Electromagnetics-Multiphysics Simulation for Emerging Electronics

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Contents

1. Background

2. Analogy of Photon and Electron

3. Governing Equations

4. Numerical Strategies

5. Conclusion
1. Background — After Moore’s law

key performance metrics at advanced nodes are plateauing

Era of the digital economy and massive connectivity leads to integrated hardware-software driven applications (5G, IOT, AI, Cloud, Big Data, …)
1. Background — Complexity of Electronics (1)

- **LEVEL 0:** Semiconductor Die/Wafer
- **LEVEL 1:** Semiconductor Packaging
- **LEVEL 2:** Device/Equipment board
- **LEVEL 3:** End Device/Equipment

Yole development

- **device/circuit/chip levels**
- **assembly or package levels**
- **board levels**
- **system levels**
1. Background — Complexity of Electronics (2)

- **Bulk Waveguide**
- **Microwave Integrated Circuits, MICs**
- **Monolithic MICs, MMICs**

**Multilayered MMIC/LTCC**

**Substrate Integration**
1. Background — Emerging Electronics

- New Materials/Tech: Organic TFT/FET
- New Architecture: 3D heterogeneous integration
- New Principle: quantum entanglement
1. Background — EM-Multiphysics Simulation

EM compatibility/ interference (EMC/EMI)  
signal integrity/ power integrity (SI/PI)  
short-channel effects  
quantum effects  
field-circuit coupling  
thermal-mechanical issue  
electro-static discharge  
parasitic effect  
packaging  
...

- AC/DC carrier transport  
- thermal conduction  
- vacuum/ thermal fluctuation  
- DFT/TB/ quantum transport  
- mechanical deformation  
- quantum tunneling/ confinement
2. Analogy — Physical Behaviors of Photons

D: object size; λ: wavelength

ray physics
D >> λ

Asymptotic solvers
PO/PTD/GO/GTD/UTD/
Ray tracing: Xpatch

wave physics
D ~ λ

Full-wave solvers
FDTD: CST
FEM: ANSYS, COMSOL
MOM: FEKO, ADS

circuit physics
D << λ

DC/AC circuit solvers
nodal equation:
SPICE, Multisim
2. Analogy — Physical Behaviors of Electrons

1. Ballistic transport limited by mean free path (coherent, \( D < L_{\text{e-e}} \)) : EM wave propagating in homogeneous media [ ATK: NEGF + DFT ]

2. Diffusive transport limited by phase coherent length (back scattering enhancement, \( D > L_{\text{e-phonon}} \)) : EM wave scattered by multiple scatterers [ Silvaco: Drift-Diffusion Model ]

3. Anderson localization (metal-insulator transitions): EM waves in random media

- time-reversal property
- disorder increase (diffusion \( \rightarrow \) localization)
- back scattering enhancement
### 3. Governing Equations — From Classical to Quantum Worlds

<table>
<thead>
<tr>
<th><strong>electron</strong></th>
<th><strong>photon</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>NEGF/ TB/ DFT equation</td>
<td>Quantized Maxwell equation</td>
</tr>
<tr>
<td>Boltzmann equation</td>
<td>Vector-scalar potential equation</td>
</tr>
<tr>
<td>Energy balance equation</td>
<td>Maxwell equation</td>
</tr>
<tr>
<td>Hydrodynamic equation</td>
<td>Parabolic wave equation</td>
</tr>
<tr>
<td>Drift-diffusion equation</td>
<td>Ray equation</td>
</tr>
</tbody>
</table>

Poisson’s equation is unique, which is valid in both classical and quantum fields!

**Level 1 (DD)**

\[
\begin{align*}
\frac{\partial n}{\partial t} &= \nabla \cdot \left( \mu_n n E_n + \frac{k_B T}{q} \nabla n \right) - (U - G) \\
\frac{\partial p}{\partial t} &= -\nabla \cdot \left( \mu_p p E_p - \frac{k_B T}{q} \nabla p \right) - (U - G) \\
\nabla \cdot \varepsilon \nabla \psi &= -q(p - n + N_D^+ - N_A^-) - \rho_s
\end{align*}
\]

**Level 2 (Level 1 + heat conduction)**

\[
\begin{align*}
\frac{\partial n}{\partial t} &= \nabla \cdot \left( \mu_n n E_n + \frac{k_B T}{q} \nabla n \right) - (U - G) \\
\frac{\partial p}{\partial t} &= -\nabla \cdot \left( \mu_p p E_p - \frac{k_B T}{q} \nabla p \right) - (U - G) \\
\nabla \cdot \varepsilon \nabla \psi &= -q(p - n + N_D^+ - N_A^-) - \rho_s \\
\frac{\rho e_0}{\partial t} &= \nabla \cdot \kappa \nabla T + J \cdot E + (E_g + 3k_B T) \cdot (U - G)
\end{align*}
\]

**Level 3 (Level 2 + energy-balance)**

\[
\begin{align*}
J_n &= q \mu_n n E_n + k_b \mu_n (n \nabla T_n + T_n \nabla n) \\
J_p &= q \mu_p p E_p - k_b \mu_p (p \nabla T_p + T_p \nabla p) \\
\frac{\partial (n \omega_n)}{\partial t} + \nabla \cdot S_n &= E_n \cdot J_n - (U - G) \cdot (E_g + \omega_n) - \frac{n(\omega_n - \omega_0)}{\tau_{on}} \\
\frac{\partial (p \omega_p)}{\partial t} + \nabla \cdot S_p &= E_p \cdot J_p - (U - G) \cdot (E_g + \omega_p) - \frac{p(\omega_p - \omega_0)}{\tau_{wp}} \\
S_n &= -\kappa_n \nabla T_n + (\omega_n + k_B T_n) \frac{J_n}{q} \\
S_p &= -\kappa_p \nabla T_p + (\omega_p + k_B T_p) \frac{J_p}{q}
\end{align*}
\]

**Level 1+ (quantum corrected DD)**

\[
\begin{align*}
E_n &= \frac{1}{q} \nabla E_n - \frac{k_B T}{q} \nabla \left( \ln(N_c) - \ln(T^{3/2}) \right) + \nabla \Lambda_n \\
E_p &= \frac{1}{q} \nabla E_p + \frac{k_B T}{q} \nabla \left( \ln(N_v) - \ln(T^{3/2}) \right) + \nabla \Lambda_p \\
\Lambda_n &= -\frac{\hbar^2 \gamma_n}{6 q m_n^*} \frac{\nabla^2 \sqrt{n}}{\sqrt{n}} \\
\Lambda_p &= \frac{\hbar^2 \gamma_p}{6 q m_p^*} \frac{\nabla^2 \sqrt{p}}{\sqrt{p}}
\end{align*}
\]

3. Governing Equations — Hybrid Solvers (1)

QM + EM + DD

Drift-diffusion Equation
\[ \rho = q(p - n + N_D - N_A) \]
\[ J_x = q\mu_x xE \pm kT\mu_x \nabla x, \ x \in \{n, p\} \]
\[ \nabla J_x \pm q \frac{\partial x}{\partial t} - q(R - G) = 0 \]

Maxwell Equation
\[ \nabla \cdot D = \rho, \ \nabla \cdot B = 0 \]
\[ \nabla \times E = -\frac{\partial B}{\partial t}, \ \nabla \times H = J + \frac{\partial D}{\partial t} \]

Ohm’s Law
\[ J = \sigma E \]
\[ \nabla \cdot J + \frac{\partial \rho}{\partial t} = 0 \]

NEGФ
\[ \sigma = -\frac{i}{2\pi} \int dE G^< (E) \]
\[ \nabla^2 V(r) = -4\pi \delta \rho(r) \]

C. Y. Yam, et al. Chemical Society Reviews
44(7): 1763-1776, 2015
3. Governing Equations — Hybrid Solvers (2)

EM-Circuit Model

3. Governing Equations — Hybrid Solvers (3)

Classical EM + Quantum EM

\[ \langle 0 | \hat{E}_S^+ (r_0, \omega_{eg}) \hat{E}_S^- (r_0, \omega_{eg}) | 0 \rangle = \frac{\hbar \omega_{eg}^2}{\pi c^2 \varepsilon_0} [ \bar{n}(\omega_{eg}, T) + 1 ] \Re \mathbf{G}(\mathbf{r}_0, \mathbf{r}_0, \omega_{eg}) \]

Fluctuation-dissipation theorem

thermal issue


MEMS


3. Governing Equations — Remarks

1. Circuit solver is fastest; EM/DD solver is fast; QM solver is slow. Hybrid QM-EM-DD-Circuit solvers are recommended.

2. For Intel corporation, quantum simulation (DFT/ TB/ NEGF) costs 90% of computer resources to carry out 10% of task. DD simulation costs 10% of computer resources to carry out 90% of task.

3. DD model can be modified for modeling new materials based electronic devices (organic, perovskite, graphene, etc). Energy-balance equation may be good for short-channel effect (velocity overshoot, thermoelectric diffusion, and ballistic transport).

4. EM + Circuit + DD solvers are still mainstream multiphysics solvers for emerging electronics. But quantum corrections should be incorporated (density-gradient theory, field-temperature-channel length dependent mobility, etc).
4. Numerical Strategies — Coupling Schemes

1. Coupling by current (resulting from carrier transport or electric circuit)

2. Coupling by constitutive parameters (permittivity and permeability)

3. Coupling by geometries and boundaries

Maxwell’s equations

\[ \nabla \times E = -\frac{\partial B}{\partial t} \quad \iff \quad \nabla \times \tilde{E} = -j\omega \tilde{B} \]

\[ \nabla \times H = J + \frac{\partial D}{\partial t} \quad \iff \quad \nabla \times \tilde{H} = \tilde{J} + j\omega \tilde{D} \]

\[ \nabla \cdot D = \rho \quad \iff \quad \nabla \cdot \tilde{D} = \tilde{\rho} \]

\[ \nabla \cdot B = 0 \quad \iff \quad \nabla \cdot \tilde{B} = 0 \]

Current continuity equation

\[ \nabla \cdot J + \frac{\partial \rho}{\partial t} = 0 \quad \iff \quad \nabla \cdot \tilde{J} + j\omega \tilde{\rho} = 0 \]
4. Numerical Strategies — General Forms

**Transient form**

\[
\begin{align*}
\frac{\partial}{\partial t} u_1 &= f_1(u_1, u_2, c_1(u_2)) \\
\frac{\partial}{\partial t} u_2 &= f_2(u_2, u_1, c_2(u_1))
\end{align*}
\]

**Steady form**

\[
\begin{align*}
f_1(u_1, u_2, c_1(u_2)) &= 0 \\
f_2(u_2, u_1, c_2(u_1)) &= 0
\end{align*}
\]

physical fields: \(u_1, u_2\) (scalar or vector)

physical parameters: \(c_1, c_2\) (scalar or vector)

**Discretization Rules**

- Electromagnetics (EM): dielectric wavelength or skin depth
- Drift-diffusion (DD): Debye length
- Quantum Mechanism (QM): electron wavelength
- Circuit: No spatial grid

**Strategies**

1. Different spatial grid sizes are adopted for different systems. From coarse-to-fine grids, lifting or interpolation is used, and from fine-to-coarse grids restriction, integration or antipolarization is used. Alternatively, the grids with basis functions of different orders are adopted.

2. Remove spatial grids in one system by the reduced eigenmode/eigenstate expansion technique ([Computer Physics Communications, 215: 63-70, 2017](#)).

**Remarks**

Stability issue and physical conservation (charge, flux, momentum, energy, etc)
4. Numerical Strategies — Multiscale in Time (1)

Discretization Rule

EM: propagation time or lifetime (for a photon)  
depends on device sizes, group velocity, absorption coefficient, quality factor, etc.

DD: relaxation time (from non-equilibrium to equilibrium states)  
depends on mean free path, coherence length, velocity of electron, etc.

QM: transition time (from an energy level to another) and decoherence time  
depends on field intensity, dipole moment, EM environment, etc.

Circuit: RLC delay time (from transient to steady states)  
depends on resistance, capacitance, and inductance.

Timescale is important!
4. Numerical Strategies — Multiscale in Time (2)

Strategies

1. When one system/process has several times faster timescale relative to another, a simple strategy is to use an integer multiple of the faster timescale for the slow timescale.

![Diagram showing time steps and intervals]

2. Explicit scheme for fast timescale or linear/non-stiff problem and implicit for the slow timescale or nonlinear/stiff problem.

\[
\text{Explicit} \quad u_1(t_{n+1}) = u_1(t_n) + \Delta_t f_1(u_1(t_n), u_2, c_1(u_2))
\]

\[
\text{Implicit} \quad u_1(t_{n+1}) = u_1(t_n) + \Delta_t f_1(u_1(t_{n+1}), u_2, c_1(u_2))
\]

4. Numerical Strategies — Multiscale in Time (3)

Strategies (Cont …)

When one system/process has an extremely (> $10^2$~$10^3$) faster timescale that the other processes, we can use the one-way non-self-consistent coupling or directly insert the faster physical quantity into the other PDE systems.

1. Electromagnetic-thermal problem (Maxwell & thermal-conduction equations) propagation of electromagnetic pulse is much faster than diffusion of thermal flux.

2. Exciton delocalization and diffusion-dissociation problem in organic electronics delocalization is ultrafast (~ fs) and diffusion-dissociation is slow (~ ps).

H. H. Zhang, etal. Scientific Reports 8: 2652, 2018

Coupled evolution of a transient multiphysics problem

\[
\begin{align*}
\frac{u_1^{n+1} - u_1^n}{\Delta_t} &= f_1(u_1^n, u_2^n, c_1(u_2^n)) \\
\frac{u_2^{n+1} - u_2^n}{\Delta_t} &= f_2(u_2^n, u_1^{n+1}, c_2(u_1^{n+1}))
\end{align*}
\]

**explicit**
No sparse matrix inversion
Stability is bad
Conditionally stable

**semi-implicit**
Sparse matrix inversion
Stability is better
Conditionally stable

**implicit**
Newton’s method in each step
Stability is best
Unconditionally stable
4. Numerical Strategies — Numerical Methods (2)

Equilibrium of a multiphysics problem (the coupling concepts are also applicable to the transient problems)

\[
\begin{align*}
\begin{cases}
f_1(u_1, u_2, c_1(u_2)) = 0 \\
f_2(u_2, u_1, c_2(u_1)) = 0
\end{cases}
\quad \Rightarrow \quad F(u, c(u)) = 0
\end{align*}
\]

- **strong coupling**
  - Newton’s method
  - \( u^{k+1} = u^k - J^{-1}(u^k)F(u^k) \)
  - DD equations

- **weak coupling**
  - self-consistent solution
  - \( f_1(u_1^{k+1}, u_2^k, c_1(u_2^k)) = 0 \)
  - EM-QM
  - EM-circuit

- **one-way coupling**
  - sequential solution
  - \( \begin{cases} f_1(u_1) = 0 \\
f_2(u_2, u_1, c_2(u_1)) = 0 \end{cases} \)
  - EM-thermal
  - organic electronics
5. Conclusion

EM-Multiphysics simulation for emerging electronics is a very challenging field. There is no universal panacea.

1. We have to understand electronics problem with a critical/deep physical insight.
2. We have to figure out the coupling strategies and numerical solutions.
3. We have to know the pros and cons of various numerical algorithms.
4. We have to identify the physical bounds of a multiphysics model.
5. We have to learn as much as possible to take a new look at governing equations.
6. We have to collaborate with mathematicians, physicists, chemists, engineers, etc.
7. We have to train our students for working in the multidisciplinary fields.
EM-Multiphysics Education in Engineering College

Knowledge Grows Like a Tree

Real-World Applications and Technologies

Application-Based Engineering

Science-Based Engineering

Mathematics, Physics, Science

Weng Cho Chew
Purdue University
“Scientists investigate that which already is; Engineers create that which has never been.”
—— Albert Einstein

Thanks for your attention!