Computer Physics Communications 185 (2014) 736–743

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

Iterative addition of parallel temperature effects to finite-difference simulation of radio-frequency wave propagation in plasmas

D.L. Green *, L.A. Berry

Oak Ridge National Laboratory, Post Office Box 2008, Oak Ridge, TN 37831-6169, USA

ARTICLE INFO

Article history:
Received 3 July 2013
Received in revised form
28 October 2013
Accepted 30 October 2013
Available online 6 November 2013

Keywords:
Radio frequency heating
FDFD
FEFD
Kinetic effects
Plasmas

ABSTRACT

Accurate simulations of how radio frequency (RF) power is launched, propagates, and absorbed in a magnetically confined plasma is a computationally challenging problem that for which no comprehensive approach presently exists. The underlying physics is governed by the Vlasov–Maxwell equations, and characteristic length scales can vary by three orders of magnitude. Present algorithms are, in general, based on finding the constitutive relation between the induced RF current and the RF electric field and solving the resulting set of Maxwell's equations. These linear equations use a Fourier basis set that is not amenable to multi-scale formulations and have a large dense coefficient matrix that requires a high-communications overhead factorization technique. Here the use of operator splitting to separate the current and field calculations, and a low-overhead iterative solver leads to an algorithm that avoids these issues and has the potential to solve presently intractable problems due to its data-parallel and favorable scaling characteristics. We verify the algorithm for the iterative addition of parallel temperature effects for a 1D electron Langmuir by reproducing the solution obtained with the existing Fourier kinetic RF code AORSA (Jaeger et al., 2008).

Published by Elsevier B.V.

1. Introduction and background

In magnetically confined, nuclear fusion devices, the injection of radio-frequency (RF) power in both the electron-cyclotron and ion-cyclotron frequency ranges is used to heat the confined plasma to the 100 M K temperatures required for significant fusion power e.g., [1,2], and to provide some control over the magnetic field configuration by driving current. Localized current drive may help control global instabilities e.g., [3,4] and lead to increased fusion energy production. The combination of high RF currents and electric fields, a poorly understood wave behavior in the edge plasma, and numerous plasma modes with a wide range of wavelengths makes it necessary for us to rely on computer simulations to understand the controlling physics and operational constraints of RF heating and current drive. This physics includes heat generation in the RF launching structure by localized currents, parasitic losses in the poorly confined edge plasma and the potential for impurity generation and wall damage; and a quantitative understanding of wave propagation and absorption in the core fusion plasma.

For accurate predictions of how launched RF power will couple to a plasma, the geometric details of the launching structure and surrounding plasma facing component (PFC)s are important [5]. However, the standard electromagnetic full-wave simulation techniques capable of accurately, and efficiently modeling complex geometric structures (e.g., finite-difference [6] and finite-element [7] methods) do not account for the non-local, kinetic response of the plasma to the RF E&M fields. For the hot plasmas considered here, the conductivity is an integral operator that depends on the integrated time–history of an ion or electron in the oscillating RF field.

Present linear kinetic full-wave simulation techniques are limited in their application to the well-confined "core" plasma, where the plasma and confining magnetic field profiles are smoothly varying, and the small-scale geometric details of the launching and PFC structures are essentially ignored. These techniques are based on the Fourier spectral method [8] in at least one dimension, and as such are not well suited to extending the core kinetic calculation to include, and resolve, the geometric and material details of the confining structures (see Section 3).

Furthermore, experiments using the ion-cyclotron range of frequencies often observe anomalous losses of RF power between the launching structure and the well-confined core plasma. These unexplained losses are a concern for present and future fusion devices [9,10], and as such, a simulation method that can efficiently model the complex geometric structures at the plasma periphery with high fidelity, and also include the kinetic physics of the target plasma is required. An important feature of any new algorithm is a formulation that localizes the simulation data in order to provide more opportunity for exploiting computing architectures with more computing power but without the corresponding increase

* Corresponding author. Tel.: +1 865 241 2752.
E-mail addresses: greendl1@ornl.gov (D.L. Green), berryla@ornl.gov (L.A. Berry).

0010-4655/$ – see front matter. Published by Elsevier B.V.
http://dx.doi.org/10.1016/j.cpc.2013.10.032

in memory or memory bandwidth that are needed for spectral algorithms. Here we present such a method.

The rest of the paper is organized as follows. Section 2 states the Vlasov–Maxwell system describing the linear RF plasma-wave problem. Section 3 discusses previous and alternate methods for determining the kinetic plasma response, with an emphasis on the limitations we are trying to remove. Section 4 describes our proposed method, and Section 4.1 presents the details of our kinetic plasma current calculation. Verification of the proposed method is presented in Section 4.2, and a complete proof-of-principle with finite-difference code, kinetic current module, and iterative scheme is demonstrated in Section 4.3. The computational and scaling advantages of the presented method are discussed in Section 5.

2. Linear kinetic RF plasma simulation

In the frequency domain, Maxwell's equations reduce to Eq. (1) for the wave electric field $\mathbf{E}_1(\mathbf{r},\omega)$

$$\begin{cases}\mathfrak{L}_1\mathbf{E}_1+\dfrac{i\omega}{c^2\epsilon_0}\mathbf{j}_1=-i\omega\mu_0\mathbf{j}_A & \text{(a)}\\ \mathbf{j}_1=\mathfrak{L}_2\mathbf{E}_1 & \text{(b)}\end{cases} \tag{1}$$

where $\mathbf{j}_A(\mathbf{r},\omega)$ is the driving antenna current at angular frequency ω and the local Maxwell operator is $\mathfrak{L}_1=-\nabla\times\nabla\times+\frac{\omega^2}{c^2}$. $\mathfrak{L}_2$ is the integral operator described by in the following. The kinetic plasma current $\mathbf{j}_1$ for a single species is

$$\mathbf{j}_1=\mathfrak{L}_2\mathbf{E}_1=q\int\mathbf{v}f_1(\mathbf{r},\mathbf{v},t)\,d\mathbf{v}. \tag{2}$$

The kinetic constituative relation is determined by solving for the oscillating piece (f_1) of the distribution function $f(\mathbf{r},\mathbf{v},t)=f_0(\mathbf{r},\mathbf{v})+f_1(\mathbf{r},\mathbf{v},t)$ which satisfies the linearized Vlasov equation as

$$\begin{aligned}\frac{df_1}{dt}&=\frac{\partial f_1}{\partial t}+\mathbf{v}\cdot\nabla f_1+\frac{q}{m}(\mathbf{v}\times\mathbf{B}_0)\cdot\nabla_v f_1\\&=-\frac{q}{m}(\mathbf{E}_1+\mathbf{v}\times\mathbf{B}_1)\cdot\nabla_v f_0.\end{aligned} \tag{3}$$

By the method-of-characteristics, and with an initial condition as $f_1(t=-\infty)=0$, f_1 is

$$\begin{aligned}f_1(\mathbf{r},\mathbf{v},t)=-\frac{q}{m}\int_{-\infty}^{t}&\Big(\mathbf{E}_1(\mathbf{r}',t')+\mathbf{v}(t')\\&\times\mathbf{B}_1(\mathbf{r}',t')\Big)\cdot\nabla_v f_0(\mathbf{r}',\mathbf{v}',t')\,dt'\end{aligned} \tag{4}$$

where the characteristic curves $(\mathbf{r}',\mathbf{v}',t')$ are given by the unperturbed particle trajectories

$$\begin{aligned}\frac{d\mathbf{r}'}{dt'}&=\mathbf{v}'\\ \frac{d\mathbf{v}'}{dt'}&=\frac{q}{m}\left(\mathbf{v}'\times\mathbf{B}_0(\mathbf{r}')\right).\end{aligned} \tag{5}$$

3. Previous and alternative approaches

The constituative relation described above is often [11] represented as

$$\mathbf{j}_1(\mathbf{r},t)=\int_{-\infty}^{t}dt'\int d\mathbf{r}'\bar{\bar{\sigma}}(\mathbf{r},\mathbf{r}',t,t')\cdot\mathbf{E}_1(\mathbf{r}',t') \tag{6}$$

where $\bar{\bar{\sigma}}$ is the plasma conductivity kernel. The convolution integral here means that the plasma response at each spatial location depends on the conductivity and wave electric field at all other locations and times. Historically in the study of RF waves in plasmas, the spatial convolution in Eq. (6) is avoided by transforming to $\mathbf{k}$ (Fourier) space. The typical analysis e.g., [11–13] applies a Fourier–Laplace transform,

$$\mathbf{E}_1(\mathbf{r},t)=\int d\omega\int d\mathbf{k}\,\mathbf{E}_1^{\mathbf{k},\omega}\exp\left(i(\mathbf{k}\cdot\mathbf{r}-\omega t)\right) \tag{7}$$

thus also assuming a time-harmonic temporal dependence (i.e., frequency-domain), and the spatial convolution is transformed to a multiplicative relationship between the wave electric field and its associated conductivity tensor for each Fourier mode, i.e., local in $\mathbf{k}$-space, rather than non-local in configuration space,

$$\mathbf{j}_1^{\mathbf{k},\omega}=\bar{\bar{\sigma}}(\mathbf{k},\omega)\cdot\mathbf{E}_1^{\mathbf{k},\omega}. \tag{8}$$

This independence of modes has allowed for the tractable analytic study of waves in hot plasmas presented in the standard texts [11–13], where expressions for $\bar{\bar{\sigma}}(\mathbf{k},\omega)$ are calculated by analytic integration of Eqs. (2)–(5) for a given single Fourier mode $\mathbf{E}_1^{\mathbf{k},\omega}$. Given that these $\mathbf{k}$ dependent (Fourier) forms for the hot plasma conductivity are the only ones in the literature, a spectral method with a Fourier basis has been the natural choice for hot plasma simulation in the frequency domain e.g., [14]. These previous approaches rely on the analytic response of $\mathbf{j}_1^{\mathbf{k},\omega}$ to $\mathbf{E}_1^{\mathbf{k},\omega}$ such that the operation of $\mathfrak{L}_2$ may be substituted into the Fourier transform of Eq. (1) and solve with $\mathfrak{L}_1$ and $\mathfrak{L}_2$ simultaneously with each row in the dense coefficient matrix of the spectral method being

$$\mathfrak{L}_1\mathbf{E}_1(\mathbf{k},\omega)+\frac{i\omega}{c^2\epsilon_0}\mathfrak{L}_2\mathbf{E}_1(\mathbf{k},\omega)=-i\omega\mu_0\mathbf{j}_A. \tag{9}$$

For analytic calculations, the decomposition of unbounded, or periodic spatial domains into a kinetic response for each $\mathbf{k}$ has proved extremely useful. However, for simulation of bounded domains with complex boundary geometries and structures, and multi-scale phenomena that include both regions where kinetic effects are, and are not important, this approach has proved troublesome. Spectral methods require the solution to a dense linear system whose work scales as $O(N^3)$ and memory requirements as $O(N^2)$, where N is the number of degrees of freedom (number of spatial points × 3 field components). Also, sharp material boundaries, such as plasma facing components, and sharp features in the plasma dielectric at resonant locations can lead to unphysical solutions stemming from Gibbs phenomena [8] and aliasing [8].

To avoid one of these issues, that associated with solving bounded problems with a periodic basis, previous kinetic simulations of RF wave propagation in fusion plasmas have either applied the Fourier spectral method only to a periodic direction, e.g., the magnetic field parallel direction along closed magnetic flux surfaces [15], or by adding artificial bounding regions to the simulation domain that allow periodicity to be enforced [16,17]. The first approach limits kinetic simulation to domains that have a periodic direction, and neither allow for a variable resolution mesh that can be conformed to real PFC structures. Without a mesh-/grid-ing solution that reduces N while preserving accuracy (i.e., variable resolution), kinetic RF simulation is restricted to leadership class supercomputing facilities where, even at the largest values of N, accurate geometry representation of plasma facing surfaces in a Tokamak device is not possible. Furthermore, the Fourier spectral method assumes the problem is completely non-local, as Eq. (6) suggests. This assumption is one of the reasons spectral kinetic methods are so costly. In practice, the spatial extent of the non-locality is limited to the trajectories traversed by particles contributing to the plasma current at $(\mathbf{r},t)$, and only back along those