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Hybridizing DSMC and Discrete Velocity Methods in Velocity Space

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Outline

1. **Brief overview of DSMC and other kinetic methods**
2. **Quasi-Particle Simulation (QUIPS)**
    1. Representation of VDF
    2. Collisions
    3. Notes on variance reduction
3. **Velocity-space Hybridization**
    1. Collisions
    2. Notes on variable-weight DSMC
4. **Numerical results**
5. **Conclusion**
6. **(if time permits) Notes on convection**

Why not use DSMC?

- Statistical fluctuations, issues with modelling of low-speed and transient flows
- Difficulty resolving low populations
  - Excited internal states
  - High-velocity particles
  - Trace species
- Difficulty resolving low-probability events (e.g. recombination reactions)
- Can use more particles, but will hit RAM limits: if molar fraction of trace species is 0.1%, means for each 1 particle of trace species we have 1000 particles of main species

Other methods for rarefied flows

- **DSMC modifications**
  - **Variance-reduced DSMC** (e.g. N. Hadjiconstantinou et al.)
  - **Variable-weight DSMC** (e.g. S. Rjasanow et al., I. Boyd et al., R. Martin et al.)
  - Distributional DSMC (e.g. C. Schrock et al.)
  - Fokker-Planck-DSMC (e.g. M. Gorji et al, P. Jenny et al., M. Torrilhon et al.)
- **Model equations** (e.g. BGK, ES-BGK, Shakhov model)
- **Spectral methods** (e.g. I. Gamba et al., A. Alexeenko et al., L. Wu et al., L. Pareschi et al.)
- **Discrete velocity methods** (e.g. F. Tcheremissine et al., V. Aristov et al., D. Goldstein et al., P. Varghese et al., L. Mieussens et al.)

Discrete Boltzmann Equation

Discrete velocity method:

- Select a fixed (discrete) set of allowed velocities
- Can replace integral collision operator with a sum
- Separate convection and collision parts

$$\frac{\partial f}{\partial t} + \boldsymbol{\eta} \cdot \nabla_{\boldsymbol{r}} f = \int \left[f(\boldsymbol{\eta}')f(\boldsymbol{\zeta}') - f(\boldsymbol{\eta})f(\boldsymbol{\zeta}) \right] g\sigma d\boldsymbol{\zeta}$$

In scaled form:

$$\frac{\partial \hat{\phi}}{\partial \hat{t}} + \hat{\boldsymbol{\eta}} \cdot \nabla_{\hat{\boldsymbol{r}}} \hat{\phi} = \frac{1}{Kn} \sum_{\hat{\zeta} \neq \hat{\eta}} \left[\hat{\phi}(\hat{\boldsymbol{\eta}}')\hat{\phi}(\hat{\boldsymbol{\zeta}}') - \hat{\phi}(\hat{\boldsymbol{\eta}})\hat{\phi}(\hat{\boldsymbol{\zeta}}) \right] \hat{g}\hat{\sigma}_t$$

Here $\hat{\phi}(\hat{\boldsymbol{\zeta}})$ is the (scaled) number of particles in a volume β^3 centered around $\boldsymbol{\zeta}$; β is the grid spacing

DVM at UT Austin: **Quasi-Particle Simulation Method (QUIPS)**

Why "QUIPS"?

DVM often (implicitly) means "discrete velocity model equation" (BGK, ES-BGK, Shakhov, modifications for multi-species, internal energies…)

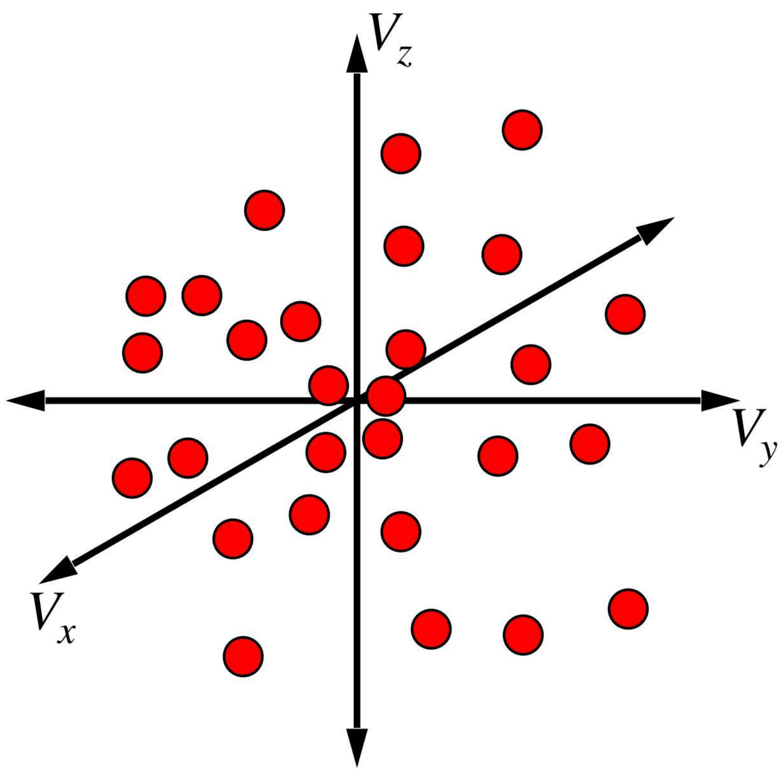
$$\frac{\partial f_i}{\partial t} + \boldsymbol{\eta}_i \cdot \nabla_{\boldsymbol{r}} f_i = \frac{f_i^{eq} - f_i}{\tau}$$

But aim of QUIPS is to accurately model the collision operator as well, without use of semi-empirical approximations

DSMC vs QUIPS

DSMC

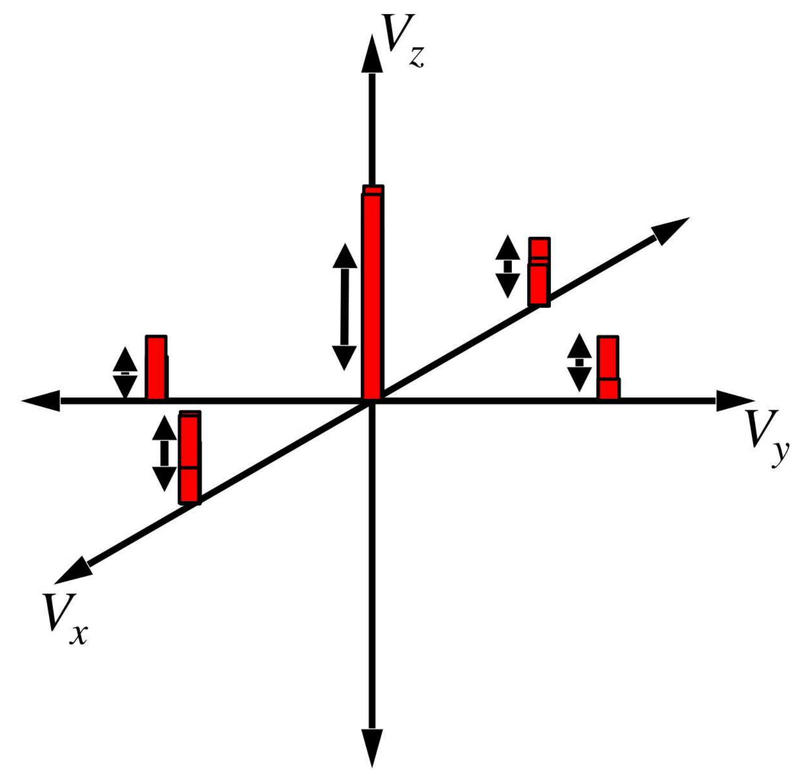
"Fixed mass, variable velocity particles."



Resolution limited by ratio of real molecules to DSMC particles

QUIPS

"Fixed velocity, variable mass quasi-particles."

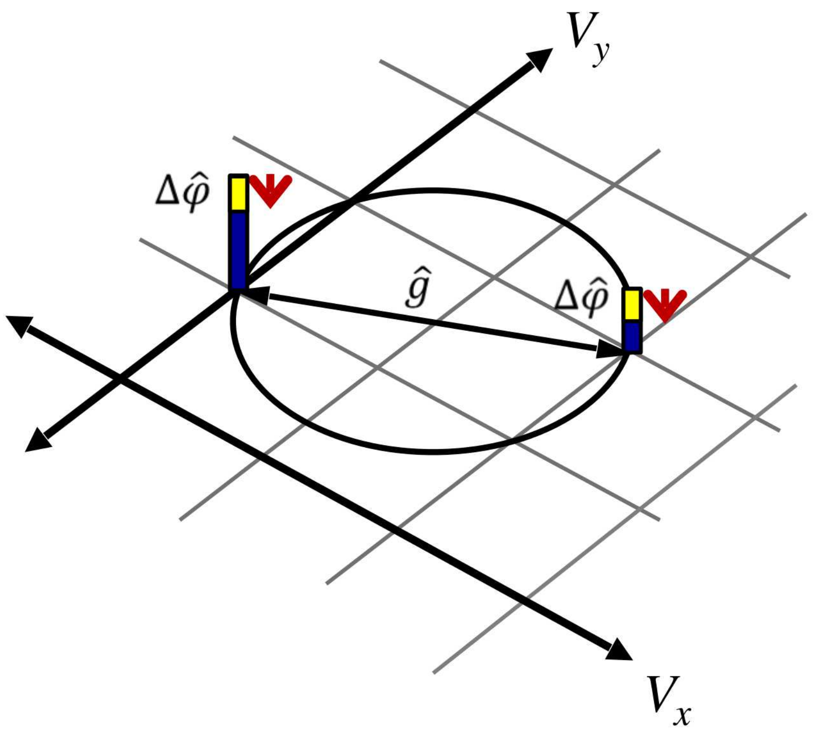


Allows resolution of tails/ trace populations up to machine precision

How to compute collision integral?

A Monte-Carlo method:

- Select two discrete velocity locations (based on their mass)
- Deplete them by a small value; replenish mass
- Repeat many times
- Parameter that controls number of collisions/noise



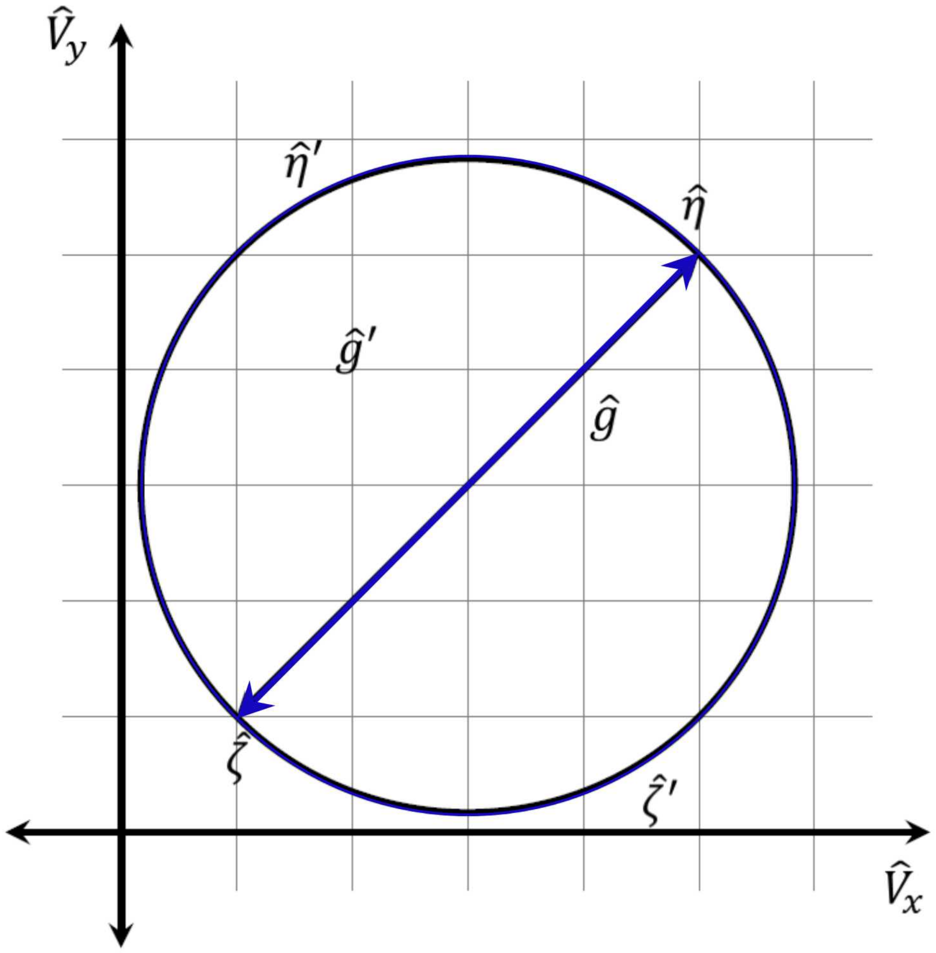
$$N_{coll} \sim \frac{1}{C_{RMS}^2}$$

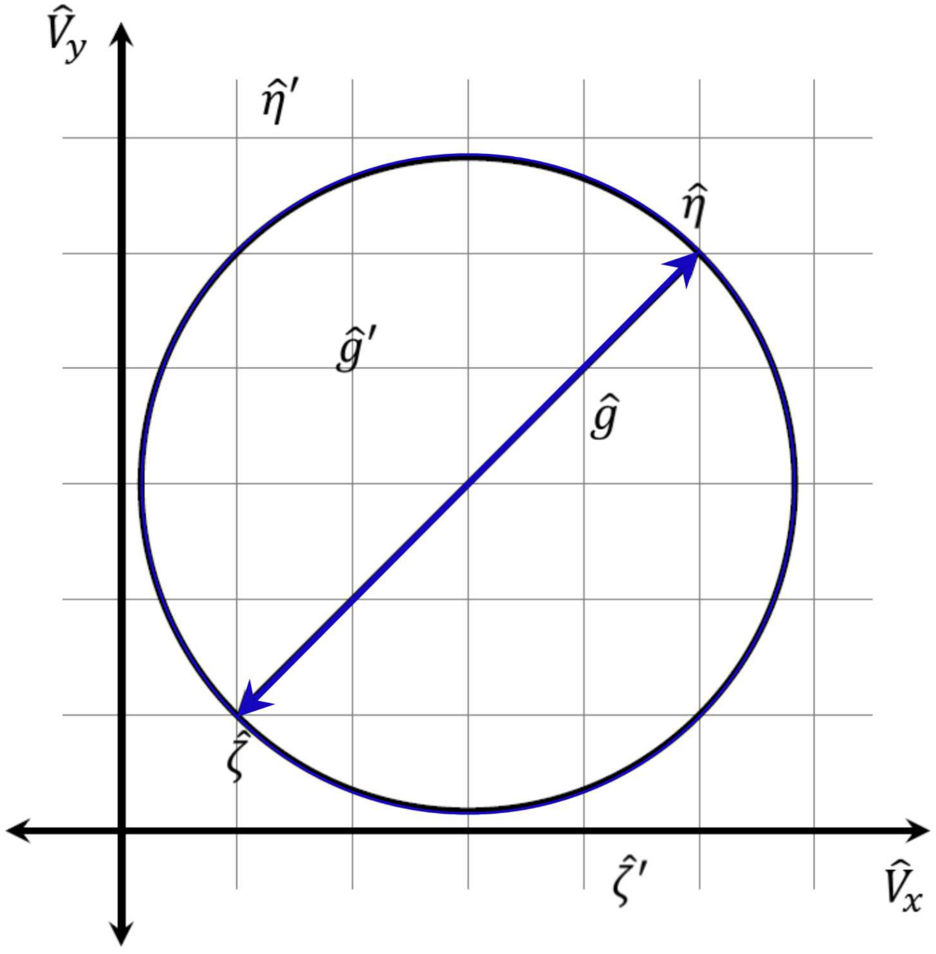
$$\Delta\hat{\phi} = \Delta\hat{t}\,\frac{(\hat{n} - 2\hat{n}_{neg})^2}{2KnN_{coll}}\, sign\left(\hat{\phi}(\hat{\boldsymbol{\eta}})\hat{\phi}(\hat{\boldsymbol{\xi}})\right)\hat{g}\hat{\sigma}_t$$

QUIPS collisions

How to compute collision integral (replenishment)?

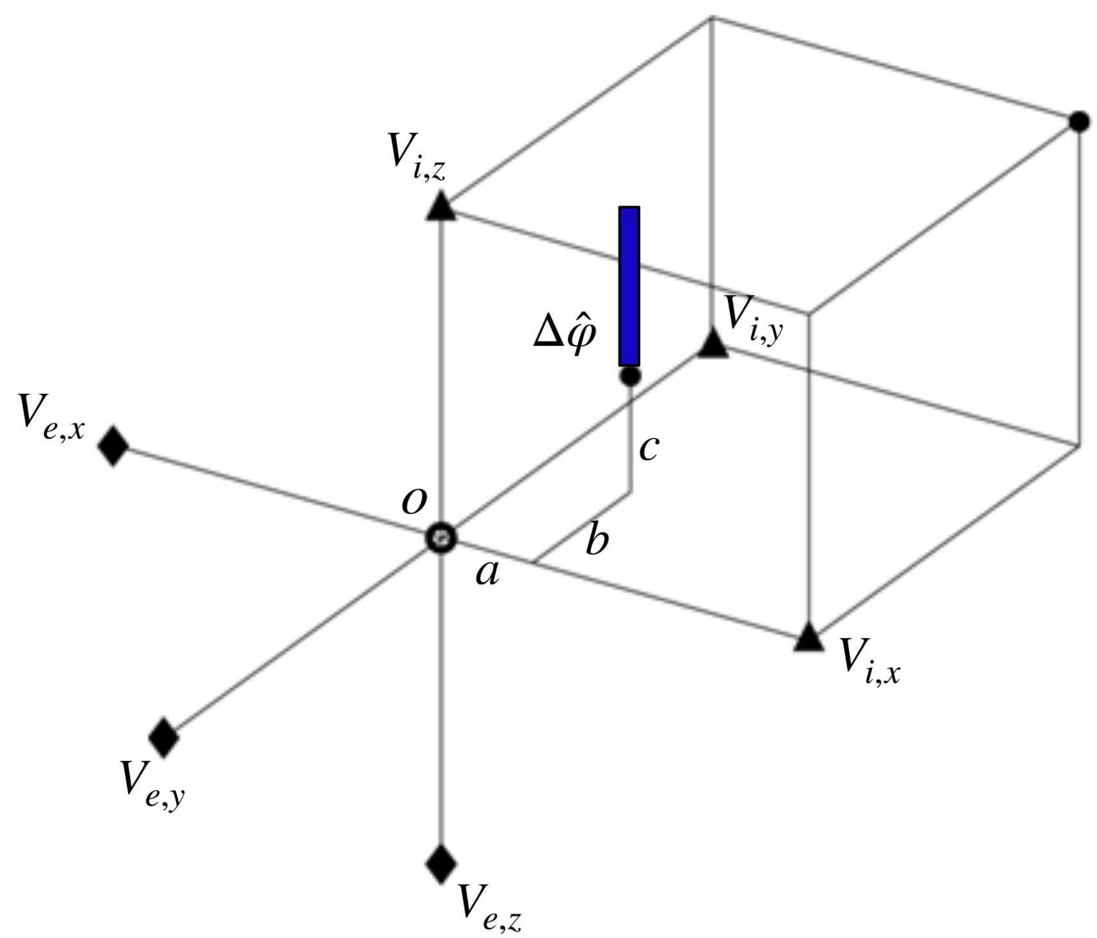
Find post-collision velocity (random point on a sphere)





But velocity does not necessarily lie on grid!

- Remap post-collision mass to 7 points on grid
- Conserves mass, momentum, energy
- Produces (small amounts of) negative mass



P. Varghese, RGD Proceedings, 2006

Remapping

Current remapping scheme

- Requires Cartesian velocity grid
- Grid can be stretched (some limits on stretching due to stability issues)
- Independent grids for different species (# of points, extents), can handle large differences in mass (e.g., in ionized flows)

QUIPS summary

QUIPS (Quasi-Particle Simulations):

- Strictly conservative
- Can handle multiple species, non-uniform velocity grids
- Can handle internal energies (rotational, vibrational)
- Can model chemical reactions
- **Variance reduction**

Variance Reduction

Under many conditions, flow is near-equilibrium (velocity and/or internal energies):

- Many collisions spent on maintaining equilibrium
- Can we focus effort on the non-equilibrium part of collisions?

$$f = f^E(T) + f^D \; (\hat{\phi} = \hat{\phi}^E + \hat{\phi}^D)$$

$$J(\hat{\eta}) = \sum_{\hat{\zeta}} \left[\left(\hat{\varphi}^E(\hat{\zeta}') + \hat{\varphi}^D(\hat{\zeta}') \right) \left(\hat{\varphi}^E(\hat{\eta}') + \hat{\varphi}^D(\hat{\eta}') \right) \right] \hat{g}\hat{\sigma} -$$

$$\sum_{\hat{\zeta}} \left[\left(\hat{\varphi}^E(\hat{\zeta}) + \hat{\varphi}^D(\hat{\zeta}) \right) \left(\hat{\varphi}^E(\hat{\eta}) + \hat{\varphi}^D(\hat{\eta}) \right) \right] \hat{g}\hat{\sigma}$$

And we have that

$$\sum_{\hat{\zeta}} \left[\hat{\varphi}^E(\hat{\zeta}')\hat{\varphi}^E(\hat{\eta}') - \hat{\varphi}^E(\hat{\zeta})\hat{\varphi}^E(\hat{\eta}) \right] \hat{g}\hat{\sigma} \equiv 0$$

Variance Reduction

Only need to compute E-D and D-D collisions – significant savings in cost (and improvement in accuracy)
Still need to compute E-E collisions for unlike species

P.S. Works (but very noisily) in case if $f^E = \delta(\zeta^\star)$!

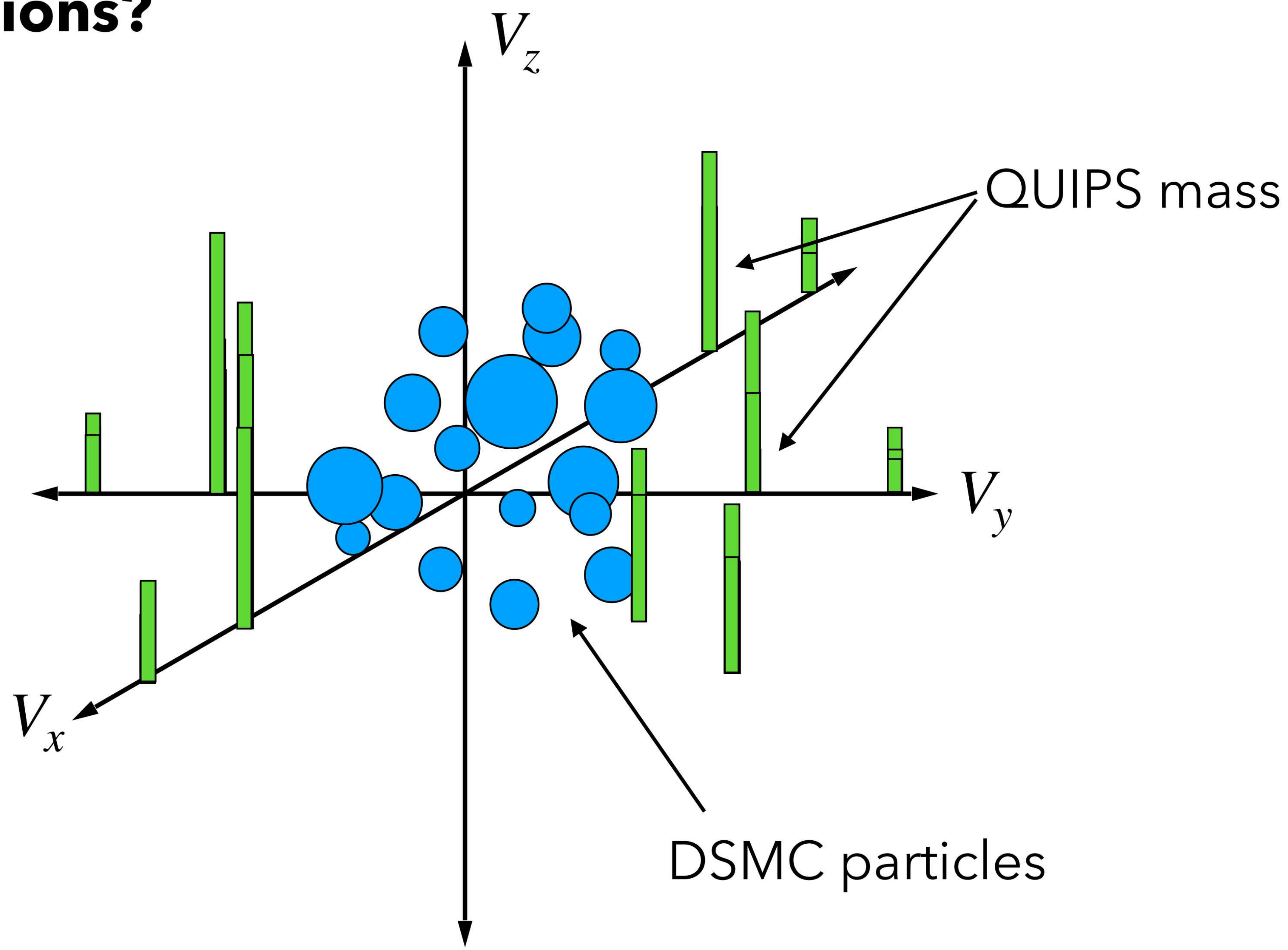
Variance Reduction in DSMC

Two different approaches:

1. LVDSMC [*Homolle, Hadjiconstantinou*]
   1. Deviational particles that are created or destroyed
   2. Difficult to implement
   3. Large variations in numbers of particles across cells
2. VRDSMC [*Al-Mohssen, Hadjiconstantinou*]
   1. Weighted particles (according to deviation from equilibrium distribution); collisions lead to re-weighting of particles and velocity updates
   2. Needs kernel smoothing to avoid uncontrolled growth of variance of weights
   3. Does not conserve mass exactly
   4. Computational speed $\sim \mathcal{O}(N_p \log N_p)$ (due to kernel smoothing)

Hybridization in velocity space

What happens if we combine DSMC and QUIPS representations?



Hybridization in velocity space

Why hybridize in velocity space?

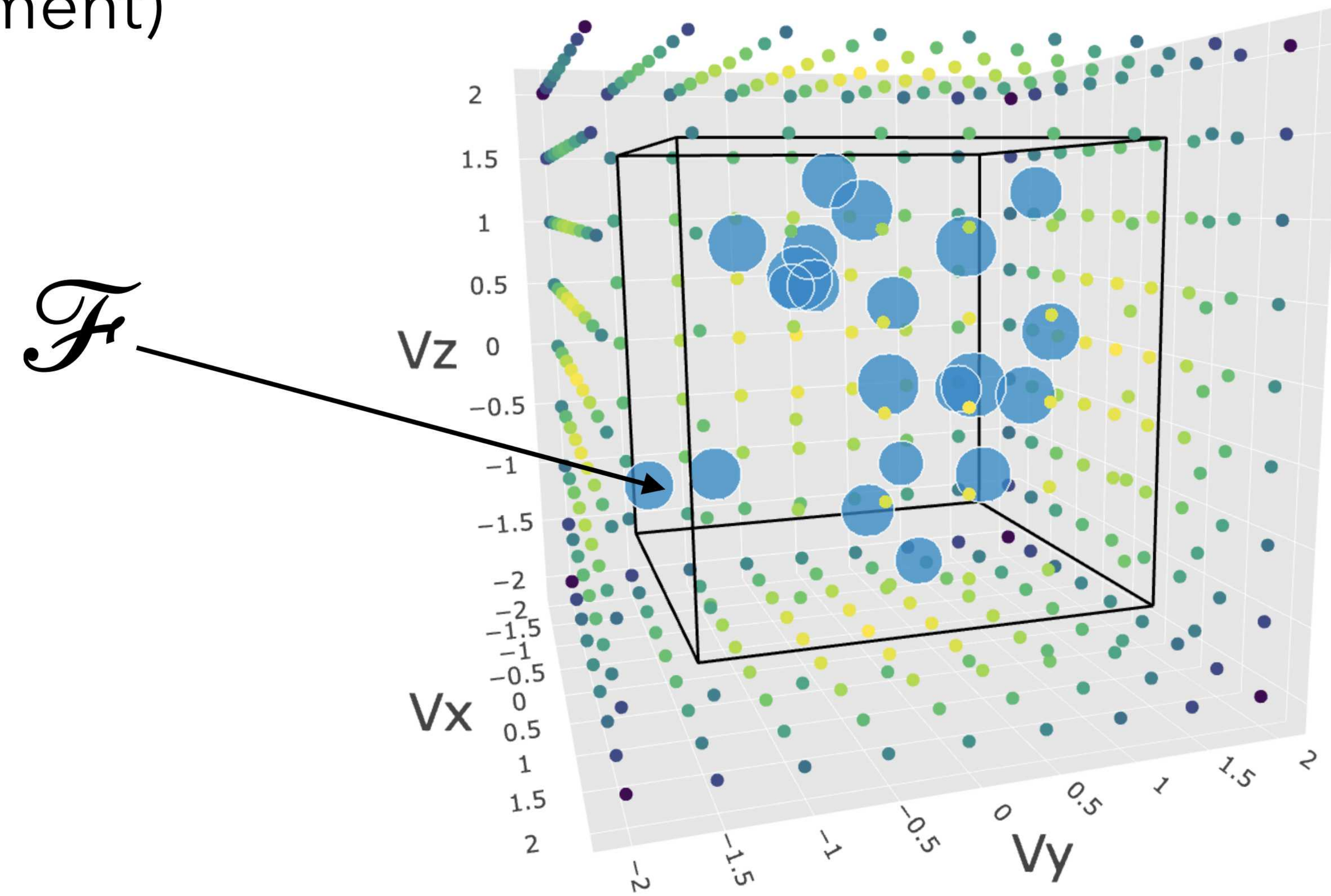
- Faster (represent bulk of distribution with a few particles)
- DVM have issues when there are discontinuities in boundary conditions

Previous work:

- G. Dimarco, L. Pareschi (2008) – BGK solver, DSMC for tails, DVM for bulk
- T. Pan, K. Stephani (2016) – DSMC for bulk, DG for tails
- T. Pan K. Stephani (2017) – DSMC for bulk, BGK for tails

How to hybridize?

- Pick region in velocity space where VDF is represented by DSMC particles
- Use DSMC collision mechanics (instead of small depletion/ replenishment)



Hybridization options

Many options possible (just in velocity space):

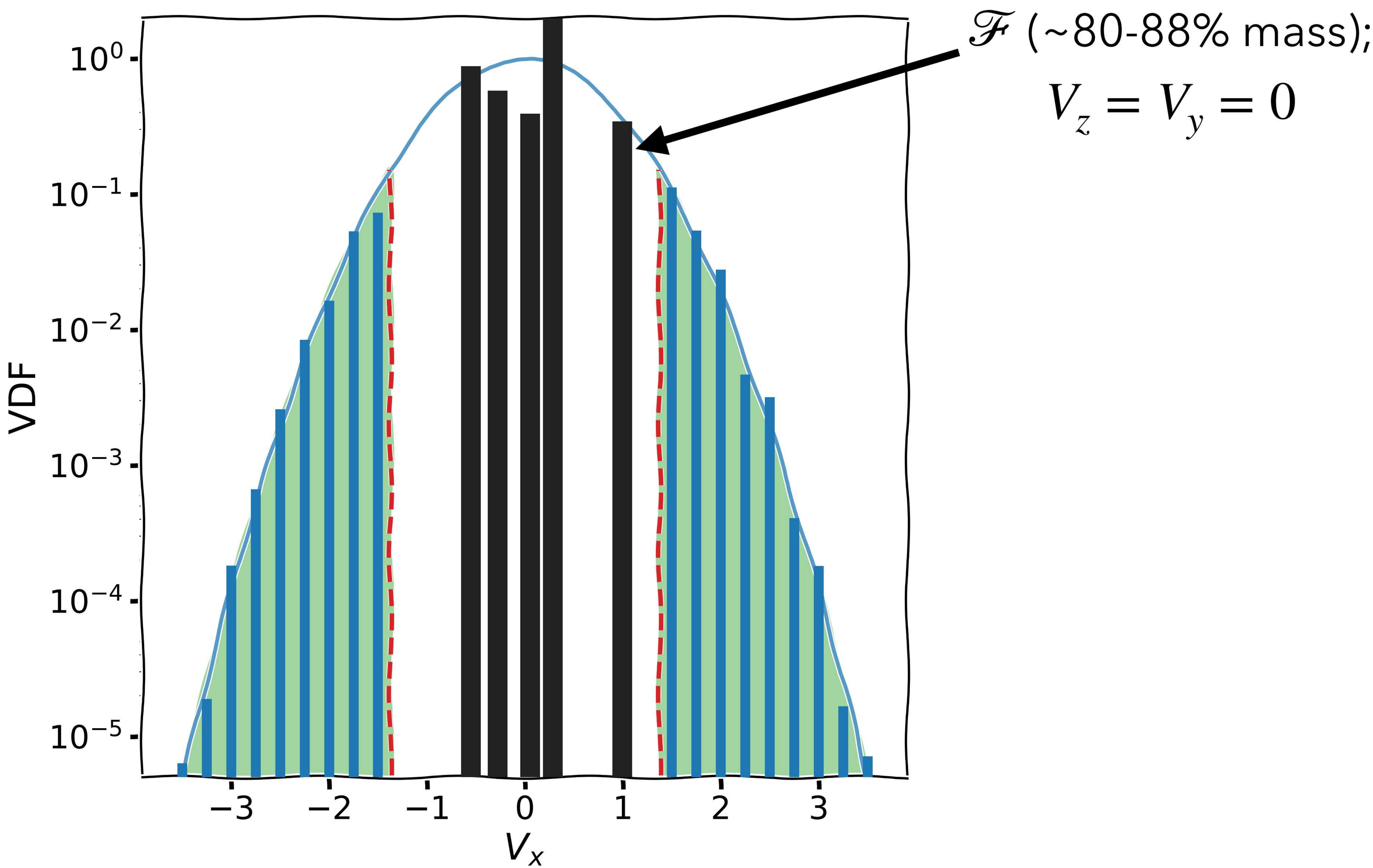
- QUIPS in bounded region $\mathcal{Q}$, DSMC in $\mathbb{R}^3/\mathcal{Q}$
- DSMC particles interspersed with QUIPS mass
- Multiple disjoint DSMC regions (bimodal VDF in shock front)
- <u>DSMC for bulk (bounded region), QUIPS in tails (bounded region)</u>

+ when considering multiple species (e.g., 2):

- QUIPS for one species, DSMC for the other (since we have a way of doing QUIPS-DSMC collisions)
- Hybrid for one species, DSMC for the other
- Hybrid for one, QUIPS for the other
- … 3^{N_s} options! → need to consider accuracy/computational expense trade-off

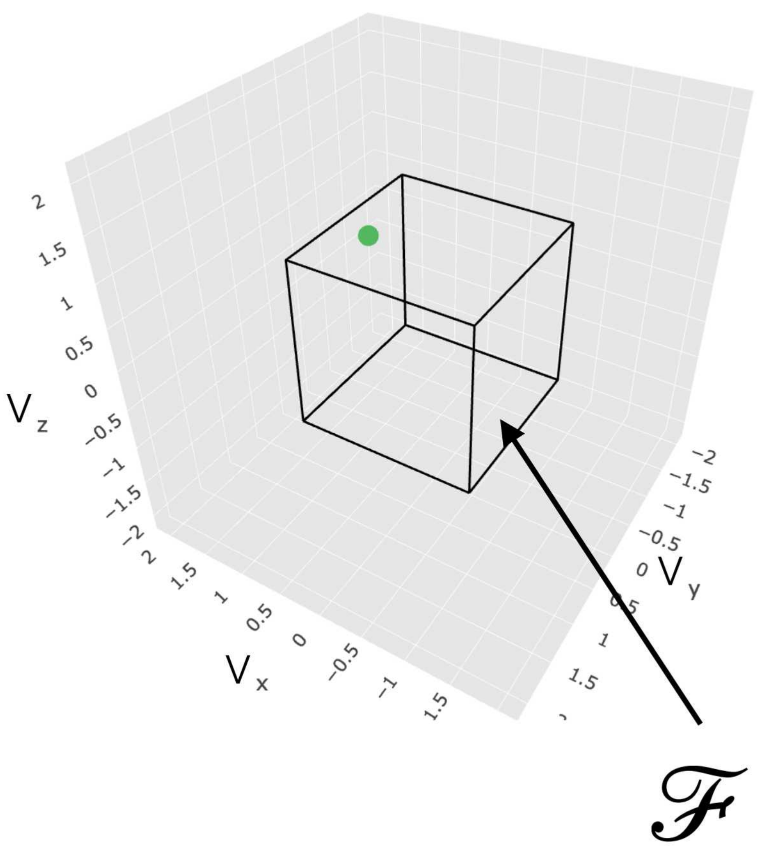
Hybridization options

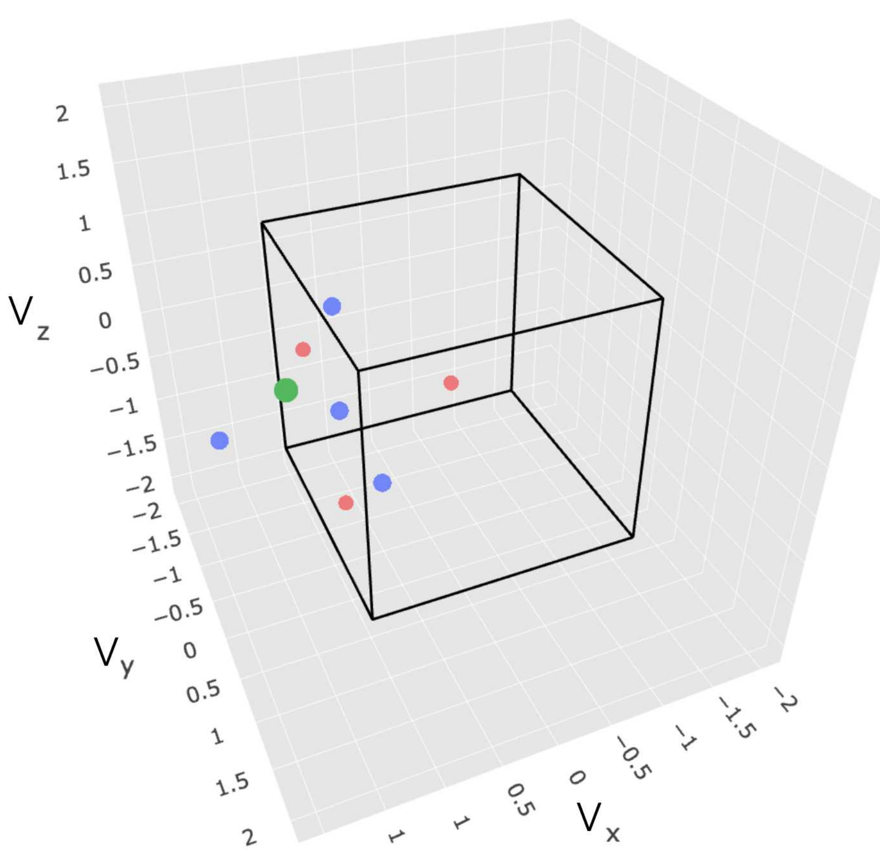
But our current goal is having quiet trace distributions:

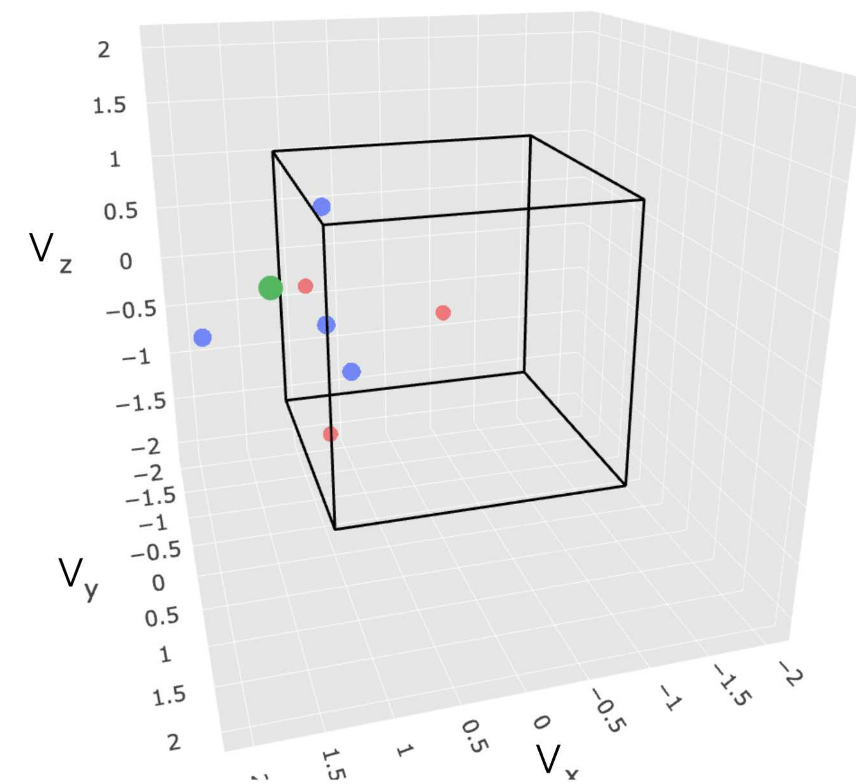


Sources of new particles in DSMC region?

1. Post-collision velocity lies inside the region
2. Remapping
3. Collision of two variable-weight DSMC particles: requires splitting

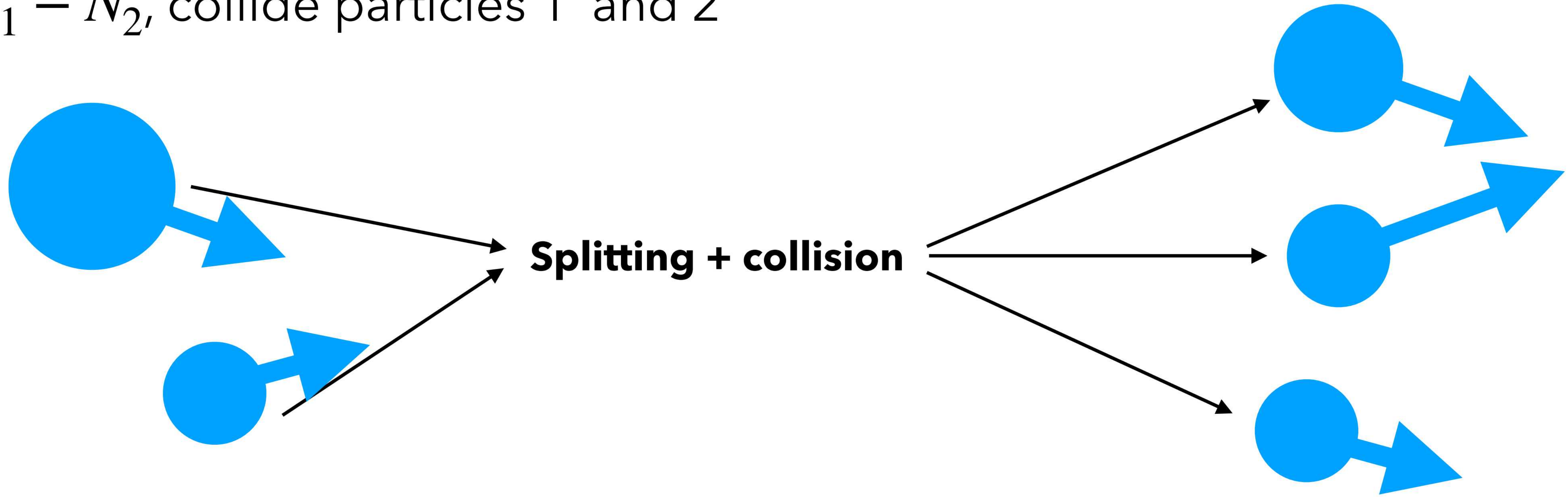






Splitting during collisions:

- If particle 1 represents N_1 molecules, particle 2 represents N_2 molecules (and $N_1 > N_2$), then during collisions only N_2 molecules actually collide
- Have to split particle 1 into two particles 1′ and 1″ with weights N_2, $N_1 - N_2$, collide particles 1′ and 2



Variable-weight NTC

Standard No-Time-Counter (Bird, 1994):

$$N_c = \Delta t F_N \frac{N_p(N_p - 1)(\sigma g)_{max}}{2V}$$

$$P = \frac{\sigma g}{(\sigma g)_{max}}$$

Variable weight No-Time-Counter (Schmidt, Rutland, 2000):

$$N_c = \Delta t \frac{N_p(N_p - 1)(w\sigma g)_{max}}{2V}$$

$$P = \frac{w\sigma g}{(w\sigma g)_{max}}$$

Variable-weight MF

Standard Majorant Frequency (Ivanov et al., 1988):

$$\nu_{max} = F_N \frac{N_p(N_p - 1)(\sigma g)_{max}}{2V}$$

sample $\delta t = -\frac{\ln \mathcal{U}(0,1)}{\nu_{max}}$; $P = \frac{\sigma g}{(\sigma g)_{max}}$; repeat while $\sum \delta t < \Delta t$

Variable weight Majorant Frequency:

$$\nu_{max} = \frac{N_p(N_p - 1)(w\sigma g)_{max}}{2V}$$

$$P = \frac{w\sigma g}{(w\sigma g)_{max}}$$

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Variable weight DSMC and surfaces

Specular reflection: no difference between standard DSMC and variable weight DSMC

Diffuse reflection: sample from half-range Maxwellian if particle hits surface; but we now need to keep track of all particles that hit surface (and store which surface they hit). After all particle moves have ended, need to renormalize particle weights ($w_i' = w_i / \sum_{i \in S_{coll}} w_i$) in order to obtain correct flux

Particle merging

Simplest (conservative) approach: 2:1 merging (Boyd, 1996):

- Merge immediately after collision: split-collide-merge split particle parts
- Non-conservative! (1 particle, 4 d.o.f., need to satisfy 5 equations) Solution: conserve momentum, keep track of change in energy in cell, change energy of next collision by this amount (conserve on average)

Particle merging

A general conservative approach: N:2 merging

2 particles have 8 d.o.f., need to satisfy 5 equations: need to add additional constraints

Usually:

1. Mass is split equally amongst the 2 particles
2. Instead of conservation of energy ($c_x^2 + c_y^2 + c_z^2$), independent conservation of c_x^2, c_y^2, c_z^2
3. May make more sense to conserve energy and some off-diagonal moment (e.g., $c_x c_y$)

N:3, N:4 merges possible, but issues with # of particles and solution of equations

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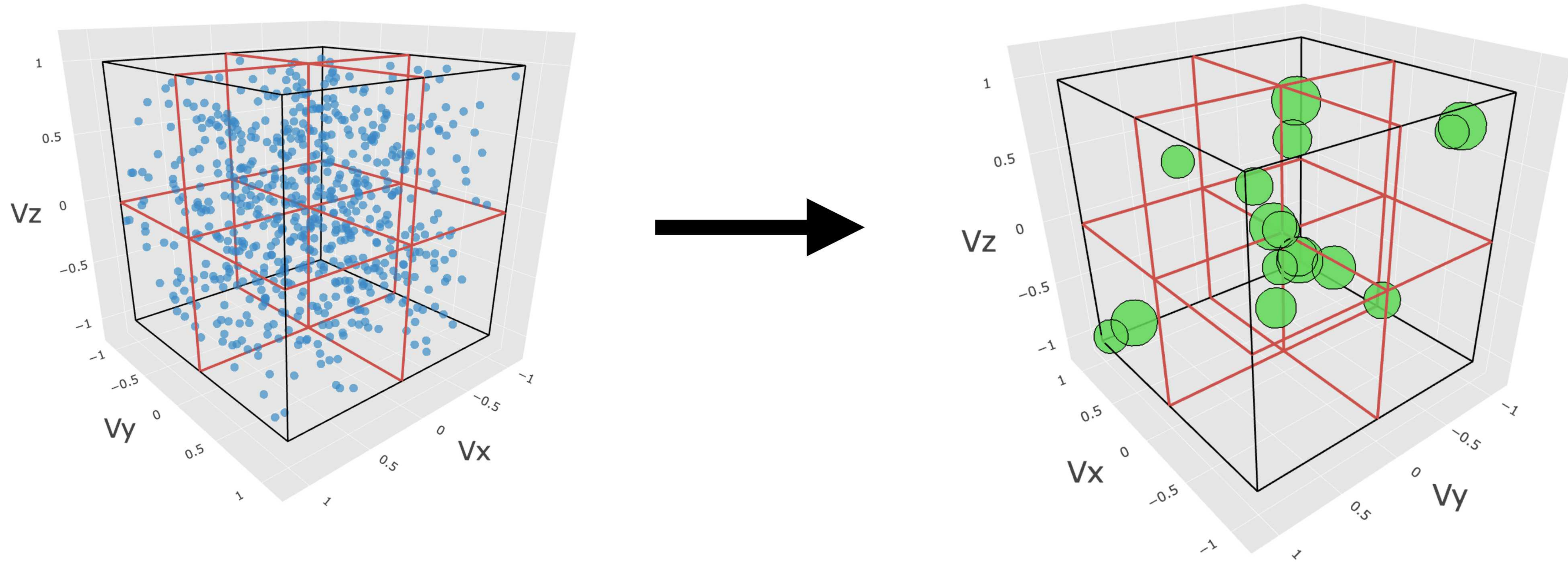
Particle merging

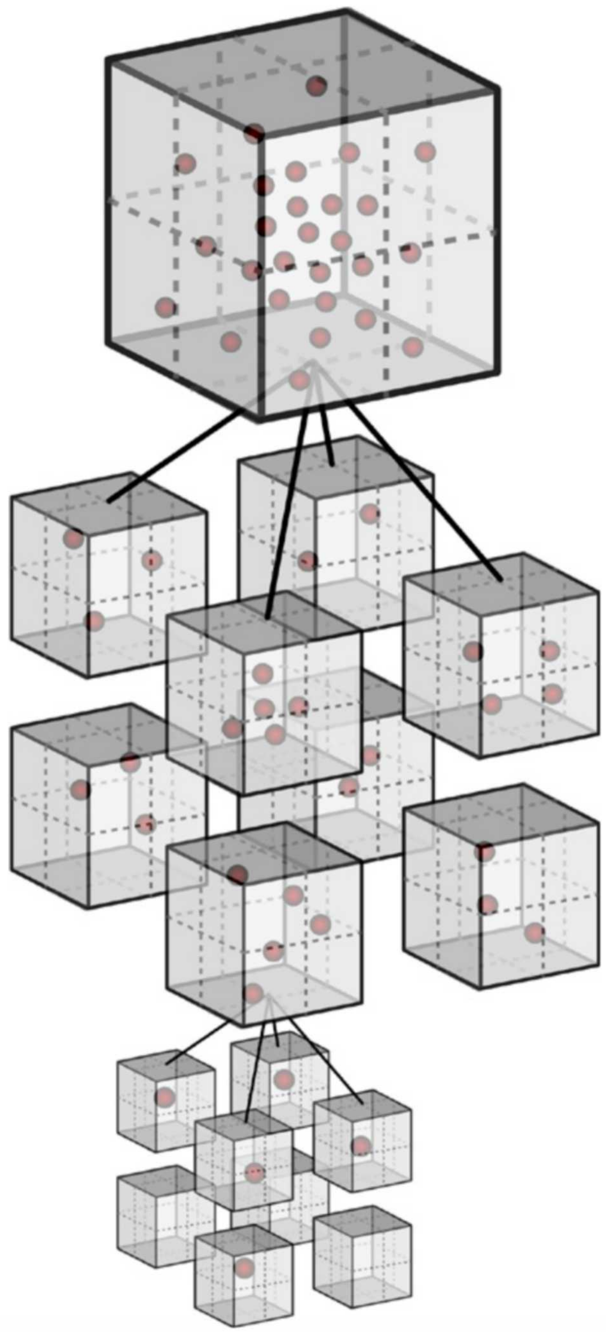
Current work utilizes a simple grid-based approach (M*M*M merging cells); CPU time $\sim \mathcal{O}(N_p + M^3)$; additional RAM $\sim \mathcal{O}(M^3)$



Particle merging

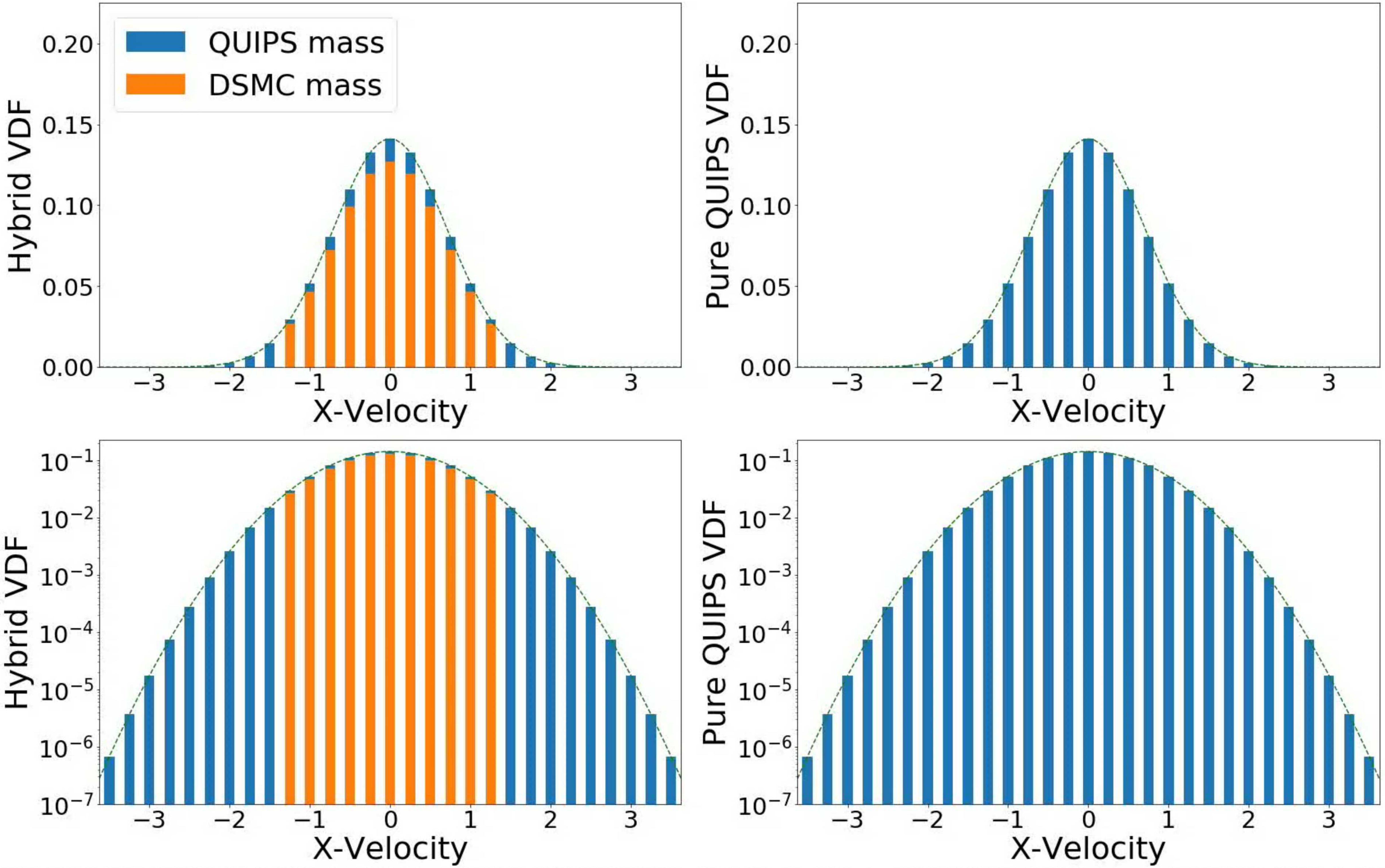
More complicated/accurate approach: Octree merging (R. Martin, J.-L. Cambier, 2016):

- Divide velocity space into octants
- Subdivide octants based on mass inside until target # of particles is reached
- Cost is $\mathcal{O}(n \log n_{c,max})$



R. Martin, J.-L. Cambier, Journ. Comp. Phys., 2016

Example of hybrid VDF representation



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Variable parameters

Variable parameters:

1. Extent of velocity grid
2. Velocity grid spacing
3. Noise parameter (C_{RMS})
4. Extent of DSMC region
5. Number of merging cells (~number of DSMC particles)

BKW relaxation

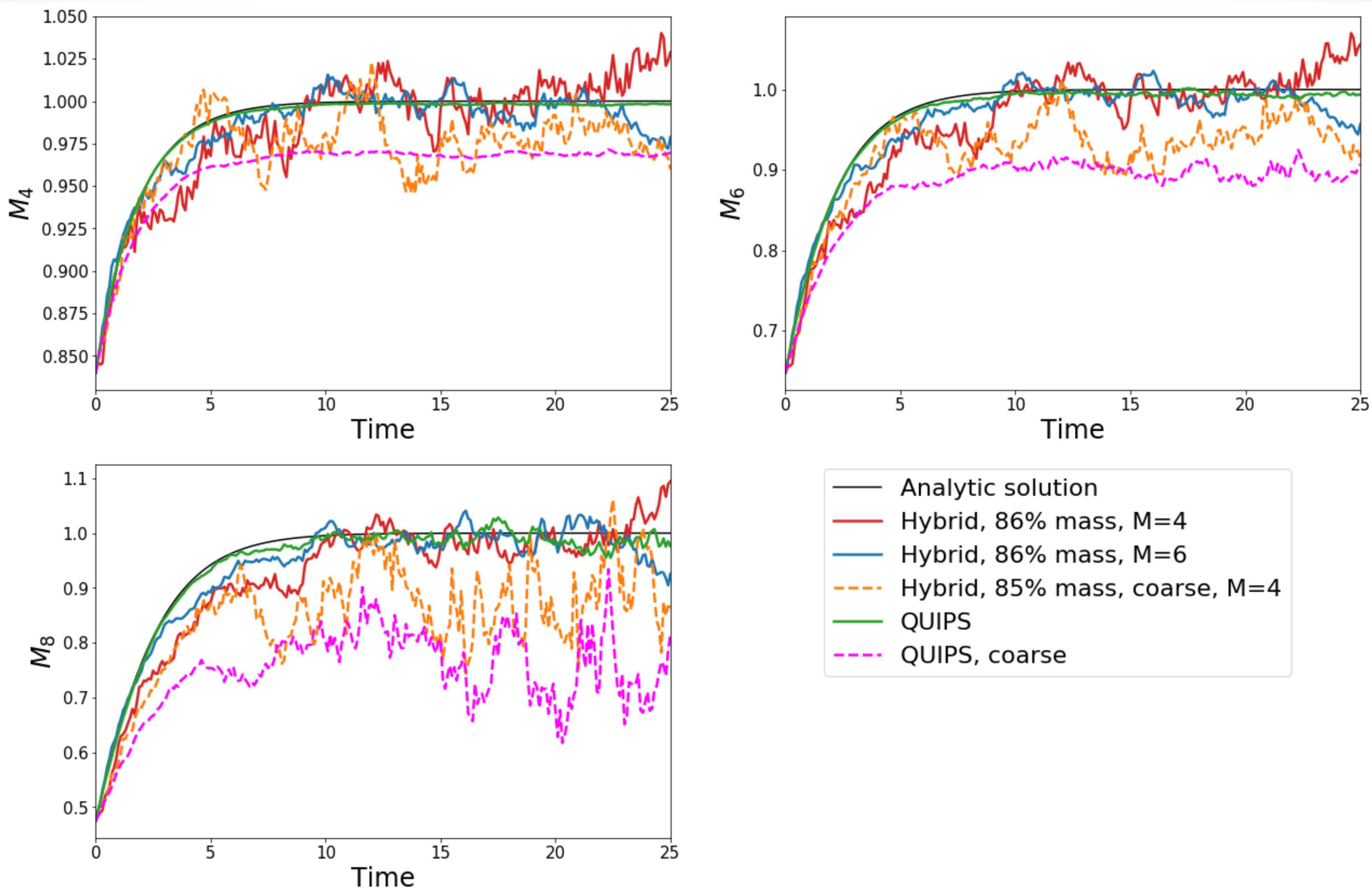
BKW relaxation: analytic solution for unsteady Boltzmann equation:

$$\hat{f}(\hat{\eta}) = \left(\frac{\hat{m}}{A\pi\hat{T}}\right)^{3/2} \frac{1}{2A}\left(5A - 3 + 2(1-A)\hat{\eta}^2\frac{\hat{m}}{A\hat{T}}\right)\exp\left(-\frac{\hat{\eta}^2\hat{m}}{A\hat{T}}\right)$$

$$A = 1 - 0.4\exp(-\hat{t}/6)$$

Requires Maxwell molecules ($\sigma(g) \propto \dfrac{1}{g} \Rightarrow \sigma g \equiv const$)

BKW relaxation



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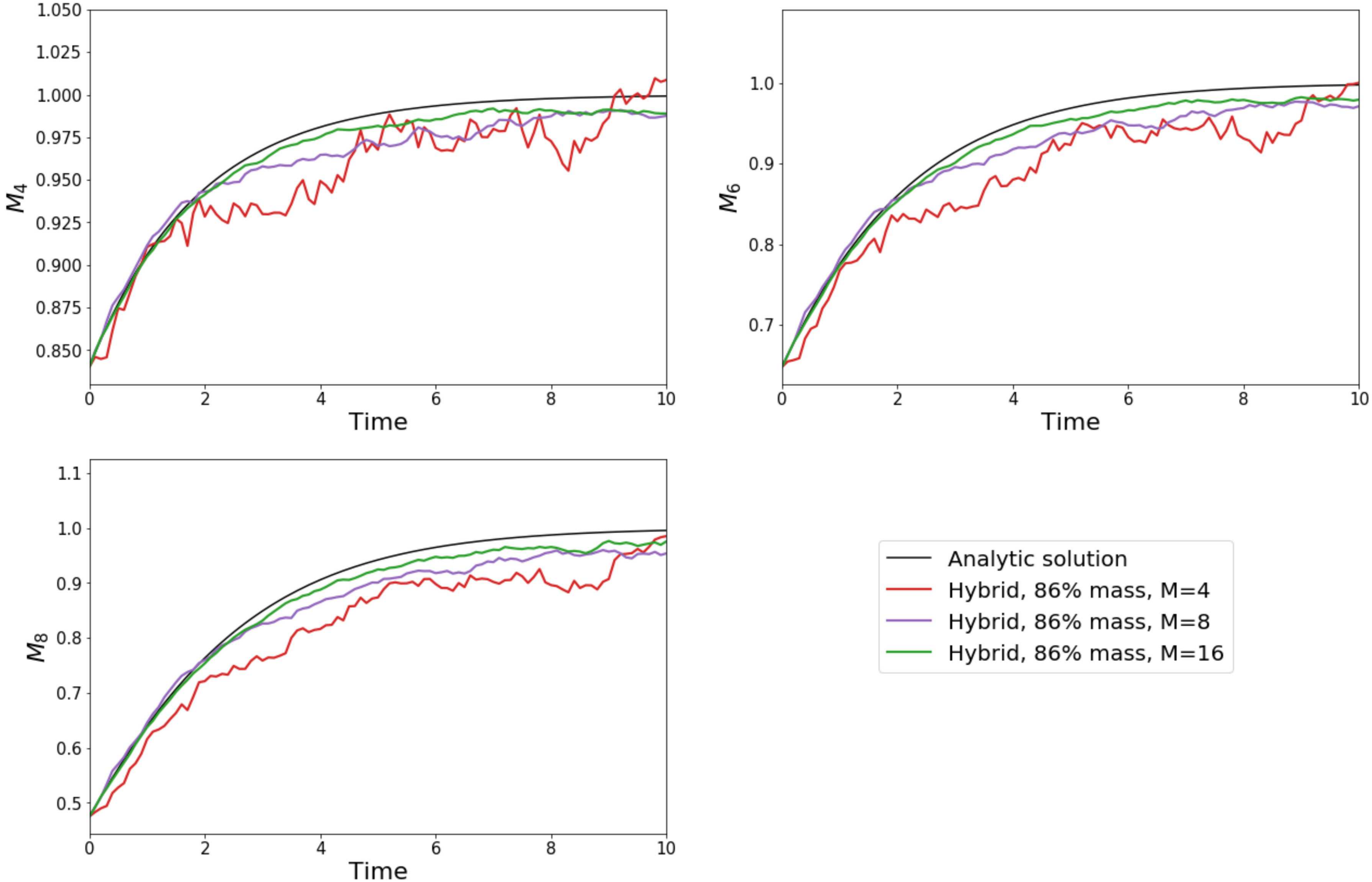
BKW relaxation



3 sources of error: grid extent, grid spacing, # of merging regions

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Numerical results

Single-species test case

- Initialize with Maxwellian distribution, look at noise (RMSE) in high-order moments (gives more weight to higher-velocity tails)
- CPU time per step vs. RMSE as measure of efficiency

$$RMSE(M_8) = \sqrt{\frac{1}{n}\sum_{t=1}^{n}\left(M_8(t) - M_8^{eq}\right)^2}$$

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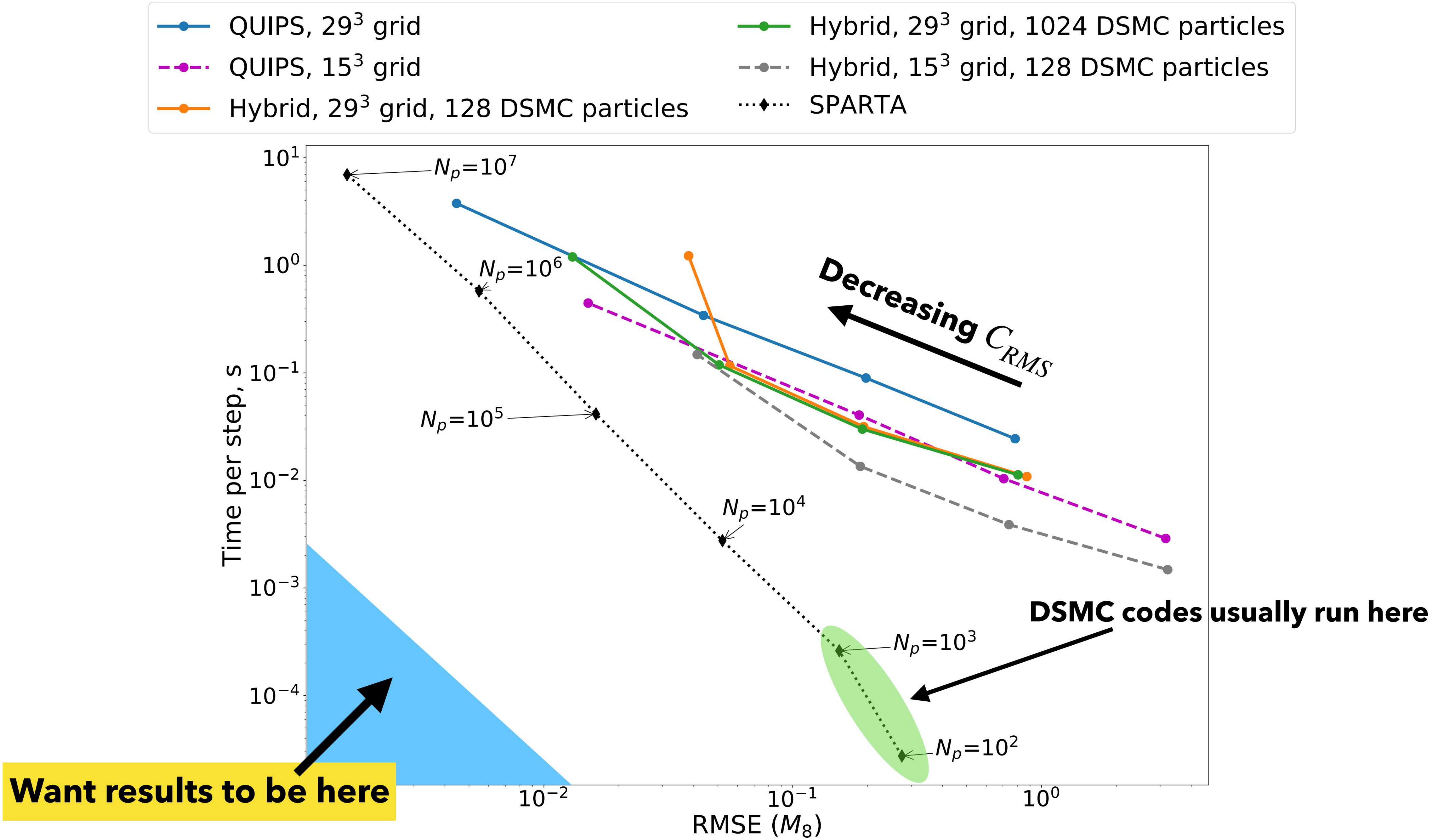
RMSE of 8th moment

Computational time per collision step vs. error in tails



Numerical results

Ionization rate computation

- Initialize with an Ar/e- mixture, compute electron-impact ionization rate coefficient (based on cross-sections given by Thompson [Lieberman and Lichtenberg, 1994])
- CPU time per step vs. error compared to analytic rate as measure of efficiency

Simulation parameters: $T_{Ar} = 300K;\ 2eV \leq T_e \leq 100eV$; 0.1% ionization
Hybrid/variable weight DSMC code uses **128** particles unless stated otherwise

Possible hybridization options:

1. Ar, e- as hybrid
2. One species as DSMC, other as pure QUIPS
3. One species as DSMC, other as hybrid

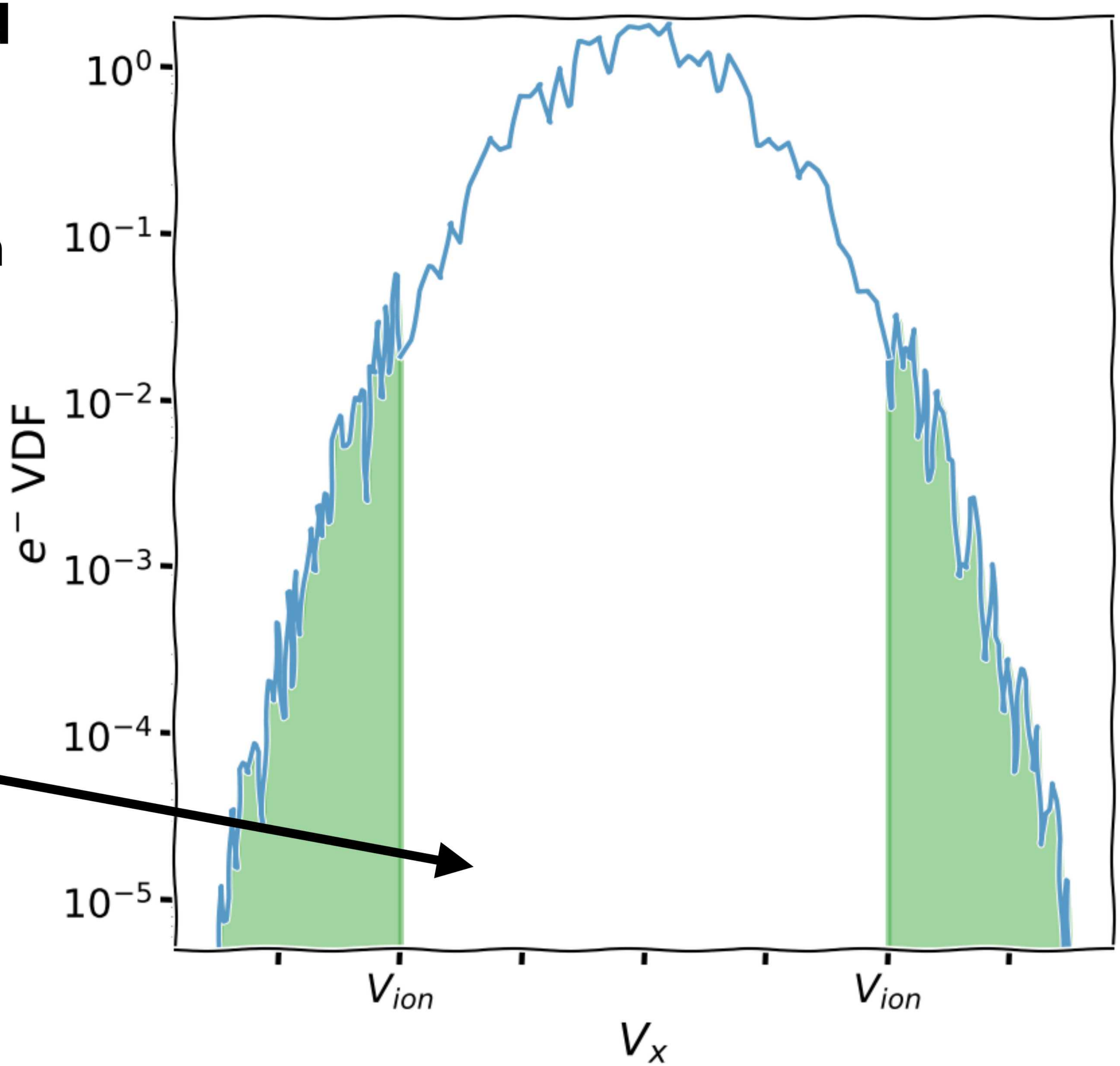
Error in ionization rate coefficient

Error in tails due to low number of particles/points on grid

Error in tails and rate coefficient due to noise in collision scheme and low event probability

Extent of DSMC region for hybrid e- VDF:

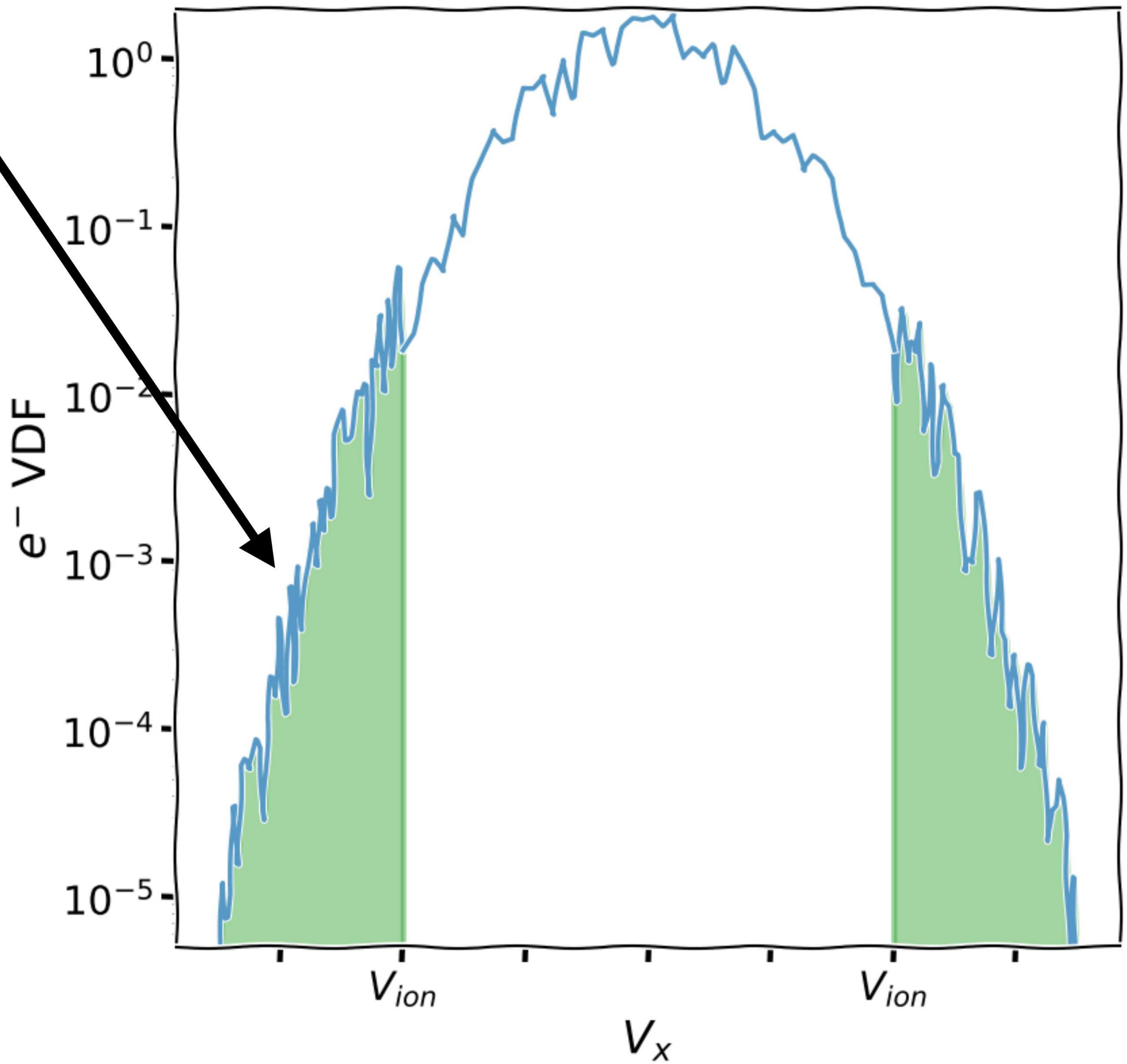
$$\left| v_i \right| \leq \frac{V_{ion}}{\sqrt{3}}, i = x, y, z$$



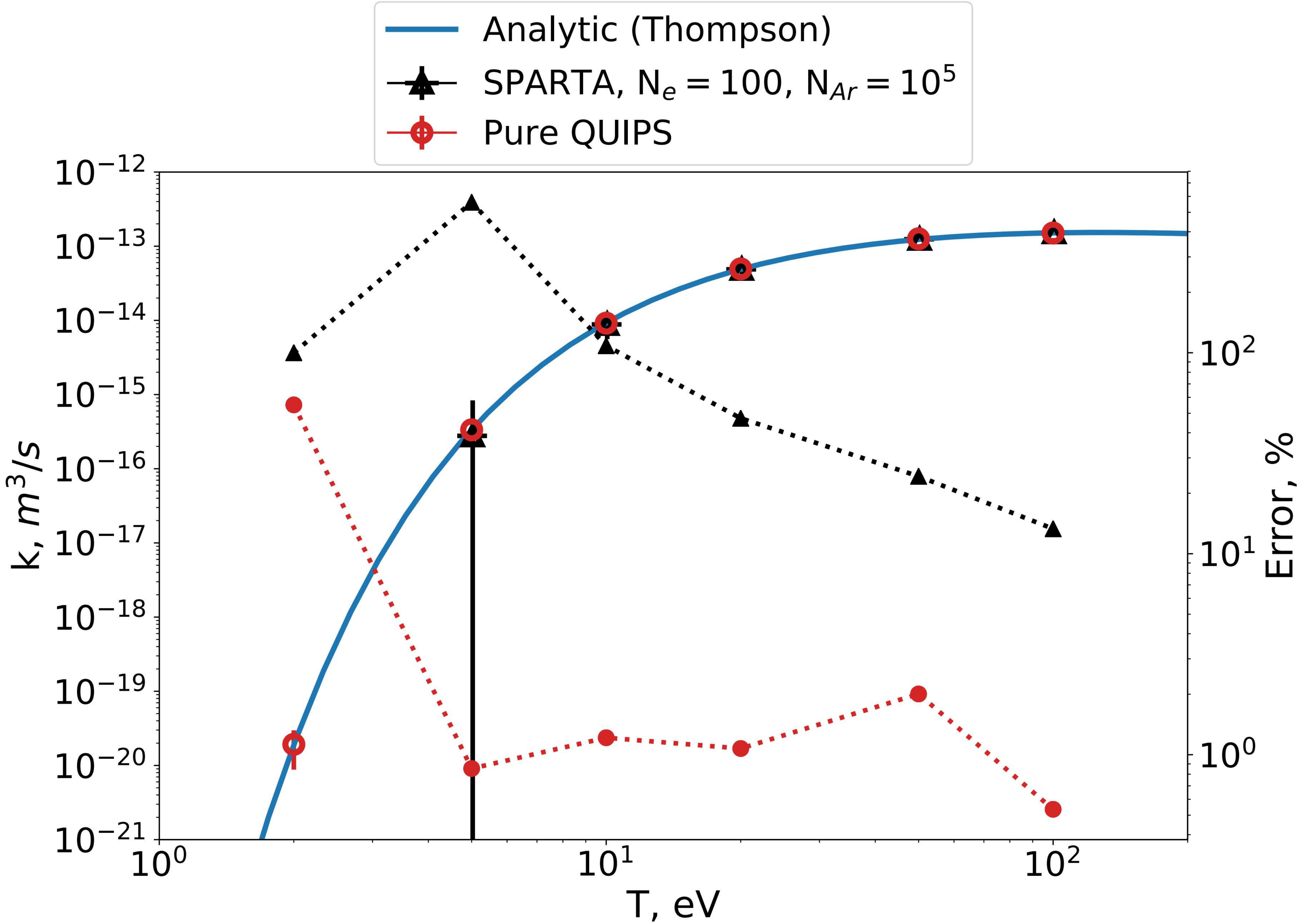
Error in ionization rate coefficient

At T=2eV, tails contain 0.2% mass; for standard DSMC need ~500 particles to get 1 particle in tail!

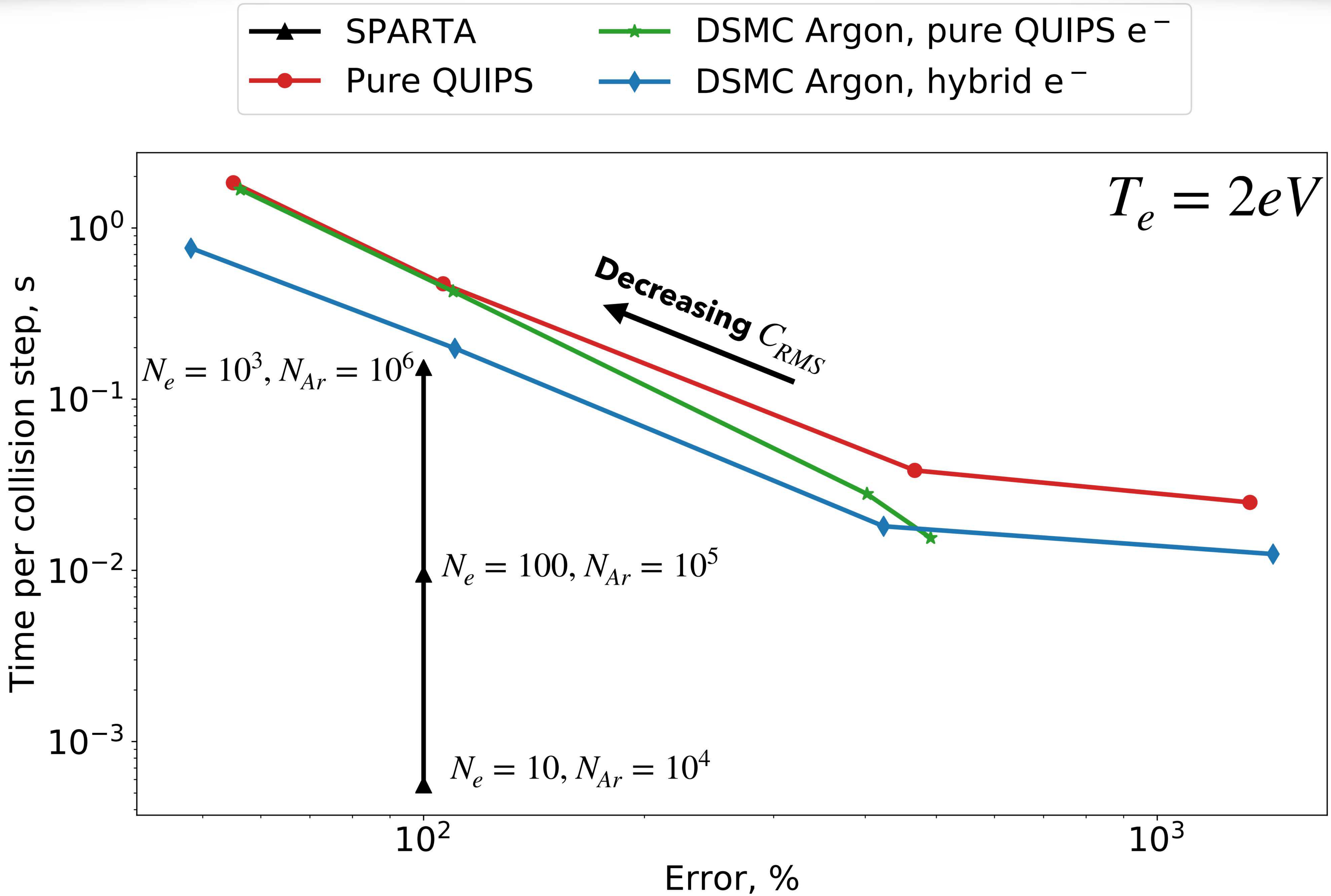
At T=5eV, 10% mass



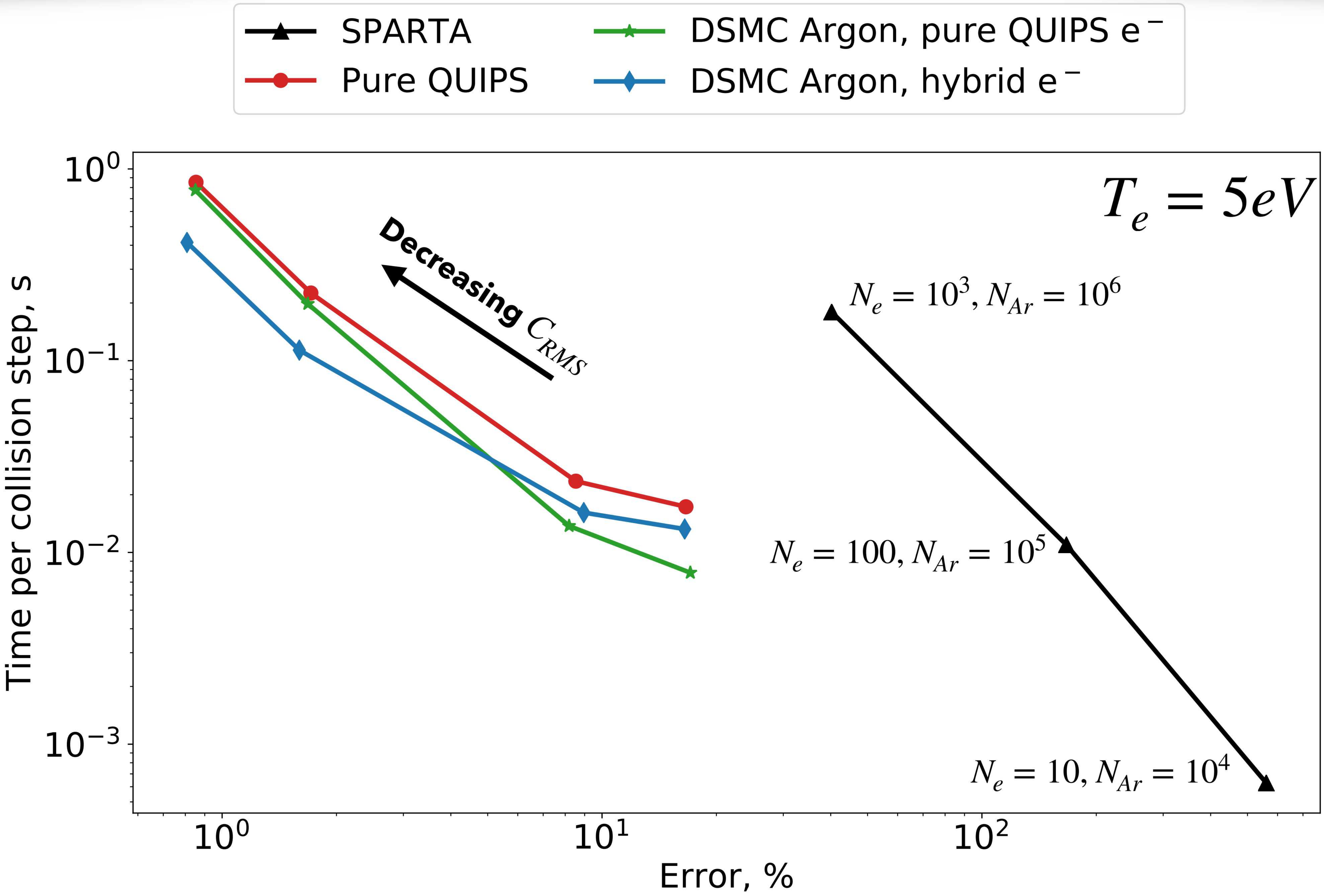
Electron-impact ionization rate



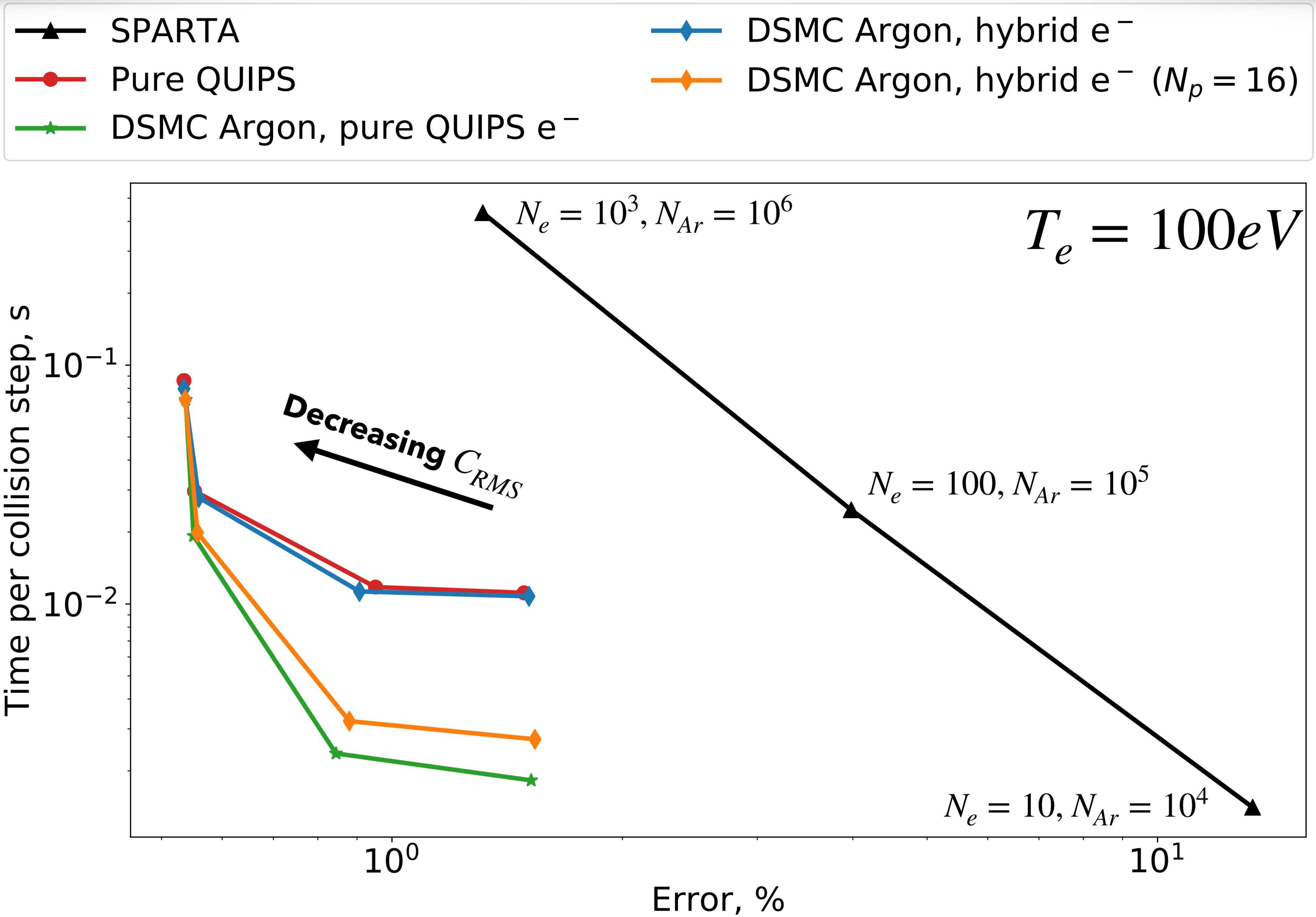
CPU vs. error, low temperature



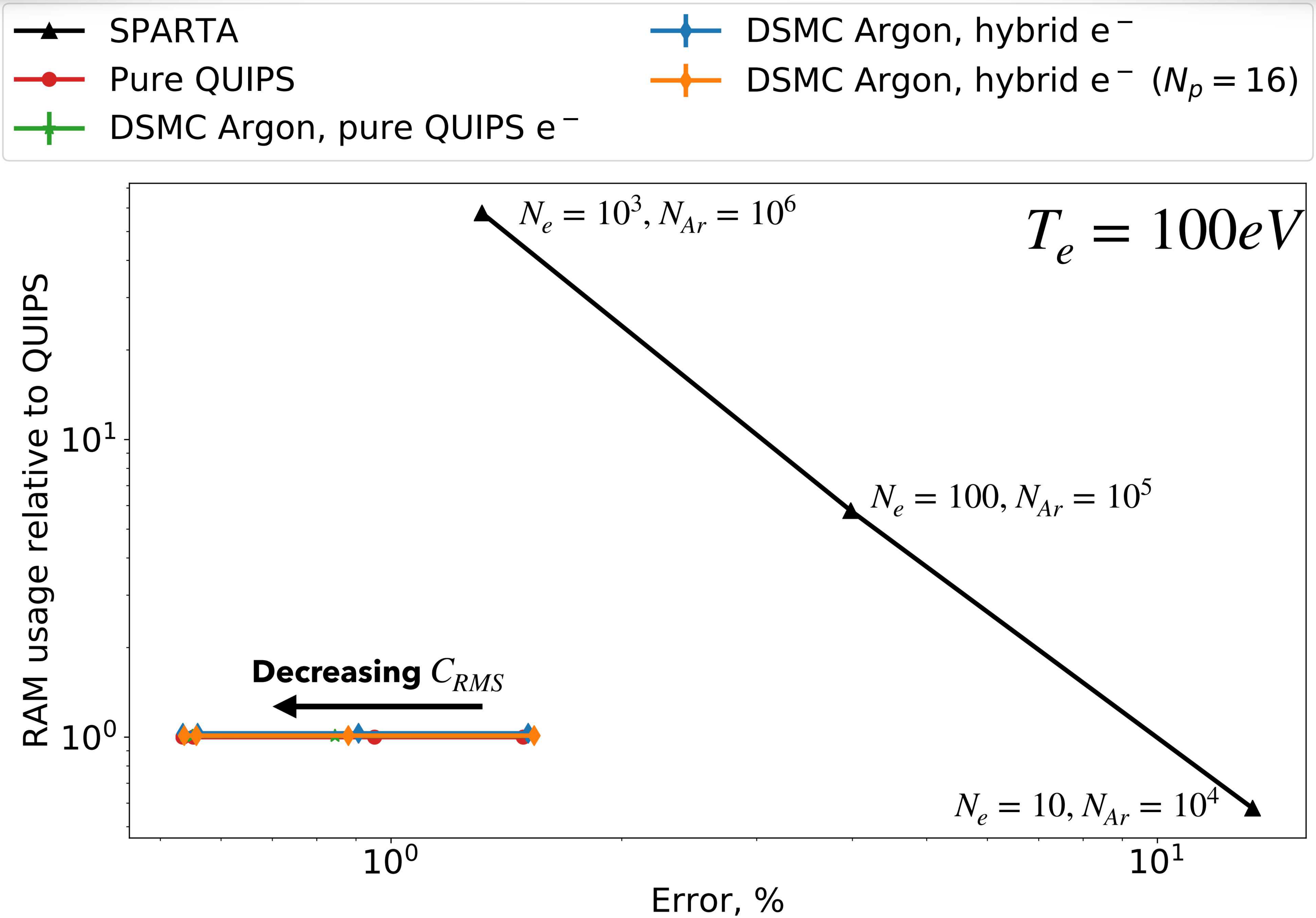
CPU vs. error, low temperature



CPU vs. error, high temperature



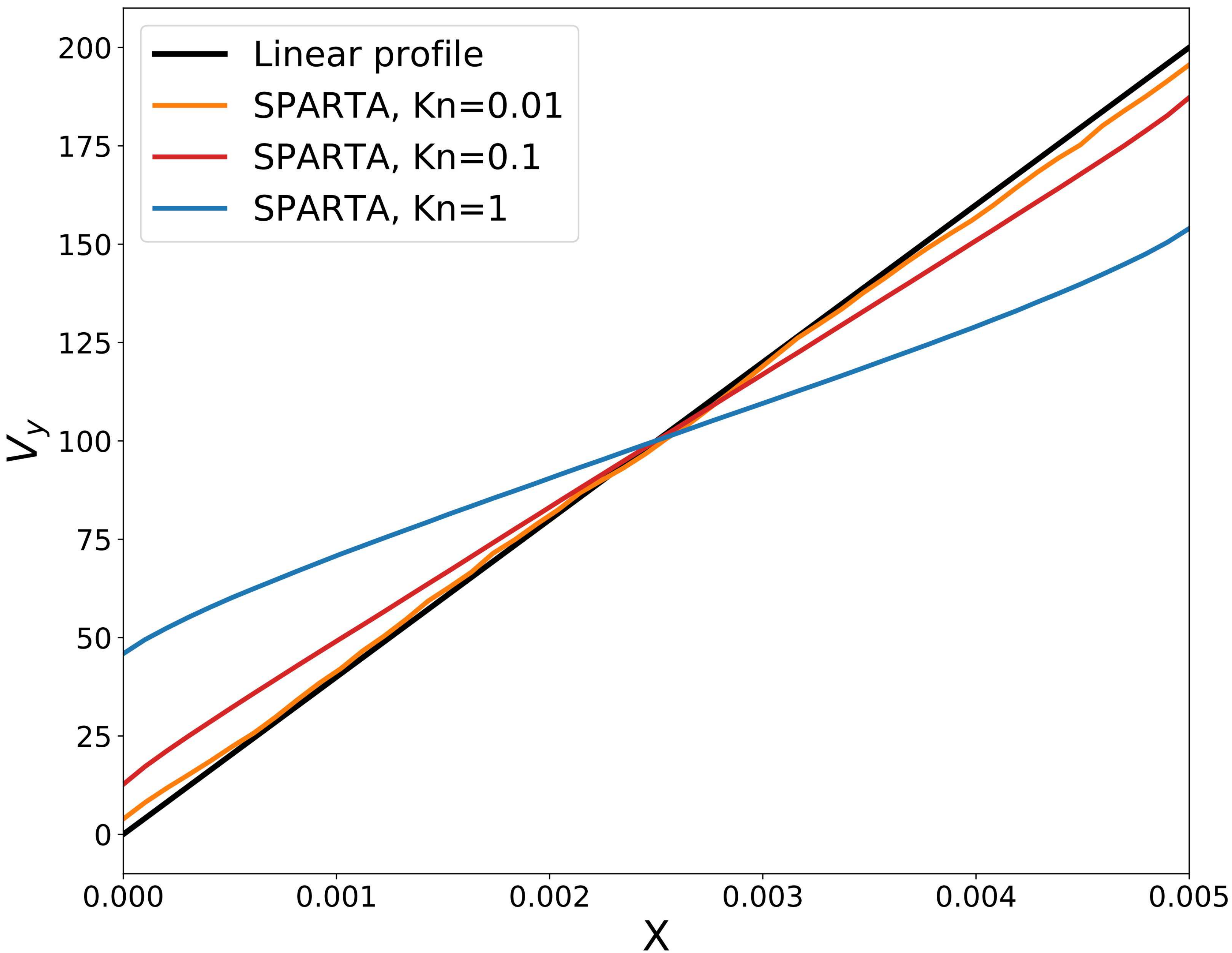
RAM vs. error, high temperature



Single-species Couette flow

- Argon gas
- Channel width 0.5 mm
- Temperature of walls 300K, right wall velocity 200 m/s ($M \approx 0.62$)
- Initial pressures:
  - 2070 Pa ($Kn \approx 0.01$)
  - 207 Pa ($Kn \approx 0.1$)
  - 20.7 Pa ($Kn \approx 1$)

Velocity profiles



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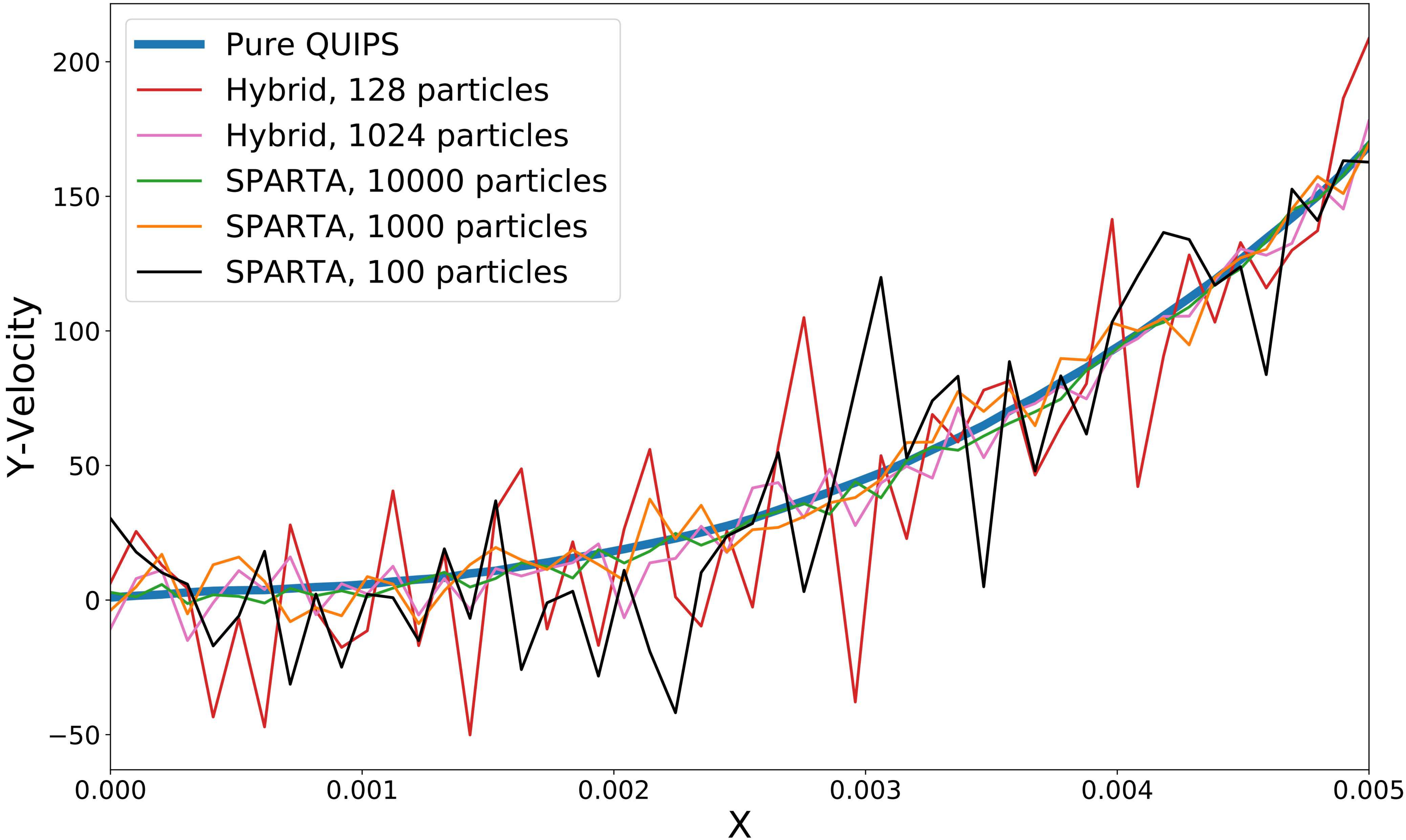
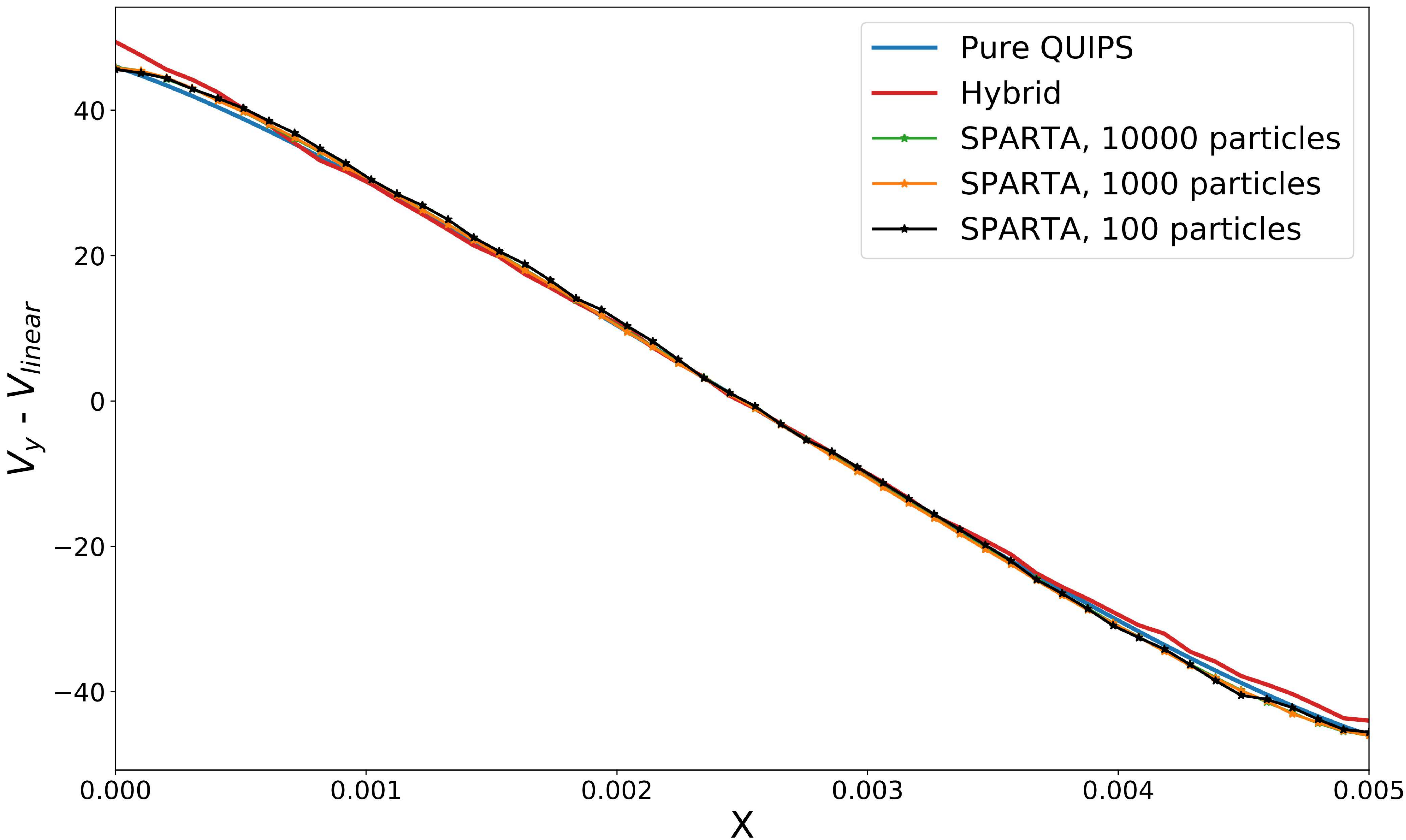
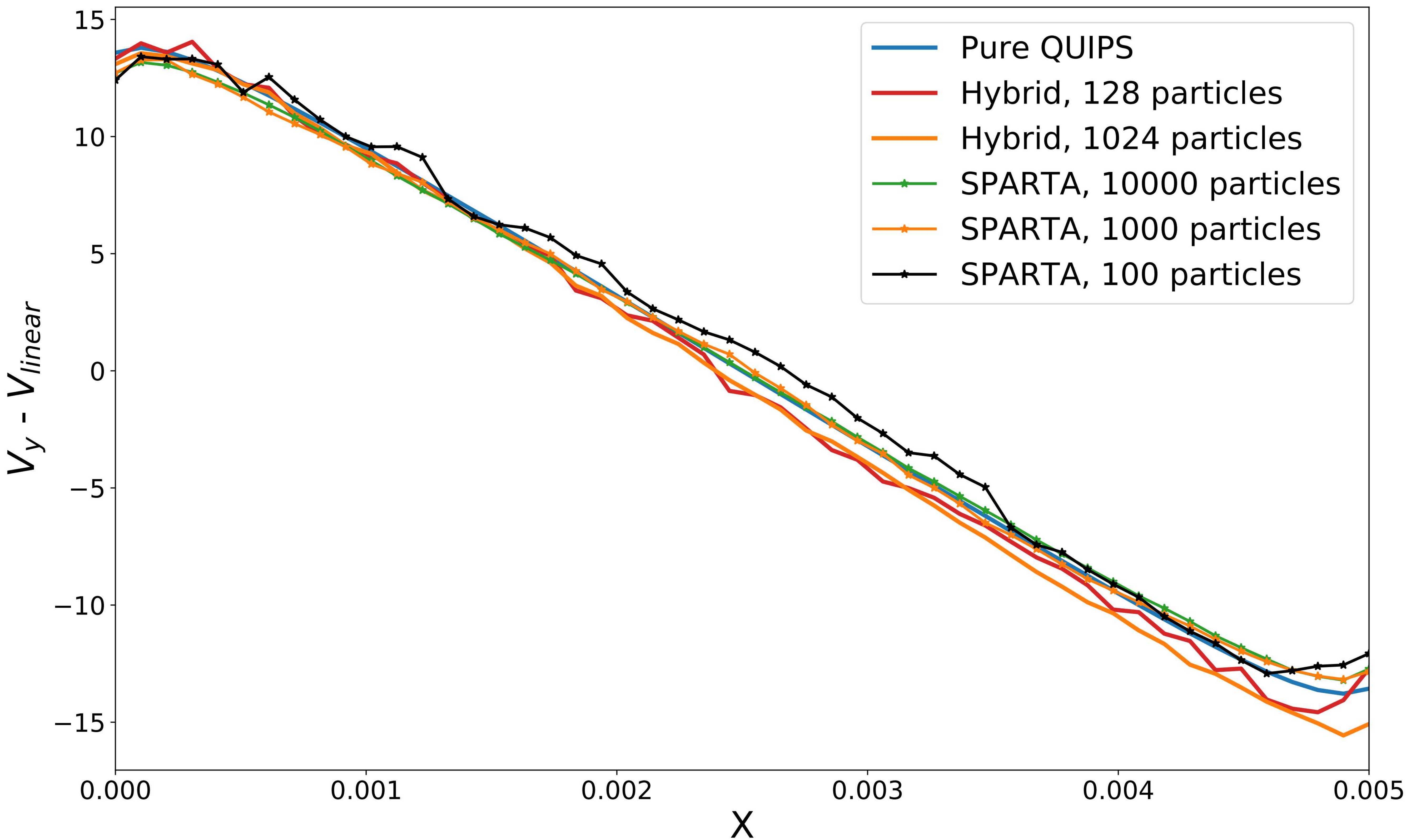
Unsteady velocity profile (Kn=0.1)



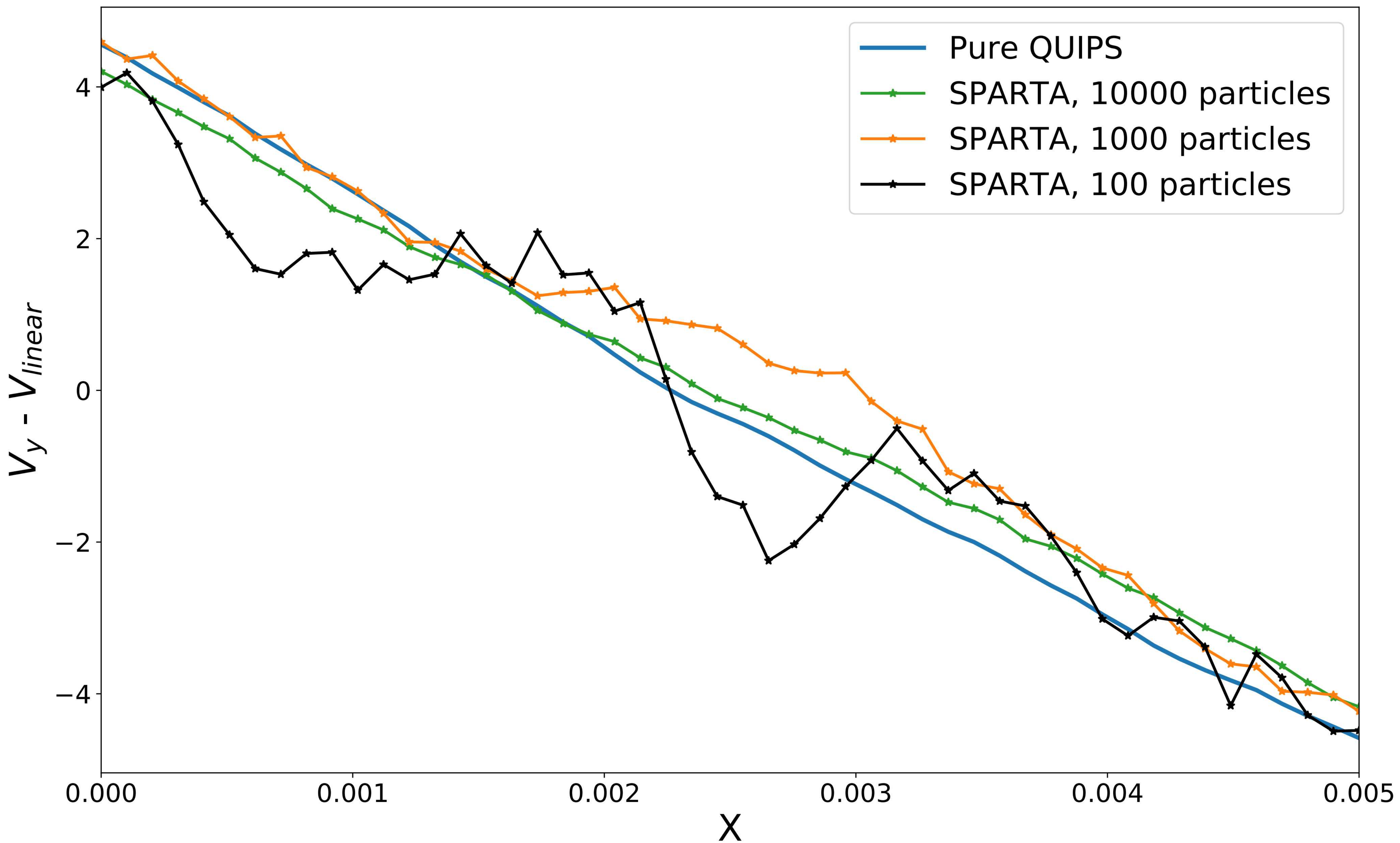
Velocity profile (Kn=1)



Velocity profile (Kn=0.1)



Velocity profile (Kn=0.01)



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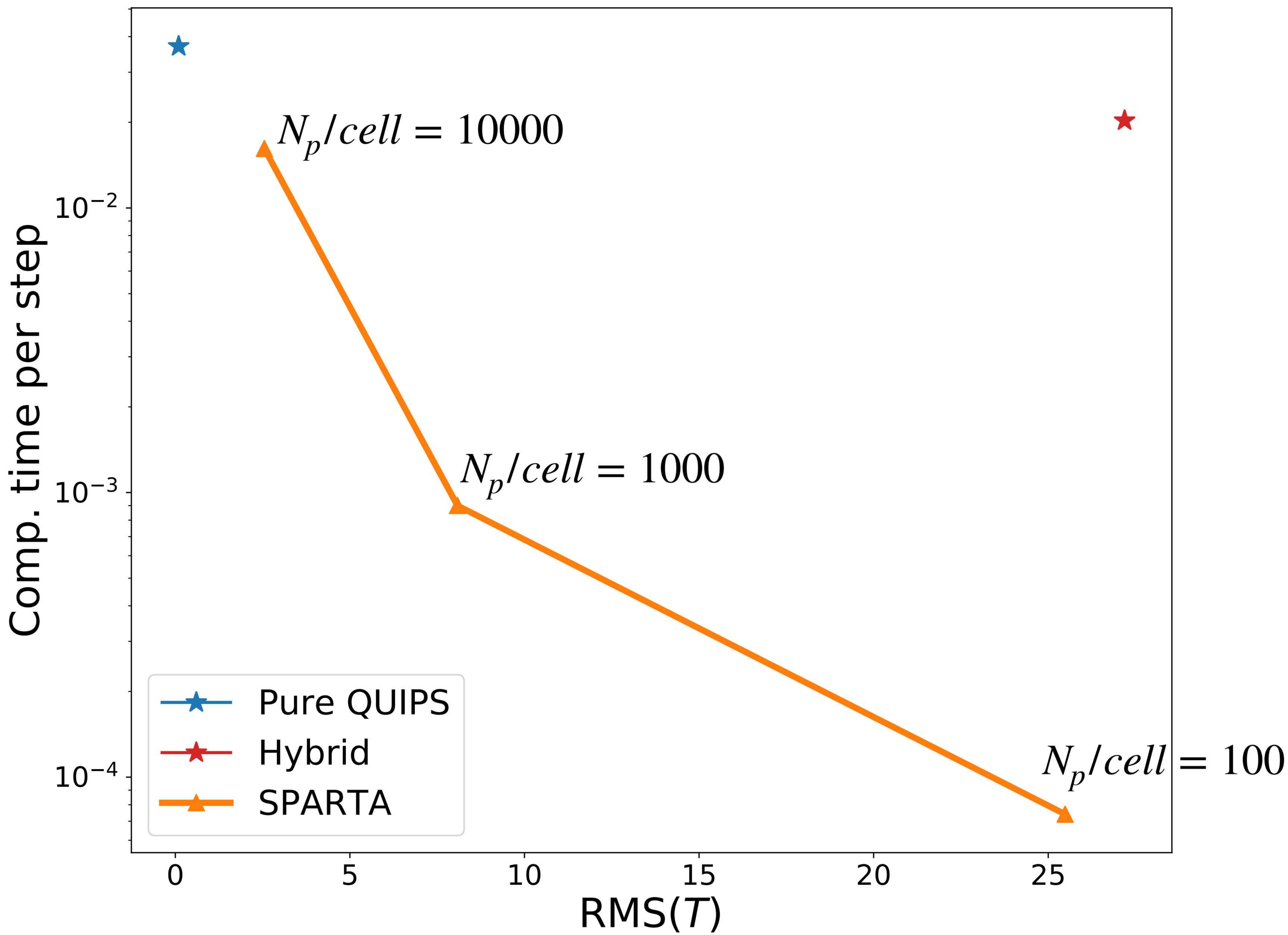
Temperature error (Kn=1)



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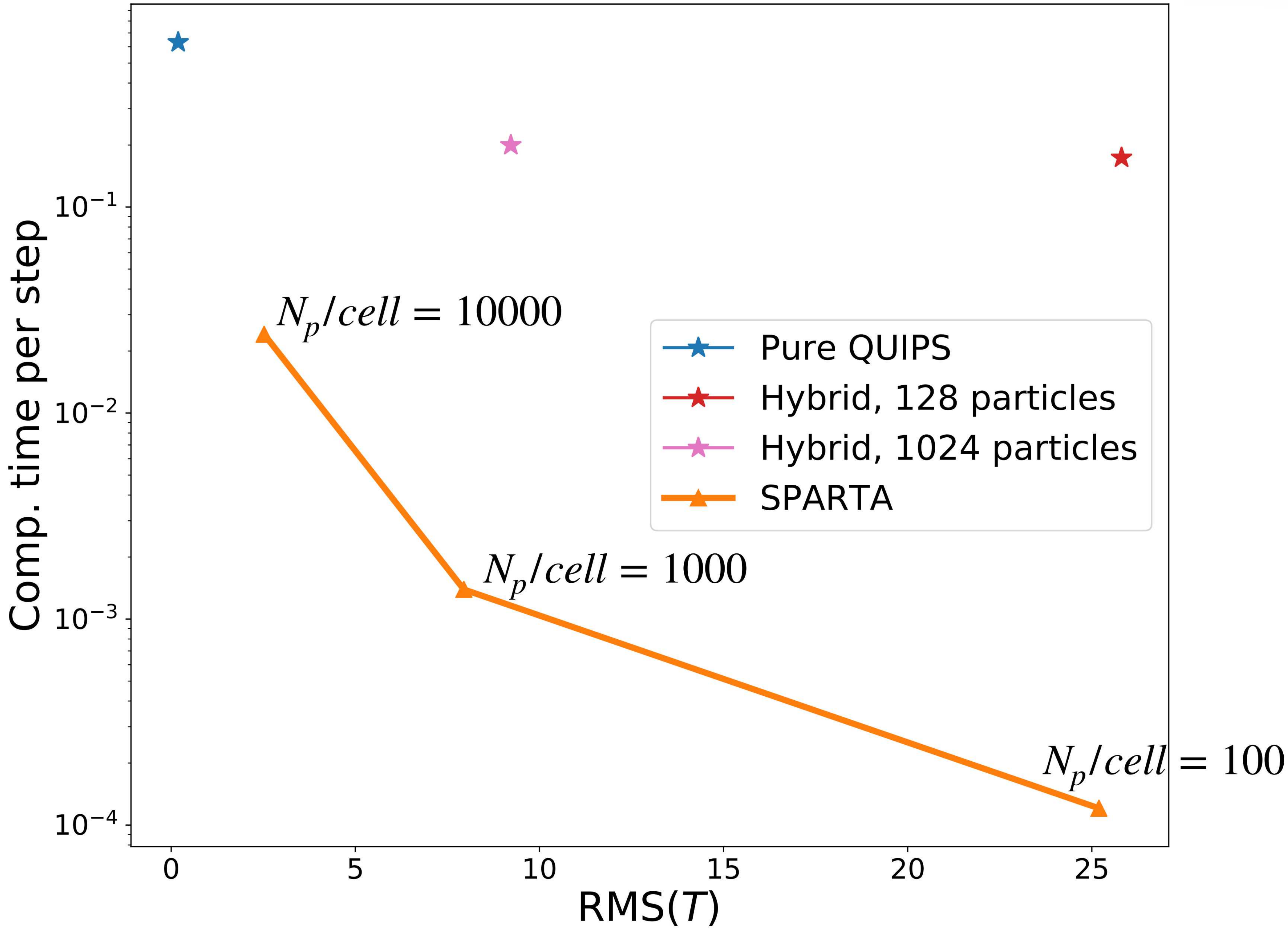
Temperature error (Kn=0.1)



Conclusions

- A new approach to modelling rarefied gas flows based on a velocity space hybridization has been developed and tested for several problems
- Such an approach can give better computational efficiency (compared to a pure QUIPS approach) and less RAM usage (compared to SPARTA), especially for flows where trace species are important
- For a 1-D single-species Couette flow, no obvious benefits due to absence of influence of trace populations, but at least approach is (somewhat) validated

Current efforts:

- 1-D and 2-D problems
- Variance reduction
- Modelling of ionization and influence of electric fields

Notes on convection

QUIPS uses a finite difference scheme:

- Timestep restricted by CFL condition: $\Delta t < \dfrac{\Delta x}{\eta_{max}}$
- Assumes that mass is located in **center of cell**

But DSMC particles have a continuous-valued position!

When creating DSMC particles during collisions, can create in cell center (thus conserving center of mass)
But when a collision involving a DSMC particle creates mass in QUIPS region (from mass depleted from DSMC particle), we shift the center of mass

Is this a problem?

Notes on convection

- Some numerical studies show that change in center of mass is not significant
- Perhaps can have an effect if coupled with a Particle-in-Cell solver (PIC solvers are stiff)

Options to avoid:

- Decrease cell size (requires decreasing timestep) (still may not fix bias towards center of cell)
- When taking mass from DSMC and putting onto QUIPS grid, use split replenishment between current cell and nearest cell (introduces numerical diffusion)