Multiscale Modeling of Transport in Optical Semiconductors

S&T Campaign: Computational Sciences
Predictive Simulation Sciences

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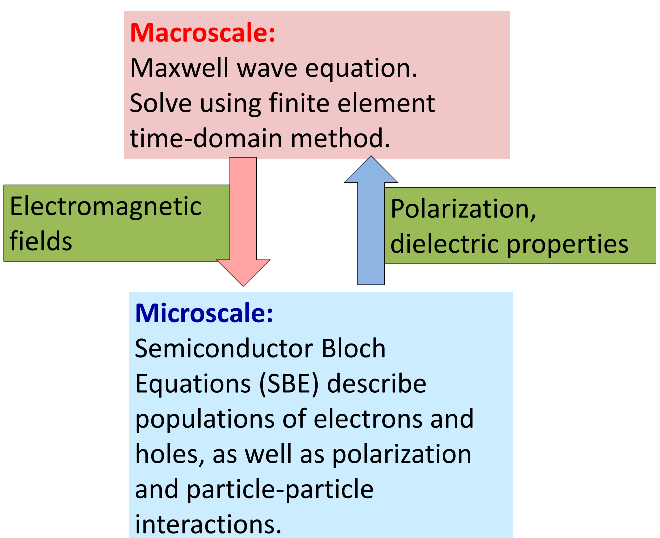
Research Objective

- We are developing the capability to do high-fidelity, scalable, multiscale computations of photo-excitation in semiconductors.
- This will assist in designing materials and heterostructures to be used in sensors and communication devices.
- We employ a two-scale, sequential multiscale method based on Semiconductor Maxwell-Bloch Equations (SMBE)
- Approach designed to allow different methods/solvers to be incorporated at either micro- or macro-scale.



Two-scale, sequential multiscale method.

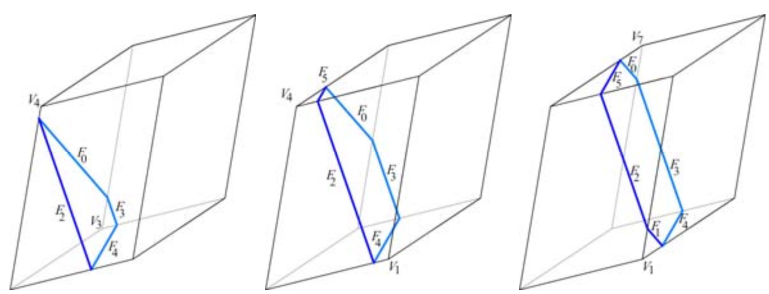
Challenges

- Relaxation-time approximation limits accuracy and choice of materials addressed.
- More accurate microscale models exist, but currently limited to homogeneous materials due to computational costs.
- More accurate physical models require significant computational cost, so efficient approaches need for use on high-performance computers.
- Limited by quality of electronic band structures for materials.

Descriptive figure caption

ARL Facilities and Capabilities Available to Support Collaborative Research

- Computation using DoD supercomputers
- Development employs hierarchical multiscale framework to allow near-drop-in use of different solution methods at microscale.
- Framework is scalable and parallelized.
- Active collaboration with semiconductor physicists in SEDD and ARL Materials Enterprise CRA.



Direct Brillouin Zone integration method under development.

Complementary Expertise/ Facilities/ Capabilities Sought in Collaboration

- We seek a variety of methods/solvers (micro and/or macroscale) to incorporate into our multiscale computational framework.
- Sought on the microscale:
  - Predictive methods for computing highly-accurate electronic band structures in any type of optically-active semiconductor.
  - Methods for computing semiconductor Bloch equations, including, but not limited to:
    - Monte Carlo
    - Direct integration methods

    (Serial methods/codes may work in this case.)
- Sought on the macroscale:
  - Electrodynamics for near- and/or far-field
  - Finite element, boundary element or finite difference (These would likely need to be parallel methods/codes.)