A general variance-reduced particle method for solving kinetic equations

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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 [1]. Hence, the variance-reduced estimate is computed via

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

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 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 the exact post-collision moments of equilibrium simulation via the functional [2]

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

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

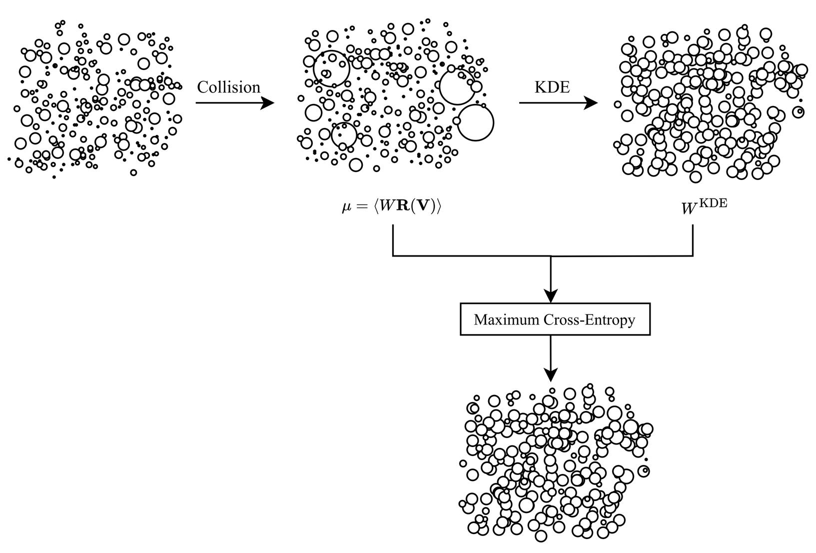
$$\mathcal{F}(\boldsymbol{v}|\boldsymbol{x},t) = \mathcal{F}^{\mathrm{prior}}(\boldsymbol{v}|\boldsymbol{x},t) \exp\left(\sum_{i=1}^{M} \lambda_i(\boldsymbol{x},t) R_i(\boldsymbol{v}) \right) .$$

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

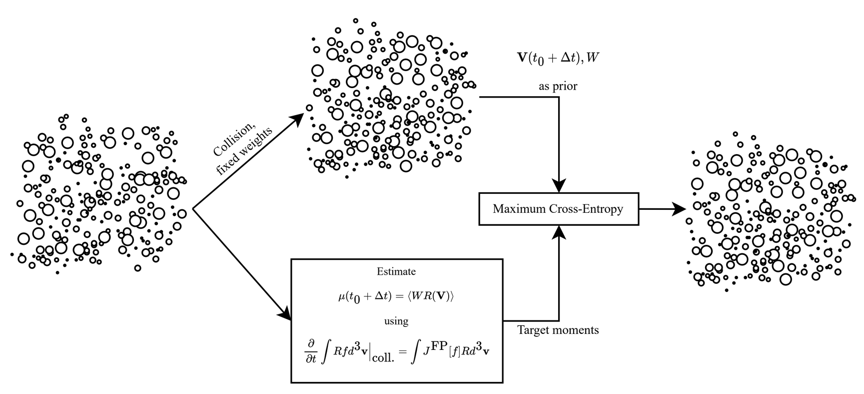
$$\boldsymbol{\lambda}^{(k+1)} = \boldsymbol{\lambda}^{(k)} - \boldsymbol{H}^{-1}(\boldsymbol{\lambda}^{(k)}) \boldsymbol{g}(\boldsymbol{\lambda}^{(k)}).$$

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

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



a) ME-VRDSMC for the Boltzmann eq.



b) ME-VR for general Fokker-Planck eq.

Guaranteed stability and conservation with the least bias.

ME-VRDSMC for Shock Tube problem

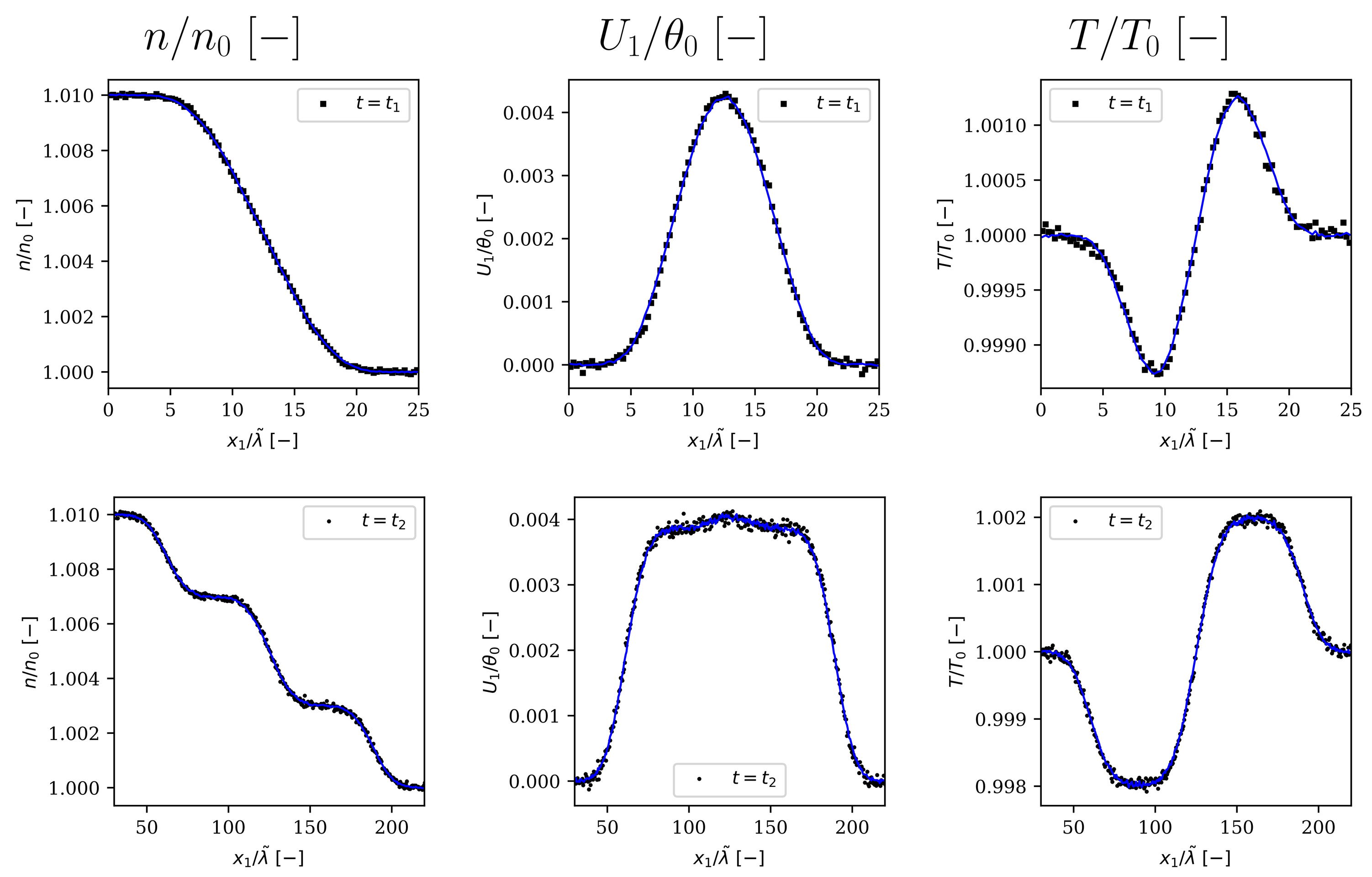


Figure 1: Solution at $t/\Delta t \in \{200, 1000\}$ with initial density $\rho_0 \in \{10^{-6}, 10^{-5}\}$ kg.m^{-3} at the right side of initial discontinuity with thermal velocity $\theta_0 = \sqrt{k_b T_0/m}$ and temperature $T_0 = 273$ K. The DSMC solution is obtained using 10^5 ensembles (black dots) and the ME-VRDSMC using 50 ensembles matching up to heat flux are shown (blue lines), respectively. Here, $\tilde{\lambda}$ denotes the mean free path of hard-sphere molecules.

ME-VR solution to cubic Fokker-Planck eq.

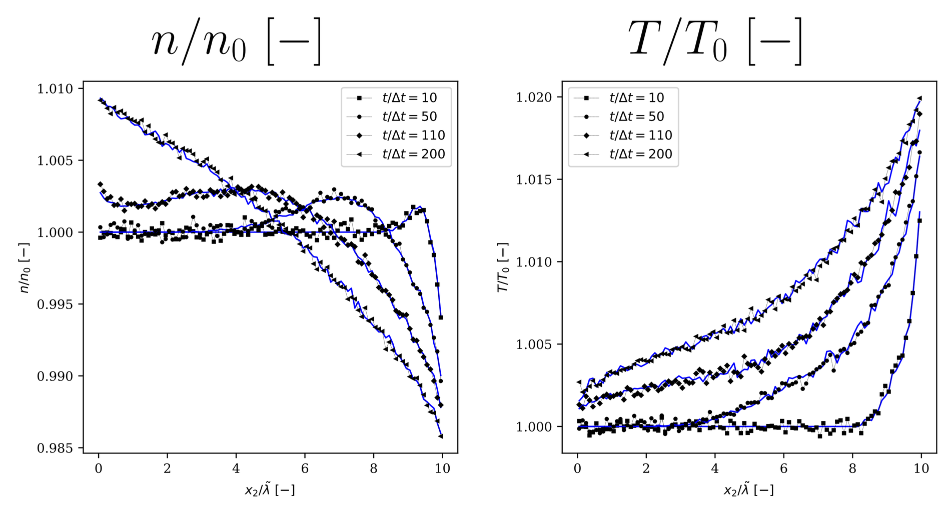


Figure 2: Solution at $t/\Delta t \in \{10, 50, 110, 200\}$ following a gradient in boundary temperature $\Delta T^{\mathrm{W}} = 7$K. The benchmark FP solution is obtained with 10^5 ensembles (black dots), and MEVR-FP solution using the maximum cross-entropy formulation with 10 ensembles (blue lines).

Performance

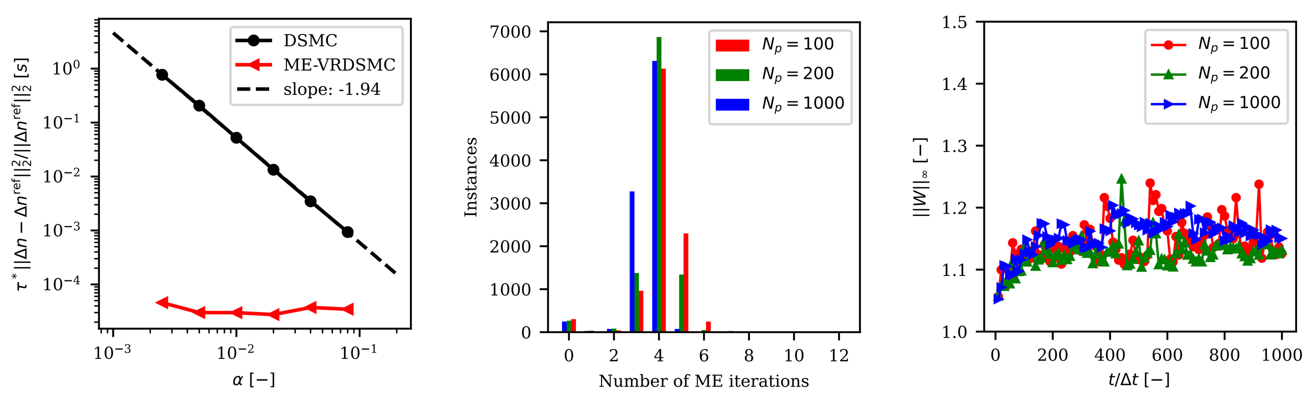


Figure 3: Performance, number of iterations for ME-VRDSMC formulation and evolution of weight in $||.||_\infty$ norm for the ME-VRDSMC solution to shock tube problem.

ME-VRDSMC for Lid-Driven Cavity problem

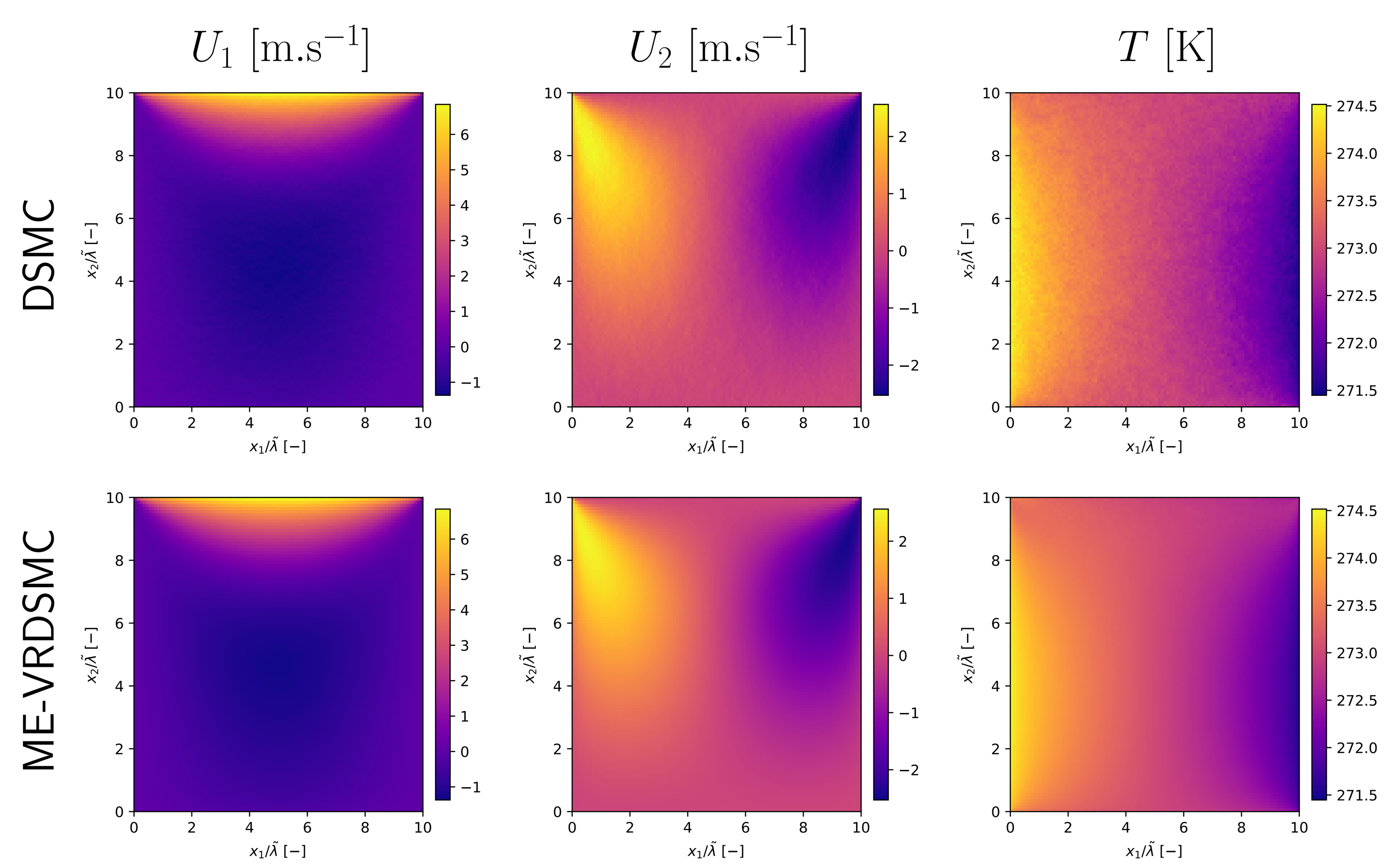


Figure 4: The steady-state solution of the Boltzmann eq. to the lid-driven Cavity problem at $\mathrm{Kn} = 0.1$ with thermal walls $(\boldsymbol{U}^{\mathrm{NW}}, T^{\mathrm{NW}}) = ([10, 0, 0]^T, 273)$, $(\boldsymbol{U}^{\mathrm{SW}}, T^{\mathrm{SW}}) = (\boldsymbol{0}, 273)$, $(\boldsymbol{U}^{\mathrm{RW}},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