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

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XXXIV General Assembly and Scientific Symposium (GASS) of the International Union of Radio Science (URSI), August 2020, Rome, Italy
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

- 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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Challenges

Total efficiency: \[ \eta = \eta_{LE} \eta_{m} \eta_{r} \]

- \( \eta_{LE} \) : optical-to-electrical, \( \eta_{m} \) : impedance matching, \( \eta_{r} \) : 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)**

1. $t = 0$
2. Initial $E_{\text{opt}}, H_{\text{opt}}, n_e, n_h, J_e, J_h$
3. $t = \tilde{t}$?
   - no
   - yes: $J \leftrightarrow E_{\text{THz}}$
5. Laser
   - no
   - yes: Update $E_{\text{opt}}, H_{\text{opt}}, n_e, n_h, J_e, J_h$
6. $t = t + \Delta t$, $t > t_{\text{max}}$?
   - no
   - yes: Postprocessing

**THz solver: Maxwell**

1. $\tilde{t} = 0$
2. Initial $E_{\text{THz}}, H_{\text{THz}}, J$
3. $t = \tilde{t}$?
   - no
   - yes: $J \leftrightarrow E_{\text{THz}}$
5. Update $E_{\text{THz}}, H_{\text{THz}}$
6. $\tilde{t} = \tilde{t} + \Delta \tilde{t}$, $\tilde{t} > \tilde{t}_{\text{max}}$?
   - no
   - yes: Postprocessing

- $E_{\text{opt}} / H_{\text{opt}}$: optical electric/magnetic field
- $n_e / n_h$: electron/hole density
- $J_e / J_h$: electron/hole current density
- $E_{\text{THz}} / H_{\text{THz}}$: THz electric/magnetic field
- $J = J_e + J_h$
Optoelectronic solver

- Maxwell-DD system

\[ \mu \partial_t \mathbf{H}_\text{opt} = -\nabla \times \mathbf{E}_\text{opt} \]
\[ \partial_t n_e = \nabla \cdot \mathbf{J}_e - R + G, \quad \mathbf{J}_e = \mu_e n_e (\mathbf{E}^s + \mathbf{E}_{THz}) + d_e \nabla n_e \]
\[ \varepsilon \partial_t \mathbf{E}_\text{opt} = \nabla \times \mathbf{H}_\text{opt} - (\mathbf{J}_e + \mathbf{J}_h) \quad \partial_t n_h = -\nabla \cdot \mathbf{J}_h - R + G, \quad \mathbf{J}_h = \mu_h n_h (\mathbf{E}^s + \mathbf{E}_{THz}) - d_h \nabla n_h \]

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

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 (2\textsuperscript{nd} level) \[\text{Typically, } M \sim 10, M' \sim 100\]

\[\begin{array}{c}
\mu \frac{\partial}{\partial t} H_{\text{THz}} = -\nabla \times E_{\text{THz}} \\
\varepsilon \frac{\partial}{\partial t} E_{\text{THz}} = \nabla \times H_{\text{THz}} - J
\end{array}\]

\[\begin{array}{c}
\mathbf{E}_{\text{opt}}^{T'}, \mathbf{H}_{\text{opt}}^{T'}, n_e^{T'}, n_h^{T'} \\
\mathbf{E}_{\text{opt}}^{T'+m'\Delta T'}, \mathbf{H}_{\text{opt}}^{T'+m'\Delta T'} \\
\mathbf{E}_{\text{opt}}^{T'+M'\Delta T'}, \mathbf{H}_{\text{opt}}^{T'+M'\Delta T'}
\end{array}\]

\[\begin{array}{c}
\mathbf{J}^{T'}(\mathbf{E}_{\text{THz}}^{T''-\Delta T''}, n_e^{T''}, n_h^{T''}) \\
to \text{DD (drift term)}
\end{array}\]

\[\begin{array}{c}
\mathbf{E}_{\text{THz}}^{T''}, \mathbf{H}_{\text{THz}}^{T''} \\
\mathbf{E}_{\text{THz}}^{T''+\Delta T''}, \mathbf{H}_{\text{THz}}^{T''+\Delta T''}
\end{array}\]

\[\begin{array}{c}
\mathbf{E}_{\text{THz}}^{T''+M\Delta T''}, \mathbf{H}_{\text{THz}}^{T''+M\Delta T''}
\end{array}\]

\[\begin{array}{c}
\mathbf{J}^{T''}(\mathbf{E}_{\text{THz}}^{T'''}, n_e^{T'''+M\Delta T'''}, n_h^{T'''+M\Delta T'''})
\end{array}\]

\[\begin{array}{c}
\mu \frac{\partial}{\partial t} H_{\text{THz}} = -\nabla \times E_{\text{THz}} \\
\varepsilon \frac{\partial}{\partial t} E_{\text{THz}} = \nabla \times H_{\text{THz}} - J
\end{array}\]

\[\begin{array}{c}
\mathbf{E}_{\text{THz}}^{T''+\Delta T''} (\Delta T'' = M'\Delta T')
\end{array}\]

Proposed dual-mesh approach

- **MPI partition**

  Initialization:
  MPI communicators, dual mesh mapping, interpolation operators, MPI buffer ...

  **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

  Time iteration

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

  J

  E_{THZ}
Proposed dual-mesh approach

- Efficient intersection test

For each THZ-element

\[ \bigcap \text{AABB of semiconductor layer?} \]

yes

\[ \bigcap \text{AABB of MPI-domain?} \]

yes

Intersection test between OPT-elements and THZ-element

For each OPT-element in semiconductor layer

\[ \bigcap \text{AABB of THZ-element?} \]

no

yes

\[ \text{OPT-element} \bigcap \text{THZ-element?} \]

tetrahedron-tetrahedron intersection test: GJK

no

yes

\[ \text{THZ-node inside OPT-element (and v.v.)?} \]

point-tetrahedron test: barycentric coordinate

no

yes

add node info

AABB: axis-aligned bounding box
Proposed dual-mesh approach

- Interpolation

\[
\overline{\mathbf{f}}_I = \overline{\mathbf{P}} \mathbf{f}
\]

nodal DG\(^{[1]}\) solutions:

\[
\overline{\mathbf{f}} = [f(r_1), \ldots, f(r_{N_p})]^T
\]

interpolated values:

\[
\overline{\mathbf{f}}_I = [f(r_{1I}), \ldots, f(r_{MI})]^T
\]

interpolation operator:

\[
\overline{\mathbf{P}} = \overline{\mathbf{V}}_I \overline{\mathbf{V}}^{-1}
\]

\[
\overline{\mathbf{V}}_I(i, j) = \phi_j(r_i^I) : \text{generalized Vandermonde matrix}
\]

\[
\overline{\mathbf{V}}(i, j) = \phi_j(r_i) : \text{generalized Vandermonde matrix}
\]

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

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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