Evaluation of the DSMC statistical error: generalization of approaches and understandable practical recommendations.

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Gas flow macroparameters

Gas flow macroparameters are expressed as the functionals of the distribution function

Number density:

$$\mathrm{n}(\mathrm{r}) = \int f(\mathrm{r}, v)\, d\, v$$

Velocity:

$$u_i(\mathrm{r}) = \frac{1}{\mathrm{n}(\mathrm{r})} \int v_i f(\mathrm{r}, v)\, d\, v$$

Temperature:

$$R\, T_i(\mathrm{r}) = \frac{1}{\mathrm{n}(\mathrm{r})} \int v_i^2\, f(\mathrm{r}, v)\, d\, v - \mathrm{v}_i^2(\mathrm{r})$$

$$i = 1, 2, 3$$

Gas flow macroparameters

Gas flow macroparameters are presented in the form of a rational functions from the mathematical expectations of random values ξ, η, ζ, which are functions of many-particle system state. Here h is cell indicator.

$$\mathrm{n}(\mathrm{r}) \approx \mathbf{E}\xi(X),$$

$$\xi(X) = \frac{1}{\Delta \mathrm{r}} \sum_{l=1}^{N} h(\mathrm{r}_l)$$

$$u_i(\mathrm{r}) \approx \frac{\mathbf{E}\eta_i(X)}{\mathbf{E}\xi(X)},$$

$$\eta_i(X) = \frac{1}{\Delta \mathrm{r}} \sum_{l=1}^{N} h(\mathrm{r}_l)\,(\mathrm{v}_l)_i$$

$$RT_i(\mathrm{r}) \approx \frac{\mathbf{E}\zeta_i(X)}{\mathbf{E}\xi(X)} - \left(\frac{\mathbf{E}\eta_i(X)}{\mathbf{E}\xi(X)}\right)^2,$$

$$\zeta_i(X) = \frac{1}{\Delta \mathrm{r}} \sum_{l=1}^{N} h(\mathrm{r}_l)\,(\mathrm{v}_l)_i^2$$

Note that random variables ξ, ηi, ζi correspond to three mechanical variables in a cell: density of mass, momentum and kinetic energy. So hydrodynamic variables (such as fluid velocity and temperature) are defined in terms of mechanical variables.

Time-averaged estimates

The DSMC method is based on the assumption that the steady process under examination is ergodic one. So the mathematical expectations are estimated by averaging a values of the functions ξ, η_i, and ζ_i taken at equal time intervals Δt :

$$\mathbf{E}\,\xi(X) \approx \tilde{\xi}_K = \frac{1}{K}\sum_{k=1}^{K}\xi(X_k) = \frac{1}{K}\sum_{k=1}^{K}\xi_k$$

X_k is state of many-particle system in time moment $t_k = k\,\Delta t$

Time-averaged estimates

The time-averaged estimates of macroparameters have the following form:

Number density:

$$n(r) \approx \tilde{\xi}_K = \frac{1}{K}\sum_{k=1}^{K} \xi_k ,$$

Velocity:

$$u_i(r) \approx \tilde{\upsilon}_{i,K} = \frac{\frac{1}{K}\sum_{k=1}^{K} \eta_{i,k}}{\frac{1}{K}\sum_{k=1}^{K} \xi_k},$$

Temperature:

$$RT_i(r) \approx \tilde{\vartheta}_{i,K} = \frac{\frac{1}{K}\sum_{k=1}^{K} \zeta_{i,k}}{\frac{1}{K}\sum_{k=1}^{K} \xi_k} - \left(\frac{\frac{1}{K}\sum_{k=1}^{K} \eta_{i,k}}{\frac{1}{K}\sum_{k=1}^{K} \xi_k} \right)^2$$

Time-averaged estimates

Estimates of hydrodynamic variables (the velocity and temperature) can be represented as a rational function of the sample averages of mechanical variables:

Velocity:

Temperature:

$$\left.\begin{matrix}\tilde{\upsilon}_{i,K} \\ \tilde{\vartheta}_{i,K}\end{matrix}\right\} = Q\left(\tilde{\xi}_K, \tilde{\eta}_{i,K}, \tilde{\zeta}_{i,K}\right),$$

Here

$$\tilde{\xi}_K = \frac{1}{K}\sum_{k=1}^{K} \xi_k,$$

$$\tilde{\eta}_{i,K} = \frac{1}{K}\sum_{k=1}^{K} \eta_{i,k},$$

$$\tilde{\zeta}_{i,K} = \frac{1}{K}\sum_{k=1}^{K} \zeta_{i,k}$$

Statistical error of DSMC method

1. **Hadjiconstantinou N, Garcia A, Bazant M, He G.** Statistical Error in Particle Simulations of Hydrodynamic Phenomena // J Comp Phys 2003.

1a. **Garcia A.** Estimating Hydrodynamic Quantities in the Presence of Microscopic Fluctuations // Commun. Appl. Math. Comput. Sci. 2006.

2. **Rogasinsky S.V., Levin D.A., Ivanov M.S.** Statistical errors of DSMC results for rarefied gas flow // Proc. of the 25-th Intern. Symp. on Rarefied Gas Dynamics, 2007.

3. **Plotnikov M.Yu., Shkarupa E.V.** Selection of sampling numerical parameters for the DSMC method // Computers & Fluids. 2012.

Equilibrium statistical mechanics

1. Hadjiconstantinou N, Garcia A, Bazant M, He G. Statistical Error in Particle Simulations of Hydrodynamic Phenomena. J Comp Phys 2003; 187: 274-297.

In the case of thermodynamic equilibrium ***variances*** of density, velocity and total temperature estimates have the following forms:

for number density estimate:

$$\mathbf{V}\,\tilde{\xi}_K = \frac{1}{K}\frac{1}{\Delta r}\,n(r),$$

for velocity estimates:

$$\mathbf{V}\,\tilde{\upsilon}_{i,K} = \frac{1}{K}\frac{1}{\Delta r}\frac{R\,T(r)}{n(r)},$$

for temperature estimate:

$$\sum_{i=1}^{3} \mathrm{V}\,\tilde{\vartheta}_{i,K} = \frac{1}{K}\frac{1}{\Delta r}\frac{2\,T^2(r)}{n(r)}$$

Equilibrium statistical mechanics

1a. Garcia A. Estimating Hydrodynamic Quantities in the Presence of Microscopic Fluctuations // Commun. Appl. Math. Comput. Sci. 2006. V.1. P.53-78.

Note that interesting connection between statistical error and fluctuations of physical variables at thermodynamic equilibrium is considered in the work 1a.

Equilibrium statistical mechanics

- Since this approach is based on the equilibrium statistical mechanics one naturally expects that it is applicable if all components of temperature are equivalent or near to equivalent.

- There is no rigorous justification of applicability of the equilibrium statistical mechanics to a non-equilibrium rarefied gas flow.

- This fact limits an application area of this approach because the flows with regions of strong non-equilibrium are of major interest in the rarefied gas dynamics.

Asymptotic behavior as $\Delta r \to 0$

2. Rogasinsky S.V., Levin D.A., Ivanov M.S. Statistical errors of DSMC results for rarefied gas flow // Proc. of the 25-th Intern. Symp. on Rarefied Gas Dynamics, 2007. P. 391-395.

The authors of the second work propose the asymptotic formulas for variances of the DSMC estimates provided that $\Delta r \to 0$.

$$\mathbf{V}\widetilde{\xi}_K \sim \frac{1}{K}\frac{1}{\Delta \mathrm{r}}\mathrm{n}(\mathrm{r}), \quad \mathbf{V}\widetilde{v}_{i,K} \sim \frac{1}{K}\frac{1}{\Delta \mathrm{r}}\frac{R\,\mathrm{T}_i(\mathrm{r})}{\mathrm{n}(\mathrm{r})},$$

$$\mathbf{V}\widetilde{\vartheta}_{i,K} \sim \frac{1}{K}\frac{1}{\Delta \mathrm{r}}\frac{1}{\mathrm{n}(\mathrm{r})}\left(-4u_i^4 - \left\langle v_i^2 \right\rangle^2 + 8u_i^2\left\langle v_i^2 \right\rangle - 4u_i\left\langle v_i^3 \right\rangle + \left\langle v_i^4 \right\rangle\right)$$

$$\left\langle v_i^j \right\rangle = \int v_i^j \, f(\mathrm{r}, v)dv \Big/ \mathrm{n}(\mathrm{r})$$

Asymptotic behavior as $\Delta r \to 0$

- This approach produces results, partially coinciding with the first one (namely for estimates of density and flow velocity).

- Note that this approach allows evaluating the variance of estimates of velocity components and temperature components.

- It requires calculating additionally third and fourth moment of distribution function for evaluation of the variance of the temperature estimates.

$$\left\langle v_i^3 \right\rangle = \int v_i^3 \, f(\mathrm{r}, v)\, dv \Big/ \mathrm{n}(\mathrm{r})$$

$$\left\langle v_i^4 \right\rangle = \int v_i^4 \, f(\mathrm{r}, v)\, dv \Big/ \mathrm{n}(\mathrm{r})$$

Central limit theorem for Markov process

The DSMC simulation process is a stationary Markov process with discrete time, so the central limit theorem for Markov processes is applicable to the method estimates.

3. Plotnikov M.Yu., Shkarupa E.V. Selection of sampling numerical parameters for the DSMC method. // Computers & Fluids. 2012. Vol. 58. P. 102-111.

Approach proposed in third work is based on the theory of Markov processes. It takes into account the time correlations of the sampled realizations.

Central limit theorem for Markov process

For example, this theorem gives the following expression for estimate of number density:

$$\mathbf{V}\tilde{\xi}_K \sim \frac{1}{K} 2\tau_\xi \mathbf{V}\xi, \quad \text{as} \quad K \to \infty$$

$$\tau_\xi = \frac{1}{2} + \sum_{k=1}^{\infty} \rho_{\xi,k}$$

is correlation time of stationary random process ξ

It characterizes the time intervals during which some dependence between states of process still remains.

$$\rho_{\xi,k} = \frac{1}{\mathbf{V}\xi} \mathbf{E}\big(\xi(s) - \mathbf{E}\xi\big)\big(\xi(s+k) - \mathbf{E}\xi\big)$$

$$2\tau_\xi = \frac{1 + \rho_{\xi,1}}{1 - \rho_{\xi,1}}$$

Common for all approaches in the case of independent samples

The asymptotic representation of variances of hydrodynamic variables in terms of variances and covariances of mechanical variables:

$$\mathbf{V}\, Q\left(\tilde{\gamma}_{1,K}, \ldots, \tilde{\gamma}_{l,K}\right)_K = \frac{1}{K} \sum_{i,j=1}^{l} F_{i,j}\left(\mathbf{E}\,\gamma_1, \ldots, \mathbf{E}\,\gamma_l\right) \operatorname{cov}\left(\gamma_i \gamma_j\right),$$

as $K \to \infty$

where $Q\left(\tilde{\xi}_K, \tilde{\eta}_{i,K}, \tilde{\zeta}_{i,K}\right)$ is general form of the estimate

Difference of approaches in the case of independent samples

Covariances of mechanical variables are evaluated

- **First approach:** in the frame of equilibrium statistical mechanics. Variances of estimates include only density and temperature in a cell.
- **Second approach:** asymptotically as $\Delta\mathbf{r} \to 0$. Third and fourth distribution function moments are to be calculated in process of the DSMC simulation.
- **Third approach** – numerically in process of the DSMC simulation.

Note that second and third approaches are available at any degree of non-equilibrium.

Theoretical analysis of approaches in the case of independent samples

The way of direct evaluation at equilibrium from the work

> Garcia A. Estimating Hydrodynamic Quantities in the Presence of Microscopic Fluctuations // Commun. Appl. Math. Comput. Sci. 2006. V.1. P.53-78.

It includes assumptions that particles are independent and distribution function is Maxwellian.

Analysis shows that all approaches give the same result for estimate of density and velocity.

Whereas the formula for variance of the temperature estimate in the second approach differs from one in the first approach. This is due to neglect of terms which is small while $\Delta \mathbf{r} \to 0$.

Conclusions
in the case of independent samples

- The first approach (equilibrium statistical mechanics) is the most promising for the approximate evaluation of the statistical errors due to its simplicity (no additional calculations). There is doubt about validity of it to a non-equilibrium rarefied gas flow. However our numerical experiments have shown the possibility of using this approach for approximate evaluation of the statistical error.

- The second (asymptotic evaluating of the variances) and the third (CLT for Markov processes) approaches to evaluation of the statistical errors are constructed in the most general assumptions. However they require additional computations.

Difference of approaches in the case of dependent samples

- In the first approach the correction factor is proposed to use for the account of dependence by analogy with the "persistent random walks".

- The second approach (asymptotic evaluating of variances) leaves out of account the dependencies of samples. So it is applicable only if samples are independent.

Difference of approaches in the case of dependent samples

The third approach (CLT for Markov processes) is available at any degree of dependence of samples. Here asymptotic representation of variances contains multiplier which allows for dependence of samples:

$$\mathbf{V}\, Q\left(\tilde{\gamma}_{1,K}, \dots, \tilde{\gamma}_{l,K}\right)_K = \frac{1}{K} \sum_{i,j=1}^{l} F_{i,j}\left(\mathbf{E}\,\gamma_1, \dots, \mathbf{E}\,\gamma_l\right) \operatorname{cov}\left(\gamma_i \gamma_j\right) 2\sqrt{\tau_i \tau_j},$$

as $K \to \infty$, where $2\tau_i = \dfrac{1+\rho_{i,1}}{1-\rho_{i,1}}$

Approximate approach

We propose to use a simple combined approach to the evaluation of the statistical error, which includes the use of formulas for the variance in the case of independent samples, based on statistical mechanics, and approximate analytical expression for the correlation ρ_{ξ}.

for number density estimate:

$$\mathbf{V}\tilde{\xi}_K = \frac{1}{K}\frac{\mathrm{n}(\mathrm{r})}{\Delta \mathrm{r}}\left(\frac{1+\rho_{\xi,1}}{1-\rho_{\xi,1}}\right),$$

for velocity estimates:

$$\mathbf{V}\,\tilde{\upsilon}_{i,K} = \frac{1}{K}\frac{R\,\mathrm{T}_i(\mathrm{r})}{\Delta \mathrm{r}\;\mathrm{n}(\mathrm{r})}\left(\frac{1+\rho_{\xi,1}}{1-\rho_{\xi,1}}\right),$$

for temperature estimates:

$$\mathbf{V}\,\tilde{\vartheta}_{i,K} = \frac{1}{K}\frac{1}{\Delta \mathrm{r}}\frac{2\,\mathrm{T}_i^{\,2}(\mathrm{r})}{\mathrm{n}(\mathrm{r})}\left(\frac{1+\rho_{\xi,1}}{1-\rho_{\xi,1}}\right)$$

Way to evaluate correlation $\rho_{\xi,1}$

It has been shown that under certain conditions, the correlation coefficient is close to the part of particles remaining in the cell after the next time step:

$$\rho_{\xi,1} \approx p$$

p denotes mathematical expectation of the fraction of particles remaining in a cell after particles motion per a time step.

Way to evaluate correlation $\rho_{\xi,1}$

The expectation p is evaluated provided that the following two assumptions are valid:

1. the particles are uniformly distributed in a cell, and the distribution function of the particle velocity is almost spatially homogeneous in the cell;
2. the distribution function of the particle velocity is the Maxwellian distribution function on each coordinates:

$$f(v) = f_1(v_1) f_2(v_2) f_3(v_3)$$

$$f_i(v_i) = \frac{\beta_i}{\sqrt{\pi}} \exp\left(-\beta_i^2 (v_i - \mathbf{v}_i)^2\right), \quad \beta_i = \frac{1}{\sqrt{2RT_i}}$$

Way to evaluate $\rho_{\xi,1}$

For simplicity we present formulas for one-dimensional problem in the case of zero flow velocity. One-dimensional cell can be denoted by the interval $[0, h]$

The fraction of particles that remain in cell is represented by the following integral

$$p = \frac{\beta_i}{h\sqrt{\pi}} \int_0^h \int_{-\frac{x}{\Delta t}}^{\frac{h-x}{\Delta t}} \exp\left(-\beta^2 v^2\right)$$

After the necessary transformations we obtain the formula:

$$p = \operatorname{erf}(s) + \frac{1}{s\sqrt{\pi}} \exp\left(-s^2\right) - \frac{1}{s\sqrt{\pi}}, \quad s = \frac{\beta h}{\Delta t}$$

Approximate approach

- The approximate approach was tested on the examples of a number of characteristic problems of the rarefied gas dynamics with different degree of non-equilibrium:
  - the Fourier problem,
  - the Couette problem,
  - the problem of supersonic flow through a permeable obstacle.

- Performed calculations have shown the possibility of using the approximate approach for the evaluation of the DSMC statistical error.

Thank you
for your attention!