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Progress Toward Robust Dynamic Particle Reweighting

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Motivation

- Flows of practical interest evolve in time, have strong gradients, trace species, or wide ranges of density and collisionality.
- DSMC and PIC place requirements on cell size and particle count to ensure overall accuracy and constrain instantaneous statistical scatter.
- For fixed particle weight, a huge number of particles is needed in some areas to get desired number elsewhere.
- Reweighting could speed up particle methods to make more applications tractable.

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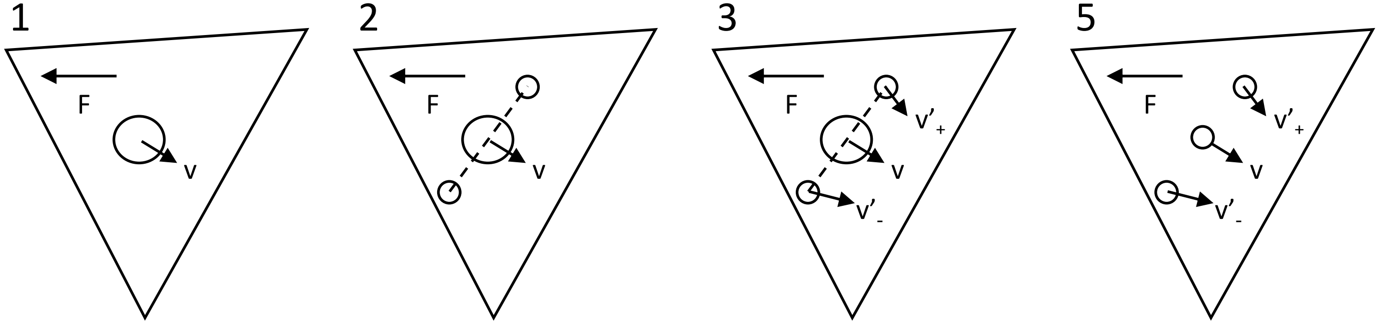
Force Aware Reweighting

- For a collisional electrostatic simulation, the reweighting method needs to preserve:
  - Net charge, as weighted to nodes.
  - Moments of the velocity distribution function, which are related to conservation of mass, momentum, and energy.
- Force Aware reweighting controls particle count by cloning and merging in cells.
  - Accounts for interaction of position and velocity.
  - Attempts to conserve total energy for particles.

Clone Procedure

- **If a cell has too few particles:**
  1. **Choose a high weight parent particle.**
  2. **Generate a pair of random positions in the cell, symmetric about the parent position.**
  3. **Compute modified velocities at the new positions by accounting for displacement in the force field.**
  4. **If unphysical velocities result, repeat 2-3.**
  5. **Adjust weights for parent and new particles.**
  6. **Repeat 1-4 until target number is met.**



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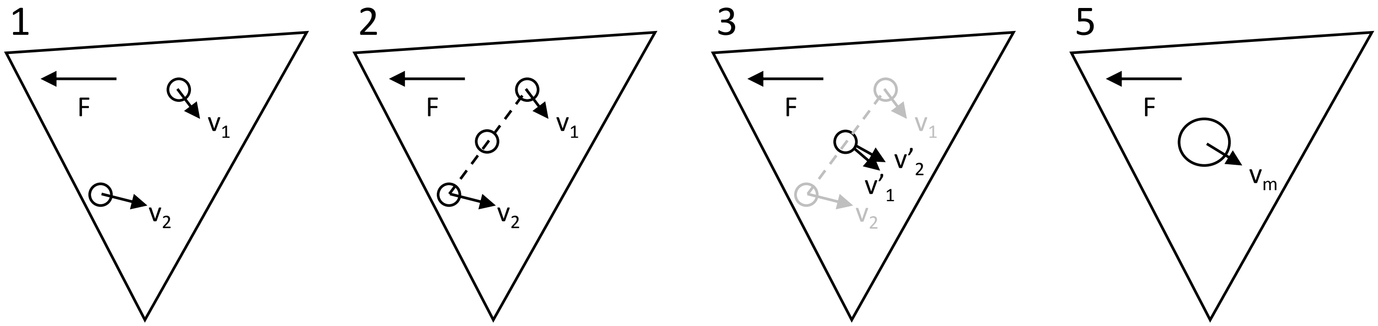
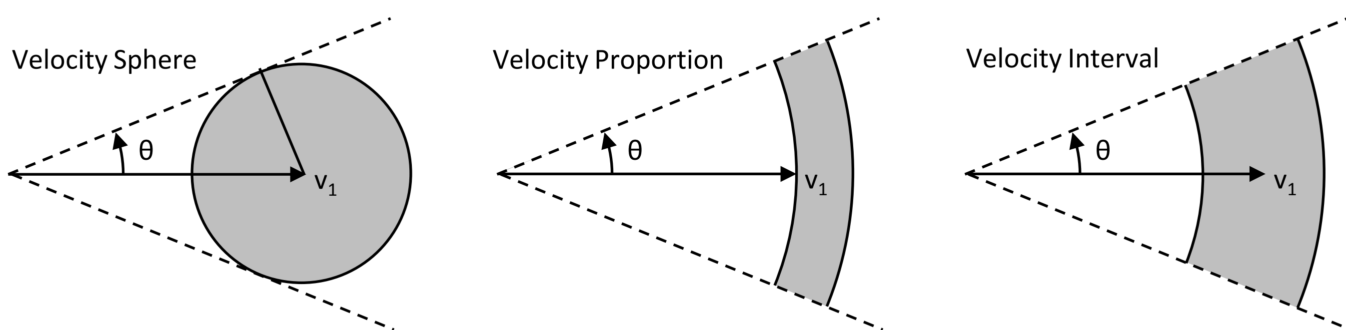
Merge Procedure

- **If a cell has too many particles:**
  1. **Choose a pair of low weight particles.**
  2. **Compute center of mass position.**
  3. **Compute modified velocities at the center of mass by accounting for displacement in the force field.**
  4. **If velocities are “too different,” reject pair and repeat 1-3.**
  5. **Calculate average velocity, conserving momentum.**
  6. **Adjust weight and record difference in kinetic energy.**
  7. **Repeat 1-6 until target number is met.**



Merge Candidate Pair Selection

- **Only approve merge pairs that are close in both position and velocity—close in phase space.**
- **The spatial bin is the cell, approves any pair.**
- **The velocity bin has many options, including:**
  - **Velocity Sphere** $|\mathbf{v}_2 - \mathbf{v}_1| < |\mathbf{v}_1| \sin(\theta)$
  - **Velocity Proportion** $\mathbf{v}_2 \cdot \mathbf{v}_1 > |\mathbf{v}_1||\mathbf{v}_2| \cos(\theta)$ $\quad |\mathbf{v}_2| \big/ |\mathbf{v}_1| < R$
  - **Velocity Interval** $\mathbf{v}_2 \cdot \mathbf{v}_1 > |\mathbf{v}_1||\mathbf{v}_2| \cos(\theta)$ $\quad |\mathbf{v}_2| - |\mathbf{v}_1| < v_c = \sqrt{\frac{k_B T}{m}}$



Restore Energy

- **Merge process cannot conserve energy.**
- **Restore energy in the cell by thermostat method.**

$$R = \sqrt{\frac{E_K - \frac{1}{2}M\mathbf{v}_m^2 + \Delta E_K}{E_K - \frac{1}{2}M\mathbf{v}_m^2}}$$

  - **E_k is total kinetic energy, M is total mass, and v_m is mean velocity, summed over particles; ΔE_k is kinetic energy to add.**
- **Then each particle velocity is rescaled.**

$$\mathbf{v}_i' = R(\mathbf{v}_i - \mathbf{v}_m) + \mathbf{v}_m$$

- **This scales the thermal component of each particle velocity, and preserves total momentum.**

Test Problem: Particles In A Box

- **Initial population in a box with specular walls**
  - Helium gas, n = 2×10^{18} cm^{-3}, v = 0 cm/μs, T = 300 K
  - Box is 0.1 cm x 0.1 cm x 1.0 cm, in 58 cells.
  - Initial weighting is 2.3×10^{11} particles/macroparticle, giving about 87,000 particles or 1500 per cell.
- **Reweighting target of 30 particles per cell.**
- **Expect average properties to be constant**
  - Mass is exactly constant
  - Velocity has instantaneous fluctuations about zero as particles bounce back and forth
  - Temperature has fluctuations as mean velocity and velocity distribution fluctuate.

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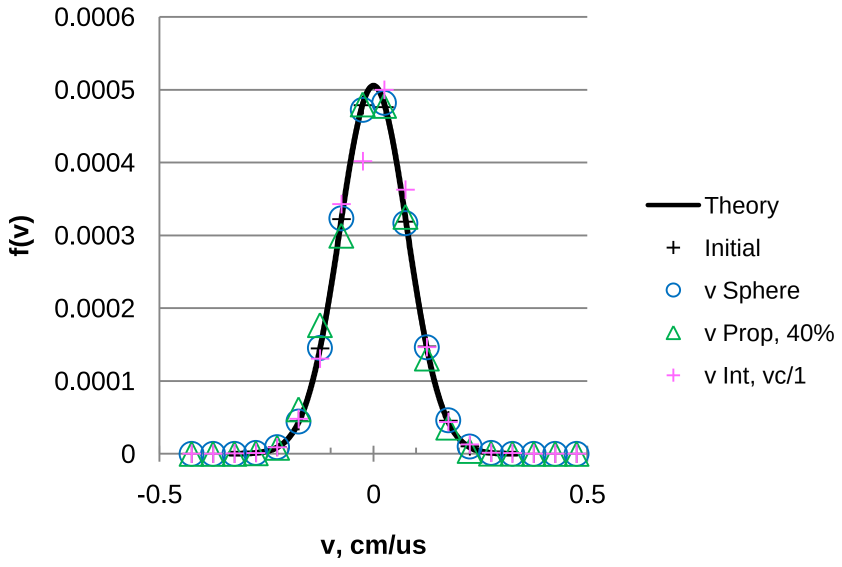
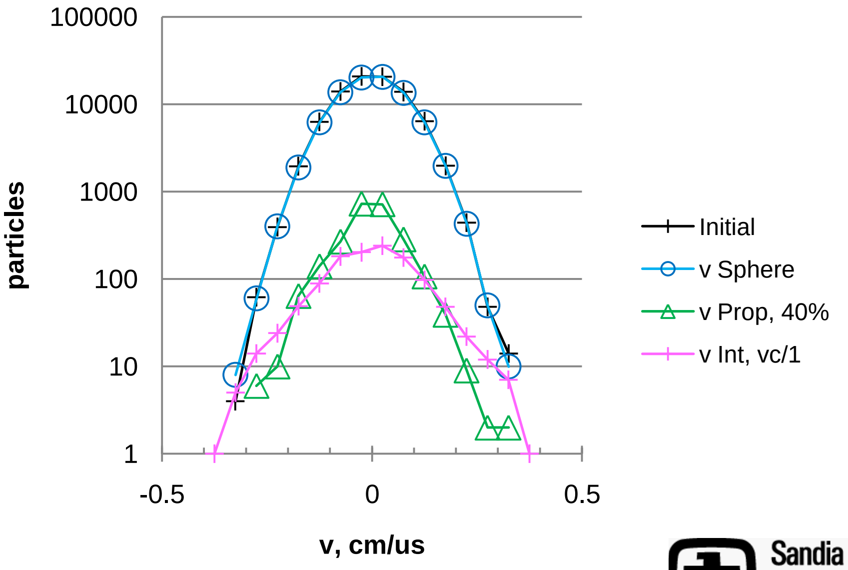
Accuracy Comparison

- **With restore energy, all methods preserve VDF and moments fairly well—even with huge bins.**
- **Less strict methods reduce the number of redundant particles near the mean velocity.**

Velocity Distribution Function



Particle Velocity Histograms



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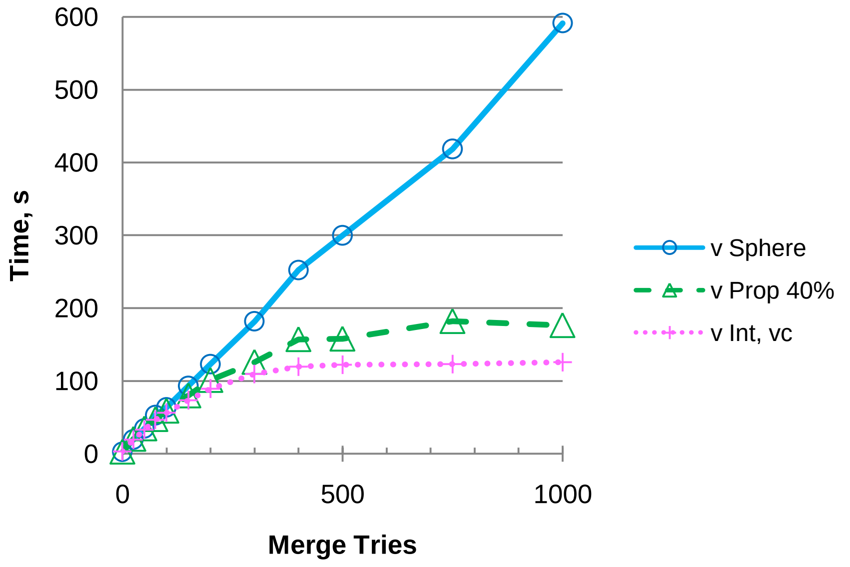
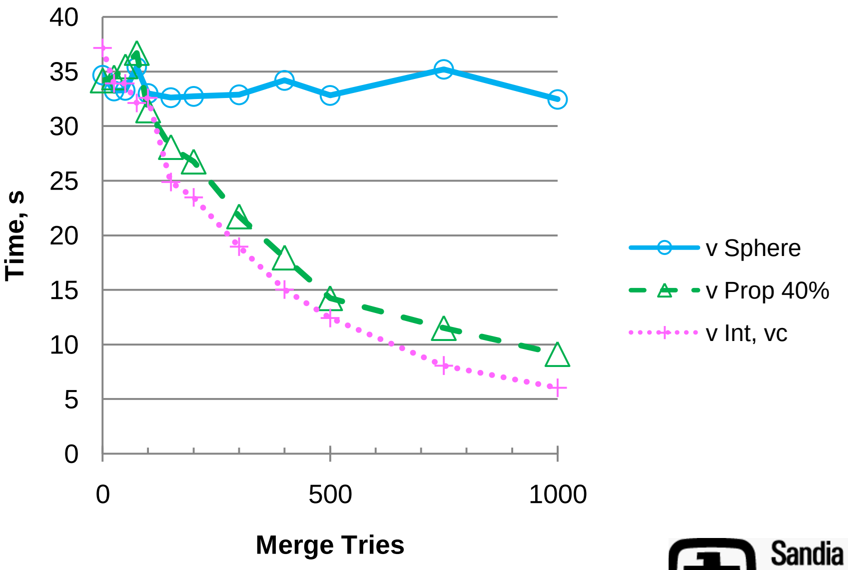
Timing Comparison

- For this example problem and these criteria, not the time benefit from reweighting is not clear.
- Varied number of merge attempts to minimize wasted effort spent testing and rejecting pairs.

Time Spent Reweighting



Time Spent Moving Particles



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Conclusions and Future Work

- Accounting for total energy makes clone and merge processes more reliable for use with PIC.
- A lenient velocity space criteria for merging can drastically reduce total particle count.
- Restore energy mitigates the numerical cooling effect of merging.

- Optimize how many merge pairs to test.
- Test reweighting on more demanding problems with fields, non-Maxwellian distributions, and collisions.

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