Fragmentation, Merging, and Internal Dynamics for PIC Simulation with Finite Size Particles

Dennis W. Hewett and David J. Larson
AX-Division
Lawrence Livermore National Laboratory
Livermore, CA 94550

Abstract

Components of a new type of "smart PIC" algorithm, intended to bridge the gap between Eulerian fluid regimes and kinetic regimes, are developed. Enlarging the scope of PIC, the CPK method (Complex Particle Kinetic) concept uses an ensemble of small, fluid-like macro-particles to represent particle distributions in phase space. These macro-particles are Gaussian-shaped in both position and velocity compared to the phase-space delta functions used in standard PIC and the spatial "sugar cube" particles used in an early version of this model. Time evolution is modeled by a combination of the Lagrangian motion and internal evolution within each individual macro-particle. An analytic term is added to each particle's shape that represents internal evolution consistent with the collision-less, free-streaming of each macro-particle. Collision-dominated, γ–law gas internal evolution is also developed to define the opposite limit of collisionality. Similar to our initial effort, macro-particles are aggressively fragmented in phase space to probe for emerging kinetic features and aggressively merged, for economy, if interesting features fail to materialize. With CPK, fragmentation in both position and velocity space can be accomplished without loss of significant phase space information. Fragmentation preserves the kinetic capabilities of PIC; merging dramatically shrinks the number of particles in non-kinetic or collisional regions. In collision-dominated regimes, merging naturally produces a few Lagrangian particles that act much as nodes in Free-Lagrangian hydrodynamics. The only interaction between neutral particles is through merging; no mesh-dependent pressure gradients are needed. Finally, a linked-list data structure significantly reduces time spent "sorting" nearest neighbors for potential merging--and should lead to straightforward MPP operation.