SAND2019-8226PE

A velocity-space hybridization approach to modelling rarefied gas flows

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Supported by **Sandia National Laboratories**

Outline

1. **Modelling of rarefied gas flows**
    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**
5. **Conclusion**

Why not use DSMC?

- Statistical fluctuations, issues with modelling of low-speed flows
- Difficulty resolving low populations
  - Excited internal states
  - High-velocity particles
  - Trace species
- Difficulty resolving low-probability events (such as recombination reactions)

Other methods for rarefied flows

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

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

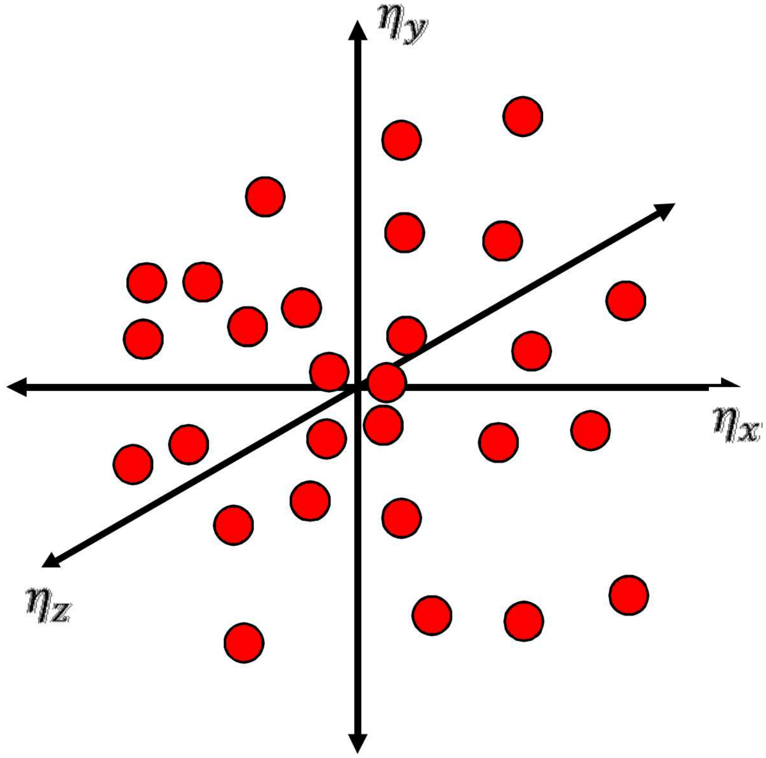
In non-dimensional form:

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

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

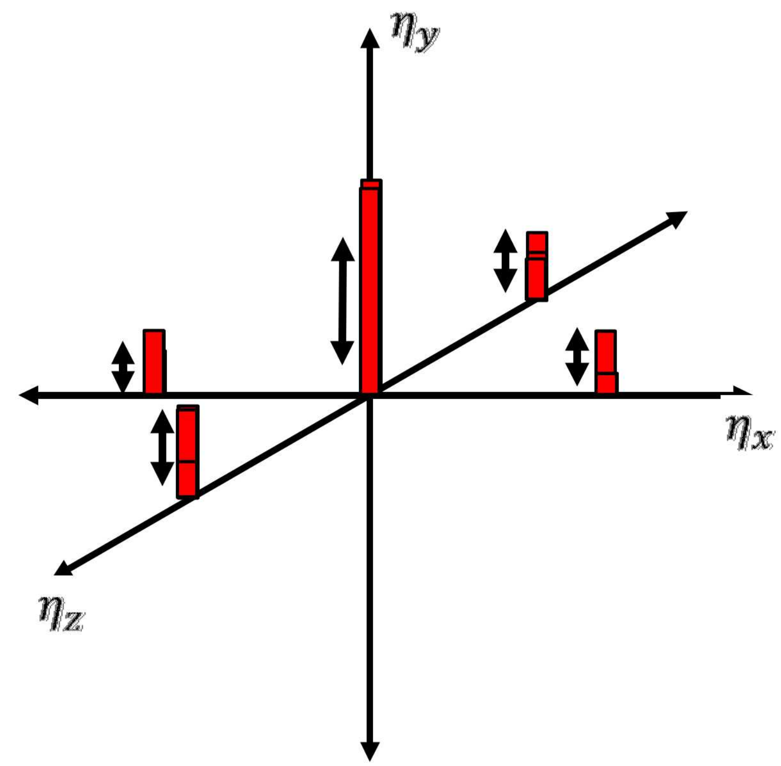
QUIPS vs DSMC

DSMC
"Fixed mass, variable velocity particles."



Resolution limited by ratio of real molecules to DSMC particles

QUIPS
"Fixed velocity, variable mass quasi-particles."



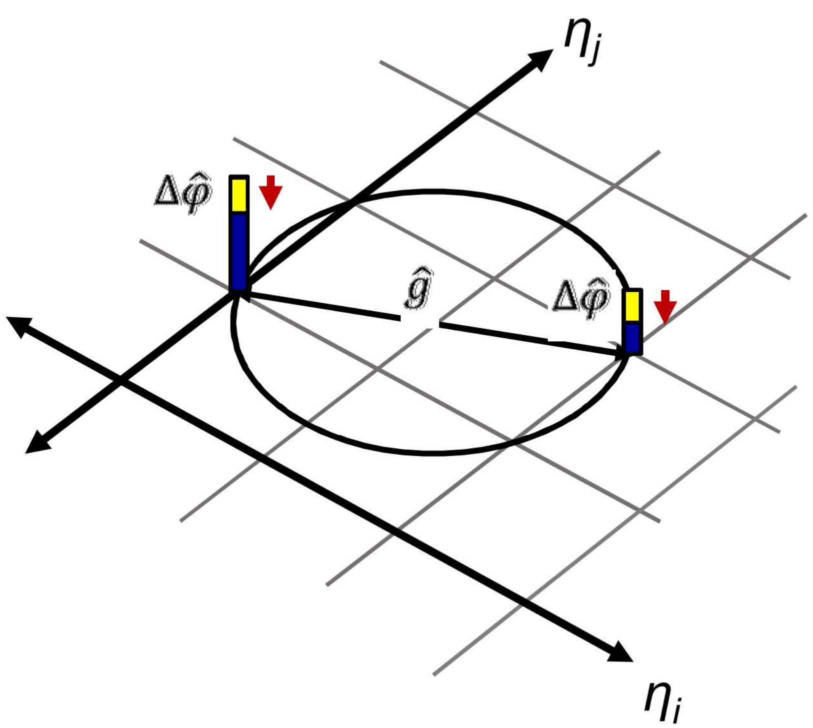
Allows resolution of tails/trace populations up to machine precision

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
- Repeat many times
- Parameter that controls number of collisions/noise



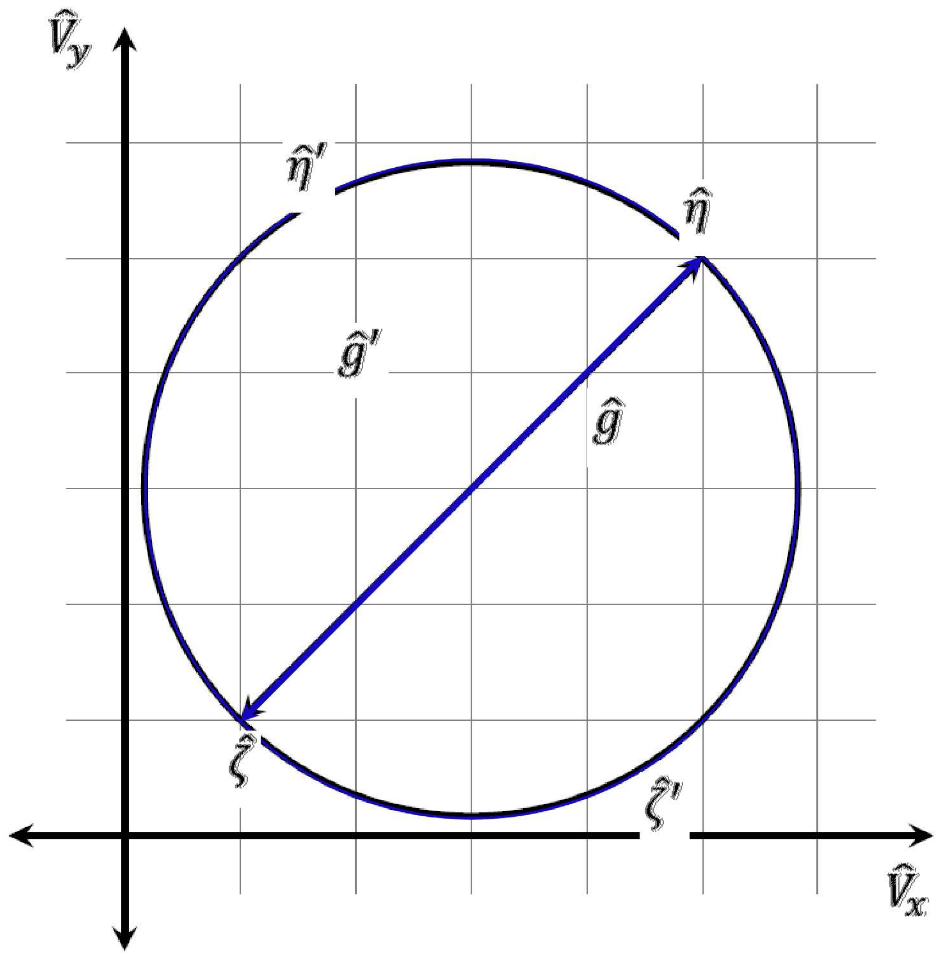
$$N_{coll} \sim \frac{1}{C_{RMS}^2}$$

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

QUIPS collisions

How to compute collision integral (replenishment)?

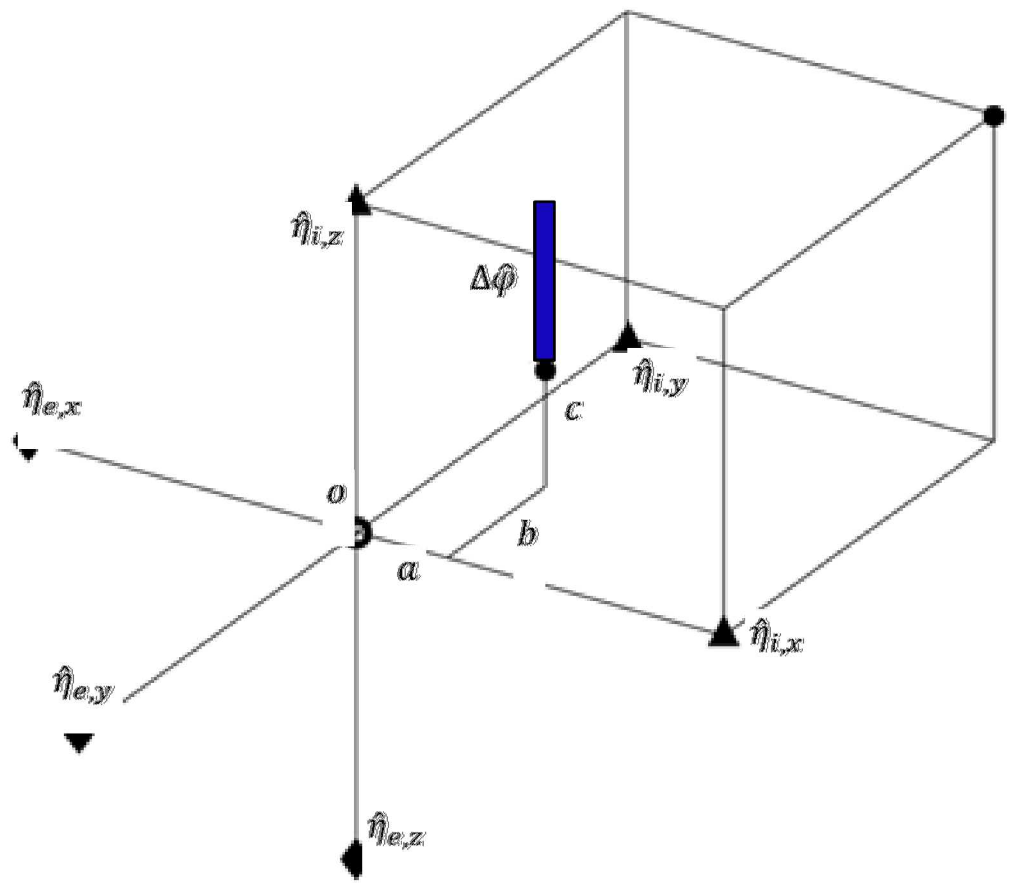
Find post-collision velocity (random point on a sphere)



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) negative mass



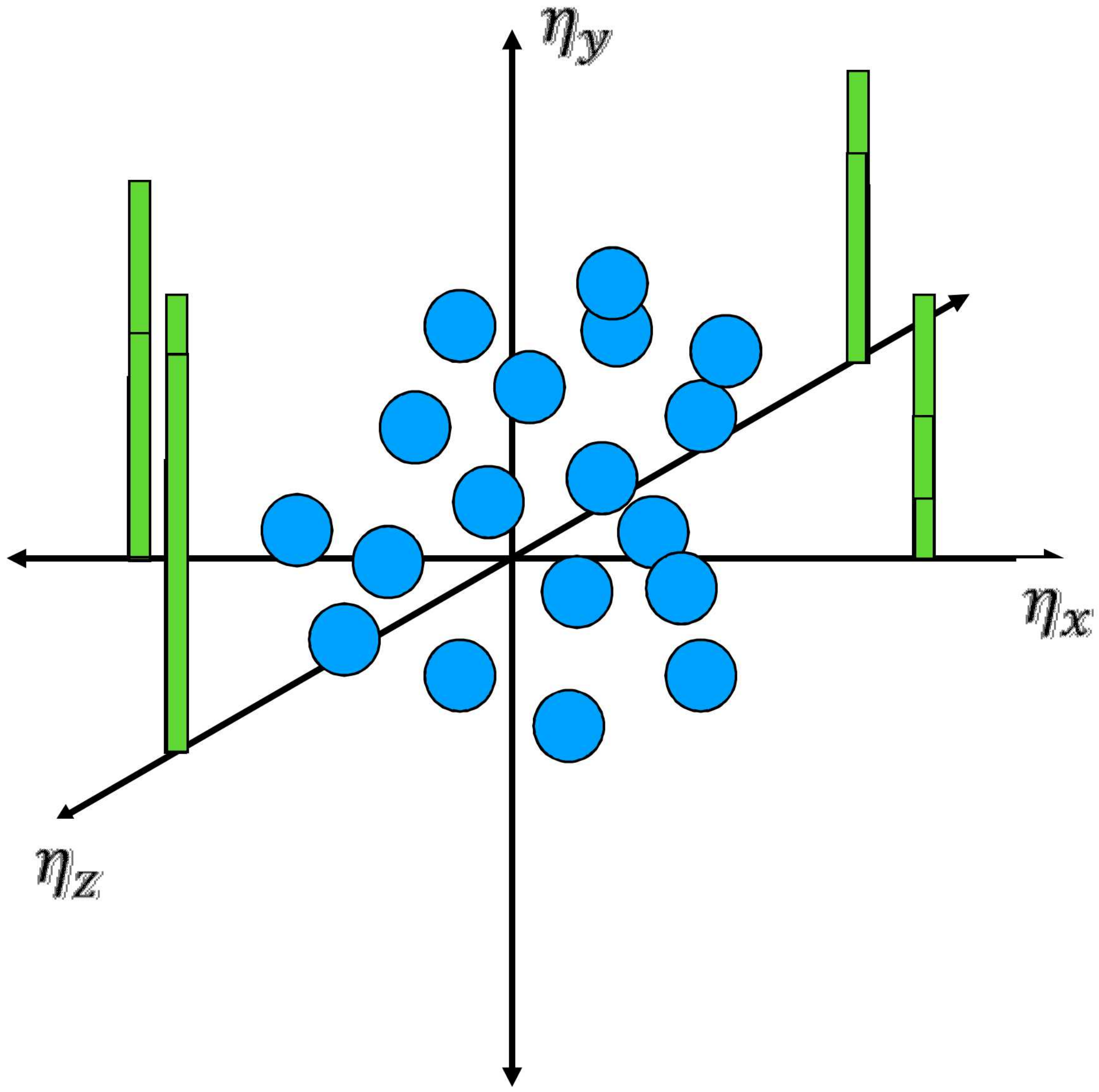
QUIPS summary

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

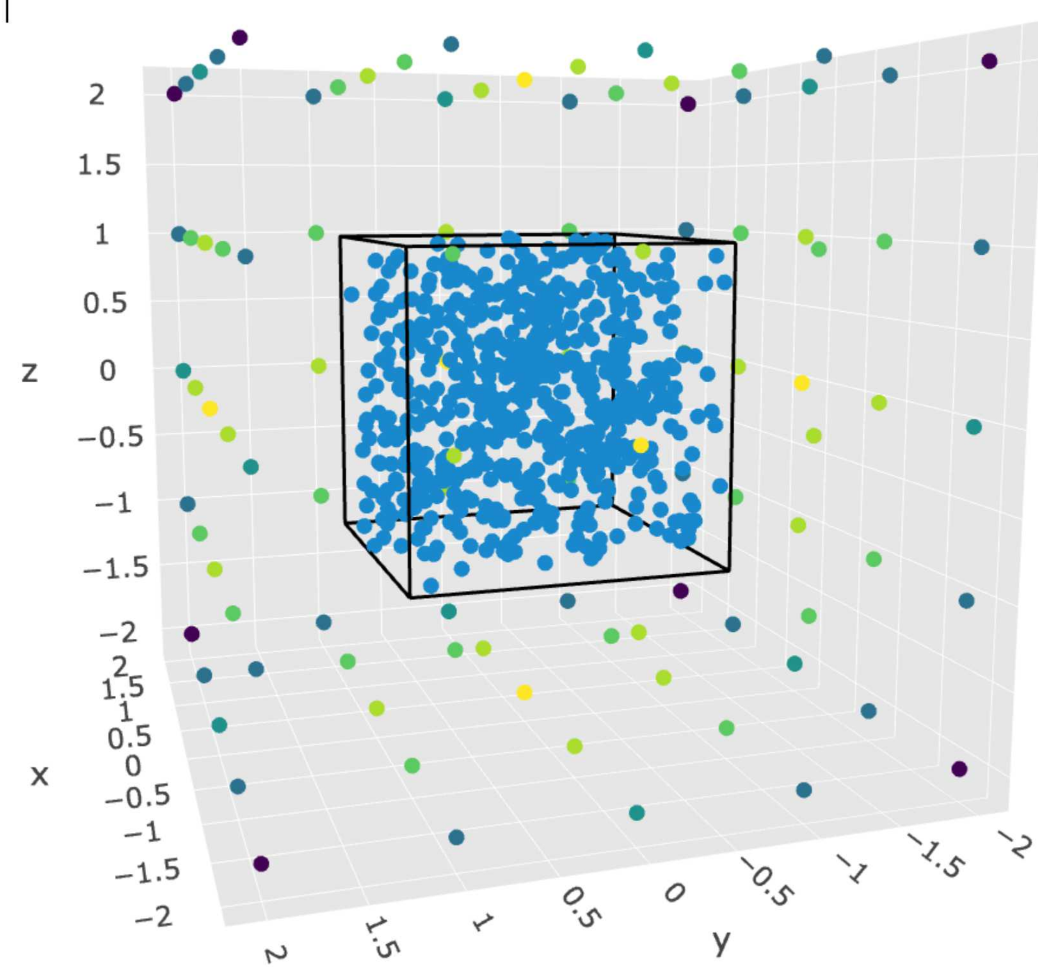
Why hybridize in velocity space?

- Easy to do convection
- Easy to do boundary conditions
- DVM have issues when there are discontinuities in boundary conditions
- Faster (represent bulk of distribution with a few particles)
- Velocity-space hybridization is a new approach

Hybrid QUIPS/DSMC

How to hybridize?

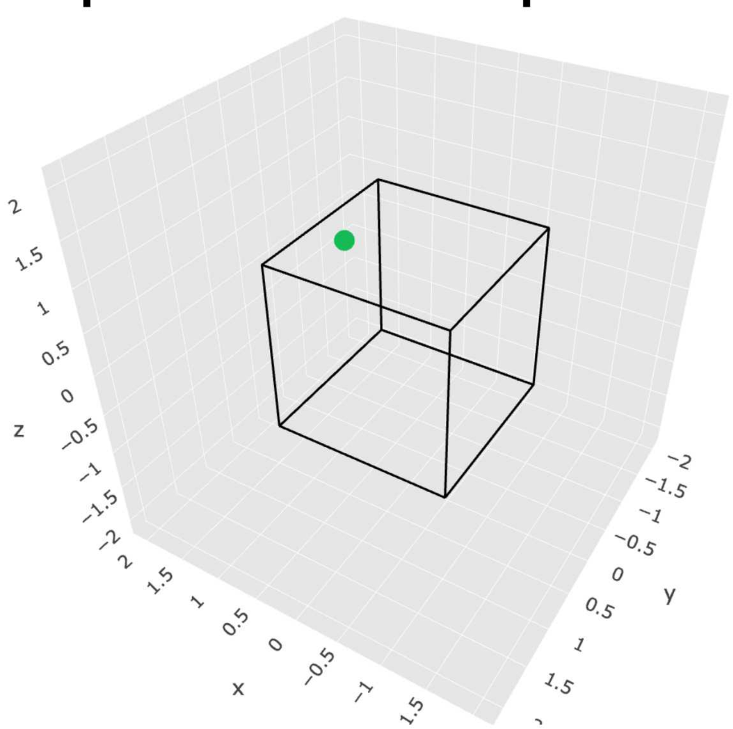
- Pick region in velocity space where particles can have any velocity
- Use DSMC collision mechanics (instead of small depletion/replenishmen

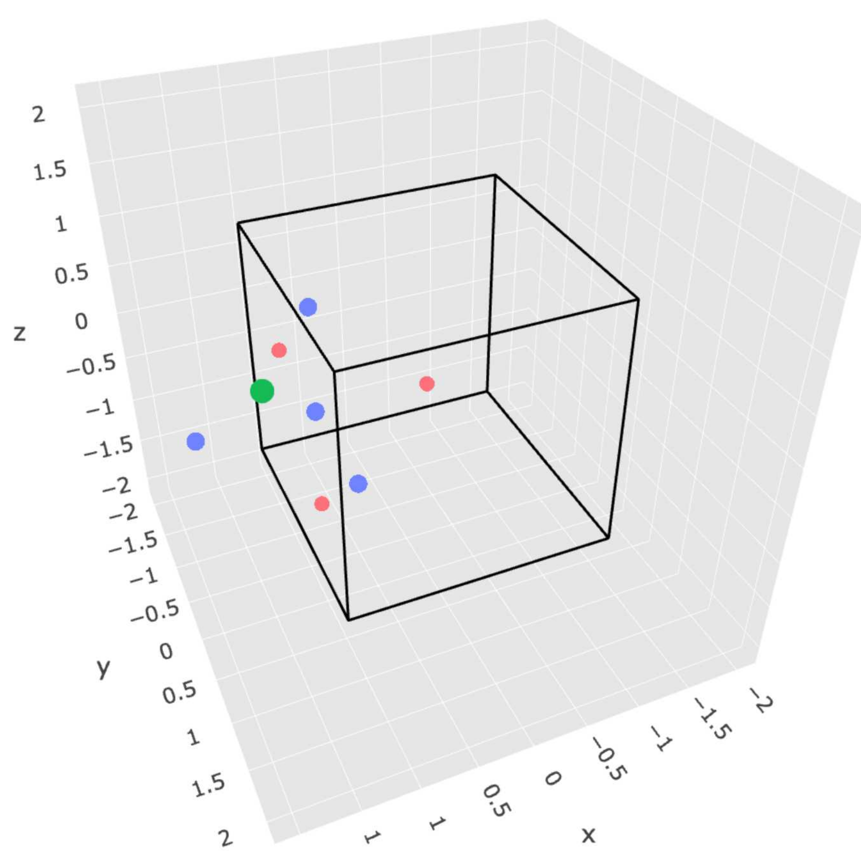


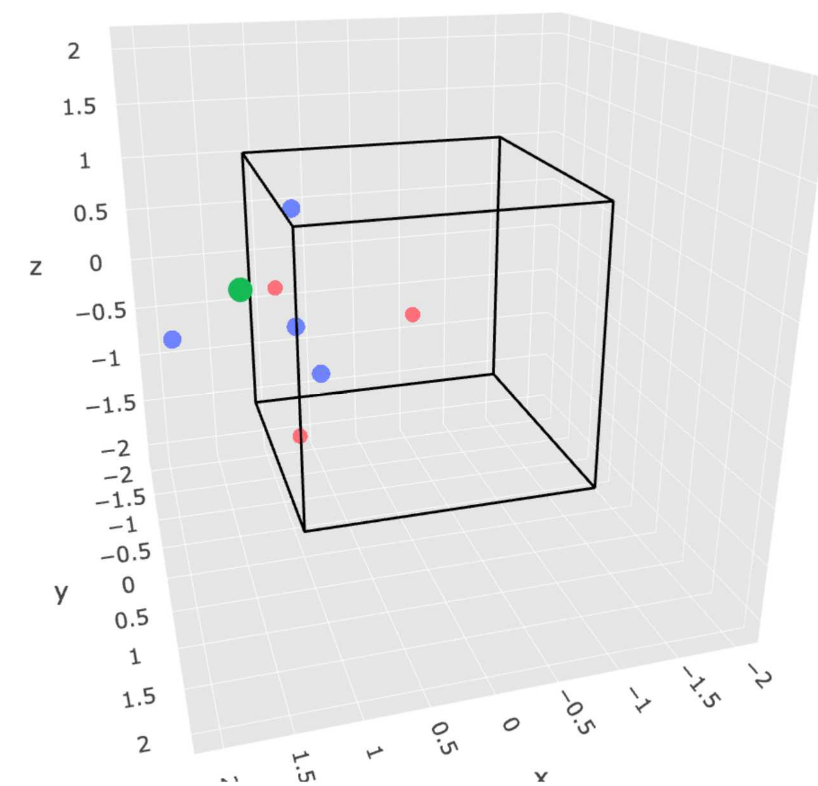
Hybrid QUIPS/DSMC

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







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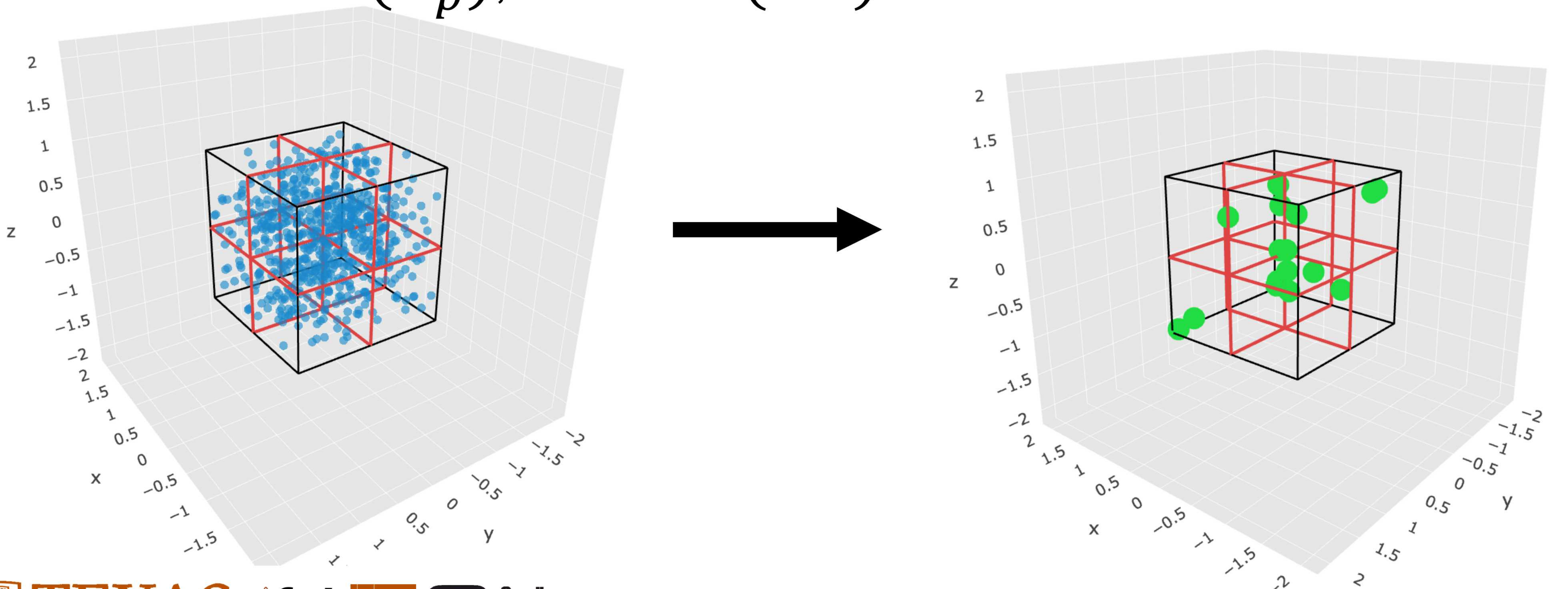
Hybrid QUIPS/DSMC

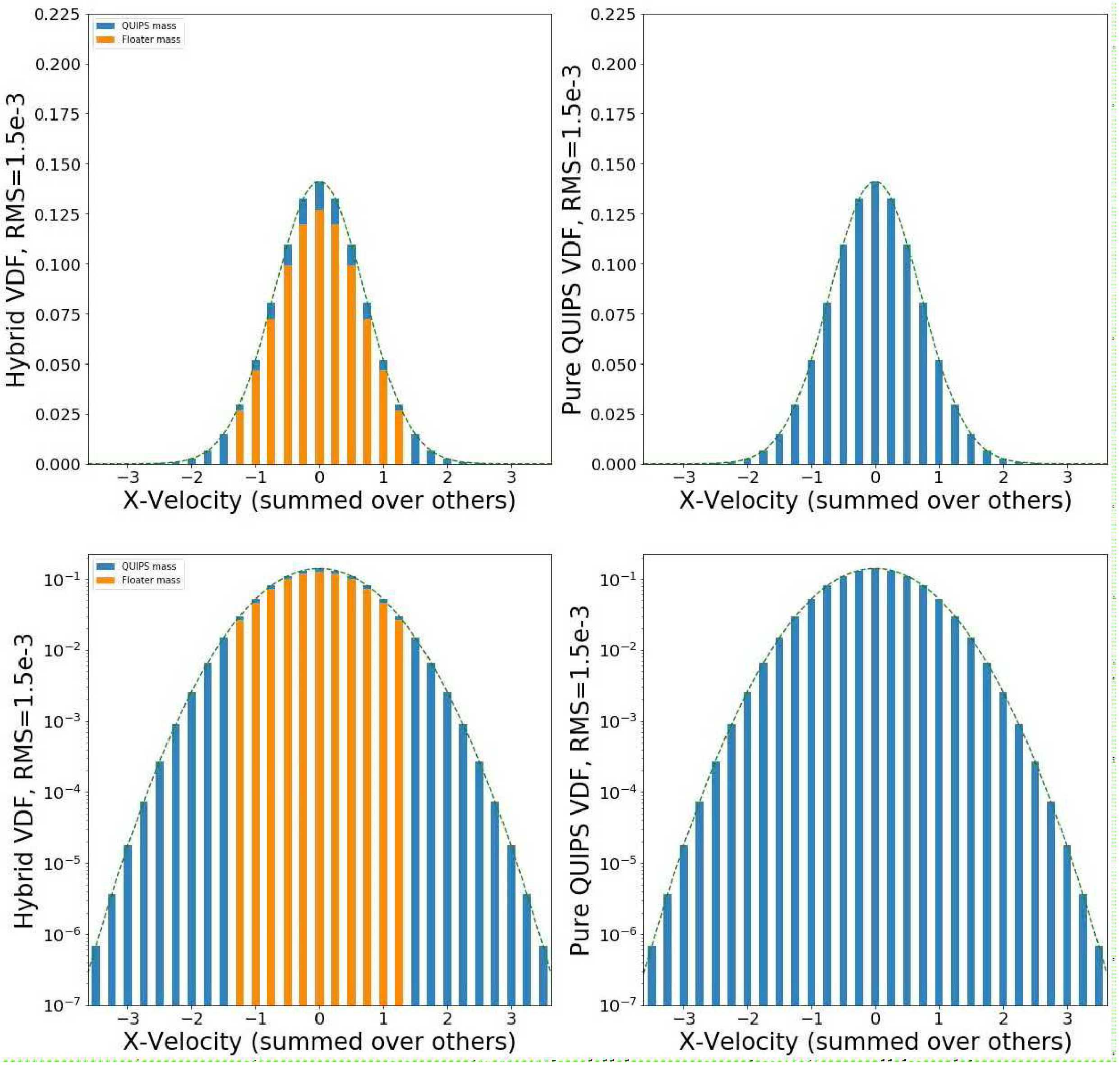
How to avoid (exponential) growth of number of particles?

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



Hybrid QUIPS/DSMC

Example of hybrid VDF representation



Hybrid QUIPS/DSMC

Numerical results

- Initialize with Maxwellian distribution, look at noise (RMSE) in tails and in high-order moments
- CPU time per step vs. RMSE as measure of efficiency

Variable parameters:

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

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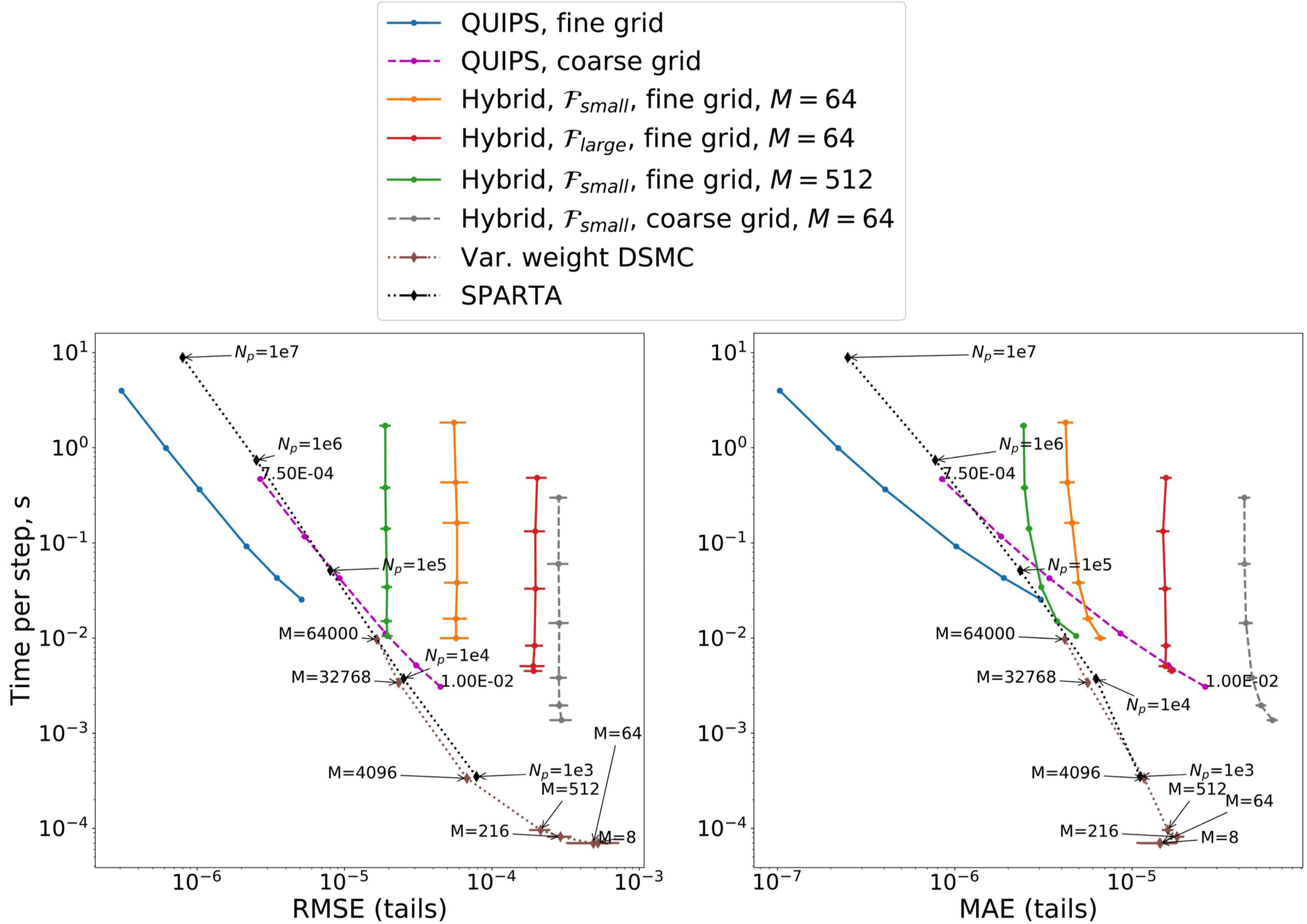
Hybrid QUIPS/DSMC

Computational time per collision step vs. error in tails



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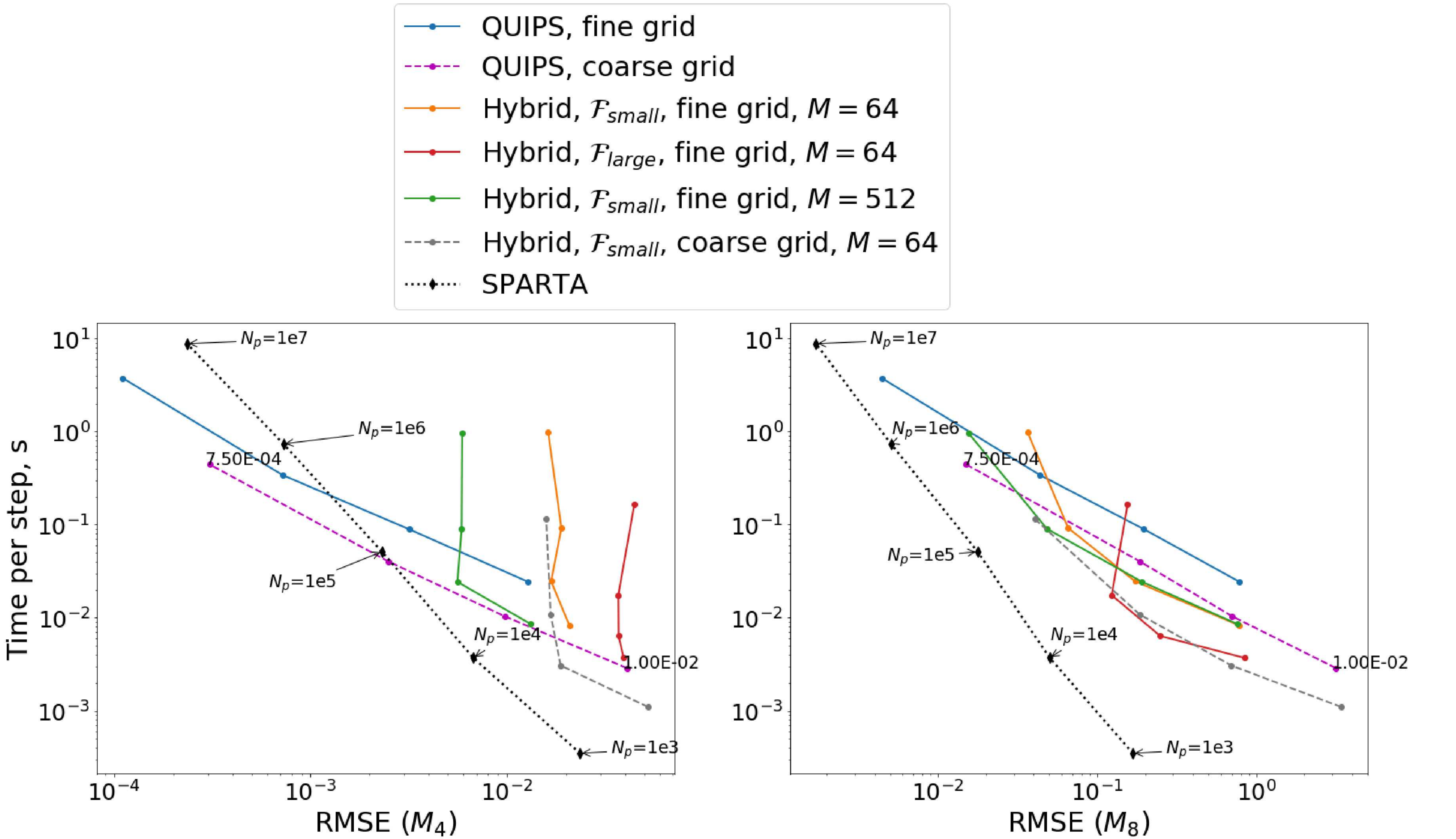
Computational time per collision step vs. error in moments



Conclusions

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

Further things to look at:

- Internal energies
- Variance reduction
- 1-D and 2-D problems
- New metrics for comparison (noise in macroscopic variables; noise in reaction rates)

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.