Time Domain modeling of plasmas at RF time-scales

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Abstract. Results from tokamak experiments such as PPPL's NSTX indicate that significant anomalous power absorption can occur in the edge of the fusion plasma. Understanding of this phenomenon is a critical issue for analysis of RF heating scenarios on the ITER fusion experiment. Two probable edge absorption candidates, rf sheath losses and parametric decay instability, are both inherently non-linear, and likely to depend significantly on non-axisymmetric geometric detail in the vicinity of the antenna structures. Analysis of these phenomena is beyond the capabilities of existing axisymmetric frequency-domain linear-solvers used for analysis of heating and current drive in core fusion plasma, and so we are augmenting our analysis capability with the time-domain 3-D general-geometry electromagnetic and particle-in-cell simulation framework, Vorpal[1]. This framework is a modern object-oriented software package, which has demonstrated fast scalable operation on clusters of over 1000 cpu's, a necessity for this type of calculation. We have successfully introduced into this framework an implicit plasma solver[2], in order to accurately treat electromagnetic plasma wave characteristics in the wide range of plasma conditions occurring from edge plasma to core plasma, including situations where the plasma frequency is not resolvable at the rf time-scales of interest, and including sharp plasma resonances and cutoff behaviours common in the rf regime. We present benchmarking of this new plasma solver for 1-D, 2-D, and 3-D scenarios. We also discuss implementation plans for non-linear sheath boundary models, non-linear edge-plasma conditions leading to parametric decay, and also tracking of high-energy particles in core-heating scenarios, where issues of finite-banana-width effects and superadiabaticity remain outside the scope of the existing frequency-domain solvers.

1. Overview
In this paper we report on the implementation within the VORPAL software of the new time-domain plasma algorithm of Reference 2. Previous tests of the algorithm were done isolated from other software in order to assess and verify the predicted robustness and stability of the algorithm in a wide variety of circumstances, and benchmark the algorithms against the existing frequency domain solutions. Especially of interest was the algorithm’s performance at intermediate ion-time scales, where electron time-scales are unresolved by the temporal grid, but still included in a physically accurate manner for ion plasma waves. With promising results from these studies, we have proceeded with the installation of the model in an existing plasma simulation framework, VORPAL, which is more suitable for large-scale parallel computations on supercomputers.

This new software capability will augment existing large-scale frequency-domain parallel software within the SciDAC Center for Wave Plasma Interactions. Its inclusion in this project reflects, in part,
a new emerging appreciation for edge-related effects in rf heating of fusion experiments, particularly ITER, which is expected to have unique and challenging rf launching scenarios.

The purpose of the time-domain plasma algorithm is to provide accurate modeling through the transition from the vacuum wall’s very low densities through to the stronger densities inside the last closed flux surface. This transition contains a very rich variety of plasma wave phenomena, including hybrid and cyclotron resonances, their associated cutoffs, surface, whispering gallery, and coaxial modes, sheaths, and perhaps most important, very complex metallic and dielectric geometrical features. Furthermore, the combination of low plasma density and high power throughput provides conditions favorable to non-linear behaviors, most notably parametric decay instability (PDI). Indeed, evidence of up to 50% parasitic power loss in the edge has occurred in existing rf heating experiments, and is thought to be due to either sheath or PDI losses. Thus, the ultimate goal of this software is to provide design-quality prediction of the power balance associated with edge physics, complimenting the core power balance analysis provided by the existing frequency domain software within the project.

2. Time Domain Plasma Algorithm

The conditions in the edge region are extremely robust in terms of physics, but the plasma is essentially cold by comparison to the core, and this aspect of the edge provides the initial path by which the time-domain plasma model is progressing. The details of the algorithm are discussed in Reference 2, resulting in the following cold-plasma wave equations for perturbed electric field, $E$, magnetic field $B$, and plasma current, $J_s$, for species, $s$,

$$\frac{\partial}{\partial t}B = -\nabla \times E$$

$$\frac{\partial}{\partial t}E = -\varepsilon_0^{-1} \sum_{\text{species}} J_s + c^2 \nabla \times B$$

$$\{\partial t + v_s\}J_s = \varepsilon_0 \omega_{ps}^2 E - \Omega_s \times J_s$$

The key innovation in this implementation is the splitting of this time integration into the traditional explicit electromagnetic solve, and an implicit solve for the plasma currents. This splitting insures that the time-step is constrained by the traditional vacuum explicit electromagnetic Courant condition, and not by any cutoff or resonance condition within the plasma. Equally important is the computational implementation in such a manner that waves which are well resolved by mesh and time step have correct dispersion, including electron effects, even if the electron plasma and gyro frequencies are not well resolved. Reference 2 discusses issues associated with the meshing of these equations, and co-location of Yee-cell electric field components for the current evolution equation, and the discrete dispersion.

To date, all benchmarks have been done as linear problems, e.g., with $\omega_{ps}^2=q^2 n_s/(m_e \varepsilon_0)$ and $\Omega_s=(q/m_s)B_0$, in order to facilitate comparison to existing analysis and linear frequency domain solvers. However, the implementation of the algorithm within the VORPAL framework is such that the plasma frequency and gyro-frequency vector are updatable fields, analogous to $E$, $B$, and the $J_s$. Thus, nonlinearity is available simply by adding in a perturbed density update, from the continuity equation, $\partial t n_s = -\nabla \cdot J_s$, and utilizing $n_0 + n_s$ and $B_0 + B$ for the plasma and gyro frequencies.

Addition of thermal effects, e.g., sound waves and Bernstein waves, is expected in future implementations, but is not present to date. In order to accomplish this, it is expected that a pressure term such as $\nabla \alpha n_s$, with the term $\alpha$ yet to be determined, will be added to the current density evolution equation. In general, we are interested in wave physics at ion time scales and faster, so that the constant, $\alpha$, will be computed from a known form of the perturbed distribution function, e.g., $\int d^3v f_s(r,v)$, rather than from a truncation of fluid moment equations, such as is done for MHD and slower time scales. In addition, for magnetized plasma, the divergence and gradient operators in a thermal term, $\nabla \alpha n_s$, would split into very different parallel and perpendicular parts. Ultimately the goal would be to reproduce finite-Larmor wave character. However, treatment of effects such as
warm plasma temperature near resonance and all-orders Larmor physics would likely require particle representation of the plasma.

Installation of an effective sheath boundary condition is a more important priority. The challenge of the sheath is its very small length scale, as compared with the macroscopic scale of the edge geometry, $\Delta \ll \delta \chi$. A multiple-scale, e.g., sub-grid, model of the sheath is required for computational efficacy, and is illustrated in Figure 1. Considerable analytic work has resulted in an effective lossy capacitance sub-grid model which is intended to be used in the time-domain calculations. This model introduces an oscillating RF sheath potential, $\phi_{\text{sheath}}$, which represents the increment to the usual DC sheath potential due to the RF, and provides an effective parallel electric field in the vicinity of a metallic surface, where normally such field would be zero. This allows real and imaginary power flow into the sheath, consistent with the sheath capacitance width, $\Delta$, and loss parameter, $\nu$. These two sheath parameters depend non-linearly on the RF electric field at the edge.

3. VORPAL Framework

The time-domain plasma model is installed in the VORPAL software framework, a pre-existing large-scale plasma simulation tool already known for its success in the areas of plasma wakefield and traditional accelerator research. VORPAL is a modern object-oriented programming framework facilitating model and algorithmic extension. The time-domain plasma model within VORPAL utilizes pre-existing Maxwell solvers, while also introducing to VORPAL its own fields and updates for its own algorithmic requirements.

The great advantage of using the pre-existing framework is the use of VORPAL’s large-scale parallel processing features. No new communication methods were required, since pre-existing communication capabilities in VORPAL provide sufficient generality for the new fields of the time-domain plasma algorithm. VORPAL has demonstrated excellent parallel speedup of the pre-existing algorithms. The speed-up with new time-domain plasma algorithm is not yet established, but is expected to also be favorable, with computation dominated by point calculations, and field communications based upon the already successful pre-existing framework.

There are other significant advantages gained from the use of the VORPAL framework. Most important among these is the availability of state-of-the-art cut-cell boundaries for metallic and dielectric surfaces in the existing Maxwell solver. As shown later in this paper, this capability is critical for accurate rendering of the complex geometry of the rf antenna launchers. Finally, two additional advantageous features of the VORPAL software are its suite of

Figure 1. Computational subgrid model for a sheath.

Figure 2. Speedup of VORPAL on the Seaborg supercomputer at NERSC.
diagnostic and visualization capabilities, and its suite of particle algorithms, including particle-in-cell (PIC), and delta-f particles.

4. Three-Dimensional Demonstration

One dimensional verification of the time-domain plasma is discussed in Reference 2. However, one of the most important advantages of the time-domain approach is the ability to treat sophisticated three-dimensional geometry. This contrasts with the frequency-domain solvers which are based upon Fourier superposition of basis modes that essentially assume smooth featureless boundaries. To demonstrate this capability, we have done a simulation of representative edge geometry containing a coupler box, loop antenna, box-limiter, and two poloidal limiters, as shown in Figure 3. The loop antenna is shorted on bottom, with an open-circuit on top, and the excitation current runs across the open circuit on top to complete the driving circuit.

Figure 3. Three-dimensional edge geometry with box antenna and limiters. The other five-of-six simulation boundaries utilize perfectly matched layer (PML) absorbers.

Figure 4. Edge density profiles, and log scale showing diverter and limiter SOLs, and shadow region.
The main vacuum wall is a section of a true torus, with toroidal and poloidal curvature. There is both toroidal and poloidal magnetic fields, with the toroidal field going as $1/R_{\text{major}}$, and the poloidal field provided by a polynomial $Q(r_{\text{minor}})$ profile. The edge density profiles are a very important aspect of the edge problem, and so particular effort is warranted in their representation. For this simulation the edge plasma consists of three exponential layers, as shown in Figure 4: a diverter scrape-off-layer (SOL), a limiter scrape-off-layer, and a shadow region, with the diverter scrape-off-layer connecting to the core profile at the last closed flux surface (LCFS).

A simulation using this geometry, magnetic field, and plasma edge density arrangement is shown in Figure 5. The frequency regime is that of lower hybrid waves, and the simulation is run long enough for fields to cross the simulation domain, and be absorbed in the surrounding PML absorbers. The radiation pattern is very noticeably tilted by the poloidal magnetic field. Also illustrated are the surface electric fields which will drive the sheath model, and are also needed to assess breakdown risk on the various components of the launcher geometry.

![Figure 5](image)

Figure 5. 3-D edge geometry, including coupler box, loop antenna, and absorbing boundary conditions. Various outputs and visualizations from the VORPAL software framework are shown.

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