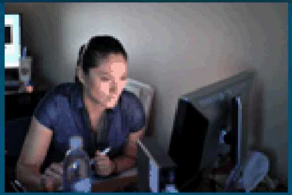
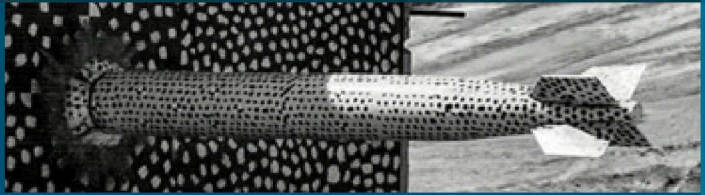
SAND2020-8934PE

Particle-to-Fluid Merge in Hybrid Plasma Simulation





PRESENTED BY

L. T. Meredith

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Outline

- Motivation
- Method
- Results
- Conclusions and outlook

EMPIRE is a next-generation hybrid plasma code

The **Boltzmann eqn** models time evolution of plasma's **distribution** f

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = \left(\frac{\partial f}{\partial t} \right)_{\text{collisions}}$$

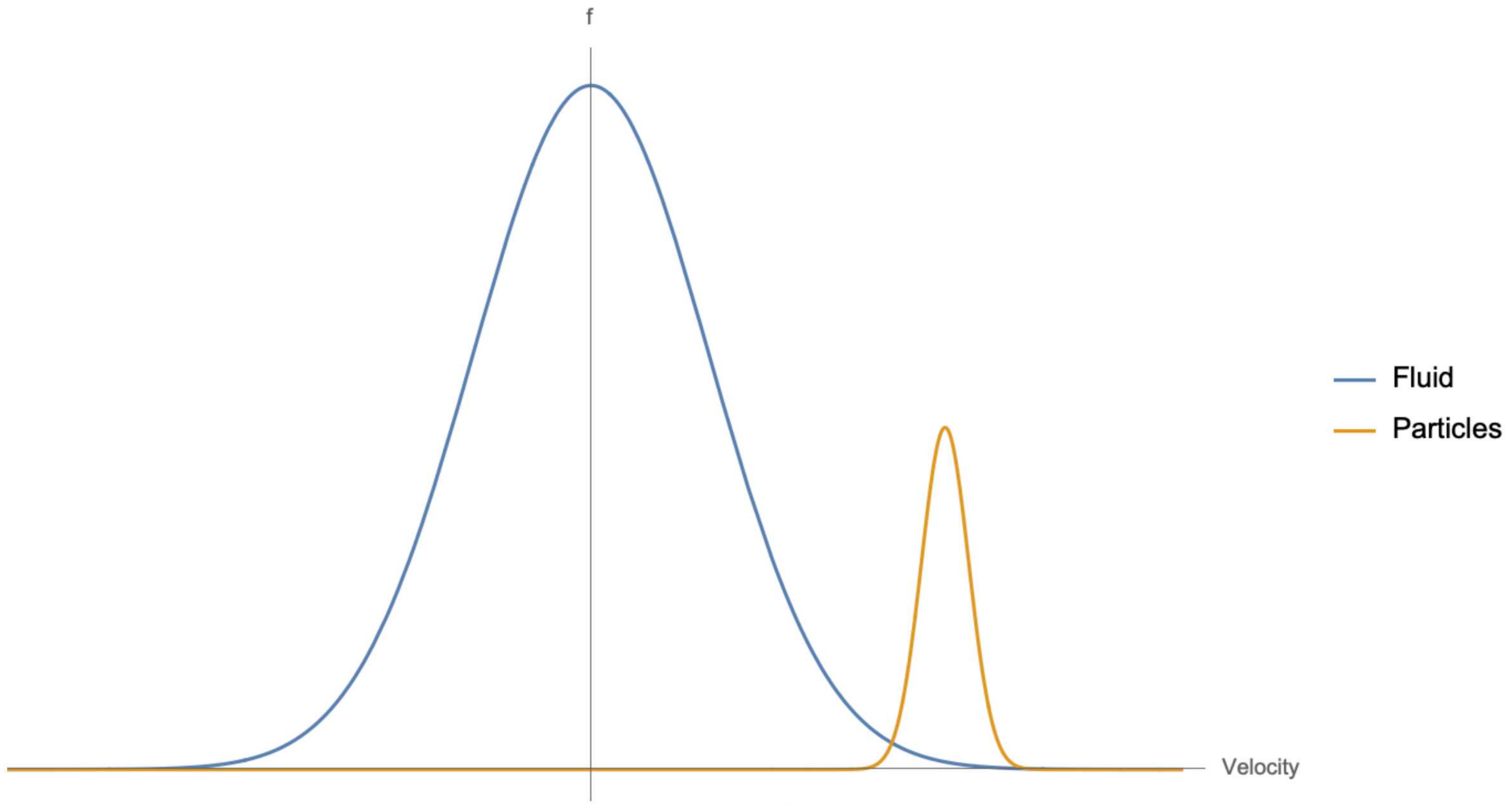
- $f = f(\mathbf{x}, \mathbf{v}, t)$ gives the number of particles near point **x** with velocities about **v** at time t
- Hybrid codes solve the Boltzmann eqn using both fluid and kinetic methods simultaneously
- **Fluid** methods solve this by taking kinetic moments
  - Multiply both sides of the eqn by $\mathbf{v}^n$ and integrate to reduce dimensionality at the cost of more equations
  - Assumes that the distribution f is drifting Maxwellian (Gaussian)* ($\sim e^{-v^2}$) (*in most cases)
  - Fast and accurate but doesn't work at low densities
- **Kinetic** methods don't integrate away the velocity information; particle-in-cell (PIC) most popular
  - Populate domain with particles representing samples of f
  - Evolve Newtonian mechanics of individual particles
  - Slow and noisy but captures more physics

Hybrid codes can be applied to many far-from-equilibrium plasmas

- Pulsed power
  - Target design: targets treated as fluids, but fluids cannot capture particle ablation
  - Power flow: electrical current treated with PIC, but particle count becomes too high for PIC alone
- Magnetic confinement fusion
  - Electrons thermalize much faster than ions, so treat electrons as a fluid and ions with PIC
- Space physics
  - Coronal mass ejections: mostly Maxwellian but with a significant fraction of highly-energetic particles
  - Cosmic rays: energetic particles on a background of a cold neutral gas

Hybrid models split a plasma into PIC and fluid parts

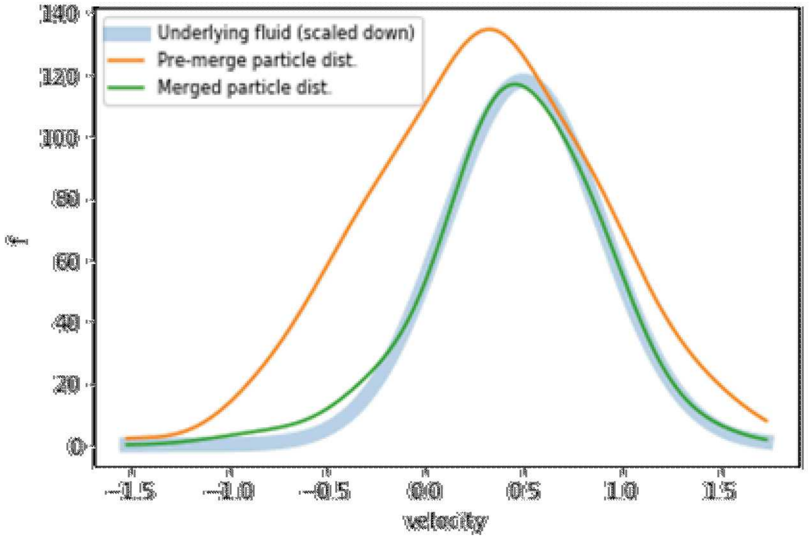
- Delta-*f* models have a well-behaved Gaussian fluid underneath a few far-from-equilibrium particles



- Particles more accurately represented by Dirac deltas, but this gives a sense of how the plasma is partitioned between fluid and PIC solvers

Tracking particles is expensive and a limiting factor

- Often, physics/numerics cause particle population to explode
- Want to reduce particles by identifying a "fluid-like" subset and merging them into the fluid
- Fluid-like means the particles won't skew the fluid away from its nice Gaussian shape
- How do we choose particles to merge such that their distribution is the same as the underlying fluid's?
- Pure statistics formulation: given a sample from some unknown distribution, how do we choose a weighted subset of the sample that represents a distribution we want?



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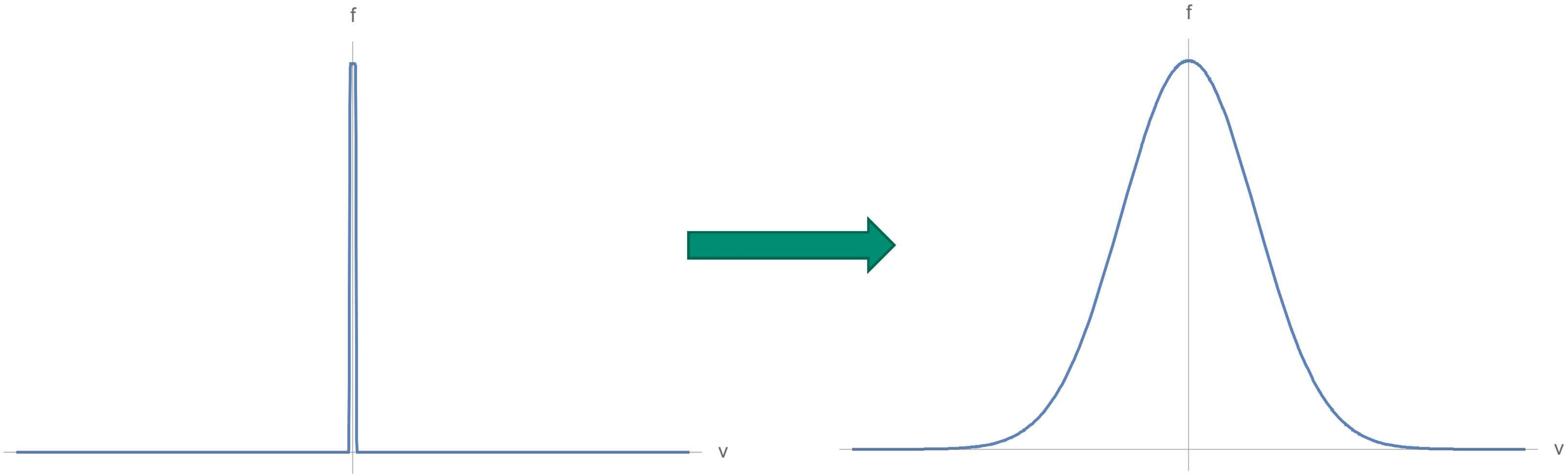
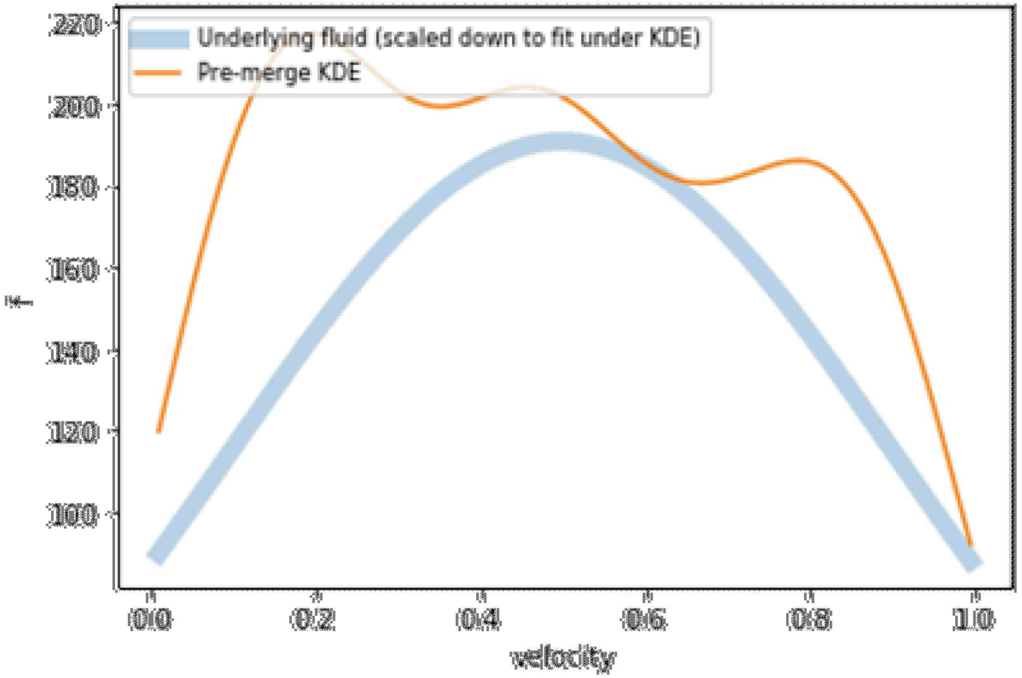
What does it mean for particles to “represent” a distribution?

- Classical particle is a Dirac delta in phase space – no uncertainty in position or velocity
- Must smooth out the delta to gain some info about what distribution the particle is from
- Generally called **kernel density estimator (KDE)**; replace the delta function with a **kernel**
- Width of kernel is determined by number of particles and sample standard deviation
- Distribution represented by the particles is just the sum of all the kernels
- Example: histograms



Select particles to merge whose KDE matches the underlying fluid

- That is, the selected particles should have a KDE with the same shape as the fluid
- Ensures that merging the particles won't skew the fluid, just scale it up a bit
- Particles can have non-integer weight (number of particles represented by macroparticle), so individual kernels can be scaled up or down to tune the KDE
- However, can't merge more weight from a particle than it originally had



The constraints on the weight suggest use of optimization techniques

- Point is to minimize some quantity representing error (**cost**) as a function of selected weights
- Choice of cost generally depends on what errors are considered significant
- In our case, KDE should equal a scaled-down version of the fluid distribution everywhere
- Too hard to enforce equality everywhere; just check at a few (**collocation**) points in phase space

$$\sum_{i=1}^{N} w_i K_h(v - v_i) = f(v)$$

KDE at point *v* Fluid distro

(v_i is velocity of particle i; w_i is its selected weight)

More important: KDE's moments should match fluid's

$$\sum_{i=1}^{N} w_i v_i^n = \int f(v)\, v^n \, \mathrm{d}v$$

- Since fluid solver evolves moments, it's important that they incur as little error as possible
- Set some threshold n and compare moments for all integers $<n$
- In three dimensions, moments should be checked in each direction

Combine moments and collocation points to get a matrix equation:

$$\begin{cases} \sum_{i=1}^{N} w_i v_i^n = \int f(v)\, v^n \, \mathrm{d}v \\ \sum_{i=1}^{N} w_i K_h(v - v_i) = f(v) \end{cases}$$

- This is linear in the weights for finitely many collocation points and moments
- Number of moments/collocation points can be chosen to suit individual problem needs
- Equivalent to $Aw = b$
- Due to constraints on weights, don't expect an exact solution
- Instead, find weights that minimize $|Aw - b|^2$ -- **constrained linear least-squares optimization**
- Very well-researched subject, lots of good optimization algorithms

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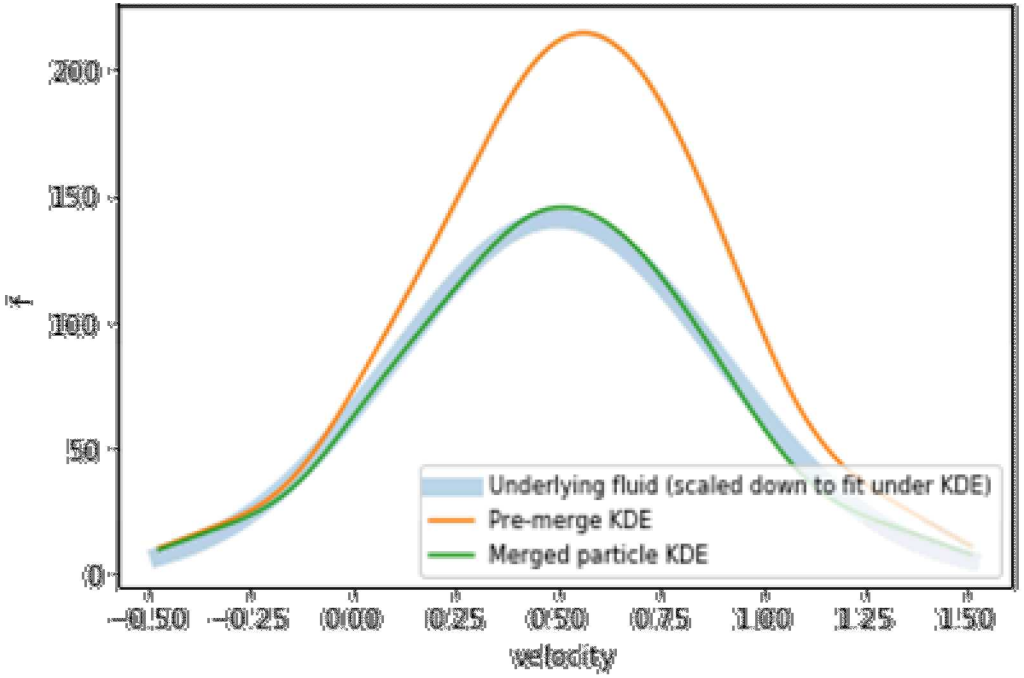
Good matching when the pre-merge particles are already fluid-like

- Match moments up to order n=4, no collocation points, 200 particles

Error in moment of order *n*

n=0	0.000000e+00
1	2.015724e-16
2	1.108475e-15
3	6.927222e-16
4	2.404612e-15

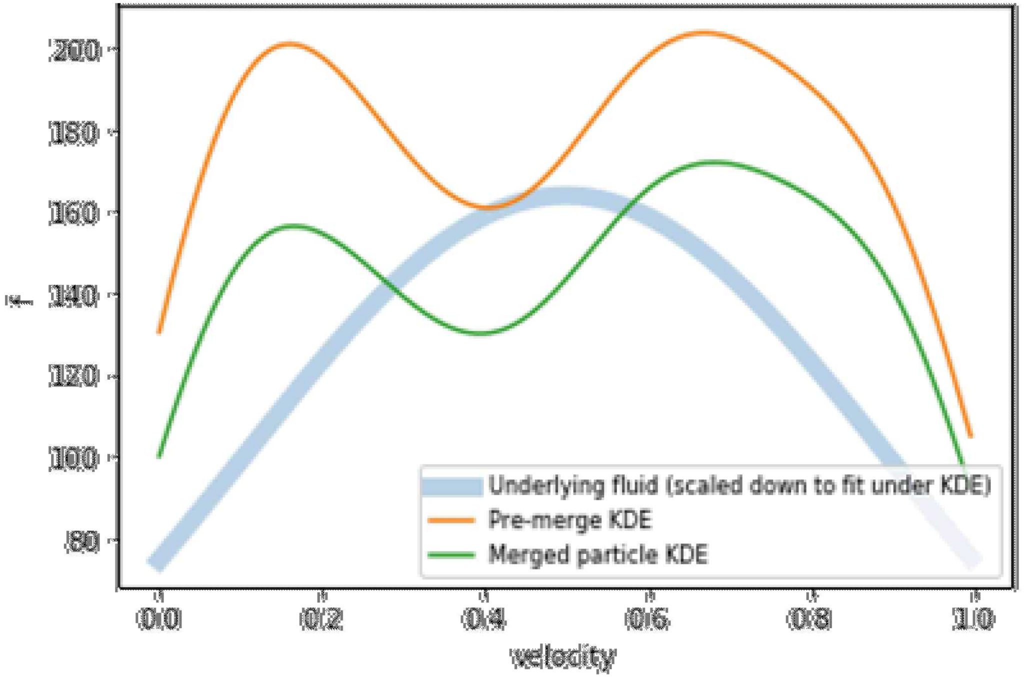


Without collocation points, algorithm struggles with uniformly distributed particles

- Match moments up to order n=4, no collocation points, 200 particles
- L2 error = 1401.81

Error in moment of order *n*

n=0	3.466062e-16
1	-1.733031e-16
2	-1.307062e-01
3	-2.259371e-01
4	-3.656592e-01

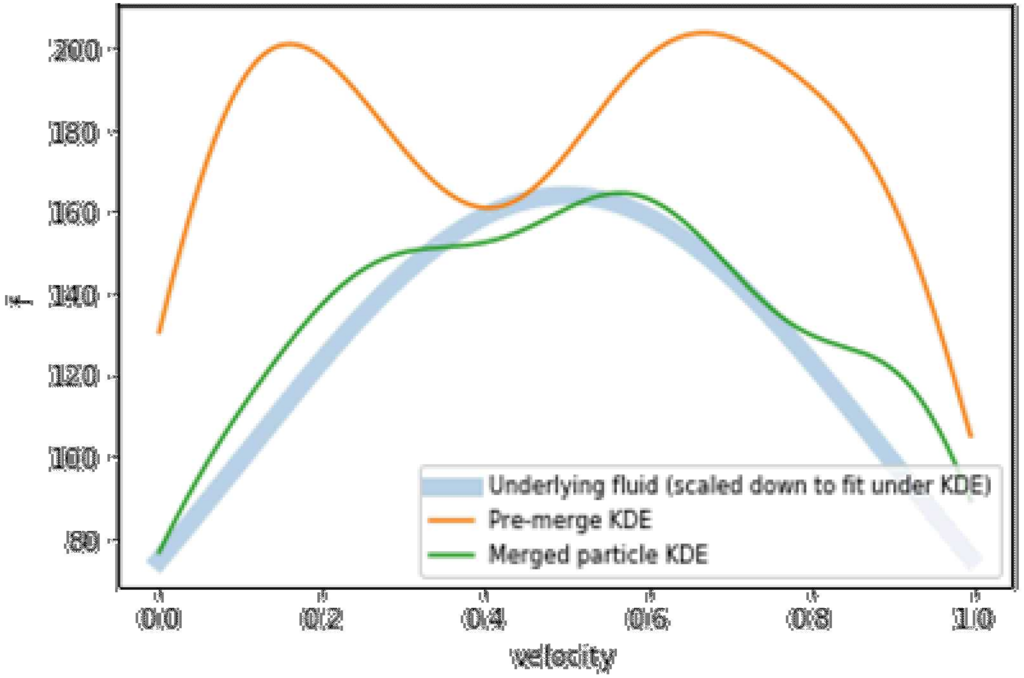


Adding collocation points sacrifices moment error for better "fit"

- Match moments up to order *n*=4, 10 collocation points, 200 particles
- Note that this is a particularly pathological particle sample; particles are expected to form a more Gaussian distribution
- Fit quantified by L2 error = 572.86

Error in moment of order *n*

n=0	6.8734e-2
1	5.9558e-2
2	1.93157e-1
3	2.85557e-1
4	4.13122e-1

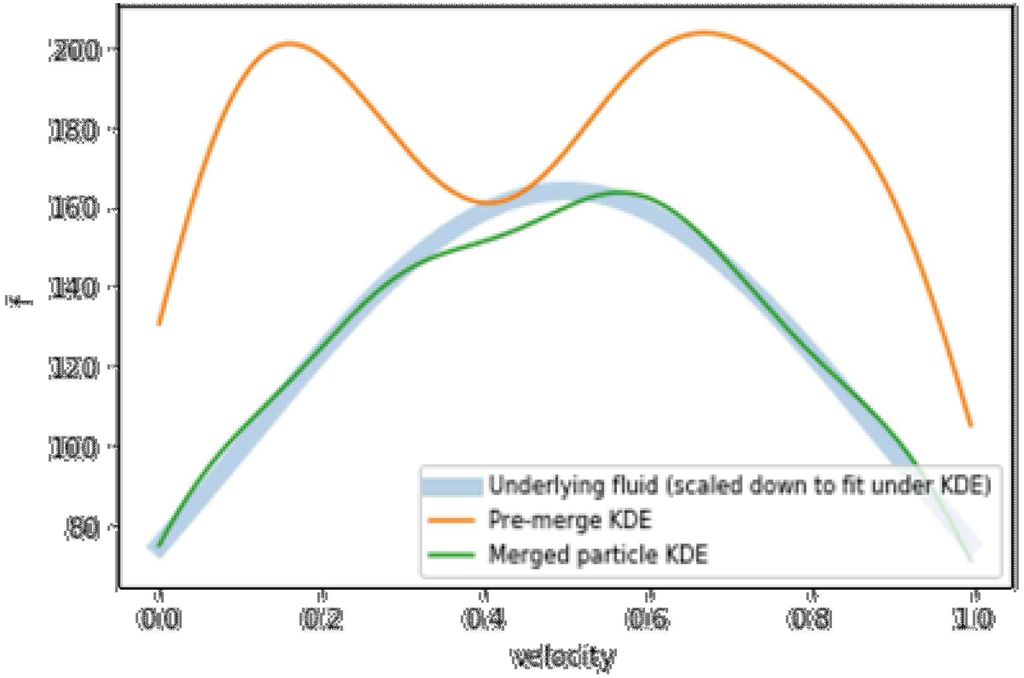


Can add arbitrarily many collocation points to improve L2 error

- Match moments up to order n=4, 100 collocation points, 200 particles
- This comes at the cost of error in moments
- L2 error = 506.62

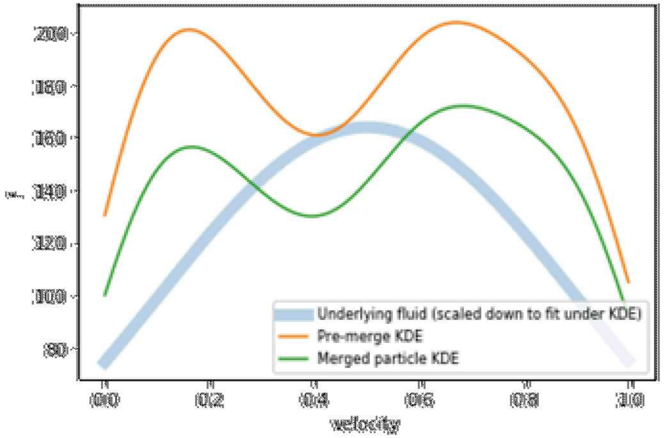
Error in moment of order *n*

n=0	-1.20741e-1
1	-1.27833e-1
2	-2.67308e-1
3	-3.64794e-1
4	-4.87790e-1

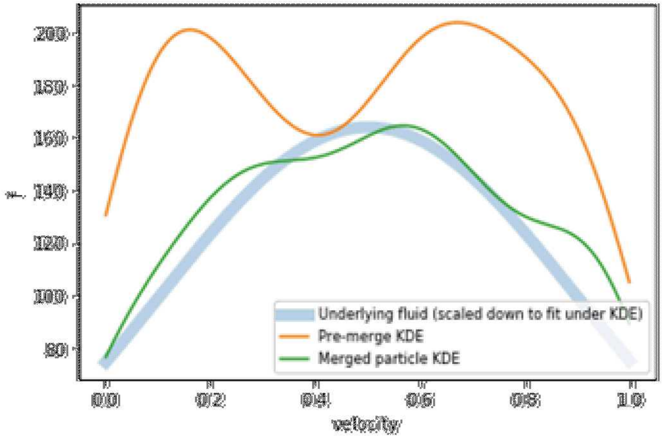


All three uniform attempts side by side

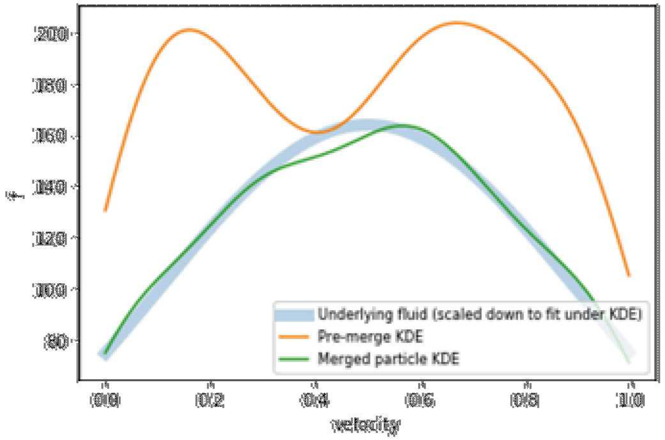
No collocation points



10 collocation points



100 collocation points



L2 errors

1401.81

572.86

506.62

Error in moment of order *n*

n=0	3.466062e-16
1	-1.733031e-16
2	-1.307062e-01
3	-2.259371e-01
4	-3.656592e-01

n=0	6.8734e-2
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The hybrid merge algorithm tries to choose particles that will not skew the fluid when merged

- Kernel density estimation used to reconstruct shape of particle distribution
- Weighted kernels are chosen that best match the shape of the fluid distribution
- Error metrics used in optimization include moments and values of KDE evaluated at certain collocation points
- Algorithm shows very low error and good qualitative agreement when particle distribution is initially approximately Gaussian
- Agreement is less good for uniformly distribution particles, and there is a tradeoff between moment error and fit to fluid distribution as quantified by L2 error
- Particles expected to be mostly Gaussian with perturbations in real simulations, so uniformly distributed particles represents a worst-case scenario for the merge algorithm