Quantum
Mechanical &
Electromagnetic
Systems
Modelling Lab

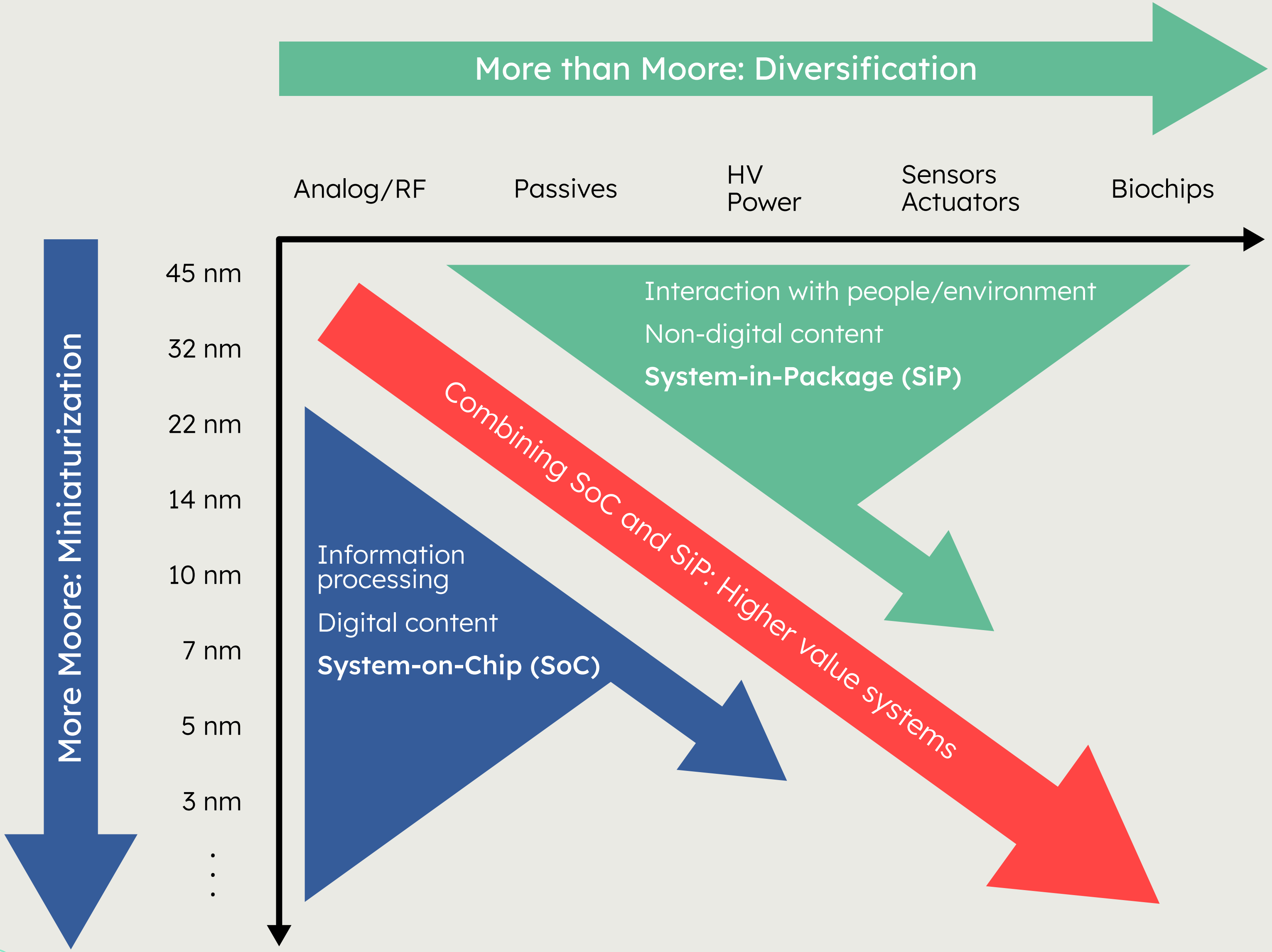
An ADHIE-TDDFT Method for the EM/QM Co-Simulation of Coupled 1-D Nanowires.

Maxim TORREELE, Pieter DECLEER, Dries VANDE GINSTE

quest.

Continuous down-scaling requires innovative solutions.

The Moore, the merrier.

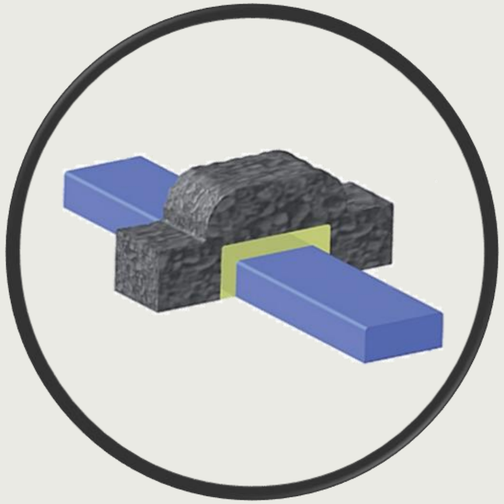


IEEE International Roadmap for Devices and Systems – IEEE IRDS™

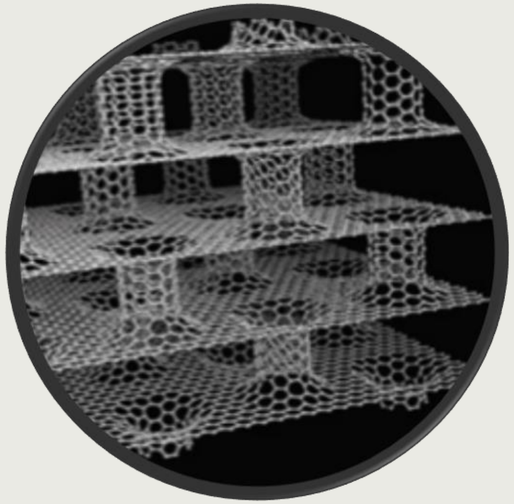
The next generation of devices benefits from the emergence of **quantum materials**.

Continuous down-scaling requires innovative solutions.

Advent of nanowire technologies.



Transistors[1]



Interconnects

Solar cells[2]

Modeling challenges: **multiscale** and **multiphysics** nature.

[1] J. Colinge *et al*, Nature Nanotechnology, 2010.
[2] A. Munkherjee *et al*, ACS Photonics, 2021.

Nanowire modeling requires multiscale approach.

The ADHIE method for EM fields.

Yee-FDTD

= explicit time stepping using a leapfrog scheme

- low memory consumption, does not require matrix inversion
- stability limited by Courant-Friedrichs-Lewy criterion: small time step

Alternating-direction implicit (ADI)

= implicit scheme based on the splitting of the curl operator in Maxwell's equations

- system is stable independent of the chosen time step (unconditionally stable)
- costly method that requires matrix inversion at each time step

Best of both worlds: the novel **Alternating-Direction Hybrid Implicit-Explicit (ADHIE) method**.

Nanowire modeling requires multiscale approach.

The ADHIE method for EM fields.

Yee-FDTD

= explicit time stepping using a leapfrog scheme

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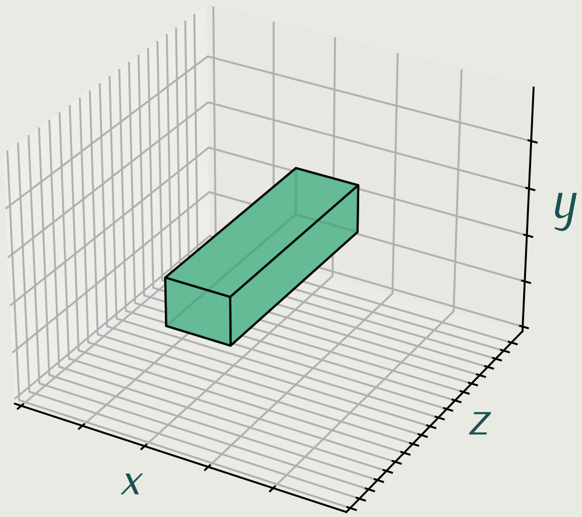
Best of both worlds: the novel **Alternating-Direction Hybrid Implicit-Explicit (ADHIE) method**.

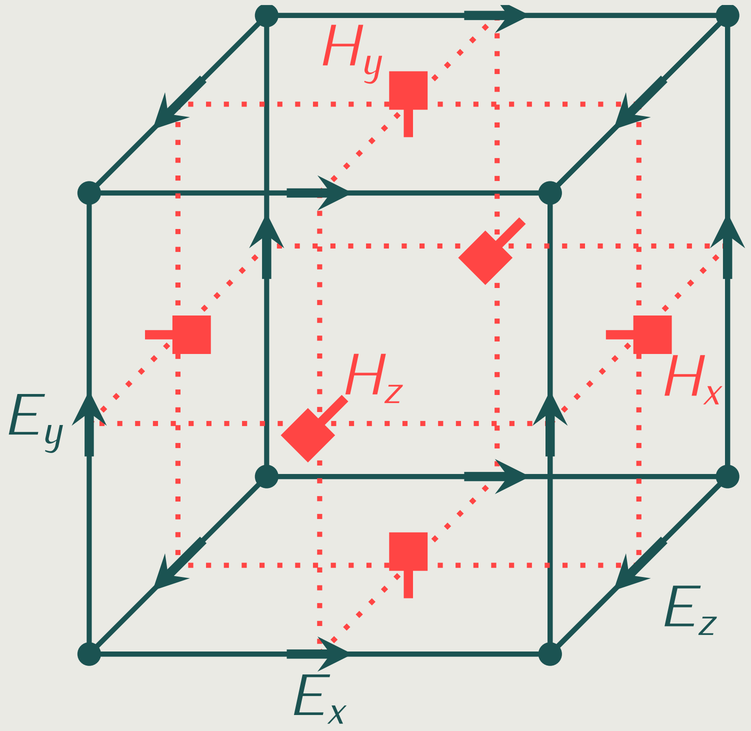


- explicit treatment of the coarsely-sampled directions
- implicitization along refinement direction eliminates small grid step from stability criterion

Nanowire modeling requires multiscale approach.

The ADHIE method for EM fields.

Yee cell



Yee update equations*

Faraday's law:

$$E_y\big|^{n}_{i,j,k} = E_y\big|^{n-1}_{i,j,k} + \frac{\Delta t}{\epsilon \Delta z^\star}\left(H_x\big|^{n-\frac{1}{2}}_{i,j,k+1} - H_x\big|^{n-\frac{1}{2}}_{i,j,k}\right) - \frac{\Delta t}{\epsilon \Delta x^\star}\left(H_z\big|^{n-\frac{1}{2}}_{i+1,j,k} - H_z\big|^{n-\frac{1}{2}}_{i,j,k}\right)$$

Ampère's law:

$$H_y\big|^{n+\frac{1}{2}}_{i,j,k} = H_y\big|^{n-\frac{1}{2}}_{i,j,k} + \frac{\Delta t}{\mu \Delta z}\left(E_x\big|^{n}_{i,j,k+1} - E_x\big|^{n}_{i,j,k}\right) - \frac{\Delta t}{\mu \Delta x}\left(E_z\big|^{n}_{i+1,j,k} - E_z\big|^{n}_{i,j,k}\right)$$

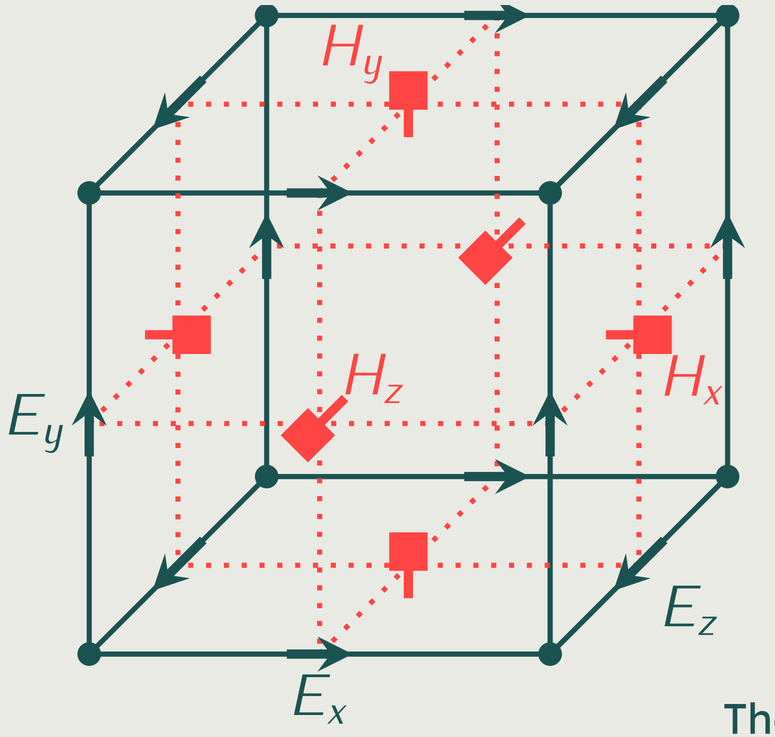
The remaining field components (E_x, E_z, H_x, H_z) are updated similarly.

* The displayed equations are written in "implementation notation".

Nanowire modeling requires multiscale approach.

The ADHIE method for EM fields.

Yee cell



ADHIE update equations

For implicitization along the *z*-direction:

Faraday's law:

$$f_1\left(E_y\big|^{n}_{i,j,k},\, E_y\big|^{n}_{i,j,k+1},\, E_y\big|^{n}_{i,j,k-1}\right) = f_1\left(E_y\big|^{n-1}_{i,j,k},\, E_y\big|^{n-1}_{i,j,k+1},\, E_y\big|^{n-1}_{i,j,k-1}\right) + \frac{1}{\Delta z^\star}\left(H_x\big|^{n-\frac{1}{2}}_{i,j,k+1} - H_x\big|^{n-\frac{1}{2}}_{i,j,k}\right) - \frac{1}{\Delta x^\star}\left(H_z\big|^{n-\frac{1}{2}}_{i+1,j,k} - H_z\big|^{n-\frac{1}{2}}_{i,j,k}\right)$$

Ampère's law:

$$f_2\left(H_y\big|^{n+\frac{1}{2}}_{i,j,k},\, H_y\big|^{n+\frac{1}{2}}_{i,j,k+1},\, H_y\big|^{n+\frac{1}{2}}_{i,j,k-1}\right) = f_2\left(H_y\big|^{n-\frac{1}{2}}_{i,j,k},\, H_y\big|^{n-\frac{1}{2}}_{i,j,k+1},\, H_y\big|^{n-\frac{1}{2}}_{i,j,k-1}\right) + \frac{1}{\Delta z}\left(E_x\big|^{n}_{i,j,k+1} - E_x\big|^{n}_{i,j,k}\right) - \frac{1}{\Delta x}\left(E_z\big|^{n}_{i+1,j,k} - E_z\big|^{n}_{i,j,k}\right)$$

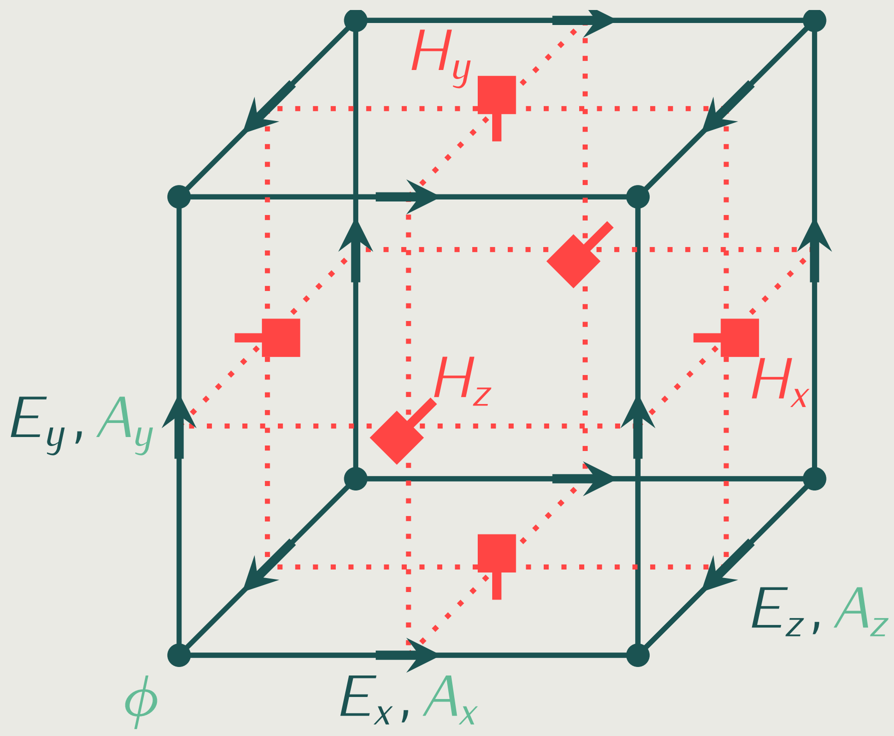
The remaining field components (E_x, E_z, H_x, H_z) are updated through the Yee scheme.

[3] A. Van Londersele *et al*, IEEE Transactions on Antennas and Propagation, 2016.

Nanowire modeling requires multiscale approach.

The ADHIE method for EM potentials.

Extended Yee cell



[4] P. Decleer *et al*, IEEE JMMCT, 2022.

Scalar and vector potential in the Lorenz gauge:

$$E = -\nabla\phi - \partial_t A,\ \nabla\cdot A + \frac{1}{c^2}\partial_t\phi = 0$$

ADHIE update equations[4]

Explicit update equations for the vector potential.

$$f\left(\phi|^{(1)}_{i,j,k},\ \phi|^{(1)}_{i,j,k+1},\ \phi|^{(1)}_{i,j,k-1}\right) = -\frac{c^2\Delta t}{\Delta x^\star}\left(A_x|^{n+\frac{1}{2}}_{i+\frac{1}{2},j,k} - A_x|^{n+\frac{1}{2}}_{i-\frac{1}{2},j,k}\right)$$
$$-\frac{c^2\Delta t}{\Delta y^\star}\left(A_y|^{n+\frac{1}{2}}_{i,j+\frac{1}{2},k} - A_y|^{n+\frac{1}{2}}_{i,j-\frac{1}{2},k}\right) - \frac{c^2\Delta t}{\Delta z^\star}\left(A_z|^{n+\frac{1}{2}}_{i,j,k+\frac{1}{2}} - A_z|^{n+\frac{1}{2}}_{i,j,k-\frac{1}{2}}\right)$$

after which $\phi|^{n+1}_{i,j,k} = \phi|^{n}_{i,j,k} + \phi|^{(1)}_{i,j,k}$

Nanowire dynamics are governed by quantum mechanics.

Beyond the Schrödinger equation: TDDFT.

Problem: *2N* electrons interacting with each other and external EM fields.

Time-dependent density functional theory (TDDFT)

Time evolution of the system described by the time-dependent Kohn-Sham (TDKS) equations for *N* orbitals:

$$\jmath\hbar \frac{\partial \psi_l(\boldsymbol{r}, t)}{\partial t} = \frac{1}{2m} \left(-\jmath\hbar\nabla - q\boldsymbol{A}\right)^2 \psi_l(\boldsymbol{r}, t) + v_{\mathrm{KS}}\psi_l(\boldsymbol{r}, t)$$

The system is described through the electron density:

$$\rho(\boldsymbol{r}, t) = \sum_{l=1}^{N} 2\left|\psi_l(\boldsymbol{r}, t)\right|^2$$

It is tractable to account for many-electron interactions through the exchange-correlation (xc) potential:

$$v_{\mathrm{KS}} = q\phi + v_{\mathrm{ext}} + v_{\mathrm{xc}}$$

Nanowire modeling requires multiphysics approach.

Coupling the EM and QM counterparts.

EM potentials:

A, ϕ

EM

QM

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

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

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

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

$$\jmath\hbar \frac{\partial \psi_l(\mathbf{r}, t)}{\partial t} = \frac{1}{2m}\left(-\jmath\hbar\nabla - qA\right)^2 \psi_l(\mathbf{r}, t) + v_{\mathrm{KS}}\psi_l(\mathbf{r}, t)$$

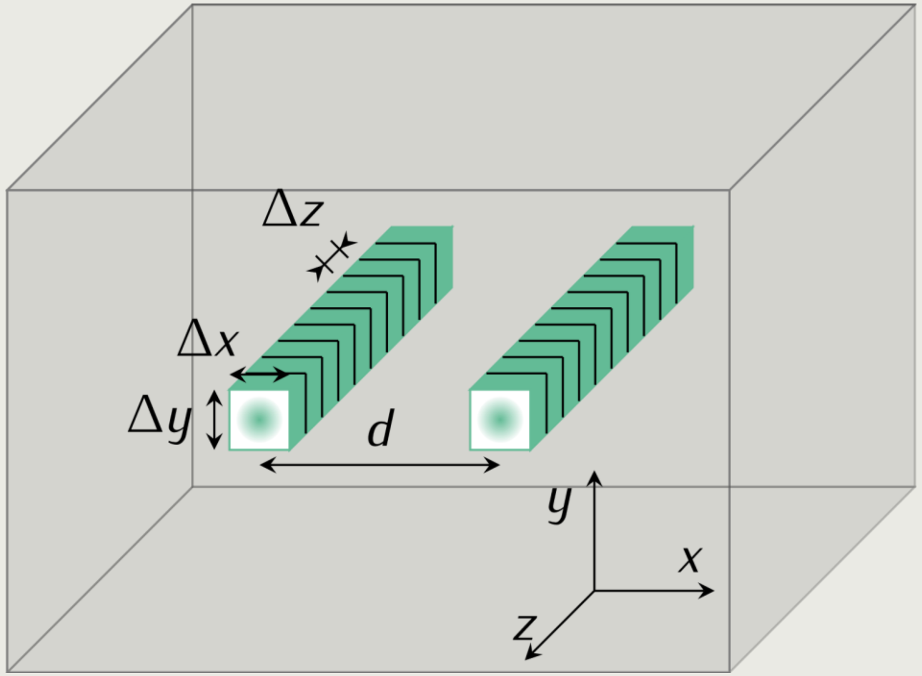
$$v_{\mathrm{KS}} = q\phi + v_{\mathrm{ext}} + v_{\mathrm{xc}}$$

Quantum current density:

$$J_q = \frac{q}{m}\sum_{l=1}^{N}\left(-\jmath\hbar\left(\psi_l^*\nabla\psi_l - \psi_l\nabla\psi_l^*\right) - 2qA\psi_l^*\psi_l\right)$$

Closely-spaced nanowires display crosstalk.

An application.



[5] M. Casula *et al*, Physical Review B, 2006.

Geometry & grid

- coarse sampling in *x*- and *y*-direction: explicit
- dense sampling in *z*-direction: implicitization
- time step: determined by EM problem

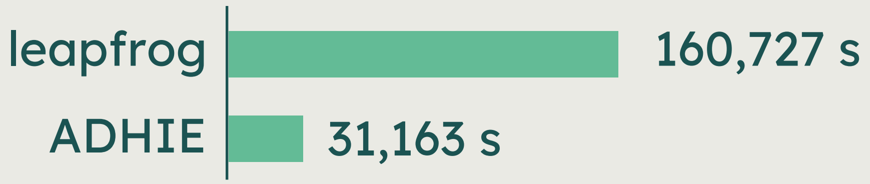
Nanowire model

- properties of GaAs
- one-dimensional: neglect transversal effects
- use parametrization for xc potential[5]

Closely-spaced nanowires display crosstalk.

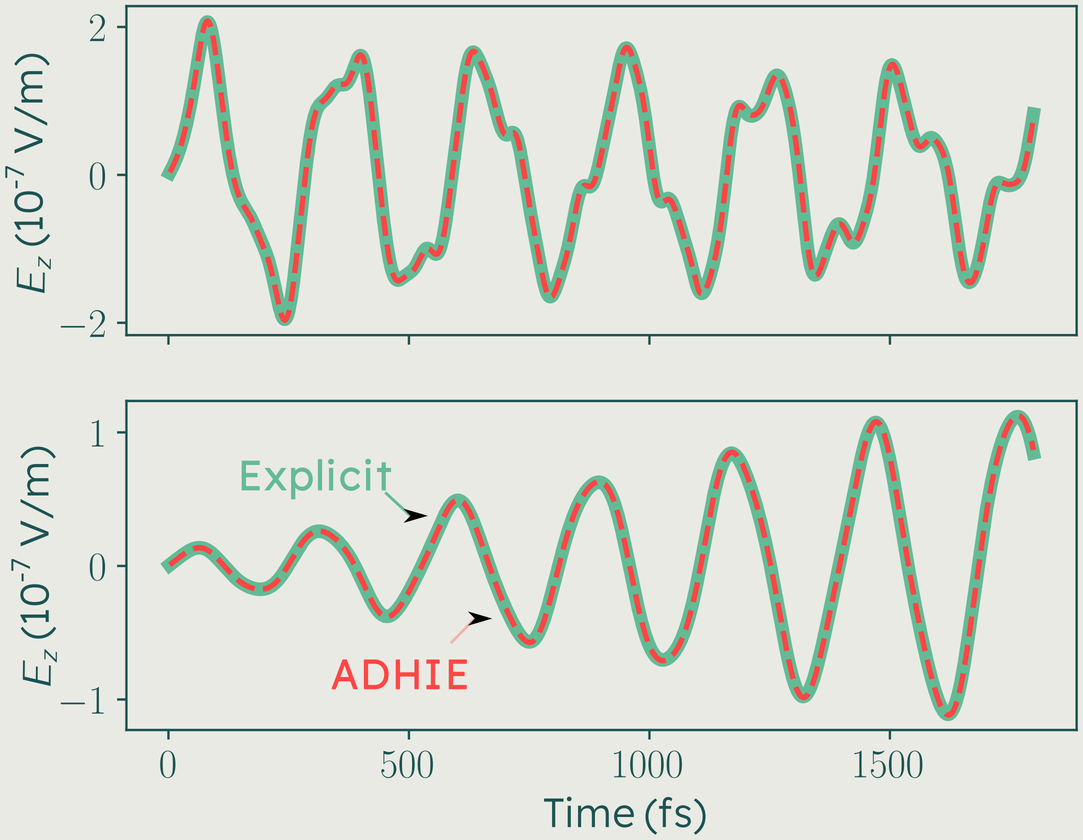
An application: explicit vs. ADHIE.

CPU results



Generator wire

Victim wire

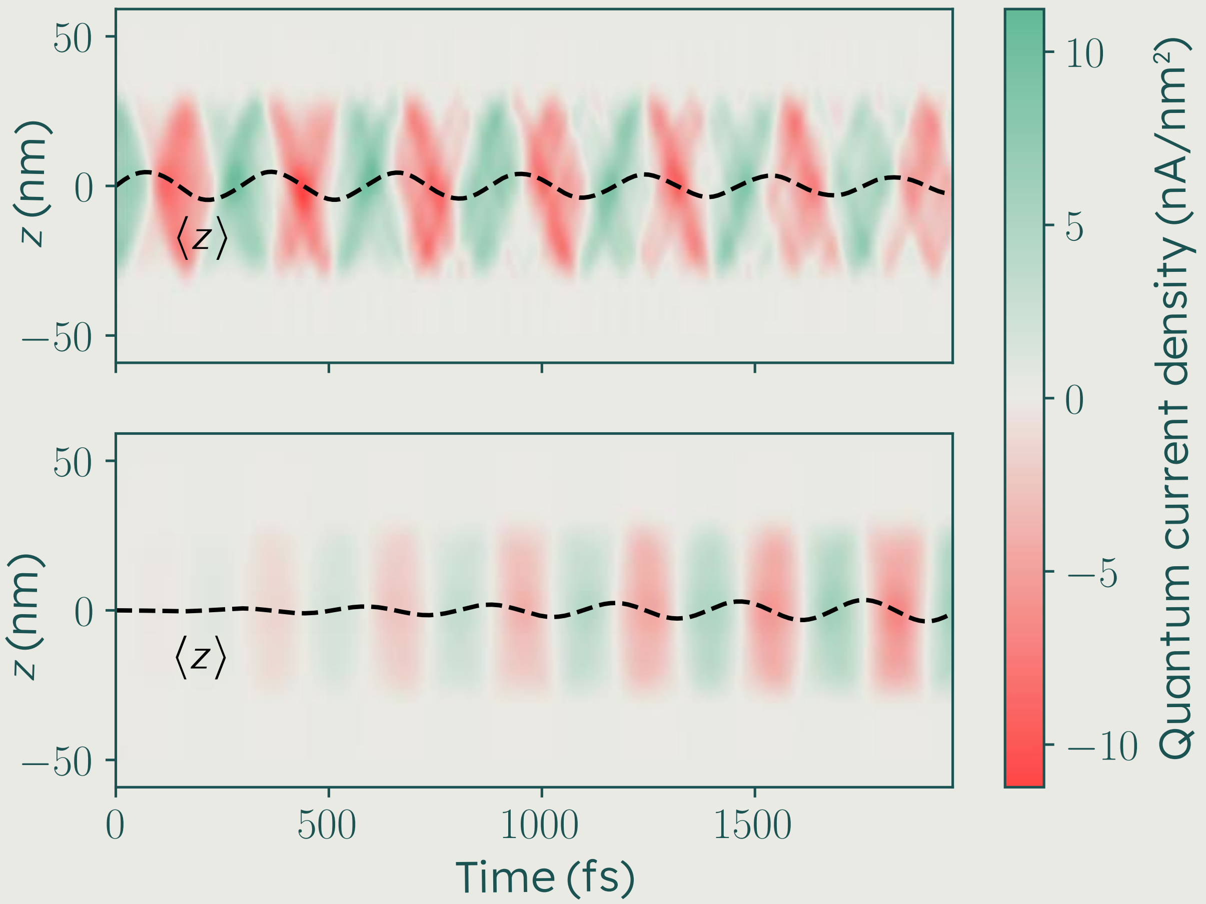


Closely-spaced nanowires display crosstalk.

An application: visualization of current dynamics.

Generator wire

Victim wire



Conclusions.

- The modeling of nanowires has a highly multiscale and multiphysics nature.
- The newly developed ADHIE method allows for faster simulations by reducing the time step of the problem.
- Many-electron effects can be accounted for by means of TDDFT.
- Real-time simulation allows for monitoring of intricate charge carrier dynamics.

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