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- Hongbo Li (ACMS/OSC)

Collaborators:

Stephan Koch (Marburg/OSC) + many more from OSC!!
ACMS Photonics Supercomputing Laboratory

Dual Opteron Workstations

46 CPU AMD Opteron Cluster

2 TB GFS Home

Infiniband

32 CPU Itanium 2 Altix 3700

1 TB XFS Home

2 TB PVFS Scratch Directory

Gigabit Network

Graphic Head

Dual Graphic Head to Prism Graphics

2 TB GFS Home

Graphic Head

Gigabit Network

Dual Graphic Head to Prism Graphics

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Talk Outline

• Femtosecond Atmospheric Light Strings

• Beyond the Nonlinear Schrödinger Equation

• Role of nanostructures in high power SCL design

• Computational Nanophotonics: Issues and Challenges

• Nanophotonics and Plasmonics Applications

• Summary
Maxwell’s Equations

\[
\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}; \quad \nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t}
\]

\[
\nabla \cdot \vec{D} = 0, \quad \nabla \cdot \vec{B} = 0
\]

Constitutive Relations:

\[
\vec{B} = \mu_0 \vec{H}, \quad \vec{D} = \varepsilon_0 \vec{E} + \vec{P}
\]

Link between E.M and material excitation

Semiconductor passive/active media - rigorous microscopic many-body model
Other material systems - phenomenological models (Lorenz, Drüde, 2-level, .)

Challenges - reliable physical models for ultra-broadband excitations
- numerical algorithms to implement them
Atmospheric Femtosecond Probe


New Scientist, February 19, 2000

The Physics

• White light continuum spectroscopic probe

• Optical breakdown creates narrow plasma filaments - RF emission/lightning control.
Light String Physics

- Nonlinear self-focusing in air – $P_{th} = 7$ GW
- Extreme self-phase modulation - remote white light supercontinuum spectroscopic source.
- Dilute plasma channel generation – THz source, remote LIBS spectroscopy.
- Light string diameters below inner turbulence scale – obscurant penetration
Nonlinear Spatial Replenishment

- Low power, radial symmetry

- Nonlinear spatial replenishment (Mlejnek et al. Optics Letters 1998)
Extended 3D NLS Model

\[ \frac{\partial A}{\partial z} = \frac{i}{2k} \nabla_T^2 A - i \frac{k}{2} \frac{\partial^2 A}{\partial t^2} + i(1 - f_R)kn_2 \left| A \right|^2 A - \frac{\sigma}{2} (1 + i \omega \tau) \rho A \]

\[ - \frac{\beta^{(N)}}{2} \left| A \right|^{2N-2} A + i f_R kn_2 \int_{-\infty}^{t} R(t') \left| A(t-t') \right|^2 dt' A \]

\[ \frac{\partial \rho}{\partial t} = \frac{1}{n_b^2 E_g} \sigma \rho \left| A \right|^2 + \frac{\beta^{(N)}}{Nh \omega} \left| A \right|^{2N} - a \rho^2 \]

- Plasma Drude Model
  
  Avalanche generation  Multi-photon generation  Plasma recombination

- Diffraction  GVD  Kerr Nonlinearity  Plasma Absorption/refraction
  
  Multi-photon absorption  Delayed Raman Response
Rigorous Carrier Resolved 3D Propagator

- Captures all relevant physics of vector Maxwell in absence of backward generated field.

- Measured absorption/refractive index spectra over relevant bandwidth can be input directly to code

- Includes extreme self-focusing down to the wavelength of light in the material.
Unidirectional Pulse Propagation Equation

\[ \partial_t \vec{D}_f(\vec{k}) = -i\omega(\vec{k}) \vec{D}_f(\vec{k}) + \frac{i}{2} \omega(\vec{k}) \left[ \vec{P}_{NL}(\{\vec{D}\}, \vec{k}) - \frac{1}{k^2} \vec{k} \cdot \vec{P}_{NL}(\{\vec{D}\}, \vec{k}) \right] \]

Equation written in spectral domain. Not a PDE in real-space representation.

Nonlinear response coupling
Contribution from self-steepening
\[ \text{div } \vec{E} \] - related term
Nonzero due to gradients.

Linear propagation,
Contains space-time focusing “terms”

Nonlinear polarization of medium calculated from material equation (Kerr effect, plasma, ...)

This equation is exact as long as \( D \) is full field

To close the system of equations for numerical simulations, we approximate:

\[ \vec{P}_{NL}(\{\vec{D}\}) \approx \vec{P}_{NL}(\{\vec{D}_f\}) \]
Shock regularization in femtosecond pulse propagation

25-fs, 8GW, 775nm light pulse propagating in air (animation records 60cm propagation):
- shock forms after 0.5m in the trailing edge of the pulse
- steep wave-form generates higher-frequency field components

Electric induction
(fully resolved by algorithm)

On-axis intensity
Shock regularization in femtosecond pulse propagation

detail: “shock” portion of the pulse

- Makes possible 3D carrier-resolved propagation over tens of meters!
- Describes fs pulse propagation with focusing to λ
- Other “envelope models” derived in seamless fashion
**Periodic** Hermitian Eigenproblems in 1d

- $k$ is periodic: $k + 2\pi/a$ equivalent to $k$
- $\varepsilon(x) = \varepsilon(x+a)$
- Band gap/stop band
- Irreducible Brillouin zone
Slowing Down Light
- engineering material properties!

\[ \frac{d\omega}{dk} \rightarrow 0: \text{slow light} \]
(e.g. bandedge lasing)

backwards slope: negative refraction

strong curvature: super-prisms, …
(+ negative refraction)
Optically-Pumped Semiconductor Laser

- OSC Expts. M. Fallahi, Li Fan, Marc Schillgalies

- Heat sinks
- Optional heat spreader
- AR Coating
- MM Pump

\[ \lambda/4 \text{ Mirror Stack} \]
\[ \text{InGaAs MQW (14-16)} \]

\text{Output}

\text{∼ 5-6 µm!}

\text{Very efficient heat extraction!}

\text{Highly efficient incoherent diode bar to coherent output converter!}
High Power OPSL Chips
Can one achieve > 1kW from a single chip?
Semiconductor Sub-Cavity
Active Mirror

- A. Zakharian, J. Hader (ACMS)

Nanostructured Sub-cavity

Active Mirror Reflectance
VECSEL/OPSL Modeling

- A. Zakharian, M. Kolesik

Optical field spectral domain propagator in the external cavity

Optical field bidirectional Bi_BPM propagator and carrier density rate eqn in active semiconductor sub-cavity

Thermal transport from active region through to heat sink
High Brightness OPSL Design Cycle

- collaboration involving UofA (ACMS/OSC), AFRL
- M. Fallahi, Li Fan, Marc Schillgalies, S.W. Koch, W. Stolz, T. Nelson, R. Bedford

Optimization of MQW Semiconductor Epi Structure

Sub-cavity optimization for pump/signal

Gain Spectra (waffe diagnostic)

3D Thermal Analysis of Optically-Pumped VCSEL

Device growth and processing

Send for growth
Sub-cavity Optimization for Bandedge Lasing

Nontrivial nonlinear optimization problem for pump absorption and signal gain!

Conventional sub-cavity design

Original reflectance spectrum

Band-edge lasing sub-cavity design

Sharper and enhanced BGE reflectance spectrum

Reflectance as seen by external cavity

- RPG-design, 360K
- BGE-design, 330K
- BGE-design, 360K

$\Gamma_{\text{opt}} = 8\, \text{nm}$

$\alpha = 2.5 - 3.5 \times 10^{12}\, \text{cm}^{-2}$, $15\, \text{meV}$
Actively Cooled kW OPLS

- Can dissipate 1 kW of heat with active cooling \( \Rightarrow \) 1kW signal power!

- Active Structure + 60°
- CVD diamond heat spreader
- Copper Mount
- Transparent single crystal diamond heat spreader
- Active Structure blowup
MIT Photonics Micropolis

**Simulation Goal:** Resolve fine nanoscale features in an otherwise featureless landscape

3D + time Maxwell solvers for time domain analysis
Vector Maxwell Simulators

Maxwell’s Equations:

\[ \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} ; \quad \nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} \]

\[ \nabla \cdot \vec{D} = 0, \quad \nabla \cdot \vec{B} = 0 \]

Constitutive relations:

\[ \vec{B} = \mu_0 \vec{H} , \quad \vec{D} = \varepsilon_0 \vec{E} + P \]

Simulation size grows as \( N^3 \) making memory and CPU prohibitive!
Layout of Computational Domain

- PML Layer
- Micro-ring add-drop filter
Example of AMR FDTD discretization for TM-mode in two space dimensions

- A.R. Zakharian, M. Brio

\[
\frac{\partial H_x}{\partial t} = -\frac{\partial E_z}{\partial y}, \quad \frac{\partial H_y}{\partial t} = \frac{\partial E_z}{\partial x}
\]

\[
\frac{\partial E_z}{\partial t} = \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y}
\]

\[
H^{n+1/2}_{x,i+1/2,j} - H^{n-1/2}_{x,i+1/2,j} = -\frac{\Delta t}{\Delta y} \left( E^n_{z,i+1/2,j+1/2} - E^n_{z,i+1/2,j-1/2} \right)
\]

\[
H^{n+1/2}_{y,i+1/2,j} - H^{n-1/2}_{y,i+1/2,j} = \frac{\Delta t}{\Delta x} \left( E^n_{z,i+1/2,j+1/2} - E^n_{z,i-1/2,j+1/2} \right)
\]

AMR refines the computational domain locally using nested rectangular grid patches. A standard FDTD update is applied to each patch.

At the coarse/fine grid interfaces the solution is interpolated. Dashed lines denote boundaries of the ghost cells around the fine region. Arrows show a sample interpolation from coarse to fine values of the electric field.
Nested Grids on a 3D PBG Structure

- A. Zakharian, C. Dineen

- confined defect mode of a 3D PBG lattice
Resolving a QD in a PBG Lattice

-Jens Foerstner - experiment Gibbs et al.

QD Wavefunction

Coupling QD to High Q Defect Mode

Energy level splitting

4-20 nm

AMR Mesh
PBG+QD Confined/Radiating Modes

Bare PBG Mode from Top

Coupled QD+PBG Energy Transfer

Radiating Pattern
Nested 3-level AMR Resolves SP on 20nm Metal Film

<table>
<thead>
<tr>
<th>z</th>
<th>Nlevels</th>
<th>Runtime ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>2nm</td>
<td>2</td>
<td>2.3</td>
</tr>
<tr>
<td>1nm</td>
<td>3</td>
<td>8.1</td>
</tr>
</tbody>
</table>
Scattering from a metal Nanosphere – 3 nested AMR Levels
Nested AMR Mesh for a Plasmon Waveguide

- shows 3 levels of mesh refinement
Summary

Why Computational Photonics?

• Provides a fast track to device design, dramatically reducing wasteful material re-growth, packaging etc

• Interactive simulation laboratory will make many future experiments redundant – computer laboratory on a bench

• Powerful tool to discover new linear and nonlinear optical phenomena on micro- and nano-scales

-Many basic research challenges remain in physics and algorithm development
Lateral ASE and Lasing

- UA, AFRL and Coherent Inc. Collaboration
- Expt data courtesy of Coherent and Robert Bedford (AFRL)