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Velocity-space Hybridization of DSMC and a Boltzmann Solver

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Outline

1. **Brief overview**
    1. Rarefied flows and DSMC
    2. DSMC drawbacks
2. **Quasi-Particle Simulation (QUIPS)**
    1. Distribution function representation
    2. Collision integral evaluation
3. **Hybridization**
    1. Why hybridize in velocity space?
    2. Velocity-space hybridization particulars
        1. Velocity space decomposition
        2. Collisions
        3. Merging
4. **Numerical results**
    1. Ionization rate computation
    2. Couette flow
5. **Conclusion**

DSMC

$Kn = \frac{\lambda}{L}$ – governs applicability of different models

When do we have to use kinetic methods?

- $Kn < 0.01$ – can use CFD
- $0.01 \leq Kn \leq 0.1$ – can use CFD with appropriate boundary conditions

- Rarefied flows (large λ)
- Meso- and nanoscale flows (small L)

DSMC (Direct Simulation Monte Carlo) – main engineering/ computational tool for transitional and rarefied regimes

DSMC

Main ideas of DSMC:

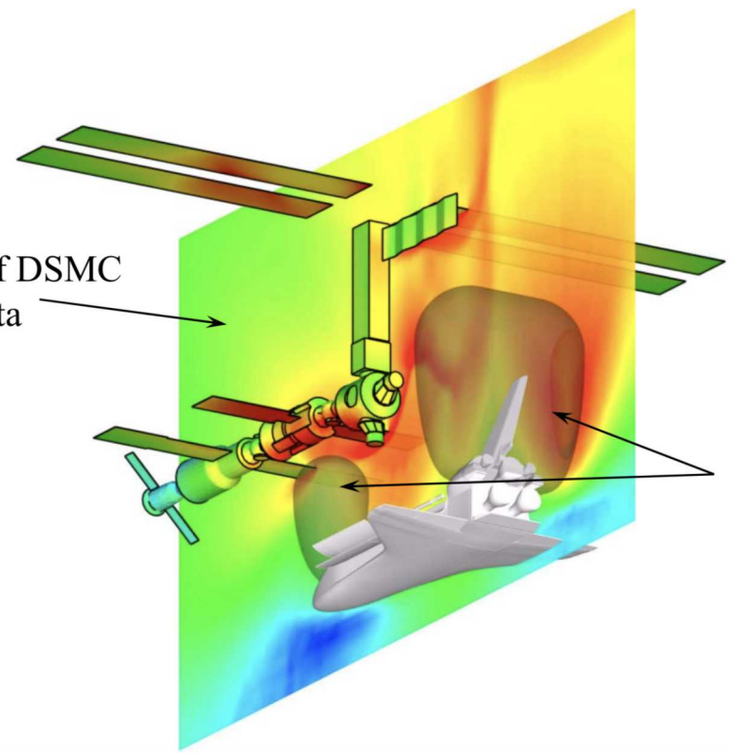
- Model many particles, each represents many ($\sim 10^{15}$) real molecules
- Separate convection and collision steps: particles move along straight lines in between collisions ($\mathbf{r}_{t+\Delta t} = \mathbf{r}_t + \mathbf{v}\Delta t$)
- Collisions are performed stochastically: computational cost $\sim \mathcal{O}(N_p)$
- Sample macroscopic parameters based on microscopic quantities of molecules in cells

DSMC can be used in a wide range of flows, but becomes very expensive at low Kn numbers!

DSMC

Main drawbacks of DSMC:

- Stochastic fluctuations lead to issues with:
  - Modelling low-speed flows (poor signal-to-noise ratio)
  - Modelling transient flows (cannot do time-averaging)
  - Hybridization with CFD (noisy boundary conditions in CFD solver)
  - Particle-in-cell codes (stiff numerically)
- Issues with modelling trace populations such as:
  - High-velocity particles
  - Excited internal states
  - Trace species



Example:

Ar/e- mixture: 0.1% ionization

For each electron, need to have 10^3 argon particles

F. Lumpkin, J. Marichalar, A. Piplica, 2007

Discrete Boltzmann Equation

Boltzmann equation:

$$\frac{\partial \phi}{\partial t} + \boldsymbol{\eta} \cdot \nabla_{\mathbf{r}} \phi = \int_{\zeta} \left[\phi(\boldsymbol{\eta}') \phi(\boldsymbol{\zeta}') - \phi(\boldsymbol{\eta}) \phi(\boldsymbol{\zeta}) \right] g \sigma_t d\boldsymbol{\zeta}$$

Discrete velocity method:

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

In scaled form:

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

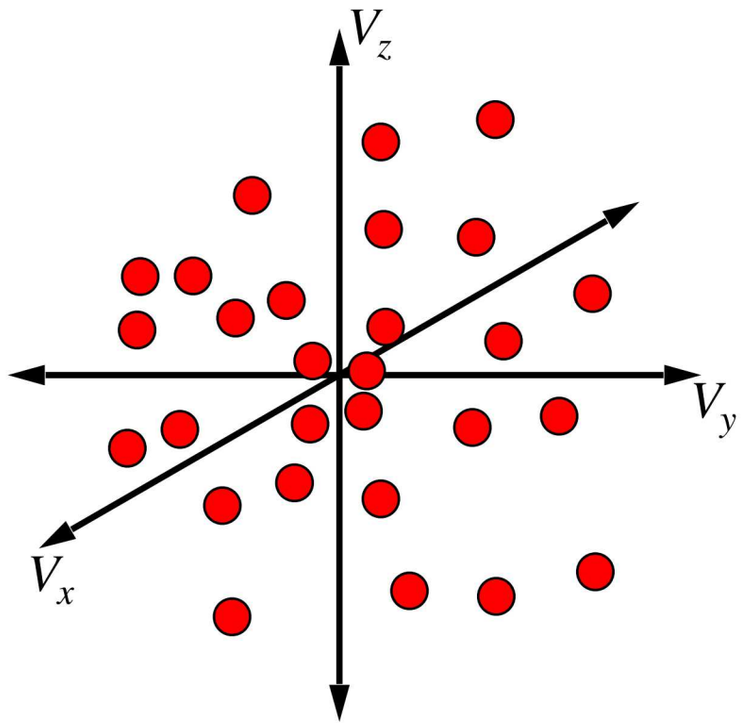
Here $\hat{\phi}(\hat{\boldsymbol{\xi}})$ is the (scaled) number of particles in a volume β^3 centered around $\boldsymbol{\xi}$; β is the grid spacing

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

DSMC vs QUIPS

DSMC

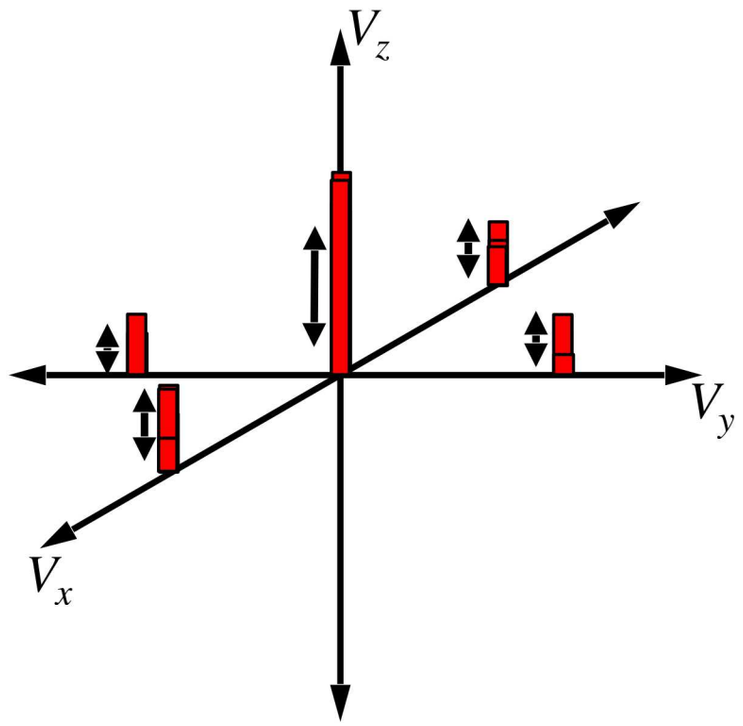
"Fixed mass, variable velocity particles."



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

Numerical scheme:

Velocity distribution function in each physical cell is a 3-dimensional array (3 velocity components) (not considering internal energies)

1. Compute change in velocity distribution function in each physical cell due to collisions
2. Perform convection
    1. Apply appropriate boundary conditions
    2. Compute convection

Convection:

In present work, a simple first-order upwind finite difference scheme is used; more accurate methods (e.g., Finite Volume) are widely used for DVM (works of Titarev, Kolobov, etc.)

$$\hat{\phi}_{n_x}^{\hat{t}+\Delta\hat{t}}(\hat{\eta}) = \hat{\phi}_{n_x}^{\hat{t}}(\hat{\eta}) - c\left(\phi_{n_x+1}^{\hat{t}}(\hat{\eta}) - \phi_{n_x}^{\hat{t}}(\hat{\eta})\right), \hat{\eta} < 0$$

$$\hat{\phi}_{n_x}^{\hat{t}+\Delta\hat{t}}(\hat{\eta}) = \hat{\phi}_{n_x}^{\hat{t}}(\hat{\eta}) - c\left(\phi_{n_x}^{\hat{t}}(\hat{\eta}) - \phi_{n_x-1}^{\hat{t}}(\hat{\eta})\right), \hat{\eta} > 0$$

Stability criterion: $c = |\hat{\eta}|\dfrac{\Delta\hat{t}}{\Delta\hat{x}} < 1$

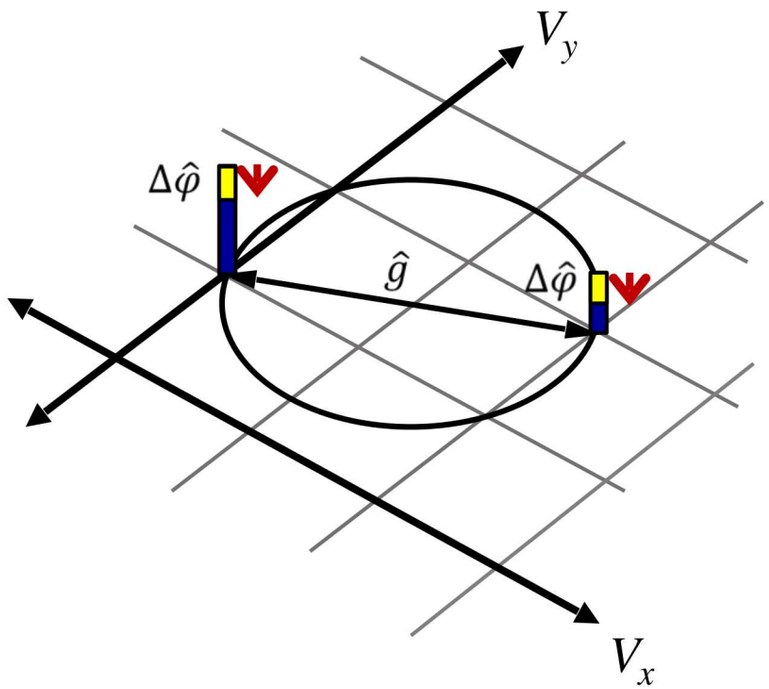
QUIPS collisions

How to compute collision integral?

$$\sum_{\hat{\xi}\neq\hat{\eta}} \left[\hat{\phi}(\hat{\eta}')\hat{\phi}(\hat{\xi}') - \hat{\phi}(\hat{\eta})\hat{\phi}(\hat{\xi})\right] \hat{g}\hat{\sigma}_t$$

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



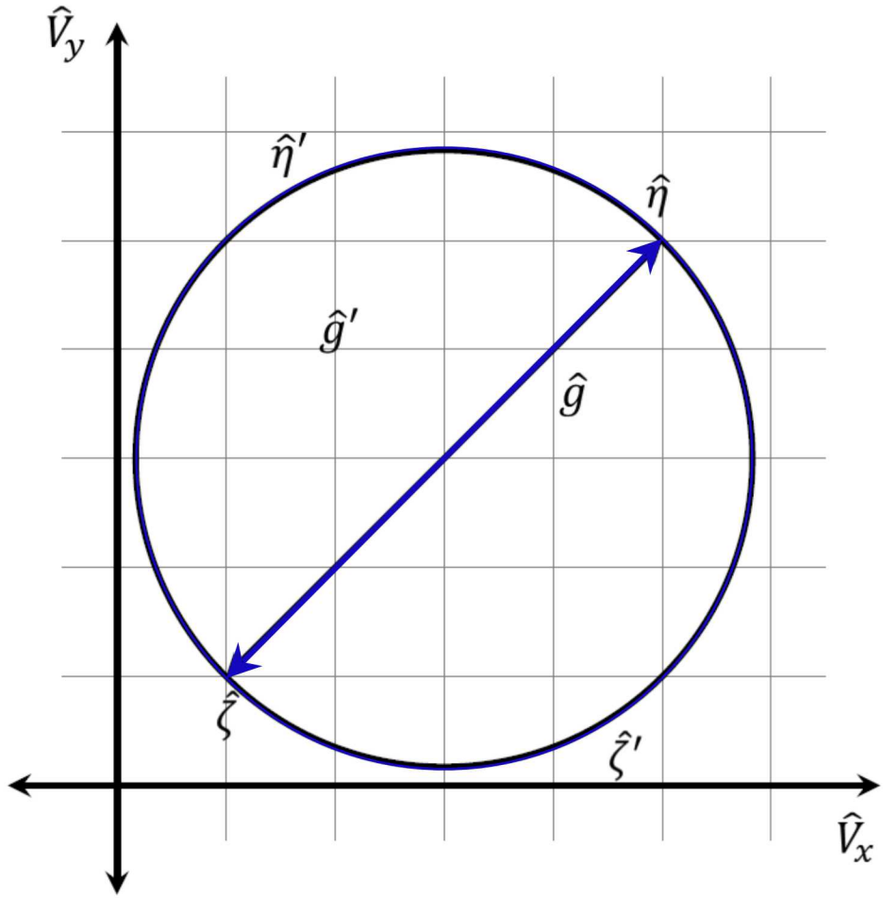
$$N_{coll} \sim \frac{1}{C_{RMS}^2}$$

Noise parameter

QUIPS collisions

How to compute collision integral (replenishment)?

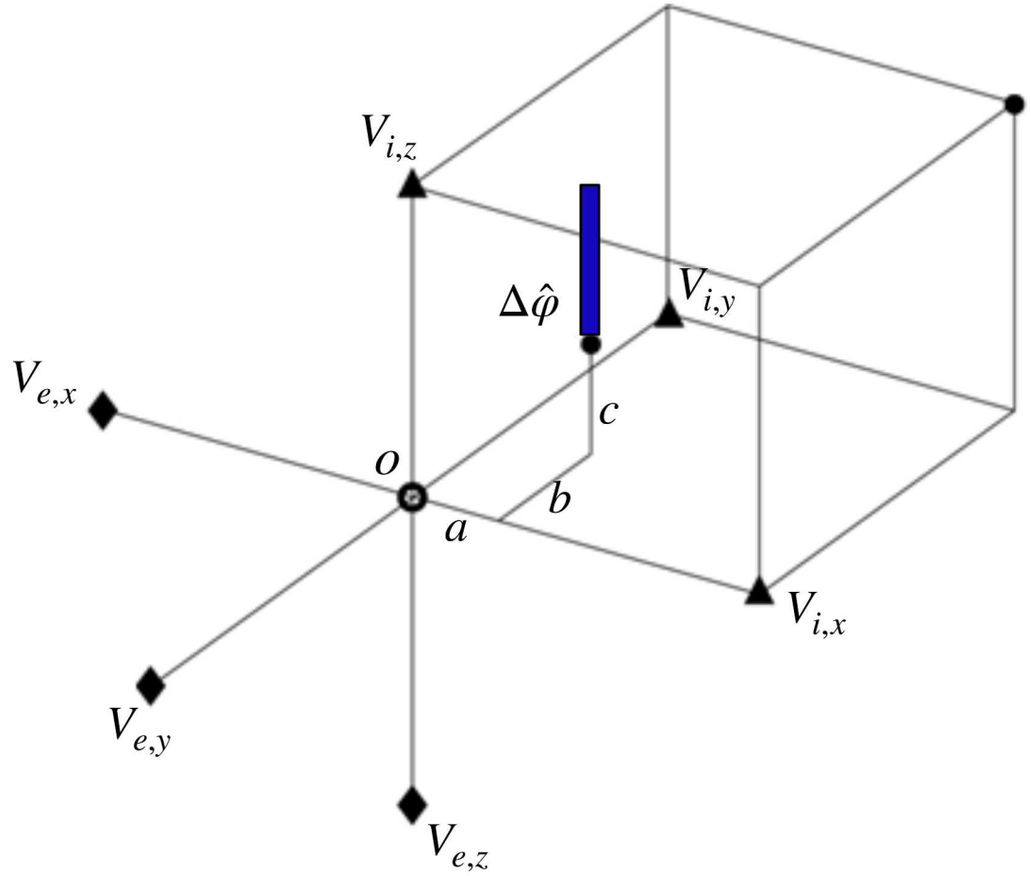
Find post-collision velocity (random point on a sphere)



QUIPS Collisions: Remapping

But velocity does not necessarily lie on grid!

- Remap post-collision mass to 7 points on grid
- Conserves mass, momentum, energy



P. Varghese, RGD Proceedings, 2006

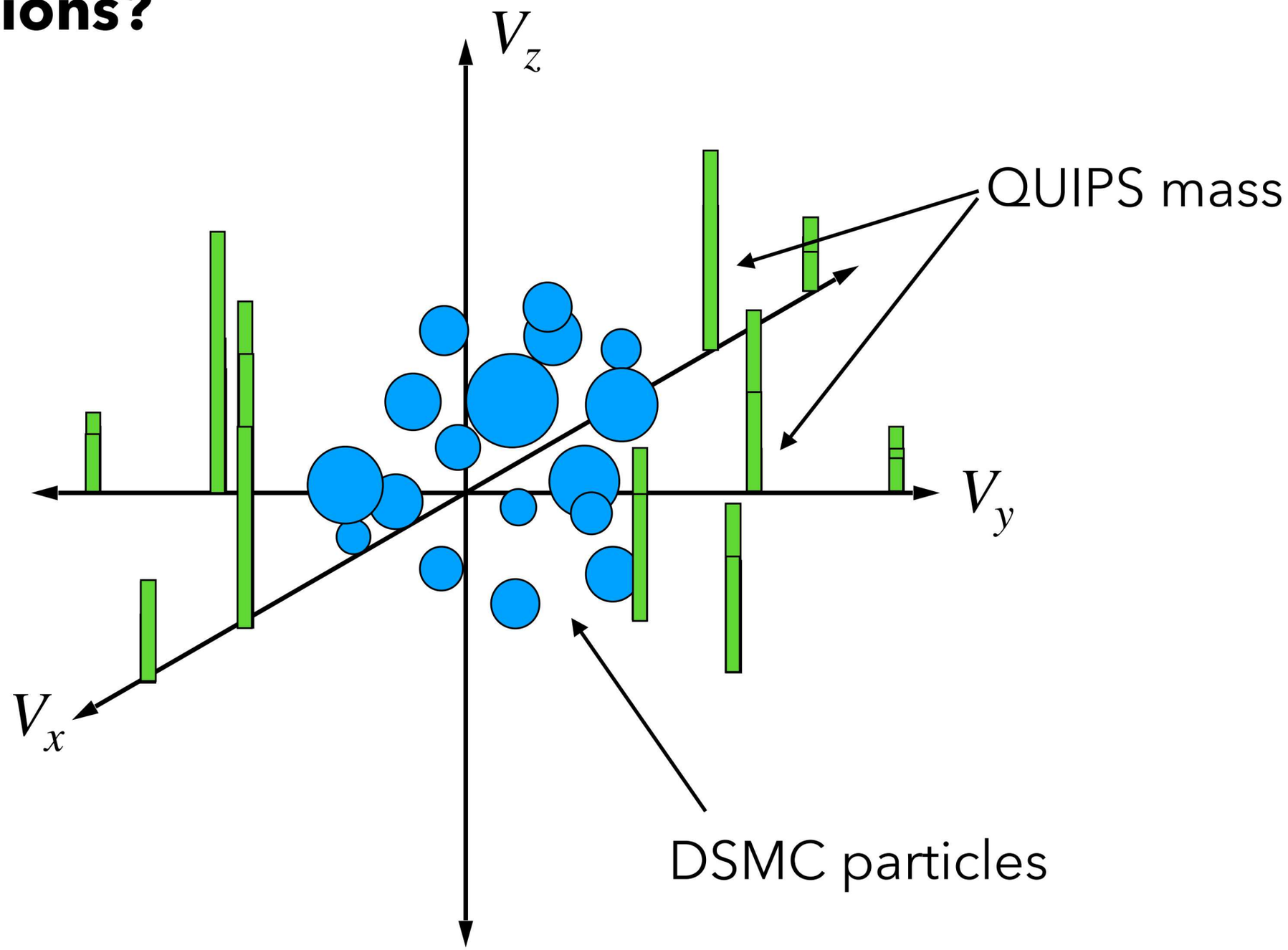
QUIPS summary

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
- Accuracy of collision integral evaluation can be adjusted without increase in RAM requirements

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 DSMC particles), while retaining accuracy in modelling of high-energy particles/trace species (use QUIPS)
- DVM have issues when there are discontinuities in boundary conditions

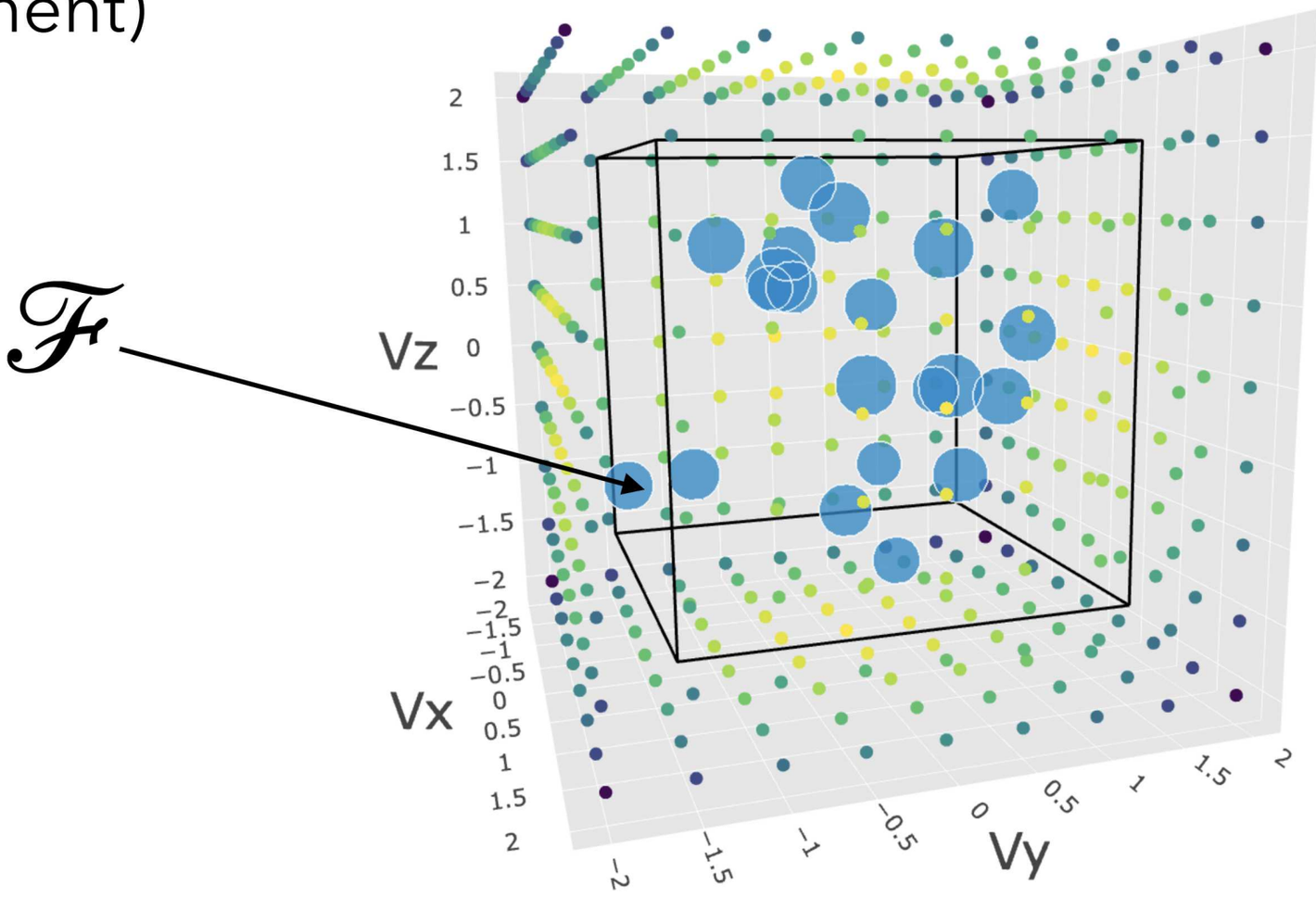
Previous work:

- 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

Hybrid QUIPS/DSMC

How to hybridize?

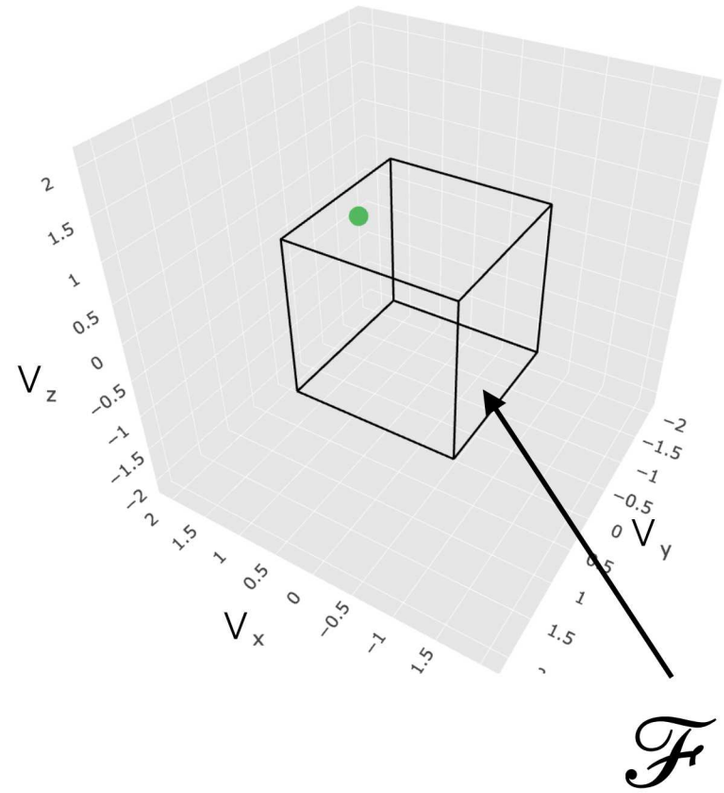
- Pick region in velocity space where VDF is represented by DSMC particles
- Use DSMC collision mechanics (instead of small depletion/ replenishment)

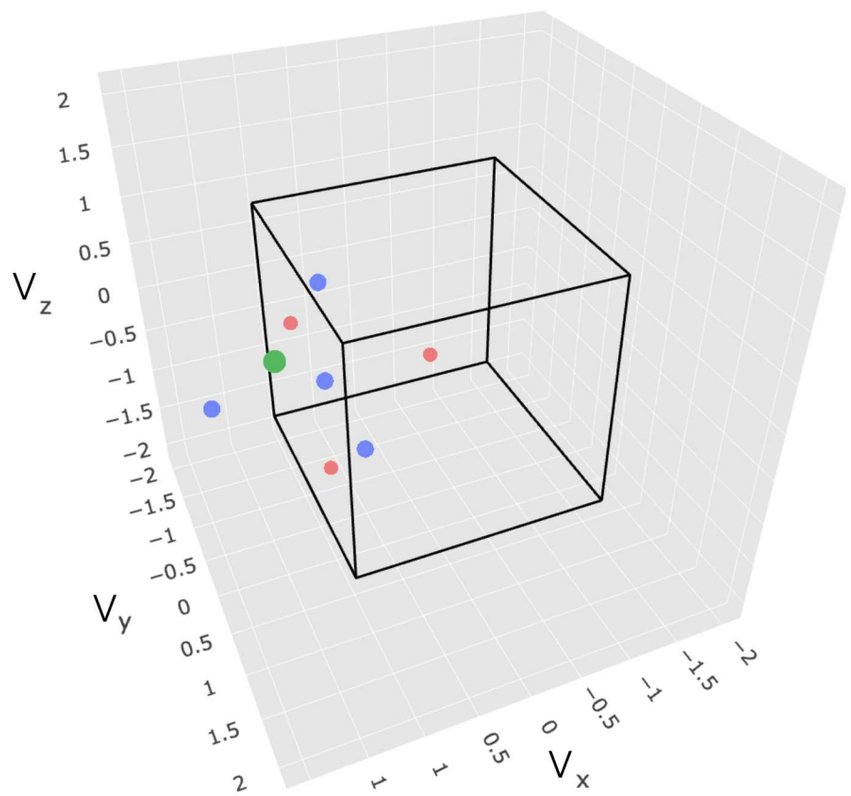


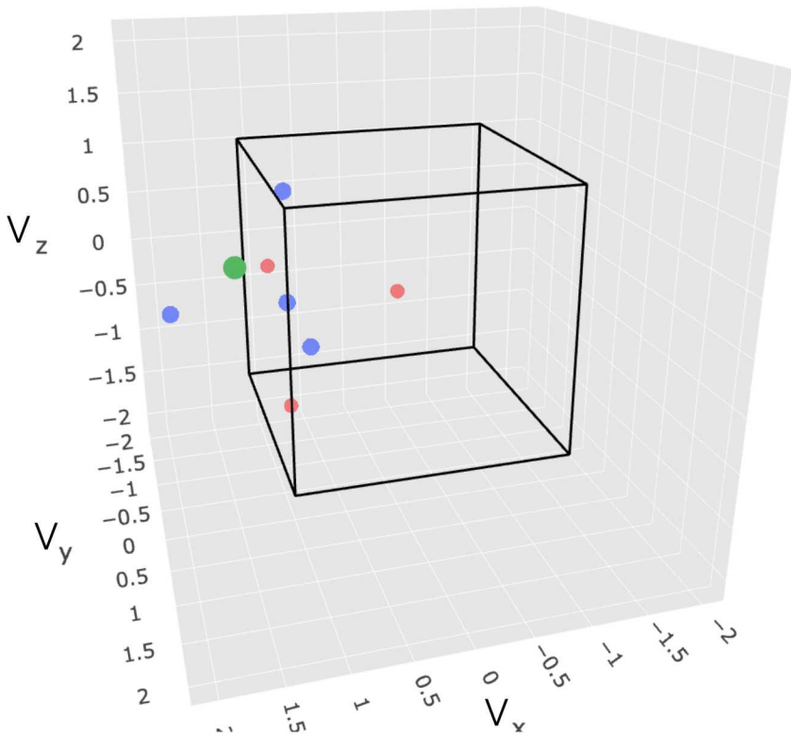
Hybrid QUIPS/DSMC

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



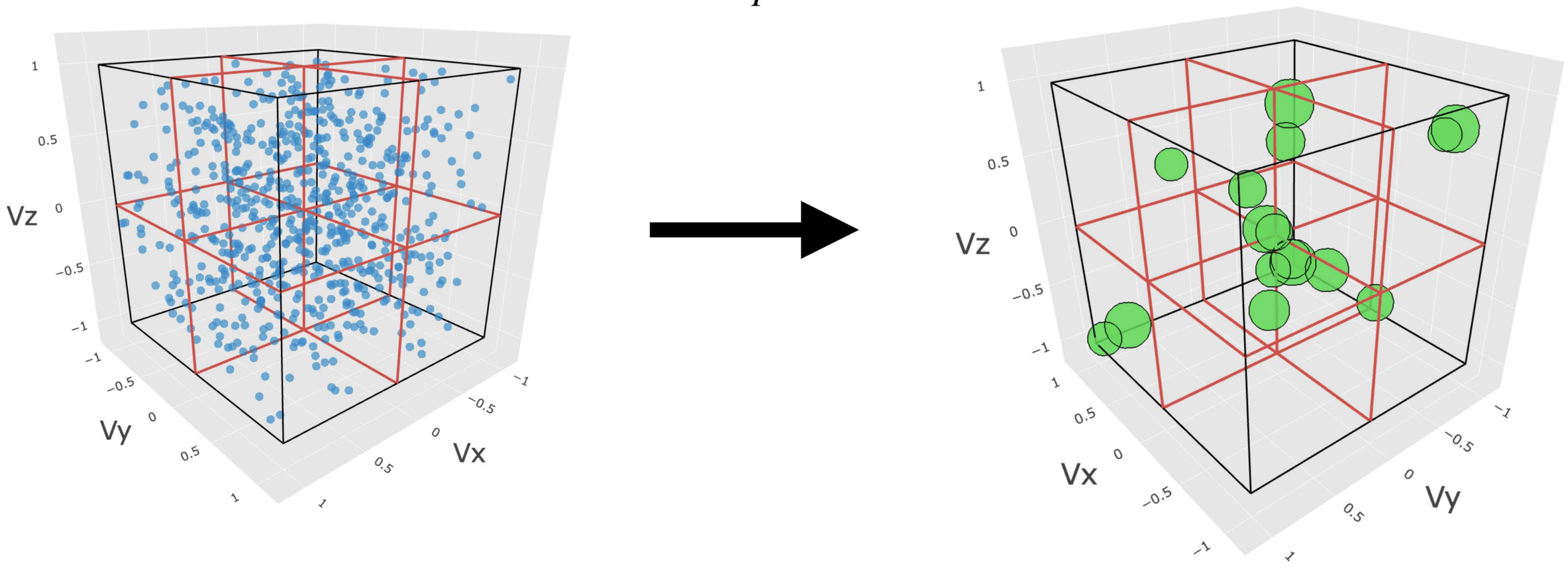




Hybrid QUIPS/DSMC

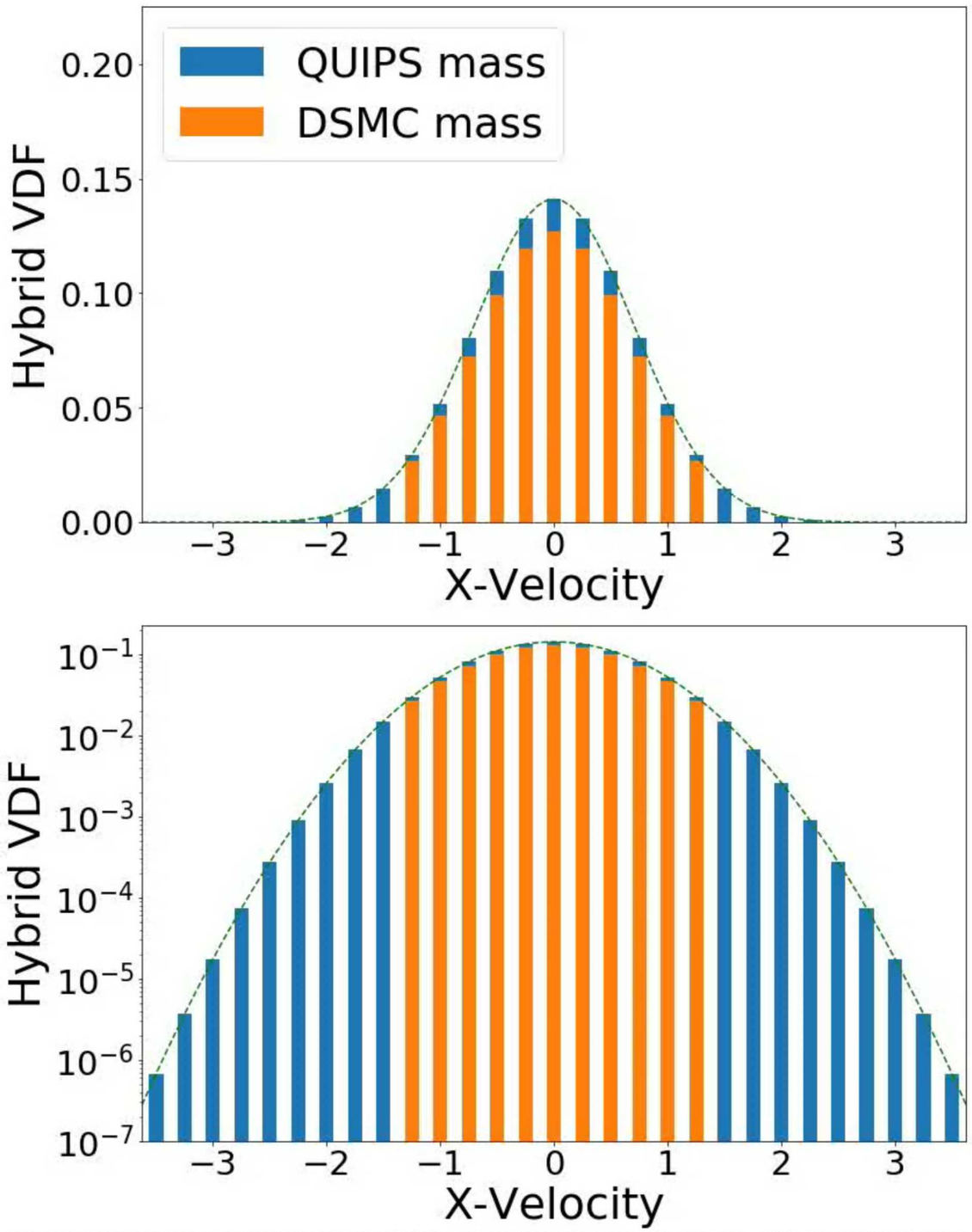
How to avoid (exponential) growth of number of particles?

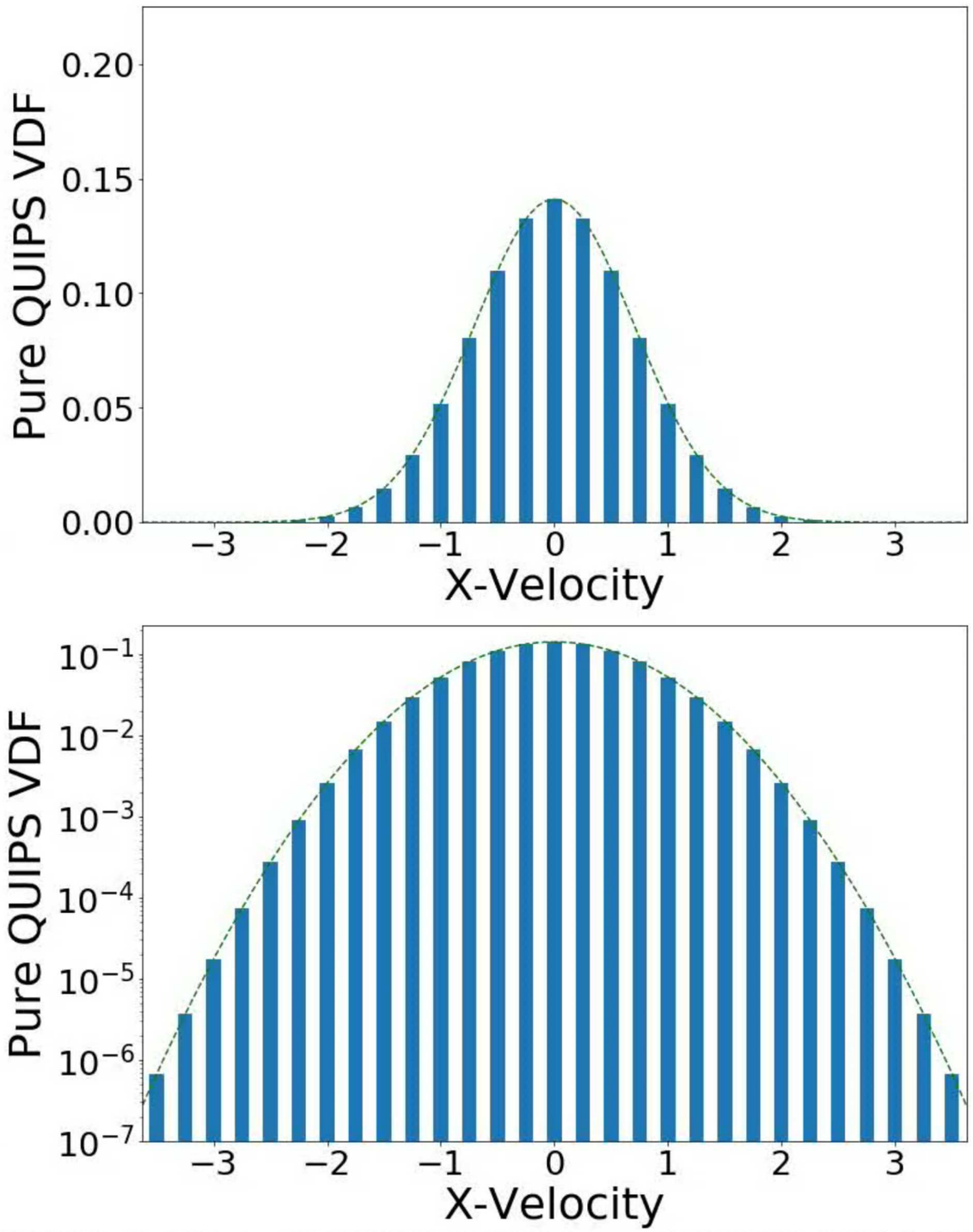
- Do conservative N:2 merging (preserve mass, momentum, energy, spatial moments)
- Current work utilizes a simple grid-based approach (M*M*M merging cells); CPU time $\sim \mathcal{O}(N_p)$; additional RAM $\sim \mathcal{O}(M^3)$



Hybrid QUIPS/DSMC

Example of hybrid VDF representation





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: $T_{Ar} = 300K;\ 2eV \leq T_e \leq 10eV$; 0.1% ionization
Hybrid/variable weight DSMC code uses **128** particles unless stated otherwise

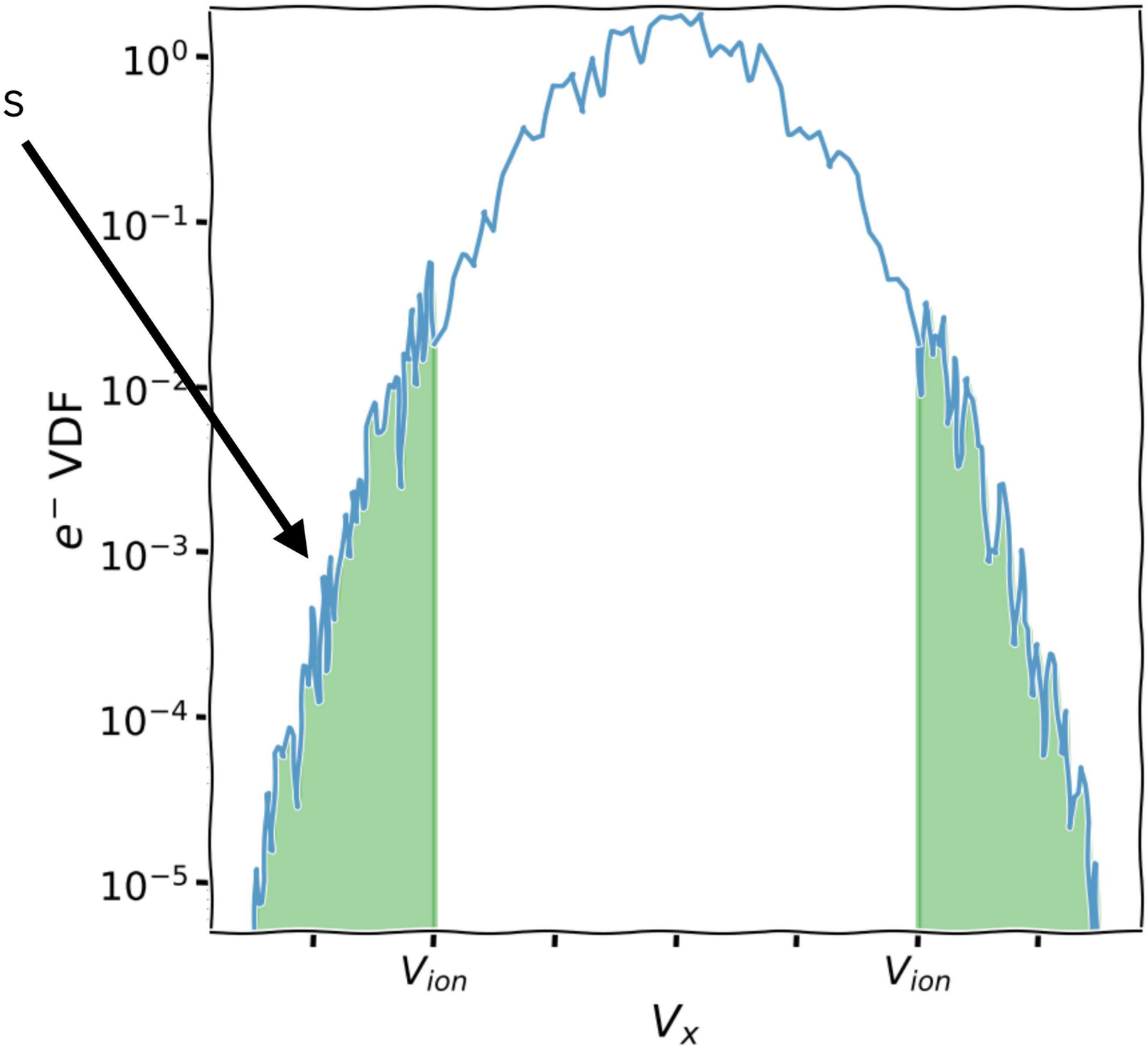
Possible hybridization options:

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

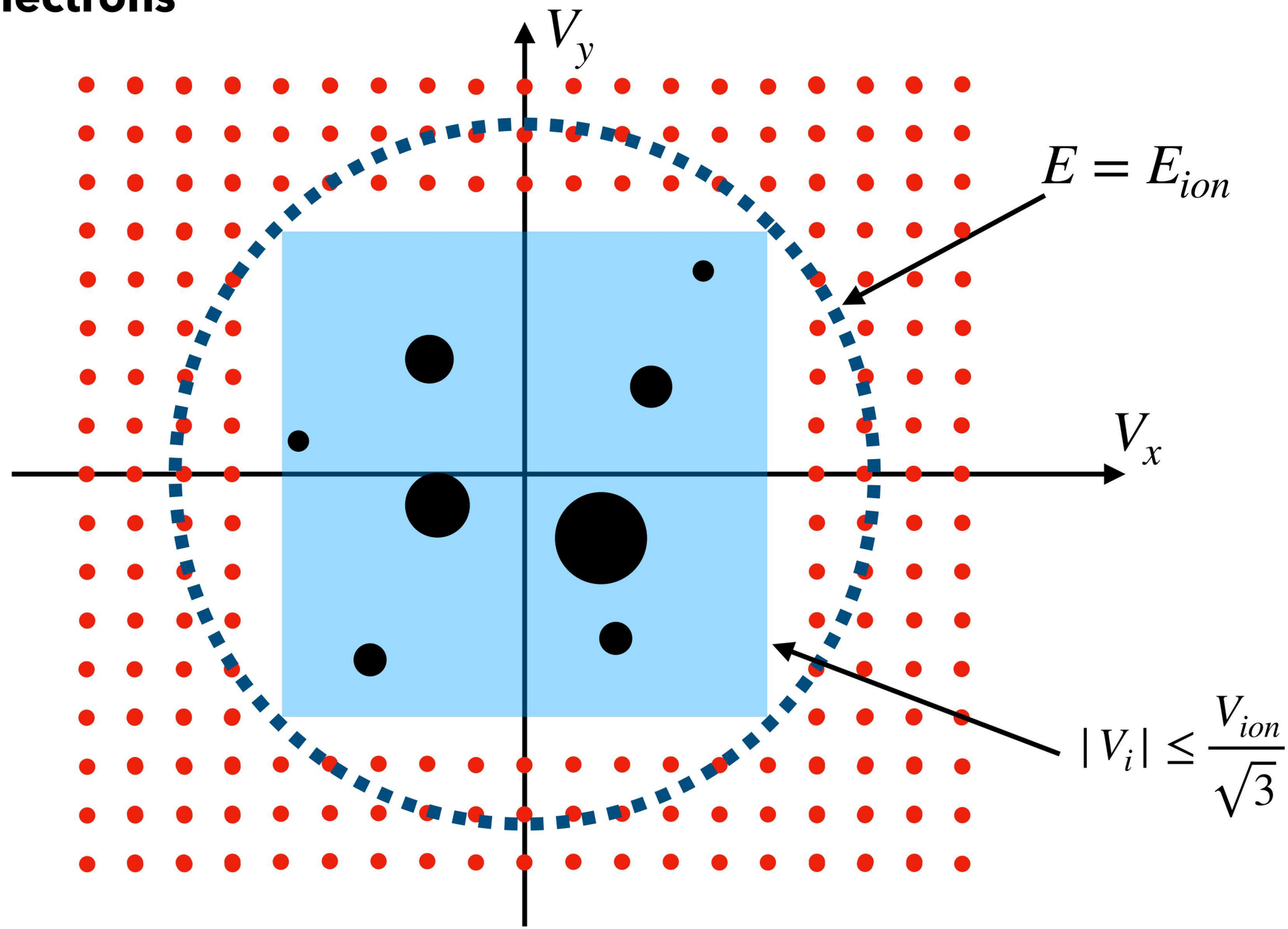
At T=2eV, tails contain 0.2% mass; for standard DSMC need ~500 particles to get 1 particle in tail!

At T=5eV, 10% mass

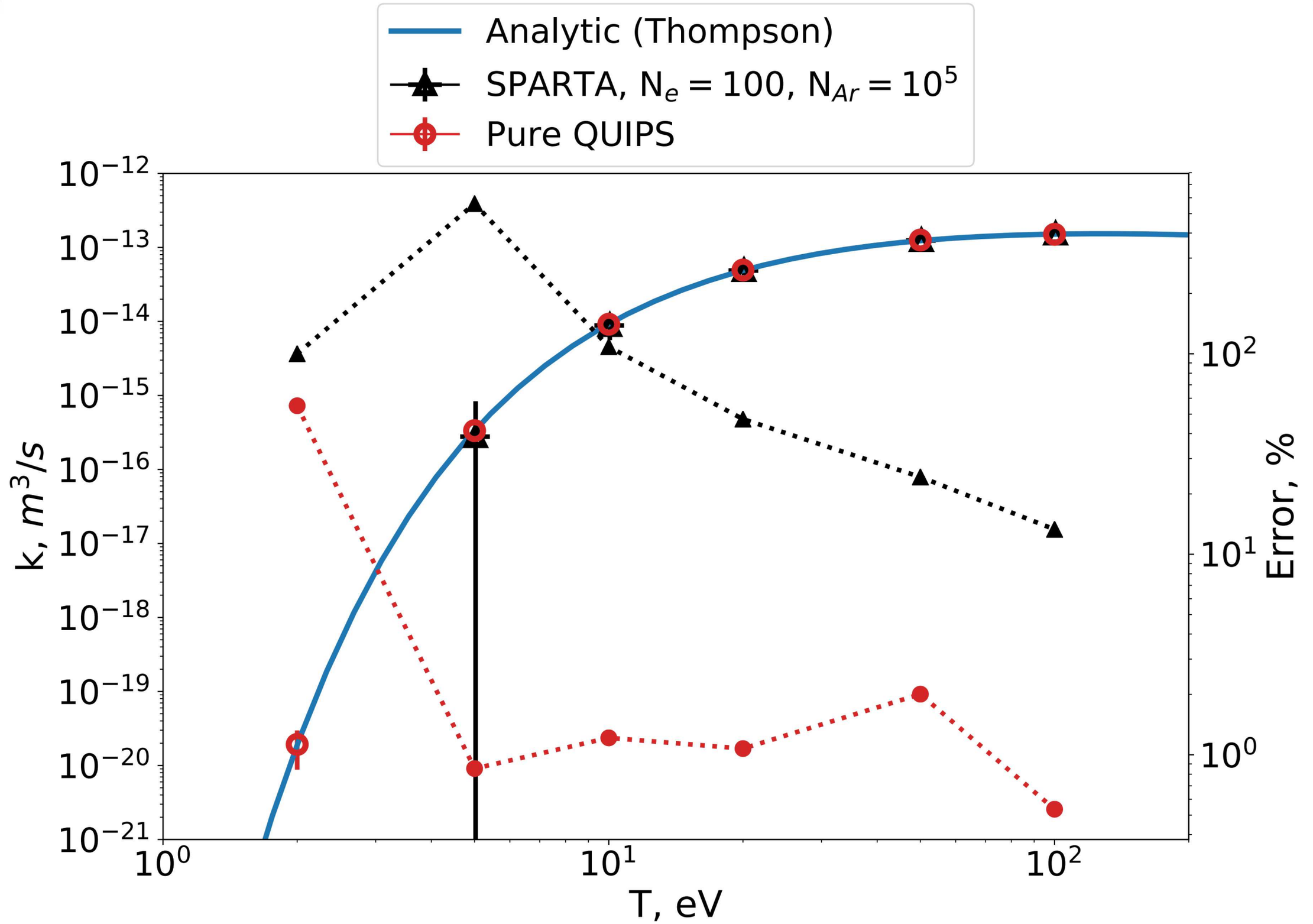


Choice of hybrid region

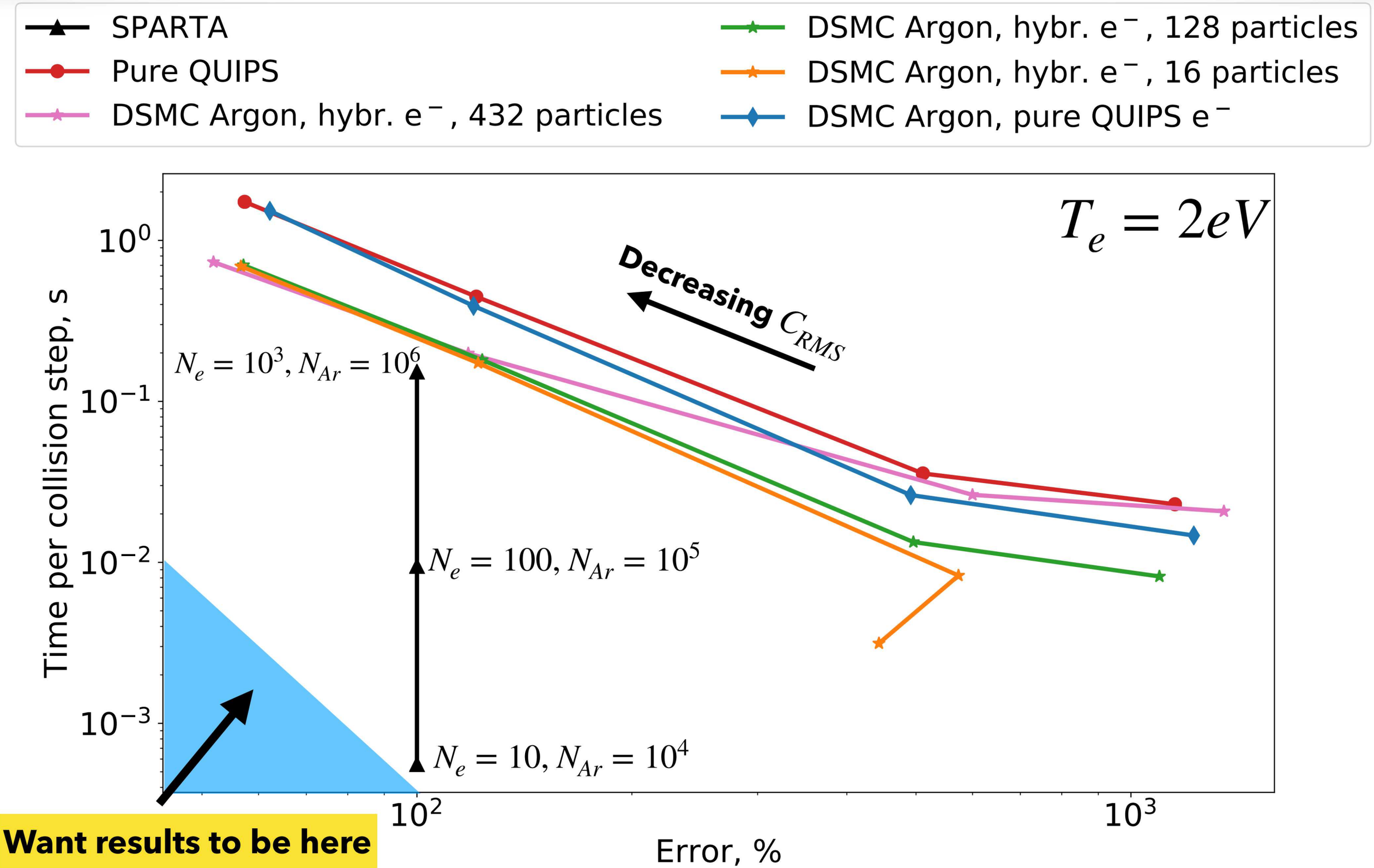
If modelling electrons with hybrid scheme, use DSMC particles for low-velocity electrons



Electron-impact ionization rate

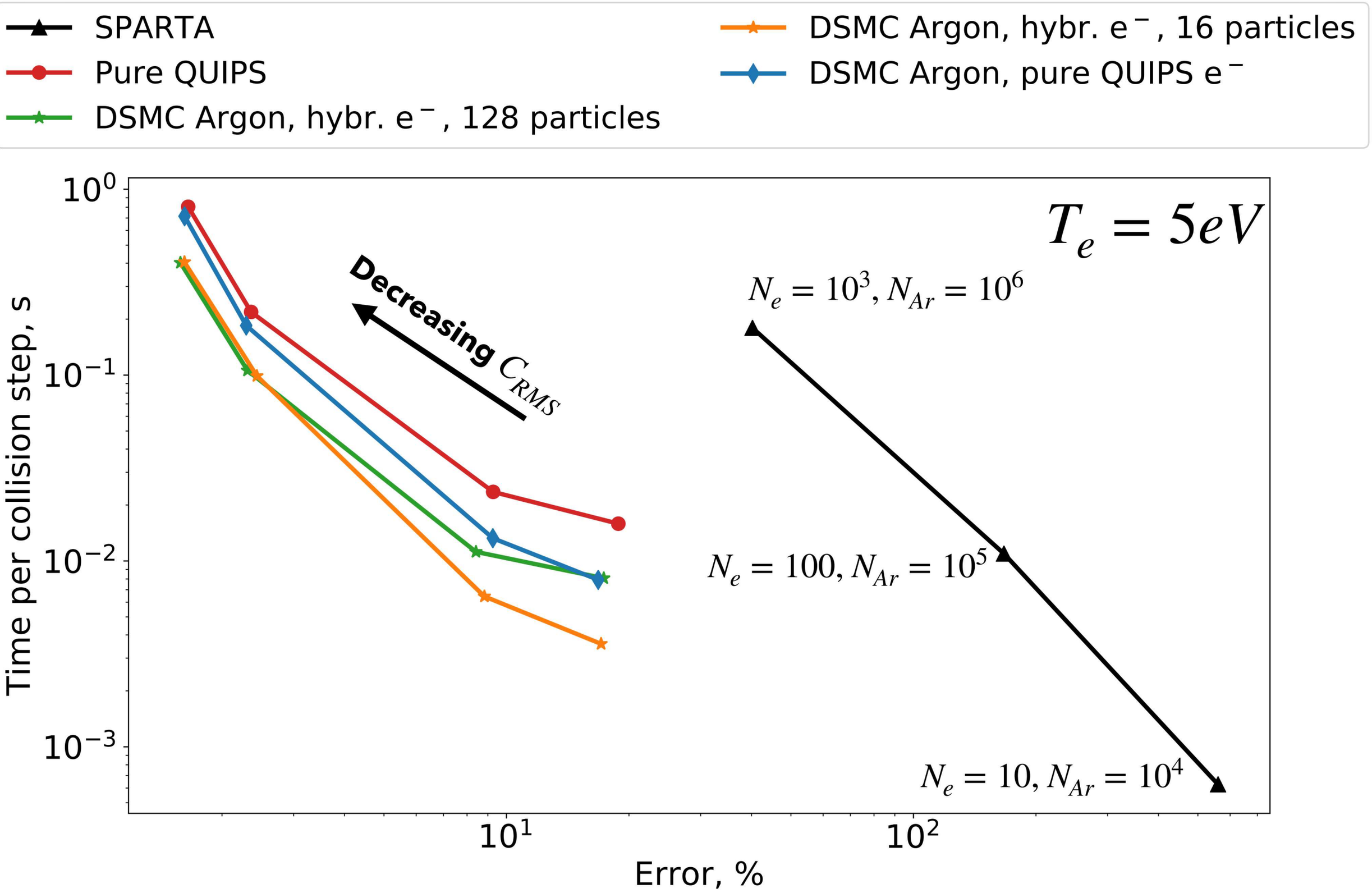


CPU vs. error

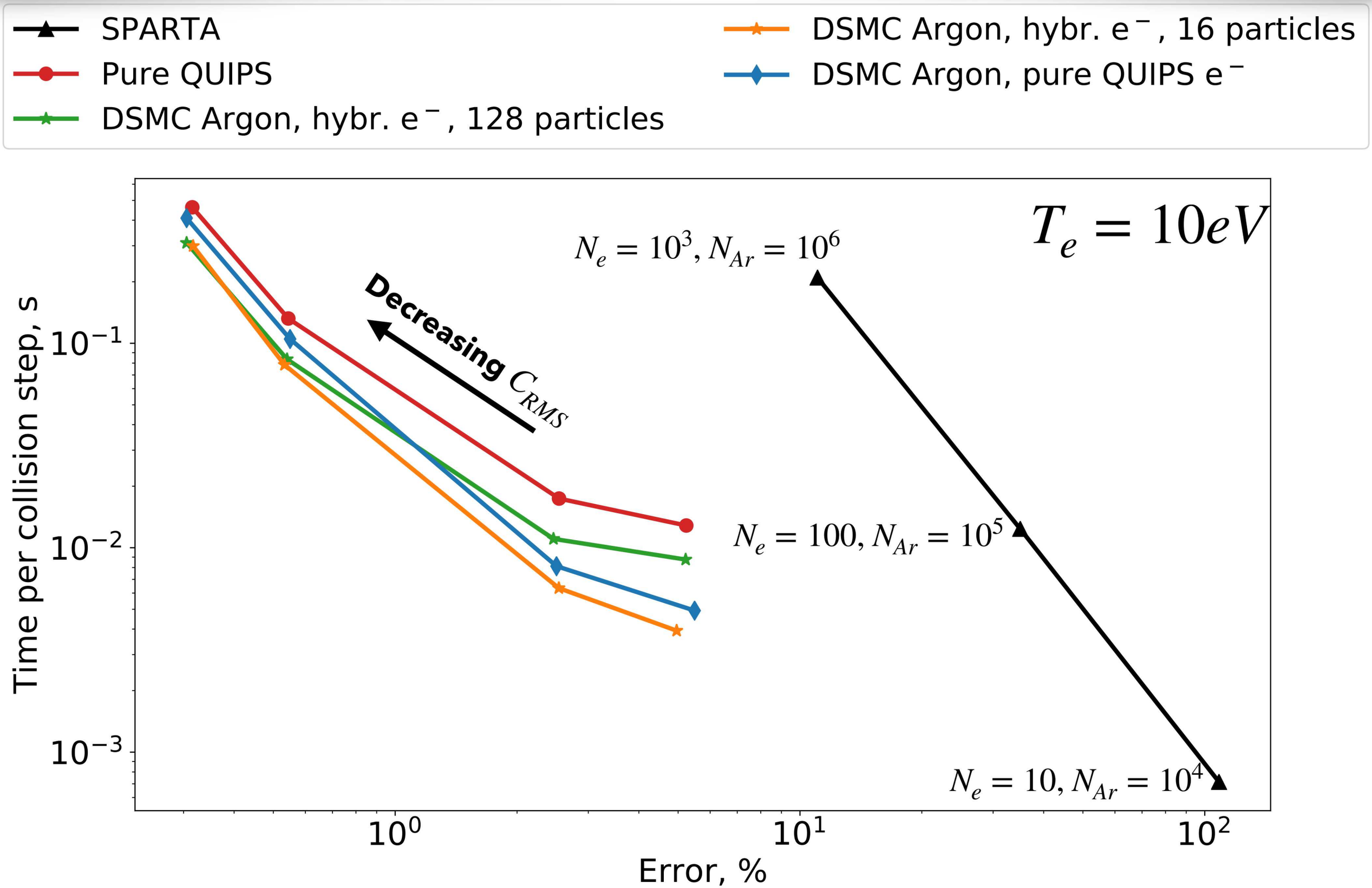


Want results to be here

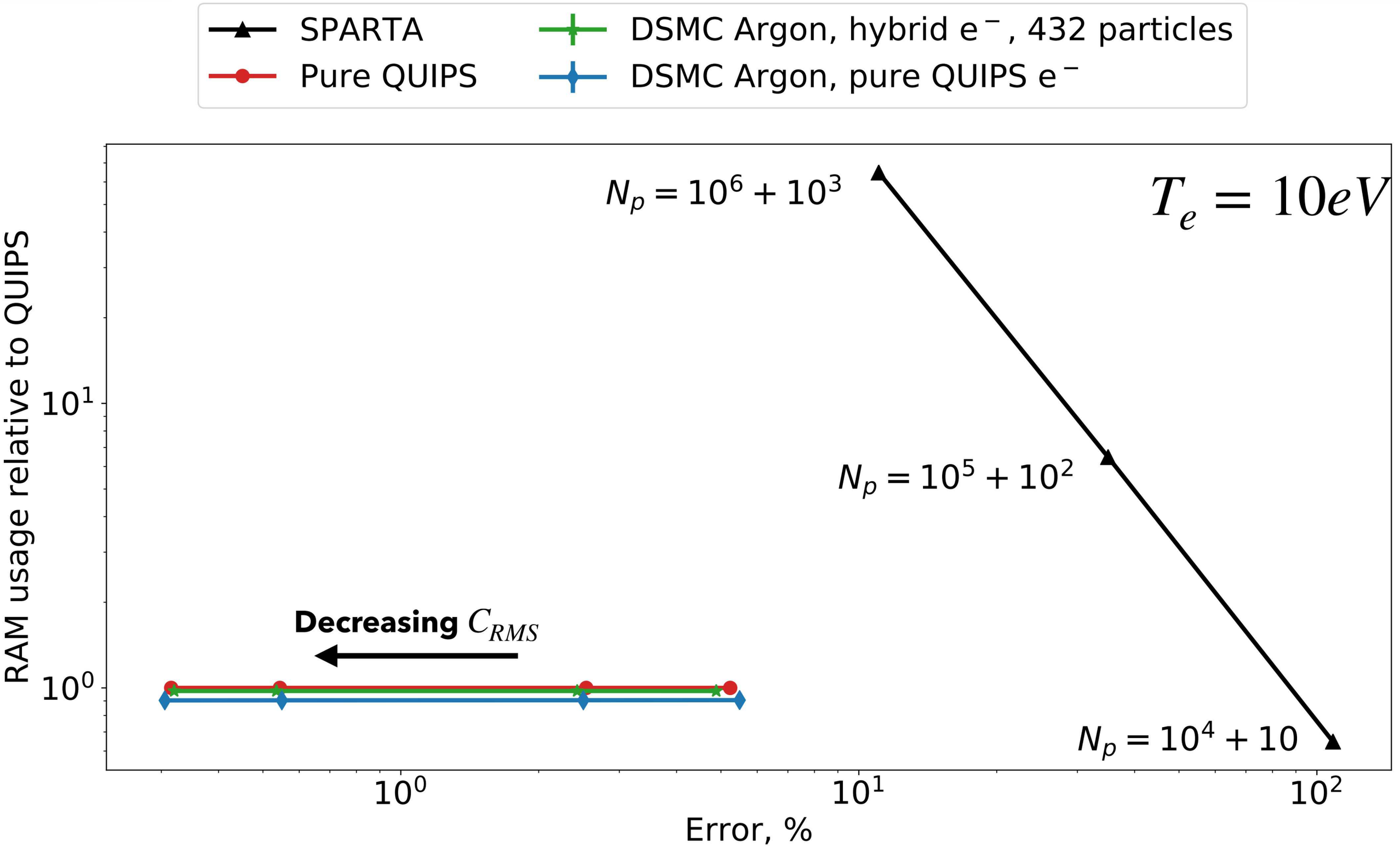
CPU vs. error


SPARTA
Pure QUIPS
DSMC Argon, hybr. e⁻, 128 particles
DSMC Argon, hybr. e⁻, 16 particles
DSMC Argon, pure QUIPS e⁻
$T_e = 5eV$
$N_e = 10^3, N_{Ar} = 10^6$
Decreasing C_{RMS}
$N_e = 100, N_{Ar} = 10^5$
$N_e = 10, N_{Ar} = 10^4$
Time per collision step, s
10^0
10^{-1}
10^{-2}
10^{-3}
10^1
10^2
Error, %

CPU vs. error


SPARTA
Pure QUIPS
DSMC Argon, hybr. e⁻, 128 particles
DSMC Argon, hybr. e⁻, 16 particles
DSMC Argon, pure QUIPS e⁻
$T_e = 10eV$
$N_e = 10^3, N_{Ar} = 10^6$
Decreasing C_{RMS}
$N_e = 100, N_{Ar} = 10^5$
$N_e = 10, N_{Ar} = 10^4$
Time per collision step, s
10^{-1}
10^{-2}
10^{-3}
10^0
10^1
10^2
Error, %

RAM vs. error


SPARTA
Pure QUIPS
DSMC Argon, hybrid e⁻, 432 particles
DSMC Argon, pure QUIPS e⁻
$N_p = 10^6 + 10^3$
$T_e = 10eV$
$N_p = 10^5 + 10^2$
$N_p = 10^4 + 10$
Decreasing C_{RMS}
RAM usage relative to QUIPS
10^1
10^0
10^0
10^1
10^2
Error, %

Numerical results

Single-species Couette flow

- Pure argon flow
- Channel width 0.5 mm, 50 cells
- Temperature of walls 300K, right wall velocity 1000 m/s ($M \approx 3.1$)
- Initial pressures:
  - 207 Pa ($Kn \approx 0.1$)
  - Higher Knudsen numbers not considered due to low number of collisions

Measures of efficiency

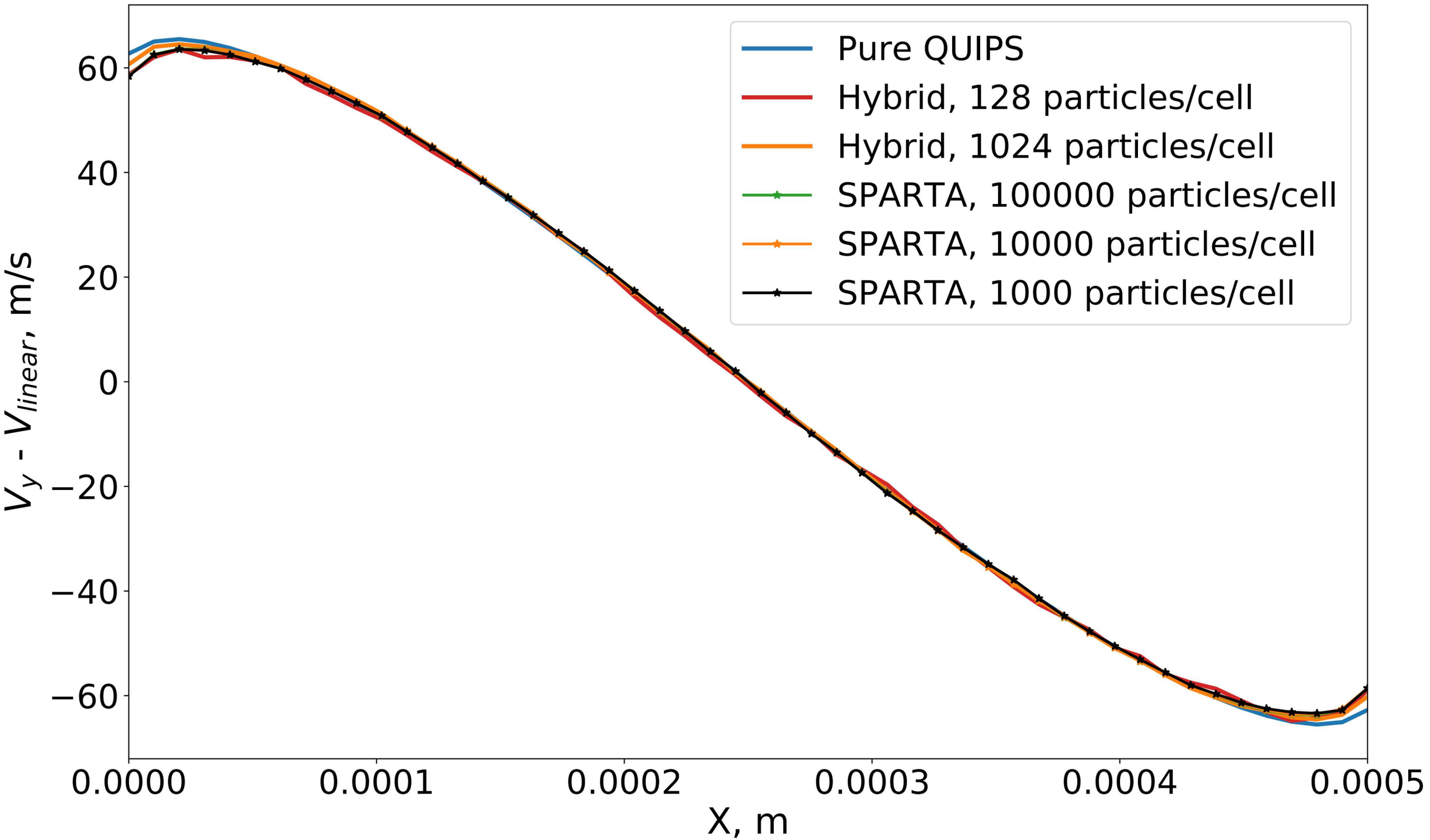
- Look at noise (RMSE) in high-order moments (gives more weight to higher-velocity tails):

$$M_8 \sim \int \left(\sqrt{v_x^2 + v_y^2 + v_z^2} \right)^8 \hat{\phi}(v_x, v_y, v_z) dv_v dv_x dv_z$$

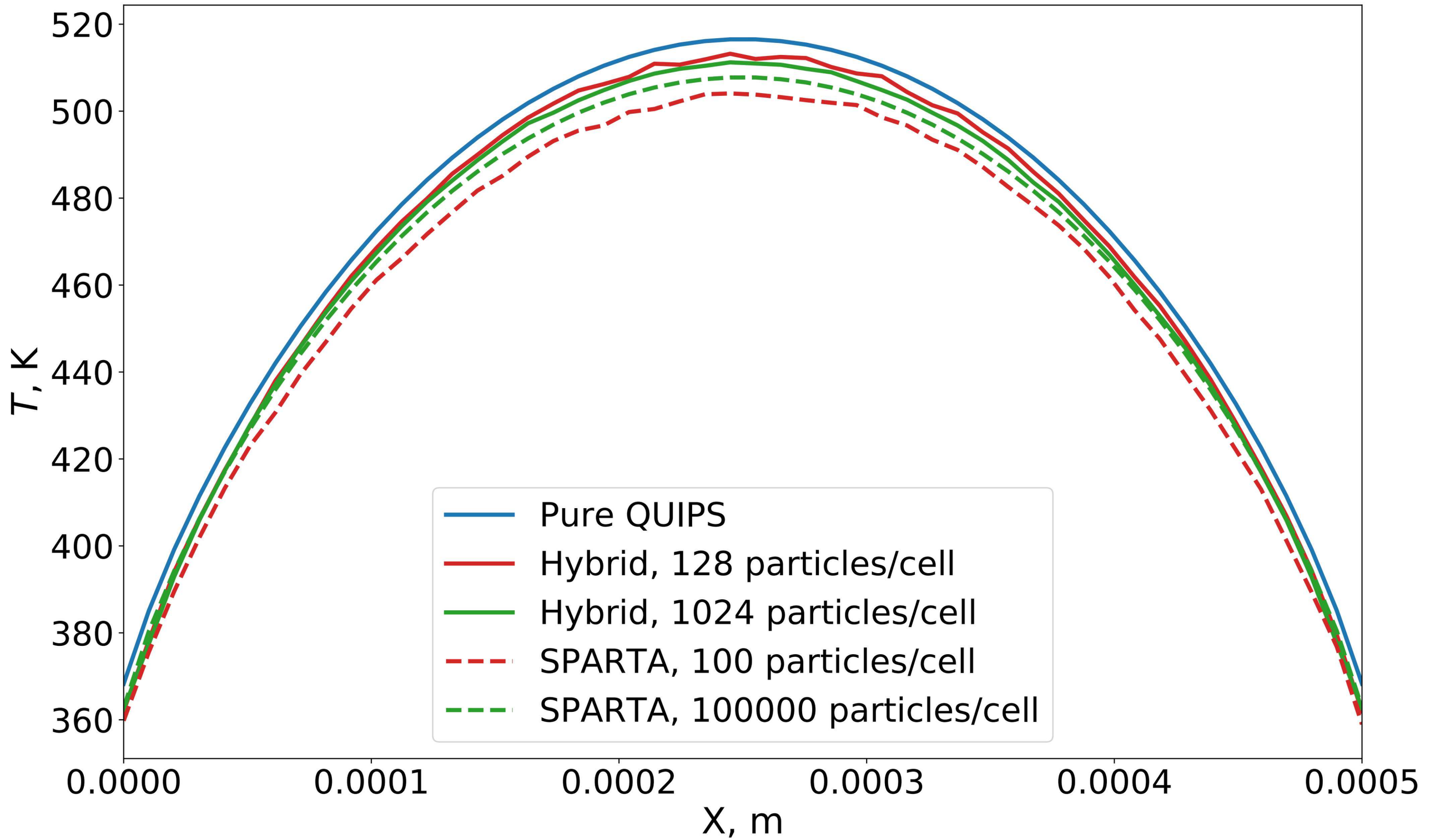
- CPU time per step vs. RMSE as measure of efficiency

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

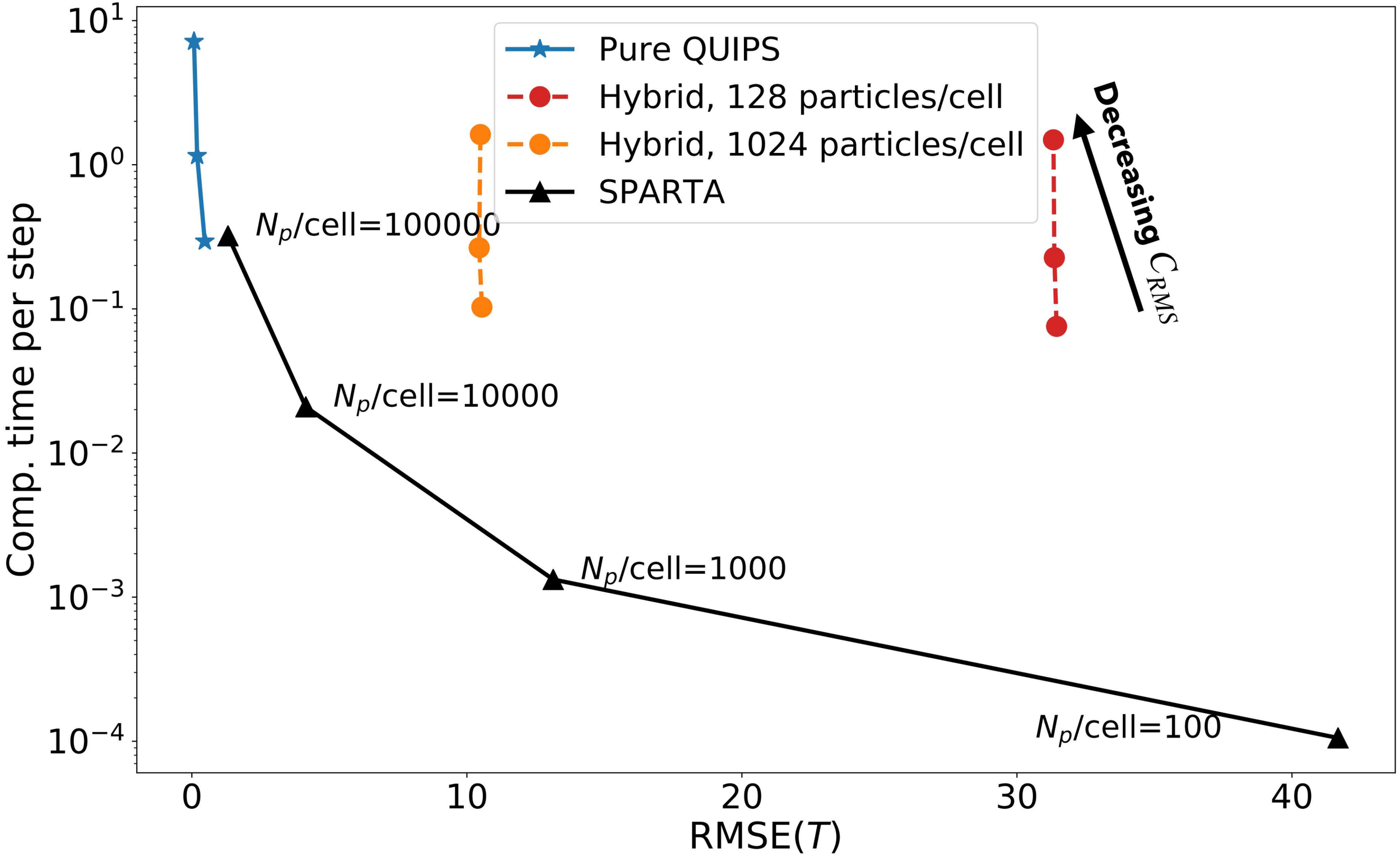
Velocity profiles



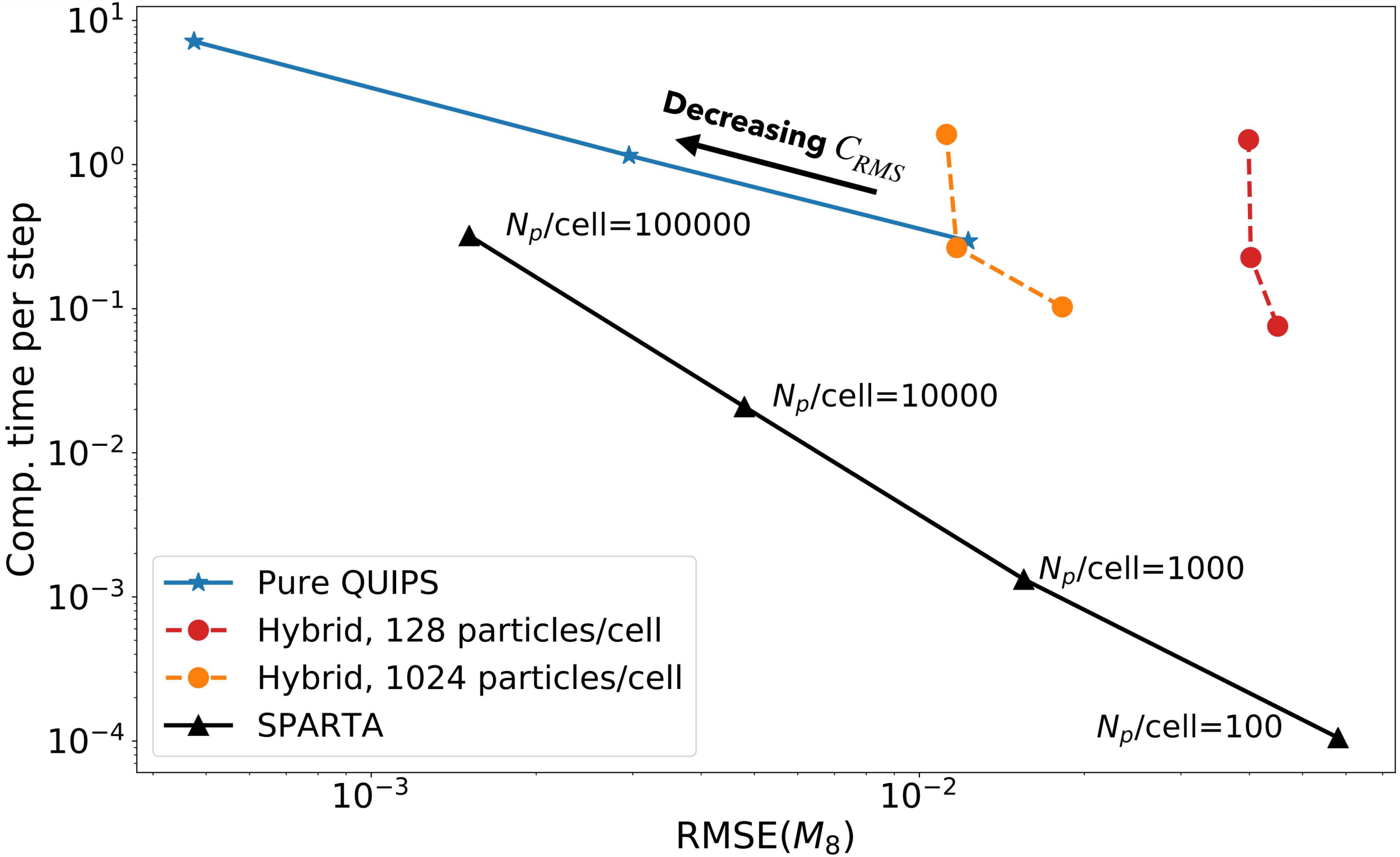
Temperature profiles



Temperature error



8th Moment error



Conclusions

- A new approach to modelling rarefied gas flows based on a velocity space hybridization has been developed
- Such an approach can give better computational efficiency (compared to a pure QUIPS approach) and less RAM usage (compared to SPARTA) 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 approach is validated

Current efforts:

- Adaptive DSMC region
- Modelling of 1-D and 2-D weakly ionized flows
- Internal energies

RMSE of 8th moment

Computational time per collision step vs. error in tails