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ADVANCED PARTICLE-IN-CELL TECHNIQUES FOR PULSED POWER DEVICE AND HEDP SIMULATION *

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Abstract

Understanding the operation of pulse power systems and components, magnetically insulated transmission lines (MITLs), plasma accelerators and high power diodes require accurate modeling of evolving electron flow and plasma motion. Challenges include gas breakdown, surface physics, high energy density plasma, interaction of energetic particles with surfaces, and complex geometries. In this paper, we will discuss the new capabilities and discuss the enabling algorithms.

I. INTRODUCTION

Realistic and accurate modeling of power flow in pulsed power systems including components, magnetically insulated transmission lines (MITLs), plasma accelerators and high power diodes is required to meet future needs for high energy density (HED) experiments. The physics involved includes gas breakdown, surface physics, high energy density plasma (HEDP), interaction of energetic particles with surfaces, and complex geometries. The sheer size of the current and planned pulsed power systems demands efficient massively parallel algorithms to follow the details of the power flow from capacitors to load. Accurate representations of complex shapes are necessary for calculation of field stresses and electron sheath motion. The ultimate goal is the development of virtual 3D accelerators which aid in the design and mitigate risk of future machines.

As these systems become increasingly more powerful, unwanted plasma dynamics can affect power flow. The production and evolution of electrode plasmas in magnetically-insulated transmission lines (MITL), plasma accelerators, and high power diodes is critical to the understanding of the operating characteristics of these devices as well as establishing scaling relations for reliable extrapolation to higher voltages. In typical pulsed power diodes with large area cathodes, electrode plasma velocities are of order 1--3 cm/μs.[1] Modeling of high density electrode plasmas is difficult given the larger range of densities from solid density (~10^{23} cm^{-3}) at the surface to that expected in monopolar flow and MITL vacuum flow (~10^{13} cm^{-3}). In such regimes, the assumption of quasi-neutrality is poor. Magnetohydrodynamics, while a powerful tool for many problems, is not applicable where sheath dynamics are dominant. Electromagnetic 2-fluid, hybrid (fluid-kinetic) and fully kinetic models yield increasing levels of accuracy.

The loads driven by the pulse power systems develop intense charged particle beams, radiation sources, and HED plasmas to interrogate matter and produce fusion energy. Tens of mega-ampere driver are being used on Z[2] to drive z-pinches for radiation and neutron production. To confine HED plasmas, plasma rail guns are being developed to produce Mach 20 plasma jets of > 10^{17} cm^{-3} density and 100 km/s velocity. The time and length scales of these devices are challenging for PIC codes.

Here, we discuss new particle-in-cell (PIC) techniques that enable more accurate simulation of these pulse power systems as well as their intense beam and HED plasma loads. Several unique algorithms have been developed for the hybrid particle-in-cell (PIC) simulation code LSP[3] to address these physical processes. For the simulation of pulsed power components, MITLs, and diodes, a locally conformal finite-difference algorithm for modeling three-dimensional perfectly conducting objects has been developed that for the first time includes charge particle emission and annihilation.[4] This cut-cell model removes most of the artifacts seen from stair stepping with orthogonal grids. Additionally, progress has been made in 3D modeling of pulse power systems including the Z

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machine and linear transformer drivers.[5] Significant progress has been made concerning the descriptions of plasmas evolving from electrodes,[6] produced in gas switches,[7] accelerated in plasma-jet guns,[8] confined in field reversed configuration,[9] and compressed in z-pinches.[10] Advance simulation techniques include detailed kinetic breakdown physics, surface interaction, and equation of state. For HEDP, more general algorithms for radiation transport and laser injection, fusion reactions and fusion-product transport algorithms have been developed.

II. SIMULATION MODEL OF VIRTUAL ACCELERATORS

Large scale virtual accelerators, including the ZR accelerator and LTD systems for z-pinch and radiographic loads, have been simulated. For example, the ZR model was composed of two parts: a 3D EM simulation region modeling the oil and water sections and a transmission-line region that models the vacuum sections. These two parts were dynamically coupled within the LSP model. The simulations were carried out in 3D cylindrical coordinates to model the ZR accelerator (the coordinate system changes to Cartesian at large radius to avoid stair steps). Models for the evolution of conductivity were used for gas and water switches. 1D transmission lines carry the power from the 3D grid at the insulator stack to the MITLs. Several computational techniques were developed to complete these large-scale simulations. These include the development of a technique to change the coordinate system of the underlying mesh from cylindrical to Cartesian at a predetermined radius, and a model for reducing non-TEM modes at the junction between the 3D PIC grid and the 1D transmission-line model. Comparison with various currents measurements validated the model.

Recently, a new technique for conformal representation of curved surfaces was developed that includes particles emission and absorption. The partial cell method makes use of the Dey-Mittra algorithm adapted to implicit electromagnetic solvers. The general management of particles in partial cells requires additional parameters associated with those cells that are precalculated and stored for later use. In addition to the values previously mentioned which are used in the field solution, the correct handling of the particles involves the following quantities: coordinate values that describe the center of the surface spanning the cell, the surface normal vector at that point, and the surface area. At any given point during the simulation, a particle can be tested after it has undergone incremental motion to determine if it should be absorbed in the conductor by constructing a vector from the surface center to the particle position and dotting this with the surface normal vector. If the value of this operation is negative, the particle is made to finish its ‘‘deferred’’ currents through the conductor and then destroyed.

Conversely, during field emission, the particle's weight is determined by the electric field strength at the surface and the saved surface area associated with the cell, and is placed on the surface after contributing to the currents due to the motion from an underlying whole conductor cell. This treatment works well without being exact and is necessary because for 3D simulations an exact formulation of current depositions cannot, in general, be implemented, as previously mentioned.

A simple example involves a 7 MA diode with a 1-cm ball cathode and a gas focusing cell (3 Torr neutral N_2). With the typical stair stepped representation of the ball surface, discrete streams of electrons develop and remain through the gas cell [see Figure 1(a)]. Using the new partial cell algorithm in (b), these numerical artifacts are avoided yielding 10x smaller density fluctuations at the focus.

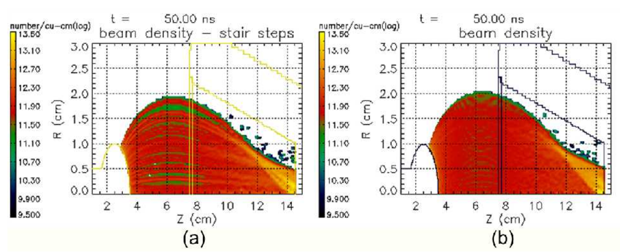


Figure 1. The simulation of a ball cathode 7-MV diode with focusing cell at z = 7.5 cm us shown. In (a), the ball was modeled with stair steps and in (b) with the new partial cell model.

III. HYBRID FLUID-KINETIC ALGORITHM

To improve understanding of plasma behavior with a co-axial gun, MITL, and diode, simulation techniques must be capable of accurately modeling the production and evolution of surface-contaminant plasmas as well as modeling the acceleration of energetic particles across the gap. The LSP simulation code makes use of a plasma injection technique that minimizes nonphysical sheath formation at the injection plane via a staged ionization of an injected neutral gas near the emitting electrode surfaces. The technique can be used in conjunction with a fluid or kinetic particle description. The electrode surface cells are initialized for plasma turn-on after a threshold field or temperature is exceeded or as a function of a thermal desorption model.

The fluid algorithm uses a Lagrangian push, Eulerian remap technique.[11] Fluid "particles" with associated mass, charge, and temperature begin a timestep on a grid node or corner. The equation of motion for the fluid particles is identical to that of kinetic particles except for scattering terms. A pressure gradient force term to model collisions within the given fluid, and a frictional force to model collisions with other particle species, are added to the equation of motion, i.e.,

$$mn_j \frac{dp_j}{dt} = qn_j \left(\mathbf{E} + \mathbf{v} \times \mathbf{B}\right) - \nabla P + mn_j \sum_i^I \gamma_j \nu_{ij} \left(u_i - u_j\right),$$

where the momentum $p_j = \gamma_j u_j / c$, P is the scalar pressure of species j, and ν_{ij} is the momentum transfer frequency between species i and j. For density n_i, velocity u_i, and temperature T_i, the new energy equation for an ideal gas is given by

$$\frac{3}{2} n_i \frac{dT_i}{dt} = -n_i T_i \nabla \cdot u_i + \sum_j \frac{2 m_i n_i}{m_j \tau_{ji}} (T_j - T_i) + \nabla \cdot \kappa \nabla T_i + \frac{3}{2} \sum_j \frac{\gamma_j \nu_{ji} m_j}{m_i + m_j} \left(u_i - u_j\right)^2,$$

where the right-hand-side terms are the *pdV*, energy exchange between species (τ_{ji} is the characteristic thermalization time between species j and i), thermal conduction (κ is the thermal conductivity), and Ohmic heating rate. Inelastic losses with neutrals can also be included. After fluid particles are advanced, their properties are interpolated back to the grid where the change in momentum and temperature (or internal energy) is calculated. This change is then interpolated back to each fluid particle where their internal quantities are updated. At the end of the time step, the fluid T, p, charge, and mass are once again remapped to the grid nodes where old particles are destroyed and new particles are constituted via linear interpolation. The remapped quantities include any new "ionized" particles and exclude particles that have transitioned to kinetic state. This technique naturally conserves all these quantities at the large time steps desired for dense thermal plasma modeling. IN addition to the ideal gas description, an equation of state can also be used.

In *dynamic* hybrid operation, LSP permits charged particles to be either fluid or kinetic. The default criterion for a fluid electron to become a kinetic one is that the particle's directed energy (½ mu^2) is much greater (10x greater) than its internal energy (3/2 kT, where k is the Boltzmann constant). For electrode plasma modeling, we find that an even simpler criterion for transition based on the magnitude of the fluid kinetic energy is sufficient. In the simulations presented here, we transition the particle when ½mu^2 reaches some fraction of the applied voltage. In the transition, the kinetic particle velocity u_k assumes the fluid particle velocity u_f with a thermal component added from sampling a Gaussian distribution in each direction, i.e., $u_k = u_f + \cos(2\pi r_1)\,(-2\ln(r_2)\,kT/m)^{1/2}$ where r_1 and r_2 are random numbers. In this way, the energy is conserved and momentum is statistically conserved over many particle transitions.

This technique has been used in the stress environment of a self-magnetic pinch diode where the operating condition observed in experiment have been explain via the hybrid simulations. In a 6.5 MV simulation of the SMP diode, the large density of ions near the top of the cathode increases the electron emission for large radius to anode-cathode gap.[12]

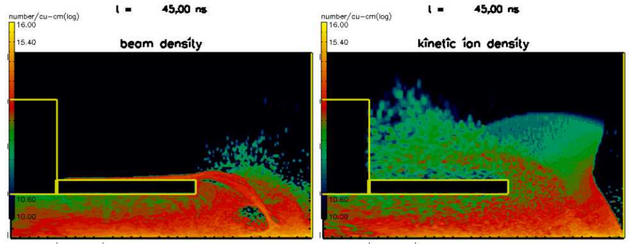
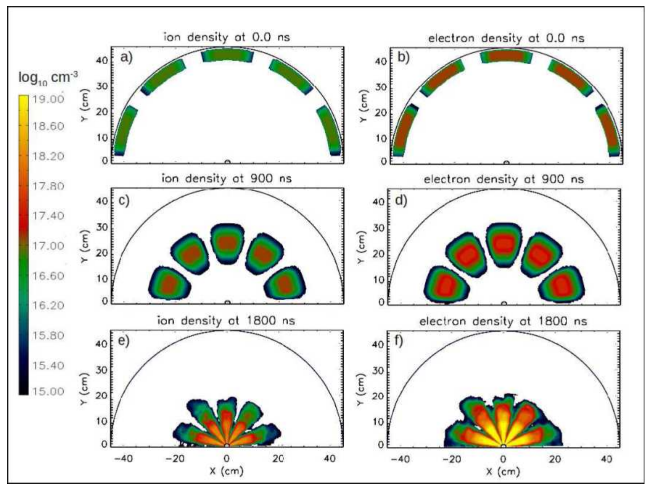


Figure 2. The (left) beam and (right) kinetic anode ion densities are plotted from a 6.5 MV SMP simulation after 45 ns.

We have also use the technique including an equation of state to simulate the transport and merging of energetic plasma jets. In the 2D spherical representation of the Plasma Liner eXperiment (PLX), five Mach 10, 2.8-eV temperature, 10^{17}-cm^{-3} density argon jets converge on axis. The electromagnetic simulation has fluid electrons and kinetic Ar ions with variable charge state.[13]



IV. ADVANCED IMPLICIT TECHNIQUE

. As plasma energy density increases, the numerical requirements on resolving both the plasma and cyclotron frequencies become severe. In low impedance pulse power components including convolutes, MITLs and z-pinch loads, resolving the cyclotron frequency Ω, is the most restrictive constraint on the explicit time step Δt. Errors of order $\Omega^2 \Delta t^2$ are incurred in modeling the particle orbits with explicit PIC leading to unphysical cyclotron radii. We have developed an algorithm that can greatly relax this constraint while maintaining accuracy while still maintaining the capability of under resolving the plasma frequency.

As described in the recent publication,**Error! Bookmark not defined.Error! Bookmark not defined.** the Magnetic Implicit (MI) technique does not employ approximations, but is an implicit (predictor-corrector) solution of the full Lorentz and EM equations. Thus, the accuracy of the particle advance is maintained in regions of small magnetic field as well large field. In our MI algorithm, the motion of a charged particle in electromagnetic fields centers the position and relativistic momentum variables of the particle at the same time level. The mirror force is added when the cyclotron orbits are under resolved. We recently have combined the field corrections of the direct-implicit technique to give an improved prediction of the future electric field and the capability of under resolving the plasma frequency. With the assumption that the magnetic field changes slowly, the susceptibility tensor $\langle \boldsymbol{S} \rangle$ accounts for the current density response of the particles $\delta \boldsymbol{J}$ to the electric field at the future time step, i.e., $\delta \boldsymbol{J} = \langle \boldsymbol{S} \rangle \cdot \delta \boldsymbol{E}$. These terms are added in an implicit electromagnetic field solve including $\delta \boldsymbol{J}$ for $\boldsymbol{E}^{n+1}$ electric fields at the future time step n+1,

$$\frac{\partial \boldsymbol{E}}{\partial t} = \nabla \times \boldsymbol{B} - \boldsymbol{J}^{n+1/2} - \langle \boldsymbol{S} \rangle \cdot \boldsymbol{E}^{n+1},$$

where $\boldsymbol{J}^{n+1/2}$ is the particle current density at the ½ step. We have benchmarked the algorithm against published results for a magnetic confinement device using rotating dipole fields to drive a field reversed configuration. The result is an algorithm with an enlarged region of both numerical accuracy and stability.

We have used the above algorithm to simulate the run down and pinch behavior of a dense plasma focus load. In the example, a 190-kA current (from the upper left) drives the acceleration of a D gas armature for 3 Torr pressure in a co-axial geometry. Gas breakdown is modeled with a Monte Carlo PIC treatment. Using fluid electron and kinetic D^+ description, high energy ions develop in 60 kV induced electric potentials. The ions accelerate due to JxB forces off the anode and pinch reaching 10^{19} cm^{-3} density and 30 keV temperature.

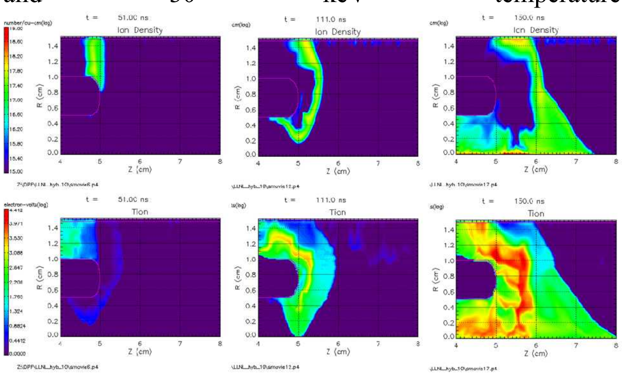


Figure 3. The ion density and temperature are plotted at 51, 111 and 150 ns into the simulation. A 190 kA current pulse is injected in the cylindrical geometry with the anode inner conductor.

IV. GAS SWITCH MODELING

Streamer and leader formation in high pressure devices such as a laser-triggered gas switch is a dynamic process involving a hierarchy of physical phenomena. These include elastic and inelastic particle collisions in the gas, radiation generation, transport and absorption, and electrode interactions. Accurate modeling of these physical processes is essential. We have developed a new 3D implicit particle-in-cell simulation model of gas breakdown leading to streamer formation in electronegative gases. The model uses a Monte Carlo treatment for all particle interactions and includes discrete photon generation, transport, and absorption for ultra-violet and soft x-ray radiation. Central to the realization of this fully kinetic particle treatment is an algorithm that manages the total particle count by species while preserving the local momentum distribution functions and conserving charge.[14] The simulation is fully electromagnetic, making it capable of following, for example, the evolution of a gas switch from the point of laser-induced localized breakdown of the gas between electrodes through the successive stages of streamer propagation, initial electrode current connection, and high-current conduction channel evolution where self-magnetic field effects are likely to be important.

For example a laser-produced plasma channel in 0.5-atm SF_6 of initial density 10^9 cm^{-3} is initialized in the simulation with a 115 kV/cm electric field.[15] The streamer propagates in both direction due to electron avalanche and photoelectric ionization.

VI. SUMMARY AND CONCLUSION

We have discussed several unique algorithms implemented in the hybrid PIC simulation code LSP to address the detailed physical processes in pulsed power applications. Example shown include large scale virtual accelerator modeling (for ZR) and intense beams (SMP diode), and HED plasma loads (z-pinch, DPF and plasma jet). For the simulation of pulsed power components, MITLs, and diodes, a locally conformal finite-difference algorithm for modeling three-dimensional perfectly conducting objects has been developed that includes charge particle emission and annihilation. Other techniques involve a new implicit algorithm that more accurately reproduces particle orbits for large time step, an advanced gas breakdown algorithm for laser-trigger gas cell modeling.

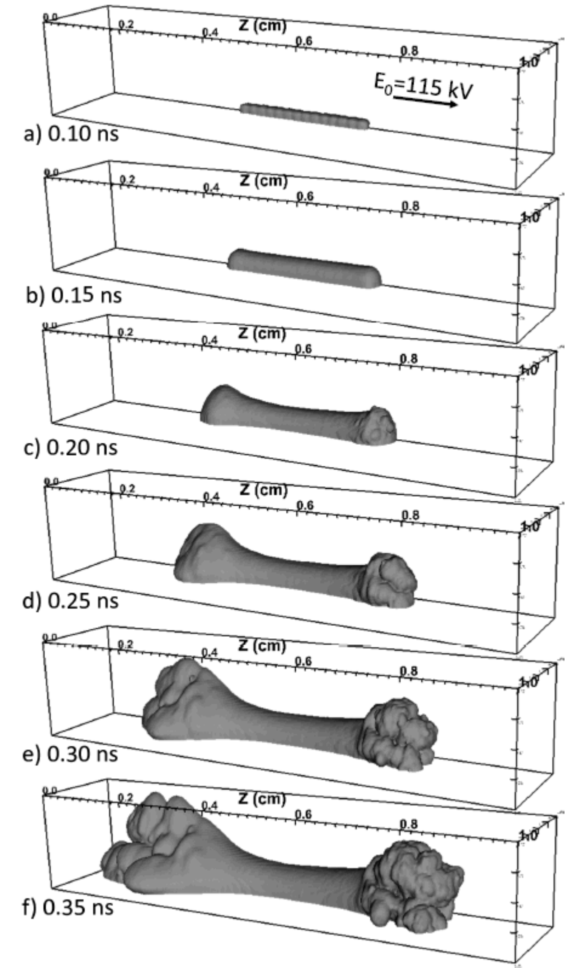


Figure 4. Isodensity contour plots of the evolving ion density of a plasma filament in a 3D simulation. All frames show the ion density contour for $n_i = 2\times10^{13}$ cm^{-3}. The first frame (top) is at t = 0.1 ns and the remaining frames are in 0.05 ns increments. The applied electric field of 115 kV/cm points to the right along the z axis.

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