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EMPIRE Beam Simulations with Particle Merge

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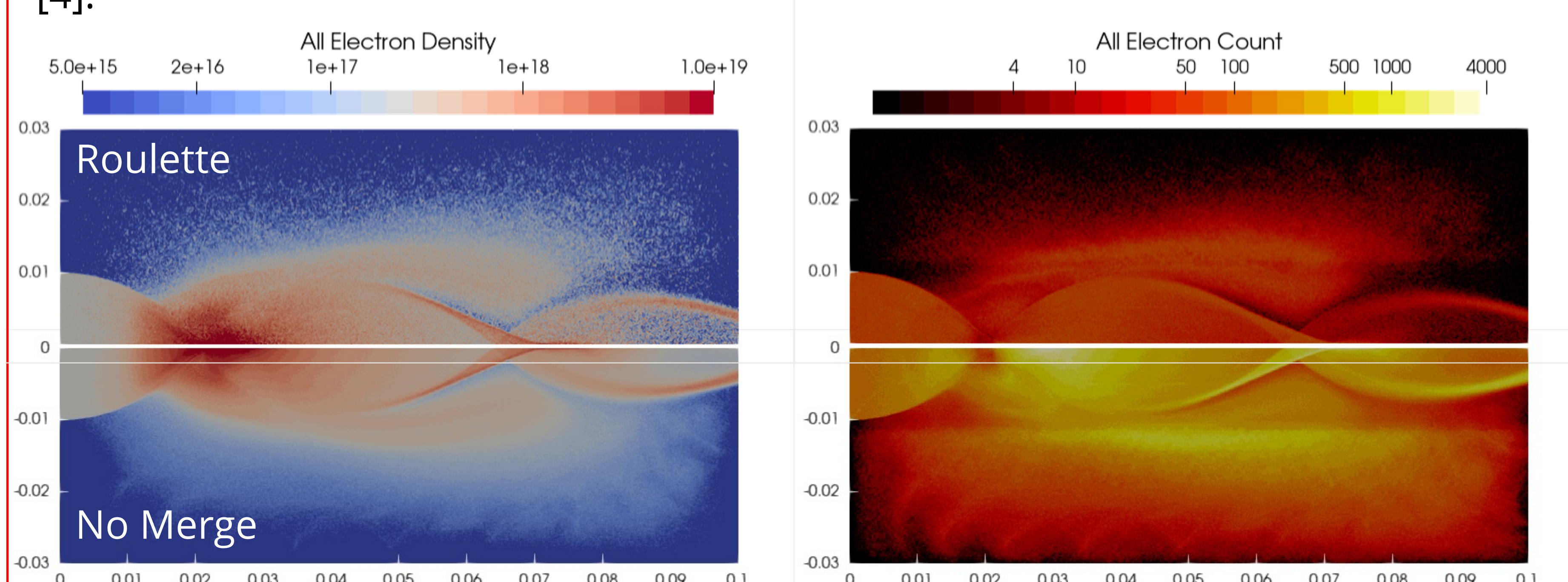
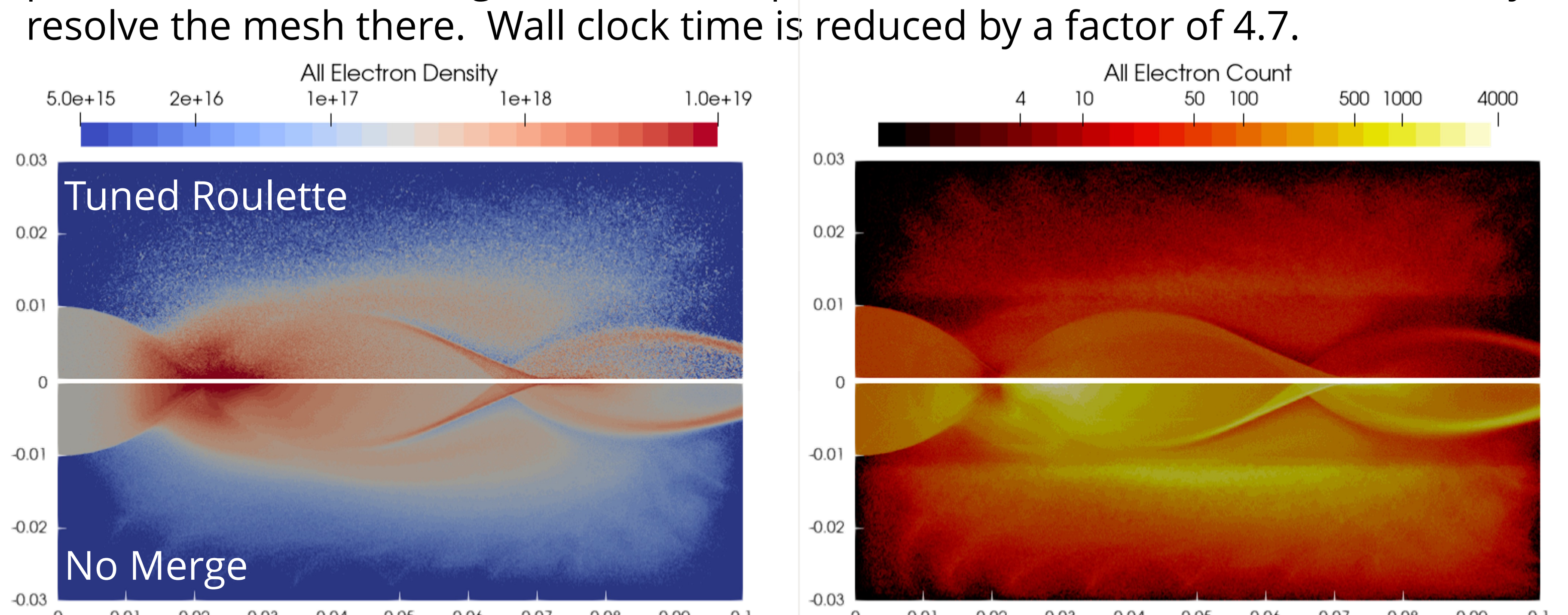
We model electron beams fired into a background gas using Sandia's plasma simulation code EMPIRE [1], which implements Direct Simulation Monte Carlo [2] collisions. In order to resolve the beam and the ions and electrons that appear due to its collisions with the background, the low-density electrons use a different macroparticle weight than the neutrals. Collisions between different-weight particles cause particle counts to grow very quickly if not constrained by, e.g., a merge. We have implemented a number of merges and here we present results for an extremely simple Roulette merge and a complex Distribution Resample merge. **Surprisingly, the Roulette merge performs extremely well, even though it does not conserve the spatial charge distribution and only conserves momentum and energy in the ensemble rather than exactly.** It compares favorably to the Distribution Resample merge and also to a momentum- and energy-conserving M-to-2 merge (not shown).

Roulette Merge:

We keep the Roulette Merge as simple as possible. To merge M particles down to N particles, we randomly assign M/N particles to each of N bins. Within each bin, one particle is chosen with probability proportional to its weight. Then its weight is changed to the total weight of the bin and the remaining particles are deleted. The only moment of the spatial and velocity distribution functions which is conserved exactly is mass. No other moment is exactly conserved, although *every* moment is conserved in expectation. More details and examples can be found in [4].



The Roulette Merge preserves important features although there is noise far from the symmetry plane and past the second pinch point. The number of particles per element is reduced significantly, in some cases from thousands to about one hundred. The number of particles at the second pinch point is a particular problem for the No Merge case; we can predict the location of the first and finely resolve the mesh there. Wall clock time is reduced by a factor of 4.7.



Tuning by distinguishing generations of electrons does not significantly affect the physical accuracy of the Roulette Merge. It is slightly less aggressive and there are more particles far from the symmetry plane. Wall clock time is still reduced by a factor of 4.1.

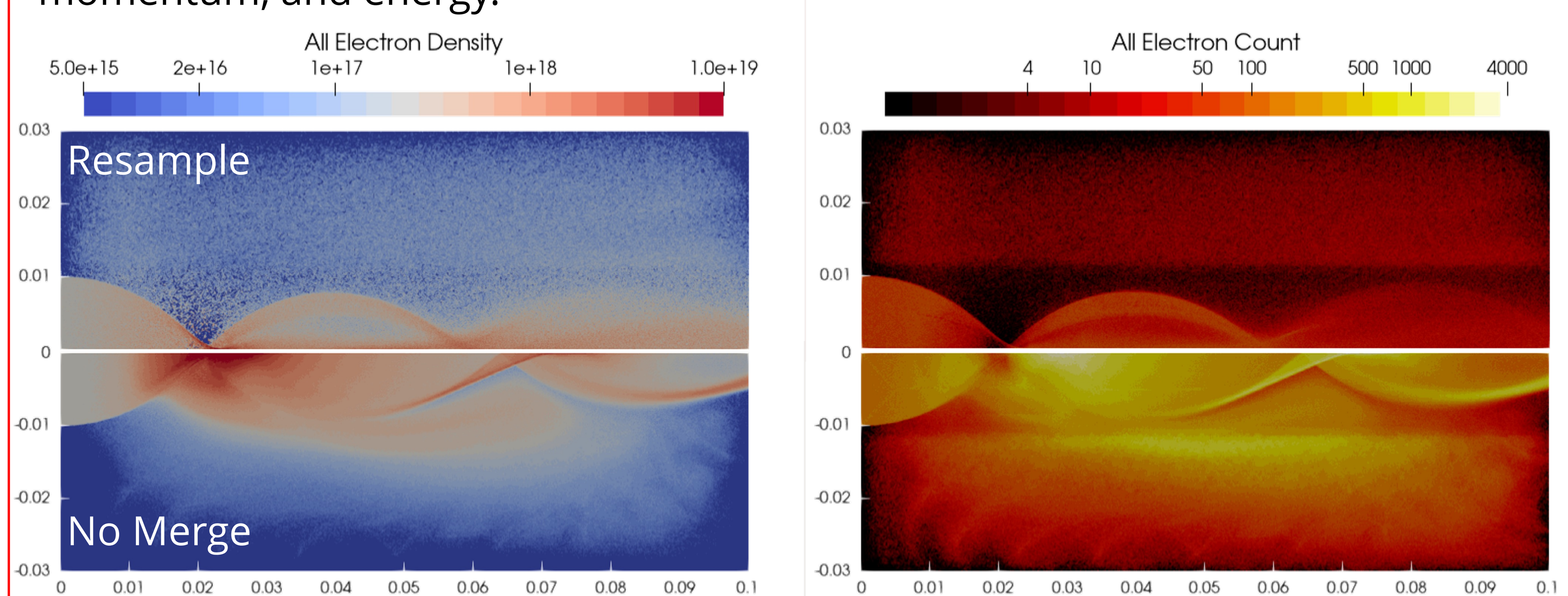
[1] Bettencourt et al., "Empire-PIC: A Performance Portable Unstructured Particle-in-Cell Code", Communications in Computational Physics, 2021.
[2] Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, 1994.
[3] Medina et al., "Verification and Benchmarking Relativistic Electron Beam Transport Through a Background Gas", Computer Physics Communication, 2023.
[4] McDoniel and Moore, "Roulette Merge With Variable Weights", 2023 Santa Fe DSMC Workshop.
[5] Watrous et al., "SGEMP Algorithm Development and Demonstration for ICEPIC", Technical Report SAND2019-3165, 2019.
[6] Welch et al., "Adaptive Particle Management in a Particle-in-Cell Code", Journal of Computational Physics, 2007.

Electrons are injected from the left wall at 500 keV and 180 kA per meter of depth into an argon background at a number density of 2.47×10^{21} m^{-3}, similar to simulations in [3]. Only ionizing collisions between the electrons and the background are considered. We run the simulation to 30 ns when the beam has developed two pinch points as shown below. We do this without any particle merge, and compare electron number density and computational particles per element to results from the Roulette Merge and from the Distribution Resample Merge. The mesh is refined where we expect the first pinch point and becomes coarser far from the symmetry plane.

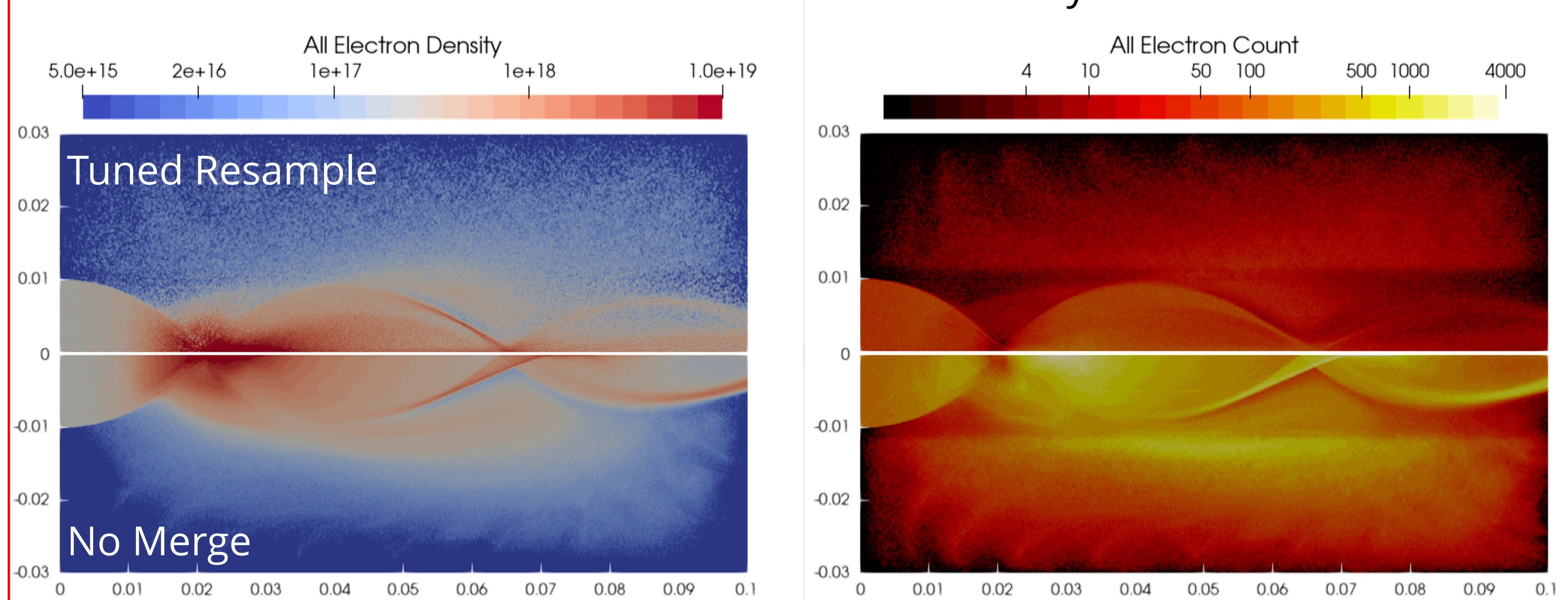
After running these merges in their simplest configuration, we tune them to the problem by separately merging the primary beam electrons and each generation of secondaries.

Distribution Resample Merge:

The Distribution Resample Merge was originally developed for the Emphasis code and uses a complex algorithm described in [5][6]. It seeks to identify a subset of the particle mass which is approximately Maxwellian, then it removes that mass from the particles and resamples new, weightier particles from a Maxwell distribution. It conserves the projected charge on mesh nodes as well as mass, momentum, and energy.



The Distribution Resample Merge fails to preserve important features such as the current density distribution on the right wall, and the second pinch point has moved, but the number of particles per element is significantly reduced. The merge struggles when asked to reduce the combined population of beam electrons and secondaries. Wall clock time is reduced by a factor of 3.8.



Tuning visibly improves the physical accuracy of the Distribution Resample Merge. The location of the second pinch point is more accurately reproduced, the secondary electron envelope above it is present although weaker than in the No Merge case, and the beam has a distinct though weak edge after the second pinch point. Wall clock time is reduced by a factor of 4.6.

Both merge schemes significantly reduce the number of particles in the simulation and therefore the total runtime required. The Roulette Merge, despite its simplicity and merely on-average conservation, accurately captures visible features of the beam simulation at the cost of only slightly increased noise. The Distribution Resample Merge does not perform well out of the box, but is much improved with some simple tuning. More problem-specific tuning would be necessary for an adequate engineering result, but it is hard to know how to tune without No Merge results to compare against.

With enough particles per element, further optimizations such as seeking to merge neighbors in velocity space and attempting to control post-merge weight distributions are promising.

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