SAND2016-10074C

Exceptional service in the national interest

Sandia National Laboratories

Evaluation of the Aleph PIC Code on Benchmark Simulations

Jeremiah J. Boerner, Jose L. Pacheco, and Anne M. Grillet,
Sandia National Laboratories, Albuquerque, New Mexico, USA

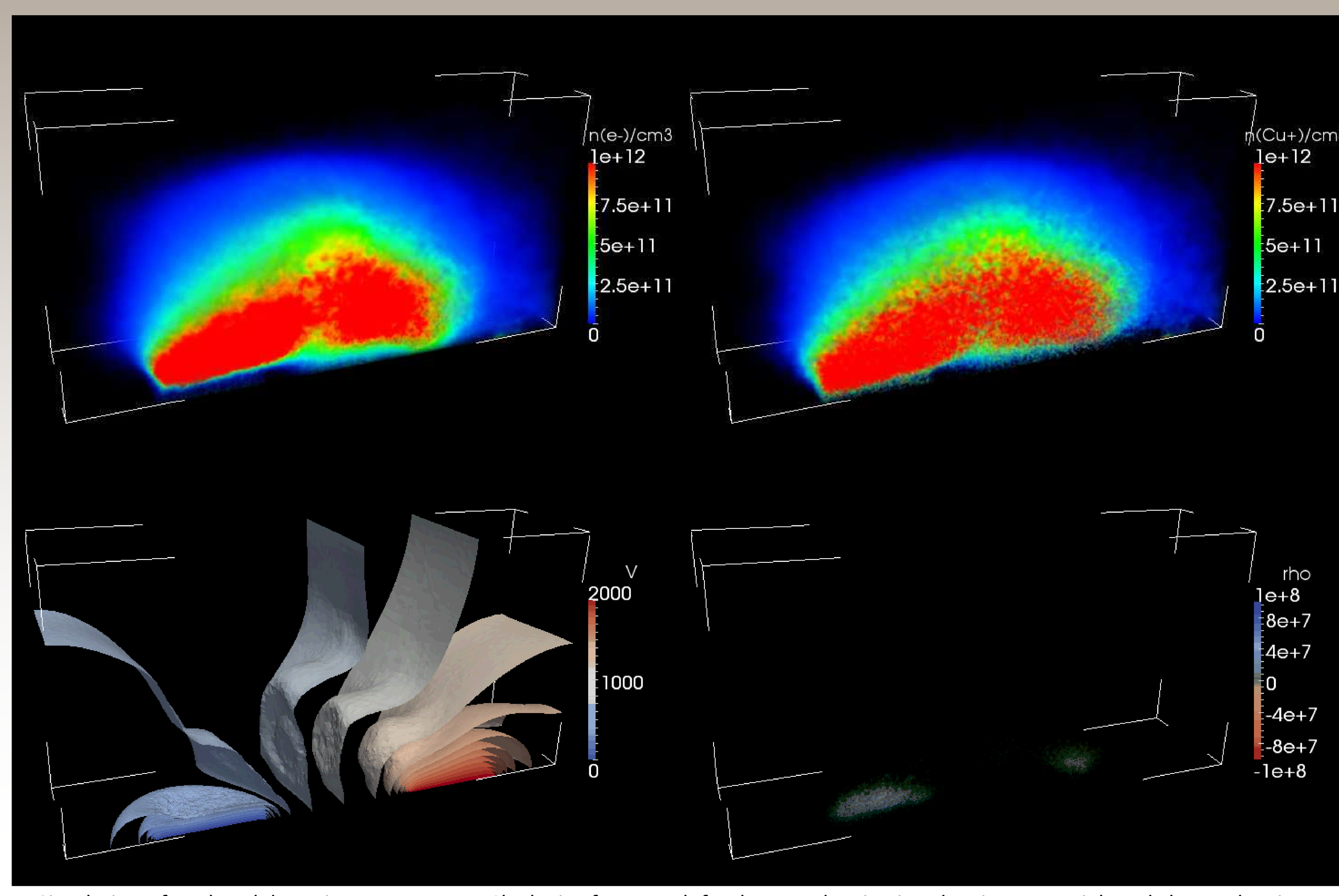
Aleph Capabilities

Numerical models

- Aleph version 1.1 in preparation, v1.0 released June 2014
- Particle-In-Cell methods for kinetic particle moves
- Finite element method for Poisson electrostatic field solves
- Direct Simulation Monte Carlo (DSMC) collisions
- 1D, 2D, 2D axisymmetric, and 3D- unstructured meshes
- Dual mesh concept for PIC model and for output
- Massively parallel, up to 64K processors or ~1B elements
- Dynamic load balancing improves parallel efficiency
- Dynamic particle reweighting adapts to density evolution
- Full restart with all particles, fields, and outputs
- Extensive verification and validation in regression suite

Physical models

- Elastic, Coulomb, excitation, ionization, reaction collisions
- Thermal and electrical emission models for electrodes
- External circuit models for potential and current BCs
- Ambipolar and Boltzmann approximations for electrons
- Photon emission, absorption, reactions, and spectra



Simulation of arc breakdown in copper vapor. Clockwise from top left: electron density, ion density, potential, and charge density. From M. M. Hopkins et al., "Challenges to Simulating Vacuum Arc Discharge", 31st ICPIG, Granada, Spain, 2013.

Research Directions

Aleph is intended for general purpose modeling of low temperature plasma applications, and is presently being used at Sandia to investigate:

- Arc breakdown in triggered vacuum gap switches
- Arc breakdown in atmospheric pressure gaps
- Ion beam extraction and transport from a source plasma
- Sheath structure in glow discharge of differing polarities
- Collisional excitation and UV generation in microcavities

Aleph is also well suited to explore topics relevant to numerical modeling.

- Solution convergence in dx, dt, and particle weight
- Uncertainty quantification and error estimation

Here Aleph is used to simulate a series of canonical plasma physics problems in order to verify its performance. These are proposed as benchmark problems in the literature, and are considered fundamental and well characterized, with complete specification of the numerical models and numerical parameters.

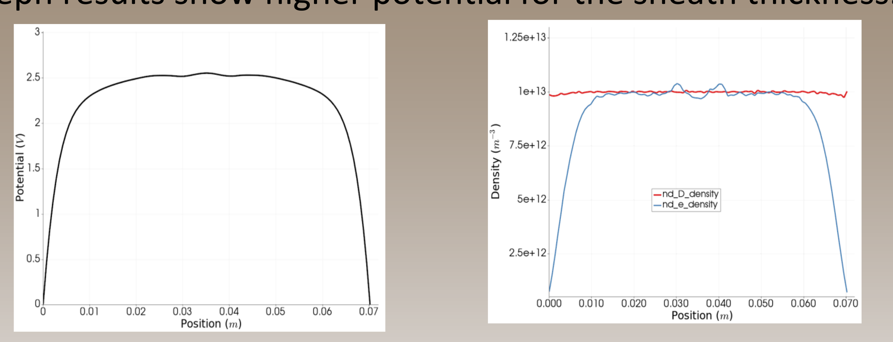
Electrostatic Sheath

The undriven electrostatic sheath tests the self-consistent Poisson field solver and particle push algorithms. Fixed ions provide a background of positive charge and electrons move through the domain. Sheaths develop as electrons escape at the boundaries, until space charge confines the remaining electrons.

Aleph simulations yield instant values for potential that appear 4-5% higher than expected, with residual fields throughout the plasma region. Potential fluctuations in the quasineutral region are of a similar magnitude. The sheath thicknesses appear to match well at ~10 mm.

The benchmark reference provides good guidance on the initial plasma conditions, but does not specify the cell size, time step or any averaging.

Aleph results show higher potential for the sheath thickness.



Benchmark results from: A. J. Christlieb et al., IEEE Trans. Plas. Sci, Vol. 34, No. 2, p. 149, April 2006

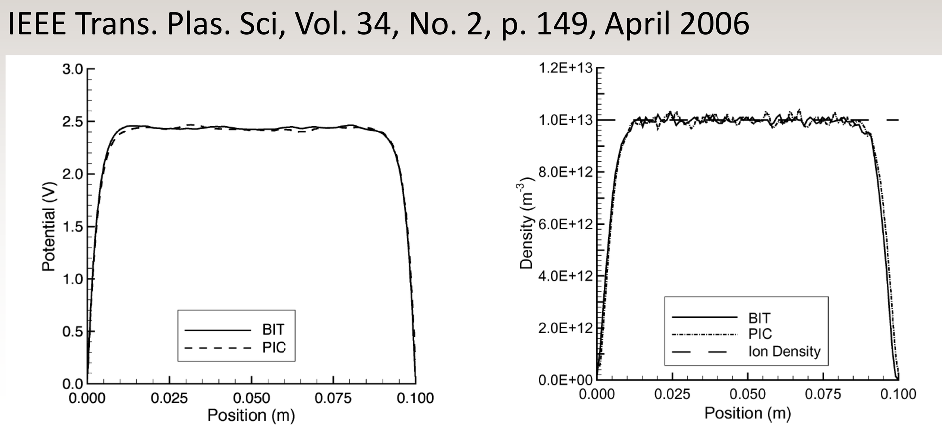


Fig. 7. Potential Φ as a function of position across domain for BIT and PIC. Fig. 8. Electron density for BIT and PIC. Ion density is also shown.

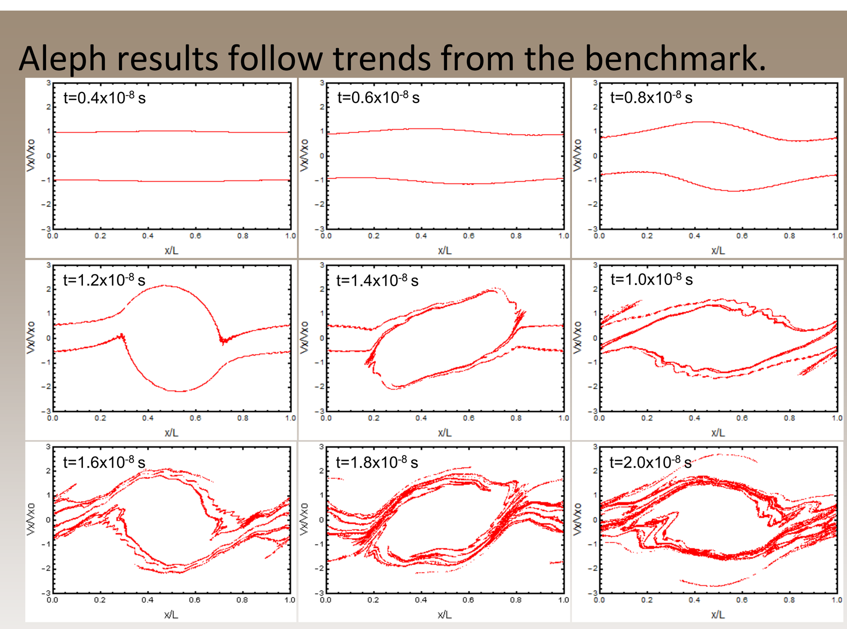
Two-stream Instability

This a more detailed test of field solver and particle push algorithms. Two cold, counter-streaming electron beams propagate in a periodic domain and fixed ions provide a background of positive charge. The beam speeds are perturbed in space, and this grows through linear and nonlinear phases. Over time, the electron VDFs form filaments and roll up in phase space.

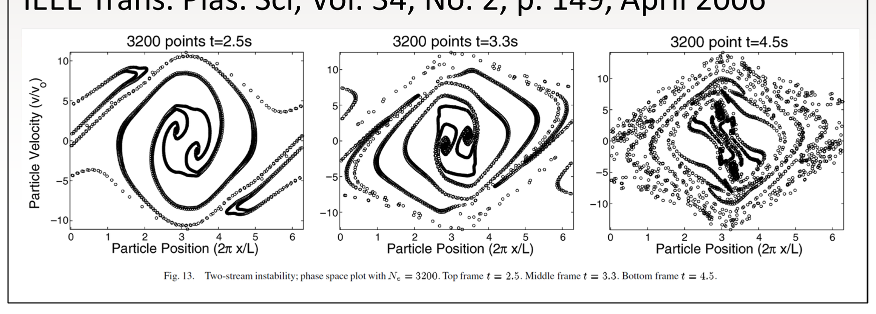
Aleph results are obtained at higher density (1×10^{13} m^{-3}) than the benchmark (4×10^{12} m^{-3}). The evolution of the phase space plots show similar trends, but the maximum speeds and details of the structure are markedly different.

A critical difference is that the benchmark reference uses non-dimensional domain length based on the wavelength of the perturbation, and non-dimensional time step based on the ratio of the cell size to the initial beam speed. However, this scaling does not hold across different plasma densities. Debye length and the plasma frequency are likely better choices for normalizing the plasma parameters.

Aleph results follow trends from the benchmark.



Benchmark results from: A. J. Christlieb et al., IEEE Trans. Plas. Sci, Vol. 34, No. 2, p. 149, April 2006

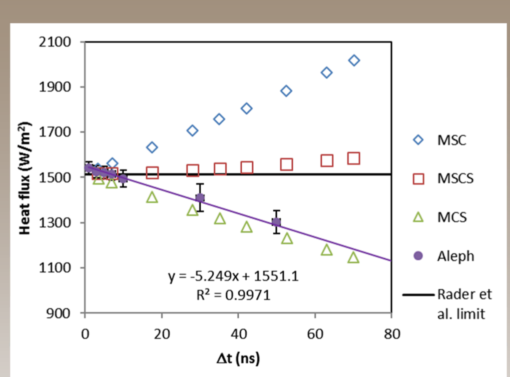


Fourier Heat Transfer

Heat transfer in kinetic simulations is mediated by particle collisions. Here 2 Torr of neutral argon is held between plates at 223 K and 323 K. Particles undergo diffuse reflection with thermal accommodation at surfaces and VHS collisions in the gap. A temperature gradient develops in the gas, and heat flux across the gap is computed.

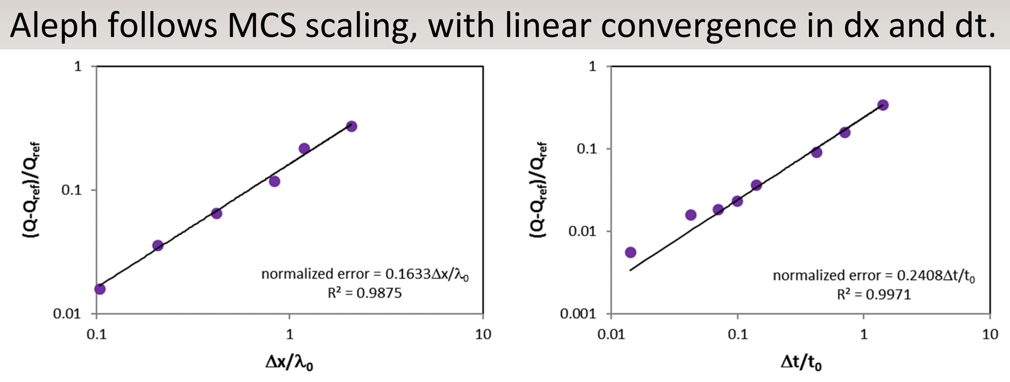
Aleph converges to a limiting value of heat flux that is 2-3% (or 30-50 W/m^2) higher than the benchmark value. Stochastic fluctuations in the heat flux are a similar magnitude (+/- 50 W/m^2).

The heat flux is computed from particle velocities in the gap and is sensitive to variation in the bulk velocity. Computing the heat flux by accumulating the change in particle kinetic energy at the surface could yield smaller fluctuations.



The order of operations affects solution convergence in DSMC. MSC (move-sample-collide) and MCS (move-collide-sample) respectively converge down and up to the limiting value as the time step is decreased.

Aleph follows MCS scaling, with linear convergence in dx and dt.



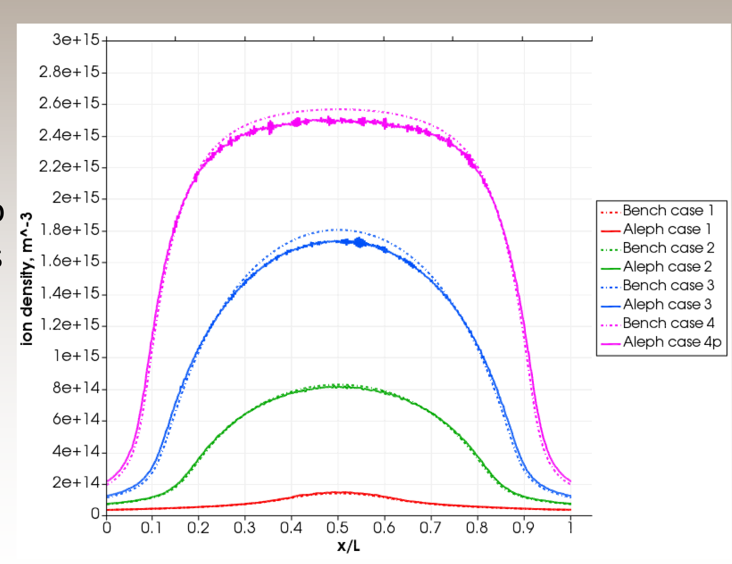
Benchmark results from: D. J. Rader et al., Phys. Fluids Vol. 18, N. 077102, 2006, http://dx.doi.org/10.1063/1.2213640

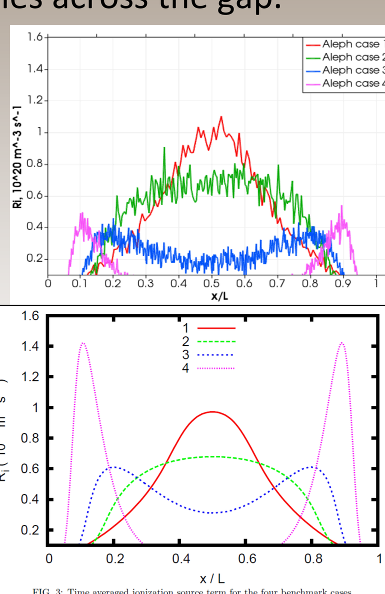
RF Discharge

A typical discharge requires coupling all the physics in the previous problems. Here a 13.56 MHz sine wave voltage is applied between two surfaces, with high pressure neutral helium at 300 K and a seed plasma of helium ions and electrons in the gap. Electron impacts can ionize more helium, while neutral collisions with electrons or ions mediate the plasma transport. Averaging over 32 cycles yields ion and electron density profiles across the gap.

Results are shown for four cases with increasing collisionality. At low pressures (case 1 at 0.03 Torr and case 2 at 0.1 Torr) Aleph reproduces the benchmark results to within stochastic noise. At higher pressures (case 3 at 0.3 Torr and case 4 at 1.0 Torr) Aleph under predicts the density by 4-5%.

The discrepancy may be due to differences in ionization rate across the domain. The Aleph instant values are significantly lower than the benchmark average values. This may be due to under sampling the number of possible collision pairs in each cell.





Benchmark results from: M. M. Turner et al., Phys. Plasmas Vol. 20, N. 013507, 2013, http://dx.doi.org/10.1063/1.4775084

Discussion

Even well-characterized benchmark problems like those shown above are challenging to reproduce solely from the literature. There is a tendency to identify the physical parameters or the numerical parameters of a simulation, but not both. Similarly, the outputs are often reduced to values or quantities that are easily displayed, but difficult to compare without tabulated values.

One item not addressed here is that there are few or no benchmark problems between the "textbook" problems and the typical "application" problem. More systematic verification problems are desired that progressively relax simplifying assumptions to move from a demonstration to an application. For example, consider DSMC collisions. A more thorough benchmark might begin with constant cross sections and cold beams, and then proceed to variable cross sections with cold beams, then variable cross sections with thermal populations, and finally a Fourier problem. Documenting this sequential approach builds confidence in each aspect of the coupled models.

It is recommended that future benchmark problems include more complete inputs and outputs as supplementary materials. The RF discharge problem described by Turner et al. is an example of an effective compromise. The input collision cross sections and output ion and electron densities are available for download as data files. Tables in the appendix describe the plasma and numerical parameters, both in formulas and explicit values. Making these available lends more confidence that inputs to a benchmark are accurately reproduced in a new simulation.

Conclusions

The Aleph simulation code demonstrates good qualitative agreement over all four benchmark problems posed today, with generally good quantitative agreement. Discrepancies at high collisionality require further investigation.

Well-characterized benchmark problems are critical for verification of modeling tools. New benchmarks should:

1) Incorporate results that demonstrate concordance among multiple models or codes.
2) Archive input data files and key outputs as supplementary data during publication.
3) Develop sequential benchmarks to progressively demonstrate a model capability.

Acknowledgements: These efforts are built on many years of contributions from a diverse team, including: Matt Hopkins, Russell Hooper, Paul Crozier, Larry Musson, Chris Moore, Stan Moore, Greg Weirs, Ed Barnat and more.