TIME-STEP STABILITY FOR SELF-CONSISTENT MONTE CARLO DEVICE SIMULATION

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ABSTRACT

An important numerical constraint on self consistent Monte Carlo device simulation is the stability limit on the time step imposed by plasma oscillations. The widely quoted stability limit for the time step between Poisson field solutions, $\Delta t<2/\omega_p$ where ω_p is the plasma frequency, is specific to the leapfrog particle advance used in collisionless plasma simulation and does not apply to typical particle advance schemes used for device simulation. We present a stability criterion applicable to several algorithms in use for solid state modeling; this criterion is verified with numerical simulation. This work clarifies the time step limitation due to plasma oscillations and provides a useful guide for the efficient choice of time step size in Monte Carlo simulation. Because frequent solution of the Poisson equation can be a sizable computational burden, methods for allowing larger time step are desirable. The use of advanced time levels to allow stability with $\omega_p\Delta t>>1$ is well known in the simulation of collisionless plasmas; we have adapted these implicit methods to semiconductor modeling and demonstrated stable simulation for time steps larger than the explicit limit.

I. TIME STEP STABILITY

One important constraint on self consistent simulations of both solid state devices and plasmas is numerical stability of plasma waves. This limitation imposes a maximum on the allowed time step interval between Poisson field solutions Δt, relative to the plasma frequency ω_p, and is particularly important for simulations of devices with high carrier concentrations, such as found in heavily doped contact regions. Motivated by analysis of numerical schemes for plasma simulation, many authors have quoted the stability limit $\omega_p\Delta t<2$ [1]. This limit of $\omega_p\Delta t<2$, however, is specific to the leapfrog particle advance used in plasma simulation and is generally not applicable to algorithms used for solid state device simulation. In contrast to the leapfrog algorithm which is centered and advances the particles with a fixed time increment equal to the time step between field solves, Δt, solid state simulations typically use non-centered algorithms with a particle time step $\delta t\neq\Delta t$. Furthermore the particle time step is often picked stochastically based on mean free collision times determined not only by physical parameters but also by details of the numerical implementation such as self-scattering.

The numerical stability of typical algorithms used for Monte Carlo device simulation has been investigated in Ref. [2]. This analysis is applied to a variety of algorithms in different regimes; here we confine our discussion to the case of $\delta t<<\Delta t$ which is generally applicable to any scheme which only uses the electric field at the old time level in advancing the particles. This situation could correspond to the case of high collision rate (perhaps due to a large self scatter rate), or simply an attempt to ensure very accurate particle orbits. In this limit the particle advance approximates an exact orbit. Then the numerical solution corresponds to solving the Boltzmann equation exactly between times t^n and $t^{n+1}=t^n+\Delta t$ with the time independent electric field, $E(t^n)$. A dispersion relation is obtained, which shows the surprising result that in the absence of collisions, instability occurs for all time steps. In practice, collisions allow stable simulation for finite time step. The appropriate collision rate is the rate of momentum transfer ν_c, defined by the first velocity moment over the Boltzmann collision operator, and may be related to the mobility by $\nu_c=e/\mu m^*$ with e and m^* the electron charge and effective mass . The amount of collisionality required to offset the tendancy for growth is determined by the threshold for stability (zero growth, $\gamma=0$),

$$\left(\frac{\nu_c}{\omega_p}\right)_{\gamma=0} = \left(\frac{1-e^{-\alpha}-\alpha e^{-\alpha}}{1-e^{-\alpha}}\right)^{1/2}, \text{ for } \alpha \equiv \nu_c \Delta t \le \alpha_c$$
$$= \left(\frac{\alpha}{2}-\frac{1-e^{-\alpha}}{1+e^{-\alpha}}\right)^{1/2}, \text{ for } \alpha \equiv \nu_c \Delta t \ge \alpha_c \quad (1)$$

and plotted in Fig. 1. Stable solutions lie above the stability threshold shown as a solid line in Fig. 1. For values of the collision rate below this threshold, unstable growth is present. $\alpha_c \approx 3.72$ corresponds to the point C in Fig. 1 where the threshold crosses the boundary between complex and real roots denoted by a dotted line. An approximate expression for the stability limit, valid for $\gamma\Delta t \ll 1$ and $\nu_c \Delta t \ll 1$, is given by,

$$\omega_p \Delta t \le 2\, \nu_c / \omega_p \quad (2)$$

This condition is plotted as a straight dashed line in Fig. 1 and comparison with the exact threshold (solid line) shows that it remains a good approximation out to values of $\omega_p \Delta t$ approaching unity.

A number of simulations have been performed to explore the stability boundary in the space of ν_c/ω_p vs. $\omega_p \Delta t$ shown in solid line in Fig. 1. The code used allows multiple nonparabolic, elliptic bands and scattering processes appropriate for simulation of GaAs or Si. The particle advance is performed as described by Hockney and Eastwood with δt picked randomly based upon the total scattering rate Γ which includes self scattering. A grid with uniform spacing Δx is used; interpolation from the particles to the grid uses standard linear weighting, and the Poisson equation is solved directly without spatial smoothing. Results from simple simulations which closely conform to the analysis are shown in Fig. 1. For these runs a single spherical parabolic band is used, and collisions correspond to elastic, isotropic scattering which is independent of energy. Simulation results are plotted as solid markers if unstable growth is observed, and as open markers if the run was observed to be stable ($\gamma\Delta t < 0.01$). The circles are from simulations with $\Gamma = \nu_c$, while triangles represent simulations with $\Gamma = 5\nu_c$. It can be seen that the stability condition implied by the boundary between solid and open markers is in reasonable agreement with the analysis, but

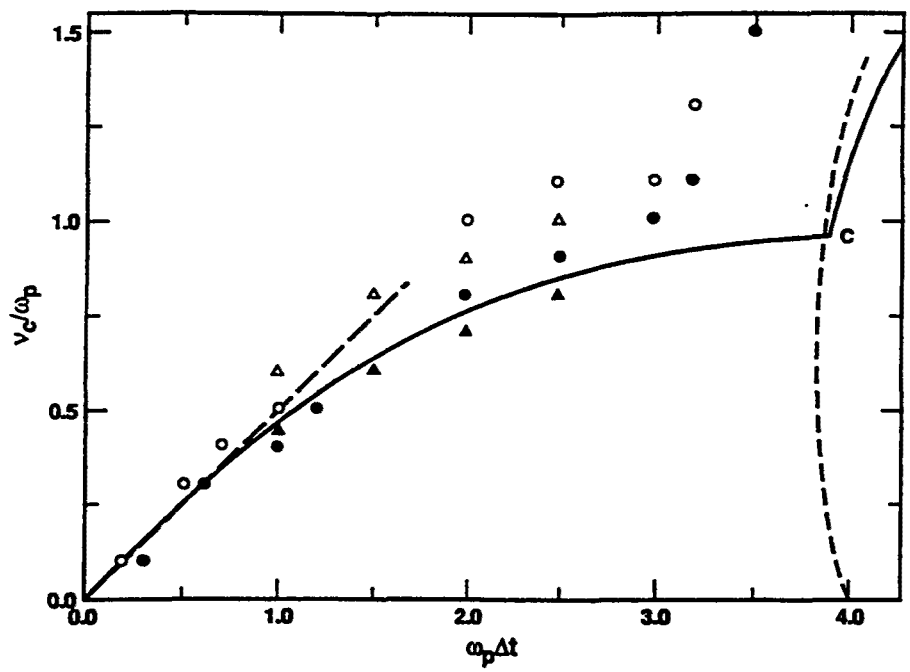

Fig. 1. Numerical stability as a function of collisionality, ν_c/ω_p, and time step between Poisson solves, $\omega_p \Delta t$. Markers represent results of simulations: open for stable, closed for unstable.

indicates a slightly more stringent stability condition; this is due to the effects of finite temperature which are neglected in the analysis.

As an example relevant to realistic device simulations, consider GaAs at a doping density of N_D=1.0×10^{17} cm^{-3}; assuming the electron density is equal to the doping density we have ω_p≈2.0×10^{13} s^{-1}. At a lattice temperature of T=300 K, the low field mobility is μ≈5.3×10^3 cm^2/V·s; this corresponds to an effective collision frequency ν_c≈5.0×10^{12} s^{-1}. Then ν_c/ω_p≈0.25, and the stable time step limit is predicted to be $\omega_p\Delta t$≈0.5 or Δt≈2.6×10^{-14} s. At a lattice temperature T=77 K, μ≈9.2×10^3 cm^2/V·s corresponding to ν_c≈2.9×10^{12} s^{-1}. Then ν_c/ω_p≈0.15 and the stability limit is $\omega_p\Delta t$≈0.3 (Δt≈1.5×10^{-14} s). Simulations of the two cases described above (T=300 K, $\omega_p\Delta t$=0.5; T=77 K, $\omega_p\Delta t$=0.3) performed using realistic models for GaAs show weak instability; stability requires somewhat smaller values of the time step consistent with the effect of finite pressure. Unstable runs were observed to saturate by heating the electrons. In some cases, mobilities were noticably reduced and significant numbers of electrons promoted to the upper valleys.

II. LARGE TIME STEP ALGORITHM

Frequent solution of the Poisson equation to resolve plasma oscillations can be a sizable computational burden. Caution suggests that the condition presented above not be approached to closely, since finite pressure effects slightly lower the stability limit. Additionally, near the stability limit unphysical heating of the carriers may be a more insidious effect than the catastrophic instability which occurs well above the limit. The necessity of using advanced time levels for numerical stability with $\omega_p\Delta t$>>1 has long been known in the case of collisionless plasma simulation, and stable large time step simulations have been achieved using time-implicit methods [3].

The key ingredient for large time step stability is to advance the particles using the *advanced* electric field E^{n+1}, such as

$$x^{n+1} = x_0 + \beta\Delta t^2 \frac{qE^{n+1}}{m^*}, \tag{3}$$

where x_0 depends only on quantities at the past time level t^n and β is the implicitness parameter. Because the new field depends on the new particle positions through the solution to the Poisson equation, however, an implicit solution for the electric field is required. The implicit field equation may be found by writing the Poisson equation at the new time level, and linearizing the charge density with respect to perturbations due to the advanced field,

$$\frac{\partial E^{n+1}}{\partial x} = \frac{4\pi}{\varepsilon}\rho^{n+1} \equiv \frac{4\pi}{\varepsilon}\{\rho_0(x_0)+\delta\rho\}. \tag{4}$$

The perturbation to the charge density, $\delta\rho$, may be expressed in terms of the perturbation to the particle position δx by,

$$\delta\rho \approx -\frac{\partial}{\partial x}(\rho_0\delta x) = -\frac{\partial}{\partial x}(\rho_0 \frac{q}{m^*}\beta\Delta t^2 E^{n+1}). \tag{5}$$

Substituting into Eq. (5), and rearranging, the field equation becomes

$$\frac{\partial}{\partial x}\left\{(1+\chi)\frac{\partial\phi}{\partial x}\right\} = -\frac{4\pi}{\varepsilon}\rho_0 \quad , \quad \chi \equiv \frac{4\pi}{\varepsilon}\rho_0\frac{q}{m^*}\beta\Delta t^2 = \beta(\omega_p\Delta t)^2, \tag{6}$$

with χ the effective susceptibility due to the partial advance of the particles to x_0. Strict implementation of such a scheme requires writing these equations with the spatial derivatives replaced by finite differences generalized to include the interpolation between the grid and particles. This leads to a matrix system for the new electric field which is completely consistent with the particle push but has a larger stencil than the original explicit system. Simplified differencing (and reduced computational stencil) can be obtained by simply writing Eq. (2) in finite difference form; this is appropriate if $\omega_p\Delta t$ is not too large.

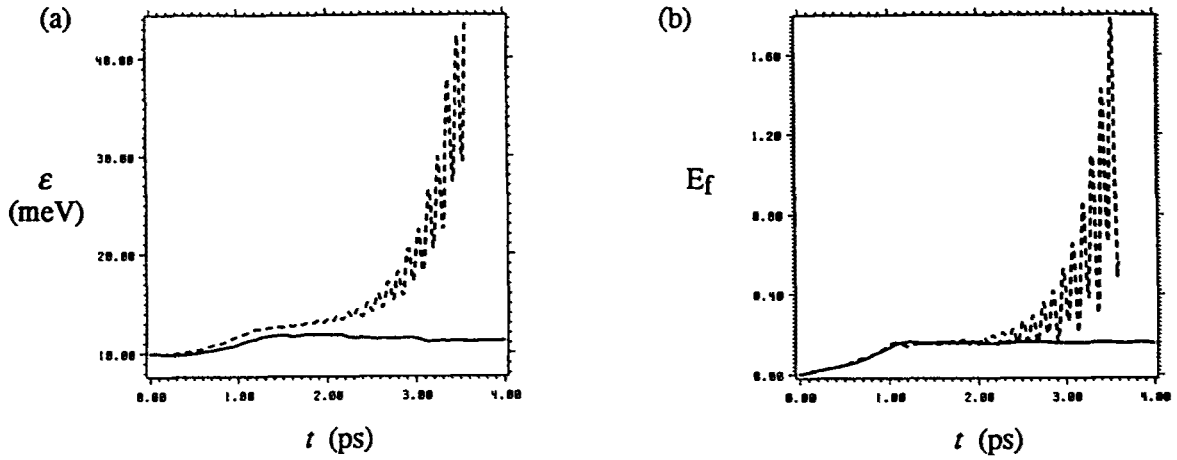

Fig. 2. Time history of (a) average particle energy and (b) electrostatic field energy (arbitrary units) from two diode calculations: explicit $\omega_p\Delta t$=0.42 (dashed line) and implicit $\omega_p\Delta t$=2.24 (solid line).

We have adapted these implicit plasma techniques to semiconductor modeling and demonstrated stable simulation for $\omega_p\Delta t$ larger than the limit given in Section I. At each time step, particles which undergo one or more collisions ($\delta t<\Delta t$) are advanced explicitly. These collisional particles contribute only to ρ_0 and not to the susceptibilities. Particles which do not undergo a collision ($\delta t\geq\Delta t$) are advanced implicitly by performing a partial push and accumulating the necessary susceptibilities. Then the implicit field equation is solved and the positions of the implicit particles corrected, completing the time step. Calculations of a submicron GaAs diode [4] have been performed as a realistic test. The diode is composed of a 0.25 μm undoped active layer between 0.35 μm n^+-layers doped at density N_D=2.0×10^{17} cm^{-3} (ω_p=2.7×10^{13} s^{-1}). The simulation model is substantially the same as used by Tomizawa et al., and for their time step, Δt=1.0×10^{-14} s, similar results are obtained. Figure 2 shows time histories of the average particle energy and electrostatic energy from simulations with an applied voltage of 0.25 volts (rising from zero in 1.0 ps) and lattice temperature of 77 K. An explicit calculation with Δt=1.5×10^{-14} s is unstable (as predicted above for $\omega_p\Delta t$≈0.42), while in contrast, the implicit calculation (β=0.75) with Δt=8.0×10^{-14} s ($\omega_p\Delta t$≈2.24) is well behaved. The increase in time step which can be realized is limited, because as Δt is increased, the fraction of particles which are treated implicitly decreases. As $\Gamma\Delta t$ becomes of order unity, most of the particles are treated explicitly, and the stability limit of Eq. (1) becomes effective. Although the time savings in one dimension is modest, appreciable gains in multi-dimensional simulation might be realized because of the increased computational burden of the Poisson solve.

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