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Propagator methods for plasma simulations: application to breakdown

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Abstract

Accurate simulation of plasmas often requires a solution of the kinetic equation, either directly by solving the Boltzmann equation (BE) or indirectly by means of 'particle' simulations. However, kinetic simulations are still too computationally intensive for many large scale 3D simulations. In this paper we examine the matching between a kinetic simulation and fluid models which we use in conjunction to form a 'hybrid' plasma model of the breakdown process. The kinetic model is tested for convergence with respect to mesh size Δx and time-step Δt. We then implement fluid models in an attempt to reproduce the results of the kinetic model. To do this it is necessary to have a fluid model which provides accurate simulations with a wide range of Δx and Δt. We accomplish this by means of a propagator (or Green's function) approach. The propagator method reduces to a finite difference scheme at small $\Delta x, \Delta t$ and gives correct results across a wide range of parameters. For intermediate $\Delta x, \Delta t$ it is necessary to take considerable care to derive the correct propagator. We apply the propagator method to two fluid models; one uses parameters which are functions of the electric field, and the other one uses parameters which are functions of the mean kinetic energy (this version also explicitly conserves energy locally). The details of the fluid models employed make a profound difference to the prediction of the breakdown.

Keywords: Plasma simulation; Kinetic model; Convective scheme; Propagator method; Fluid model; Energy-conserving scheme

1. Introduction

The purpose of this paper is to examine the effectiveness of numerical techniques for the simulation of electrical breakdown of a gas. Breakdown is in some regards more difficult to simulate than other aspects of plasma behavior. During the initial phases of breakdown the electron density is expected to grow exponentially in time (and sometimes in space). Modest differences in the predicted ionization rate [1,2] can lead to

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very large differences in density in this phase. Alternatively, near the threshold for the onset of breakdown there is a sensitive region where we may predict growth or decay in the density, and only small changes in parameters or models are needed to make the difference between one or the other.

The most accurate simulation of breakdown calls for a kinetic treatment, such as the solution of the Boltzmann equation (BE) for the charged particle distribution function, or the numerical simulation of motions of charged particles. There are numerous plasma simulations using kinetic treatments such as [3–8]. However, kinetic simulation describes the plasma in great detail and is very computationally intensive in practical situations so it is desirable to have a fluid equation for the charged particle density which approximates the behavior predicted by the BE. Fluid simulations have been abundantly described; [17–21]. Such simulation is frequently attempted using a variety of 'hybrid' codes [9]. In a hybrid code, detailed calculations at the level of the BE are done to calibrate a fluid calculation (providing values for quantities such as the diffusion coefficient D, the mobility μ, the ionization rate S, and so on).

A key parameter in the fluid model employed here is the fraction, α, of the energy which is put into ionization, as opposed to excitation or other inelastic processes (or radiation losses). In effect, the solution of the BE provides the local value of α, as a function of the other variables. α can vary significantly, and this variation is largely what provides the range of possible final densities.

Any model which conserves energy, even approximately, and which uses the correct α (which may mean using an approach in which α is never explicitly employed, but which nevertheless results in the right fraction of the energy being put into ionization) will give roughly the right amount of electrons. This is especially true in a homogeneous plasma. Inert gases (Xe, Ne, Ar, etc.) should have a very high α which makes modeling them more straightforward.

We have examined the capability of fluid models to reproduce the behavior of the BE, in order to assess how accurate a fluid model of breakdown can be made. One issue of some concern was the value of the Δx and the Δt which can be used. The BE solution requires very small values of Δx and Δt, because the natural scales of the problem are rather short. It is of some concern whether the fluid equation must be restricted to the same range of Δx and Δt. We thus employed a 'propagator' (Green's function) method [38–41] to solve the fluid equations (similar to our BE solution technique) which works well for a wide range of Δx and Δt.

The propagator method is of some interest in itself. It provides a simple scheme for solving a discretized fluid equation, which can be reduced to a finite difference scheme for small $\Delta x, \Delta t$ but which works equally well for a wide range of $\Delta x, \Delta t$ since the propagator does not necessarily obey the Courant limit. One version of the scheme has been implemented in a form which explicitly and locally conserves particles and energy. The finite difference forms of the fluid equations involve evaluating derivatives; in this problem those derivatives are not necessarily well described by finite differences because the gradients are very steep indeed. The propagator does not require the calculation of derivatives and is easier to implement than the finite difference scheme.

Eastwood [39,40] has presented a rather general treatment of methods of characteristics, including Lagrangian schemes, applied to a one dimensional fluid flow. Eastwood distinguished a number of different ways of handling the problem, and although our methods do not entirely fall within his framework, there are some aspects of his categorization which are illuminating. The most pertinent distinction between schemes, from our point of view, reflects whether the scheme (a) takes an initial density defined on mesh points and propagates it forward in time, along the characteristics, or (b) if the scheme focuses on a final cell and looks back along the trajectory to find the initial density. In case (b), when looking back along the trajectory one is (in general) forced to interpolate between mesh points to find the 'old' density on the trajectory/characteristic. Case (a) requires that density from an 'old' mesh point be propagated forward and then shared between mesh points. Eastwood prefers case (b) for reasons of accuracy in the problem he was studying. We find compelling reasons to use case (a) which we shall point out shortly. The review paper by Staniforth and Cote [44] considers Eastwood's work, but their discussion is limited to case (b), as their Figs. 1 and 2 show. These figures define what we mean by 'looking back along a trajectory' very clearly. The