A general variance-reduced particle method for solving kinetic equations

Mohsen Sadr and Nicolas Hadjiconstantinou

Department of Mechanical Engineering, MIT, Cambridge, MA 02139, USA

Variance reduction with importance weights

The idea is to reduce the variance of non-equilibrium simulation using its correlation to an equilibrium simulation with known analytical moments. Let us rewrite $R(\boldsymbol{v}) \in \{1, \boldsymbol{v}, ...\}$ moments of particle distribution f as

$$\int R(\boldsymbol{v}) f(\boldsymbol{v}|\boldsymbol{x},t) d^3\boldsymbol{v} = \int R(\boldsymbol{v}) \left(1 - w(\boldsymbol{v}|\boldsymbol{x},t)\right) f(\boldsymbol{v}|\boldsymbol{x},t) d^3\boldsymbol{v} + \int R(\boldsymbol{v}) f^{\mathrm{eq}}(\boldsymbol{v}|\boldsymbol{x},t) d^3\boldsymbol{v}$$

$$\text{where} \quad w(\boldsymbol{v}|\boldsymbol{x},t) = \frac{f^{\mathrm{eq}}(\boldsymbol{v}|\boldsymbol{x},t)}{f(\boldsymbol{v}|\boldsymbol{x},t)} \, .$$

Instead of explicitly performing the parallel equilibrium simulation, the weight w allows computing its moments using particles of non-equilibrium simulation. The variance-reduced estimate is computed via [1]

$$\Big\langle R(\boldsymbol{v}) f(\boldsymbol{v}|\boldsymbol{x},t) \Big\rangle_{\mathrm{VR}} = N_{\mathrm{eff}} \sum_{i=1}^{N_p} R(\boldsymbol{V}^{(i)})(1 - W^{(i)}) + \underbrace{\int R(\boldsymbol{v}) f^{\mathrm{eq}}(\boldsymbol{v}|\boldsymbol{x},t) d^3\boldsymbol{v}}_{\text{analytical computation}} \, .$$

Orders of magnitude speed-up with the minimal change in the base code

VR for stochastic collision operator

Unfortunately, weight evolution for most collision operators, e.g. the Boltzmann eq.

$$\frac{\partial f^{\mathrm{eq}}}{\partial t}\Big|_{\mathrm{col}} = \frac{1}{2} \int\int\int (\delta_1' + \delta_2' - \delta_1 - \delta_2) w_1 w_2 f_1 f_2 v_r \sigma d\Omega d\boldsymbol{v}_1 d\boldsymbol{v}_2$$

becomes **unstable** due to its unbounded multiplicative process with diverging fixed points.

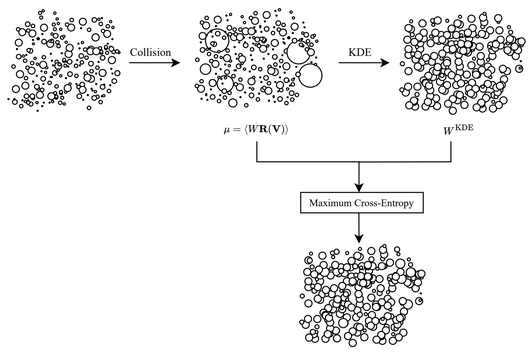
Maximum cross-entropy formulation

The stability and conservation laws can be enforced by combining a stabilized estimate of post-collision weight distribution $\mathcal{F}^{\mathrm{prior}}$ with exact post-collision moments of equilibrium simulation with the functional [2]

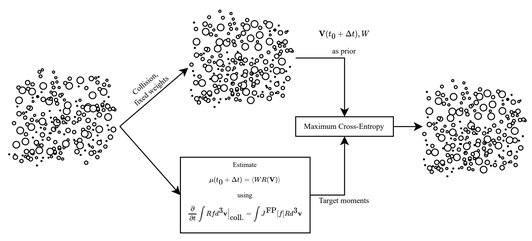
$$C[\mathcal{F}(\boldsymbol{v}|\boldsymbol{x},t)] := \int \mathcal{F}(\boldsymbol{v}|\boldsymbol{x},t) \log\left(\mathcal{F}(\boldsymbol{v}|\boldsymbol{x},t)/\mathcal{F}^{\mathrm{prior}}(\boldsymbol{v}|\boldsymbol{x},t)\right) d^3\boldsymbol{v} + \sum_{i=1}^{M} \lambda_i \left(\int R_i(\boldsymbol{v}) \mathcal{F}(\boldsymbol{v}|\boldsymbol{x},t) d^3\boldsymbol{v} - \mu_i(\boldsymbol{x},t) \right).$$

The extremum of this objective functional gives the maximum cross-entropy formulation

$$\mathcal{F}(\boldsymbol{v}|\boldsymbol{x},t) = \mathcal{F}^{\mathrm{prior}}(\boldsymbol{v}|\boldsymbol{x},t) \exp\left(\sum_{i=1}^{M} \lambda_i(\boldsymbol{x},t) R_i(\boldsymbol{v}) \right).$$



a) ME-VR for DSMC



b) ME-VR for FP eq.

The Lagrange multipliers can be found using the unconstrained dual formulation $D(\boldsymbol{\lambda})$ with the gradient $\boldsymbol{g} = \nabla D(\boldsymbol{\lambda})$ and Hessian $\boldsymbol{H}(\boldsymbol{\lambda}) = \nabla^2 D(\boldsymbol{\lambda})$ leading to an iterative scheme

$$\boldsymbol{\lambda}^{(k+1)} = \boldsymbol{\lambda}^{(k)} - \boldsymbol{H}^{-1}(\boldsymbol{\lambda}^{(k)}) \boldsymbol{g}(\boldsymbol{\lambda}^{(k)}).$$

Having computed the Lagrange multipliers, the weight of particles can be evaluated as

$$W^{(k)} = W^{\mathrm{prior},\,(k)} \exp\left(\sum_{i=1}^{M} \lambda_i R_i(\boldsymbol{V}^{(k)}) \right) \quad \text{for } k = 1, ..., N_p.$$

Guaranteed stability and conservation with the least bias.

ME-VRDSMC for Shock Tube problem

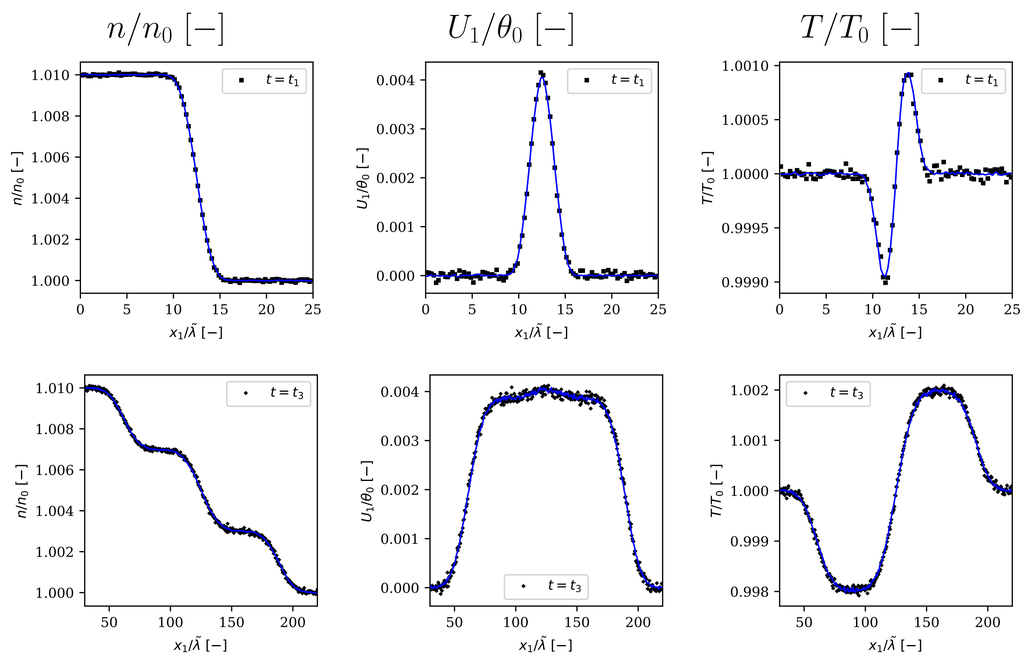


Figure 1: Solution at $t/\Delta t \in \{50, 200\}$ with initial right density $\rho_0 = 10^{-5}$ kg.m^{-3}, thermal velocity $\theta_0 = \sqrt{k_b T_0/m}$ and temperature $T_0 = 273$ K. The DSMC solution obtained using 10^5 ensembles is shown in black dots and the ME-VRDSMC solutions obtained using 50 ensembles matching up to heat flux are shown in blue lines, respectively. Here, $\tilde{\lambda}$ denotes the mean free path.

ME-VRFP for Fourier problem

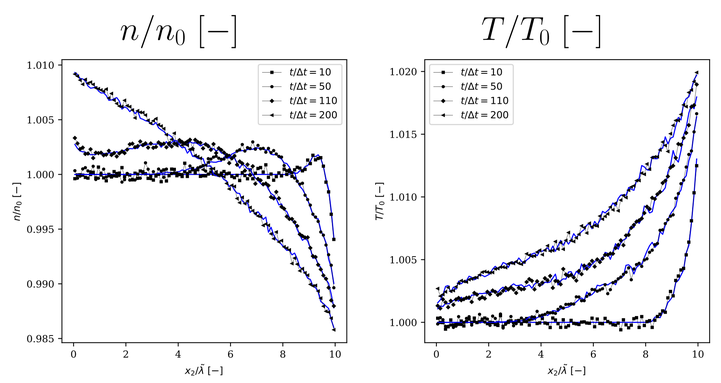


Figure 2: Solution at $t/\Delta t = 10, 50, 110$ and 200 following an impulsive change in the boundary temperature $\Delta T = 7$K. The benchmark FP solution averaged over 10^5 ensembles is denoted by black dots, and MEVR-FP solution using the maximum cross-entropy formulation averaged over 10 ensembles is shown in blue lines.

Performance

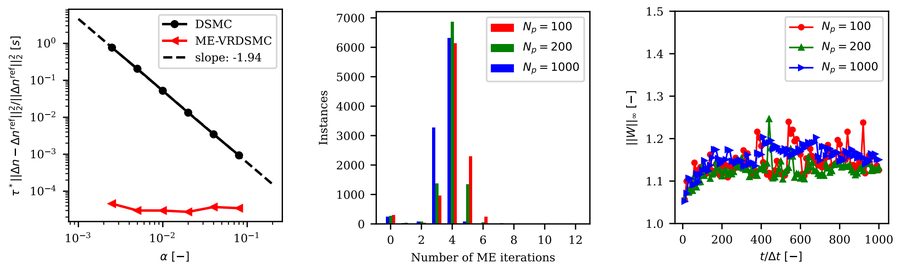


Figure 3: Performance, number of iterations for ME-VRDSMC formulation and evolution of maximum weight.

ME-VRDSMC for Lid-Driven Cavity problem

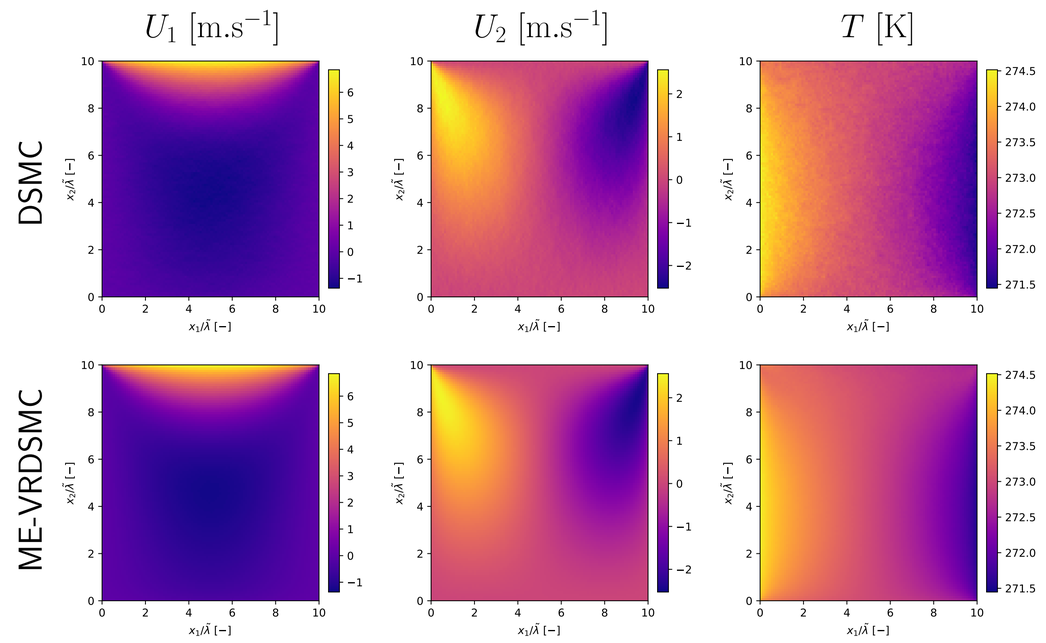


Figure 4: The steady-state solution of the Boltzmann eq. to the lid-driven Cavity problem at $\mathrm{Kn} = 0.1$ with thermal walls $(\boldsymbol{U}^{\mathrm{NW}}, T^{\mathrm{NW}}) = ([10, 0, 0]^T, 273)$, $(\boldsymbol{U}^{\mathrm{SW}}, T^{\mathrm{SW}}) = (\boldsymbol{0}, 273)$, $(\boldsymbol{U}^{\mathrm{RW}}, T^{\mathrm{RW}}) = (\boldsymbol{0}, 273)$, $(\boldsymbol{U}^{\mathrm{LW}}, T^{\mathrm{NW}}) = (\boldsymbol{0}, 275)$. DSMC result is obtained using 10^5 and ME-VRDSMC using 1000 ensembles.

References

[1] Husain A. Al-Mohssen & Nicolas G Hadjiconstantinou, Esaim Math Model Numer Anal, Vol. 44, (2010).

[2] Mohsen Sadr & Nicolas G. Hadjiconstantinou, J. Comput. Phys. Vol. 472, (2023).