PROGRESS SIMULATING LOW TEMPERATURE COLLISIONAL PLASMAS WITH A PIC-DSMC METHOD

*Matthew M. Hopkins¹, Paul S. Crozier², Russell Hooper³, Polly L. Hopkins¹, Steven J. Plimpton⁴, and Alan B. Williams⁵

¹ Nanoscale and Reactive	² Multiscale Dynamic Material	³ Applied Math and
Processes, Sandia National	Modeling, Sandia National	Applications, Sandia National
Laboratories [†] , M.S. 0836, P.O.	Laboratories [†] , M.S. 1322,	Laboratories [†] , M.S. 1318,
Box 5800, Albuquerque, NM	P.O. Box 5800, Albuquerque,	P.O. Box 5800, Albuquerque,
87185-0836, USA	NM 87185-1322, USA	NM 87185-1318, USA
mmhopki@sandia.gov	pscrozi@sandia.gov	rhoope@sandia.gov
⁴ Scalable Algorithms, Sandia ⁵ Computational Thermal and National Laboratories [†] M S Eluid Mechanics, Sandia		
		* * > 5 @

1316, P.O. Box 5800, Albuquerque, NM 87185-1316, USA sjplimp@sandia.gov ⁵Computational Thermal and Fluid Mechanics, Sandia National Laboratories[†], M.S. 0382, P.O. Box 5800, Albuquerque, NM 87185-0382, USA william@sandia.gov

Key Words: Plasmas, Computational methods, Parallel, DSMC, PIC.

ABSTRACT

In this work we will present the current state of our low temperature plasma simulation code, Aleph. Its target application regime is low temperature plasmas that straddle the non-continuum to continuum regime, specifically including collisional effects and chemistry. Of particular importance to us is that the code be production quality, applicable to industrial problems. In pursuit of that goal, Aleph is based on unstructured meshes, is massively parallel, and includes dynamic load balancing.

Our plasma model consists of weighted particles for each constituent present (ions and neutrals of differing species, and electrons) coupled to an electrostatic (ES) field. The ES field is computed via the finite element method (FEM) every time step by aggregating particle charges on an element-by-element basis. Particles within an element interpolate the electric field to their position for use in the particle move algorithm. Thus, we are performing a very simple particle-in-cell (PIC) simulation. Subsequent to particle moves, collisions are accounted for via a direct simulation Monte Carlo (DSMC) method. And subsequent to collisions, chemistry events are accounted for. Of special relevance to plasma simulation is charge exchange.

To address realistic problems, we operate on 3D unstructured meshes in a massively parallel environment (to thousands of processors). To improve scaling of the overall

[†] Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

method we employ advanced solvers (including preconditioning) and dynamic load balancing. Because the mesh decomposition that optimally balances the FEM is in general different from the one that optimally balances particle calculations, we use multiple decompositions of the same mesh.

This presentation will relate our experiences in applying the simulation technique to test and application problems, including scaling efficiency and the impact of improvements to solving the coupled particle/field problem.

REFERENCES

- [1] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Clarendon, 1994.
- [2] C. K. Birdsall and A. B. Langdon, *Plasma Physics via Computer Simulation*, McGraw-Hill, 1985.
- [3] R. W. Hockney and J. W. Eastwood, *Computer Simulation Using Particles*, Institute of Physics Publishing, 1988.
- [4] J.-S. Wu, K.-H. Hsu, F.-L. Li, C.-T. Hung, and S.-Y. Jou, "Development of a parallelized 3D electrostatic PIC-FEM code and its applications", *Comput. Phys. Comm.*, vol. **177**, pp. 98-101, (2007).