The Challenges and Remedies of Multiphysics Modeling — A Personal View

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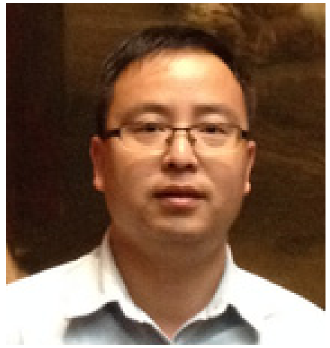

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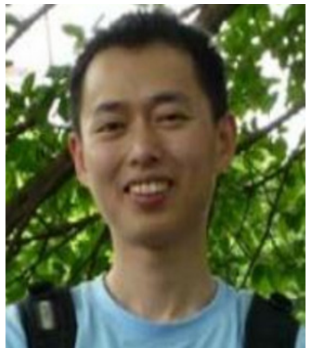

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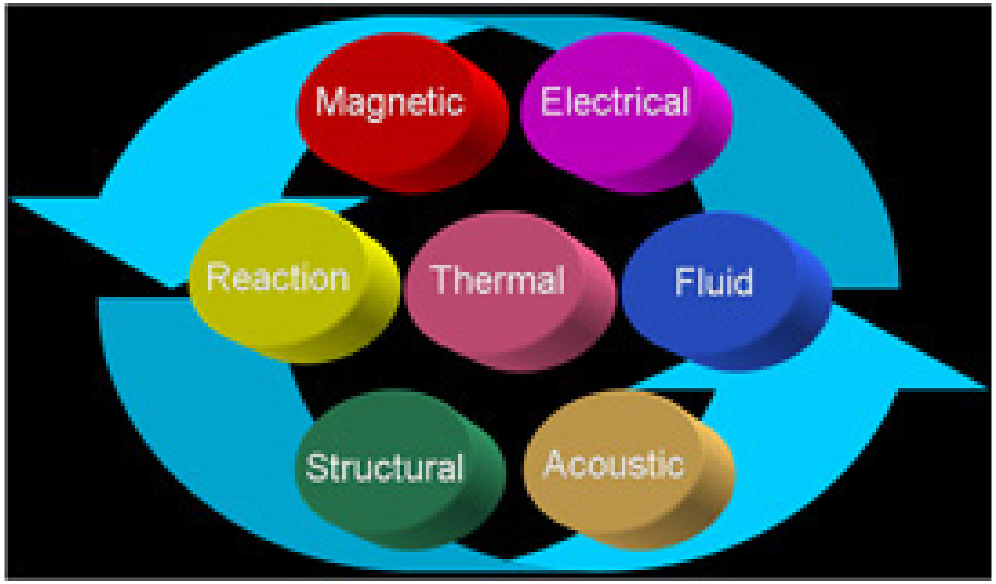
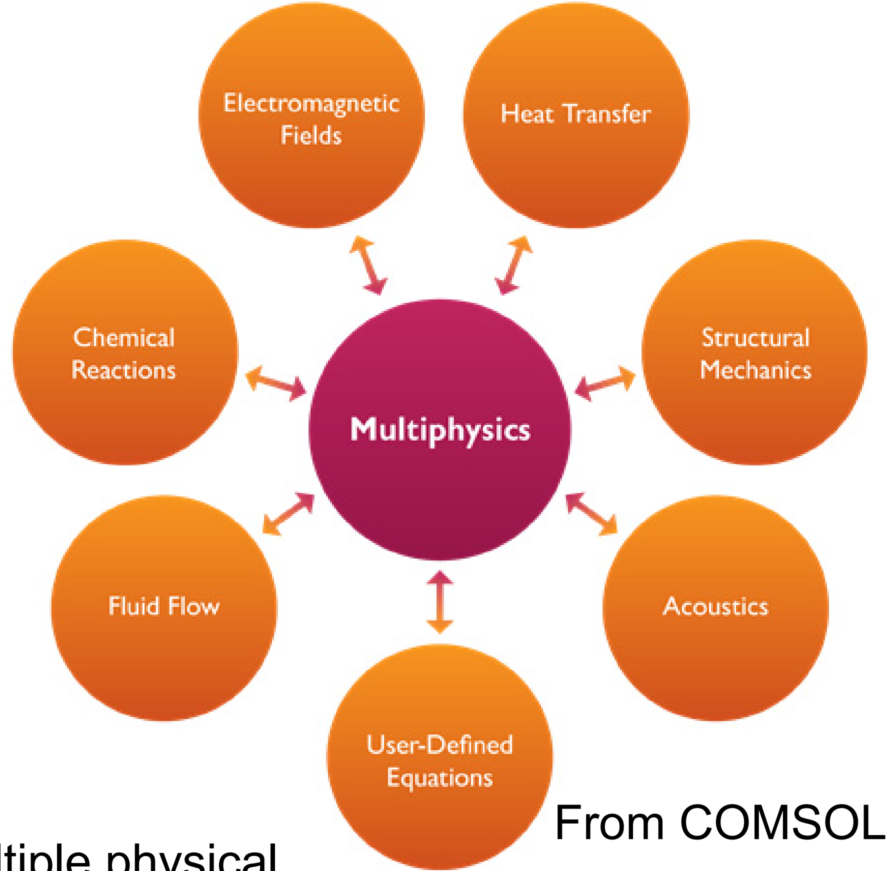
INTRODUCTION TO MULTIPHYSICS

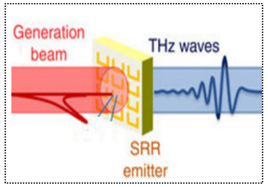




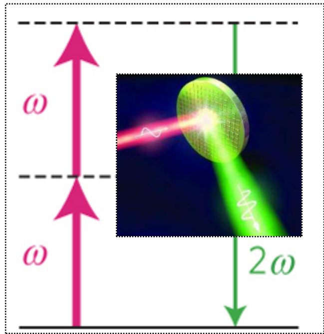
From COMSOL

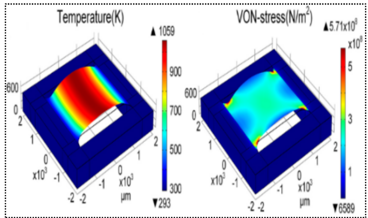
Multiphysics treats simulations that involve multiple physical models or multiple simultaneous physical phenomena. Multiphysics typically involves solving coupled systems of partial differential equations (PDEs). We lived in a multiphysical world!

MAXWELL EQUATION IN MULTIPHYSICS



Boltzmann Equation for **Electron**
[drift-diffusion, current continuity, energy balance]
(electronics and optoelectronics)

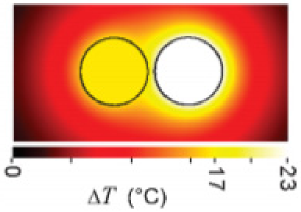




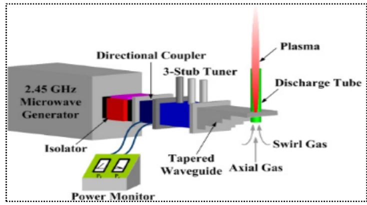
Heat Equation for **Phonon**
(acoustic and elastic waves)

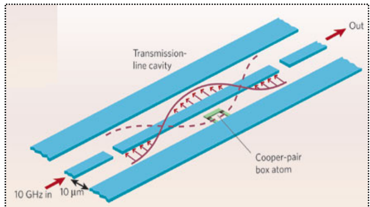
Maxwell Equation for **Photon**
(electromagnetics and optics)

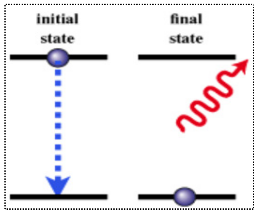
Hydrodynamic Equation
(nonlinear optics & plasma)

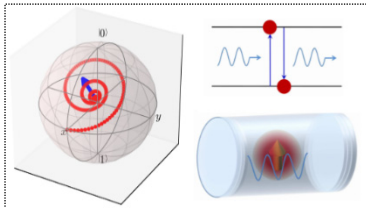


Schrödinger Equation & Density Functional Theory
for **Quantum** Effect









CHALLENGES IN MULTIPHYSICS SIMULATION

- Multiscale (in Space and Time Domains)
- Floating Point Overflow/Underflow (Scale Difference of Units)
- Stability in Transient Simulation (Explicit, Implicit, and Semi-implicit Schemes)
- Strong and Weak Coupling (Newton's Method, Self-Consistent, One-Way Coupling)
- Benchmark Issue (Analytical Solution and Physical Conservation Law)
- Prediction Capability (Maxwell equation v.s. Semiconductor equation)
- Breakdown of Model (Classical, Semi-Classical, and Quantum)

MULTISCALE (1)

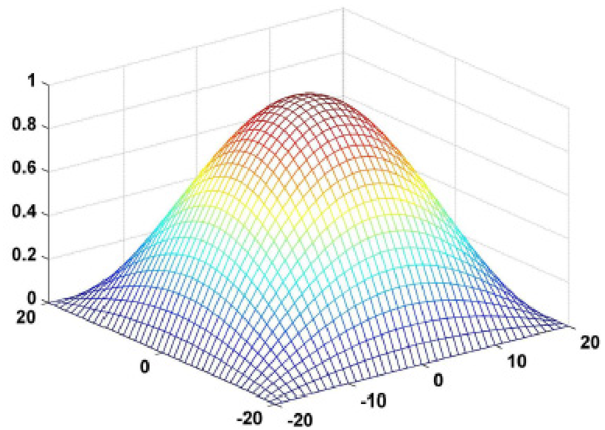
How to determine the grid size in a multiphysics system (multiscale in space)?

Electromagnetics (EM): dielectric wavelength or skin depth

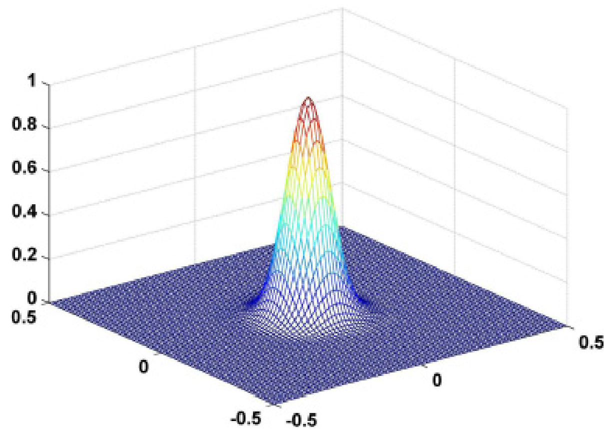
Semiconductor Physics: Debye length

Quantum Mechanism (QM): electron wavelength

electron in a cavity



EM system



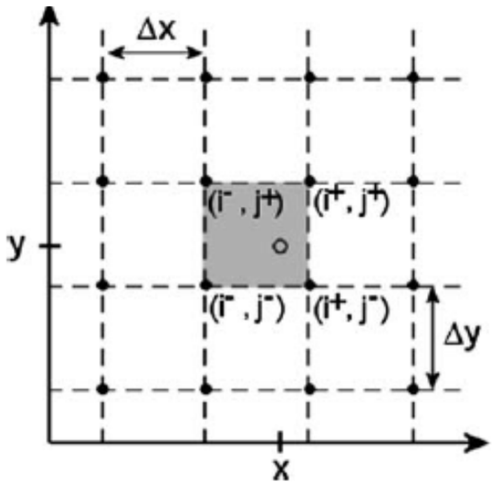
QM system

MULTISCALE (2)

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

K. J. Willis, J.S. Ayubi-Moak, S.C. Hagness, I. Knezevic, "Global modeling of carrier-field dynamics in semiconductors using EMC–FDTD," J Comput Electron, DOI: 10.1007/s10825-009-0280-4.

S. Yan, A. D. Greenwood, and J.-M. Jin, IEEE Journal on Multiscale and Multiphysics Computational Techniques, vol. 1, pp. 2-13, 2016.



Stability is maintained?
Mass, charge, energy is conserved?
Current (flux) continuity is satisfied?

Our Remedy:

Remove spatial grids in one PDE system by the eigenmode/eigenstate expansion technique.

Reference: Y. P. Chen, W. E. I. Sha, L. Jiang, M. Meng, Y. M. Wu, and W. C. Chew, "A Unified Hamiltonian Solution to Maxwell-Schrödinger Equations for Modeling Electromagnetic Field-Particle Interaction," Computer Physics Communications, Accepted. DOI: 10.1016/j.cpc.2017.02.006

MULTISCALE (3)

Total Hamiltonian of Maxwell-Schrödinger system (Coulomb gauge) $\nabla \cdot \mathbf{A} = 0$

$\mathbf{Y} = -\epsilon_0 \mathbf{E}$

$$H^s(\mathbf{A}, \mathbf{Y}, \psi, \psi^*) = H^{em}(\mathbf{A}, \mathbf{Y}) + H^q(\psi, \psi^*, \mathbf{A})$$

$$H^{em}(\mathbf{A}, \mathbf{Y}) = \int_v \left(\frac{1}{2\epsilon_0} |\mathbf{Y}|^2 + \frac{1}{2\mu_0} |\nabla \times \mathbf{A}|^2 \right) d\mathbf{r}$$

electrodynamics

$$H^q(\psi, \psi^*, \mathbf{A}) = \int_v \left[\psi^* \frac{(\hat{\mathbf{p}} - q\mathbf{A})^2}{2m} \psi + \psi^* V \psi \right] d\mathbf{r}$$

quantum mechanics

Hamiltonian's equations

$$\frac{\partial \mathbf{A}}{\partial t} = \frac{\partial H^s}{\partial \mathbf{Y}} = \frac{\mathbf{Y}}{\epsilon_0}$$

$$\frac{\partial \mathbf{Y}}{\partial t} = -\frac{\partial H^s}{\partial \mathbf{A}} = -\frac{\nabla \times \nabla \times \mathbf{A}}{\mu_0} + \mathbf{J}$$

$$\frac{\partial \psi}{\partial t} = \frac{1}{i\hbar} \frac{\partial H^s}{\partial \psi^*} = \frac{1}{i\hbar} \left[\frac{(\hat{\mathbf{p}} - q\mathbf{A})^2}{2m} + V \right] \psi$$

$$\frac{\partial \psi^*}{\partial t} = \frac{-1}{i\hbar} \frac{\partial H^s}{\partial \psi} = -\frac{1}{i\hbar} \left[\frac{(\hat{\mathbf{p}} + q\mathbf{A})^2}{2m} + V \right] \psi^*$$

$$\mathbf{J} = \frac{q}{2m} \left[\psi^* (\hat{\mathbf{p}} - q\mathbf{A}) \psi + \psi (-\hat{\mathbf{p}} - q\mathbf{A}) \psi^* \right]$$

quantum current

MULTISCALE (4)

Numerical difficulties in the self-consistent solution by the FDTD method

$\lambda_q \ll \lambda_{em}$ wavelength mismatch between electrons and photons

$\psi(\mathbf{r},t) \sim \exp(-i\omega_g t),\ \exp(-i\omega_e t)$ fast oscillation of wave function

$\psi(\mathbf{r},t) \approx a(t)\exp(-i\omega_g t)\psi_g(\mathbf{r}) + b(t)\exp(-i\omega_e t)\psi_e(\mathbf{r})$ reduced eigenstate expansion (two-level atomic system)

$$\frac{\partial \psi}{\partial t} = \frac{1}{i\hbar}\frac{\partial H^s}{\partial \psi^*} = \frac{1}{i\hbar}\left[\frac{(\hat{\mathbf{p}} - q\mathbf{A})^2}{2m} + V\right]\psi$$

$$\left\langle \psi_g, \frac{\partial \psi}{\partial t}\right\rangle = \left\langle \psi_g, \frac{1}{i\hbar}\frac{\partial H^s}{\partial \psi^*}\right\rangle$$

$$\left\langle \psi_e, \frac{\partial \psi}{\partial t}\right\rangle = \left\langle \psi_e, \frac{1}{i\hbar}\frac{\partial H^s}{\partial \psi^*}\right\rangle$$

Galerkin strategy

$$i\hbar\frac{\partial a(t)}{\partial t} = -\frac{q\mathbf{A}}{m}\langle\psi_g|\hat{\mathbf{p}}|\psi_e\rangle b(t)e^{i(\omega_g-\omega_e)t} + \frac{q^2\mathbf{A}^2}{2m}a(t)$$

$$i\hbar\frac{\partial b(t)}{\partial t} = -\frac{q\mathbf{A}}{m}\langle\psi_e|\hat{\mathbf{p}}|\psi_g\rangle a(t)e^{i(\omega_e-\omega_g)t} + \frac{q^2\mathbf{A}^2}{2m}b(t)$$

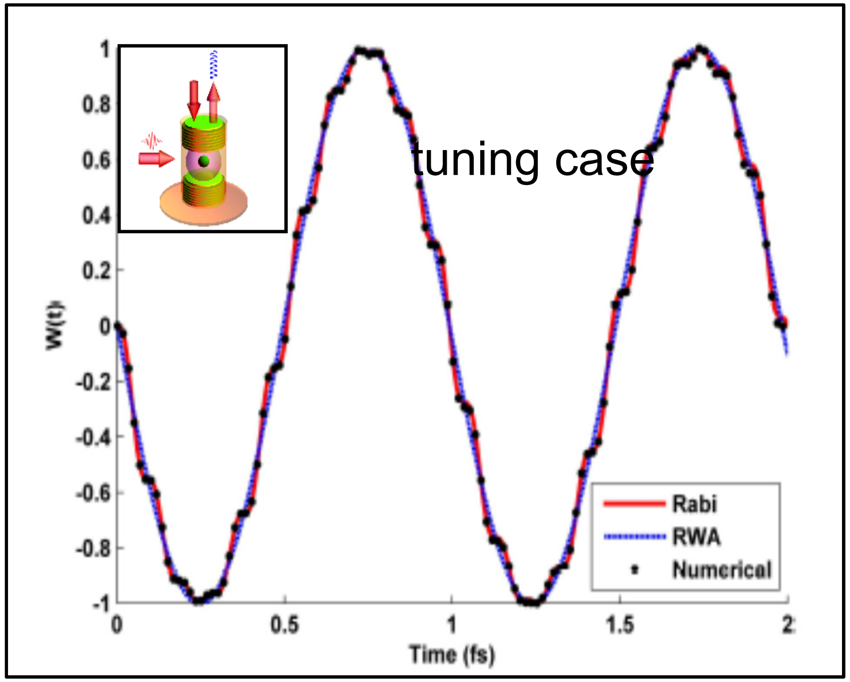
$\Longleftrightarrow$

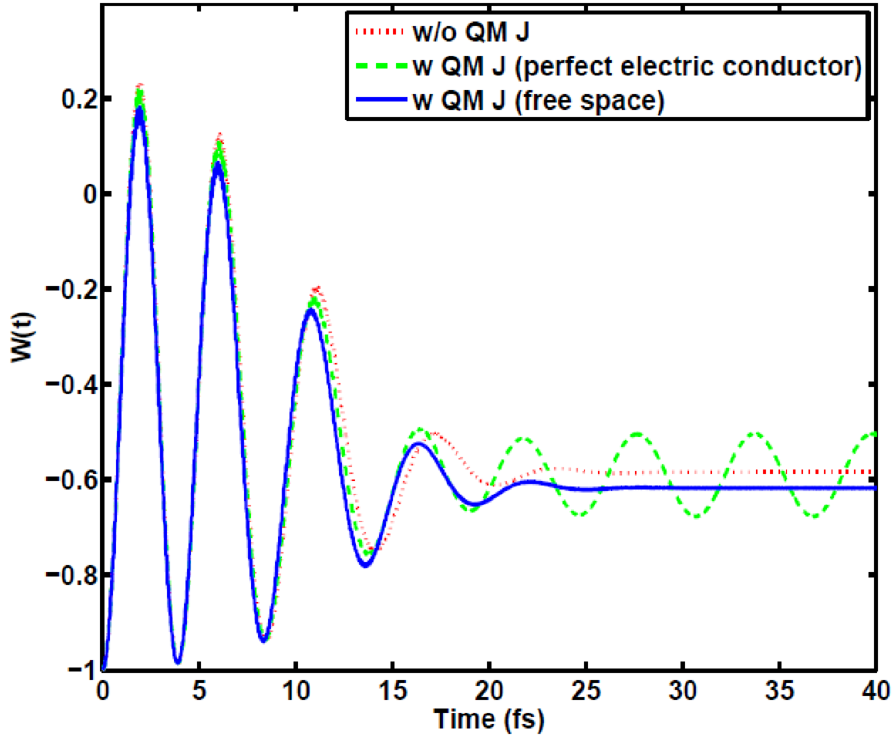
$$\frac{\partial \mathbf{A}}{\partial t} = \frac{\partial H^s}{\partial \mathbf{Y}} = \frac{\mathbf{Y}}{\epsilon_0}$$

$$\frac{\partial \mathbf{Y}}{\partial t} = -\frac{\partial H^s}{\partial \mathbf{A}} = -\frac{\nabla\times\nabla\times\mathbf{A}}{\mu_0} + \mathbf{J}$$

$$\langle\mathbf{J}\rangle = \frac{-q^2}{m}\mathbf{A}\left(|a|^2 + |b|^2\right) + \frac{q}{m}\left[a^*(t)b(t)e^{i(\omega_g-\omega_e)t}\langle\psi_g|\hat{\mathbf{p}}|\psi_e\rangle + b^*(t)a(t)e^{i(\omega_e-\omega_g)t}\langle\psi_e|\hat{\mathbf{p}}|\psi_g\rangle\right]$$

MULTISCALE (5)





rabi oscillation for a particle in a cavity
(RWA: rotating wave approximation)

radiative decay for a particle in air
(self consistent: w QM J)

For self-consistent solution with a back coupling of QM current, the particle is driven by an external field and induced field generated by the QM current.

MULTISCALE (6)

How to determine the time step size in a multiphysics system (multiscale in time)?

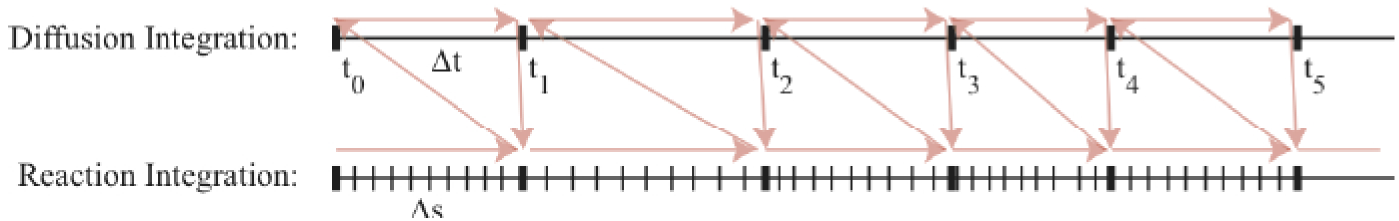
Electromagnetics (EM): Propagation time or Lifetime (for a photon)
It relates to device dimension, group velocity, absorption coefficient, quality factor, etc.

Semiconductor Physics: Relaxation time (from non-equilibrium to equilibrium states)
It relates to mean free path, coherence length, mean velocity of electron, etc.

Quantum Mechanism (QM): Coherent time (from a pure quantum to a mixed system)
It relates to inhomogeneous broadening, radiative decay, etc.

MULTISCALE (7)

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 $$u(t_{n+1}) = u(t_n) + \Delta t f(u(t_n))$$

Implicit $$u(t_{n+1}) = u(t_n) + \Delta t f(u(t_{n+1}))$$

Reference: David E. Keyes, etal., Multiphysics Simulations: Challenges and Opportunities.

MULTISCALE (8)

Our Remedy:

When one system/process has an extremely ($>10^2 \sim 10^3$) 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. Solar cell or THz generation problem (Maxwell & Drift-Diffusion equations)

The light speed is much faster than electron speed and thus propagation (absorption) time of photons is much faster than relaxation time of electrons.

2. Exciton delocalization and diffusion-dissociation problems in organic solar cells

The delocalization process is at ultrafast time scale (~fs) and the diffusion-dissociation process is at slow time scale (~ps).

Reference: Z. S. Wang, W. E. I. Sha, and W. C. H. Choy, "Exciton Delocalization Incorporated Drift-Diffusion Model for Bulk-Heterojunction Organic Solar Cells," Journal of Applied Physics, vol. 120, no. 21, pp. 213101, Dec. 2016.

MULTISCALE (9)

permittivity

$$\nabla\times\mathbf{E}=-j\omega\mu_0\mathbf{H}\,,\quad \nabla\times\mathbf{H}=j\omega\varepsilon(\omega)\mathbf{E}$$

optical E-field

$$G(\mathbf{r})=\int_{400}^{800}\frac{\lambda}{hc}A(\mathbf{r},\lambda)d\lambda\,,\quad A(\mathbf{r},\lambda)=\omega\varepsilon_0 n_r k_i\,|\,\mathbf{E}(\mathbf{r})\,|^2$$

electrostatic potential

electron density

$$\nabla\cdot(\varepsilon\nabla\varphi)=-q(p-n)$$

$$\frac{\partial n}{\partial t}=\eta_d G+\frac{1}{q}\nabla\cdot(q\mu_n nE_n+qD_n\nabla n)+k_d X_l-R(n,p)$$

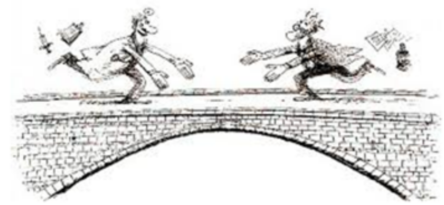
hole density *mobility* *diffusion coef.* *recombination*

$$\frac{\partial p}{\partial t}=\eta_d G-\frac{1}{q}\nabla\cdot(q\mu_p pE_p-qD_p\nabla p)+k_d X_l-R(n,p)$$

Ex density *Ex diffusion coef.* *Ex dissociation & decay*

$$\frac{\partial X}{\partial t}=(1-\eta_d)G+\nabla\cdot(D_X\nabla X_l)-k_d X_l-k_f X_l+\eta_s R(n,p)$$

Electrodynamics Semiconductor Physics



Maxwell's equations

Generation rate

Poisson equation

Drift-diffusion equation & Current-continuity equation

Exciton diffusion-dissociation equation

FLOATING POINT OVERFLOW/UNDERFLOW

When time and space scales are quite different for the multiphysics system, it is better to rescale or redefine all the international units.

rescale or redefine units in semiconductor equations

cm	$\max\{\mathrm{DOS}\}^{1/3}$
s	10^{12}
V	1
C	$\frac{1}{1.602\times 10^{-19}}$
K	$\frac{1}{300}$

DOS: density of states

Reference: W. E. I. Sha, W. C. H. Choy, Y. Wu, and W. C. Chew, "Optical and Electrical Study of Organic Solar Cells with a 2D Grating Anode," *Optics Express*, vol. 20, no. 3, pp. 2572-2580, Jan. 2012.

STABILITY IN TRANSIENT SIMULATION

Coupled evolution of a multiphysics problem

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

explicit

$$\frac{u_1^n - u_1^{n-1}}{\Delta_t} = f_1(u_1^{n-1}, u_2^{n-1})$$

$$\frac{u_2^n - u_2^{n-1}}{\Delta_t} = f_2(u_1^n, u_2^{n-1})$$

No sparse matrix inversion
Stability is bad
Conditionally stable

semi-implicit

$$\frac{u_1^n - u_1^{n-1}}{\Delta_t} = f_1(u_1^n, u_2^{n-1})$$

$$\frac{u_2^n - u_2^{n-1}}{\Delta_t} = f_2(u_1^n, u_2^n)$$

Sparse matrix inversion
Stability is better
Conditionally stable

implicit

$$\frac{u_1^n - u_1^{n-1}}{\Delta_t} = f_1(u_1^n, u_2^n)$$

$$\frac{u_2^n - u_2^{n-1}}{\Delta_t} = f_2(u_1^n, u_2^n)$$

Newton method in each step
Stability is best
Unconditionally stable

STRONG AND WEAK COUPLING

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

$$F(u) = \begin{pmatrix} F_1(u_1, u_2) \\ F_2(u_1, u_2) \end{pmatrix} = 0$$

strong coupling

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

$$J = \begin{bmatrix} \frac{\partial F_1}{\partial u_1} & \frac{\partial F_1}{\partial u_2} \\ \frac{\partial F_2}{\partial u_1} & \frac{\partial F_2}{\partial u_2} \end{bmatrix}$$

Newton's method

weak coupling

Gauss-Seidel approach

$$F_1(u_1^{k+1}, u_2^k) = 0$$

$$\Downarrow \quad \Uparrow$$

$$F_2(u_1^{k+1}, u_2^{k+1}) = 0$$

Self-consistent solution

1. Maxwell-Schrödinger
2. Maxwell-hydrodynamic

one-way (forward) coupling

$$F_1(u_1) = 0$$

$$F_2(f(u_1), u_2) = 0$$

Solve one PDE equation F_1 and then solve another PDE F_2 by substituting a post-processed physical quantity $f(u_1)$.

1. Solar cell & THz generation
2. Second harmonic generation (undepleted-pump approximation)

BENCHMARK ISSUE (1)

Is it a correct solution?
Can be the analytical or semi-analytical solution found?
Is the deviation caused by numerical error or by real physical effects?
Could we believe our new findings?

Our Remedy:

Validate physical conservation law: **mass, charge, energy, momentum, angular momentum, parity ….**

Reference:

M. Fang, Z. Huang, W. E. I. Sha, X. Y. Z. Xiong, and X. Wu, "Full Hydrodynamic Model of Nonlinear Electromagnetic Response in Metallic Metamaterials (Invited Paper)," Progress In Electromagnetics Research, vol. 157, 63-78, Oct. 2016.

BENCHMARK ISSUE (2)

When electromagnetic waves strongly interact with metallic structures, it can couple to free electrons near the metal surface resulting in complex linear and nonlinear responses. Interestingly, the complex motion of electrons within metallic structures resembles that of fluids.

Maxwell equation

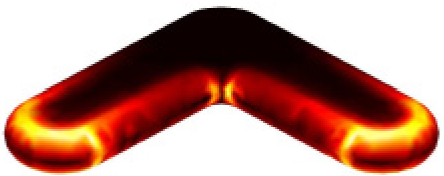
$$\varepsilon_0 \frac{\partial \boldsymbol{E}}{\partial t} = \nabla \times \boldsymbol{H} - \frac{\partial \boldsymbol{P}}{\partial t} \qquad \mu_0 \frac{\partial \boldsymbol{H}}{\partial t} = -\nabla \times \boldsymbol{E}$$

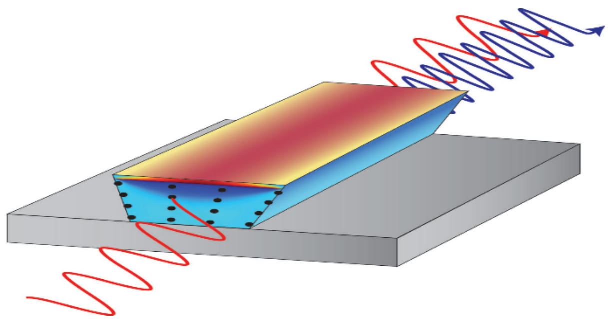
$$m_e n \left(\frac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{v} \cdot \nabla \boldsymbol{v} \right) + \gamma m_e n \boldsymbol{v} = -q_e n (\boldsymbol{E} + \boldsymbol{v} \times \mu_0 \boldsymbol{H})$$

hydrodynamic equation

current continuity

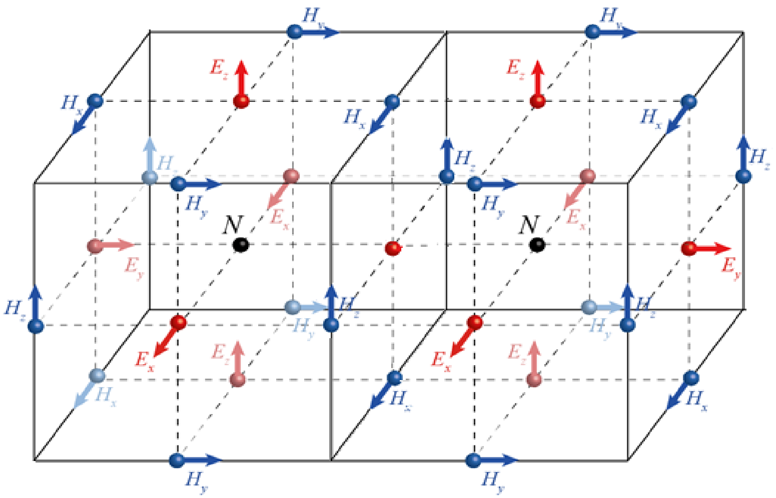
$$\frac{\partial n}{\partial t} + \nabla \cdot (n \boldsymbol{v}) = 0 \qquad \frac{\partial \boldsymbol{P}}{\partial t} = -q_e n \boldsymbol{v}$$

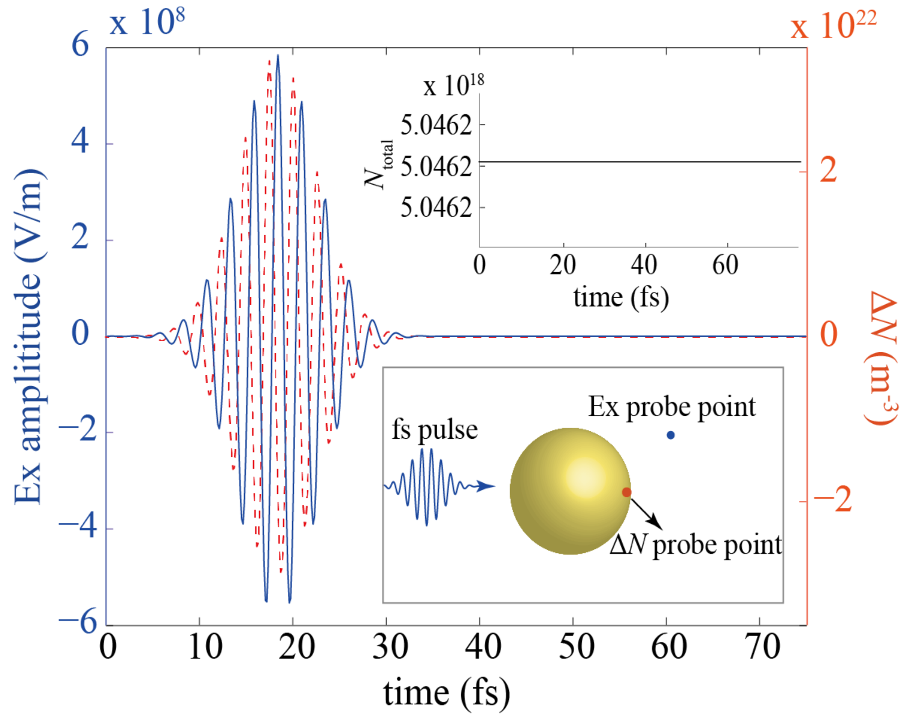




BENCHMARK ISSUE (3)

Charge conservation





At each point, the electron density fluctuates. However, the total charge within the sphere is conserved.

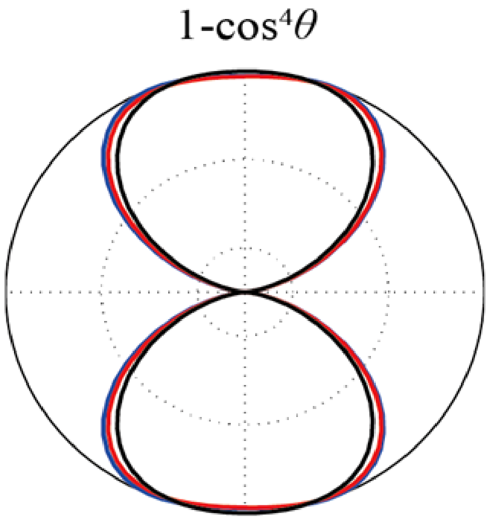
$$
\begin{aligned}
&n^{l+3/2}(i+1/2,j+1/2,k+1/2) = n^{l+1/2}(i+1/2,j+1/2,k+1/2)\\
&-\Bigg[\frac{\Delta t}{\Delta x}\left(\bar{n}^{l+1/2}(i{+}1,j{+}1/2,k{+}1/2)v_x^{l+1}(i{+}1,j{+}1/2,k{+}1/2)-\bar{n}^{l+1/2}(i,j{+}1/2,k{+}1/2)v_x^{l+1}(i,j{+}1/2,k{+}1/2)\right)\\
&+\frac{\Delta t}{\Delta y}\left(\bar{n}^{l+1/2}(i{+}1/2,j{+}1,k{+}1/2)v_y^{l+1}(i{+}1/2,j{+}1,k{+}1/2)-\bar{n}^{l+1/2}(i{+}1/2,j,k{+}1/2)v_y^{l+1}(i{+}1/2,j,k{+}1/2)\right)\\
&+\frac{\Delta t}{\Delta z}\left(\bar{n}^{l+1/2}(i{+}1/2,j{+}1/2,k{+}1)v_z^{l+1}(i{+}1/2,j{+}1/2,k{+}1)-\bar{n}^{l+1/2}(i{+}1/2,j{+}1/2,k)v_z^{l+1}(i{+}1/2,j{+}1/2,k)\right)\Bigg]
\end{aligned}
$$

Angular momentum conservation

The incident wave is left-circularly polarized wave carrying the spin angular momentum of *s*=1. If the size of a metallic sphere is well controlled, according to angular momentum conservation, we have

$l=m=2s=2$

$Y_\ell^m(\theta,\varphi) \quad \ell \geq |m|$



Red: E-plane (FDTD)
Blue: H-plane (FDTD)
Black: Analytical

second-harmonic pattern of a metallic sphere

PREDICTION CAPABILITY (1)

1. Styer wrote in 2012 that the accuracy of Maxwell equation had been improved to a few parts in a trillion: such an error is equivalent to a few human hair widths in the distance from the Earth to the Moon [“calculation of the anomalous magnetic moment of the electron”]. The strong prediction capability is due to the only needed physical parameter (permittivity) in most problems.

2. Compared to linear Maxwell equation, the nonlinear semiconductor equation (drift-diffusion equation) has much weaker prediction capability. The physics parameters include field, carrier density and geometry dependent mobility, band gap, work function, valance band, conduction band, density of states, applied voltage, generation rate, recombination coefficients (direct, SRH, Auger), etc. For a complex polymer system, we have to add exciton radius, lifetime and diffusion coefficient, dissociation probability, etc.

3. Can we believe the simulation results in the semiconductor-Maxwell system?

References: W. E. I. Sha, X. Li, and W. C. H. Choy, “Breaking the Space Charge Limit in Organic Solar Cells by a Novel Plasmonic-Electrical Concept,” Scientific Reports, vol. 4, pp. 6236, Aug. 2014.

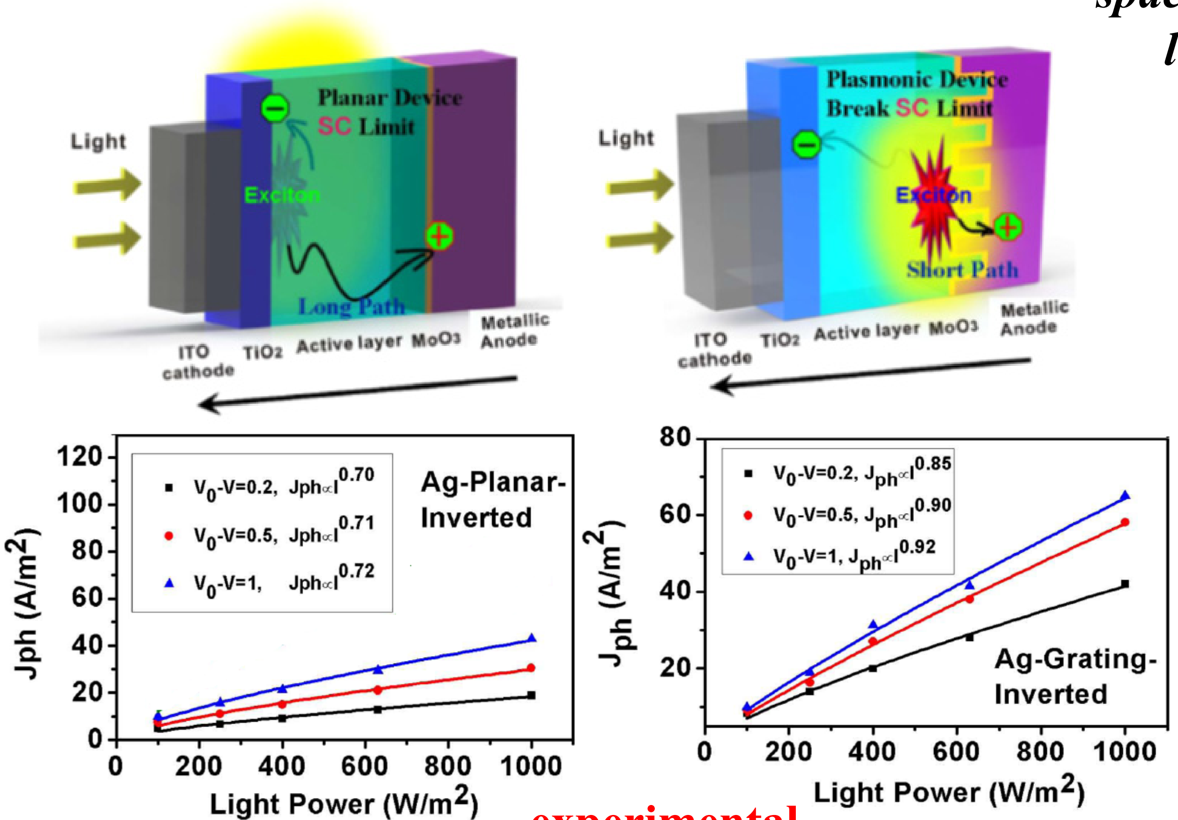
PREDICTION CAPABILITY (2)

Our Remedy:

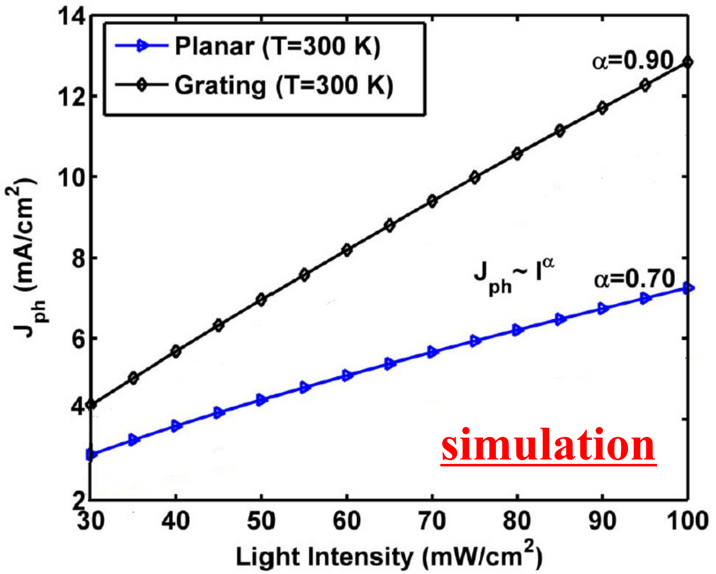
Even if a quantitative prediction is not allowed/possible, the qualitative prediction is still critically important to engineering designs.

space charge limited
$$J_{ph} = \left(\frac{9\varepsilon_0\varepsilon_r\mu_h}{8}\right)^{1/4}(qG)^{3/4}V_e^{1/2}$$

normal
$$J_{ph} = qGL$$

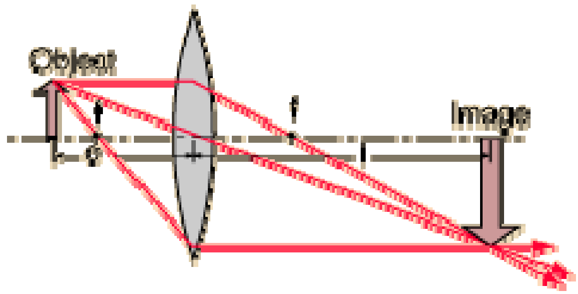


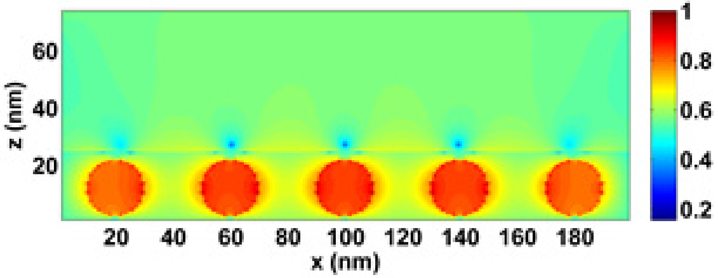
experimental

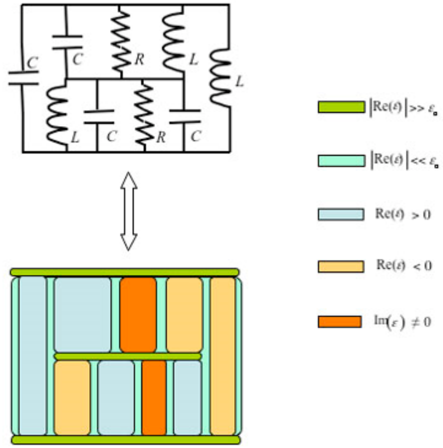


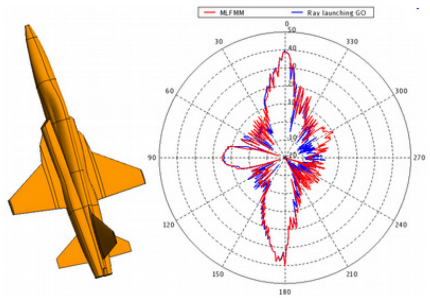
simulation

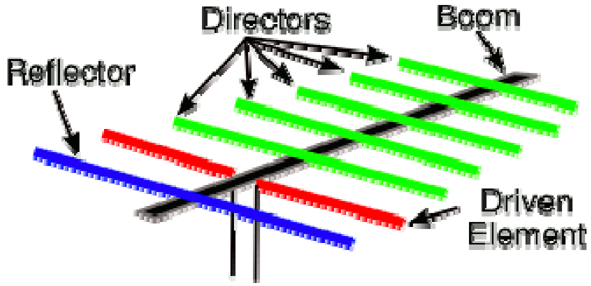
BREAKDOWN OF CLASSICAL MAXWELL EQUATION (1)

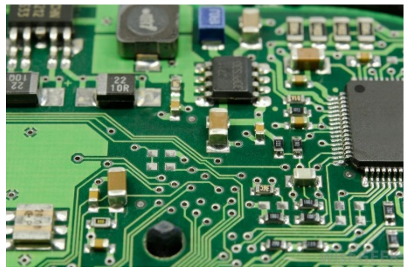












classical optics
ray physics
D>>λ

nano-optics
wave physics
D~λ

nano-circuit
circuit physics
D<<λ

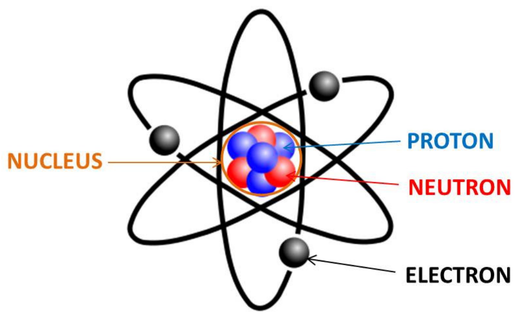
BREAKDOWN OF CLASSICAL MAXWELL EQUATION (2)

Quantum regime $|E| \gg \frac{\sqrt{\hbar c}}{(c\Delta t)^2}.$ strong field condition

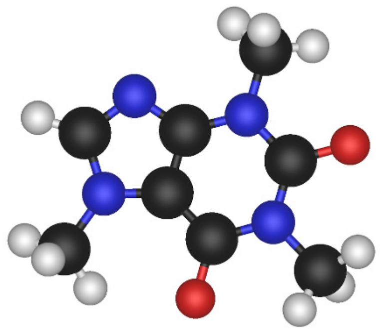
At the quantum regime, when the object size is tiny small (<10 nm) so that the "homogenized" permittivity and permeability of Maxwell equation is invalid or meaningless.

If the field intensity is strong or the number of photons are large, semi-classical Maxwell-Schrödinger system is required to describe the EM-particle interaction, where Maxwell equation is still classical.

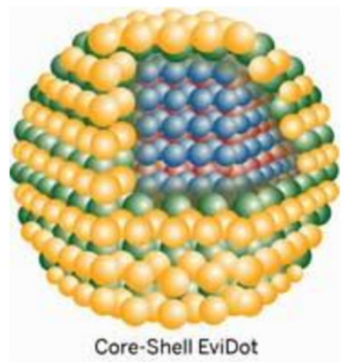
If the field intensity is very weak and the number of photons is quite small (vacuum fluctuation, single photon source, etc), Maxwell's equations should be quantized and classical Maxwell's equations is invalid.



atoms



molecules



- Nanocrystals
- 2-10 nm diameter
- semiconductors

quantum dots

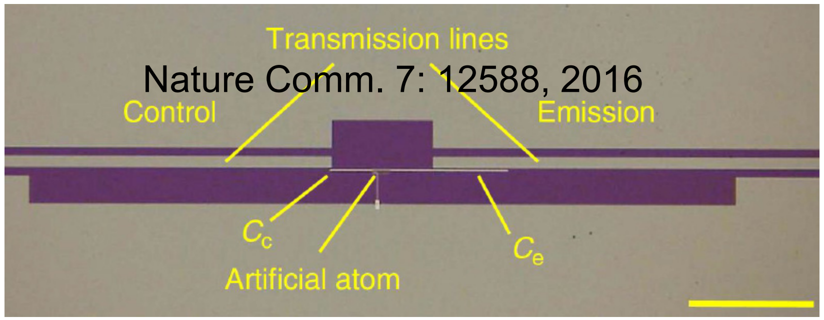
BREAKDOWN OF CLASSICAL MAXWELL EQUATION (3)

Why quantized Maxwell equation is required?

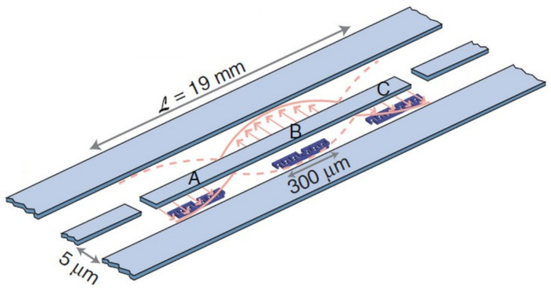
Nanofabrication techniques allow the construction of artificial atoms such as quantum dots that are microscopic in scale. In this case, semi-classical calculations do not suffice to support many of the emerging technologies, when the number of photons is limited, such as single photon devices/photodetectors.

Another interesting example is the circuit quantum electrodynamics at microwave frequencies where a superconducting quantum interference device based artificial atom is entangled with coplanar waveguide microwave resonators. For these situations, Maxwell equation should be quantized.

single photon source



circuit quantum electrodynamics



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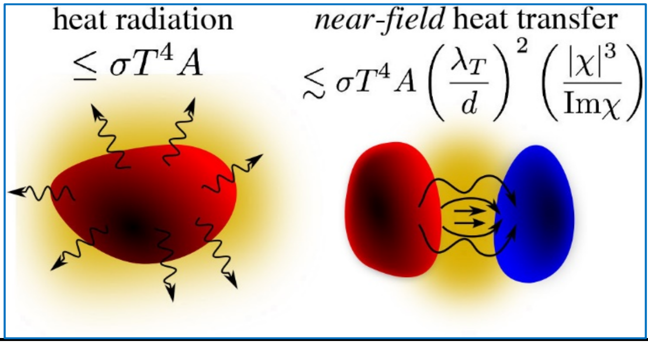
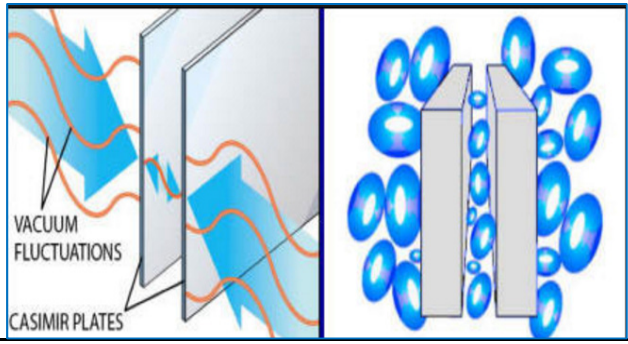
BREAKDOWN OF CLASSICAL MAXWELL EQUATION (4)

Why quantized Maxwell equation is required? Cont…

Nano-fabrication also induces the quantum effects in heat transfer. While phonons require material media for heat transfer, photons can account for near-field heat transfer through vacuum where classical heat conduction equation and Kirchhoff law of thermal radiation are invalid.

Experiments confirmed that Casimir force is real, and entirely quantum: it can be only explained using quantum theory of electromagnetic field in its quantized form. Also, Casimir force cannot be explained by classic electromagnetics theory that assumes null electromagnetic field in vacuum.





BREAKDOWN OF CLASSICAL MAXWELL EQUATION (5)

Our Remedy:

The use of the ubiquitous Green's function is still present in many quantum calculations. Hence, the knowledge and effort in computational electromagnetics for computing the Green's functions of complicated systems have not gone obsolete or in vain. Therefore, the development of computational electromagnetics (CEM), which has been important for decades for the development of many classical electromagnetics technologies all across the electromagnetic spectrum, will be equally important in the development of quantum technologies.

$$\hat{\mathbf{A}}(\mathbf{r},t) = \int d\mathbf{r}\overline{\mathbf{G}}(\mathbf{r},\mathbf{r}',t) \circledast \hat{\mathbf{J}}_{\mathrm{ext}}(\mathbf{r}',t)$$

$$\hat{\Phi}(\mathbf{r},t) = \int d\mathbf{r}g(\mathbf{r},\mathbf{r}',t) \circledast \hat{\varrho}_{\mathrm{ext}}(\mathbf{r}',t)$$

Quantized Maxwell Equation

$$\nabla \times \hat{\mathbf{H}}(\mathbf{r},t) - \partial_t \hat{\mathbf{D}}(\mathbf{r},t) = \hat{\mathbf{J}}_{\mathrm{ext}}(\mathbf{r},t), \qquad \nabla \times \hat{\mathbf{E}}(\mathbf{r},t) + \partial_t \hat{\mathbf{B}}(\mathbf{r},t) = 0,$$

$$\nabla \cdot \hat{\mathbf{D}}(\mathbf{r},t) = \hat{\varrho}_{\mathrm{ext}}(\mathbf{r},t), \qquad \nabla \cdot \hat{\mathbf{B}}(\mathbf{r},t) = 0.$$

BREAKDOWN OF CLASSICAL MAXWELL EQUATION (6)

Quantized Hamiltonian for Maxwell-Schrödinger equation

$$\hat{H}\left(\hat{\mathbf{A}},\hat{\mathbf{Y}},\hat{\mathbf{p}}\right)=\hat{H}^{em}\left(\hat{\mathbf{A}},\hat{\mathbf{Y}}\right)+H_0^q\left(\hat{\mathbf{p}},\hat{\mathbf{A}}\right)+H_I^q\left(\hat{\mathbf{p}},\hat{\mathbf{A}}\right) \qquad \hat{H}\Psi(t)=i\hbar\frac{\partial\Psi(t)}{\partial t}$$

electromagnetic part — atomic part — interaction part

$$\hat{H}^{em}\left(\hat{\mathbf{A}},\hat{\mathbf{Y}}\right)=\int_\Omega\left(\frac{1}{2\epsilon_0}\left|\hat{\mathbf{Y}}\right|^2+\frac{1}{2\mu_0}\left|\nabla\times\hat{\mathbf{A}}\right|^2\right)d\mathbf{r} \qquad H_0^q\left(\hat{\mathbf{p}},\hat{\mathbf{A}}\right)=\frac{\hat{\mathbf{p}}^2}{2m}+V \qquad H_I^q\left(\hat{\mathbf{p}},\hat{\mathbf{A}}\right)\approx\frac{q\hat{\mathbf{p}}\cdot\hat{\mathbf{A}}}{m}$$

quantized field

$$\hat{\mathbf{A}}=\sum_k\frac{\alpha_k}{\omega_k}\left(\mathbf{U}_k(\mathbf{r})\hat{a}_k+\mathbf{U}_k^*(\mathbf{r})\hat{a}_k^+\right),\ \alpha_k=\sqrt{\frac{\hbar\omega_k}{2\epsilon_0}}$$

wave-particle duality

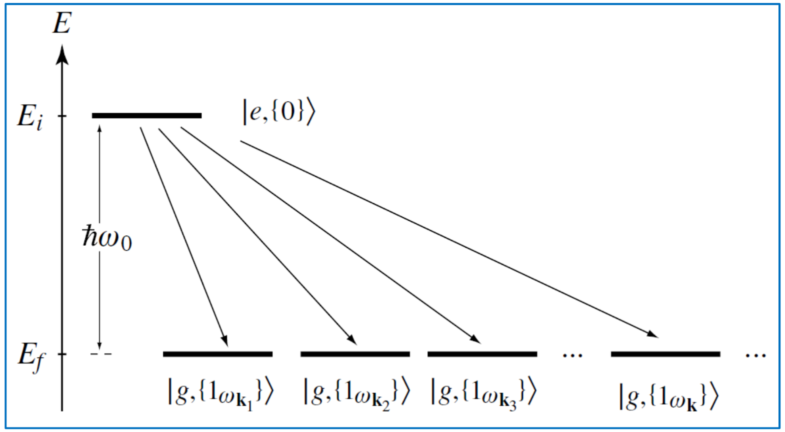
wave function expansion

$$\Psi(t)=a(t)|e,0>+\sum_k b_k(t)|g,1_k>$$

e: excited state of atom, 0: no photon; g: ground state of atom, 1: one photon

BREAKDOWN OF CLASSICAL MAXWELL EQUATION (7)

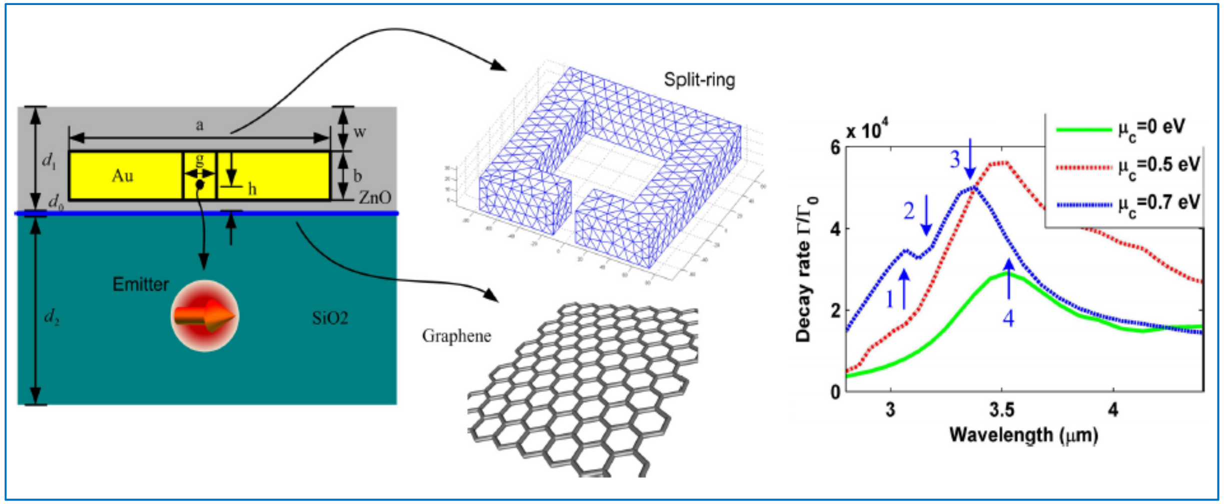
equivalent principle (PMCHWT) & multilayer Green's function



spontaneous emission rate

$$\gamma(\mathbf{r}_0,\omega_0) = \frac{\pi\omega_0}{\epsilon_0\hbar}\sum_k[\mathbf{p}\cdot(\mathbf{u}_\mathbf{k}\mathbf{u}_\mathbf{k}^*)\cdot\mathbf{p}]\delta(\omega_\mathbf{k}-\omega_0)$$

$$\gamma(\mathbf{r}_0,\omega_0) = \frac{2\omega_0^2}{\epsilon_0\hbar c^2}\langle\mathbf{p}\cdot\mathrm{Im}[\bar{\mathbf{G}}(\mathbf{r}_0,\mathbf{r}_0,\omega_0)]\cdot\mathbf{p}\rangle$$



CONCLUSION

Multiphysics simulation is a very challenging field. There is no universal panacea.

1. We have to understand multiphysics problem with a critical/deep physical insight.
2. We have to determine how to couple these multiphysical equations.
3. We have to know the pros and cons of various algorithms.
4. We have to be aware that when the model will break down.
5. We have to learn as much as possible to have a new look at Maxwell equation.
6. We have to collaborate with mathematicians, physicists, chemists, engineers, etc.
7. We have to train our students for working in the multidisciplinary fields.

ACKNOWLEDGEMENT

Thanks for Your Attention!