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Thermal Lattice Boltzmann Simulations for Multi-Species Fluid Equilibration

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One of the goals of divertor physics is to model the interaction between neutrals and the plasma by a coupled UEDGE/Navier-Stokes system of solvers. An inverse statistical mechanics approach is to replace these highly nonlinear two-fluid macroscopic equations by two coupled linear lattice BGK kinetic equations – which, in the Chapman-Enskog limit, will recover the original nonlinear two-fluid system. While the dimensionality has been increased from (x, t) to the kinetic phase space, the thermal lattice Boltzmann (TLBM) approach seeks to minimize (and discretize) the required degrees of freedom that must be preserved in ξ -space. For example, on a 2D hexagonal lattice one can recover the nonlinear conservation equation of mass, momentum and energy with just 13 bits of ξ -space information for each spatial grid point. Thus while the storage requirements for TLBM is increased by a factor of 3 over conventional CFD, there are substantial computational gains by moving to this linear kinetic representation: (a) Lagrangian free-streaming kinetic codes will local operations, and (b) the avoidance of the nonlinear Riemann problem of CFD. The immediate parallelization and vectorization of TLBM codes makes them ideal for multi-PE platforms like T3E. There are also physics reasons for pursuing this kinetic imbedding. In the tokamak divertor one encounters time varying regimes in which the neutral collisionalities range from the highly collisional (and hence fluid regime) to the weakly collisional (well treated by Monte Carlo methods). The coupling of fluid-kinetic does is a numerically stiff problem. However, by replacing the fluid representation by TLBM, one will be coupling two kinetic codes with non-disparate length and time scales.

Here we shall present some 2D thermal simulations of interacting double shear layers in two species system with mass ratios of 10 and density ratios of 3. As expected, the shear layers in the lighter species break up into vortices first. These layers soon lose their identity – while for the heavier species the vortex layers retain their identity. The merging vortices of the lighter species are rotated into planes parallel to the heavier species vortex layers which are themselves dominated by 2 large vortices within the layers. The equilibration of the temperature differences in the two species is about 3.3 times that for the mean velocity difference equilibration – in good agreement with theoretical estimates.

Particle-in-Cell Simulation of Plasma Immersion Ion Implantation (PIII) of Industrial Gears

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Plasma immersion ion implantation (PIII) has emulates conventional beam-line ion implantation in that the implantation time is independent of the sample size and large industrial components of an irregular shape can be treated relatively easily due to its non-line-of-sight characteristic. For example, due to the non-planar and periodic structure of industrial gears, conventional deposition and beam-line treatment techniques are not easily implemented. In addition, as they are used in space, typically as a component in a satellite, conventional coatings may not function desirably either, and PIII is the ideal technique in this case. In this work, we employ a theoretical model to investigate the PIII process of this important industrial component. To simulate implantation into the three-dimensional structure of a commercial gear, we work in cylindrical coordinates. Due to the periodic structure of the saw-teeth, we only need to simulate the volume of one tooth. 2D simulation along the $(r-\theta)$ plane is carried out by the particle-in-cell (PIC) method. The incident dose and impact angle along the surface of the tooth are derived and our results indicate that a long implantation pulse will implant more ions at the bottom of tooth at normal angle since the momentum of the incoming ions accelerated at the middle and end period of the pulse will overcome the attractive force from the sidewall of the tooth. Therefore, shorter pulse duration will implant the whole surface of the tooth more uniformly. We will also provide an estimation on the preferred pulse duration for different tooth dimensions.