Quantum Mechanical & Electromagnetic Systems Modelling Lab

A Hybrid EM/QM Framework Based on the ADHIE-FDTD Method for the Modeling of Nanowires.

Pieter Decleer and Dries Vande Ginste.

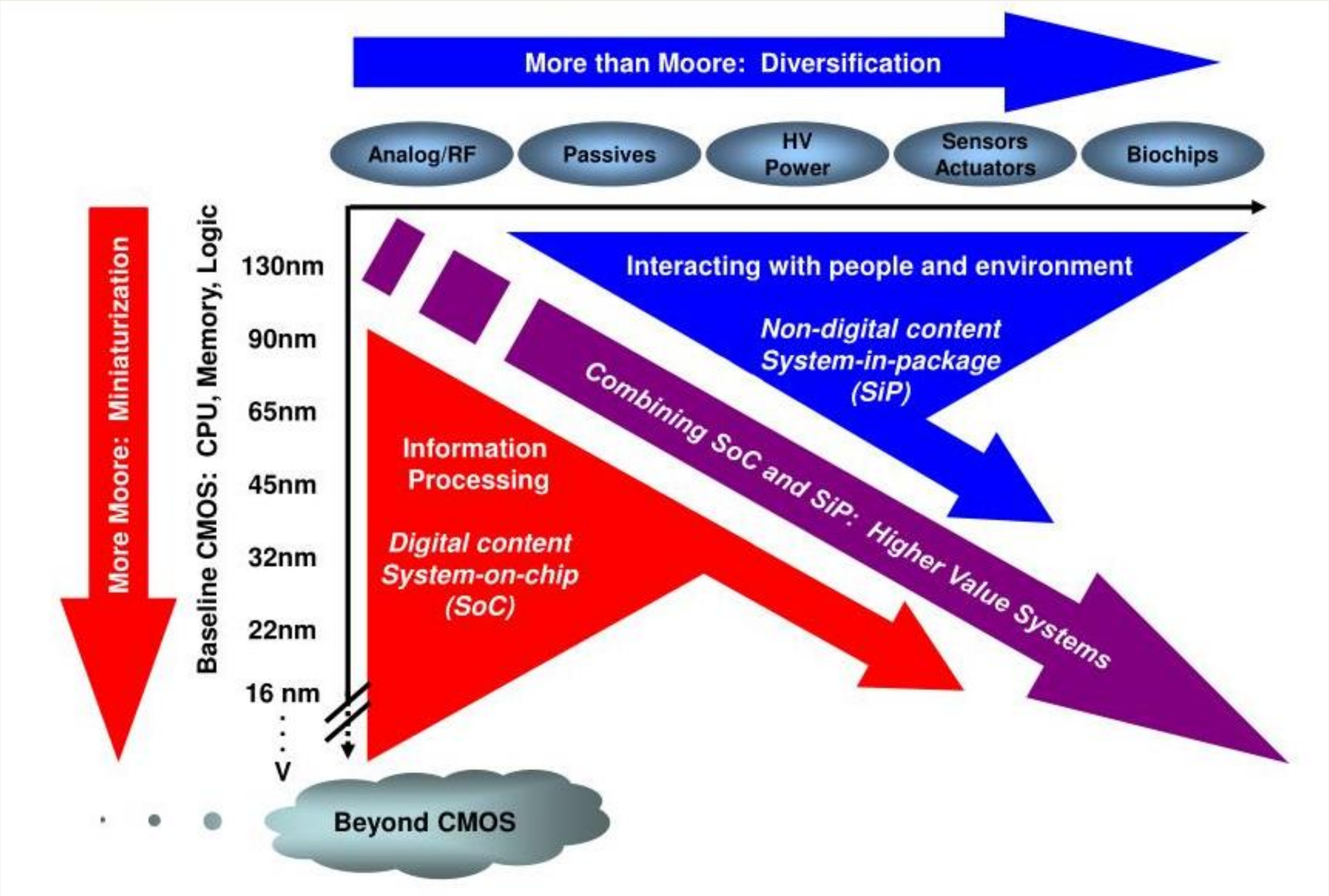
quest.

Outline.

Introduction.

Context and motivation.

Moore, Moorer, Moorest.

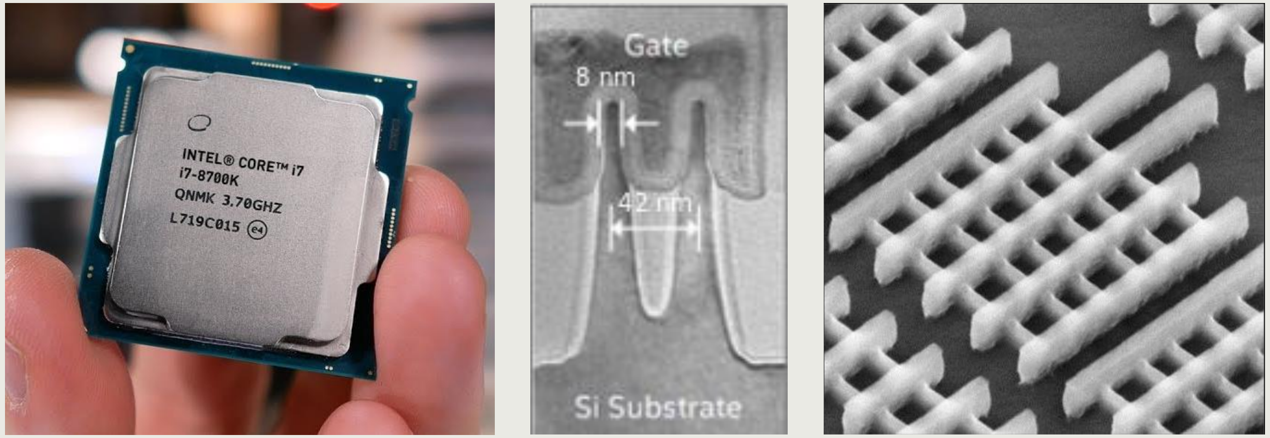


IEEE International Roadmap for Devices and Systems - IEEE IRDS™

Context and motivation.

Moore, Moorer, Moorest.

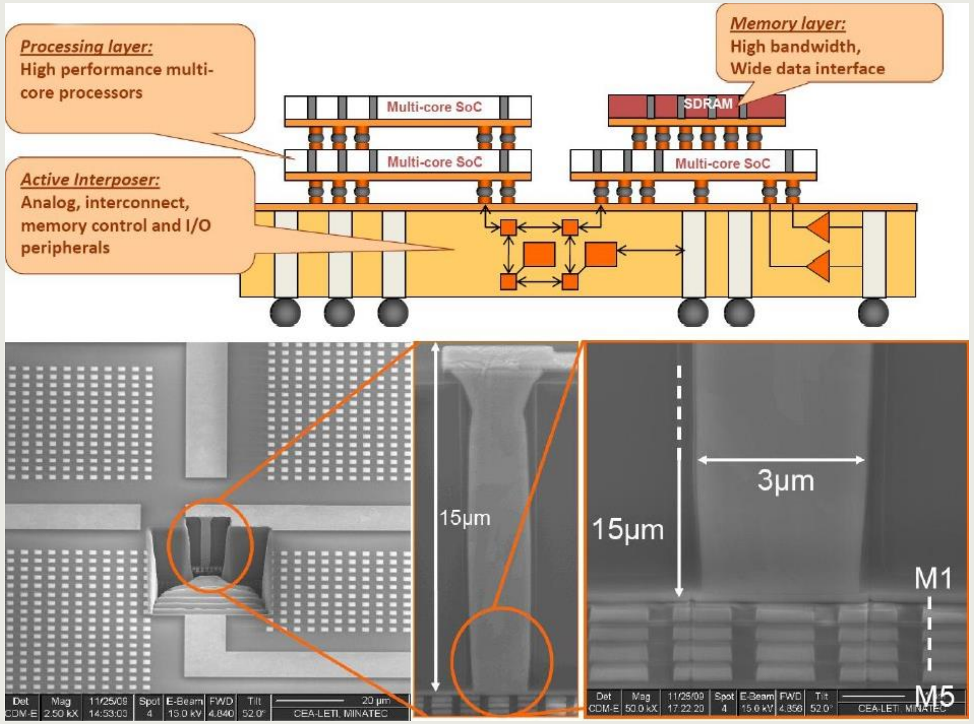
Example 1: Intel’s Core i7-8700K processor with tri-gate transistor technology



Modeling challenges

- Electromagnetic (EM) full-wave
- Heterogeneity
- Highly **multiscale**

Example 2: 3-D integration (source: CEA-Leti’s 2015 roadmap)



Context and motivation.

Moore, Moorer, Moorest.

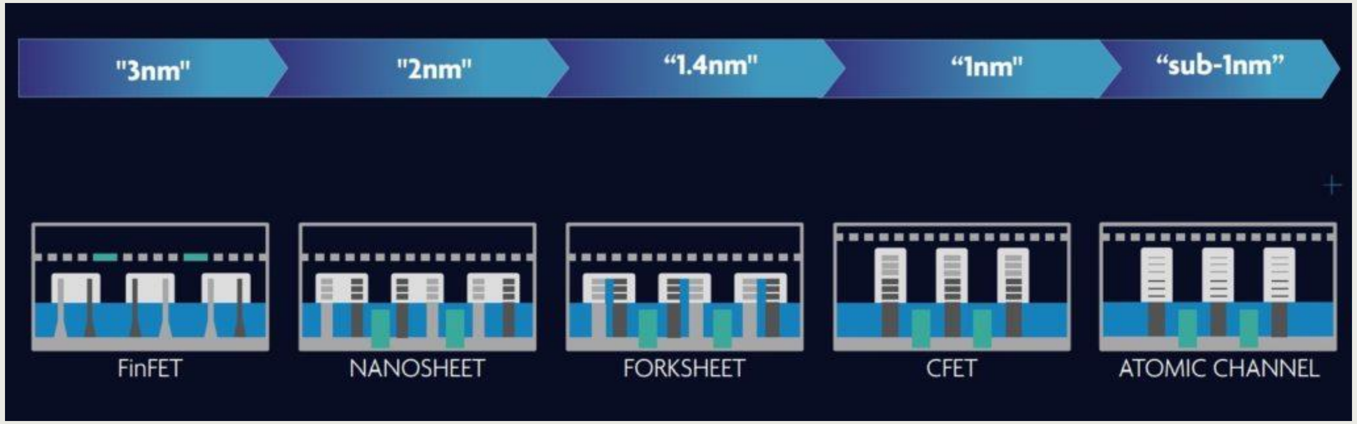
Physical phenomena

- Charge carrier confinement, ballistic transport
- Tunnel effect, Klein effect, …

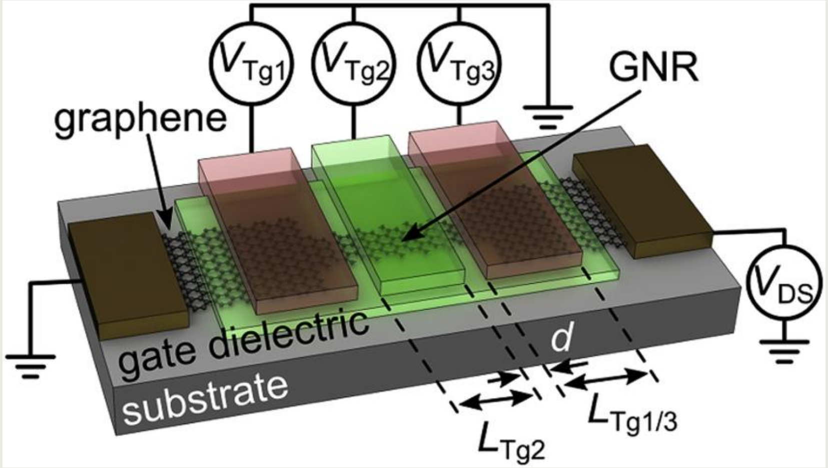
Modeling challenges

- Quantum mechanical (QM) aspects
- *Ab Initio* (↔ macroscopic conductivity models)
- **Multiphysics** (EM/QM)

Example 3: imec's Transistor Technology Roadmap (Source: imec, 2022)



Example 4: Sub-10 nm graphene nano-ribbon tunnel field-effect transistor [1]



[1] A.M.M. Hammam *et al*, Carbon, 2018

Context and motivation.

Why do we construct (multiscale and multiphysics) computational techniques?

Nano(electronic) and quantum devices: heavily researched (applications / manufacturability)

Physical phenomena occurring in these devices are not always well-understood

Computational tools and models lead to

> a more **thorough insight** in the functioning of these novel devices and systems;
>
> **computer aided design software**, avoiding trial and error during development.

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> a more **thorough insight** in the functioning of these novel devices and systems;
>
> **computer aided design software**, avoiding trial and error during development.

Additionally, it's fun! 🤓

Hybrid EM/QM modeling.

General approach.

Electromagnetic (EM) phenomena

Maxwell's equations

$$\nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t}$$

$$\nabla \times \boldsymbol{H} = \frac{\partial \boldsymbol{D}}{\partial t} + \boldsymbol{J}$$

$$\nabla \cdot \boldsymbol{B} = 0$$

$$\nabla \cdot \boldsymbol{D} = \rho$$

Continuity equation
(conservation of charge)

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

Vector potential
and scalar potential

$$\boldsymbol{B} = \nabla \times \boldsymbol{A}$$

$$\boldsymbol{E} = -\frac{\partial \boldsymbol{A}}{\partial t} - \nabla \phi$$

Lorenz gauge condition

$$\nabla \cdot \boldsymbol{A} + \frac{1}{c^2}\frac{\partial \phi}{\partial t} = 0$$

Hybrid EM/QM modeling.

General approach.

Quantum mechanical (QM) phenomena

The Schrödinger equation(*): $$\jmath\hbar\frac{\partial\psi}{\partial t} = \hat{\mathrm{H}}\,\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + v\right)\psi$$

- ψ : wave function (probability amplitude)
- m : particle's (effective) mass
- $\hat{\mathrm{H}}$: Hamiltonian operator
- v : scalar potential energy (e.g., confining potential)
- $\hbar$: reduced Plank's constant

(*) other "choices" for QM equation of motion: Dirac, Kohn-Sham, quantum transport, ...

Hybrid EM/QM modeling.

General approach.

Quantum mechanical (QM) phenomena

The Schrödinger equation
$$\jmath\hbar\frac{\partial\psi}{\partial t} = \hat{\mathrm{H}}\,\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + v\right)\psi$$

Position probability density
$$n = \psi^*\psi$$
$$\int_V n\,\mathrm{d}\boldsymbol{r} = 1$$

Probability current density
$$\boldsymbol{J}_p = \mathrm{Re}\left\{\psi^*\frac{-\jmath\hbar\boldsymbol{\nabla}}{m}\psi\right\}$$

Continuity equation for probability
$$\boldsymbol{\nabla}\cdot\boldsymbol{J}_p + \frac{\partial n}{\partial t} = 0$$

x q →

For a particle with charge q:

$$\rho_q = qn$$ *quantum charge density*

$$\boldsymbol{J_q} = q\boldsymbol{J}_p$$ *quantum current density*

$$\boldsymbol{\nabla}\cdot\boldsymbol{J}_q + \frac{\partial\rho_q}{\partial t} = 0$$
conservation of charge

Hybrid EM/QM modeling.

General approach.

Self-consistent forward-backward coupling of light and matter

Maxwell's equations

$$\nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t}$$

$$\nabla \times \boldsymbol{H} = \frac{\partial \boldsymbol{D}}{\partial t} + \boldsymbol{J}_f + \boldsymbol{J}_c + \boldsymbol{J}_q$$

$$\boldsymbol{E} = -\frac{\partial \boldsymbol{A}}{\partial t} - \nabla \phi$$

$$\nabla \cdot \boldsymbol{A} + \frac{1}{c^2}\frac{\partial \phi}{\partial t} = 0$$

forward via EM potentials

backward via quantum current density

Minimally-coupled Schrödinger equation
(spinless particle with charge q)

$$\jmath\hbar\frac{\partial \psi}{\partial t} = \left(\frac{1}{2m}(-\jmath\hbar\nabla - q\boldsymbol{A})^2 + q\phi + v\right)\psi$$

Quantum current density: $\boldsymbol{J}_q = q\boldsymbol{J}_p = q\,\mathrm{Re}\left\{\psi^* \frac{-\jmath\hbar\nabla - q\boldsymbol{A}}{m}\psi\right\}$

Conduction current density: $\boldsymbol{J}_c = \sigma \boldsymbol{E}$

Free current density: $\boldsymbol{J}_f$

Hybrid EM/QM modeling.

Choices.

Traditionally

Real-space methods in time domain, e.g., [2]

→ nonlinear coupling between EM and QM

In this seminar

Also finite-difference time-domain (FDTD) methods on a real-space grid

Full solution of the EM fields

→ inclusion of dielectric and magnetic materials

→ compatible with legacy software

EM potentials derived from EM fields

→ Lorenz gauge, but other choices possible

Multiscale aspects

→ partial implicitization

→ trade-off between efficiency and accuracy

[2] C.J. Ryu *et al*, IEEE J-MMCT, 2016

Modeling framework.

Preliminary.

Update equations and stability.

Leapfrog update equations in matrix form $$A\begin{bmatrix}\hat{\mathbf{e}}|^{n}\\ \hat{\boldsymbol{h}}|^{n+\frac{1}{2}}\end{bmatrix} = B\begin{bmatrix}\hat{\mathbf{e}}|^{n-1}\\ \hat{\boldsymbol{h}}|^{n-\frac{1}{2}}\end{bmatrix} + \begin{bmatrix}\hat{\mathbf{s}}|^{n-\frac{1}{2}}\\ 0\end{bmatrix}$$

n : time step index
$\hat{\mathbf{s}}$: source term

matrices A and B are sparse

not for implementation

(e.g., for Yee-FDTD, use *explicit* update equations, instead of solving the linear system)

compact notation

algebraic properties

System is stable [3]

if $A = E + F$ and $B = E - F$

with E real, symmetric and positive definite

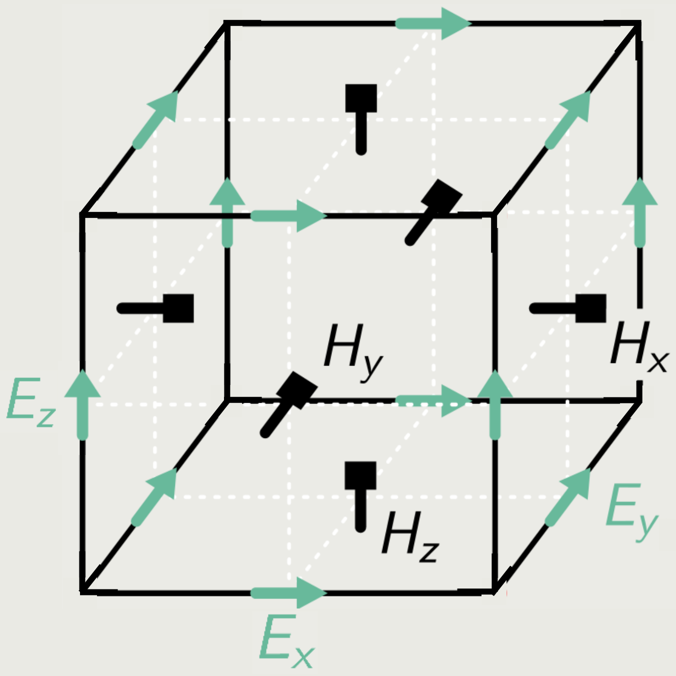
F real and $F + F^T$ positive semidefinite

[3] B. Denecker *et al*, Int. J. Electron. Commun., 2004

Two traditional FDTD methods for the EM fields.

Yee's finite-difference time-domain method (Yee-FDTD) [4].

Yee cell



E and H also staggered in time

$$\nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t}$$

$$\nabla \times \boldsymbol{H} = \frac{\partial \boldsymbol{D}}{\partial t} + \boldsymbol{J}$$

discretization on tensor-product grid
&
central finite differences

$$\begin{bmatrix} \frac{M_\epsilon}{\Delta t} & 0 \\ C^T & \frac{M_\mu}{\Delta t} \end{bmatrix} \begin{bmatrix} \hat{\mathbf{e}}|^n \\ \hat{\boldsymbol{h}}|^{n+\frac{1}{2}} \end{bmatrix} = \begin{bmatrix} \frac{M_\epsilon}{\Delta t} & C \\ 0 & \frac{M_\mu}{\Delta t} \end{bmatrix} \begin{bmatrix} \hat{\mathbf{e}}|^{n-1} \\ \hat{\boldsymbol{h}}|^{n-\frac{1}{2}} \end{bmatrix} + \begin{bmatrix} \hat{\mathbf{s}}|^{n-\frac{1}{2}} \\ 0 \end{bmatrix}$$

[4] K. Yee, IEEE T-AP, 1966

Two traditional FDTD methods for the EM fields.

Yee-FDTD.

$$\begin{bmatrix} \frac{M_\epsilon}{\Delta t} & 0 \\ C^T & \frac{M_\mu}{\Delta t} \end{bmatrix} \begin{bmatrix} \hat{\mathbf{e}}|^{n} \\ \hat{\mathbf{h}}|^{n+\frac{1}{2}} \end{bmatrix} = \begin{bmatrix} \frac{M_\epsilon}{\Delta t} & C \\ 0 & \frac{M_\mu}{\Delta t} \end{bmatrix} \begin{bmatrix} \hat{\mathbf{e}}|^{n-1} \\ \hat{\mathbf{h}}|^{n-\frac{1}{2}} \end{bmatrix} + \begin{bmatrix} \hat{\mathbf{s}}|^{n-\frac{1}{2}} \\ 0 \end{bmatrix}$$

Material matrices M_ϵ and M_μ : contain the (averaged) permittivity and permeability

Dimensionless curl matrix:

$$C = \begin{bmatrix} 0 & -I_{n_x} \otimes I_{m_y} \otimes D_z & I_{n_x} \otimes D_y \otimes I_{m_z} \\ I_{m_x} \otimes I_{n_y} \otimes D_z & 0 & -D_x \otimes I_{n_y} \otimes I_{m_z} \\ -I_{m_x} \otimes D_y \otimes I_{n_z} & D_x \otimes I_{m_y} \otimes I_{n_z} & 0 \end{bmatrix}$$

Discrete differentiator:

$$D_u = \begin{bmatrix} -1 & 1 & & & & \\ & -1 & 1 & & & \\ & & \ddots & \ddots & & \\ & & & -1 & 1 & \\ & & & & -1 & 1 \end{bmatrix}_{m_u \times n_u}, \quad u \in \{x, y, z\}$$

$\otimes$: Kronecker product

Two traditional FDTD methods for the EM fields.

Yee-FDTD.

Stability?

- Uniform gridding and homogeneous material

$$\Delta t \leq \frac{1}{\frac{1}{\sqrt{\epsilon\mu}}\sqrt{\frac{1}{\Delta x^2}+\frac{1}{\Delta y^2}+\frac{1}{\Delta z^2}}}$$

(Courant-Friedrichs-Lewy (CFL) criterion)

- Nonuniform gridding or inhomogeneities [5]

$$\Delta t < \frac{2}{\left\| M_\epsilon^{-\frac{1}{2}} C M_\mu^{-\frac{1}{2}} \right\|_2}$$

- Multiscale geometry with (albeit only one) tiny cell => very small Δt => long CPU time

[5] A. Van Londersele *et al*, J. Comput. Phys., 2017

Two traditional FDTD methods for the EM fields.

One-step leapfrog alternating-direction-implicit (ADI) FDTD [6].

Formulation

$$\begin{bmatrix} \frac{M_\epsilon}{\Delta t} + \frac{\Delta t}{4} C_1 M_\mu^{-1} {C_1}^T & 0 \\ C^T & \frac{M_\mu}{\Delta t} + \frac{\Delta t}{4} {C_2}^T M_\epsilon^{-1} C_2 \end{bmatrix} \begin{bmatrix} \hat{\mathbf{e}}|^n \\ \hat{\mathbf{h}}|^{n+\frac{1}{2}} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{M_\epsilon}{\Delta t} + \frac{\Delta t}{4} C_1 M_\mu^{-1} {C_1}^T & C \\ 0 & \frac{M_\mu}{\Delta t} + \frac{\Delta t}{4} {C_2}^T M_\epsilon^{-1} C_2 \end{bmatrix} \begin{bmatrix} \hat{\mathbf{e}}|^{n-1} \\ \hat{\mathbf{h}}|^{n-\frac{1}{2}} \end{bmatrix} + \begin{bmatrix} \hat{\mathbf{s}}|^{n-\frac{1}{2}} \\ 0 \end{bmatrix}$$

[6] S.-C. Yang *et al*, IEEE T-AP, 2012

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Complete curl splitting $C = C_1 + C_2$

$$C_1 = \begin{bmatrix} 0 & 0 & I_{n_x} \otimes D_y \otimes I_{m_z} \\ I_{m_x} \otimes I_{n_y} \otimes D_z & 0 & 0 \\ 0 & D_x \otimes I_{m_y} \otimes I_{n_z} & 0 \end{bmatrix}$$

$$C_2 = \begin{bmatrix} 0 & -I_{n_x} \otimes I_{m_y} \otimes D_z & 0 \\ 0 & 0 & -D_x \otimes I_{n_y} \otimes I_{m_z} \\ -I_{m_x} \otimes D_y \otimes I_{n_z} & 0 & 0 \end{bmatrix}$$

[6] S.-C. Yang *et al*, IEEE T-AP, 2012

Two traditional FDTD methods for the EM fields.

One-step leapfrog ADI-FDTD.

Properties

- Unconditionally stable
- Fully implicit
  - time-stepping requires inversion of (band) matrices => slower than explicit (e.g., Yee) schemes
- Splitting error
  - extra blue terms: perturbation of the Yee-scheme
  - error increases with increasing time step and for EM fields with large gradient

Two traditional FDTD methods for the EM fields.

Main drawbacks in the context of multiscale modeling.

Yee-FDTD

One small grid cell

=> small time step

=> long CPU times

ADI-FDTD

Full implicitization is overkill

=> high splitting error and long CPU time

Two traditional FDTD methods for the EM fields.

Main drawbacks in the context of multiscale modeling.

Yee-FDTD

One small grid cell

=> small time step

=> long CPU times

ADI-FDTD

Full implicitization is overkill

=> high splitting error and long CPU time

Alternative (this work)

Alternating-direction hybrid implicit-explicit (ADHIE) method

partial implicitization: remove only the smallest grid cells

The ADHIE-FDTD method for the EM fields.

General formulation.

$$\begin{bmatrix} \frac{M_\epsilon}{\Delta t} + \frac{\Delta t}{4\alpha^2}\tilde{C}_1 M_\mu^{-1} \tilde{C}_1{}^T & 0 \\ C^T & \frac{M_\mu}{\Delta t} + \frac{\Delta t}{4\alpha^2}\tilde{C}_2{}^T M_\epsilon^{-1} \tilde{C}_2 \end{bmatrix} \begin{bmatrix} \hat{\mathbf{e}}|^{n} \\ \hat{\mathbf{h}}|^{n+\frac{1}{2}} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{M_\epsilon}{\Delta t} + \frac{\Delta t}{4\alpha^2}\tilde{C}_1 M_\mu^{-1} \tilde{C}_1{}^T & C \\ 0 & \frac{M_\mu}{\Delta t} + \frac{\Delta t}{4\alpha^2}\tilde{C}_2{}^T M_\epsilon^{-1} \tilde{C}_2 \end{bmatrix} \begin{bmatrix} \hat{\mathbf{e}}|^{n-1} \\ \hat{\mathbf{h}}|^{n-\frac{1}{2}} \end{bmatrix} + \begin{bmatrix} \hat{\mathbf{s}}|^{n-\frac{1}{2}} \\ 0 \end{bmatrix}$$

Adaptations

- Splitting parameter $\alpha \in]0, 1[$
- Different curl splitting matrices $\tilde{C}_1$ and $\tilde{C}_2$
  → two illustrative examples on next slides

The ADHIE-FDTD method for the EM fields.

Implicitization of the entire *z*-direction.

$$\tilde{C}_1 = \begin{bmatrix} 0 & 0 & 0 \\ I_{m_x} \otimes I_{n_y} \otimes D_z & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Incomplete curl splitting $C \neq \tilde{C}_1 + \tilde{C}_2$

$$\tilde{C}_2 = \begin{bmatrix} 0 & -I_{n_x} \otimes I_{m_y} \otimes D_z & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

remainder $C_0 = C - \tilde{C}_1 - \tilde{C}_2 = \begin{bmatrix} 0 & 0 & I_{n_x} \otimes D_y \otimes I_{m_z} \\ 0 & 0 & -D_x \otimes I_{n_y} \otimes I_{m_z} \\ -I_{m_x} \otimes D_y \otimes I_{n_z} & D_x \otimes I_{m_y} \otimes I_{n_z} & 0 \end{bmatrix}$

With this choice:

all derivatives along x and y are explicit (Yee-style)

all derivatives along z are implicitized (ADI-style)

=> All grid steps Δz_k along z are removed from the stability criterion (see further)

The ADHIE-FDTD method for the EM fields.

Partial (local) implicitization along the z-direction.

Even more incomplete curl splitting

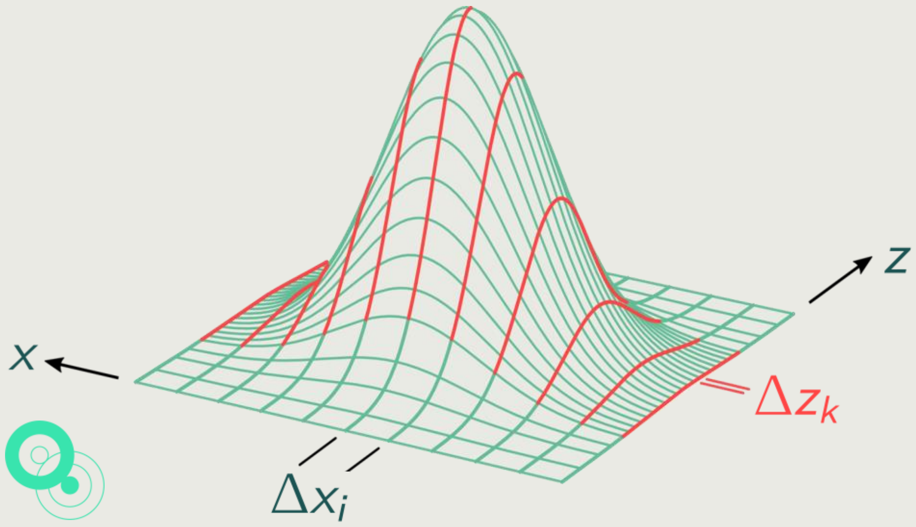
$$C \neq \tilde{C}_1 + \tilde{C}_2$$

$$\tilde{C}_1 = \begin{bmatrix} 0 & 0 & 0 \\ I_{mx} \otimes I_{ny} \otimes D_z (I_{nz} - P_z) & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\tilde{C}_2 = \begin{bmatrix} 0 & -I_{nx} \otimes I_{my} \otimes D_z (I_{nz} - P_z) & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

remainder

$$C_0 = C - \tilde{C}_1 - \tilde{C}_2 = \begin{bmatrix} 0 & -I_{nx} \otimes I_{my} \otimes D_z P_z & I_{nx} \otimes D_y \otimes I_{mz} \\ I_{mx} \otimes I_{ny} \otimes D_z P_z & 0 & -D_x \otimes I_{ny} \otimes I_{mz} \\ -I_{mx} \otimes D_y \otimes I_{nz} & D_x \otimes I_{my} \otimes I_{nz} & 0 \end{bmatrix}$$



P_z is a diagonal matrix with entries:

$$[P_z]_{k,k} = p_{z,k} = \begin{cases} 0, & \text{if } \Delta z_k \text{ should be implicit,} \\ 1, & \text{if } \Delta z_k \text{ should be explicit.} \end{cases}$$

Locally, some well-chosen (small) grid steps along z are removed!

The ADHIE-FDTD method for the EM fields.

Properties.

Stability criterion: $$\Delta t < \frac{2\left(1-\alpha^2\right)}{\left\| M_\epsilon^{-\frac{1}{2}} C_0 M_\mu^{-\frac{1}{2}} \right\|_2}$$

Special cases

Yee-FDTD : $\tilde{C}_1 = \tilde{C}_2 = 0$ and thus $C_0 = C$ → $\Delta t < \frac{2}{\left\| M_\epsilon^{-\frac{1}{2}} C M_\mu^{-\frac{1}{2}} \right\|_2}$

ADI-FDTD: $\tilde{C}_1 = C_1, \tilde{C}_2 = C_2, C_0 = 0\,,\ \alpha = 1$ → unconditionally stable ($\Delta t < \infty$), but large splitting error

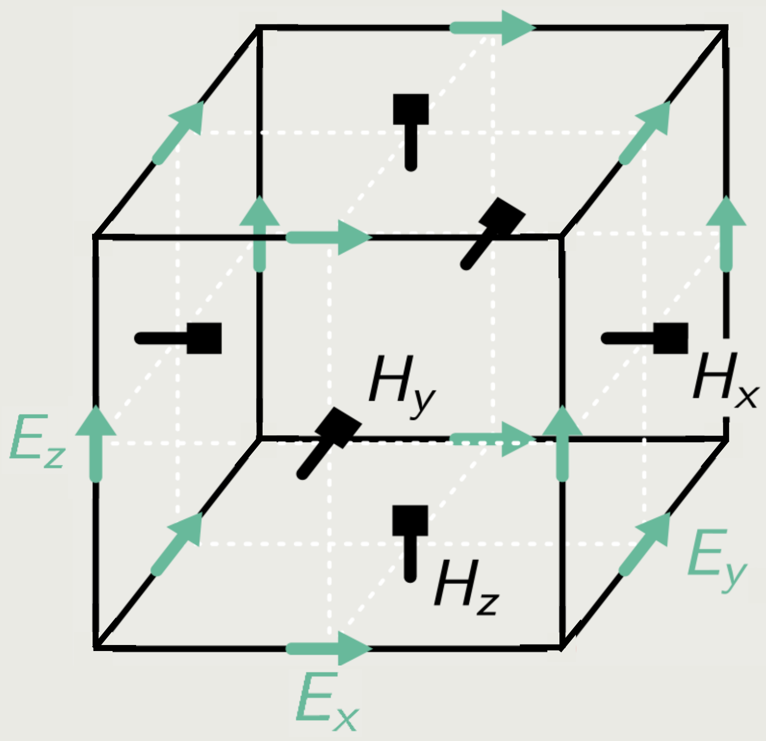
ADHIE splitting parameter $\alpha \in \left]0,1\right[$

trade-off between efficiency (time step) and splitting error

The ADHIE-FDTD method for the EM potentials.

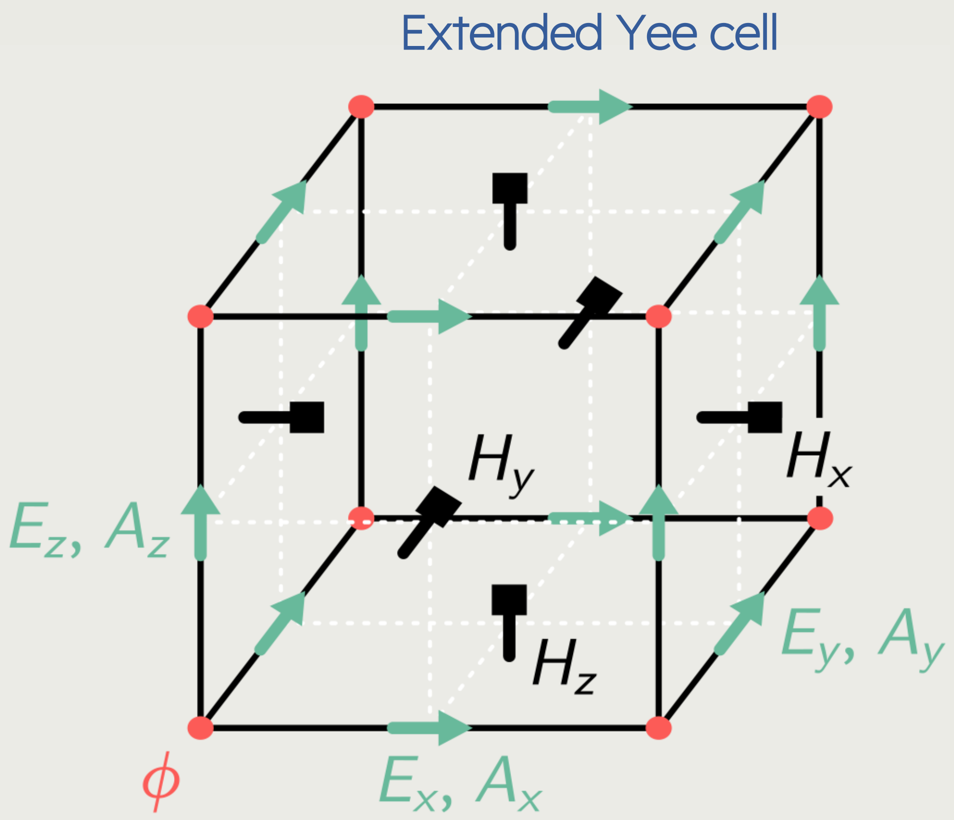
Formulation.

Yee cell



The ADHIE-FDTD method for the EM potentials.

Formulation.



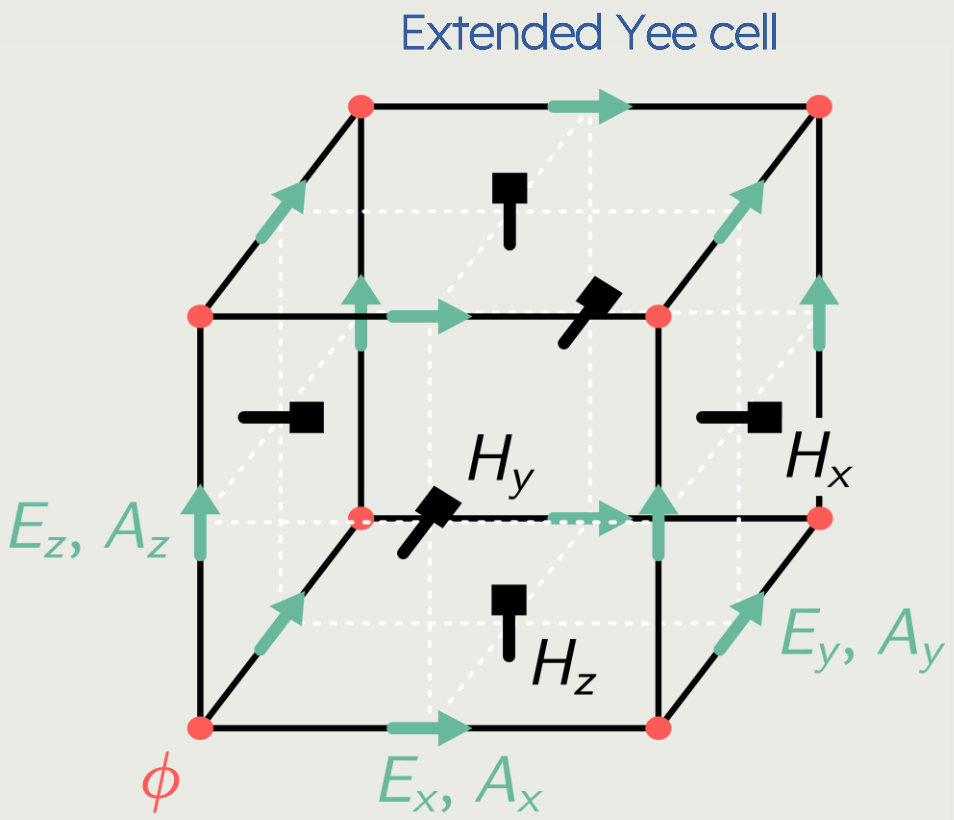
Temporal:

E and A at integer time indices

H and ϕ at half-integer time indices

The ADHIE-FDTD method for the EM potentials.

Formulation.



Temporal:

E and A at integer time indices

H and ϕ at half-integer time indices

$$\boldsymbol{E} = -\frac{\partial \boldsymbol{A}}{\partial t} - \nabla \phi$$

$$\nabla \cdot \boldsymbol{A} + \frac{1}{c^2}\frac{\partial \phi}{\partial t} = 0$$

ADHIE

$$\begin{bmatrix} I_{ne} & 0 \\ c\Delta t D^\star & G \end{bmatrix} \begin{bmatrix} \mathbf{a}|^{n+\frac{1}{2}} \\ \frac{1}{c}\phi|^{n+1} \end{bmatrix} = \begin{bmatrix} I_{ne} & c\Delta t D^T \\ 0 & G \end{bmatrix} \begin{bmatrix} \mathbf{a}|^{n-\frac{1}{2}} \\ \frac{1}{c}\phi|^{n} \end{bmatrix} - \begin{bmatrix} \mathbf{e}|^{n} \\ 0 \end{bmatrix}$$

$$G = G_x \otimes G_y \otimes G_z$$

$$G_u = \left(I_{m_u} + \frac{c^2 \Delta t^2}{4\alpha^2} \delta_u^{\star -1} D_u^\star (1 - P_u) \delta_u^{-1} D_u^T \right), \quad u \in \{x, y, z\}$$

The ADHIE-FDTD method for the EM potentials.

Properties.

Stability criterion: $$\Delta t < \frac{2}{c\sqrt{\left\| D^{\star} P D^{T} \right\|_2}}$$

ADHIE scheme: tunable between fully explicit and fully implicit

Stability does **not** depend on splitting parameter α, which can be chosen arbitrarily close to one

→ drastic reduction of splitting error

Implicit system can be solved using tridiagonal matrix algorithm

→ complexity of linear order $\mathcal{O}(n)$

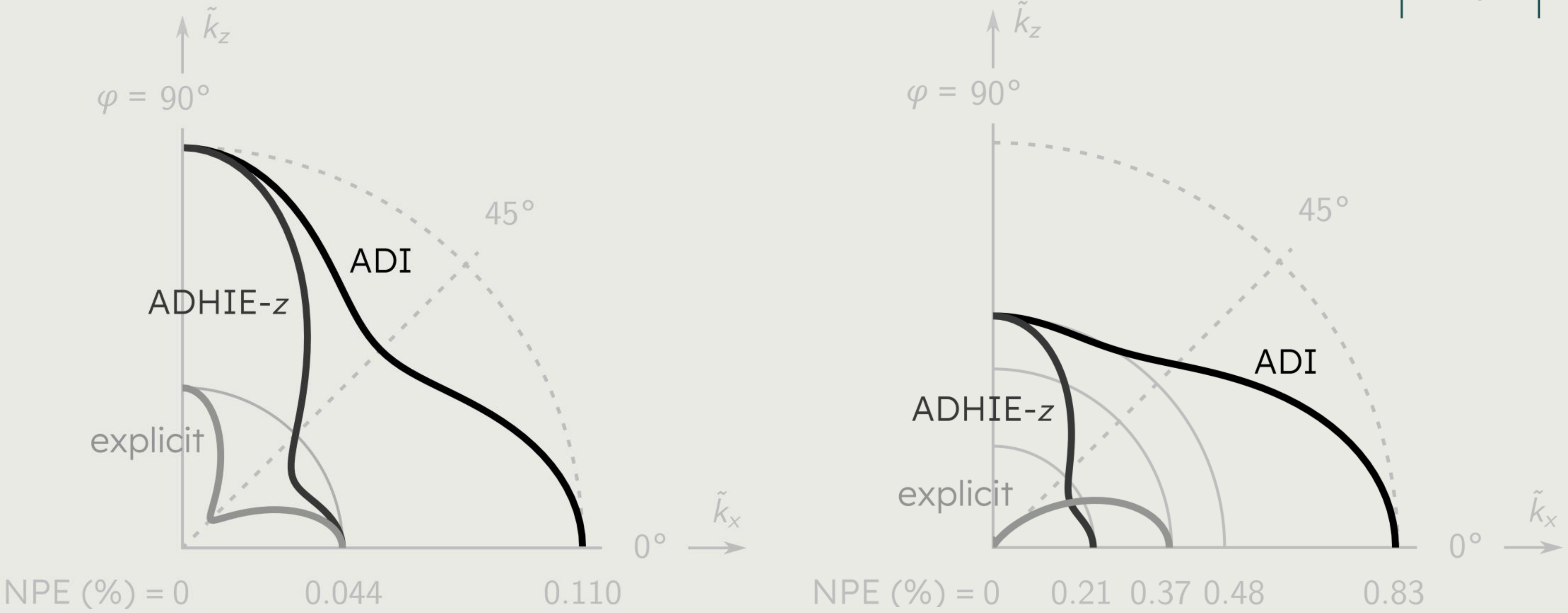
Stability of the complete Maxwellian system for $(\boldsymbol{e}, \boldsymbol{h}, \boldsymbol{a}, \boldsymbol{\phi})$ is also guaranteed!

The ADHIE-FDTD method.

Dispersion.

Plane wave traveling in the first quadrant of the *(x,z)*-plane under angle φ with *x*-axis

Comparison between exact k_0 and numerical wavenumber $\tilde{k}$ → numerical phase error: $\text{NPE}(\%) = 100 \left| \frac{\tilde{k} - k_0}{k_0} \right|$



uniform, fine spatial discretization
time step: CFL limit

fine sampling along *z* / coarse along *x* and *y*
explicit: CFL limit / ADI & ADHIE: 2 x CFL limit

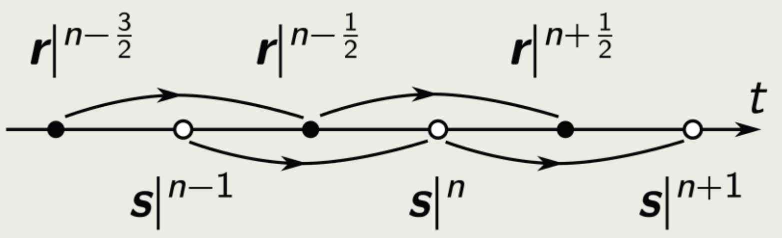
A leapfrog FDTD method for the minimally-coupled Schrödinger equation.

Formulation (extension of [7]).

$$\jmath\hbar\frac{\partial\psi}{\partial t} = \hat{\mathrm{H}}\psi = \left(\frac{1}{2m}\left(-\jmath\hbar\boldsymbol{\nabla} - q\boldsymbol{A}\right)^2 + q\phi + v\right)\psi$$

Split in real and imaginary parts $\quad \psi = r + \jmath\, s \qquad \hat{\mathrm{H}} = \hat{\mathrm{H}}_0 + \jmath\, \hat{\mathrm{H}}_1$

Temporal discretization



Spatial discretization $\quad \hat{\mathrm{H}}_0\,,\ \hat{\mathrm{H}}_1 \ \rightarrow\ H_0\,,\ H_1$

$$\begin{bmatrix} I - \frac{\Delta t}{2\hbar}H_1\big|^{n-\frac{1}{2}} & 0 \\ -\frac{\Delta t}{\hbar}H_0\big|^{n} & I - \frac{\Delta t}{2\hbar}H_1\big|^{n} \end{bmatrix}\begin{bmatrix} \boldsymbol{s}\big|^{n} \\ \boldsymbol{r}\big|^{n+\frac{1}{2}} \end{bmatrix} = \begin{bmatrix} I + \frac{\Delta t}{2\hbar}H_1\big|^{n-\frac{1}{2}} & -\frac{\Delta t}{\hbar}H_0\big|^{n-\frac{1}{2}} \\ 0 & I + \frac{\Delta t}{2\hbar}H_1\big|^{n} \end{bmatrix}\begin{bmatrix} \boldsymbol{s}\big|^{n-1} \\ \boldsymbol{r}\big|^{n-\frac{1}{2}} \end{bmatrix}$$

[7] P. Decleer *et al*, J. Comput. Appl. Math., 2021

A leapfrog FDTD method for the minimally-coupled Schrödinger equation.

Properties.

Temporal part: 2^{nd}-order accurate

Spatial part (in this work): uniform grid, 6^{th}-order accurate differences and averages

→ good balance between accuracy and efficiency

Stability criterion (for time-independent EM potentials): $\Delta t < \dfrac{2\hbar}{\left\|H_0\right\|_2}$

Self-consistent forward-backward coupled scheme.

Reminder.

forward via EM potentials

$$\nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t}$$

$$\nabla \times \boldsymbol{H} = \frac{\partial \boldsymbol{D}}{\partial t} + \boldsymbol{J}_f + \boldsymbol{J}_c + \boldsymbol{J_q}$$

$$\boldsymbol{E} = -\frac{\partial \boldsymbol{A}}{\partial t} - \nabla \phi$$

$$\nabla \cdot \boldsymbol{A} + \frac{1}{c^2}\frac{\partial \phi}{\partial t} = 0$$

$$\jmath\hbar\frac{\partial \psi}{\partial t} = \left(\frac{1}{2m}(-\jmath\hbar\nabla - q\boldsymbol{A})^2 + q\phi + v\right)\psi$$

backward via quantum current density $\boldsymbol{J_q} = q\,\mathrm{Re}\left\{\psi^* \frac{-\jmath\hbar\nabla - q\boldsymbol{A}}{m}\psi\right\}$

Self-consistent forward-backward coupled scheme.

Discretization of quantum current density.

forward via EM potentials

$$\nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t}$$

$$\nabla \times \boldsymbol{H} = \frac{\partial \boldsymbol{D}}{\partial t} + \boldsymbol{J}_f + \boldsymbol{J}_c + \boldsymbol{J}_q$$

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backward via quantum current density $\boldsymbol{J_q} = q\,\mathrm{Re}\left\{\psi^* \frac{-\jmath\hbar\boldsymbol{\nabla} - q\boldsymbol{A}}{m}\psi\right\}$

$$= \frac{q\hbar}{m}\left(r\boldsymbol{\nabla} s - s\boldsymbol{\nabla} r - \frac{q}{\hbar}(r^2 + s^2)\boldsymbol{A}\right)$$

wave function split in real and imaginary part

apply 6^{th}-order accurate averages and differences

Self-consistent forward-backward coupled scheme.

Flowchart.

$$\boldsymbol{s}|^{n} \longrightarrow \boldsymbol{j}_q|^{n-\frac{1}{2}} \longrightarrow \hat{\boldsymbol{e}}|^{n} \longrightarrow \hat{\boldsymbol{h}}|^{n+\frac{1}{2}} \longrightarrow \boldsymbol{a}|^{n+\frac{1}{2}} \longrightarrow \boldsymbol{r}|^{n+\frac{1}{2}} \longrightarrow \phi|^{n+1}$$

Self-consistent forward-backward coupled scheme.

Flowchart.

$$\boldsymbol{s}|^{n} \longrightarrow \boldsymbol{j}_q|^{n-\frac{1}{2}} \longrightarrow \hat{\boldsymbol{e}}|^{n} \longrightarrow \hat{\boldsymbol{h}}|^{n+\frac{1}{2}} \longrightarrow \boldsymbol{a}|^{n+\frac{1}{2}} \longrightarrow \boldsymbol{r}|^{n+\frac{1}{2}} \longrightarrow \boldsymbol{\phi}|^{n+1}$$

Note on **stability** of the entire scheme:

> not rigorously proven (nonlinear)
>
> choose smallest time step (usually, Maxwellian one)
>
> no issues in all practical examples we tested

Numerical examples.

Example 0: flying qubit interferometer (Schrödinger system).

Setup.

laterally tunnel-coupled quantum wires
with small geometrical details

wires separated by thin barrier
of variable length and height

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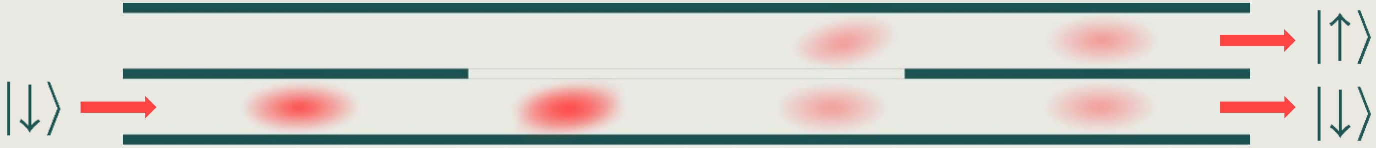
quantum superposition



Note: no harm was done to animals during the research; Vande Ginste's cat is very much in the alive state!

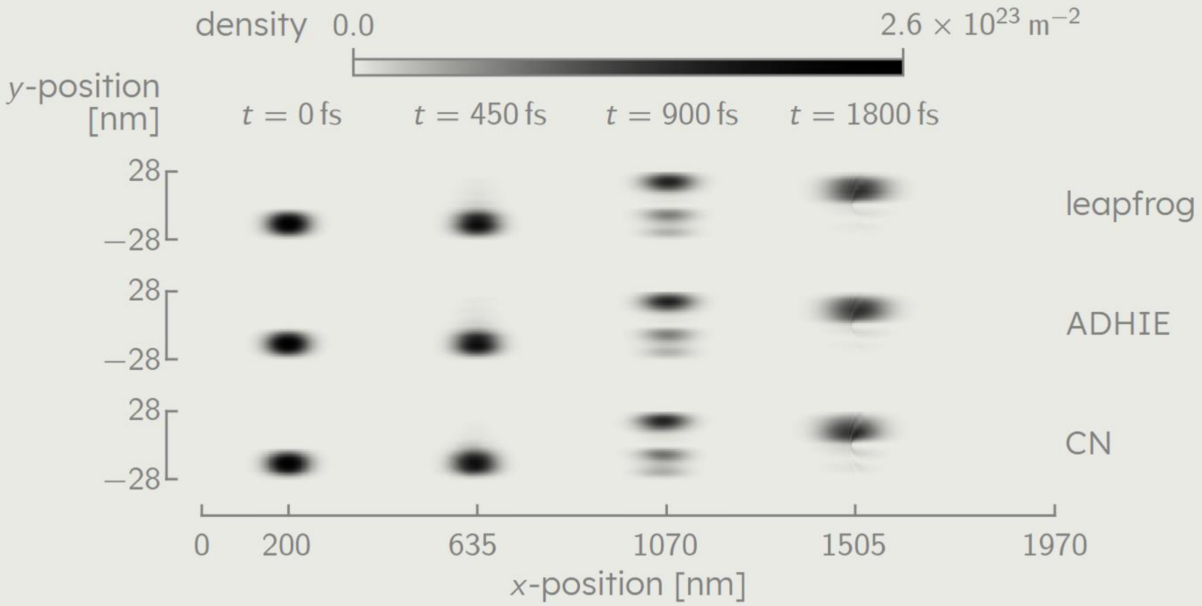
Example 0: flying qubit interferometer (Schrödinger system).

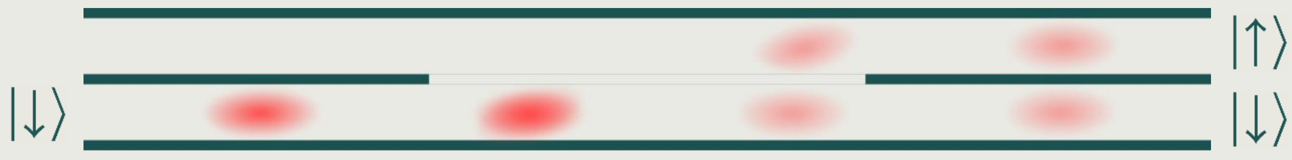
Results: comparison of three methods [8].

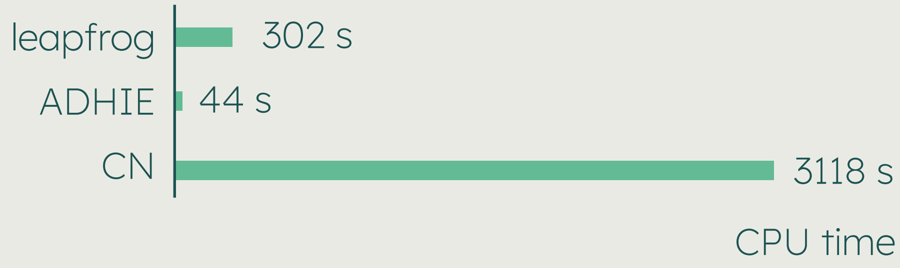
laterally tunnel-coupled quantum wires
with small geometrical details

wires separated by thin barrier
of variable length and height

quantum superposition





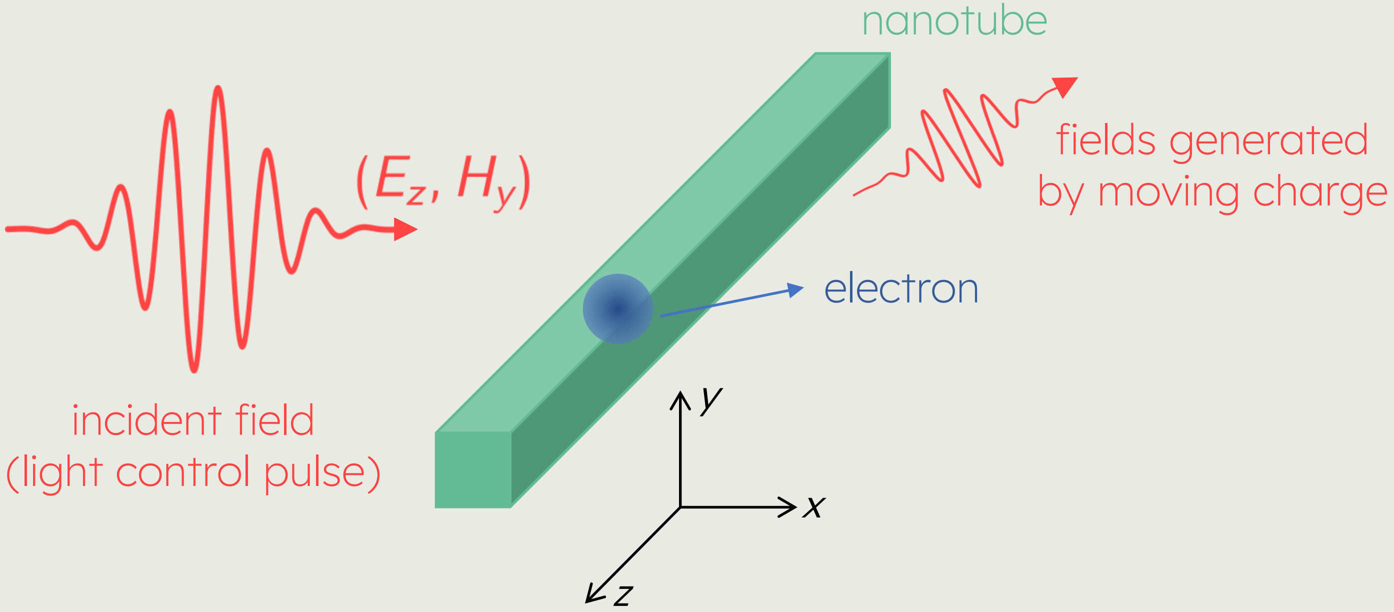


[8] P. Decleer *et al*, J. Comput. Appl. Math., 2022

CN: Crank-Nicolson

Example 1: quantum state controller [9] (Maxwell-Schrödinger system).

Setup.



[9] T. Takeuchi *et al*, Phys. Rev. A, 2015

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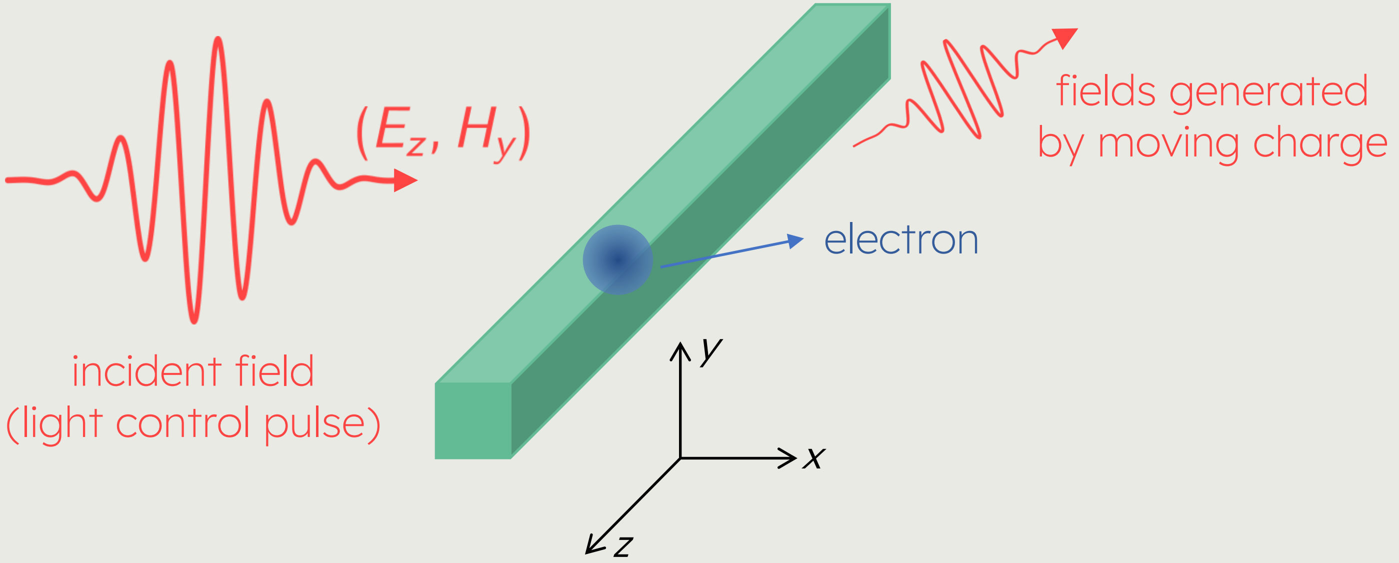
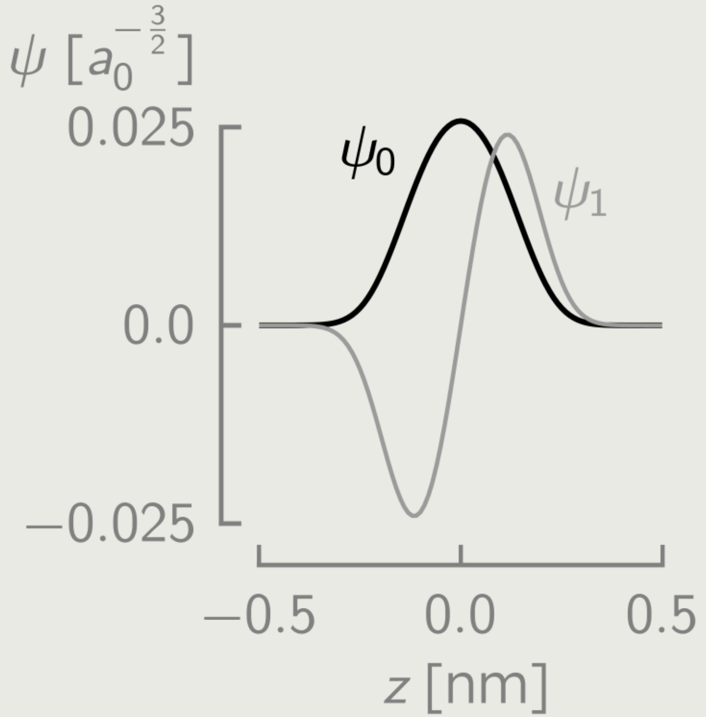




anharmonic confining potential in the nanotube:

$$v(z) = v_0 \left(\frac{z}{z_{\max}} \right)^4, \ v_0 = 5 \times 10^3\,\mathrm{eV}, \ z_{\max} = 1.0\,\mathrm{nm}$$

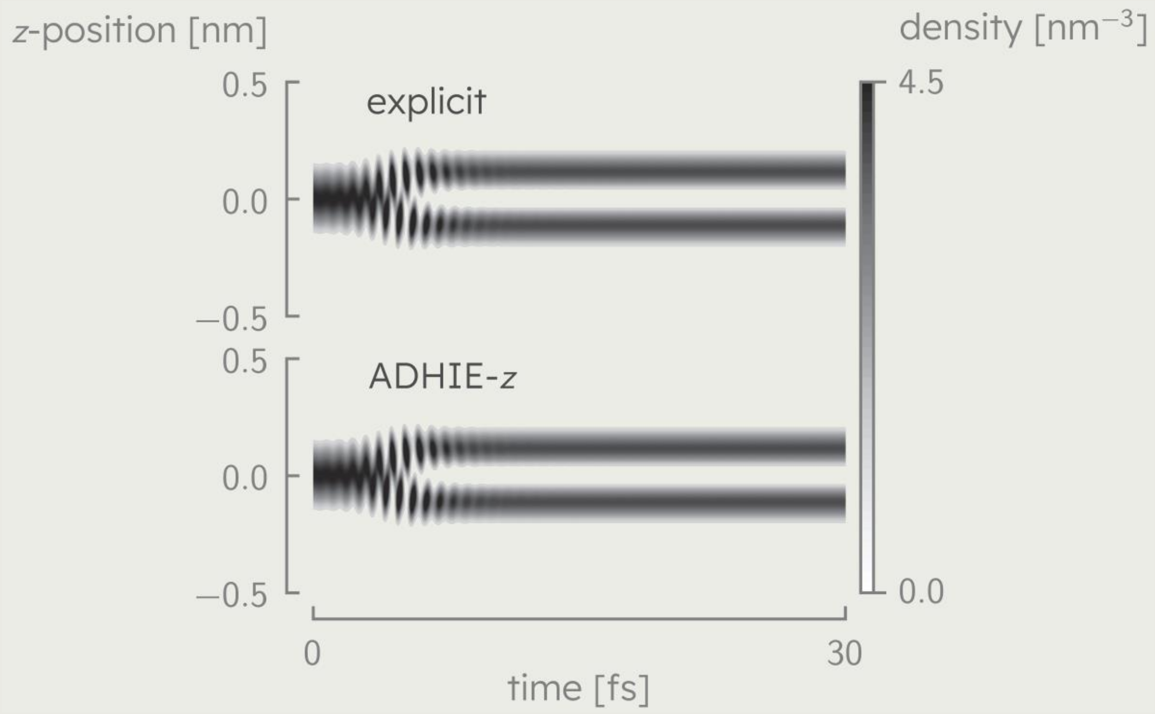
ψ_0 : initial (ground) state

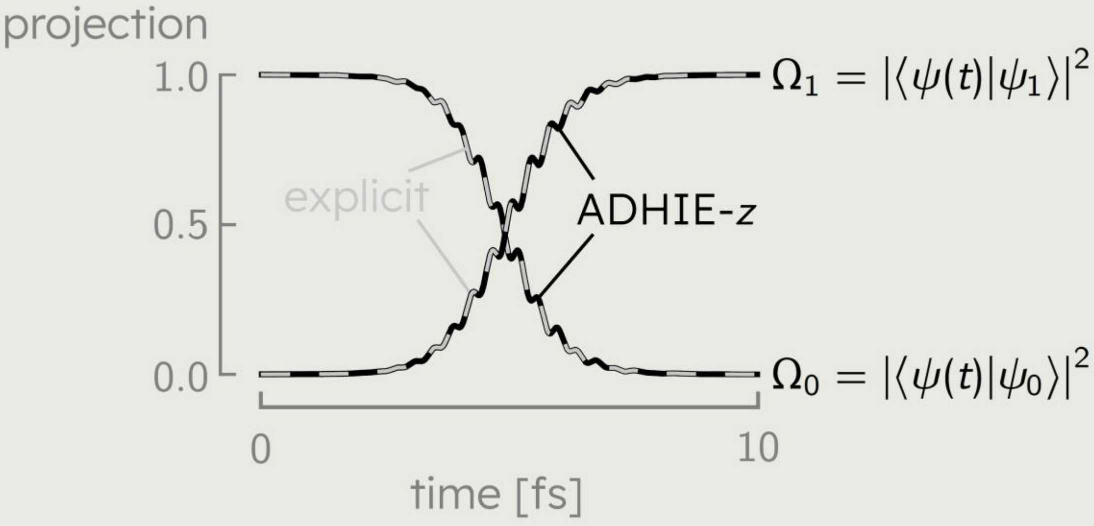
ψ_1 : desired (first excited) state

[9] T. Takeuchi *et al*, Phys. Rev. A, 2015

Example 1: quantum state controller (Maxwell-Schrödinger system).

Results.





time steps

$\Delta t_{\text{exp}} = 3.3 \times 10^{-5}$ fs $> \Delta t_{\text{ADHIE}} = 4.5 \times 10^{-4}$ fs

Intermezzo: Kohn-Sham equations

The shortest description ever.

Why?

One single time-dependent Schrödinger equation for N interacting electrons

this is a many-body problem => huge computational efforts!

Solution

Replace many-body Schrödinger equation by *N Kohn-Sham equations* subject to time-dependent EM fields [10]

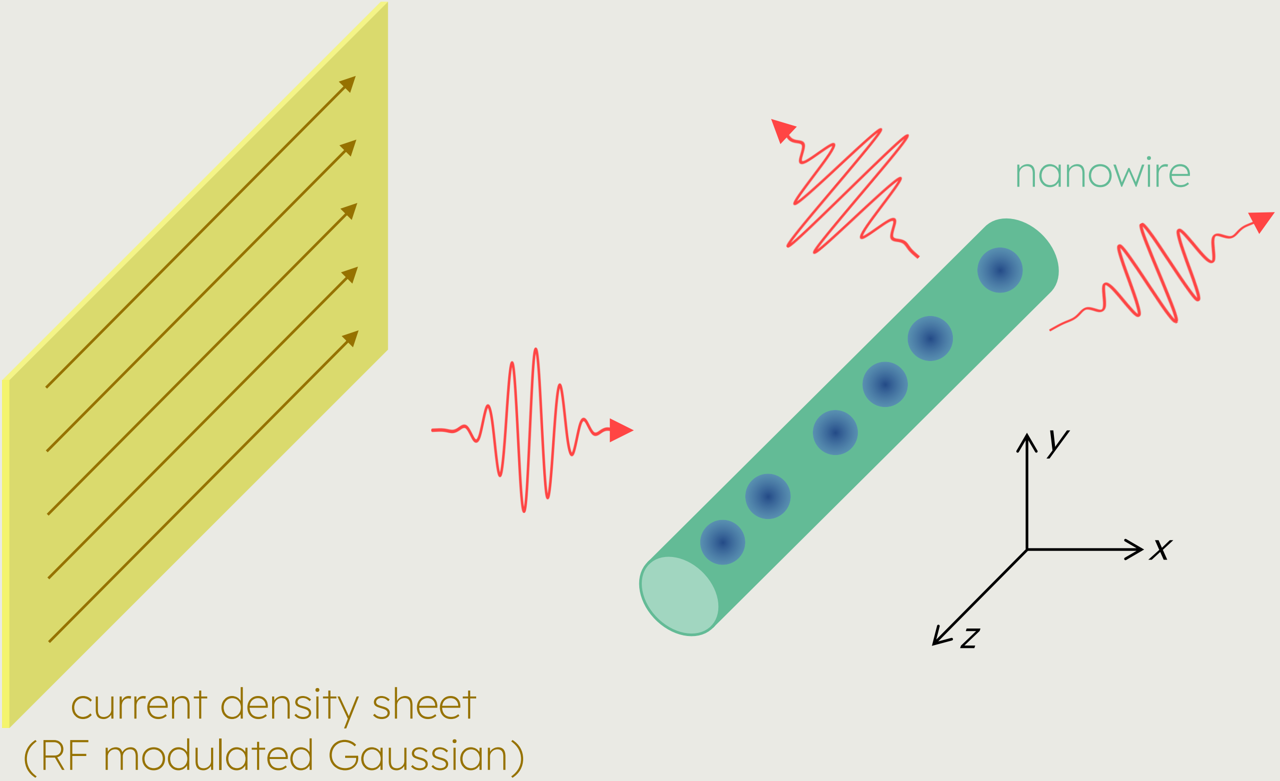
each Kohn-Sham equation models one electron and their mutual interaction is taken care of in an approximate way

the good news: each Kohn-Sham equation has the form of a single-particle Schrödinger equation

[10] S.K. Gosh and A.K. Dhara, Phys. Rev. A, 1988

Example 2: nanowire with six electrons [11] (Maxwell-Kohn-Sham system).

Setup.



[11] J. Grossi *et al*, J. Phys.: Condens. Matter, 2020

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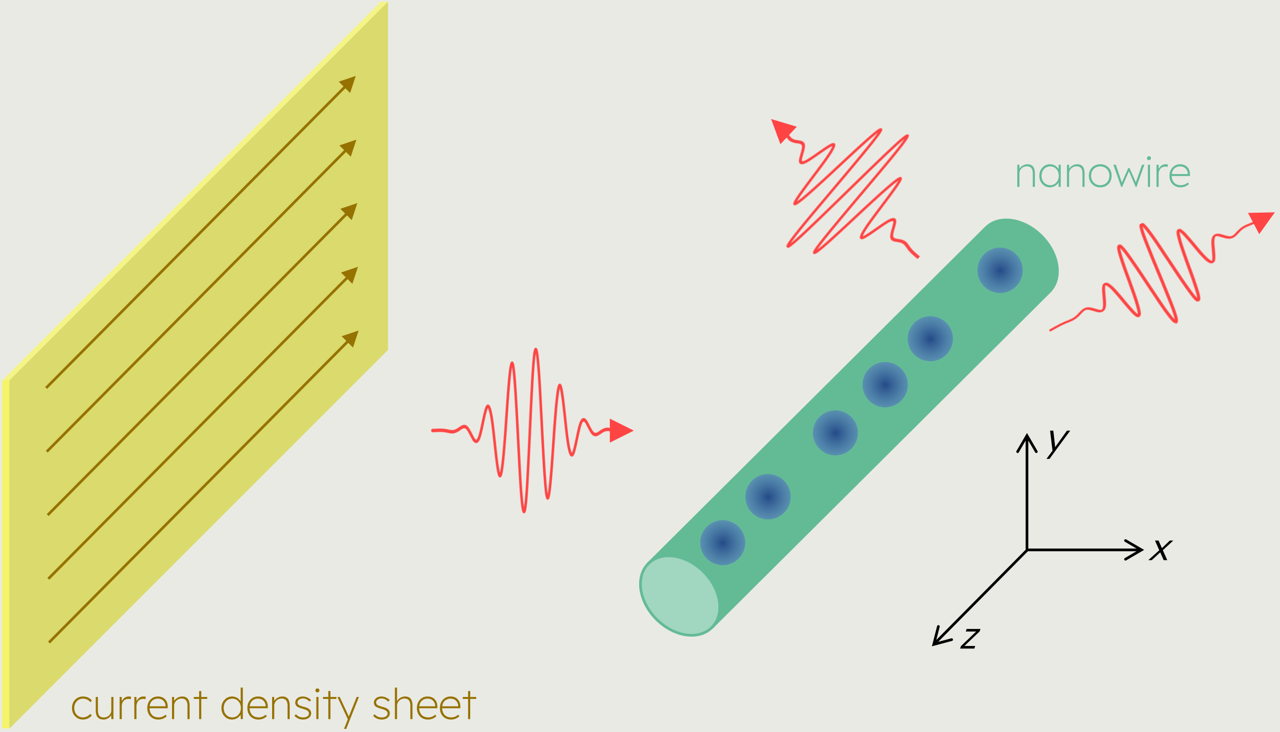
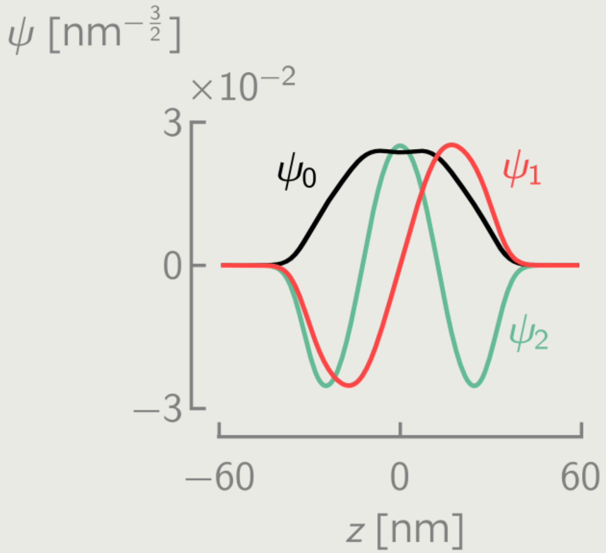
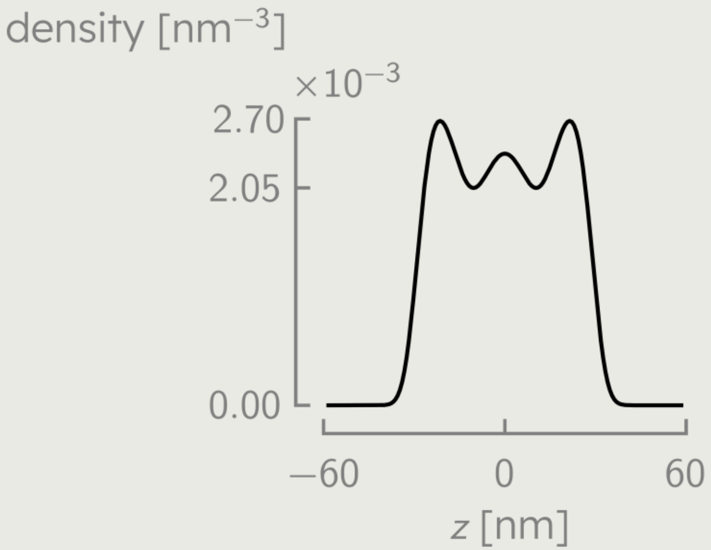




initial Kohn-Sham orbitals



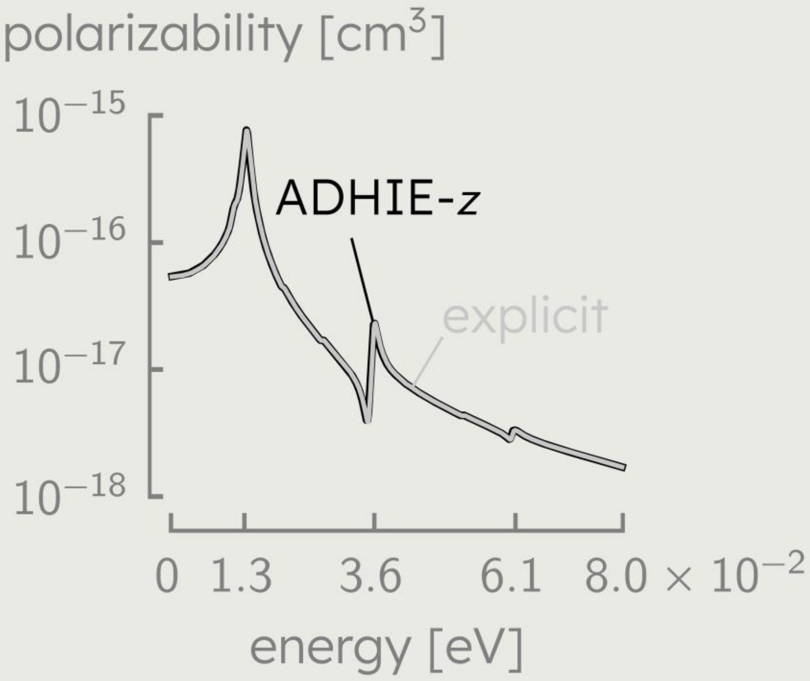
ground state density

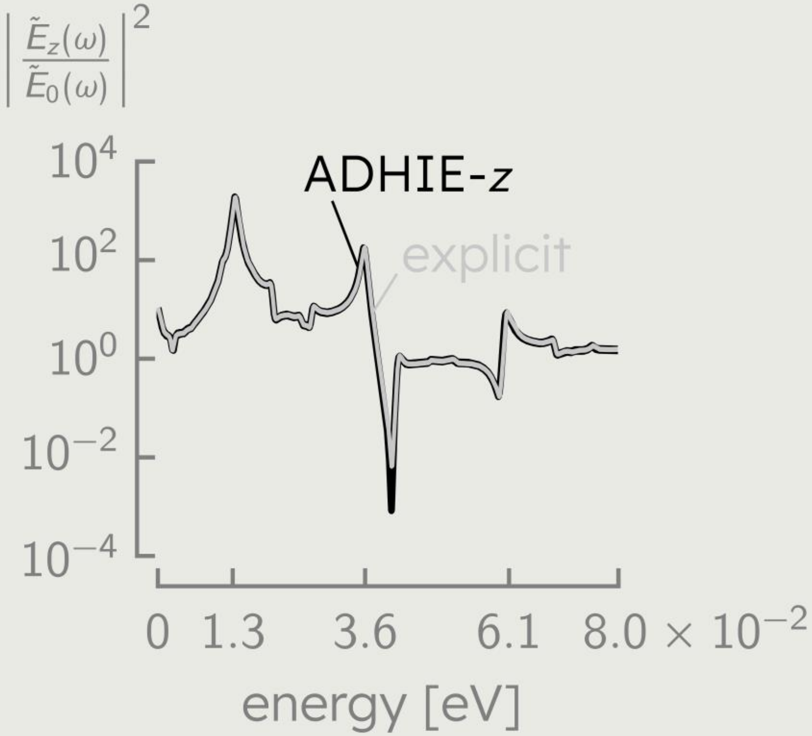
confining potentials:
transverse harmonic and longitudinal anharmonic

[11] J. Grossi *et al*, J. Phys.: Condens. Matter, 2020

Example 2: nanowire with six electrons (Maxwell-Kohn-Sham system).

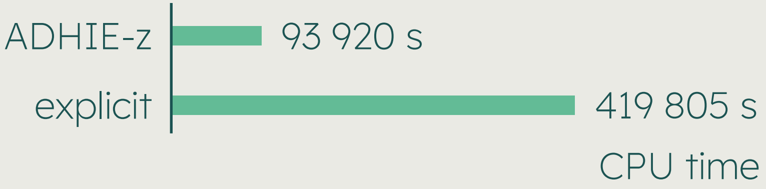
Results.





time steps

$\Delta t_{\text{exp}} = 2.43 \times 10^{-3}$ fs $> \Delta t_{\text{ADHIE}} = 14.05 \times 10^{-3}$ fs



Conclusions.

Conclusions.

Key takeaway points.

assist (quantum) electronic device **design**ers

hybrid EM/QM modeling framework

tailored toward **multiscale** geometries

- partial implicitization in preferred directions
- upper bounds for stability
- increased time step
- linear scaling

"modest" **Maxwell-Schrödinger** and **Maxwell-Kohn-Sham** applications

Conclusions.

Ongoing and future endeavors.

alternative discretization schemes

- higher-order accuracy on nonuniform grids
- subgridding
- multi-time stepping
- generalized Lorenz and other gauge conditions

applications

- intricate devices
- contacts
- Dirac materials [12,13]

[12] E. Vanderstraeten *et al*, J. Comput. Appl. Math., 2023
[13] J. Van den Broeck *et al*, Appl. Math. Model., 2023

quest.

Quantum Mechanical &
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