SAND2019-10944C

Hybridizing DSMC and Discrete Velocity Methods in Velocity Space

Georgii Oblapenko[1], David Goldstein[1], Philip Varghese[1,2], Christopher Moore[3]

[1]Oden Institute for Computational Engineering and Sciences, **UT Austin**
[2]Department of Aerospace Engineering and Engineering Mechanics, **UT Austin**
[3]Sandia National Laboratories

Supported by **Sandia National Laboratories**

This work has been supported by Sandia National Laboratories. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Outline

1. **Brief overview**
    1. Why not use DSMC?
    2. What other methods are there?
2. **Quasi-Particle Simulation (QUIPS)**
    1. Distribution function representation
    2. Collision integral evaluation
    3. Remapping scheme
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. Single species
    2. Ionization rate computation
5. **Conclusion**

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)

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

In scaled form:

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

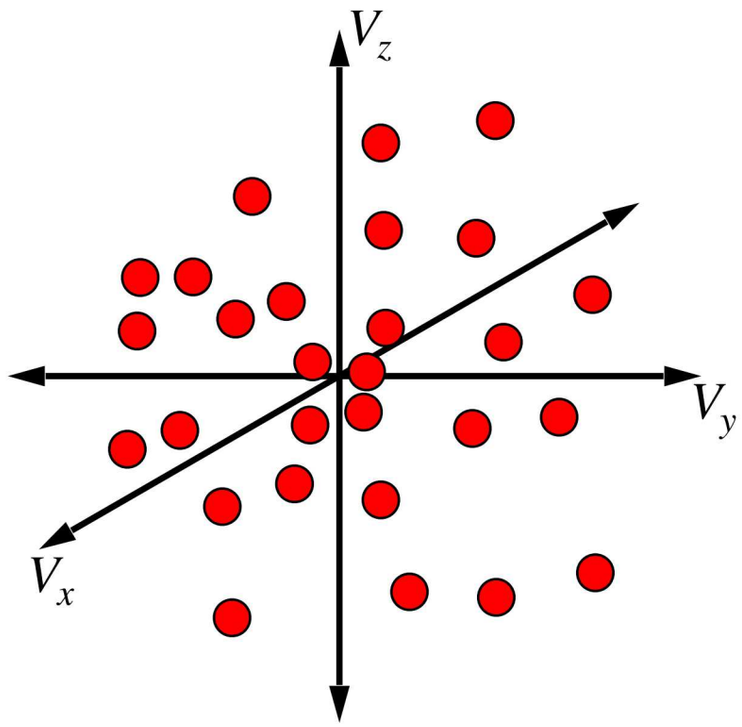
Here $\hat{\phi}(\hat{\boldsymbol{\xi}})$ is the (scaled) number of particles in a volume β^3 centered around $\boldsymbol{\xi}$; β is the grid spacing

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

DSMC vs QUIPS

DSMC

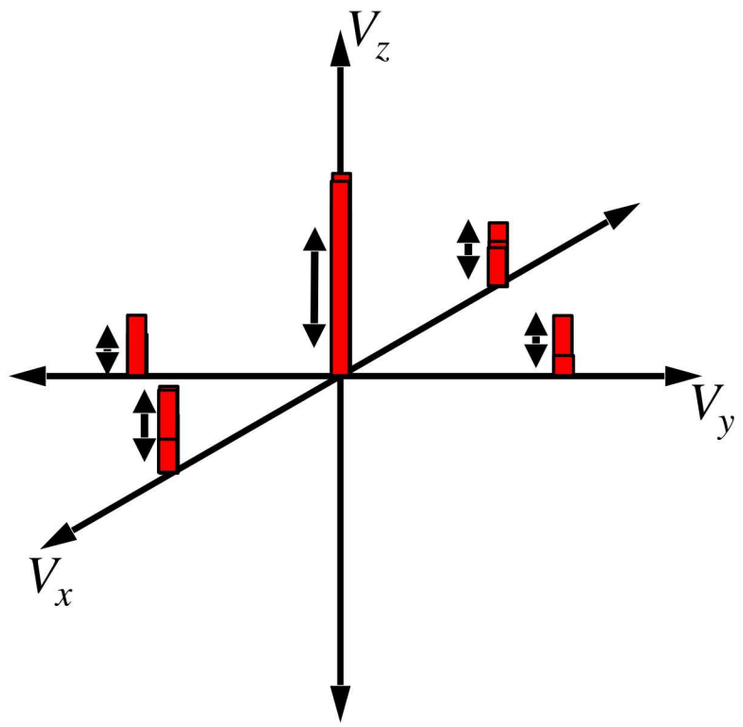
"Fixed mass, variable velocity particles."



Resolution limited by ratio of real molecules to DSMC particles

QUIPS

"Fixed velocity, variable mass quasi-particles."



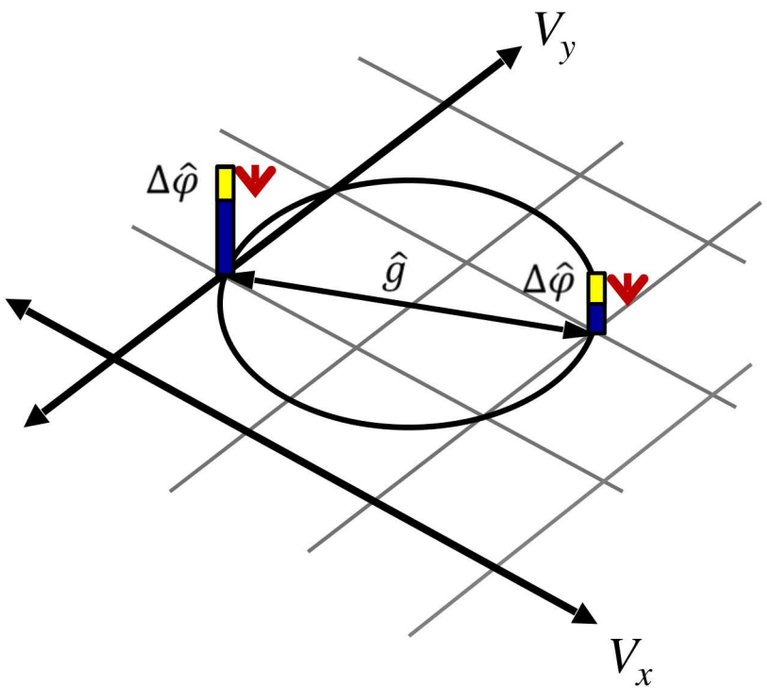
Allows resolution of tails/ trace populations up to machine precision

QUIPS collisions

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



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

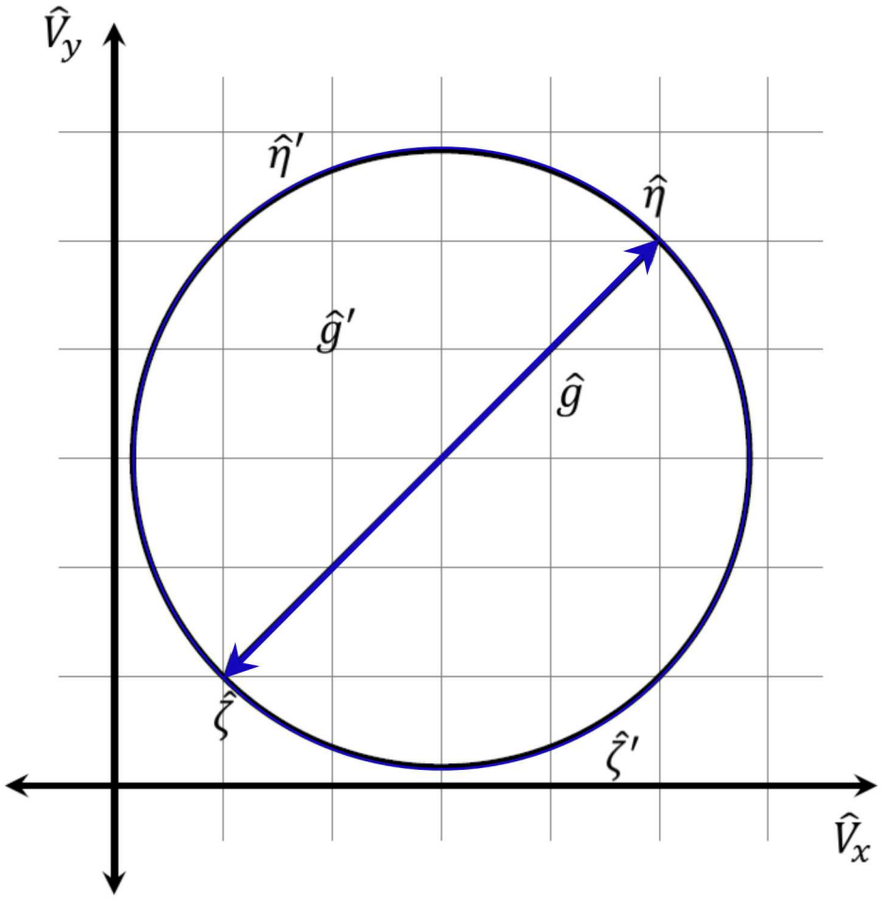
Noise parameter

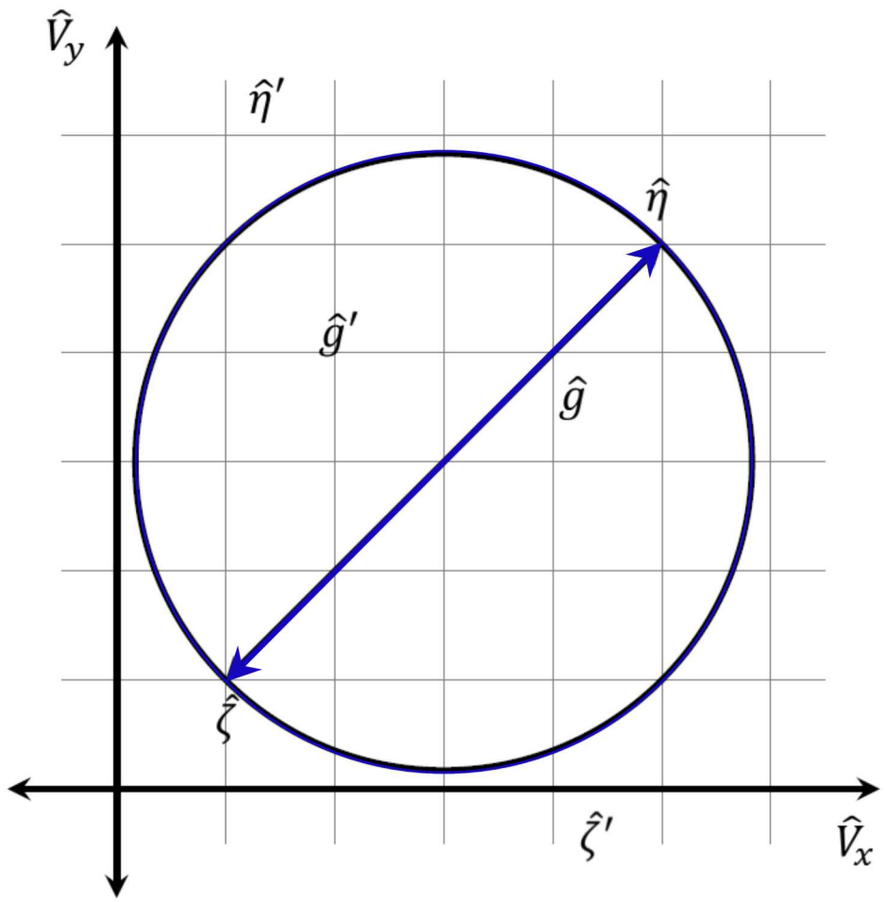
$$\Delta\hat{\phi} = \Delta\hat{t}\frac{(\hat{n} - 2\hat{n}_{neg})^2}{2KnN_{coll}} sign\left(\hat{\phi}(\hat{\eta})\hat{\phi}(\hat{\xi})\right)\hat{g}\hat{\sigma}_t$$

QUIPS collisions

How to compute collision integral (replenishment)?

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

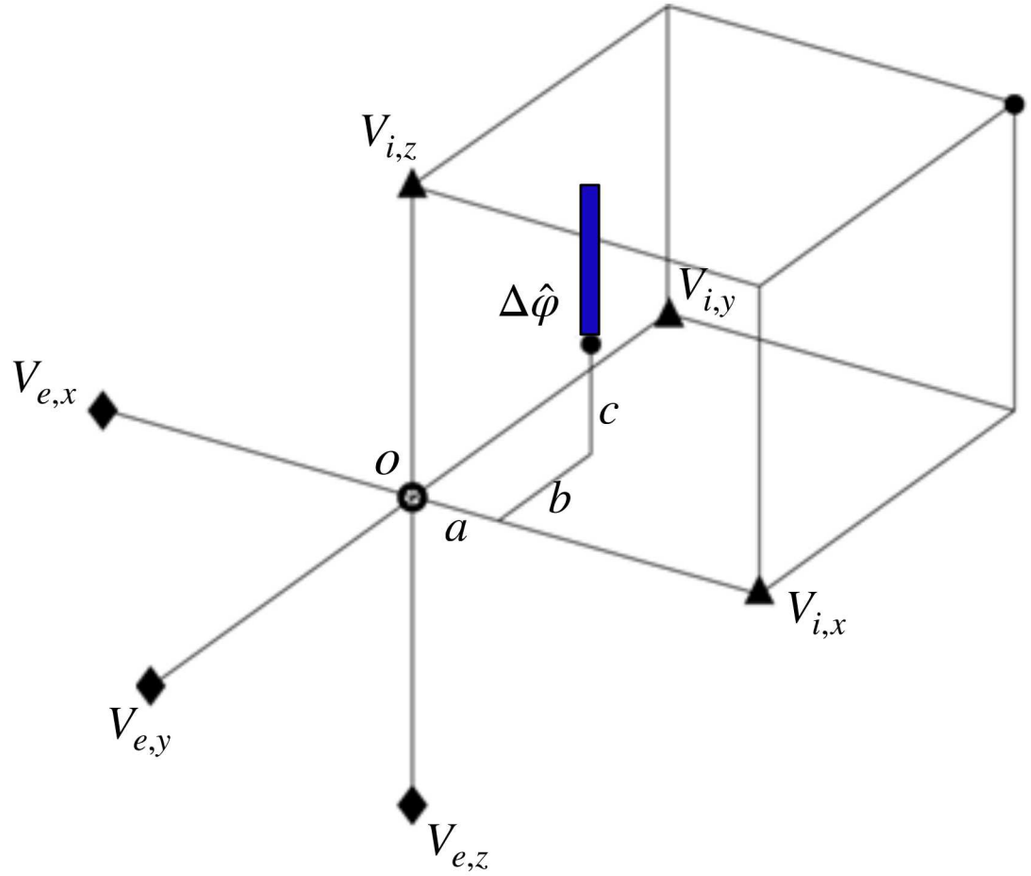




QUIPS Collisions: Remapping

But velocity does not necessarily lie on grid!

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



P. Varghese, RGD Proceedings, 2006

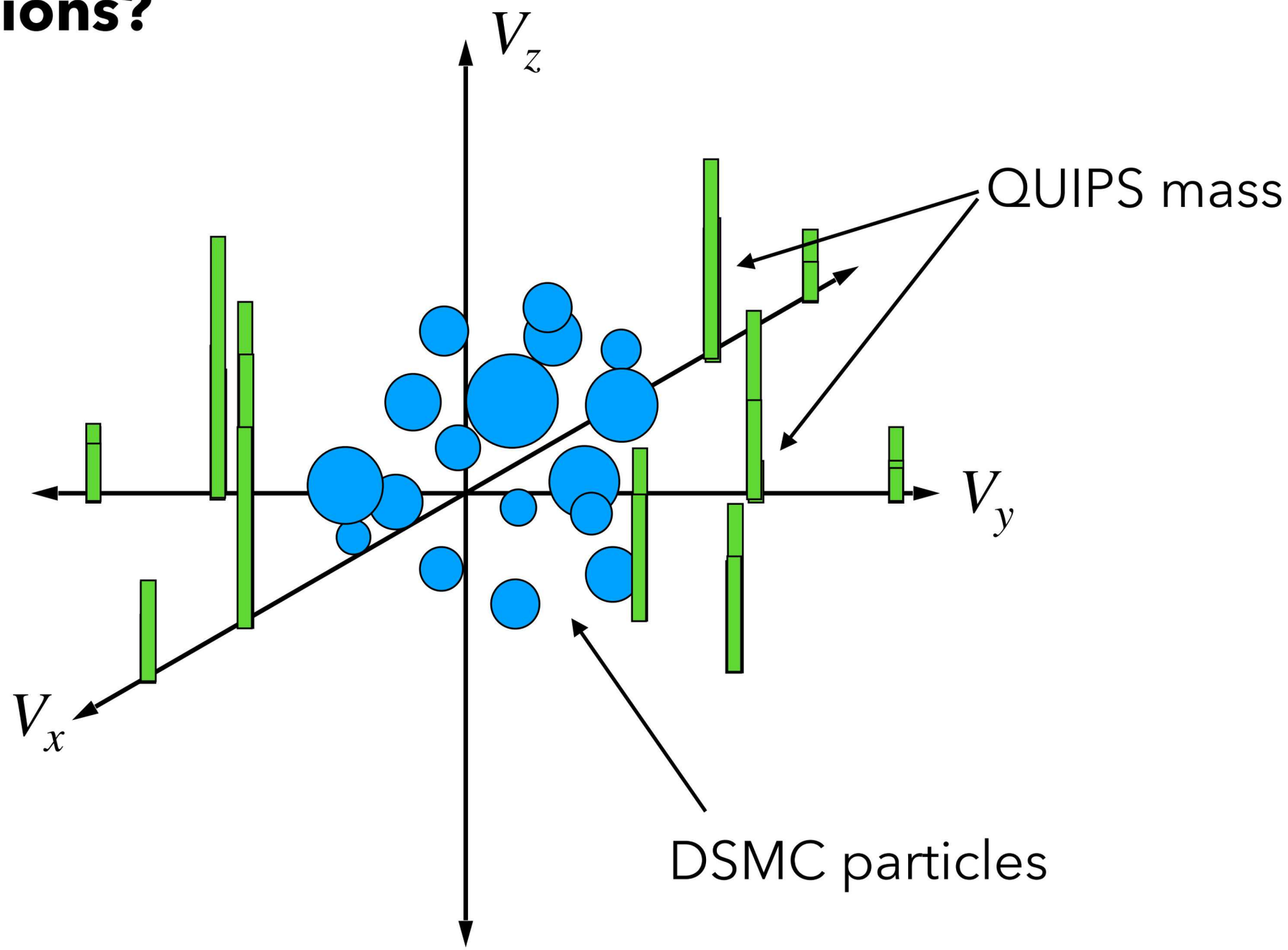
QUIPS summary

QUIPS (Quasi-Particle Simulations):

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

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

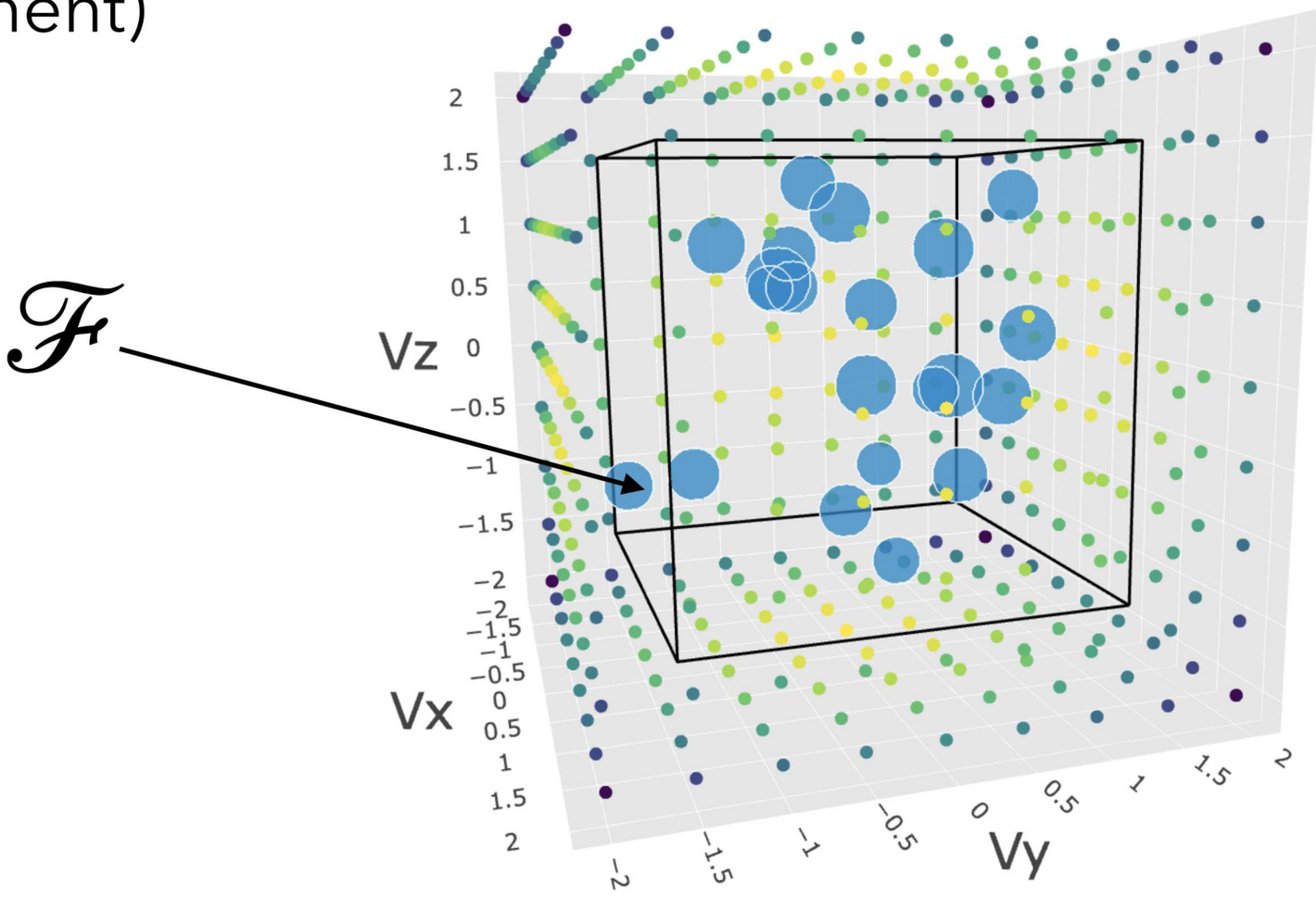
Previous work:

- 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

Hybrid QUIPS/DSMC

How to hybridize?

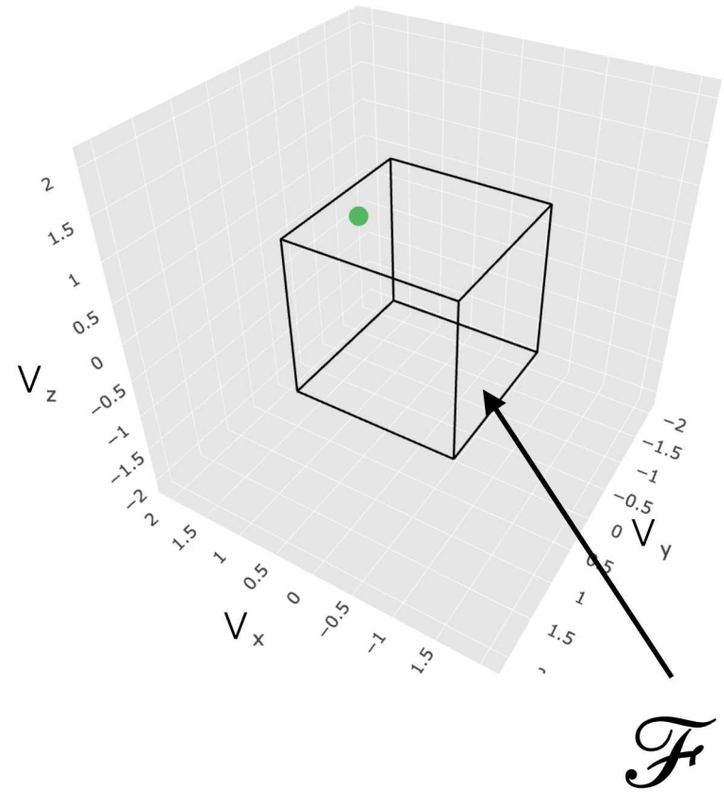
- Pick region in velocity space where VDF is represented by DSMC particles
- Use DSMC collision mechanics (instead of small depletion/ replenishment)

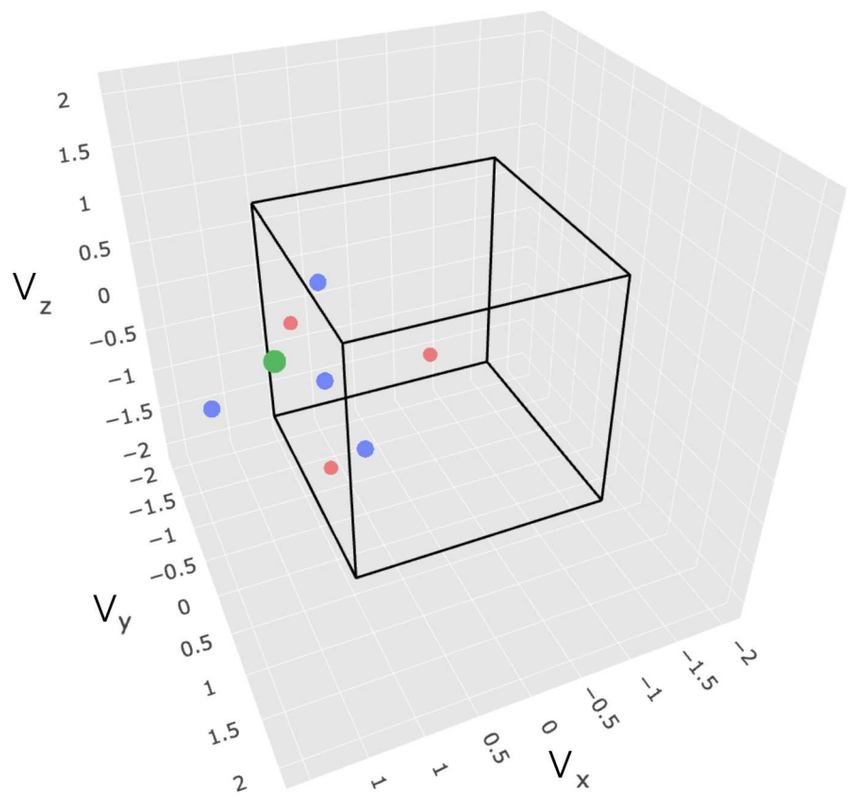


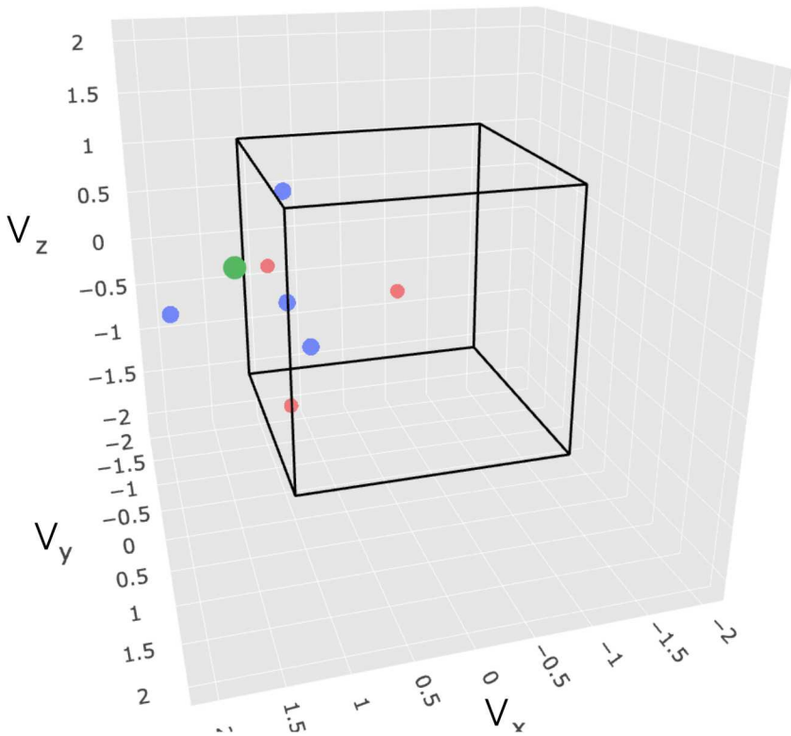
Hybrid QUIPS/DSMC

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



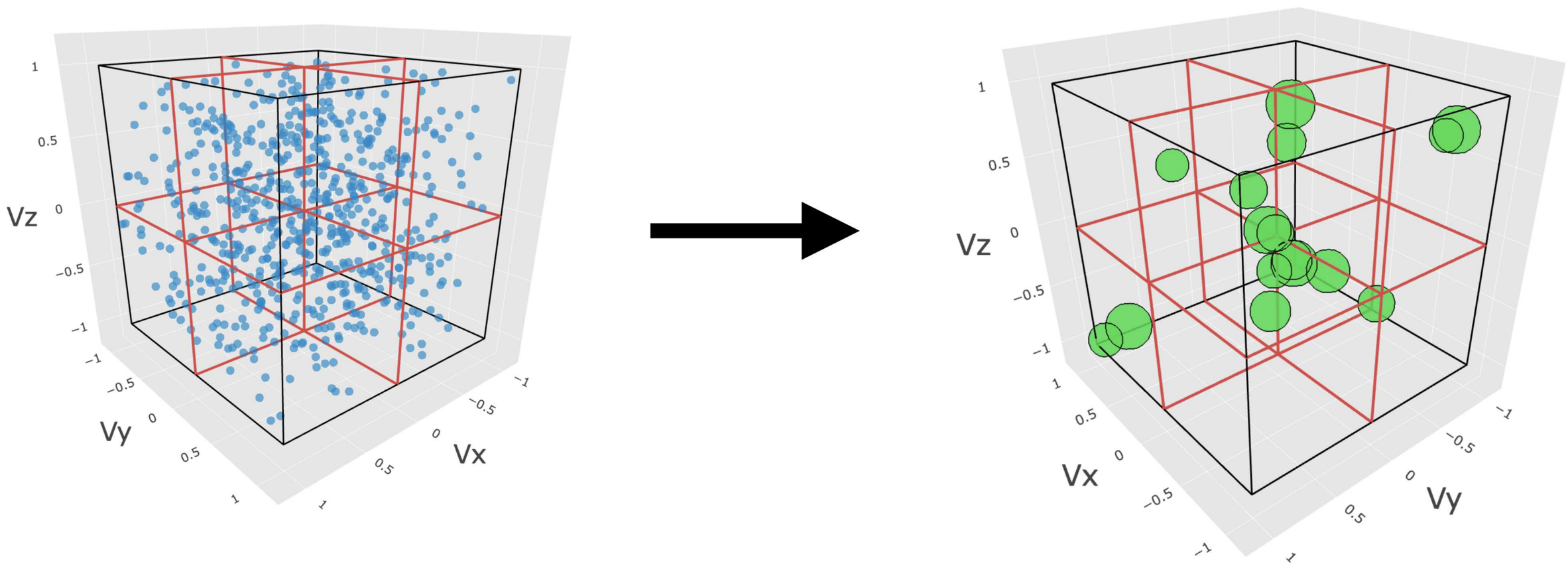




Hybrid QUIPS/DSMC

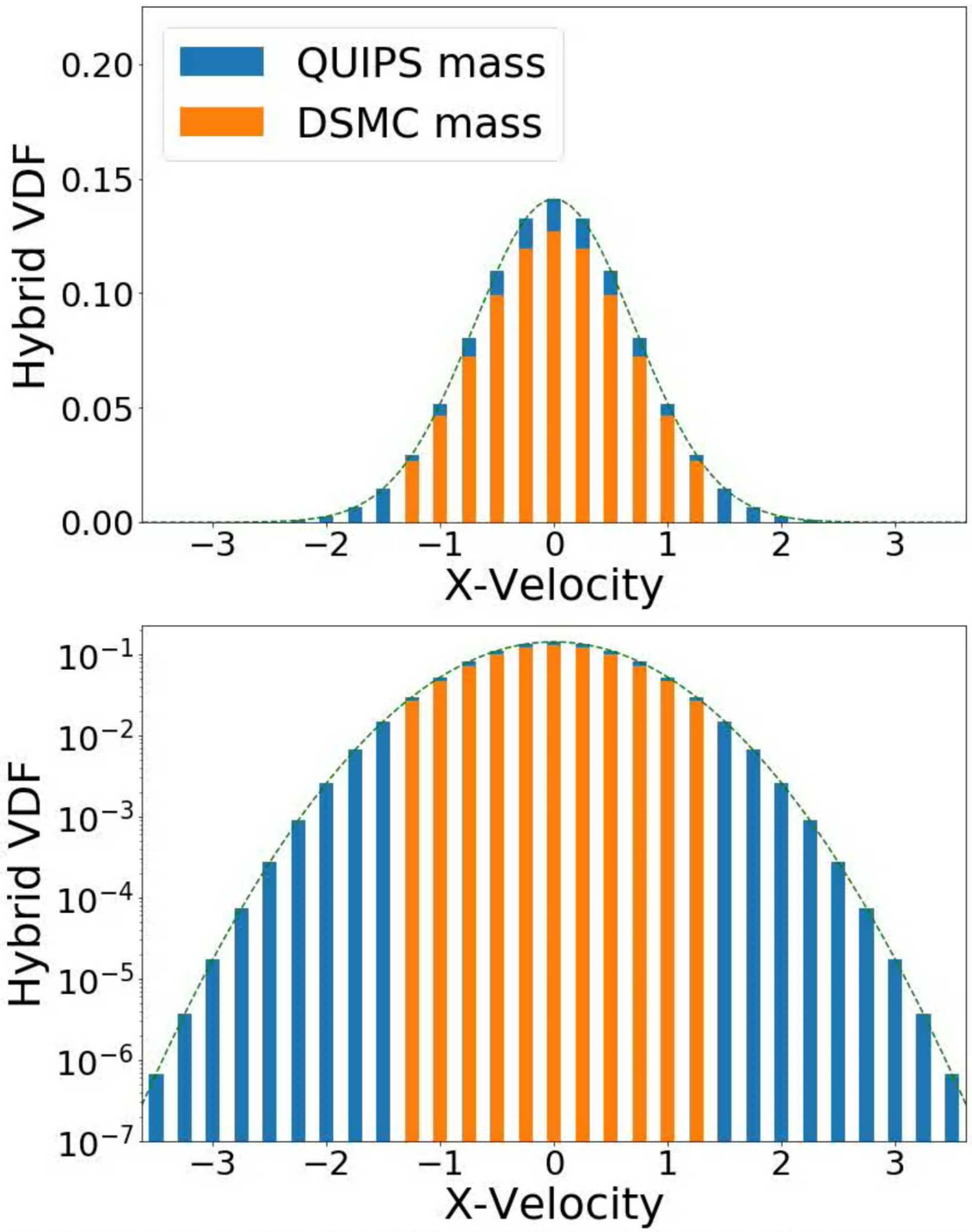
How to avoid (exponential) growth of number of particles?

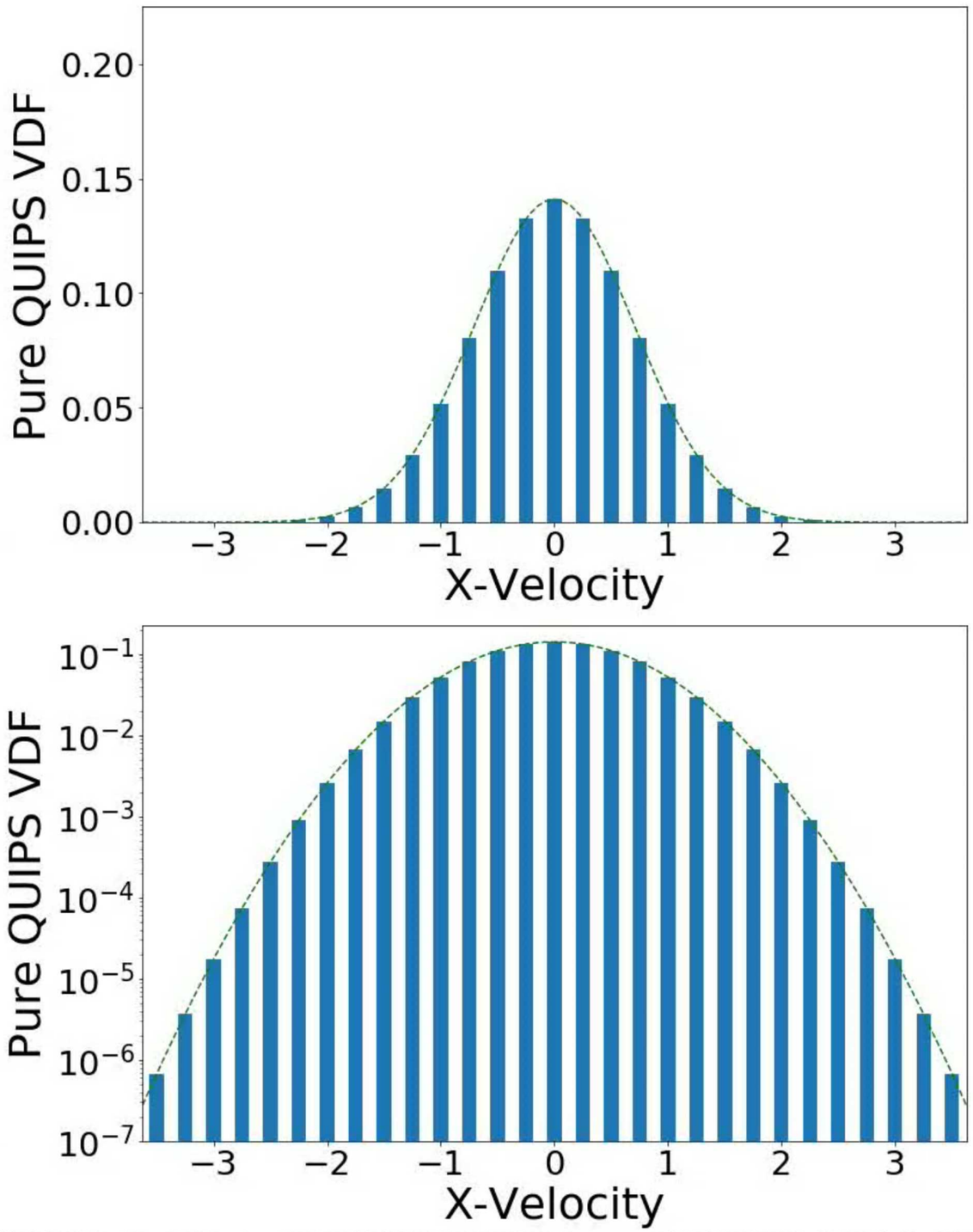
- Do conservative N:2 merging
- Current work utilizes a simple grid-based approach (M*M*M merging cells); CPU time $\sim \mathcal{O}(N_p + M^3)$; additional RAM $\sim \mathcal{O}(M^3)$



Hybrid QUIPS/DSMC

Example of hybrid VDF representation





Numerical results

Single-species test case

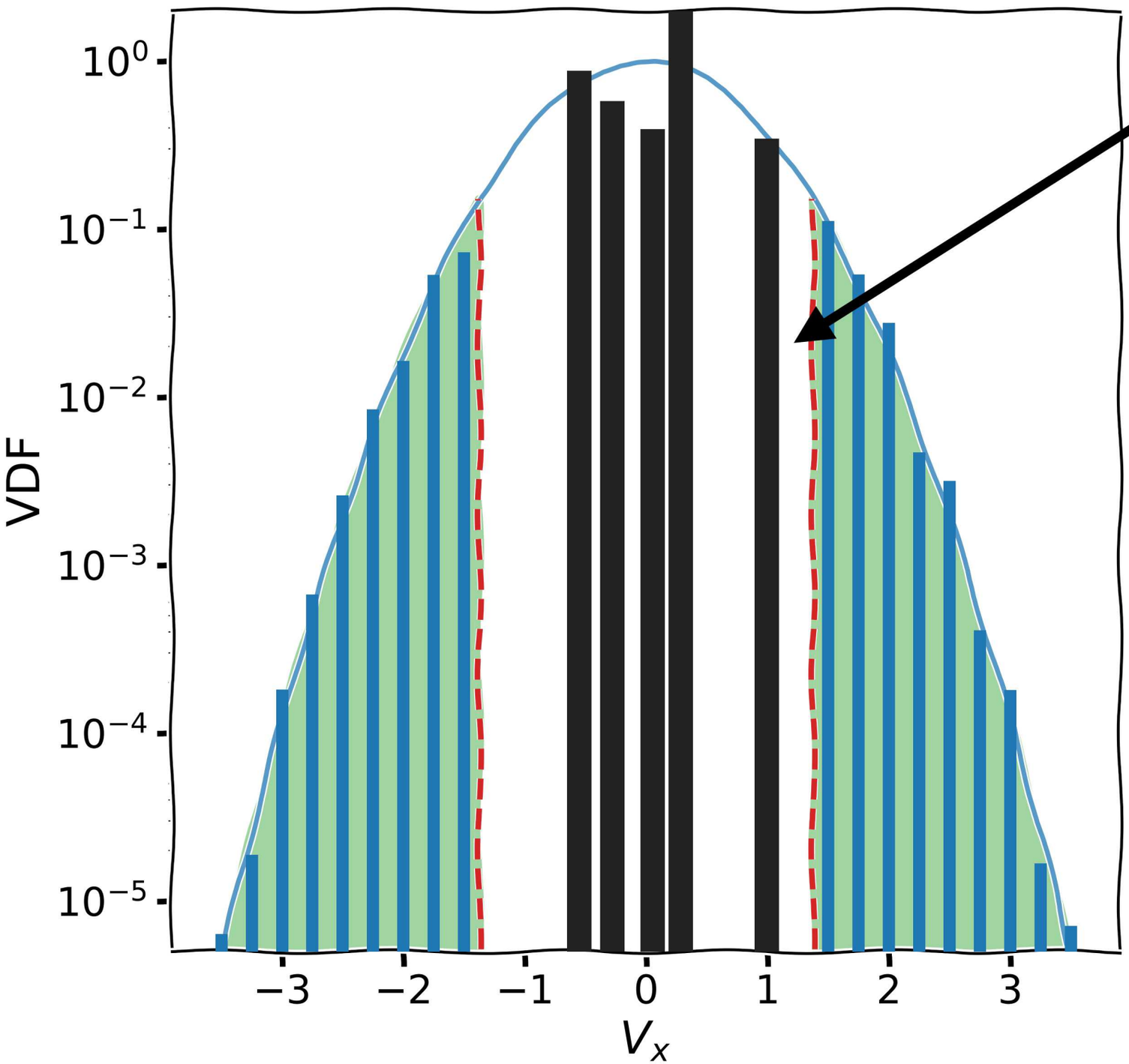
- Initialize with Maxwellian distribution, look at noise (RMSE) in high-order moments (gives more weight to higher-velocity tails)
- CPU time per step vs. RMSE as measure of efficiency

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

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)

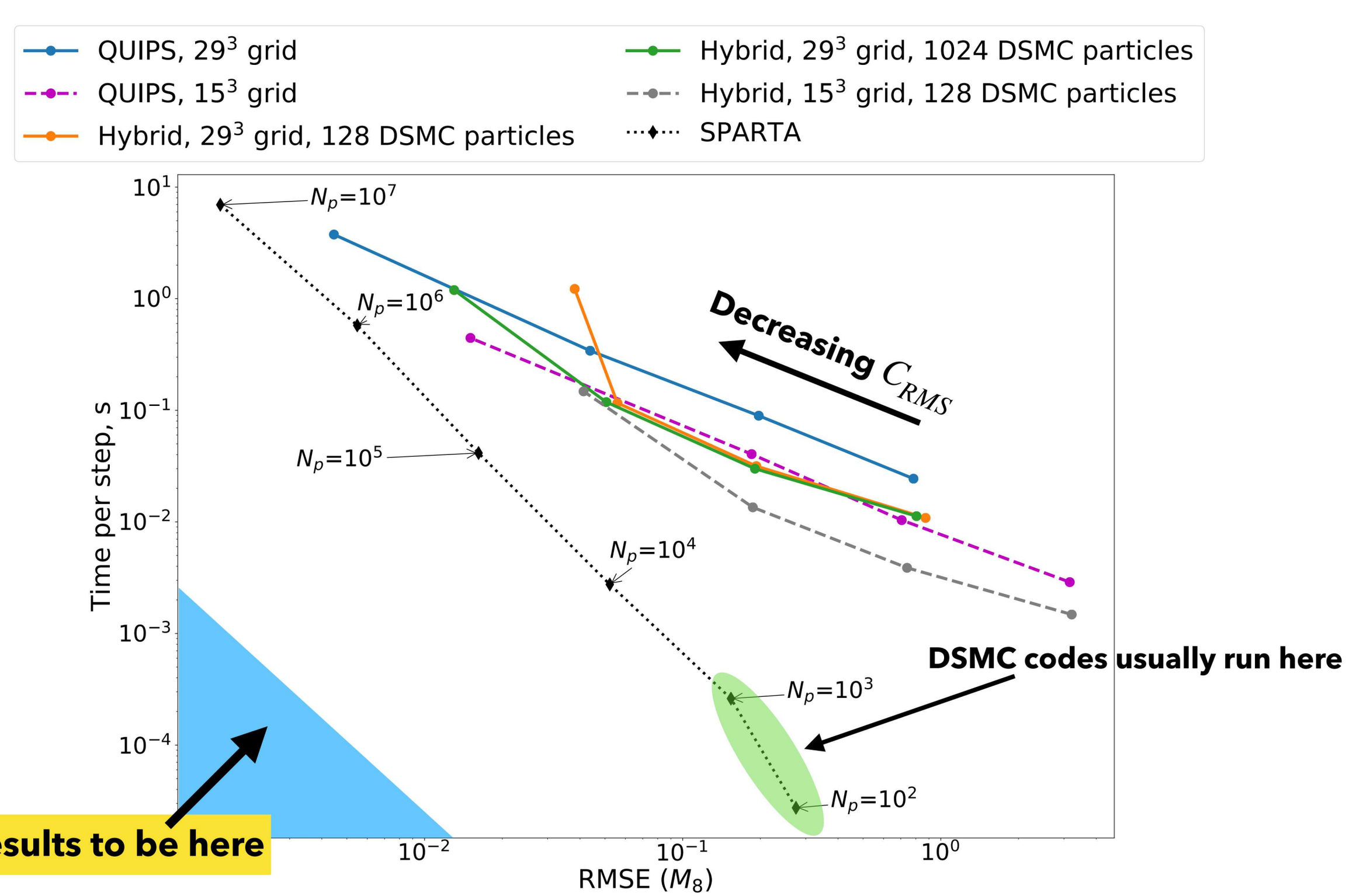
Hybridization options



$\mathcal{F}_{\text{target}}$ (~80-88% mass)

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, Smirnov [Lieberman and Lichtenberg, 1994])
- CPU time per step vs. RMSE as measure of efficiency

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

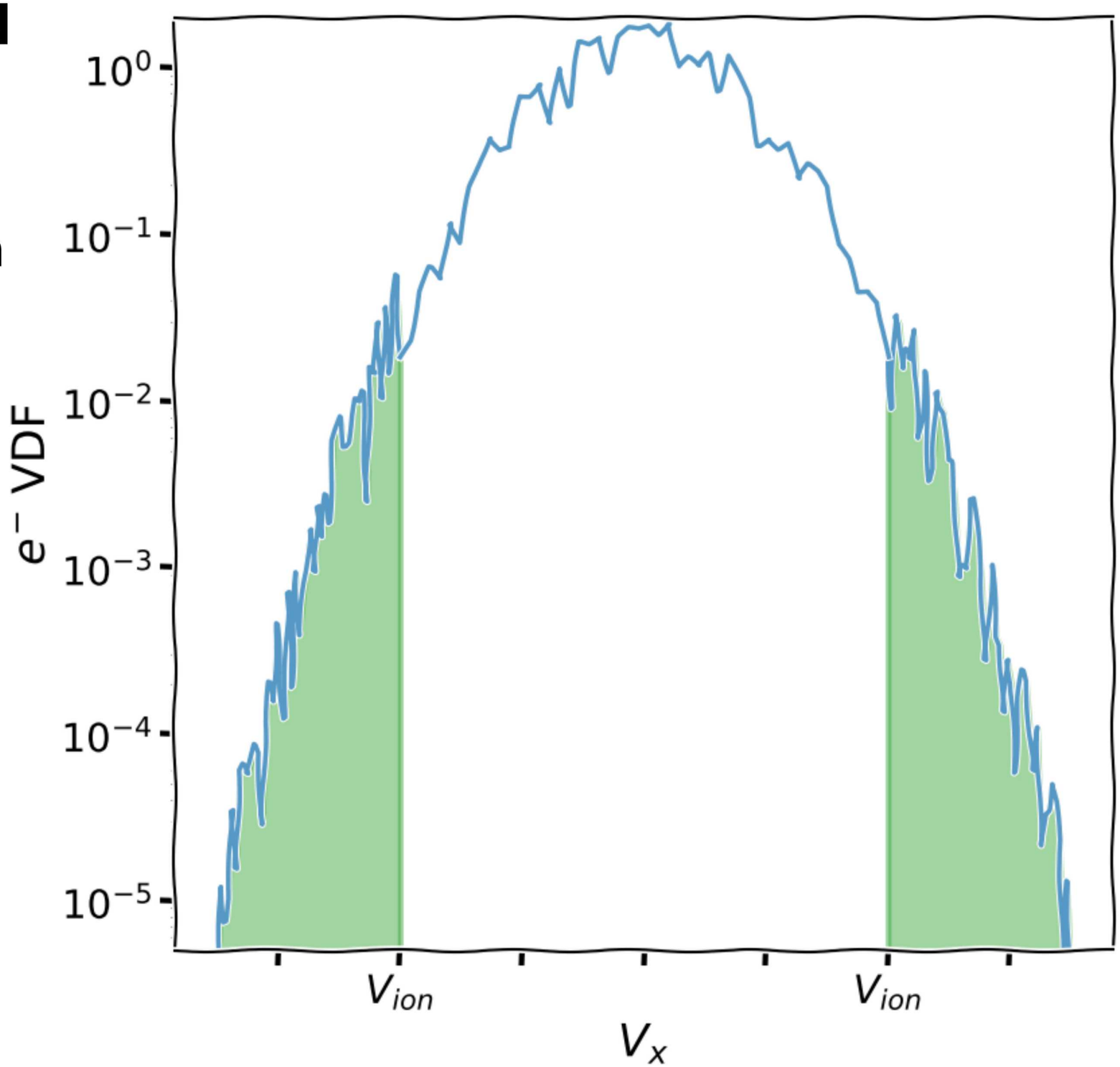
Possible hybridization options:

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

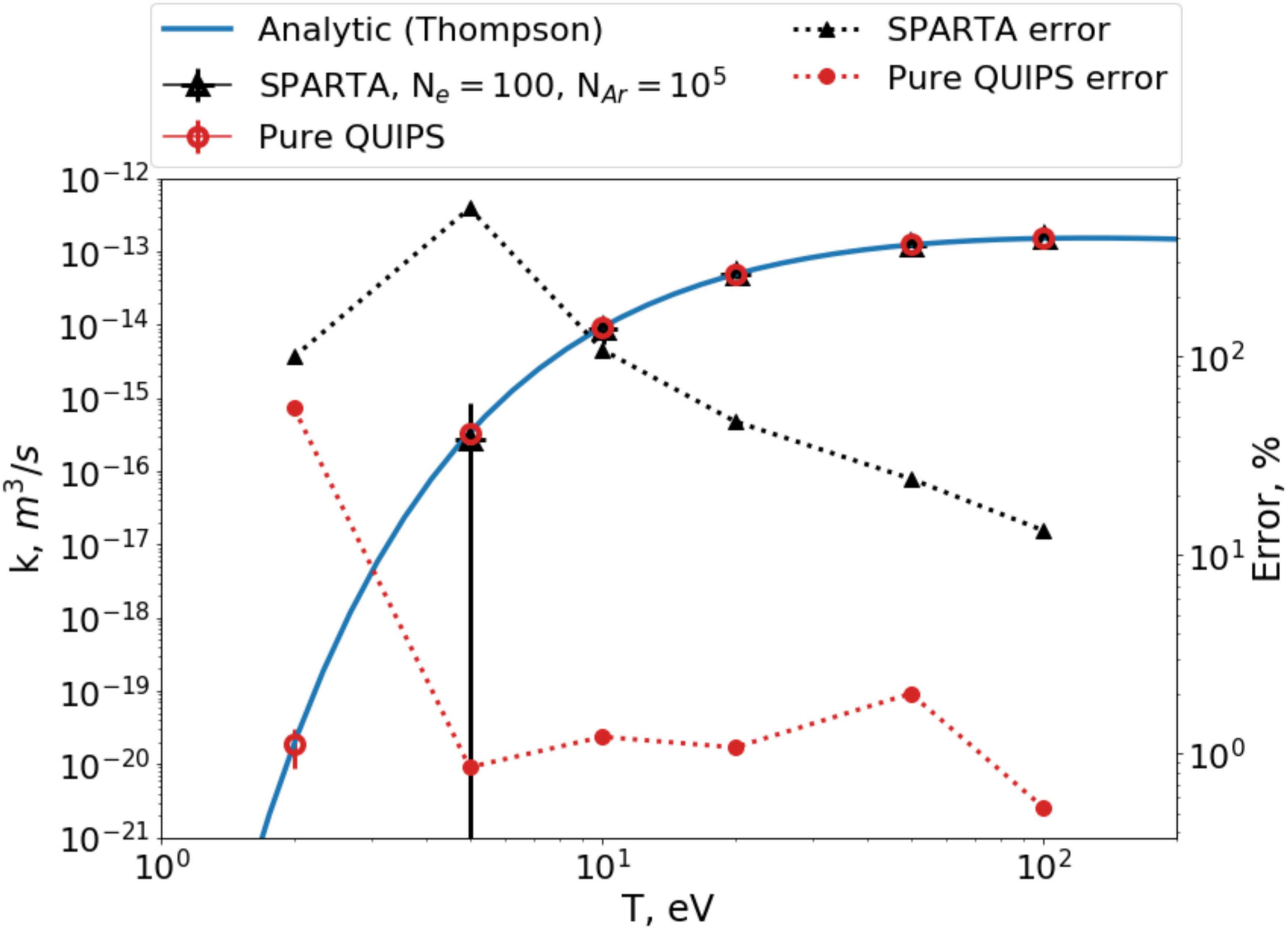
Error in ionization rate coefficient

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

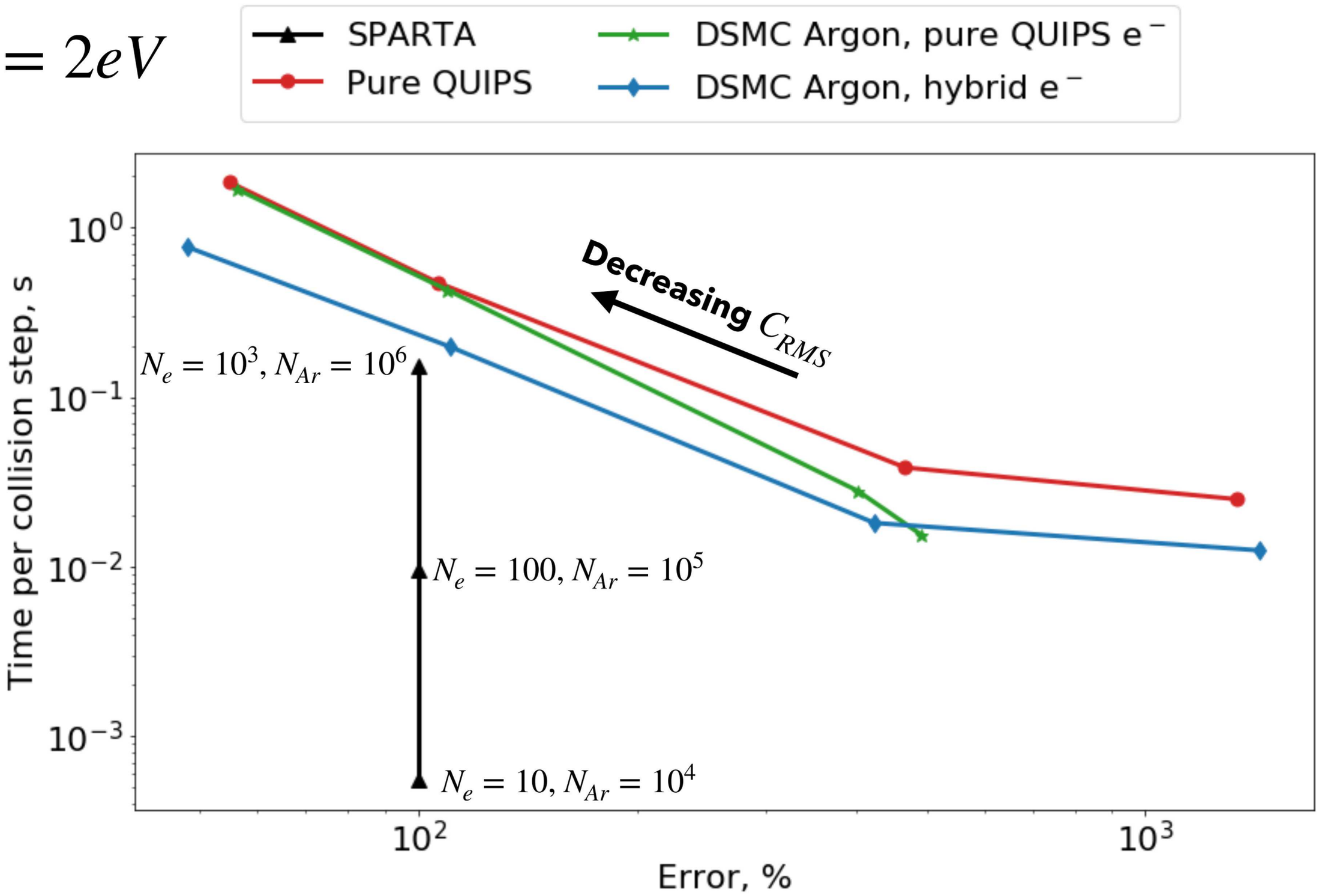


Electron-impact ionization rate



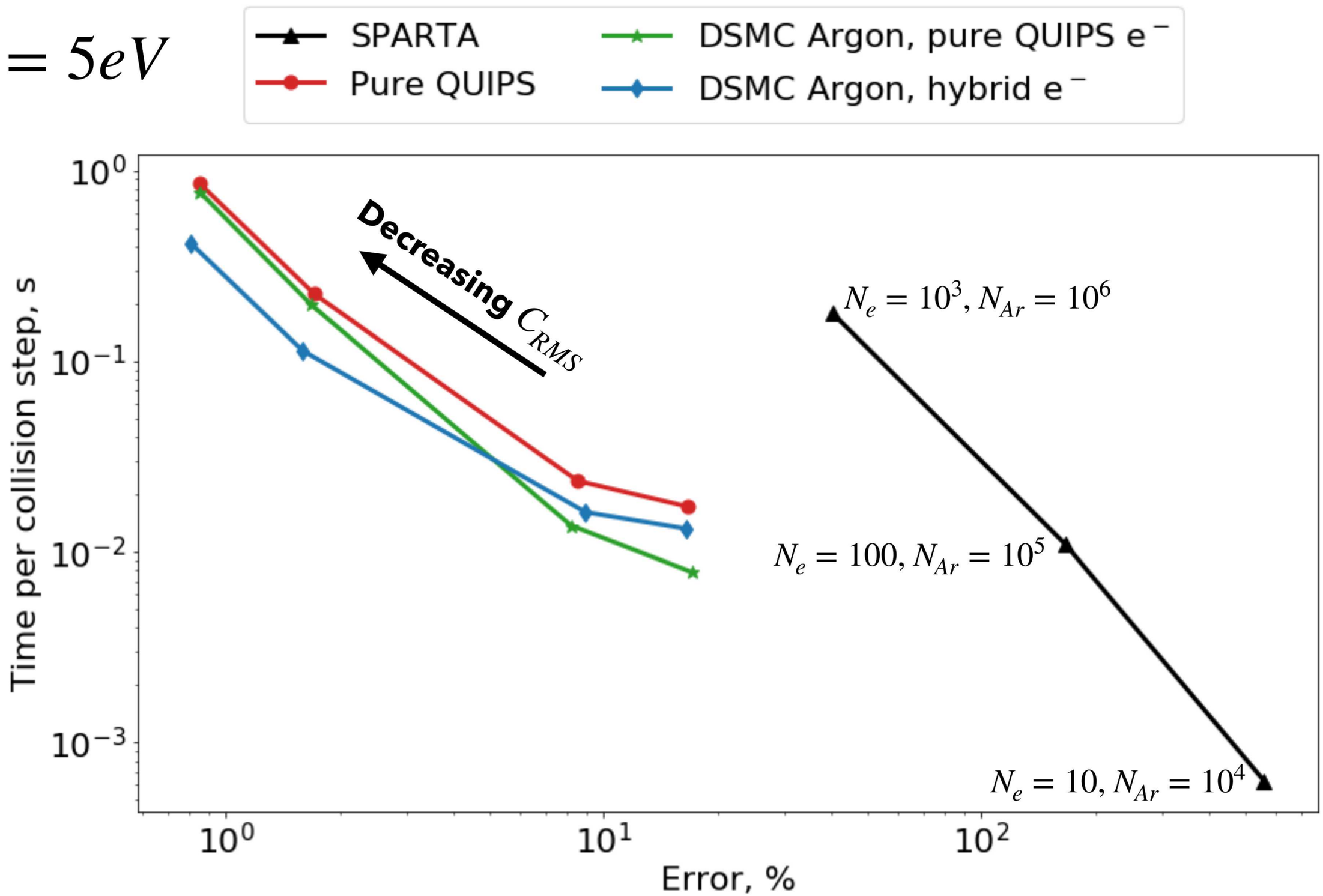
CPU vs. error, low temperature

$T_e = 2eV$



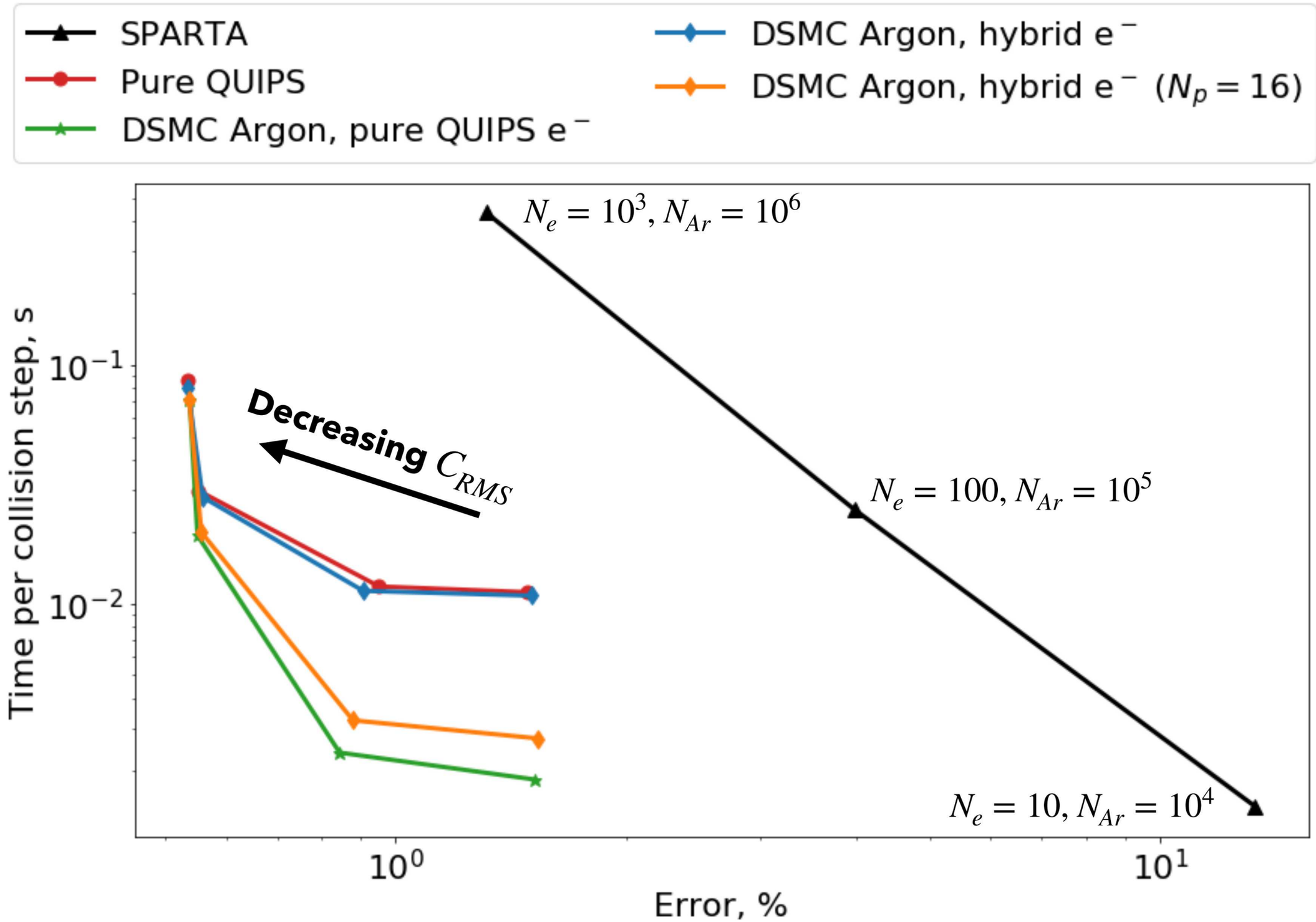
CPU vs. error, low temperature

$$T_e = 5eV$$



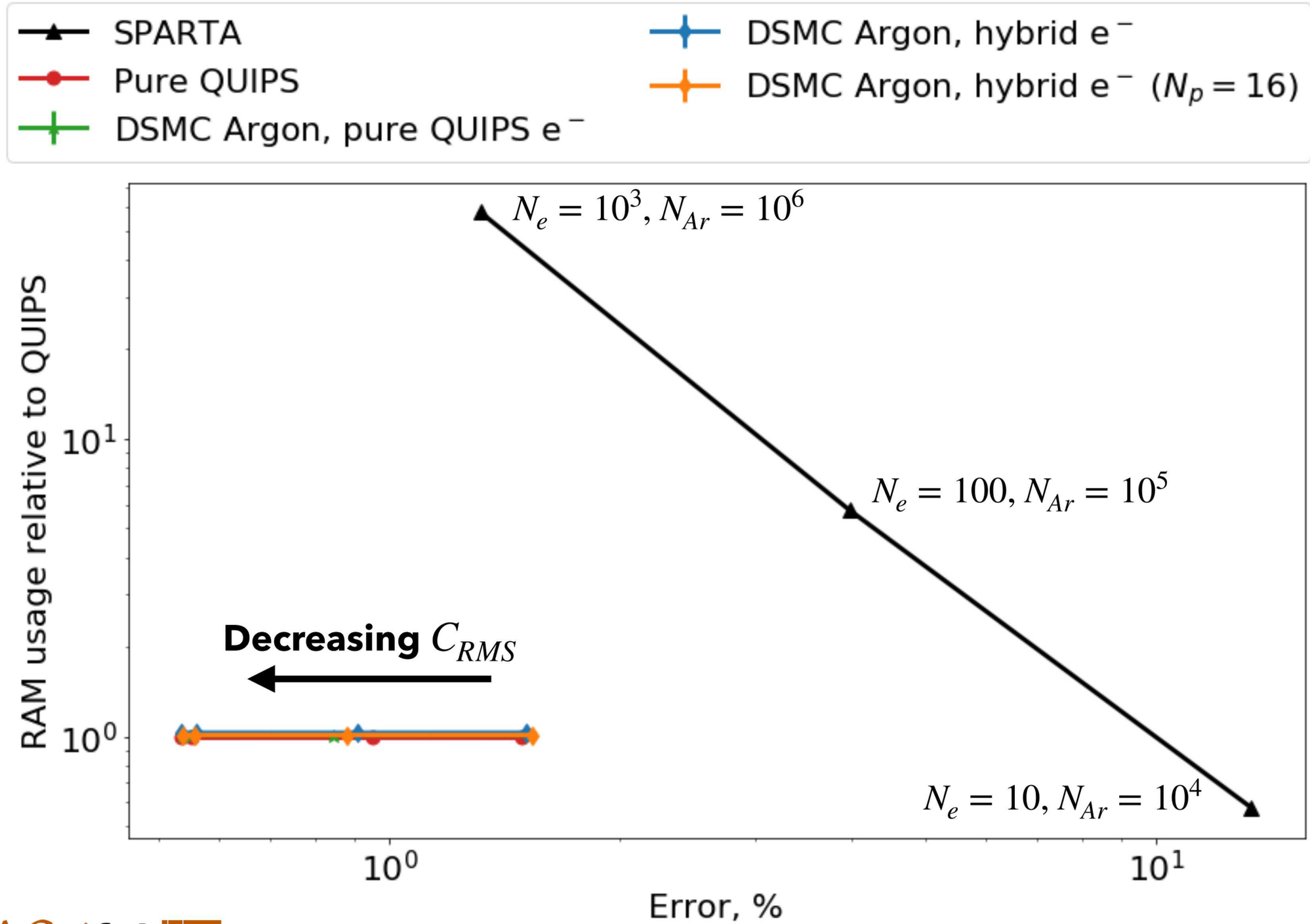
CPU vs. error, high temperature

$T_e = 100eV$



RAM vs. error, high temperature

$$T_e = 100eV$$



Conclusions

- A new approach to modelling rarefied gas flows based on a velocity space hybridization has been developed and tested for 0-D 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

Current efforts:

- 1-D and 2-D problems
- Internal energies
- Variance reduction