Electromagnetics-Multiphysics Simulation for Emerging Electronics

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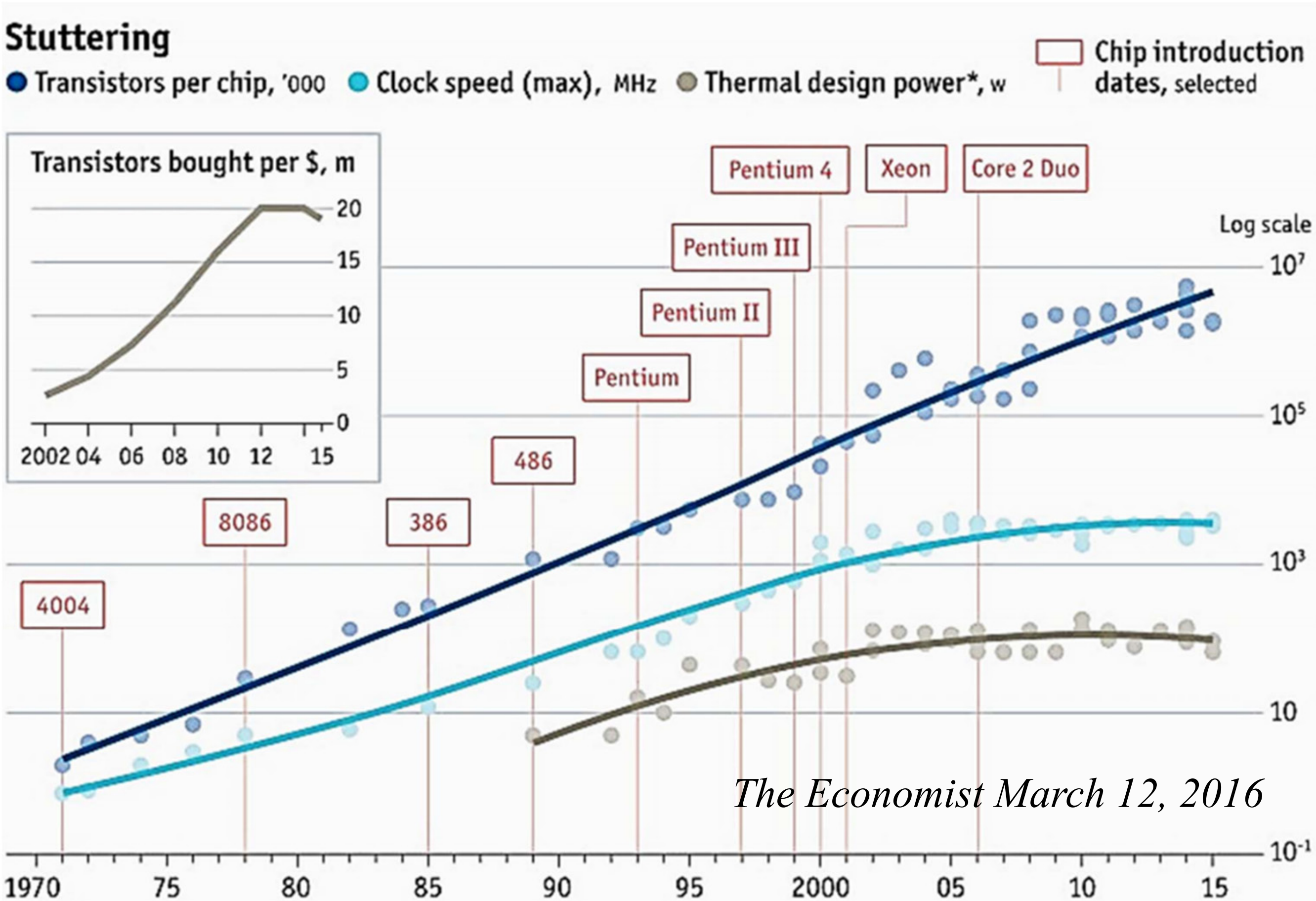
Contents

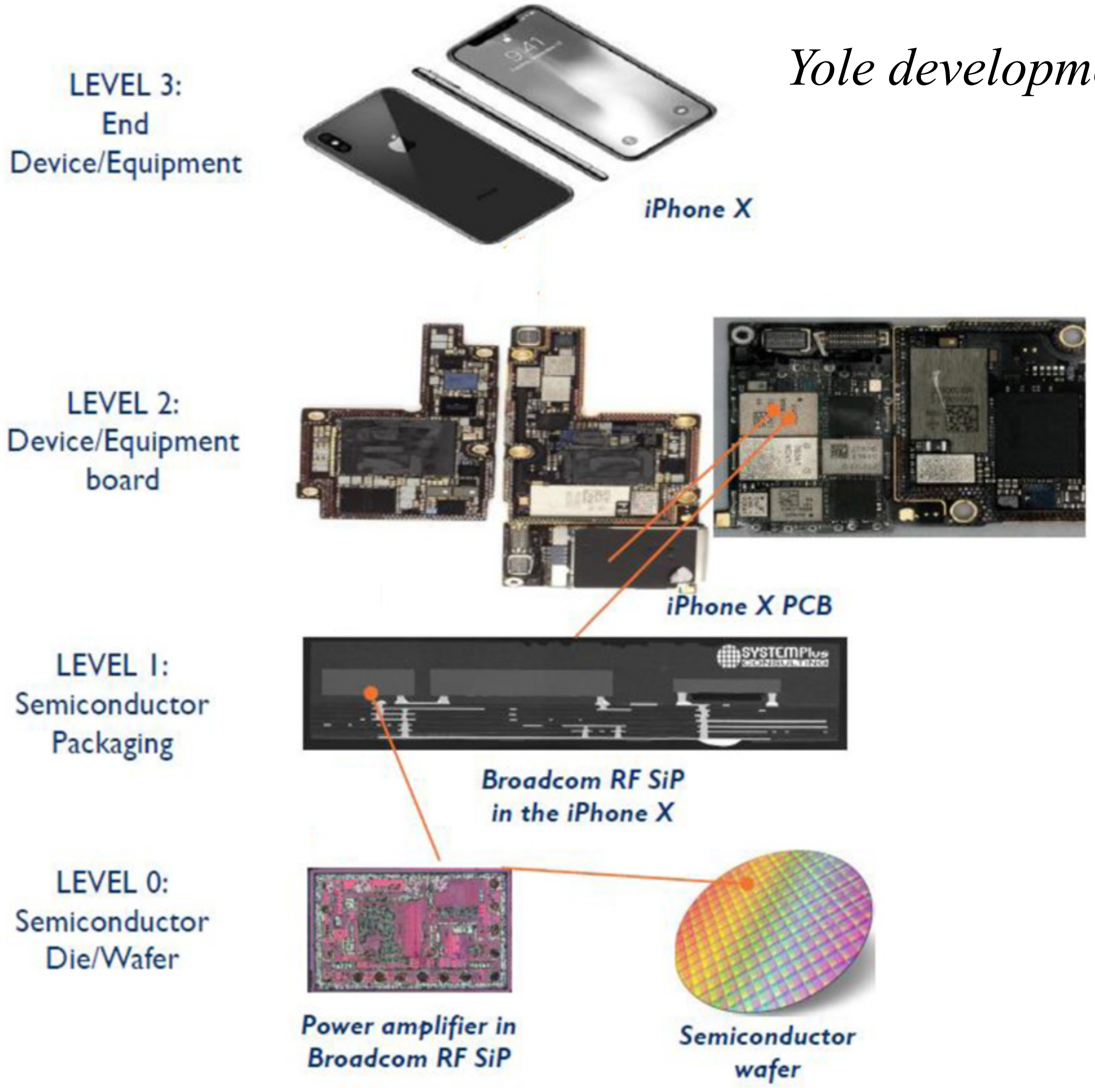
1. Background — After Moore's law

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)



Yole development

system levels

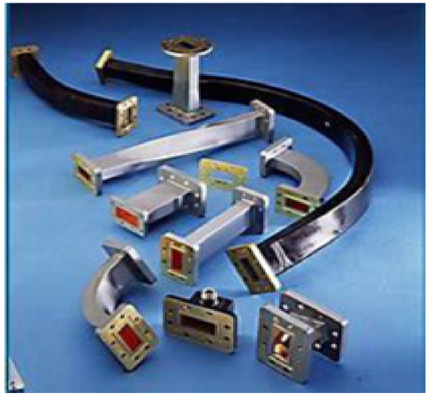
board levels

assembly or package levels

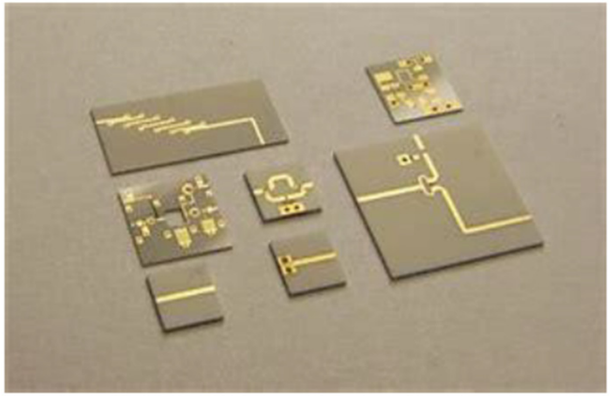
device/circuit/chip levels

1. Background — Complexity of Electronics (2)

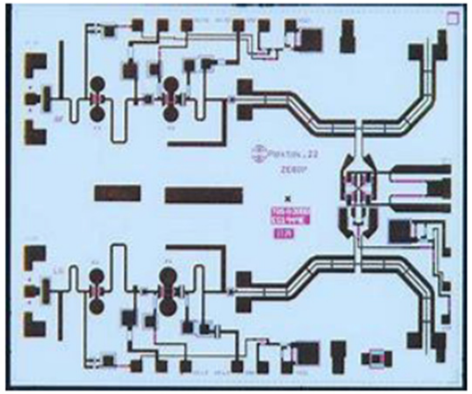
Bulk Waveguide

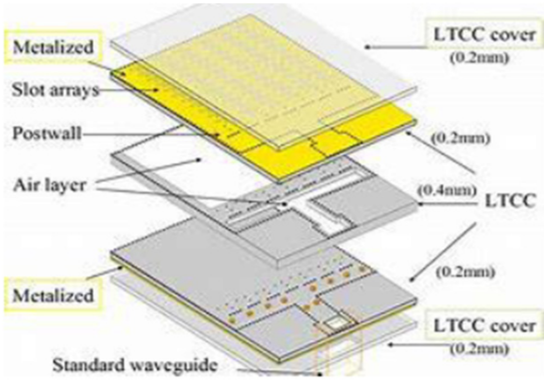


Microwave Integrated Circuits, MICs

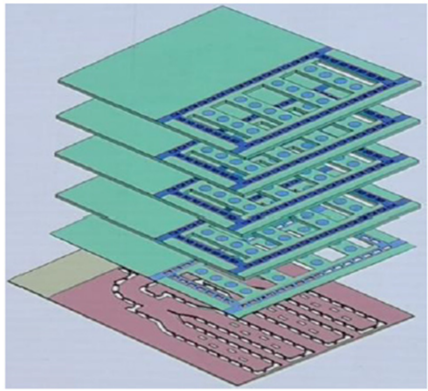


Monolithic MICs, MMICs





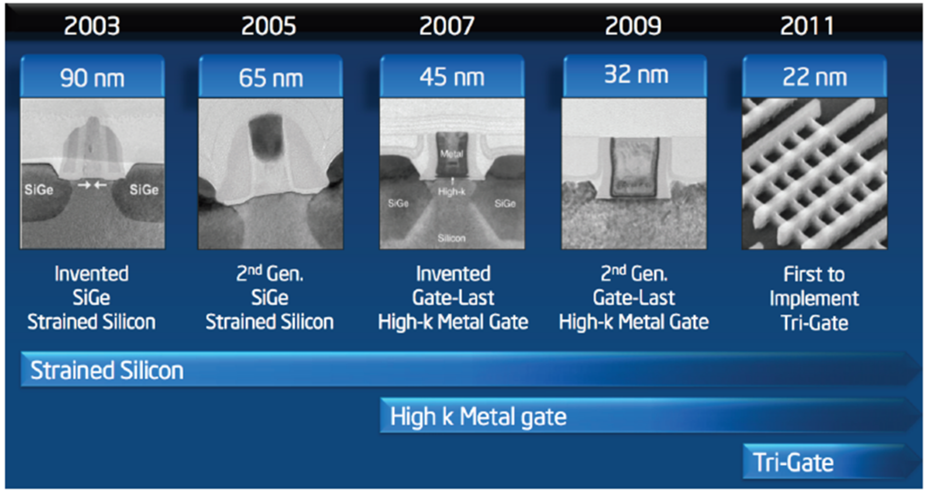
Multilayered MMIC/LTCC

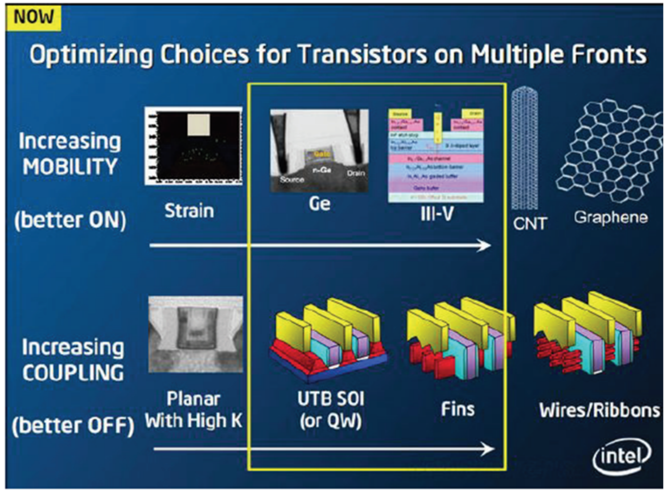


Substrate Integration

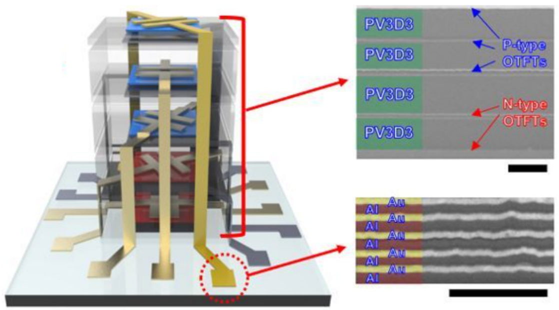
Sheng Sun
UESTC

1. Background — Emerging Electronics



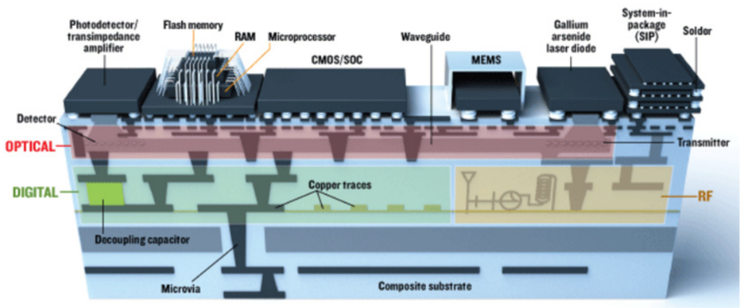


New Materials/ Tech



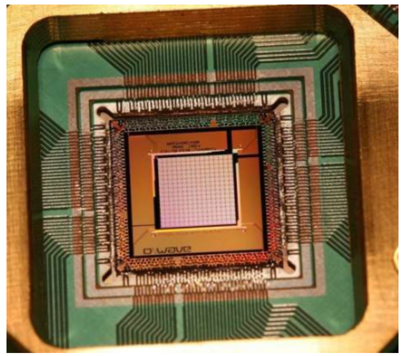
Organic TFT/FET

New Architecture



3D heterogeneous integration

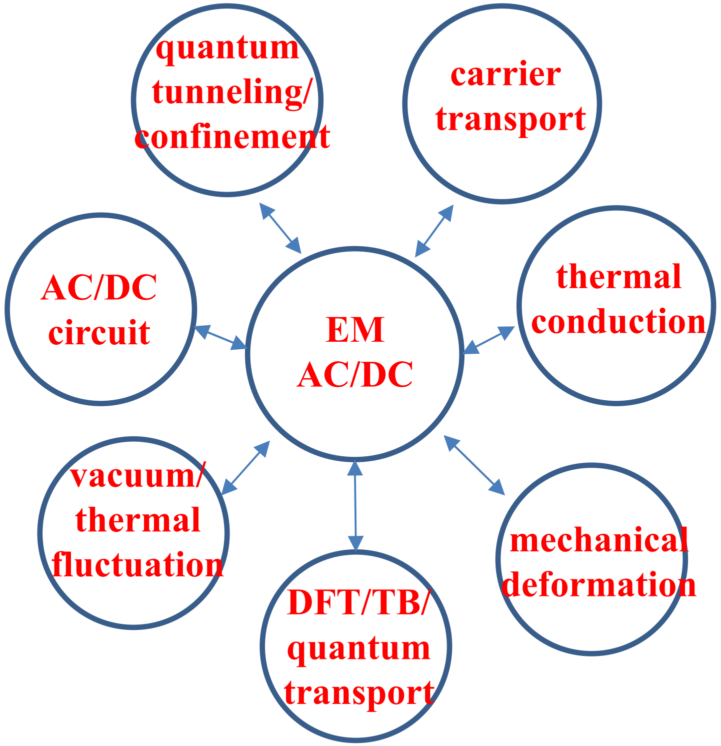
New Principle



quantum entanglement

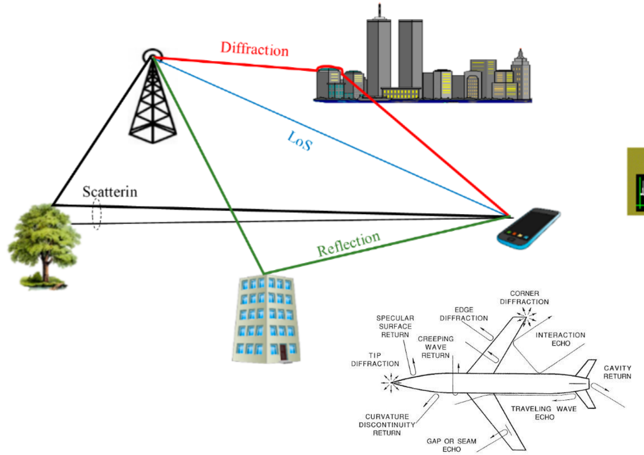
1. Background — EM-Multiphysics Simulation

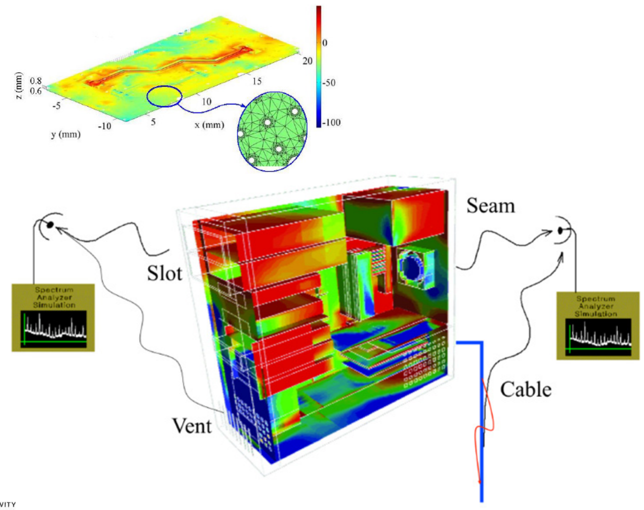
EM compatibility/ interference (EMC/EMI)
signal integrity/ power integrity (SI/PI)
short-channel effects
quantum effects
field-circuit coupling
thermal-mechanical issue
electro-static discharge
parasitic effect
packaging
…

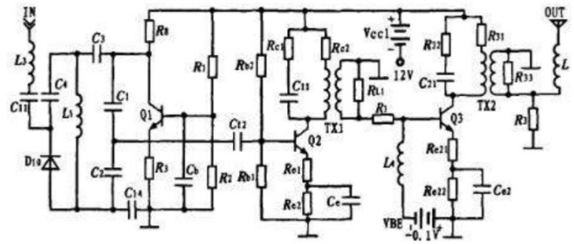


2. Analogy — Physical Behaviors of Photons

D: object size; λ: wavelength



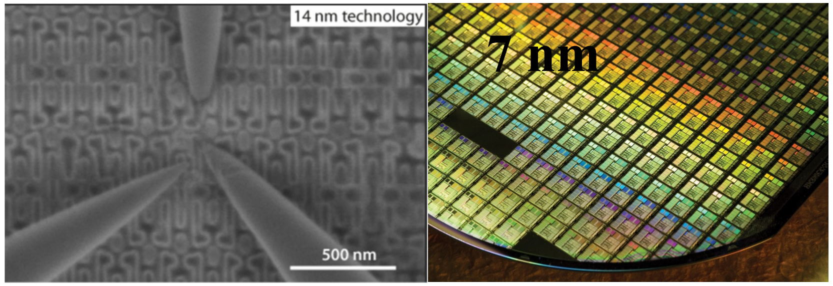




ray physics	wave physics	circuit physics
D>>λ	D~λ	D<<λ
Asymptotic solvers PO/PTD/GO/GTD/UTD/ Ray tracing: Xpatch	Full-wave solvers FDTD: CST FEM: ANSYS, COMSOL MOM: FEKO, ADS	DC/AC circuit solvers nodal equation: SPICE, Multisim

2. Analogy — Physical Behaviors of Electrons

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

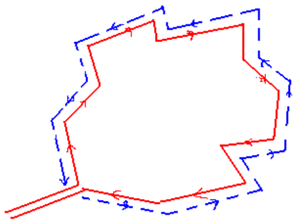


mesoscopic physics
quantum hydrodynamics

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

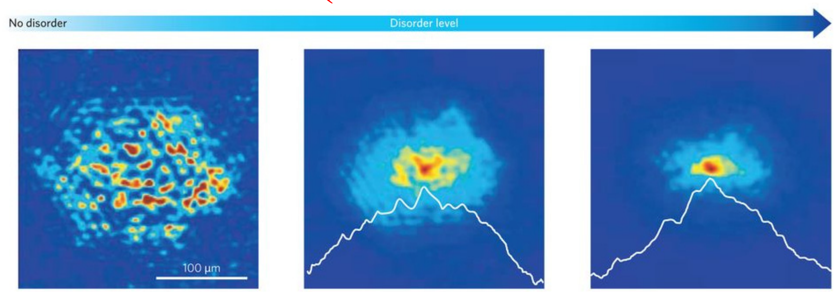
3. Anderson localization (metal-insulator transitions): EM waves in random media

time-reversal property



back scattering enhancement

disorder increase (diffusion → localization)



3. Governing Equations — From Classical to Quantum Worlds

quantum ↑ classical

electron	photon
NEGF/ TB/ DFT equation	Quantized Maxwell equation
Boltzmann equation	Vector-scalar potential equation
Energy balance equation	Maxwell equation
Hydrodynamic equation	Parabolic wave equation
Drift-diffusion equation	Ray equation

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

3. Governing Equations — Drift-Diffusion (DD) Equations Revisited

Level 1 (DD)

$$\begin{cases} \dfrac{\partial n}{\partial t} = \nabla \cdot \left(\mu_n n \mathbf{E}_n + \mu_n \dfrac{k_b T}{q} \nabla n \right) - (U - G) \\ \dfrac{\partial p}{\partial t} = -\nabla \cdot \left(\mu_p p \mathbf{E}_p - \mu_p \dfrac{k_b T}{q} \nabla p \right) - (U - G) \\ \nabla \cdot \varepsilon \nabla \psi = -q(p - n + N_D^+ - N_A^-) - \rho_s \end{cases}$$

Level 2 (Level 1 + heat conduction)

$$\begin{cases} \dfrac{\partial n}{\partial t} = \nabla \cdot \left(\mu_n n \mathbf{E}_n + \mu_n \dfrac{k_b T}{q} \nabla n + \mu_n \dfrac{k_b \nabla T}{q} n \right) - (U - G) \\ \dfrac{\partial p}{\partial t} = -\nabla \cdot \left(\mu_p p \mathbf{E}_p - \mu_p \dfrac{k_b T}{q} \nabla p - \mu_p \dfrac{k_b \nabla T}{q} p \right) - (U - G) \\ \nabla \cdot \varepsilon \nabla \psi = -q\left(p - n + N_D^+ - N_A^-\right) - \rho_s \\ \rho c_p \dfrac{\partial T}{\partial t} = \nabla \cdot \kappa \nabla T + \mathbf{J} \cdot \mathbf{E} + (E_g + 3k_b T) \cdot (U - G) \end{cases}$$

Level 3 (Level 2 + energy-balance)

$$\begin{cases} \mathbf{J}_n = q\mu_n n \mathbf{E}_n + k_b \mu_n (n \nabla T_n + T_n \nabla n) \\ \mathbf{J}_p = q\mu_p p \mathbf{E}_p - k_b \mu_p \left(p \nabla T_p + T_p \nabla p\right) \\ \dfrac{\partial (n\omega_n)}{\partial t} + \nabla \cdot \mathbf{S}_n = \mathbf{E}_n \cdot \mathbf{J}_n - (U - G) \cdot (E_g + \omega_n) - \dfrac{n(\omega_n - \omega_0)}{\tau_{\omega n}} \\ \dfrac{\partial \left(p\omega_p\right)}{\partial t} + \nabla \cdot \mathbf{S}_p = \mathbf{E}_p \cdot \mathbf{J}_p - (U - G) \cdot (E_g + \omega_p) - \dfrac{p(\omega_p - \omega_0)}{\tau_{\omega p}} \\ \mathbf{S}_n = -\kappa_n \nabla T_n - (\omega_n + k_b T_n) \dfrac{\mathbf{J}_n}{q} \qquad \omega_c = \dfrac{3}{2} k_b T_c \\ \mathbf{S}_p = -\kappa_p \nabla T_p + \left(\omega_p + k_b T_p\right) \dfrac{\mathbf{J}_p}{q} \qquad \omega_0 = \dfrac{3}{2} k_b T \\ \rho c_p \dfrac{\partial T}{\partial t} = \nabla \cdot \kappa \nabla T + \left(E_g + \omega_n + \omega_p\right) \cdot (U - G) + \dfrac{n(\omega_n - \omega_0)}{\tau_{\omega n}} + \dfrac{p(\omega_p - \omega_0)}{\tau_{\omega p}} \end{cases}$$

Level 1+ (quantum corrected DD)

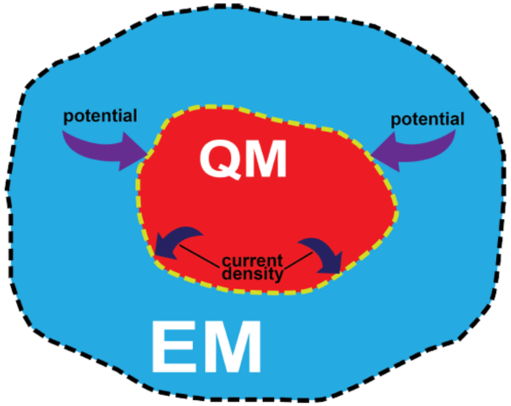
$$\begin{cases} \mathbf{E}_n = \dfrac{1}{q} \nabla E_c - \dfrac{k_b T}{q} \nabla \left(\ln(N_c) - \ln(T^{3/2}) \right) + \nabla \Lambda_n \\ \mathbf{E}_p = \dfrac{1}{q} \nabla E_v + \dfrac{k_b T}{q} \nabla \left(\ln(N_v) - \ln(T^{3/2}) \right) + \nabla \Lambda_p \\ \Lambda_n = -\dfrac{\hbar^2 \gamma_n}{6qm_n^*} \dfrac{\nabla^2 \sqrt{n}}{\sqrt{n}} \\ \Lambda_p = \dfrac{\hbar^2 \gamma_p}{6qm_p^*} \dfrac{\nabla^2 \sqrt{p}}{\sqrt{p}} \end{cases}$$

density-gradient

M. Lundstrom, Fundamentals of Carrier Transport, Cambridge University Press, 2000.

3. Governing Equations — Hybrid Solvers (1)

QM + EM + DD



NEGF

$$\sigma = -\frac{i}{2\pi}\int dEG^{<}(E)$$

$$\nabla^2 V(r) = -4\pi\delta\rho(r)$$

Ohm's Law

$$J = \sigma E$$

$$\nabla \cdot J + \frac{\partial \rho}{\partial t} = 0$$

Drift-diffusion Equation

$$\rho = q(p - n + N_D - N_A)$$

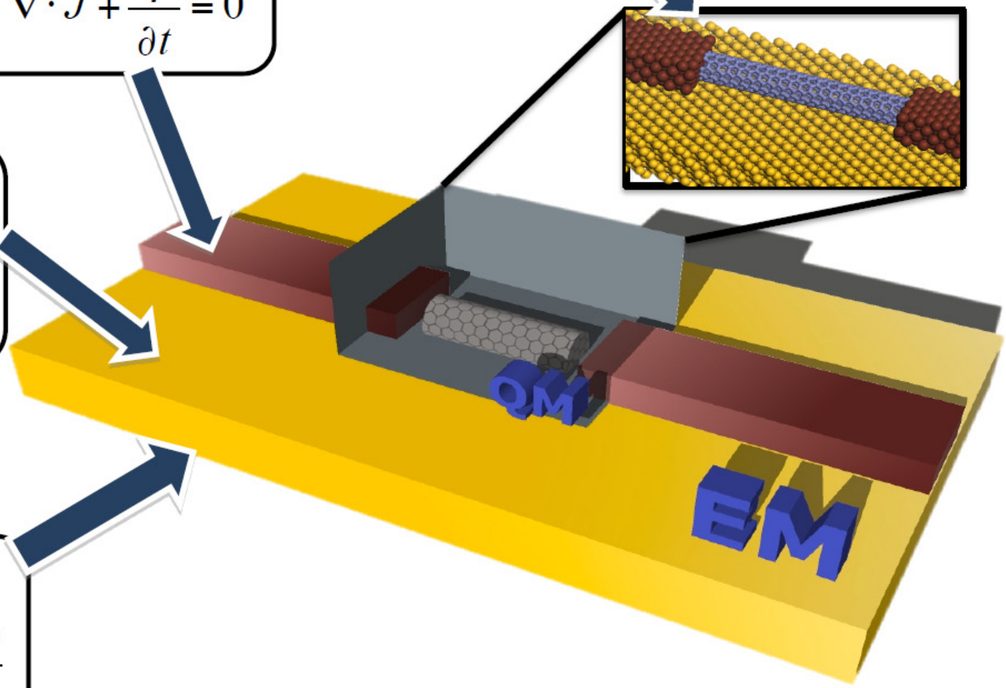
$$J_x = q\mu_x x E \pm kT\mu_x \nabla x,\ x \in \{n, p\}$$

$$\nabla J_x \pm q\frac{\partial x}{\partial t} - q(R - G) = 0$$

Maxwell Equation

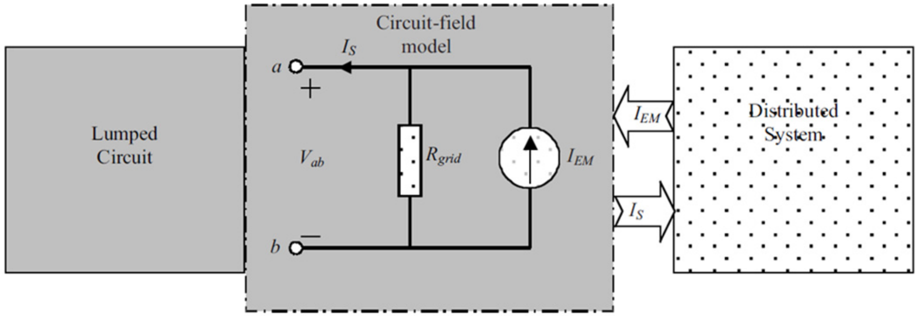
$$\nabla \cdot D = \rho,\ \nabla \cdot B = 0$$

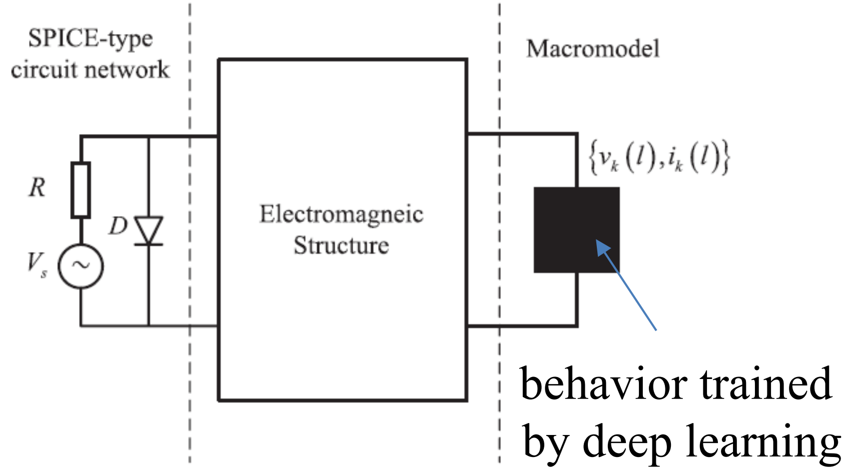
$$\nabla \times E = -\frac{\partial B}{\partial t},\ \nabla \times H = J + \frac{\partial D}{\partial t}$$

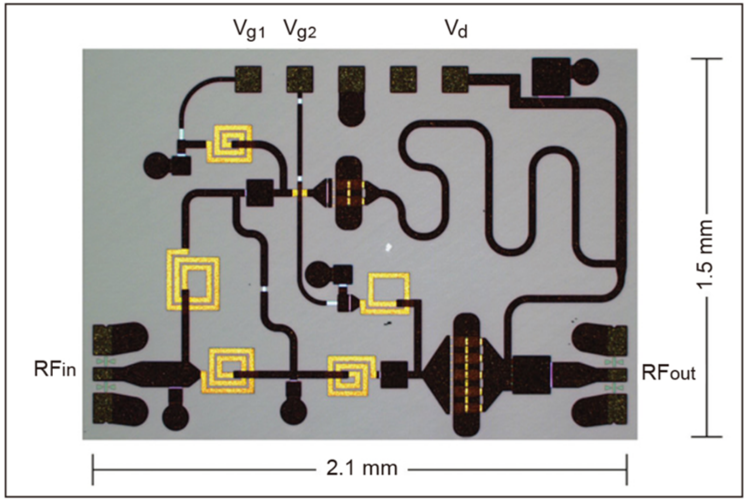


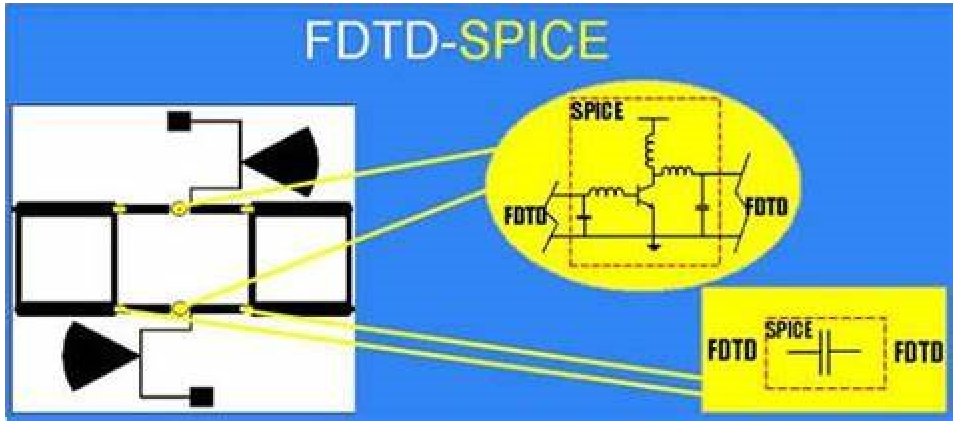
C. Y. Yam, etal. Chemical Society Reviews 44(7): 1763-1776, 2015

EM-Circuit Model









H. H. Zhang, etal. IEEE Transactions on Antennas and Propagation 64(7): 3233-3238, 2016
W. Sui, Time-Domain Computer Analysis of Nonlinear Hybrid Systems, CRC Press, 2002

3. Governing Equations — Hybrid Solvers (3)

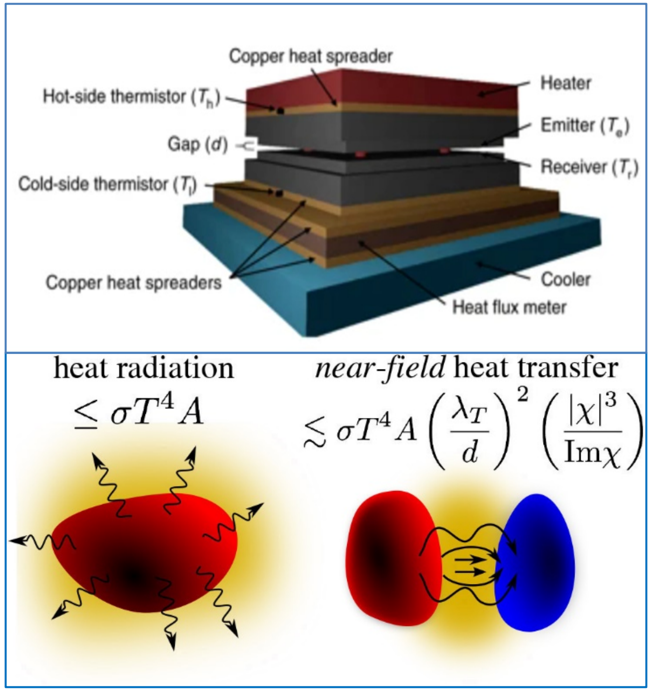
Classical EM + Quantum EM

W. E. I. Sha, IEEE Journal on Multiscale and Multiphysics Computational Techniques, 3: 198-213, 2018.

$$\langle 0|\hat{\mathbf{E}}_S^+(\mathbf{r}_0,\omega_{eg})\hat{\mathbf{E}}_S^-(\mathbf{r}_0,\omega_{eg})|0\rangle = \frac{\hbar\omega_{eg}^2}{\pi c^2 \epsilon_0}[\bar{n}(\omega_{eg},T)+1]\Im\overline{\mathbf{G}}(\mathbf{r}_0,\mathbf{r}_0,\omega_{eg})$$

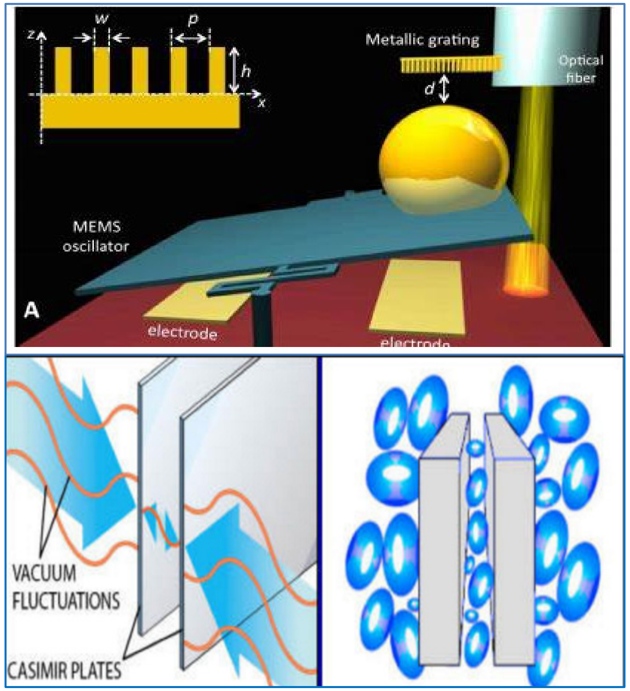
Fluctuation-dissipation theorem

thermal issue



J. DeSutter, etal. Nature Nanotechnology 14: 751-755, 2019

MEMS



F. Intravaia, etal. Nature Communications 4: 2515, 2013

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).

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

$$\nabla\times\mathbf{E}=-\frac{\partial\mathbf{B}}{\partial t}\quad\leftrightarrow\quad\nabla\times\tilde{\mathbf{E}}=-j\omega\tilde{\mathbf{B}}$$

$$\nabla\times\mathbf{H}=\mathbf{J}+\frac{\partial\mathbf{D}}{\partial t}\quad\leftrightarrow\quad\nabla\times\tilde{\mathbf{H}}=\tilde{\mathbf{J}}+j\omega\tilde{\mathbf{D}}$$

$$\nabla\cdot\mathbf{D}=\boldsymbol{\rho}\quad\leftrightarrow\quad\nabla\cdot\tilde{\mathbf{D}}=\tilde{\boldsymbol{\rho}}$$

$$\nabla\cdot\mathbf{B}=0\quad\leftrightarrow\quad\nabla\cdot\tilde{\mathbf{B}}=0$$

Current continuity equation

$$\nabla\cdot\mathbf{J}+\frac{\partial\rho}{\partial t}=0\quad\leftrightarrow\quad\nabla\cdot\tilde{\mathbf{J}}+j\omega\tilde{\rho}=0$$

4. Numerical Strategies — General Forms

Transient form

$$\begin{cases} \dfrac{\partial}{\partial t} u_1 = f_1\left(u_1, u_2, c_1(u_2)\right) \\ \dfrac{\partial}{\partial t} u_2 = f_2\left(u_2, u_1, c_2(u_1)\right) \end{cases}$$

Steady form

$$\begin{cases} f_1\left(u_1, u_2, c_1(u_2)\right) = 0 \\ f_2\left(u_2, u_1, c_2(u_1)\right) = 0 \end{cases}$$

physical fields: u_1, u_2 (scalar or vector)

physical parameters: c_1, c_2 (scalar or vector)

4. Numerical Strategies — Multiscale in Space

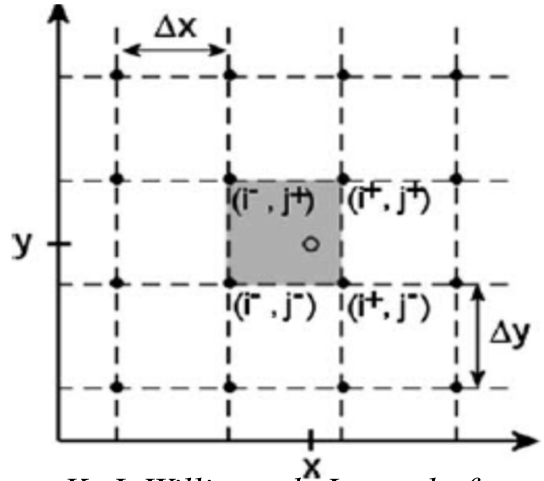
Discretization Rules

Electromagnetics (EM): dielectric wavelength or skin depth

Drift-diffusion (DD): Debye length

Quantum Mechanism (QM): electron wavelength

Circuit: No spatial grid



K. J. Willis, etal. Journal of Computational Electronics 8: 153, 2009

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 anterpolartion 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

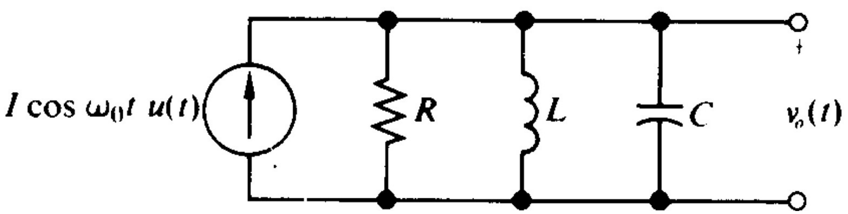
EM: propagation time or lifetime (for a photon)
depends on device sizes, group velocity, absorption coefficient, quality factor, etc.

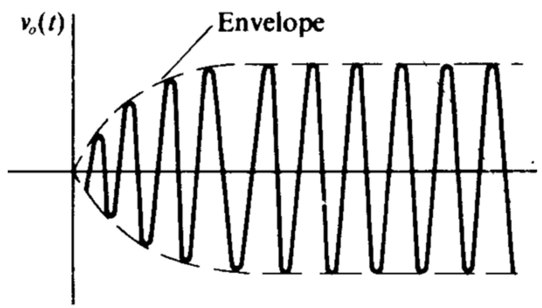
DD: relaxation time (from non-equilibrium to equilibrium states)
depends on mean free path, coherence length, velocity of electron, etc.

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 !

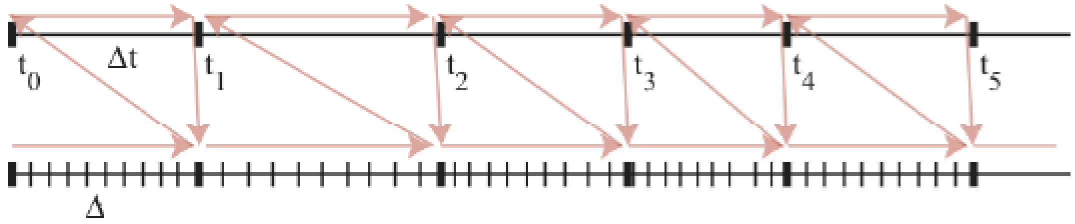




4. Numerical Strategies — Multiscale in Time (2)

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.



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

Explicit $u_1(t_{n+1}) = u_1(t_n) + \Delta_t f_1\left(u_1(t_n), u_2, c_1(u_2)\right)$

Implicit $u_1(t_{n+1}) = u_1(t_n) + \Delta_t f_1\left(u_1(t_{n+1}), u_2, c_1(u_2)\right)$

D. E. Keyes, etal. International Journal of High Performance Computing Applications 27(1): 4-83, 2013

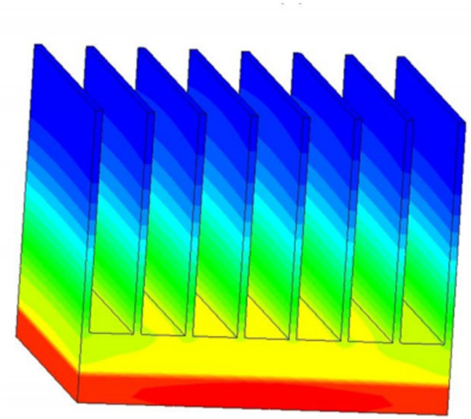
4. Numerical Strategies — Multiscale in Time (3)

Strategies (Cont …)

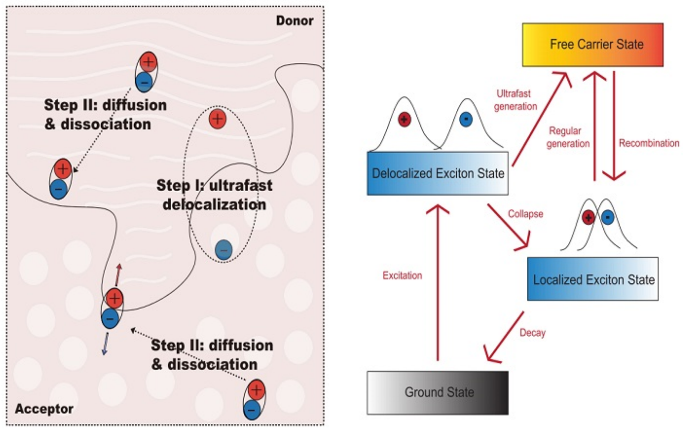
When one system/process has an extremely (> 10^2 ~10^3) faster timescale that the other processes, we can use the one-way non-self-consistent coupling or directly insert the faster physical quantity into the other PDE systems.

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



Z. S. Wang, etal. Journal of Applied Physics 120(21): 213101, 2016

4. Numerical Strategies — Numerical Methods (1)

Coupled evolution of a transient multiphysics problem

$$\begin{cases} \frac{\partial}{\partial t} u_1 = f_1\left(u_1, u_2, c_1(u_2)\right) \\ \frac{\partial}{\partial t} u_2 = f_2\left(u_2, u_1, c_2(u_1)\right) \end{cases}$$

explicit	semi-implicit	implicit
$\frac{u_1^{n+1} - u_1^n}{\Delta_t} = f_1\left(u_1^n, u_2^n, c_1(u_2^n)\right)$	$\frac{u_1^{n+1} - u_1^n}{\Delta_t} = f_1\left(u_1^{n+1}, u_2^n, c_1(u_2^n)\right)$	$\frac{u_1^{n+1} - u_1^n}{\Delta_t} = f_1\left(u_1^{n+1}, u_2^{n+1}, c_1(u_2^{n+1})\right)$
$\frac{u_2^{n+1} - u_2^n}{\Delta_t} = f_2\left(u_2^n, u_1^{n+1}, c_2(u_1^{n+1})\right)$	$\frac{u_2^{n+1} - u_2^n}{\Delta_t} = f_2\left(u_2^{n+1}, u_1^{n+1}, c_2(u_1^{n+1})\right)$	$\frac{u_2^{n+1} - u_2^n}{\Delta_t} = f_2\left(u_2^{n+1}, u_1^{n+1}, c_2(u_1^{n+1})\right)$
No sparse matrix inversion Stability is bad Conditionally stable	Sparse matrix inversion Stability is better Conditionally stable	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)

$$\begin{cases} f_1\left(u_1, u_2, c_1(u_2)\right) = 0 \\ f_2\left(u_2, u_1, c_2(u_1)\right) = 0 \end{cases} \dashrightarrow \mathbf{F}\left(\mathbf{u}, c(\mathbf{u})\right) = 0$$

strong coupling

Newton's method

$$\mathbf{u}^{k+1} = \mathbf{u}^k - J^{-1}(\mathbf{u}^k)\mathbf{F}(\mathbf{u}^k)$$

$$J = \frac{\partial \mathbf{F}}{\partial \mathbf{u}} = \begin{bmatrix} \frac{\partial f_1}{\partial u_1} & \frac{\partial f_1}{\partial u_2} \\ \frac{\partial f_2}{\partial u_1} & \frac{\partial f_2}{\partial u_2} \end{bmatrix}$$

DD equations

weak coupling

self-consistent solution

$$f_1\left(u_1^{k+1}, u_2^k, c_1(u_2^k)\right) = 0$$

$$f_2\left(u_2^{k+1}, u_1^{k+1}, c_2(u_1^{k+1})\right) = 0$$

EM-QM

EM-circuit

one-way coupling

sequential solution

$$\begin{cases} f_1\left(u_1\right) = 0 \\ f_2\left(u_2, u_1, c_2(u_1)\right) = 0 \end{cases}$$

EM-thermal

organic electronics

Wei SHA

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.

Knowledge Grows Like a Tree

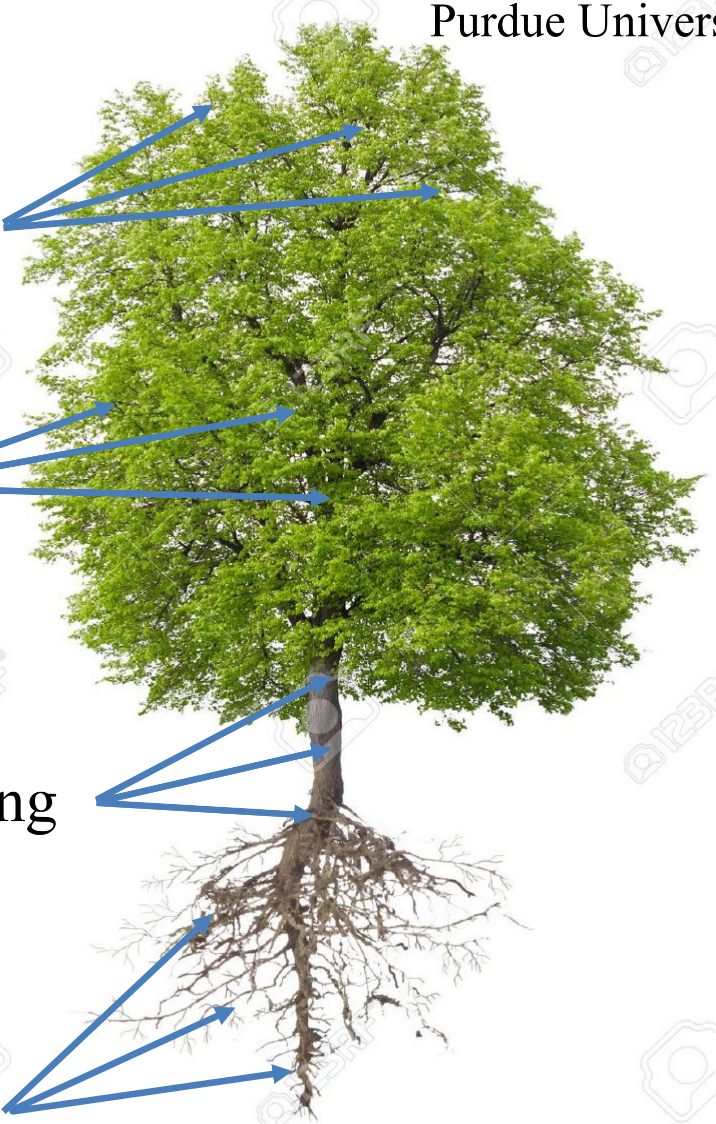
Weng Cho Chew
Purdue University

Real-World Applications and Technologies

Application-Based Engineering

Science-Based Engineering

Mathematics, Physics, Science



Thanks for your attention !

"Scientists investigate that which already is;
Engineers create that which has never been."
—— Albert Einstein