An Efficient Method for the Coupling of a Fully-Explicit Time-Domain Solid-State Hydrodynamic simulator with FDTD EM Solvers

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***Abstract* — This paper examines the implications of decoupling the FDTD grids between and FDTD Electromagnetic (FDTD-EM) and an FDTD Hydrodynamic semiconductor simulator. Excitation methods and responses are examined to determine feasibility for decoupling the space and time grids for significant computational savings. Additionally, a new fully-explicit leap-frog discretization of the Hydrodynamic model is is benchmarked with respect to several well known discretization methods.**

***Index Terms* — FDTD methods, Time-Domain, Hydrodynamics, Boltzmann equation, electromagnetic coupling, Magnetohydrodynamics.**

I. Introduction

The advent of nanostructures and the integration of exotic solid state devices in state-of-the-art RF, microwave and optoelectronic devices have dictated the integration of electromagnetic solvers with solid-state simulators. Despite the numerous efforts in the past, there are still issues remaining with the numerical accuracy and stability of the coupled schemes. The dominant challenge is the fact that the time and space gridding requirements usually differ by several orders of magnitude for the two systems. This paper will demonstrate an effective method for decoupling the time and space discretization of the two systems. The hydrodynamic simulator was chosen as it provides a wider set of submicron or nano-scale effects that can be included in the simulation gaining a more accurate result of the device or circuit characteristics *in-situ*.

A. Model Description

The hydrodynamic model (HDM) approximates the semiconductor as a highly charged gas or plasma flowing through the semiconductor lattice. The model is typically used when a Monte-Carlo approximation is not practical, such as in time-domain simulations. The original mathematical model was developed by Blotekjaer [1] for two-valley GaAs semiconductors and was extended to single-band silicon semiconductors later [2].

The mathematical model is derived by taking the first several moments of the Boltzmann Transport Equation (BTE) producing equations (1) - (3) [3]. The collision terms in each of these equations describe the average carrier-carrier, carrier-lattice interaction. In a multi-band device the collision term in the conservation of mass would allow for the loss or gain of mass due to the carriers' transition from one energy band to another, re-combination, and generation effects. The collision terms in equations (2), (3) describe the average momentum or energy lost or gained via interactions with the lattice or carrier interaction [4]. The process of taking the mathematical moments of the BTE always leaves undefined variables that need to be approximated. As a result of the calculation of the moments of the BTE, two variables are left undefined: Heat flux and Electrostatic forces. The Heat flux is approximated using Fourier's Law (4) and Wiedemann-Franz Law (5) to express the internal thermal conductivity [2,3]. Poisson's Equation (6) is used to approximate the internal electrostatic effects of the plasma. With equations (1-6) the hydrodynamic (HD) model is fully defined and mathematically self-consistent and ready for discretization and simulation prior to integration into an FDTD-EM solver.

Conservation of Mass:

$$\frac{\partial n}{\partial t} = -\nabla \cdot (\vec{v}_d n) + \left(\frac{\partial n}{\partial t}\right)_C \tag{1}$$

Conservation of Velocity

$$\frac{\partial \vec{v}_d}{\partial t} = -\frac{\vec{v}_d}{m^*}\nabla \cdot (\vec{p}_d) + \frac{e\vec{F}}{m^*} - \frac{2}{3nm^*}\nabla\left(nw - \frac{1}{2}m^* n(\vec{v}_d)^2\right) + \left(\frac{\partial(\vec{v}_d)}{\partial t}\right)_C \tag{2}$$

Conservation of Energy

$$\frac{\partial w}{\partial t} = -\vec{v}_d \cdot \nabla w - \frac{2}{3n}\nabla \cdot \left[\left(n\vec{v}_d - \frac{\kappa}{k_B}\nabla\right)\left(w - \frac{1}{2}m^*(\vec{v}_d)^2\right)\right] + e\vec{F}\cdot\vec{v}_d + \left(\frac{\partial(w)}{\partial t}\right)_C \tag{3}$$

Heat Flux Approximation: Fourier's Law

$$n\vec{q} = -\kappa \nabla T \tag{4}$$

Wiedemann–Franz law

$$\kappa = \frac{5k_B nT}{2m^* v_p(w)} \tag{5}$$

Poisson's Equation

$$\frac{\nabla^2 \varphi}{\partial x^2} = \frac{q}{\varepsilon_o \varepsilon_r}(N_D - n_i) \tag{6}$$

B. Previous Efforts

The HDM model itself is non-trivial to discretize and achieve stable, consistent and convergent results. Previous

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approaches to discretize the highly coupled non-linear model shown in (1)-(6) were typically based on the staggering of the scalars and vector parameters at full and half nodal points or setting all variables at the nodal points at the same time step. This approximation is based on the assumption the variables are unable to be decoupled in time causing the model to be 2nd order accurate in space, but only 1st order accurate in time. This discretization fails to provide a numerically stable model. To correct for this problem advanced discretization techniques are typically used in time. As examples, Tomizawa used a Crank-Nicolson semi-implicit method [3], Aste & Vahldieck used a weighted upwind scheme [5], and El-Ghazaly used a hybrid method that included both a standard upwind method and a Lax-Wendroff method [2].

II. New HDM Methodology

The novel method shown here extends the basic tenets of Yee's Leapfrog method in space and time Maxwell's Curl equation discretization to the HDM [6,7]. If one accepts that the equations can be sufficiently decoupled to stagger the gridding in space, the staggering of these variables in time is the next natural extension. The developed simulator staggers the scalar variables on the full nodal points and the vector variables on the half nodal points of the HDM grid in time and space as seen in Fig. 1.

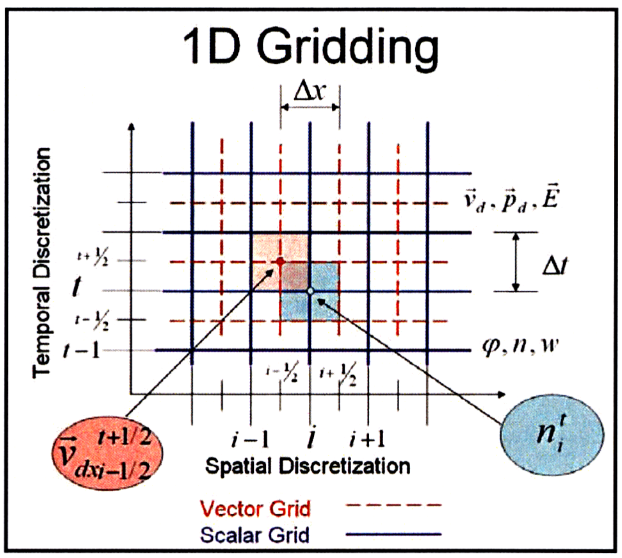

Fig. 1. Staggered Gridding technique showing vector and scalar offsets in time and space.

III. Model Comparison

Typically any new HD model is tested against the well publicized *n-i-n* diode case. Several of the previously discussed methods were implemented and compared by the author.

Three separate models were implemented. A reproduction of the time-domain discretization as described by Tomizawa was used for the *Lax-Wendroff*. The asymmetric *Upwind* scheme described by Aste & Valhdieck. And the *Leap Frog* discretization described in the previous section. All models used the same physical constants, and included El-Ghazaly's effective mass approximation [2].

Evaluating a model for integration into the FDTD-EM lattice requires the model to be stable, convergent, and consistent with physics. At a minimum the models need to produce valid results for zero bias, DC ramp to some reasonable DC bias voltage, and for the DC bias plus a sine excitation of reasonable amplitude.

A. Zero DC Bias Steady State

All hydrodynamic models provided reasonable results at the input and output ports of the ballistic diode for zero DC bias. The *Upwind* model has excessive carrier velocities at the transitions regions between the highly doped areas and the non-doped transition regions; however, when a DC bias was applied the results improve.

B. Ramp Excitation to 1VDC Steady State

The next test excited each of the implemented discretization methods for the same *n-i-n* diode with a basic DC ramp from 0V steady state to 1V. Ramp times were varied from 100ns to 10ps. Fig 2 shows the results for the fastest excitation rate each model could support for stability up to some reasonable time and acceptable convergence.

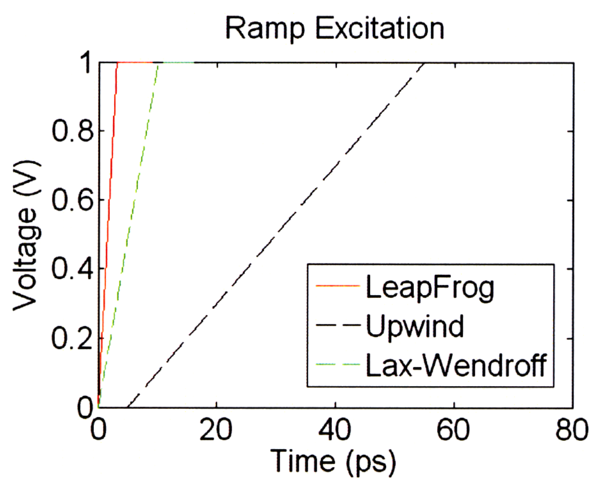

Fig. 2. Maximum stable ramp excitations showing the maximum ramp rates the produced reasonably stable or convergent solutions.

The results of this test provide unique insight into each model's behavior. The *Lax-Wendroff* discretization provides stable and convergent results provided the ramp rate is either slow enough or the steady state time is limited. Fig 3 shows

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good results. However, Fig 4 shows the effects of allowing for longer execution time. The model begins to oscillate in a divergent manner.

The *Upwind* method shows other unique results. Upon closer examination of Fig 3, the results show the non-physical effects of using an asymmetric upwind method. The device becomes a perfect current sink at both the input and output ports as the carrier velocity is positive at one end and negative at the other end. The result was convergent even for excessive simulation time (large number of time-steps). Fig 4 shows that increasing the Zero DC Bias time and slowing the ramp rate valid results can be obtained for *Upwind* model; however, the *Lax-Wendroff* method's tendency to oscillate and subsequently diverge.

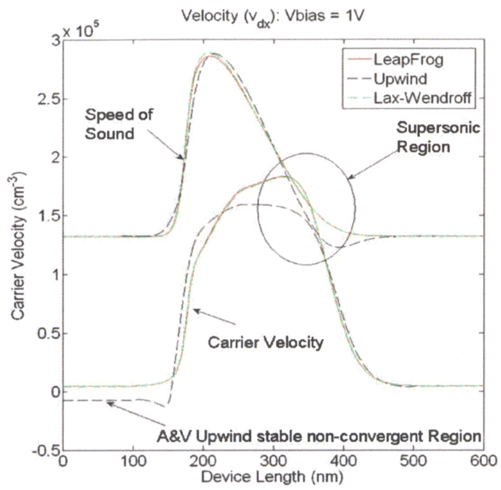

Fig. 3. Steady-state Velocity profile of *n-i-n* diode models showing the non-physical convergent results for the *Upwind* method when the ramp excitation rate is too steep.

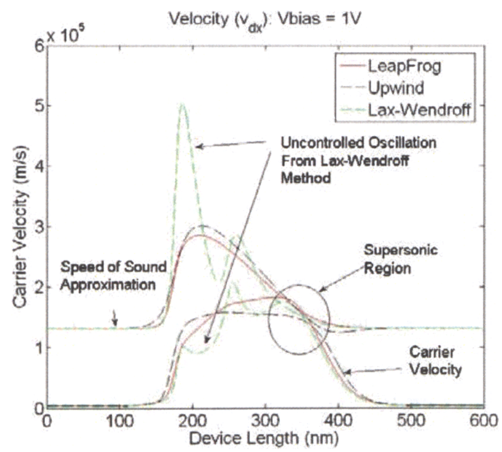

Fig. 4. Steady-state Velocity profile of *n-i-n* diode for a much slower ramp excitation and much longer execution time. The *Lax-Wendroff* method tends to oscillate when sufficient execution time has elapsed.

C. AC Excitation Plus 1V DC-Bias

The unstable *Lax-Wendroff* method results were omitted as the results were omitted due to the fact that this technique is not convergent. A 20GHz sine wave was used to validate and compare the initial results the excitation was a piecewise linear approximation similar results and the DC excitation to the ramp in which the excitation step size was dependent upon the HDM timestep, effectively making the excitation quite smooth. Both models show similar and good results the resultant curves are shown in Fig 5 with the results for the method for coupling the system.

IV. Coupling Methodology

El-Ghazaly's approach for coupling the systems included a unified grid in time and space between the two models. The two models CFL conditions have disparate space and time stepping requirements as shown in Table 1, with a maximum frequency of interest in the FDTD-EM simulator of 100 GHz. Eliminating the unified grid requirement significantly reduces the computational requirements of an integrated simulator.

TABLE I
SPACE AND TIME STEP DISPARITY

	Space Step (m)	Time Step(s)
FDTD-EM	0.150e-3	5.0e-13
FDTD-HDM	4.08e-10	4.08e-17

Decoupling the time and space grids requires an effective method of exchanging energy between the models at the HDM input and output ports. Picket-May [8] described a straightforward method for introducing Thevenin and Norton equivalent circuits into the FDTD-EM lattice and SPICE models. The previous section demonstrated the stability of the HD models under test to a very smooth excitation with *a-priori* knowledge of the excitation in a Thevenin circuit equivalent. To evaluate coupling methodologies, the AC excitation (*Smooth-HDM*) used in the previous section will be discretized in a stepwise (*Step-EMS*) and piecewise linear (*Linear-EMS*) approximation with a time step for an FDTD-EM with a maximum frequency of 100 GHz.

V. Results

Fig 5 shows the current density response of the HDM models to the excitation. Both models under investigation provide similar results that are expected and consistent with previous published results [2,3,5] and theory; thereby, validating the new discretization method.

The models were excited with three approximations of the piecewise continuous signal. The best approximation was the *Smooth* signal that is considered the reference as the piecewise approximation is based on the HDM time step. The results are shown in red and both models have smooth and valid results. The next best approximation is the piecewise linear approximation. This method, while it is slightly sensitive to the relative quick change in slope of the excitation, has acceptable results that are consistent with the reference results. Applying a single-step excitation voltage to the HDM yields unacceptable oscillations in comparison to the reference solutions.

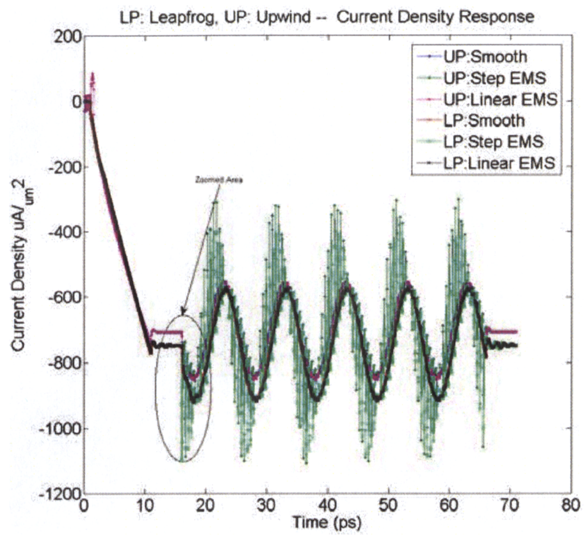

Fig. 5. Current density response to the reference excitation, a piecewise linear approximation and a stepwise linear approximation. The piecewise linear approximation and the reference excitation are similar; however the stepwise approximation shows significant overestimation in the change induced by the excitation.

VI. CONCLUSION

A novel method for coupling a FDTD-EM and FDTD-HDM models has been presented removing the previous requirement for a unified spatial and temporal grid between the models. Decoupling the grids leads to significant computational savings. For practical RF devices (<200 GHz) the computational savings is approximately 10 orders of magnitude per FDTD-EM cell per FDTD-EM time step as the HDM can be typically embedded in a single FDTD-EM cell. This reduces each of the models to their respective CFL conditions instead of imposing the smallest CFL condition on both models.

Coupling the energy between the models can be easily implemented by using Norton or Thevenin equivalent circuits if a piecewise linear approximation is used to excite the HDM model embedded in the FDTD-EM lattice.

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