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A Dual-mesh Framework for Multiphysics Simulation of Photoconductive Terahertz Devices

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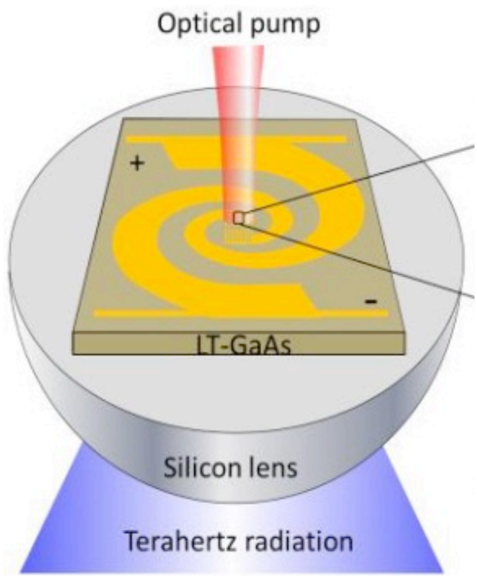
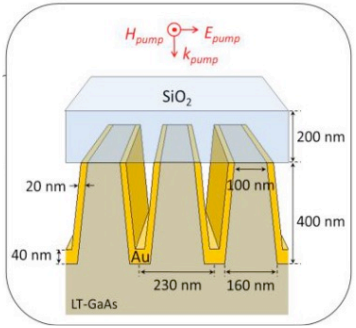
Outline

- Motivation
  - Photoconductive terahertz devices
  - Existing numerical approaches
- Proposed dual-mesh framework
  - Coupling between optoelectronic and terahertz solvers
  - MPI partition strategy
  - Efficient intersection test
- Examples
- Summary

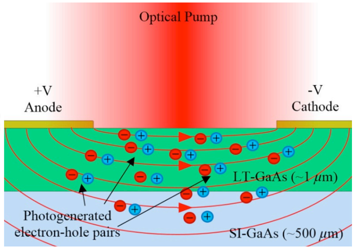
Photoconductive Terahertz (THz) Devices

- Photoconductive antennas/detectors

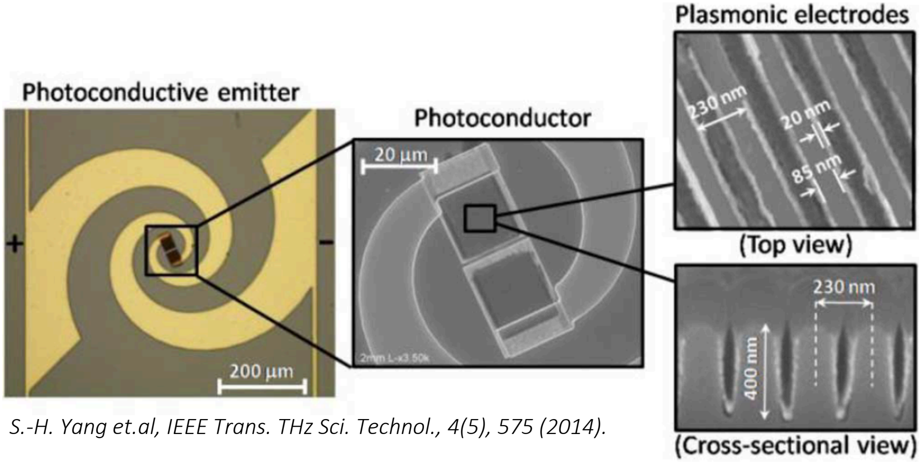




S.-H. Yang et.al, IEEE Trans. THz Sci. Technol., 4(5), 575 (2014).



N. Burforda, M. El-Shenaweeb, Opt. Eng. 56(1), 010901 (2017).



S.-H. Yang et.al, IEEE Trans. THz Sci. Technol., 4(5), 575 (2014).

- THz wave
  - 1 mm
  - 1 ps
- Laser:
  - 100 nm
  - 1 fs
- Carrier
  - 10 nm
  - 0.1 ps

- *Scales (length and time) in the THz antenna and the optoelectronic device differ by several orders of magnitude*
- *Nanostructures make the simulation more challenging*

Existing numerical approaches

- Equivalent circuit model[1-3]:

  simplified model with empirical parameters, mostly for conventional devices, not accurate

- THz antenna: Maxwell; Optoelectronic: circuit model, lumped port[4]

  no optical wave, simplified carrier dynamics model, only work for conventional devices

- THz antenna: Maxwell; Optoelectronic: analytical generation + drift-diffusion[5,6]

  no optical wave, generation models only work for conventional devices

- Nanostructured optoelectronic device

  Optical wave: frequency-domain FEM; Carrier: time-domain TCAD, analytical time-dependency for carrier generation[7,8]; Fully-coupled time-domain discontinuous Galerkin scheme[9]

  obtained photocurrent density can be used to feed the THz antenna
  need to record the space-time-dependent photocurrent density
  ignore the coupling between the THz antenna and the optoelectronic device

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[1] O. A. Castaneda-Uribe, et. al., "Comparative study of equivalent circuit models for photoconductive antennas," Opt. Express, vol. 26, no. 22, pp. 29017, 2018.

[2] N. Khiabani, et. al., "Theoretical modeling of a photoconductive antenna in a terahertz pulsed system," IEEE Trans. Antennas Propag., vol. 61, no. 4, pp. 1538, 2013.

[3] C. W. Berry and M. Jarrahi. "Principles of impedance matching in photoconductive antennas." J. Infrared Millim. Terahertz Waves, vol. 33, no. 12, pp. 1182, 2012.

[4] J. C. Young, et. al., "A DGFETD port formulation for photoconductive antenna analysis," IEEE Antennas Wirel. Propag. Lett., vol. 14, pp. 386–389, 2014.

[5] P. Kirawanich, et. al., "Study of high-power wideband terahertz-pulse generation using … photoconductive semiconductor switches," IEEE Trans. Plasma Sci., vol. 37, no. 1, pp. 219, 2008.

[6] E. Moreno, et. al., "Time-domain numerical modeling of THz photoconductive antennas," IEEE Trans. THz Sci. Technol., vol. 4, no. 4, pp. 490–500, 2014.

[7] N. Burford, et. al., "Computational modeling of plasmonic thin-film terahertz photoconductive antennas," J. Opt. Soc. Am. B, vol. 33, no. 4, pp. 748–759, 2016.

[8] M. Bashirpour, et. al., "Significant performance improvement of a terahertz photoconductive antenna using a hybrid structure," RSC Advances, vol. 7, no. 83, pp. 53 010–53 017, 2017.

[9] L. Chen, et. al., "Multiphysics modeling of plasmonic photoconductive devices using discontinuous Galerkin methods," arXiv preprint arXiv:1912.03639, 2019.

Challenges

Total efficiency: $\eta = \eta_{LE}\eta_m\eta_r$

η_{LE} : optical-to-electrical, η_m : impedance matching, η_r : THz antenna radiation

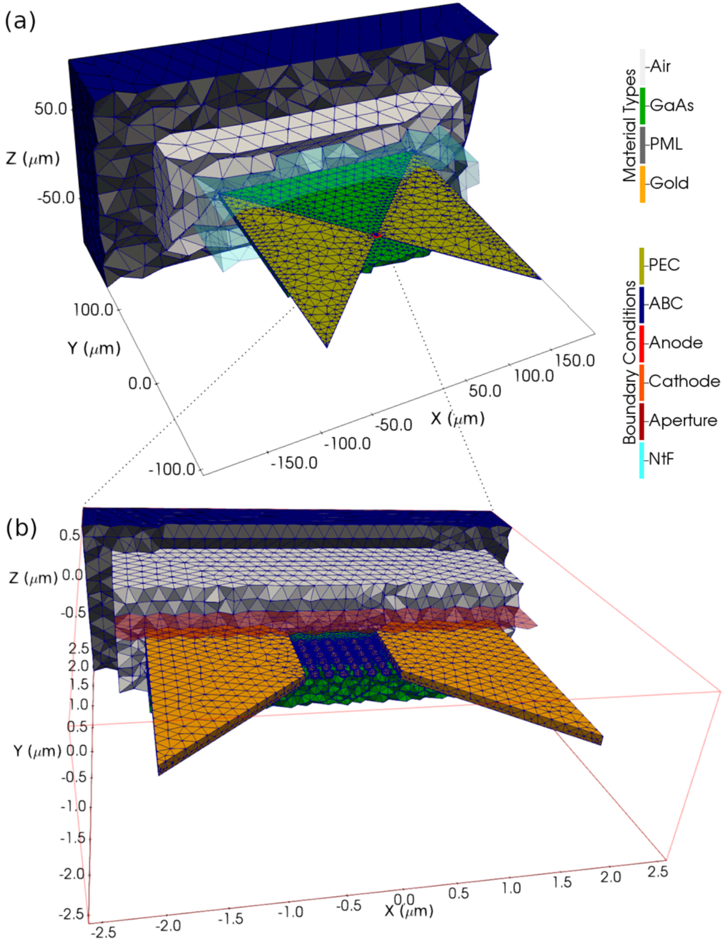
- Time-dependent impedance: difficult to develop accurate equivalent circuit models, different devices usually need very different models/parameters.
- Nanostructures are now extensively used for increasing the optical-to-electrical efficiency, making photocarriers vary strongly in space and time.
  - analytical carrier generation model does not work anymore
  - impedance matching becomes much more difficult
- Coupling between the THz radiation and the optoelectronic response is ignored in previous approaches, e.g., the radiation screening effect resulting from the THz radiation is not modeled (which is known to be important in many devices).
- Directly model both the THz radiation and the optoelectronic response in a single simulation is too expensive because of the scale differences.

Proposed dual-mesh framework

- Two solvers using two independent meshes
  - overlapped in space
  - coupled in explicit time-marching
- Optoelectronic solver:
  - fine meshes (~10nm)
  - optical wave, carrier generation/dynamics
  - simulation domain truncated near the devices
  - space-time-dependent photocurrent density

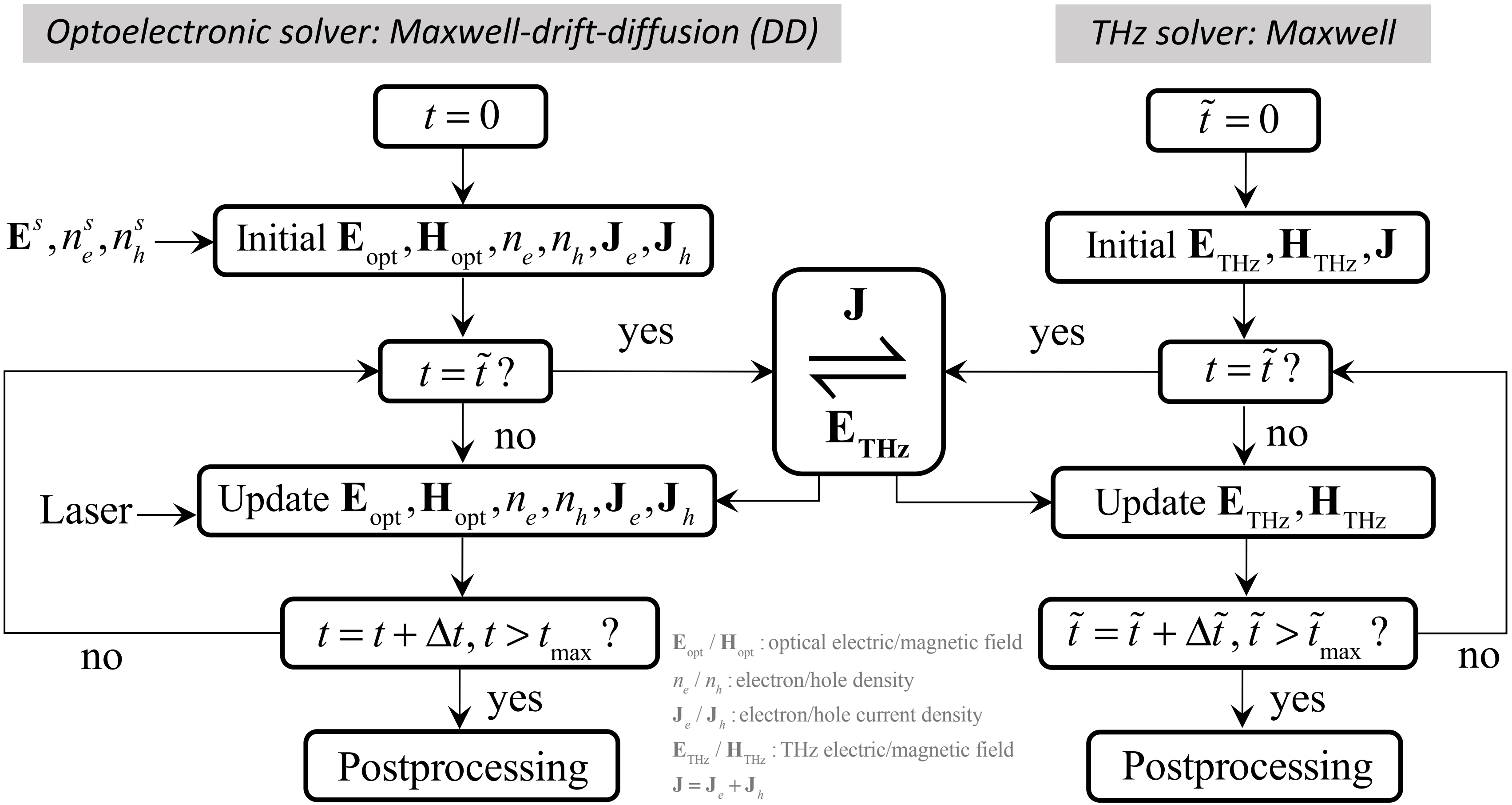
    → THz solver: feed THz antenna, affect THz wave propagation
- THz solver:
  - coarse meshes (~10um)
  - THz wave radiation/propagation
  - THz electromagnetic (EM) fields

    → optoelectronic solver: carrier dynamics



Proposed dual-mesh framework

- Flowchart



Optoelectronic solver: Maxwell-drift-diffusion (DD)

$t = 0$

$\mathbf{E}^s, n_e^s, n_h^s \rightarrow$ Initial $\mathbf{E}_{\text{opt}}, \mathbf{H}_{\text{opt}}, n_e, n_h, \mathbf{J}_e, \mathbf{J}_h$

$t = \tilde{t}\,?$ yes / no

Laser $\rightarrow$ Update $\mathbf{E}_{\text{opt}}, \mathbf{H}_{\text{opt}}, n_e, n_h, \mathbf{J}_e, \mathbf{J}_h$

$t = t + \Delta t,\ t > t_{\max}\,?$ no / yes

Postprocessing

$\mathbf{J} \rightleftharpoons \mathbf{E}_{\text{THz}}$

THz solver: Maxwell

$\tilde{t} = 0$

Initial $\mathbf{E}_{\text{THz}}, \mathbf{H}_{\text{THz}}, \mathbf{J}$

$t = \tilde{t}\,?$ yes / no

Update $\mathbf{E}_{\text{THz}}, \mathbf{H}_{\text{THz}}$

$\tilde{t} = \tilde{t} + \Delta\tilde{t},\ \tilde{t} > \tilde{t}_{\max}\,?$ no / yes

Postprocessing

$\mathbf{E}_{\text{opt}} / \mathbf{H}_{\text{opt}}$: optical electric/magnetic field

n_e / n_h : electron/hole density

$\mathbf{J}_e / \mathbf{J}_h$: electron/hole current density

$\mathbf{E}_{\text{THz}} / \mathbf{H}_{\text{THz}}$: THz electric/magnetic field

$\mathbf{J} = \mathbf{J}_e + \mathbf{J}_h$

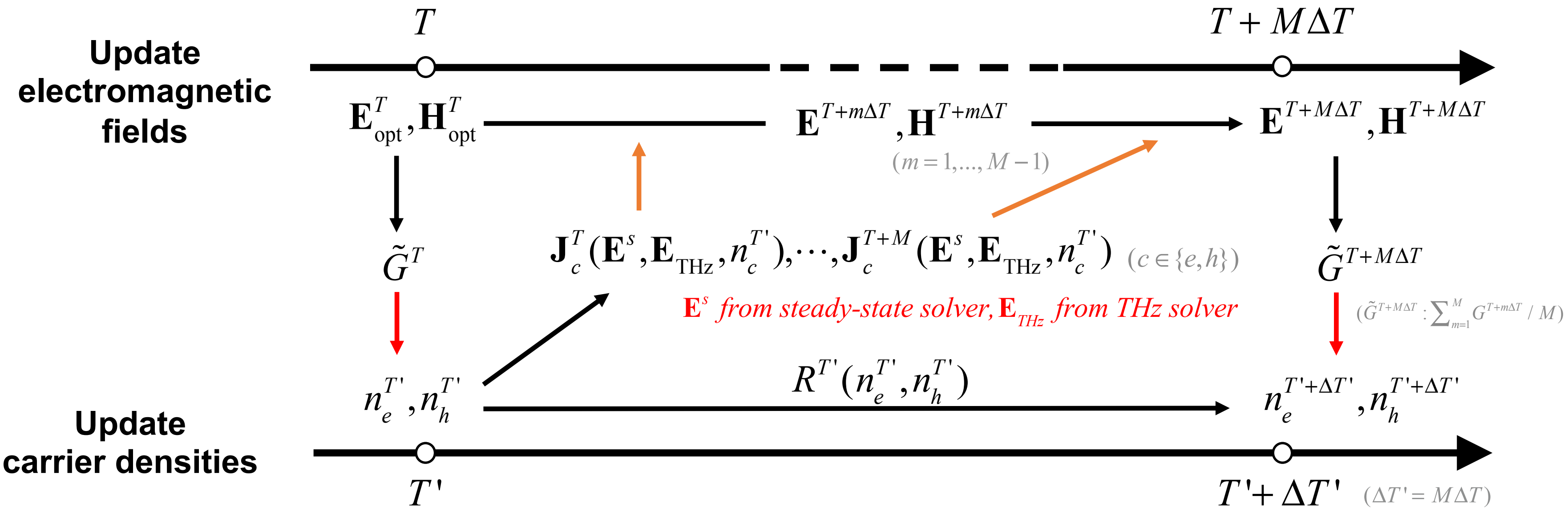
Optoelectronic solver

- Maxwell-DD system

$$\mu\partial_t \mathbf{H}_{\text{opt}} = -\nabla\times\mathbf{E}_{\text{opt}} \qquad \partial_t n_e = \nabla\cdot\mathbf{J}_e - R + G,\ \ \mathbf{J}_e = \mu_e n_e(\mathbf{E}^s+\mathbf{E}_{\text{THz}}) + d_e\nabla n_e$$

$$\varepsilon\partial_t\mathbf{E}_{\text{opt}} = \nabla\times\mathbf{H}_{\text{opt}} - (\mathbf{J}_e+\mathbf{J}_h) \qquad \partial_t n_h = -\nabla\cdot\mathbf{J}_h - R + G,\ \ \mathbf{J}_h = \mu_h n_h(\mathbf{E}^s+\mathbf{E}_{\text{THz}}) - d_h\nabla n_h$$

- Discontinuous Galerkin (DG) discretization, multiple-step time marching [1]



Update electromagnetic fields

T $\quad T + M\Delta T$

$\mathbf{E}^{T}_{\text{opt}},\mathbf{H}^{T}_{\text{opt}}$ $\quad \mathbf{E}^{T+m\Delta T},\mathbf{H}^{T+m\Delta T}$ $\quad \mathbf{E}^{T+M\Delta T},\mathbf{H}^{T+M\Delta T}$

$(m=1,\ldots,M-1)$

$\tilde{G}^{T}$ $\quad \mathbf{J}^{T}_{c}(\mathbf{E}^s,\mathbf{E}_{\text{THz}},n^{T'}_{c}),\cdots,\mathbf{J}^{T+M}_{c}(\mathbf{E}^s,\mathbf{E}_{\text{THz}},n^{T'}_{c})$ $\ (c\in\{e,h\})$ $\quad \tilde{G}^{T+M\Delta T}$

$\mathbf{E}^s$ *from steady-state solver,* $\mathbf{E}_{THz}$ *from THz solver*

$(\tilde{G}^{T+M\Delta T}:\sum_{m=1}^{M} G^{T+m\Delta T}/M)$

$R^{T'}(n^{T'}_{e},n^{T'}_{h})$

$n^{T'}_{e},n^{T'}_{h}$ $\quad n^{T'+\Delta T'}_{e},n^{T'+\Delta T'}_{h}$

Update carrier densities

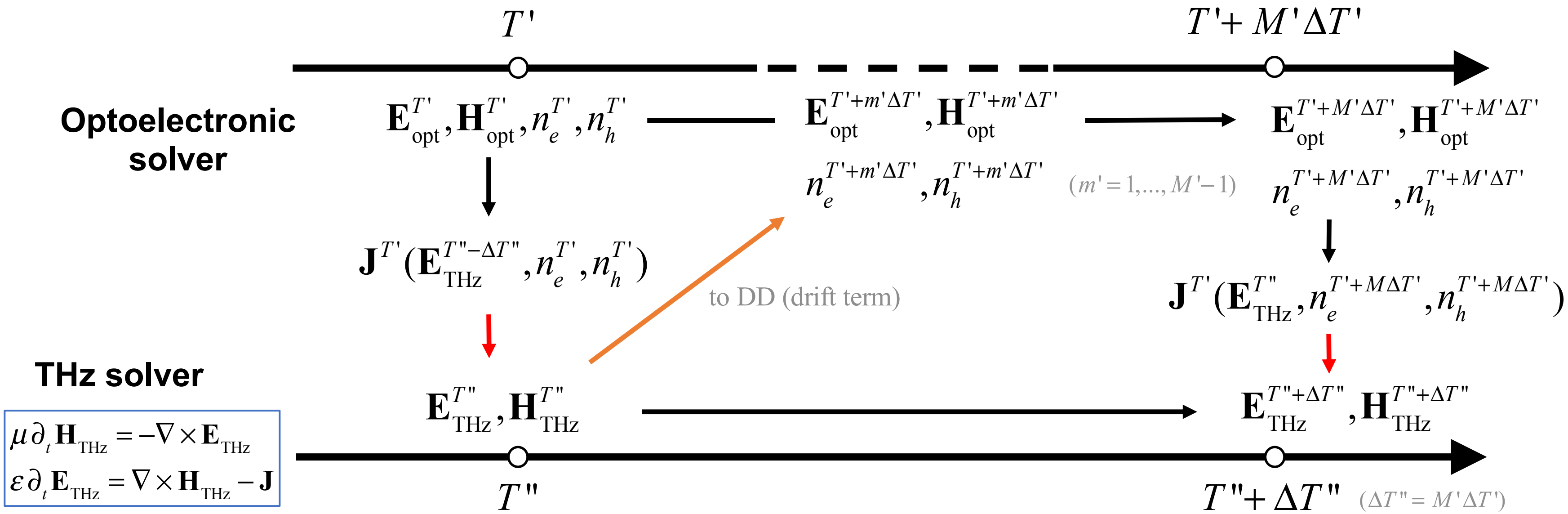
T' $\quad T'+\Delta T'$ $\ (\Delta T' = M\Delta T)$

[1] L. Chen and H. Bagci, "Multiphysics modeling of plasmonic photoconductive devices using discontinuous Galerkin methods," arXiv preprint arXiv:1912.03639, 2019.

THz solver

- DG time-domain method for Maxwell equations [1]
- Model THz wave radiation/propagation/scattering in the THz solver only

  (Optical wave propagation and carrier generation/dynamics are only modeled in the optoelectronic solver.)
- "Smooth" photocurrent density from the optoelectronic solver
- Multiple-step time marching (2nd level) Typically, $M \sim 10, M' \sim 100$



T'

$T' + M'\Delta T'$

Optoelectronic solver

$\mathbf{E}_{\text{opt}}^{T'}, \mathbf{H}_{\text{opt}}^{T'}, n_e^{T'}, n_h^{T'}$

$\mathbf{E}_{\text{opt}}^{T'+m'\Delta T'}, \mathbf{H}_{\text{opt}}^{T'+m'\Delta T'}$

$n_e^{T'+m'\Delta T'}, n_h^{T'+m'\Delta T'}$

$(m' = 1, \ldots, M'-1)$

$\mathbf{E}_{\text{opt}}^{T'+M'\Delta T'}, \mathbf{H}_{\text{opt}}^{T'+M'\Delta T'}$

$n_e^{T'+M'\Delta T'}, n_h^{T'+M'\Delta T'}$

$\mathbf{J}^{T'}(\mathbf{E}_{\text{THz}}^{T''-\Delta T''}, n_e^{T'}, n_h^{T'})$

to DD (drift term)

$\mathbf{J}^{T'}(\mathbf{E}_{\text{THz}}^{T''}, n_e^{T'+M\Delta T'}, n_h^{T'+M\Delta T'})$

THz solver

$$\mu \partial_t \mathbf{H}_{\text{THz}} = -\nabla \times \mathbf{E}_{\text{THz}}$$
$$\varepsilon \partial_t \mathbf{E}_{\text{THz}} = \nabla \times \mathbf{H}_{\text{THz}} - \mathbf{J}$$

$\mathbf{E}_{\text{THz}}^{T''}, \mathbf{H}_{\text{THz}}^{T''}$

$\mathbf{E}_{\text{THz}}^{T''+\Delta T''}, \mathbf{H}_{\text{THz}}^{T''+\Delta T''}$

T''

$T'' + \Delta T''$ $(\Delta T'' = M'\Delta T')$

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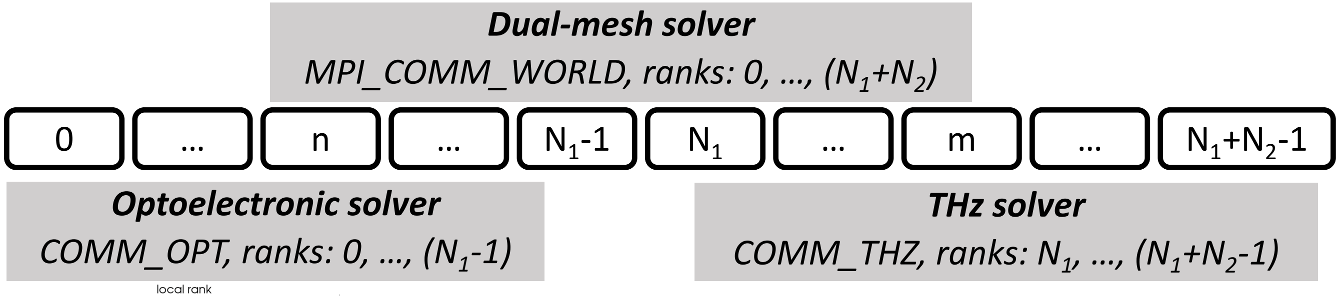
[1] L. Chen and H. Bagci, "Multiphysics modeling of plasmonic photoconductive devices using discontinuous Galerkin methods," arXiv preprint arXiv:1912.03639, 2019.

Proposed dual-mesh approach

- MPI partition



Dual-mesh solver

MPI_COMM_WORLD, ranks: 0, …, (N_1+N_2)

0 | … | n | … | N_1-1 | N_1 | … | m | … | N_1+N_2-1

Optoelectronic solver

COMM_OPT, ranks: 0, …, (N_1-1)

THz solver

COMM_THZ, ranks: N_1, …, (N_1+N_2-1)

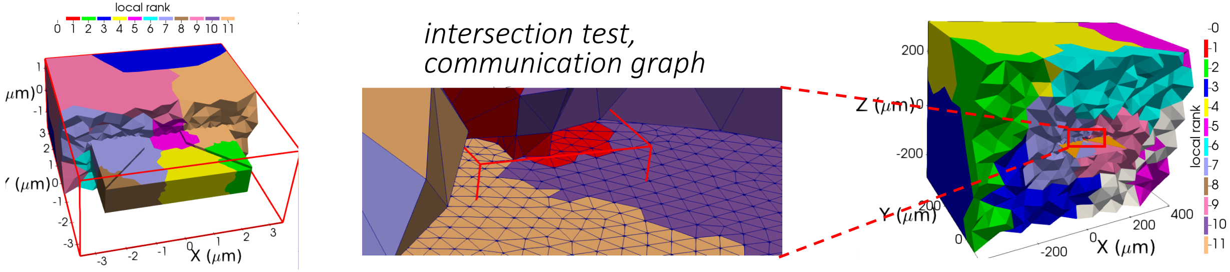
Initialization:

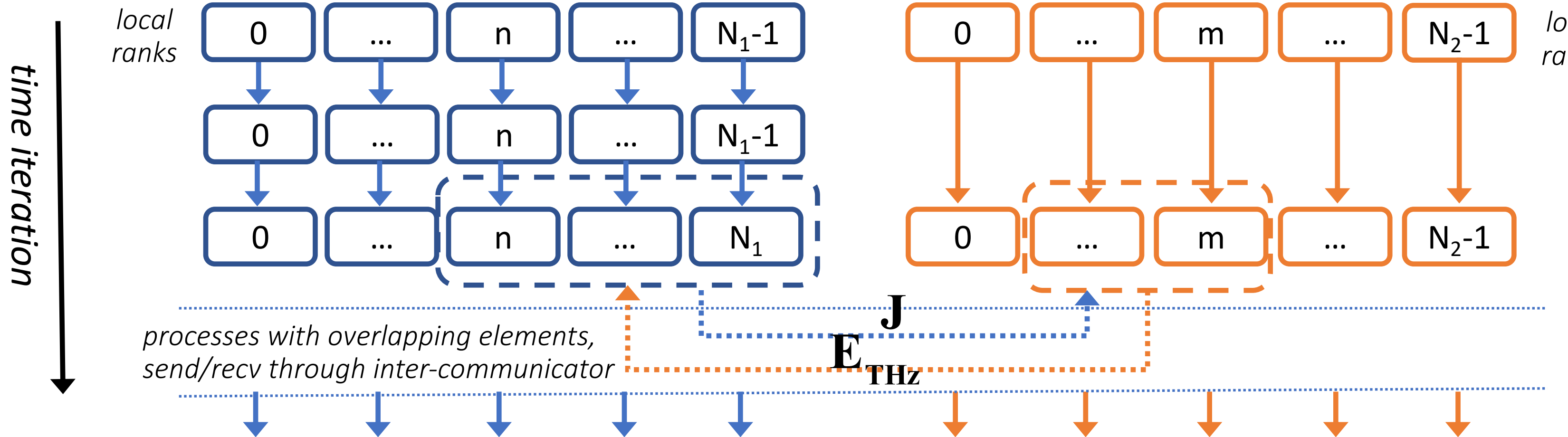
MPI communicators,
dual mesh mapping,
interpolation operators,
MPI buffer …

ParMetis partition 1

intersection test,
communication graph

ParMetis partition 2





local ranks

0 | … | n | … | N_1-1

0 | … | n | … | N_1-1

0 | … | n | … | N_1

local ranks

0 | … | m | … | N_2-1

0 | … | m | … | N_2-1

time iteration

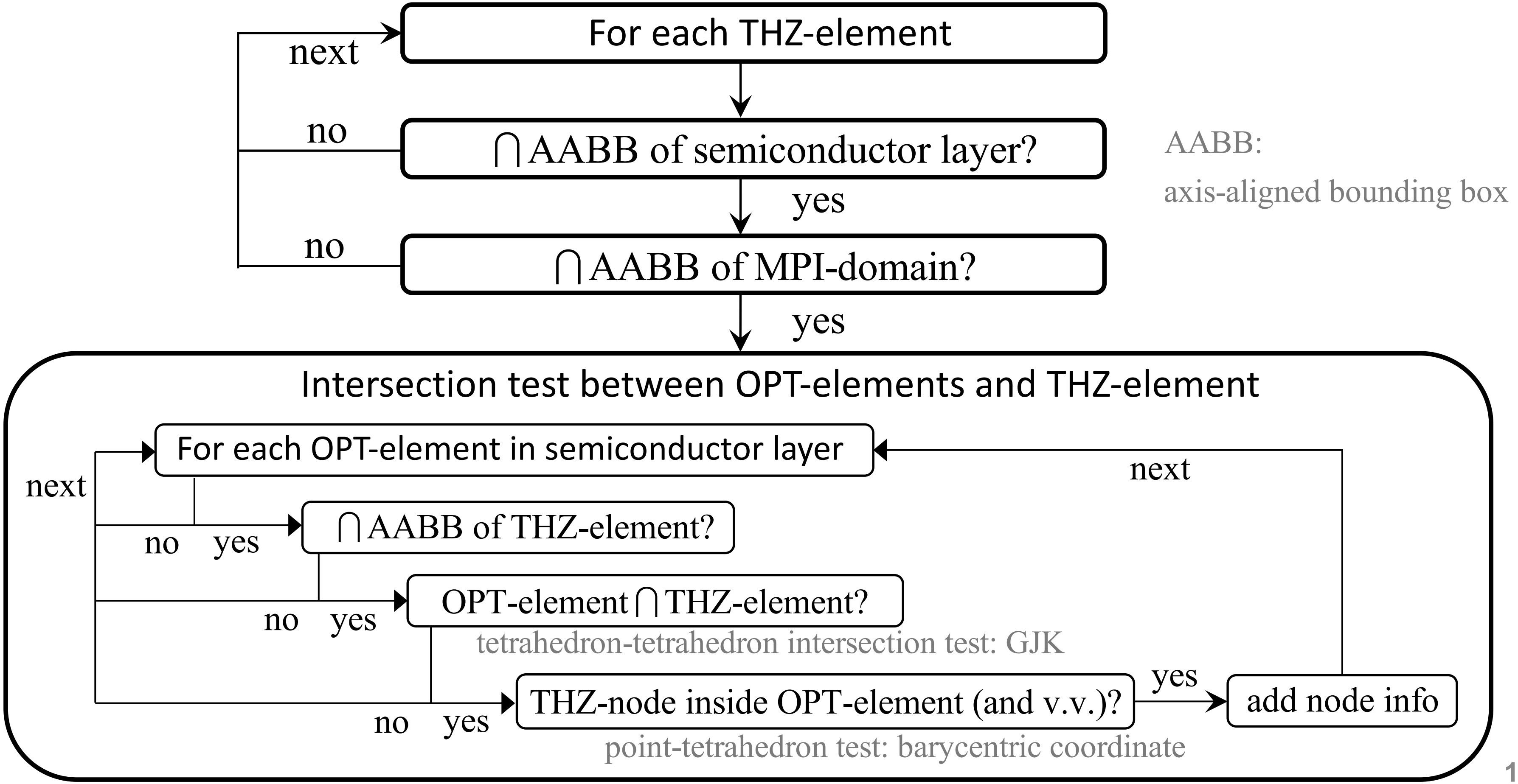
processes with overlapping elements,
send/recv through inter-communicator

$\mathbf{J}$

$\mathbf{E}_{\mathbf{THz}}$

Proposed dual-mesh approach

- Efficient intersection test



tetrahedron-tetrahedron intersection test: GJK

point-tetrahedron test: barycentric coordinate

AABB:

axis-aligned bounding box

Proposed dual-mesh approach

- Interpolation

$$\bar{f}_I = \bar{P}\bar{f}$$

nodal DG[1] solutions:

$$\bar{f} = [f(\mathbf{r}_1),\dots,f(\mathbf{r}_{N_p})]^T$$

N_p : number of nodes per element

$\mathbf{r}_i (i = 1,\dots,N_p)$: coordinate of the nodes

interpolated values:

$$\bar{f}_I = [f(\mathbf{r}_1^I),\dots,f(\mathbf{r}_M^I)]^T$$

M : number of interpolation nodes in the element

$\mathbf{r}_i^I (j = 1,\dots,M)$: coordinate of the interpolation nodes

interpolation operator:

$$\bar{P} = \bar{V}_I \bar{V}^{-1}$$

$\bar{V}_I(i,j) = \phi_j(\mathbf{r}_i^I)$: generalized Vandermonde matrix

$\bar{V}(i,j) = \phi_j(\mathbf{r}_i)$: generalized Vandermonde matrix

$\phi_j(\mathbf{r})$: the $j-th$ orthonormal polynomial basis in nodal DG[1]

[1] *J. S. Hesthaven and T. Warburton, Nodal Discontinuous Galerkin Methods, Algorithms, Analysis and Applications (2008)*

Examples

- MPI partition

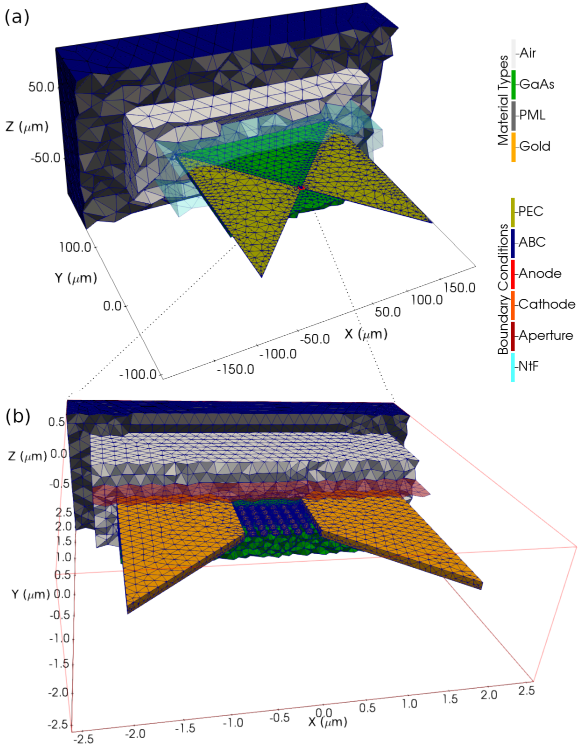
THz solver

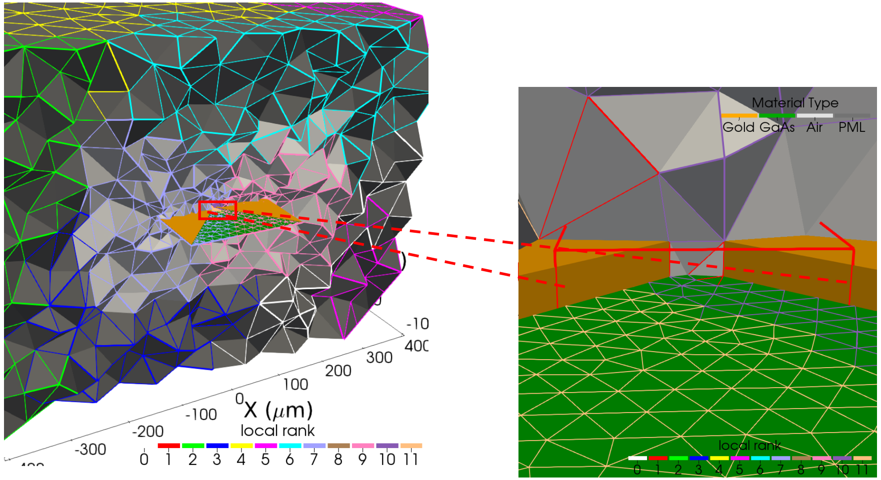
bowtie antenna, volumetric current density in the photoconductive layer, PML

Optoelectronic solver

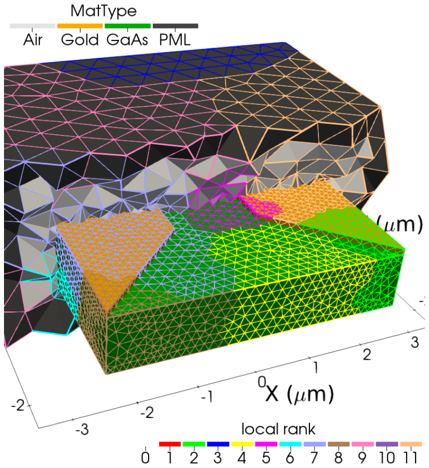
photoconductive layer, electrodes under bias voltage, laser source, PML,

possibly nanostructures on/between electrodes



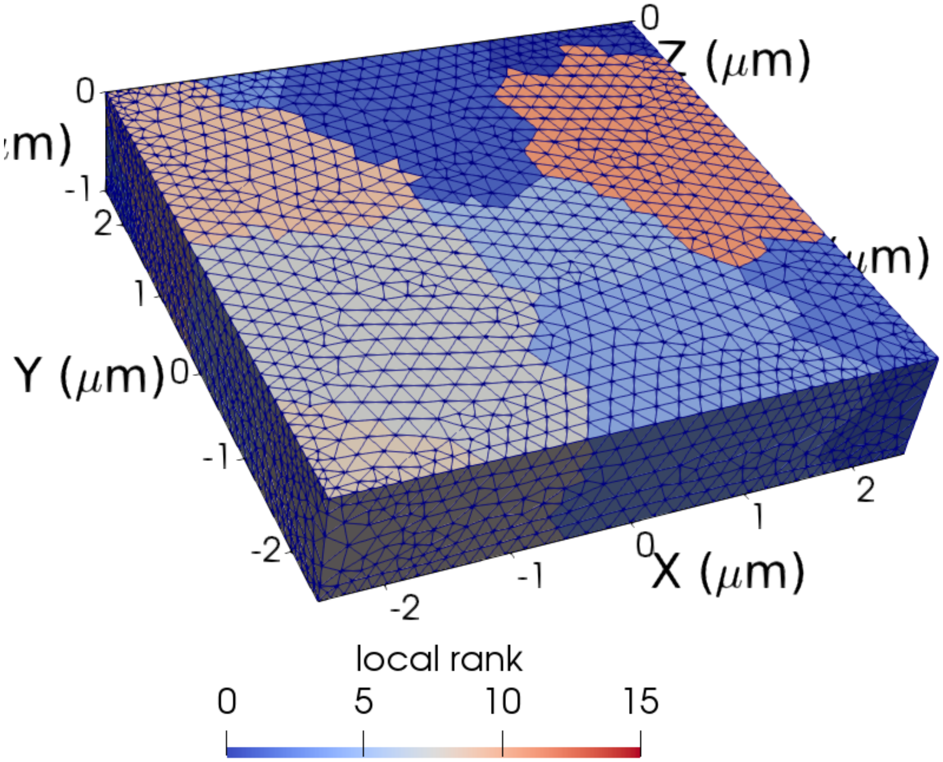


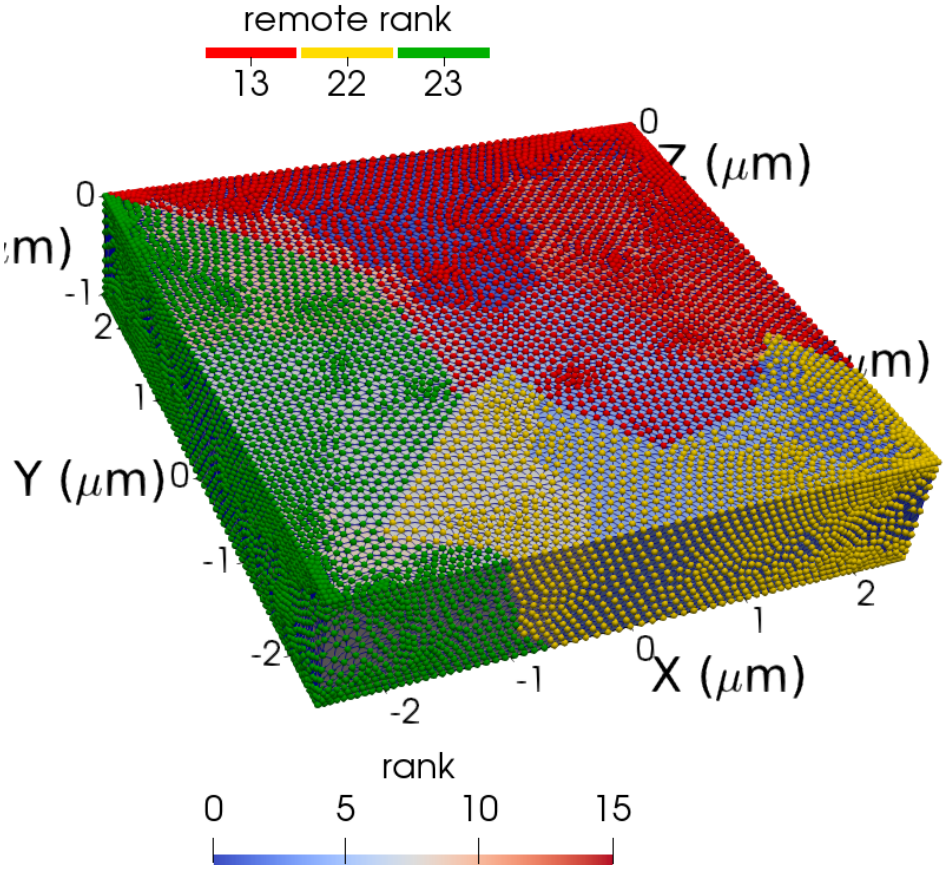
computation domain of the optoelectronic solver viewed in the THz solver



Examples

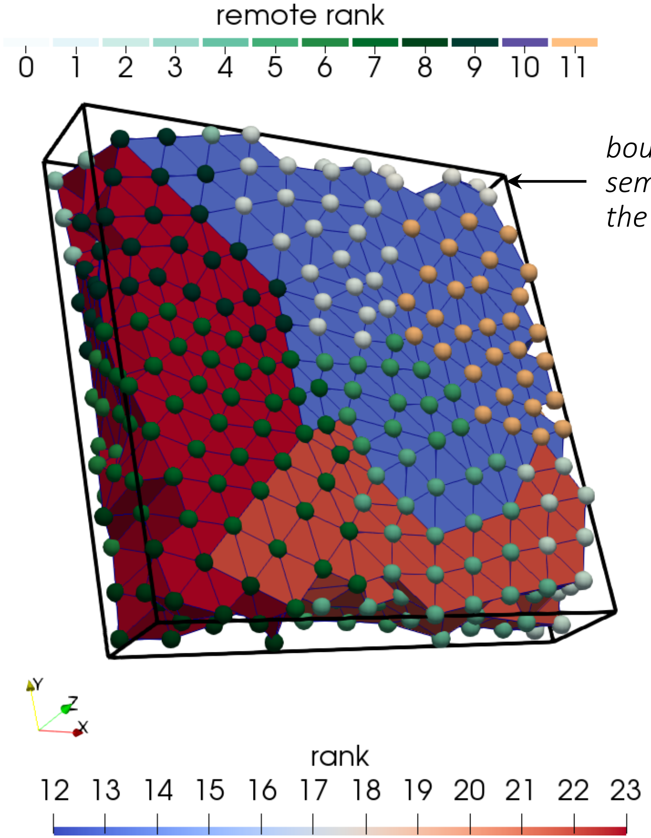
- Optoelectronic solver: intersection test and process mapping





Examples

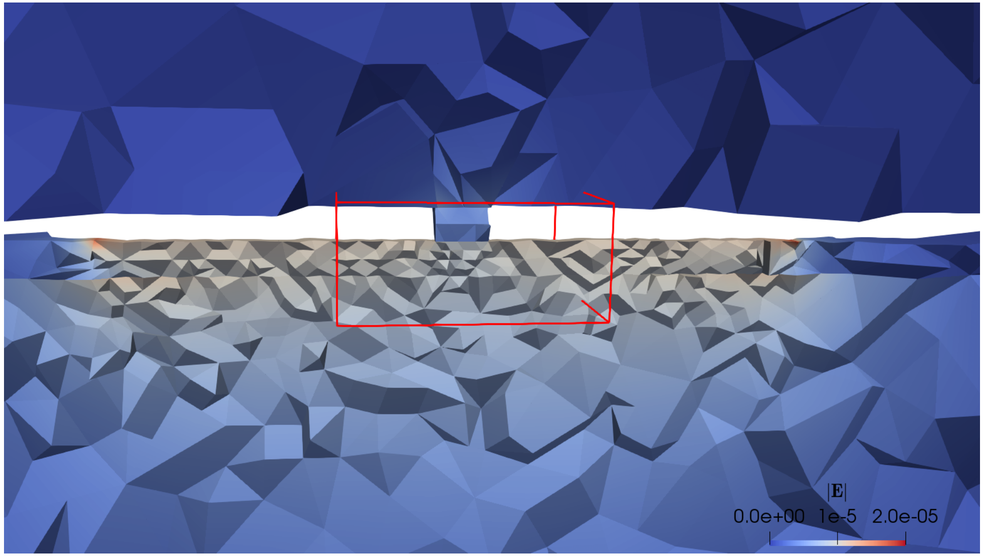
- THz solver: intersection test and process mapping



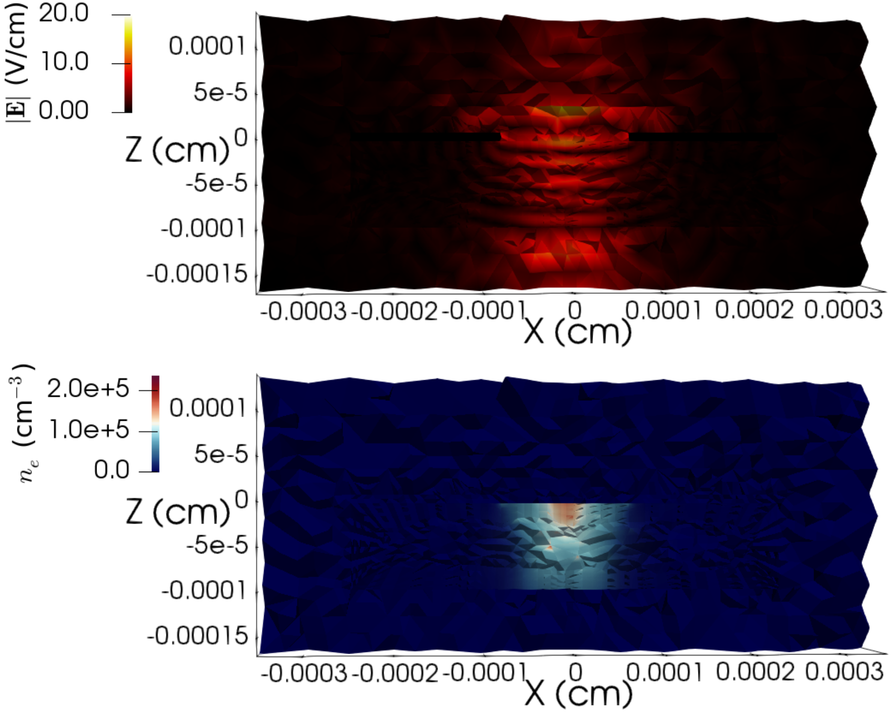
bounding box of the semiconductor layer in the optoelectronic solver

Examples

- Field distribution



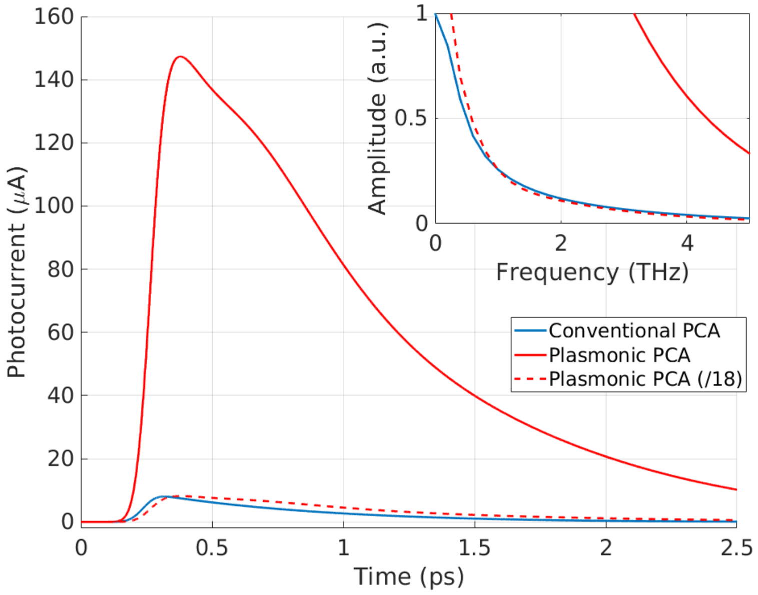
THz solver: electric field



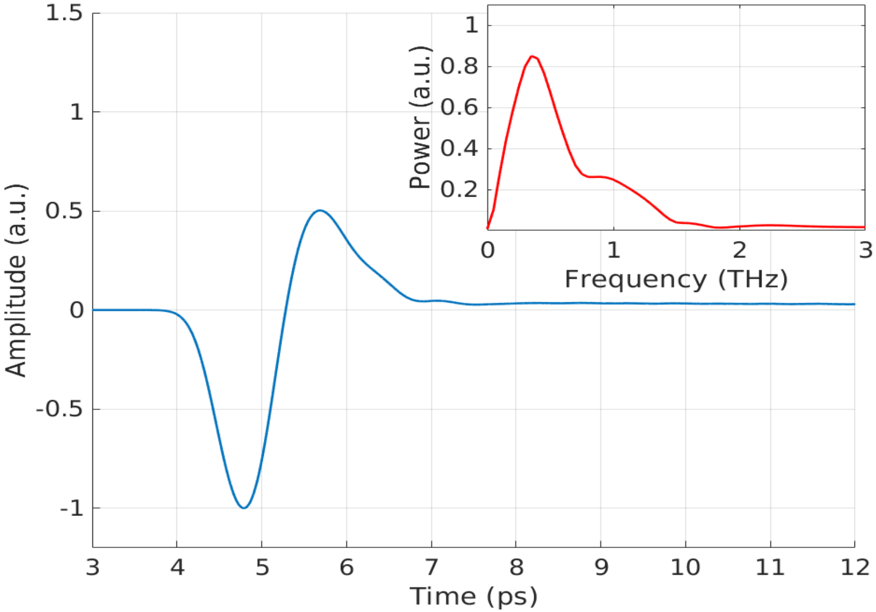
Optoelectronic solver:
electric field and electron density

Examples

- Radiation (preliminary results)



Photocurrent and power spectrum



Detected THz signal and power spectrum

Summary

- Dual-mesh framework for direct modeling optoelectronic response and THz radiation and their couplings in a single simulation
- Two-level multiple-step time-marching scheme
- Efficient implementation of an MPI-parallelized dual-mesh solver, including the MPI partition strategy and the intersection test algorithm
- To do:
  - impedance matching in nanostructured photoconductive devices
  - identify the radiation screening effect
  - advanced models for the semiconductor-electrode interface: Schottchy contact, surface recombination

Thank you!

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