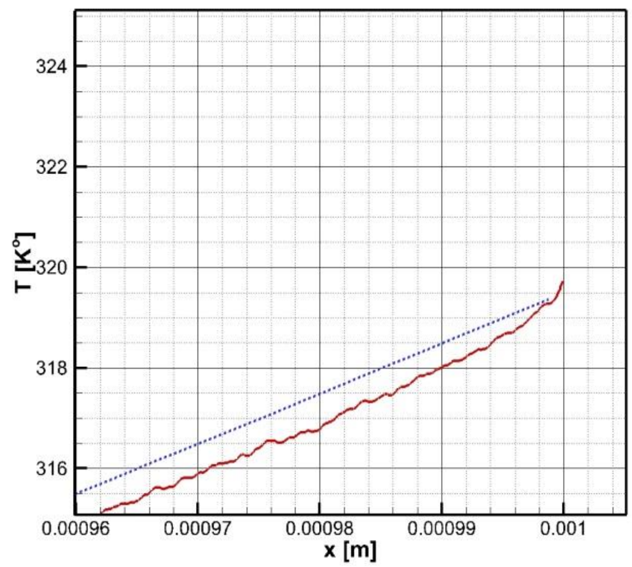
M (cells)	$\bar{N}^{(l)}$ (simulators)	$\lvert c'_m \Delta t \rvert / \Delta \mathbf{r}^{(l)}$	Q_{SBT}	Q_{NTC}	Q_{NN}	Samples
400	200	0.5	1511	1512	1513	500000
400	30	1.0	1514	1514	1515	1000000
400	10	1.0	1522	1501	1487	1500000
400	5	1.0	1536	1439	1430	3000000

Heat flux Q (computed at walls) with various number of cells M between walls and constant total number of simulators $N = 12000$ (a test with respect to the limit $\Delta t \to 0, \Delta r^{(l)} \to 0$ and $N = \sum_{l=1}^{M} N^{(l)}$ fixed).

M (cells)	$\bar{N}^{(l)}$ **(simulators)**	$\frac{\lvert c'_m \Delta t \rvert}{\Delta \mathbf{r}^{(l)}}$	Q_{SBT}	Q_{NTC}	Q_{NN}	$\frac{t_{SBT}}{t_{ref}}$	$\frac{t_{NTC}}{t_{ref}}$	$\frac{t_{NN}}{t_{ref}}$	Samples
400	30.0	1.0	1514	1514	1515	1.3	1.0	1.7	1000000
1200	10.0	1.0	1513	1504	1462	1.5	1.2	1.8	1000000
2400	5.0	1.0	1512	1501	1423	1.6	1.4	1.9	1000000
12000	1.0	1.0	1514	1265	1403	2.0	2.0	2.5	1000000
24000	0.5	1.0	1514			2.7			1000000
120000	0.1	1.0	1514			5.6			1000000

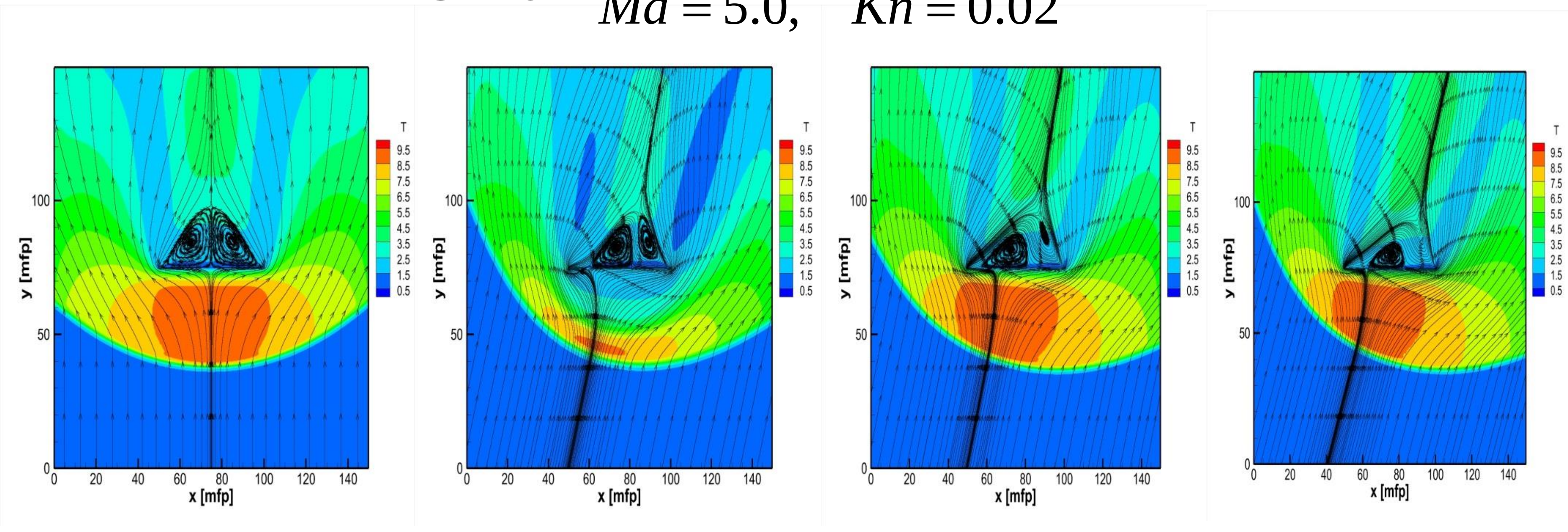

SBT, N_{cell}=120000
NTC, N_{cell}= 400
T [K°]
x [m]
320
300
280
260
240
220
0
0.0002
0.0004
0.0006
0.0008
0.001


T [K°]
x [m]
230
229
228
227
226
225
224
0
1E-05
2E-05
3E-05

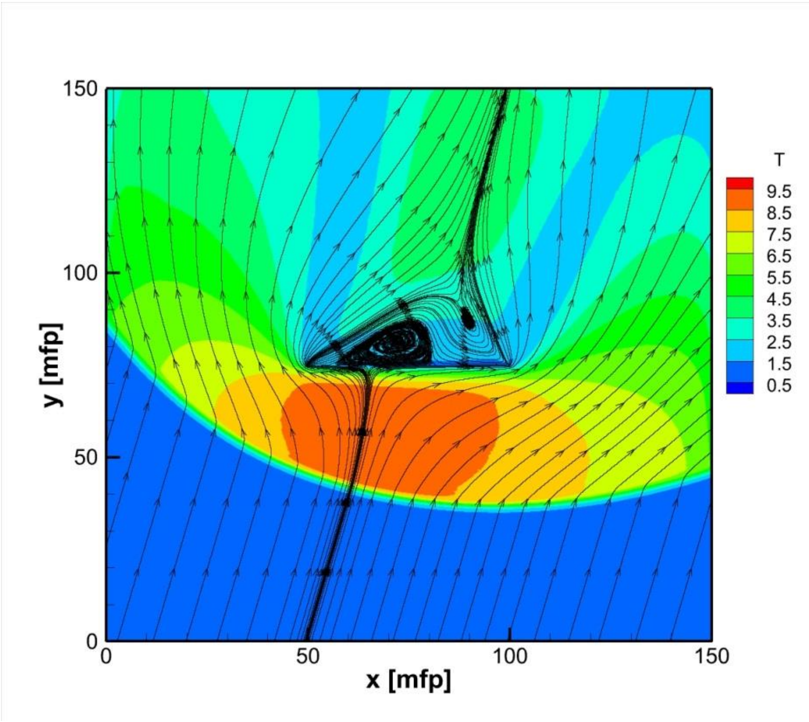

T [K°]
x [m]
324
322
320
318
316
0.00096
0.00097
0.00098
0.00099
0.001

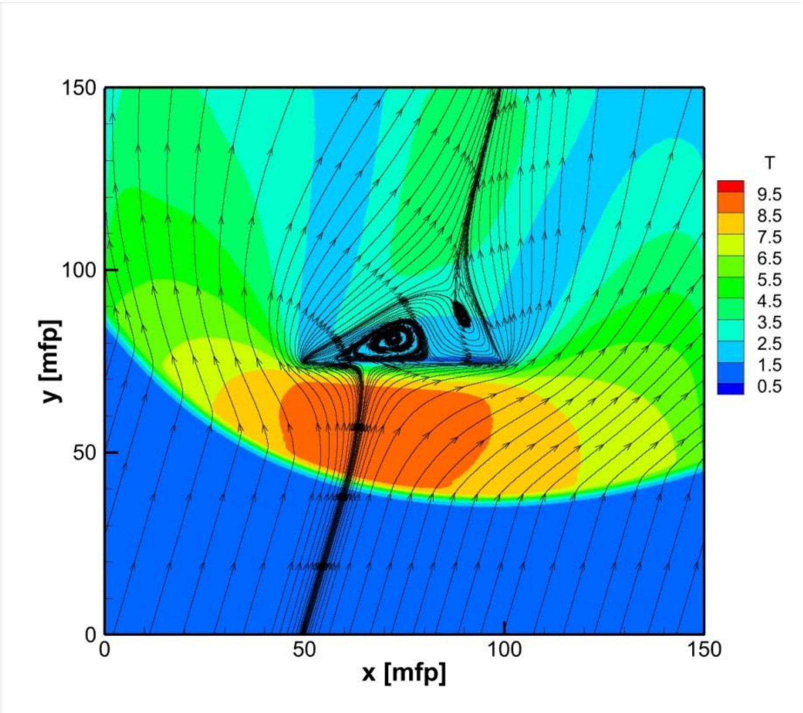
- **Two-dimensional supersonic flow around a cold flat plate at incidence angle** θ

$$Ma = 5.0, \quad Kn = 0.02$$



$\theta = 90^o$ $\theta = 80^o$ $\theta = 75^o$ $\theta = 70^o$

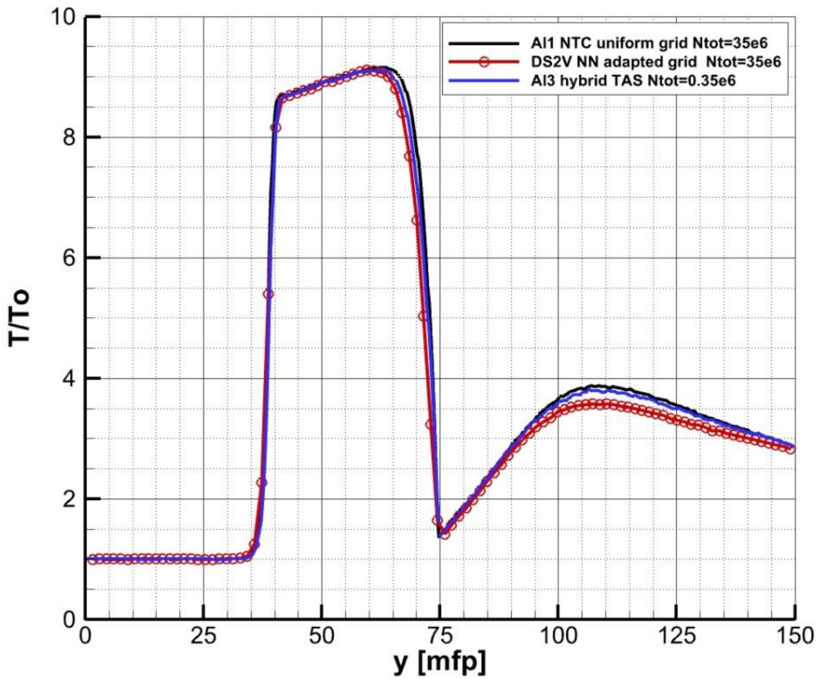




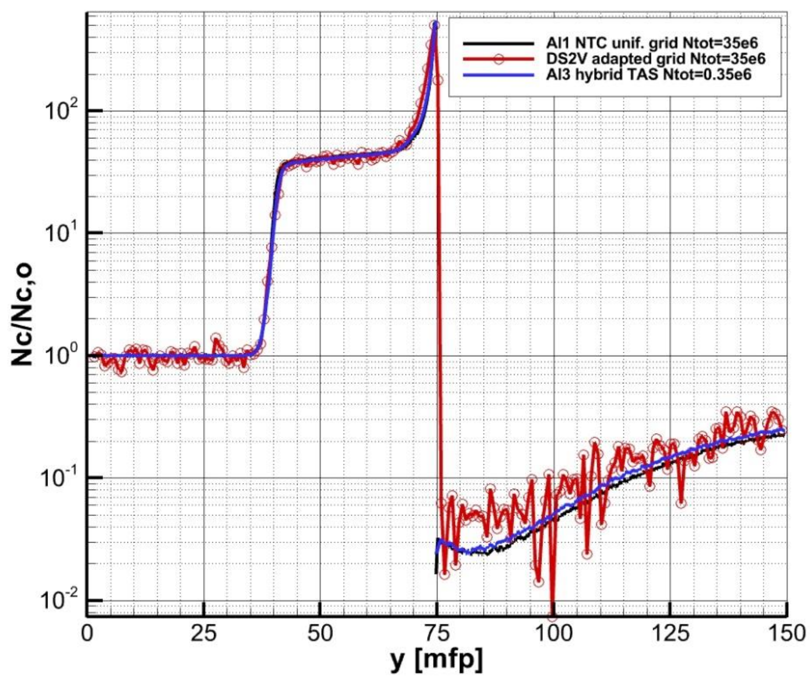
$$\theta = 75^o$$

Uniform grid, 800x800,
N=35 000 000

Hybrid TAS, 400x400
N= 350 000



Temperature profile $T(y)$ at $x=75$



Binary collision rate $N_c / N_{c,0}(y)$ at $x=75$

Conclusions

- A novel non-homogeneous N-particle kinetic equation has been derived. Its local 3D- character in physical space and 3N- dimensions in velocity space have required introduction of a randomized model of particle sets in cells of the mesh covering the computational domain. It has been found that the new equation asymptotically approximated the Boltzmann equation properties under specific conditions.
- The general transition operator describing the evolution of the randomized model during the collision process has been used to proof the derivation of all known DSMC collision schemes, including the standard NTC, from the collision operator of the randomized model.
- A new hybrid transient adaptive grid algorithm was created and tested on several benchmarks problems. The results showed that the hybrid TAS algorithm keeps accuracy within wide range of the total number of simulators.

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ACKNOWLEDGMENTS

- This work has been accomplished with the financial support by the Bulgarian Ministry of Education and Science by the Grant No BG05M2OP001-1.001-0003, provided by the SESG Operational Program (2014-2020) and co-financed by the European structural and investment funds.

Thank you for your attention!