Computer Aided Approaches for Nanophotonic Researches

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Overview

• Numerical approaches in nanophotonics research
  – Introduction to “Computer Aided R & D”
    • requirement, future direction

• Examples: nanophotonics researches enabled by HPC simulations
  – Quasi-3D plasmonic crystals for sensing application
  – Coherent control of local plasmons for decoding/encoding of digitally mastered optical signals

• Concluding remarks
  – CCT, a firm foundation for computer aided R & D environment
Intro. to Computer Aided R & D (CARD)

• Computational background
  – Low cost PCs are doing better job nowadays and will be much better in the future
  – Development of message passing interface (MPI) allows us to acquire unlimited computing power from high performance computing (HPC) environments where many cheap PCs are assembled as a cluster.
  – Techniques for rigorous and realistic numerical simulations are developed and adopted for HPC environments.

• Demands in nanophotonics
  – Light interactions are complex and unpredictable
  – Rigorous and realistic description of nanophotonics system is necessary to capture all the complexities inherent in the nanophotonics systems.
Research environment with CARD

- novel device concept
- feasibility test
- underlying physics
- HPC simulation
- provide optimal design
- fabrication of prototype
- feedback
- production
Research environment with CARD

- **Feasibility test**
  - novel device concept
  - underlying physics

- **HPC simulation**
  - provide optimal design
  - feedback

- **Fabrication of prototype**
  - production

Scientific research (discovery, exploration, …)

Engineering development (design, optimization, …)
Establishing CARD

- **Computational requirements**
  - Simulation tools and techniques must be rigorous so that one can safely rely on simulation results.
  - Simulation must be capable of efficiently handling realistic full size 3-D problems.

  ➡️ **HPC based simulations**

- **General research direction**
  - Leading role: explore novel scientific phenomena and systems which might result in subsequent research projects.
  - Supporting role: provide tools to analyze theoretically predicted and/or experimentally observed physical phenomena.

  ➡️ **Strong collaborations with theory and experiment**
Example 1: quasi-3D plasmonic crystals

- Collaborative work: computer modeling + experimental works
  - Experimental work: John A. Rogers’ group at UIUC

- Problem of interest

![Cross-sectional view of one cell (sealed structure)](image_url)
Example 1: quasi-3D plasmonic crystals

- FDTD Modeling setup and HPC computing
Example 1: quasi-3D plasmonic crystals

- FDTD Modeling setup and HPC computing

  - Numerical specs
    - Computational domain size:
      grid resolution: 5 nm
      lateral: 142 ~ 160 grid cells / dimension
      height: 1200 grid cells
    - Computational requirements
      memory: 7 ~ 10 GB
      # of CPUs: 72 ~ 128
      Wall clock time: 2 ~ 3 hrs / 350 fs
    - Computing resource:
      Jacquard @ nersc (4.4 GFlops/sec)
Example 1: quasi-3D plasmonic crystals

- Result: transmittance spectrum
  - Period = 710 nm, Hole diameter = 450 nm, Relief depth = 350 nm, metal thickness = 64 nm

FDTD simulations

experimental measurement
(John A. Rogers at UIUC)

slight pile up of gold grain on disk edge
Example 1: quasi-3D plasmonic crystals

3-D Intensity distributions at specific wavelengths of interest

- Strong coupling between bottom disk and top hole resonance is responsible for highly sensitive transmittance peak of B
- Feasible for bio-sensing application

For more info. – *Proceedings of National Academy of Science*, 103, 17143 (2006)
Example 2: coherent control of local plasmons for encoding/decoding optical signals

- Metal nanoparticle system

- Specs
  \[ d_1 \text{ (20 nm)} < d_2 \text{ (140 nm)} \]
  Length = 250 nm

- Chirped optical pulses
  \[ E_{\text{inc}}(t) = f(t)\sin(\omega t(1 + \alpha t / \tau)) \]
  \( f(t) \): pulse envelope
  \( \tau \): pulse width
  \( \alpha \): chirp parameter

Field intensities at A and B are monitored in time simultaneously through a FDTD simulation.
Local plasmons in the system

\[ \lambda_0 = 350 \text{ nm} \]

\[ \lambda_0 = 365 \text{ nm} \]

- Shorter resonant wavelength for A (smaller cross section) compared to B (bigger cross section)
Spatiotemporal observation of local hot spot

Local intensity peaks are delayed in time
Application: encode/decode digitally mastered optical signals

1 0 1
original signal

1 ? 1
optical fiber
after spreading by dispersion

Photodetector - convert to electric signal

after converted to electric signal
Application: encode/decode digitally mastered optical signals

original signal

optical fiber

after spreading by dispersion

Photodetector - convert to electric signal

proposed NPN photodetector with nanosystem

Note, e-h pair generation is not directly included but assumed to be proportional to light intensity. Capacitance effect and response time of photodetector are treated as a local average of signals.
Application: encode/decode digitally mastered optical signals

1 0 1
original signal

1 ? 1
optical fiber

1 ? 1
after spreading by dispersion

Photodetector - convert to electric signal

Conventional photodetector

Photodetector with nanosystem

For more info. – Physical Review B, 71, 035423 (2005)
Summary for examples of CARD

• Two examples of HPC enabled nanophotonics research outcomes were presented
  – Quasi 3-D plasmonic crystal:
    • Sensitivity of the system was identified by matching simulation and experimental measurement
    • Further in-depth analysis revealed underlying sensing mechanism
  – Spatiotemporal control of local plasmon excitation:
    • Engineered nanoparticle was investigated in terms of spatiotemporal plasmon response to chirped pulses
    • A new way of decoding/encoding digitally mastered optical signal was proposed
Concluding remarks: Intro.to CCT

• Center for Computation and Technology (CCT) at Louisiana State University
  – Firm infrastructure for HPC enabled scientific and engineering researches
  – Mission statement
    
    The Center for Computation & Technology at Louisiana State University is an innovative and interdisciplinary research environment, advancing computational sciences, technologies, and the disciplines they touch…
  
  – Bottom line:
    
    • CCT emphasis HPC related projects through collaborative work environment with other disciplinary areas
HPC resources of CCT

• Clusters on duty
  – Super Mike:
    6.27 TFlops, 512 nodes, dual 3.06 GHz intel Xeon processor,
  – Super Helix:
    1.02 TFlops, 128 nodes, dual 2.0 GHz intel Xeon processor,
  – And, many small clusters

• New systems under construction
  – Tezpur:
    15.32 TFlops, 360 nodes, dual-core 64 bit 2.66 GHz intel Xeon processor, 4 GB ram / node
  – Pelican 2:
    1.95 TFlops, 16 nodes, 16 processors / nodes, IBM POWER5+ processor, 32 GB / node
HPC resources of CCT

- CCT is a part of Louisiana Optical Network Initiative (LONI)

LONI maximizes an efficiency and usage of HPC resources in Louisiana
CCT designed for collaboration

CCT

HPC system

staff

joint faculty appointment

academic departments

Physics
ECE
CS
Math
Art

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