

Computational Photonics: Modeling Ultrashort Pulse Propagation and Interaction with Nanophotonics Structures.

J.V. Moloney

Arizona Center for Mathematical Sciences

and

Optical Sciences Center

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FA9550-04-1-0213; FA9550-04-1-0355
NSF DMS0335101

ACMS Research Team

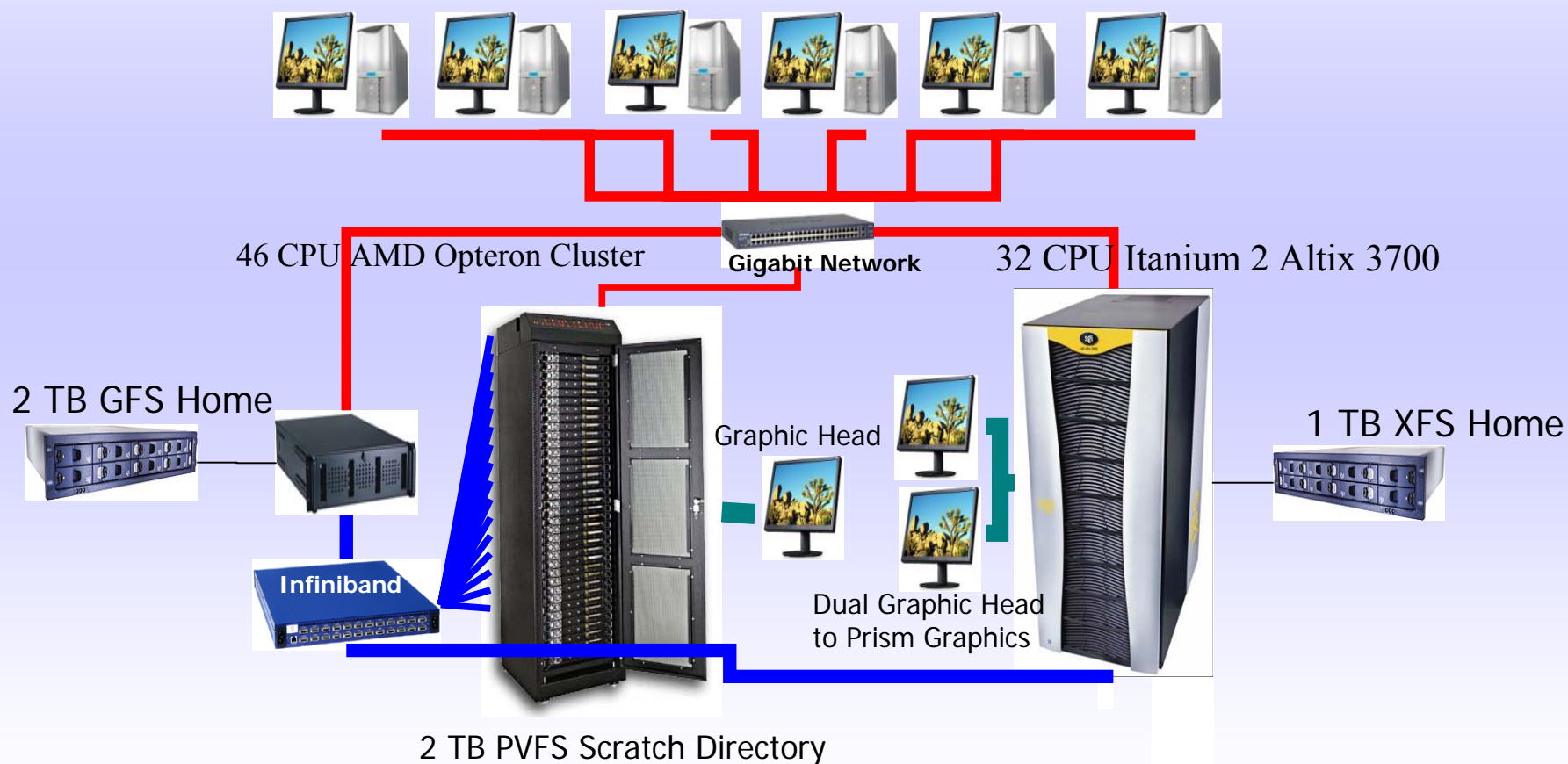
- Moysey Brio (ACMS/Mathematics)
- Miro Kolesik (ACMS/OSC)
- Joerg Hader (ACMS/OSC)
- Armis Zakharian (ACMS/OSC)
- Arash Mafi (ACMS/OSC)
- Walter Hoyer (ACMS/Mathematics)
- Jens Foerstner (ACMS/Mathematics)
- Colm Dineen (ACMS/Mathematics)
- Patrick Kano(Mathematics)
- Krishna Mohan Gundu (ACMS/OSC)
- Marcelo Matus (ACMS/ECE)
- Yong Xie (ACMS/OSC)
- Hongbo Li (ACMS/OSC)

Collaborators:

Stephan Koch (Marburg/OSC) + many more from OSC!!

ACMS Photonics Supercomputing Laboratory

Dual Oteron Workstations

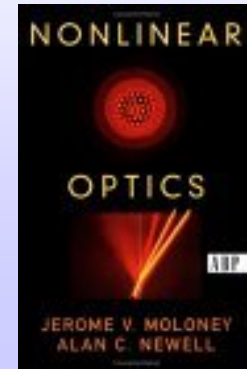


Talk Outline

- 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:

$$\vec{B} = \mu_0 \vec{H}, \quad \vec{D} = \epsilon_0 \vec{E} + \vec{P}$$

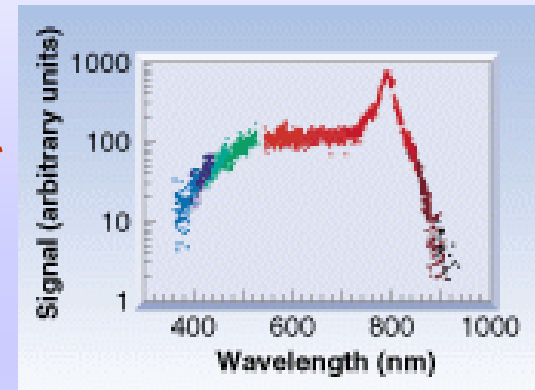
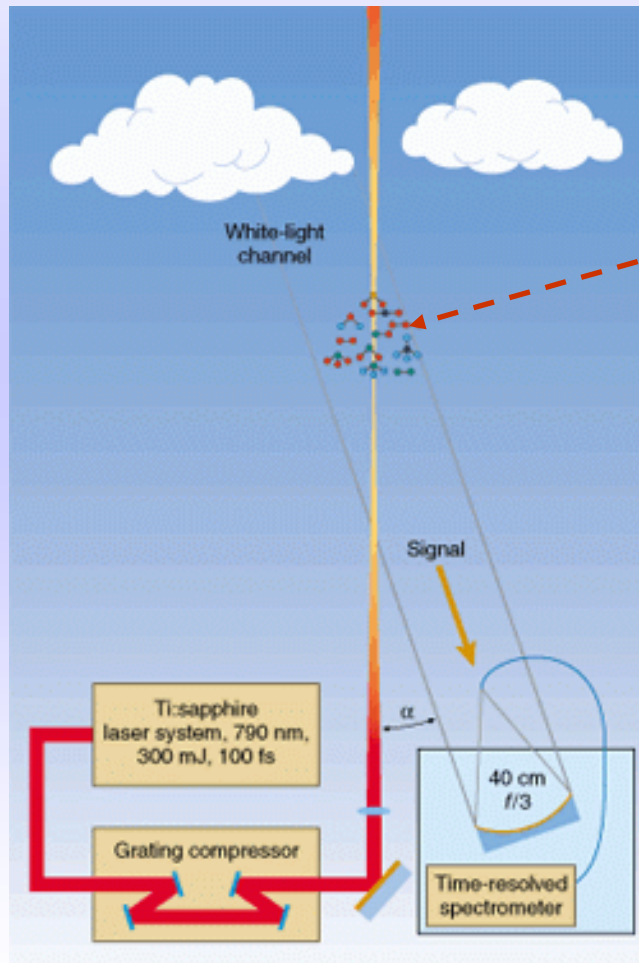
Link between E.M
and material excitation

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

Wöste et al., *Laser und Optoelektronik*, Vol. 29, p51 1997.



White Light Continuum

The Physics

- White light continuum spectroscopic probe
- Optical breakdown creates narrow plasma filaments - RF emission/lightning control.

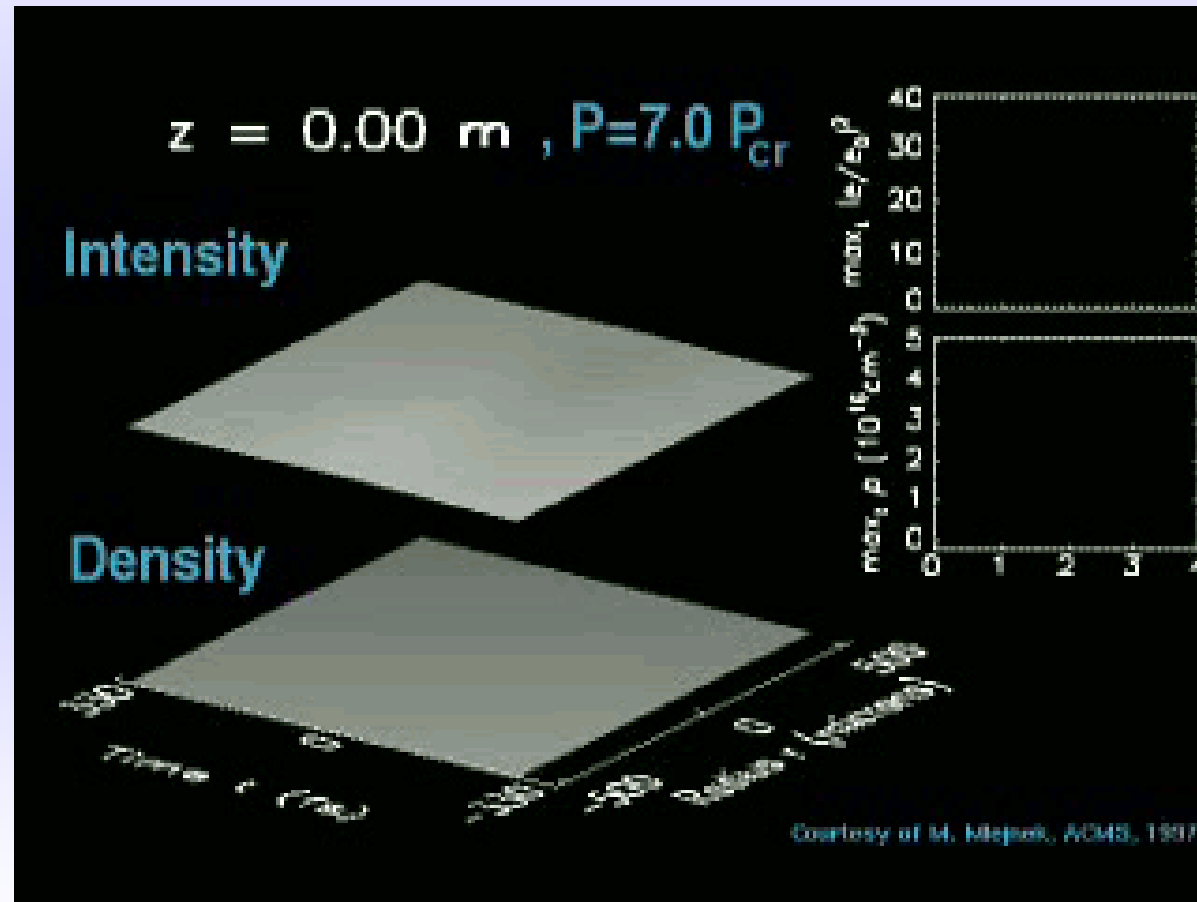
New Scientist, February 19, 2000

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

$$\frac{\partial A}{\partial z} = \frac{i}{2k} \nabla_T^2 A - i \frac{k''}{2} \frac{\partial^2 A}{\partial t^2} + i(1 - f_R)kn_2 |A|^2 A - \frac{\sigma}{2}(1 + i\omega\tau)\rho A$$

Diffraction
GVD
Kerr Nonlinearity
Plasma Absorption/refraction

$$- \frac{\beta^{(N)}}{2} |A|^{2N-2} A + if_R kn_2 \int_{-\infty}^t R(t') |A(t-t')|^2 dt' A$$

Multi-photon absorption
Delayed Raman Response

$$\frac{\partial \rho}{\partial t} = \frac{1}{n_b^2} \frac{\sigma}{E_g} \rho |A|^2 + \frac{\beta^{(N)} |A|^{2N}}{N\hbar\omega} - a\rho^2$$

- Plasma Drude Model

Avalanche generation
Multi-photon generation
Plasma recombination

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

Nonlinear Dispersion unknown!

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

Nonlinear response coupling
Contribution from self-steepening

$\text{div } \cdot \mathbf{E}$ - related term
Nonzero due to gradients.

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

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

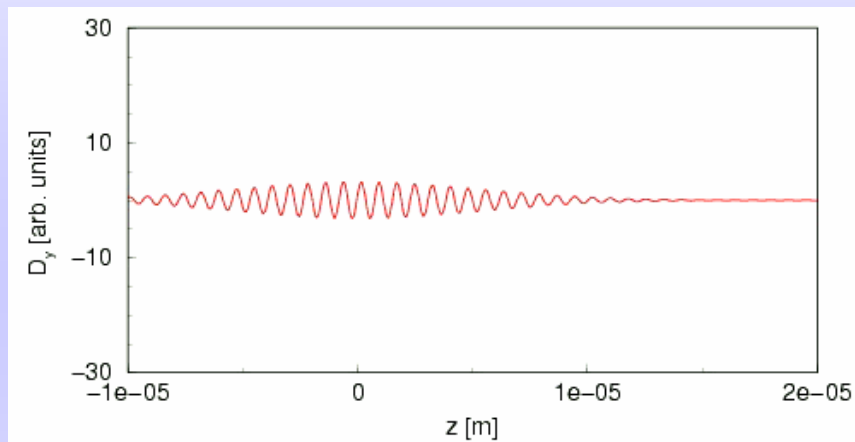
To close the system of equations for numerical simulations, we approximate:

$$\vec{P}_{\text{NL}}(\{\vec{D}\}) \approx \vec{P}_{\text{NL}}(\{\vec{D}_f\})$$

Shock regularization in femtosecond pulse propagation

25-fs, 8GW, 775nm light pulse propagating in air (animation records 60cm propagation):

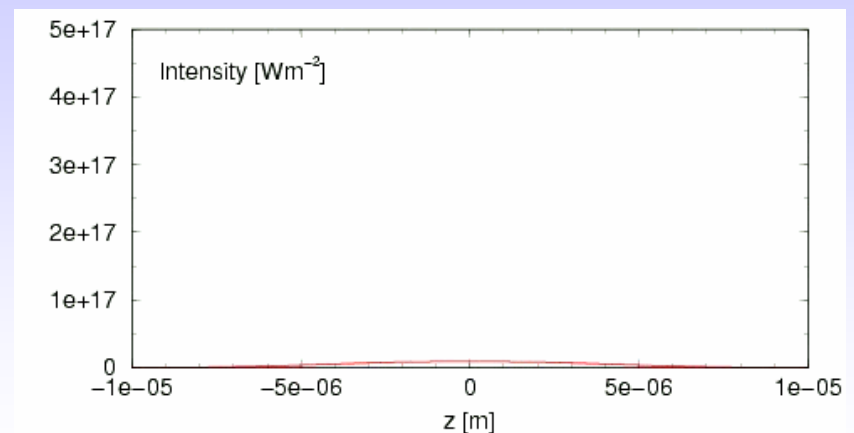
- shock forms after 0.5m in the trailing edge of the pulse
- steep wave-form generates higher-frequency field components



Electric induction

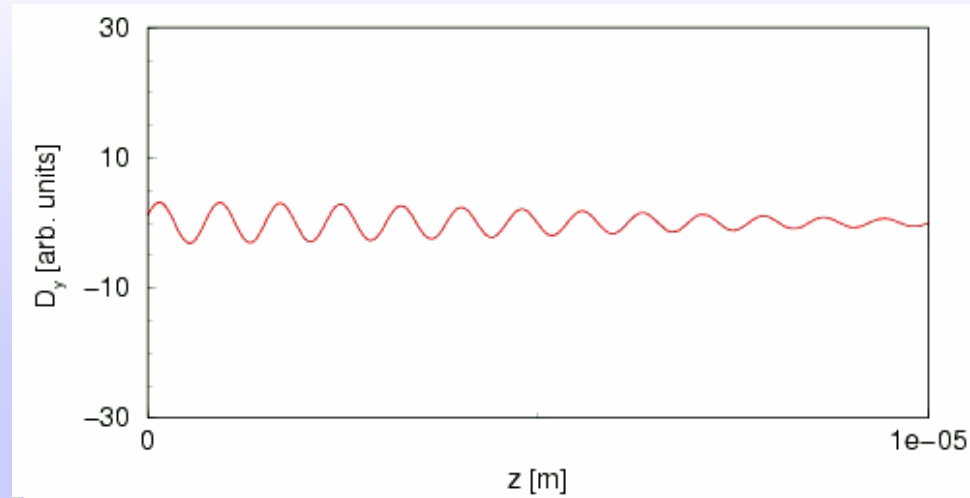
(fully resolved by algorithm)

On-axis intensity



Shock regularization in femtosecond pulse propagation

detail: "shock" portion of the pulse

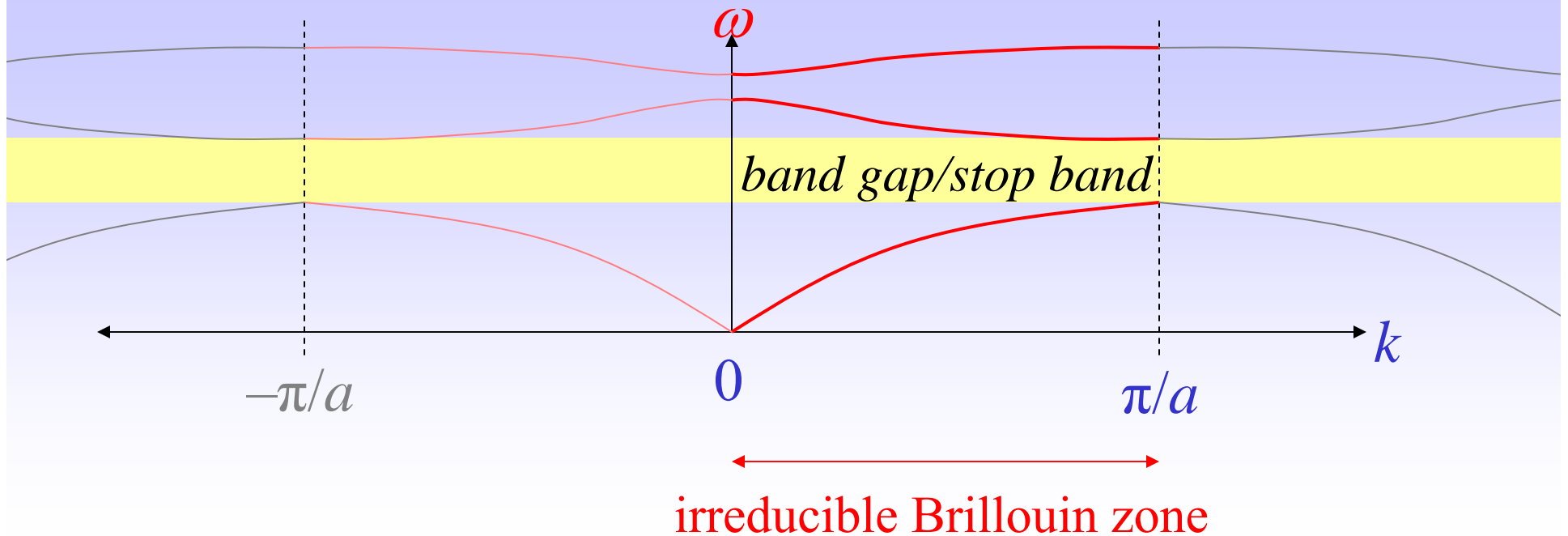
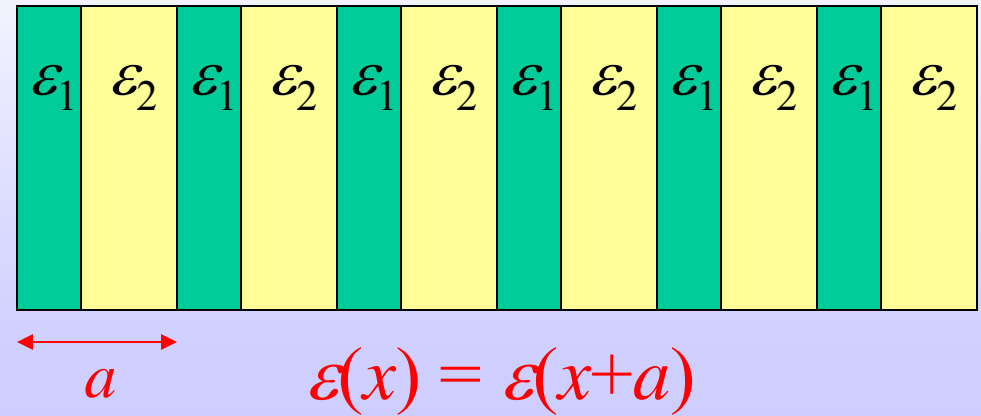


-
- *Makes possible 3D carrier-resolved propagation over tens of meters!*
 - *Describes fs pulse propagation with focusing to λ*
 - *Other "envelope models" derived in seamless fashion*

Periodic Hermitian Eigenproblems in 1d

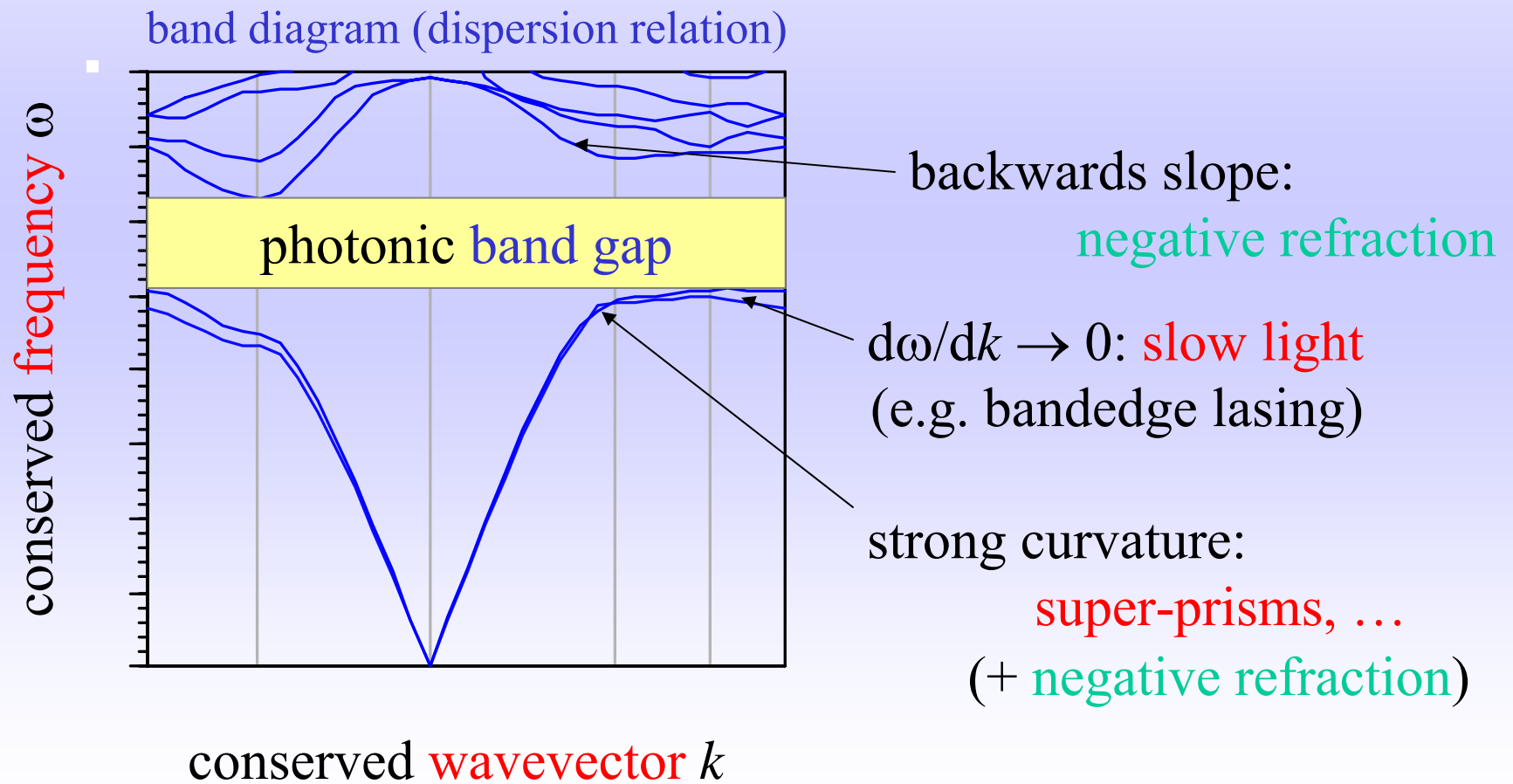
Bragg Grating

k is periodic:
 $k + 2\pi/a$ equivalent to k



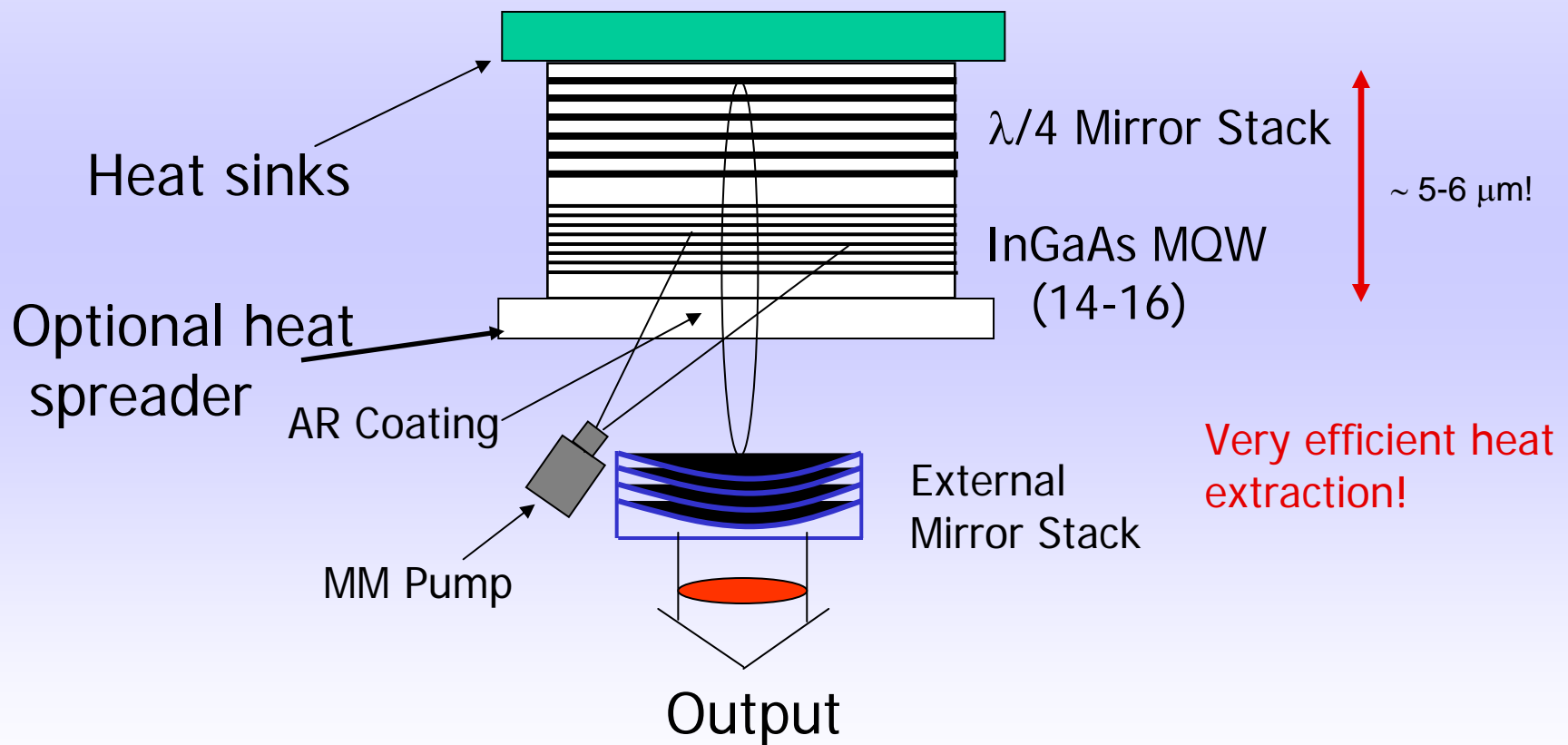
Slowing Down Light

- engineering material properties!



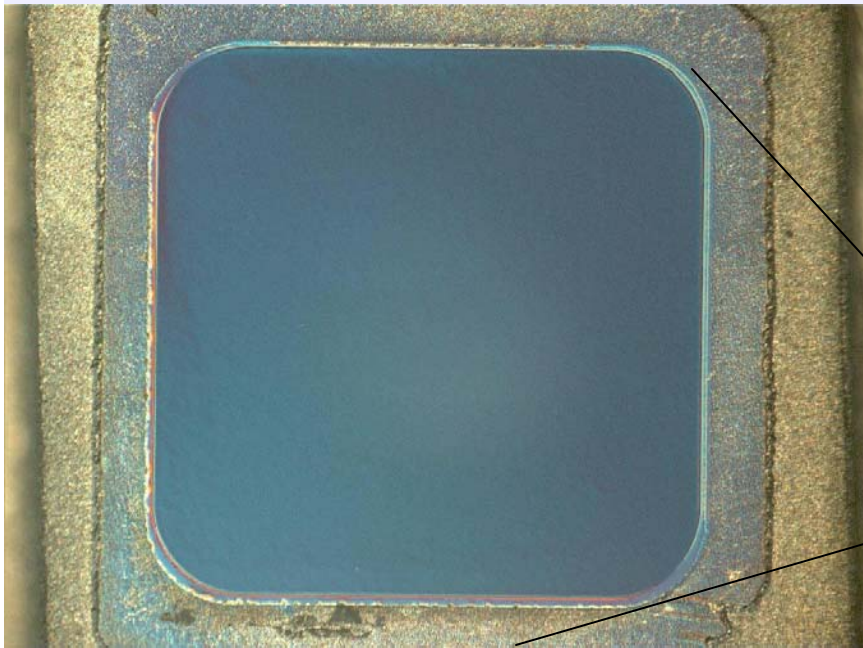
Optically-Pumped Semiconductor Laser

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

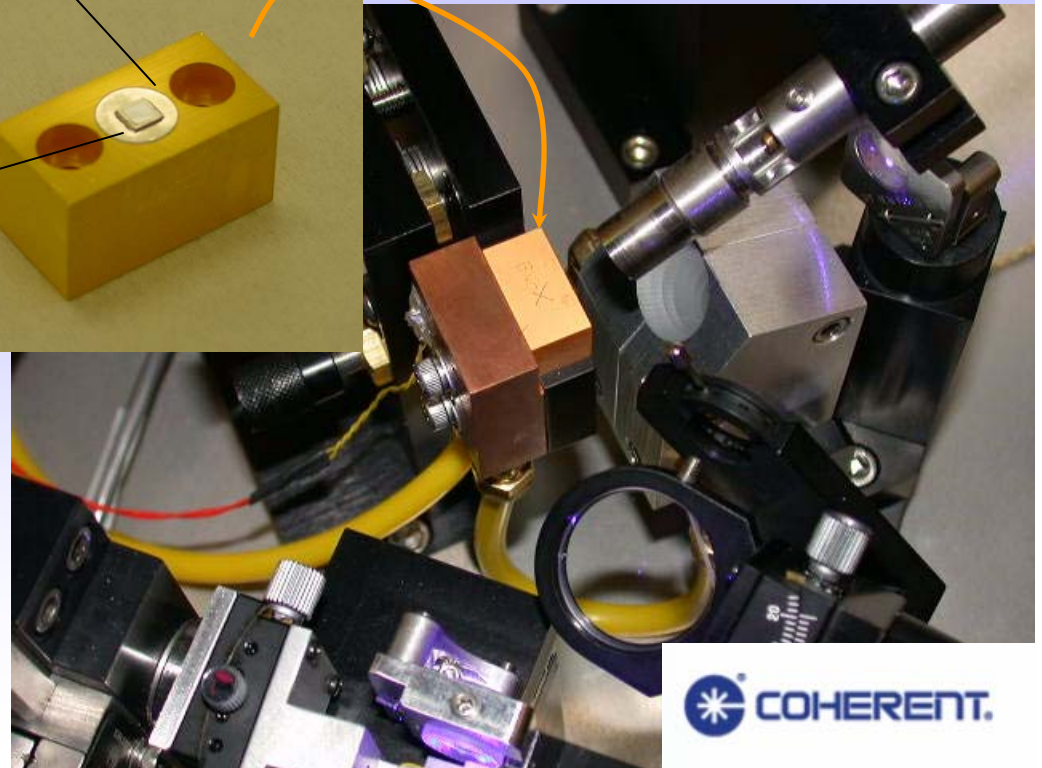
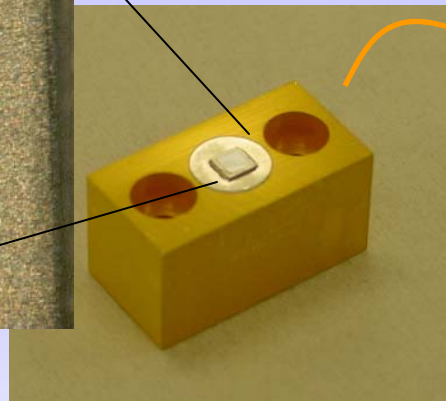


Highly efficient incoherent diode bar to coherent output converter!

High Power OPSL Chips



2 mm

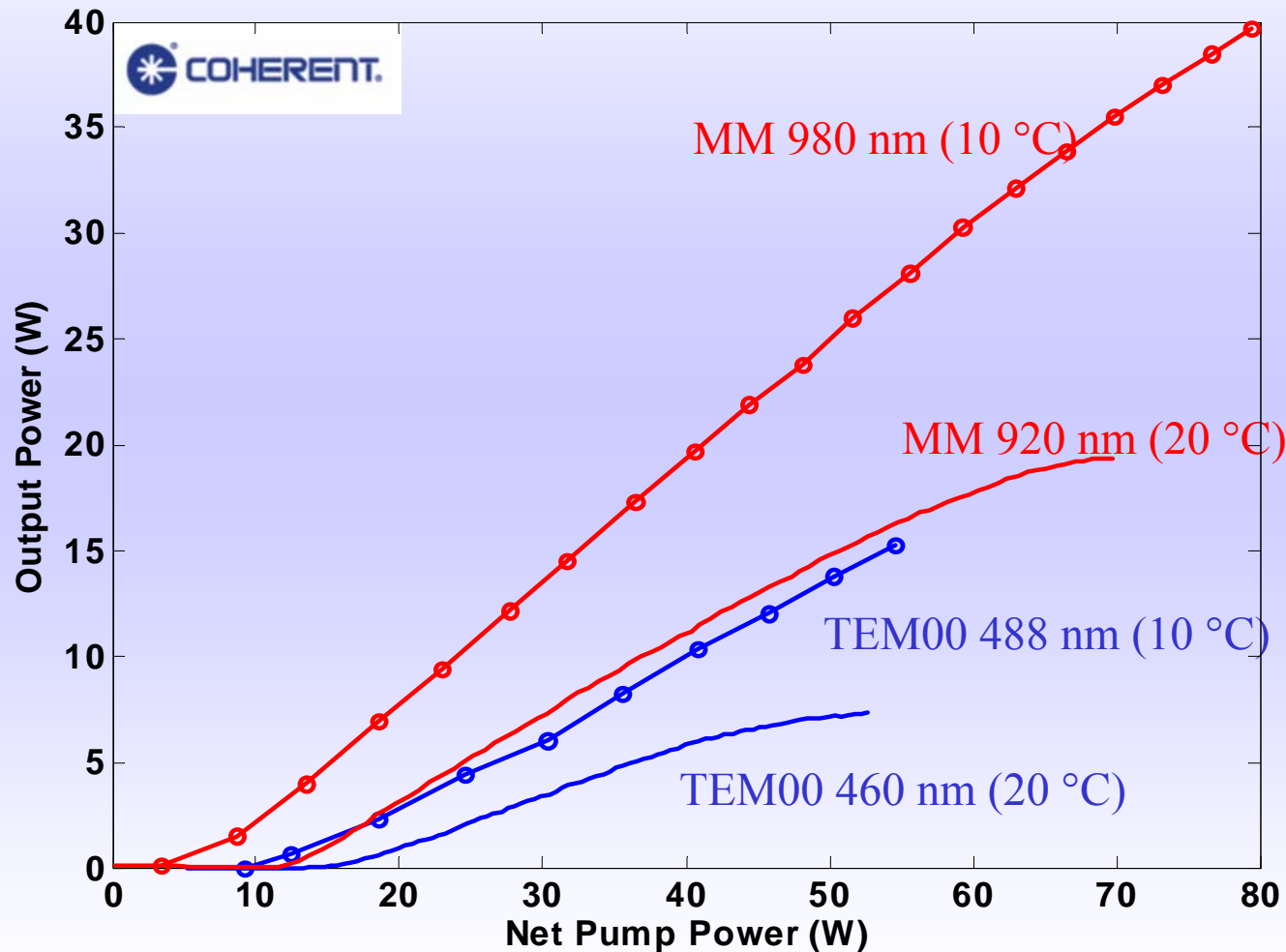


US Patent # 6298076



Record High Brightness OPSL

- Pump spot 500 – 600 μm .

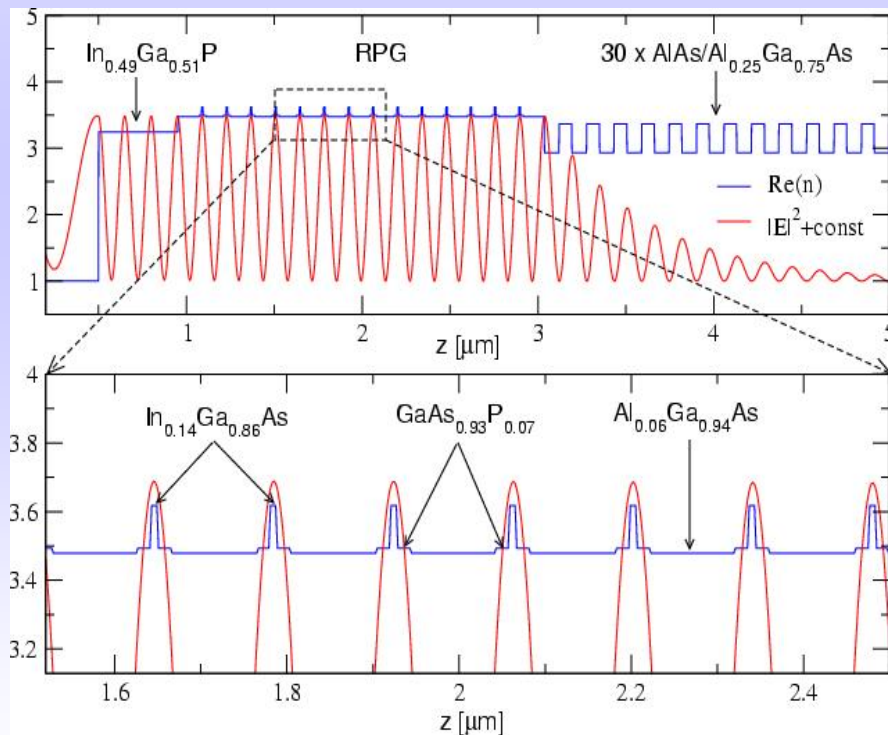


Can one achieve $> 1\text{kW}$ from a single chip?

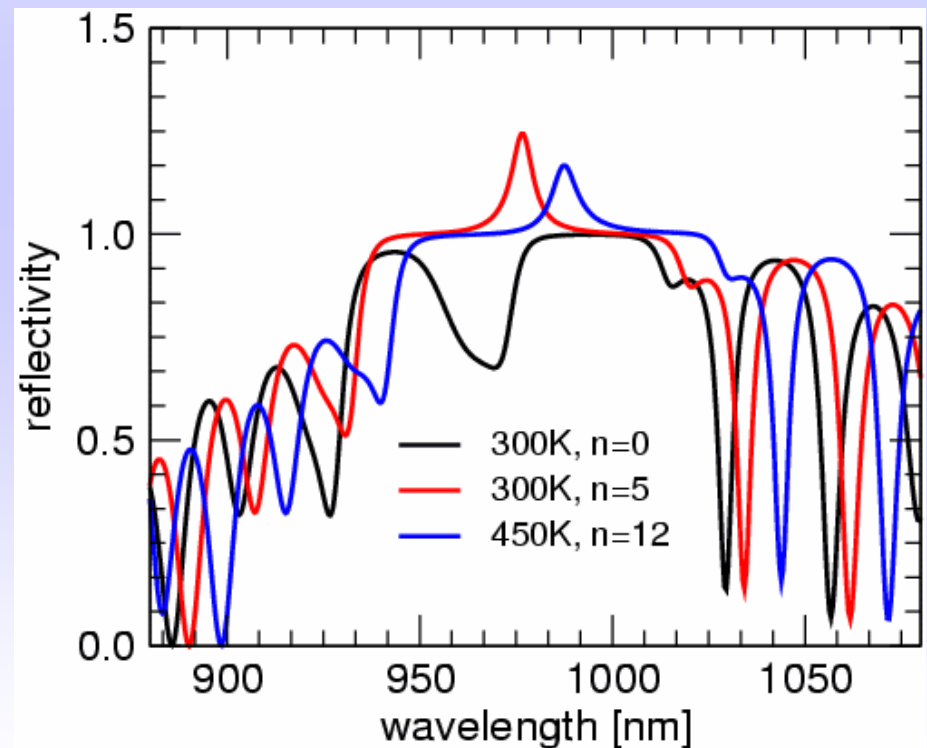
Semiconductor Sub-Cavity Active Mirror

- A. Zakharian, J. Hader(ACMS)

Nanostructured Sub-cavity

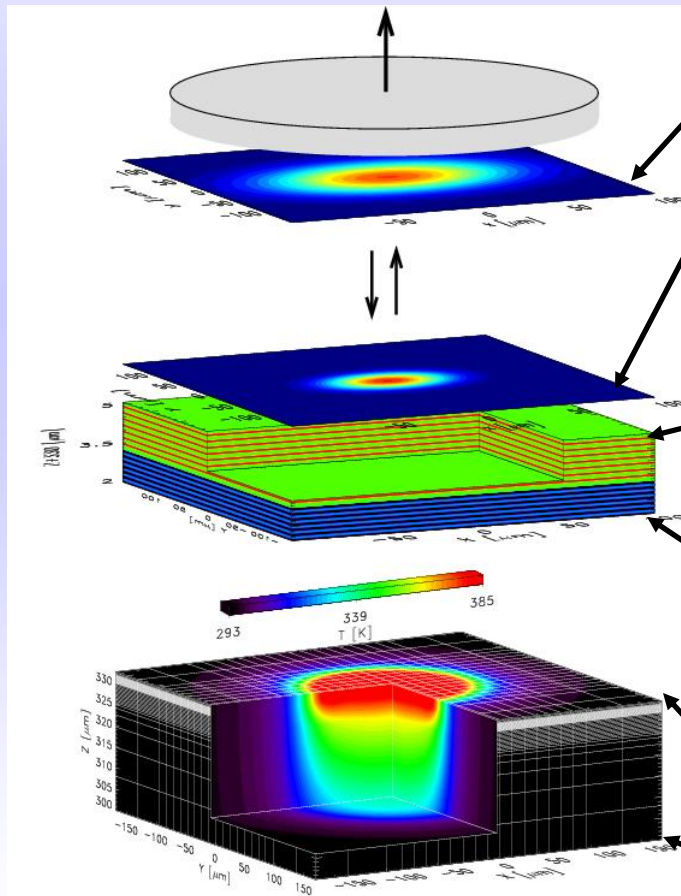


Active Mirror Reflectance



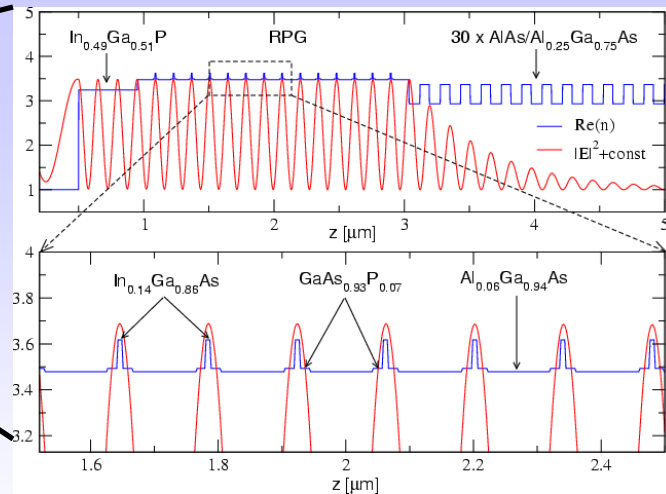
VECSEL/OPSL Modeling

- 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



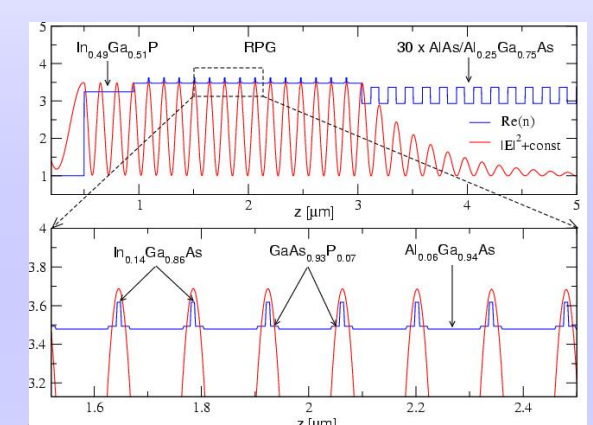
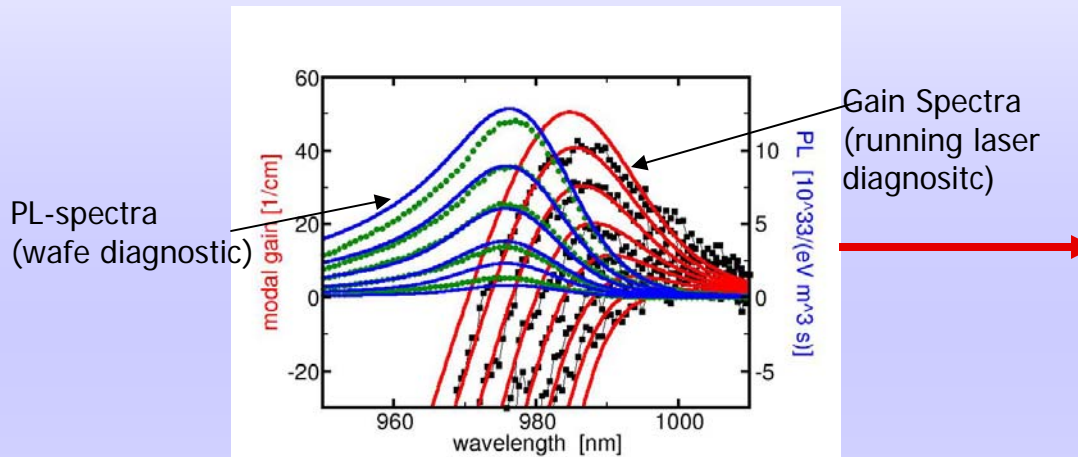
Thermal transport from active region through to heat sink

High Brightness OPSEL Design Cycle

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

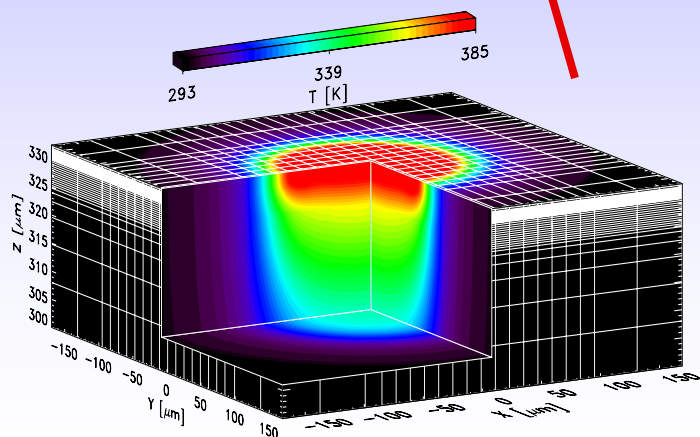
Optimization of MQW Semiconductor Epi Structure

Sub-cavity optimization for pump/signal

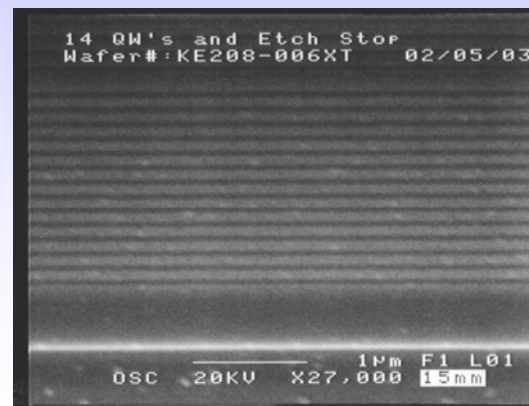


3D Thermal Analysis of Optically-Pumped VCSEL

Device growth and processing



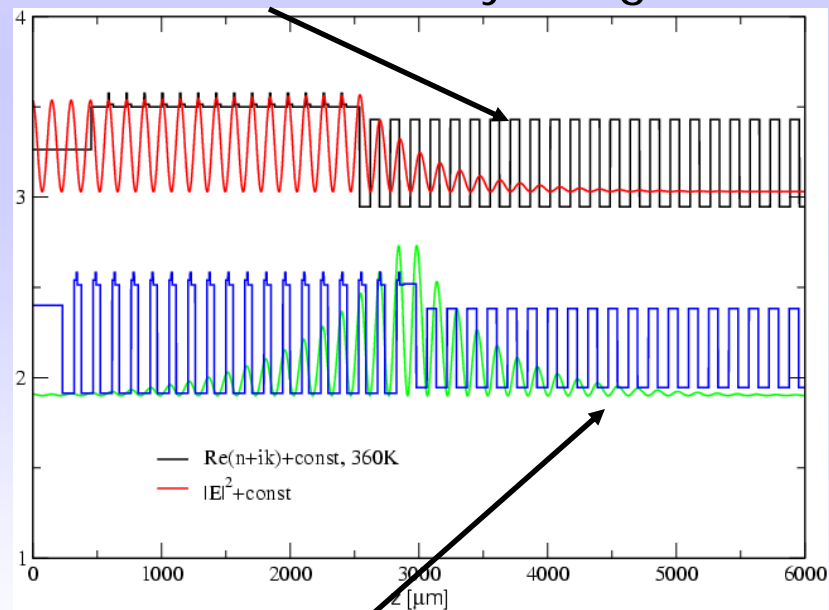
Send for growth



Sub-cavity Optimization for Bandedge Lasing

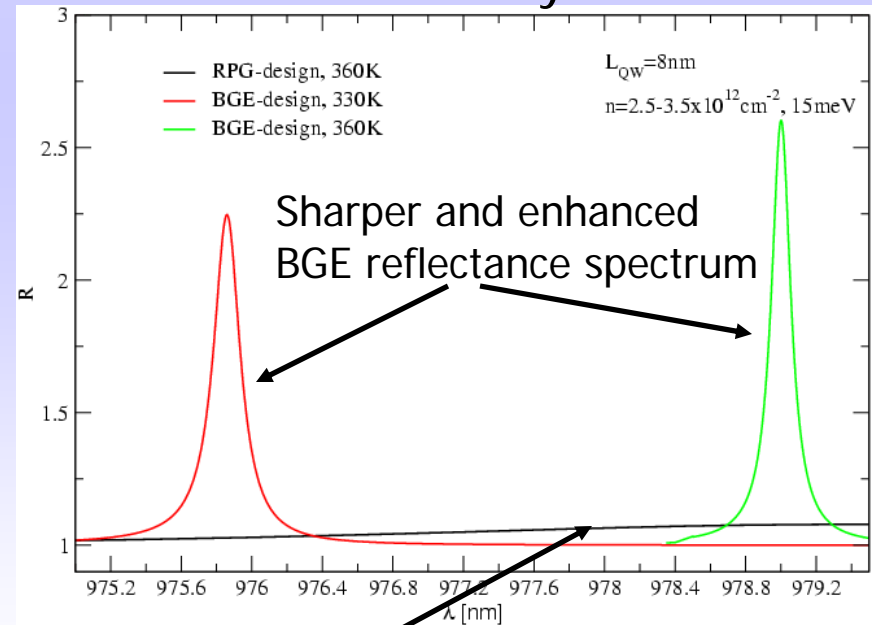
Nontrivial nonlinear optimization problem for pump absorption and signal gain!

Conventional sub-cavity design



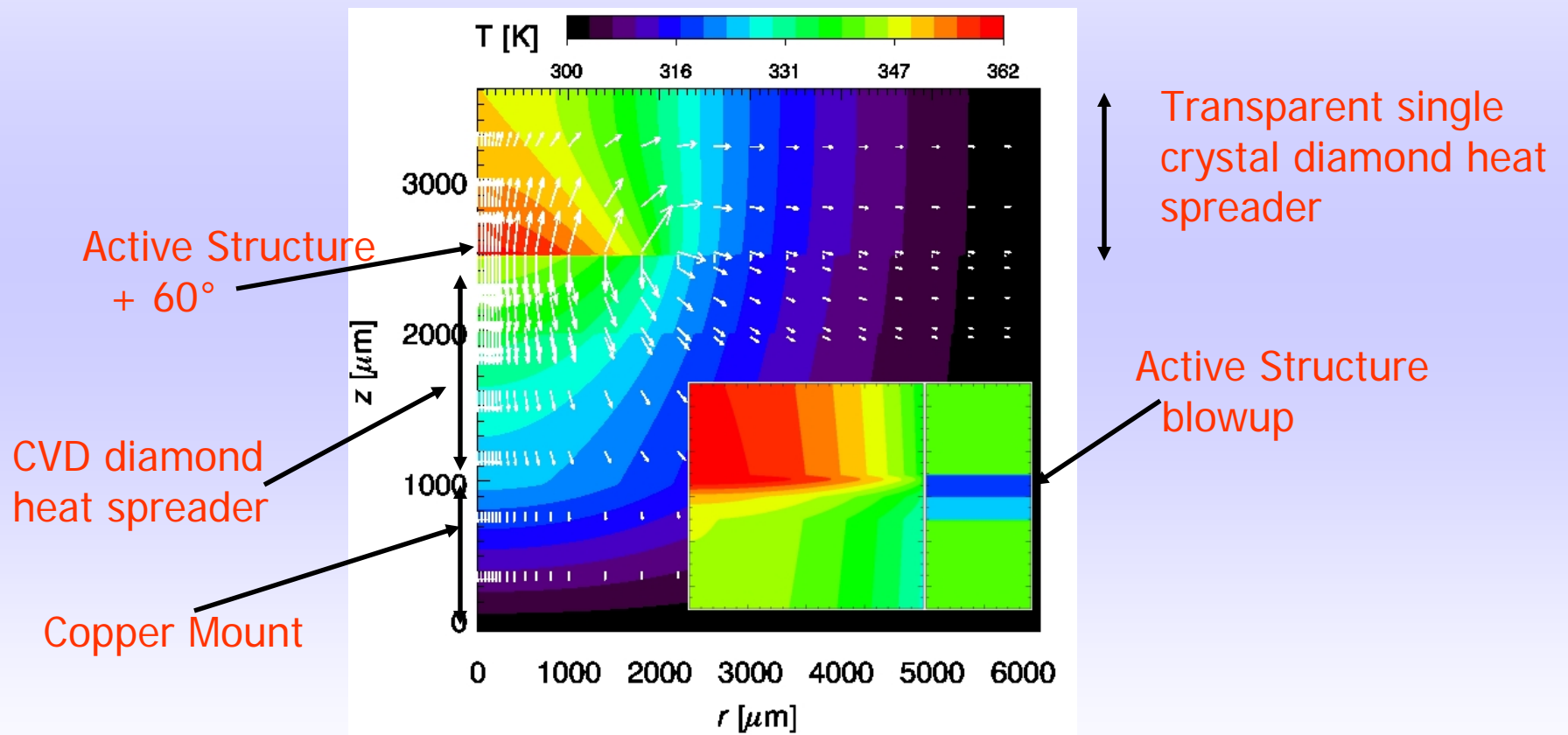
Band-edge lasing sub-cavity design

Reflectance as seen by external cavity



Original reflectance spectrum

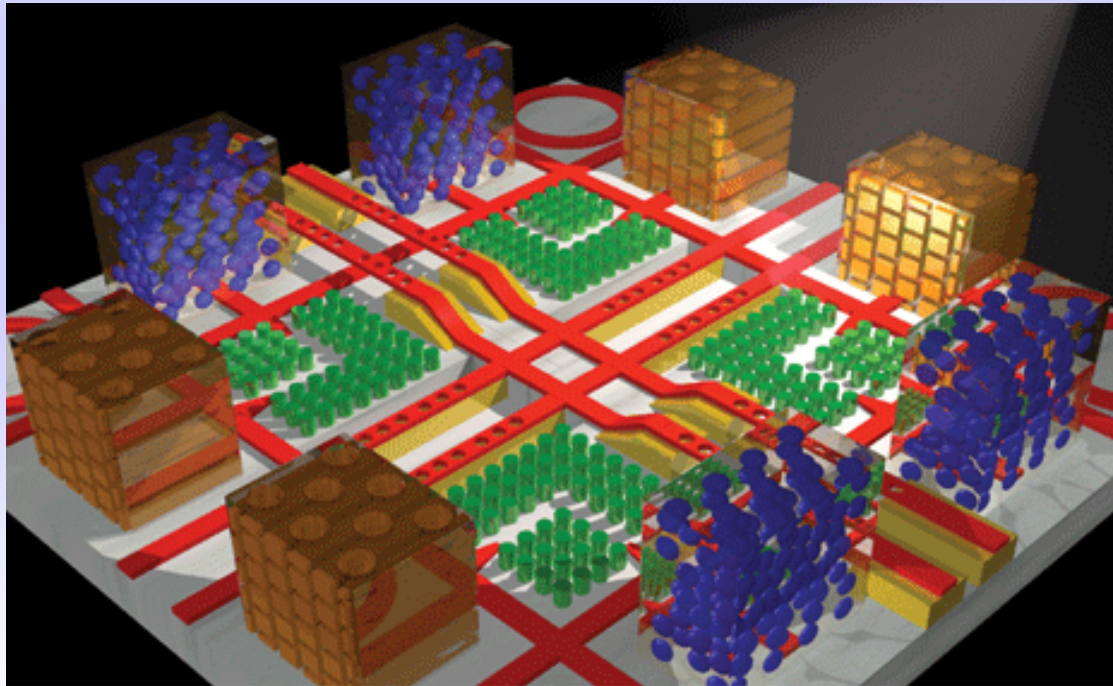
Actively Cooled kW OPSL



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

MIT Photonics Micropolis

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



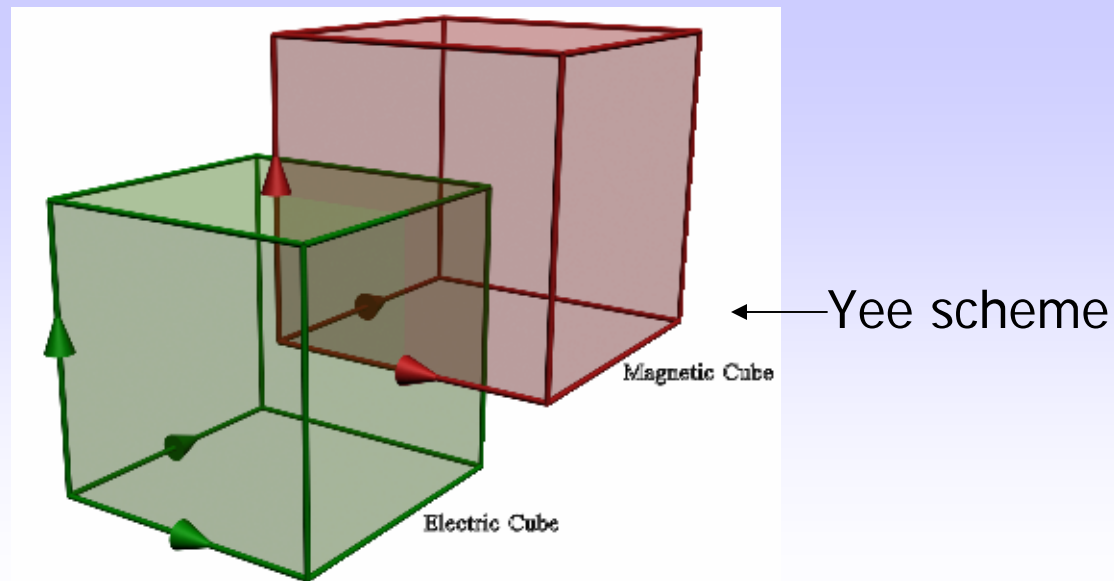
3D + time Maxwell solvers for time domain analysis

Vector Maxwell Simulators

Maxwell's Equations: $\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}; \quad \nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t}$
 $\nabla \cdot \vec{D} = 0, \quad \nabla \cdot \vec{B} = 0$

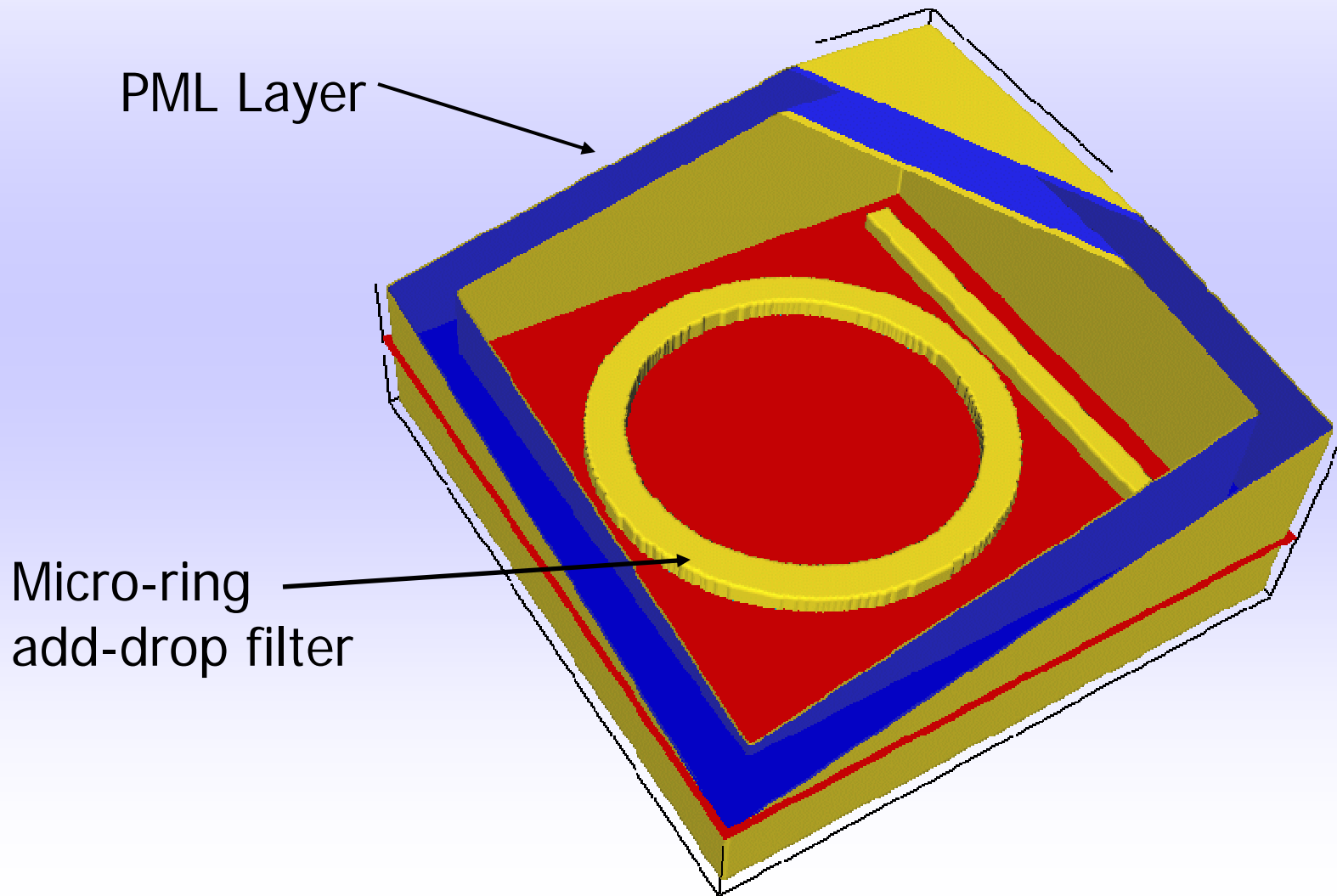
Constitutive relations: $\vec{B} = \mu_0 \vec{H}, \quad \vec{D} = \epsilon_0 \vec{E} + \vec{P}$

FDTD Method



Simulation size grows as N^3 making memory and CPU prohibitive!

Layout of Computational Domain



Example of AMR FDTD discretization for TM-mode in two space dimensions

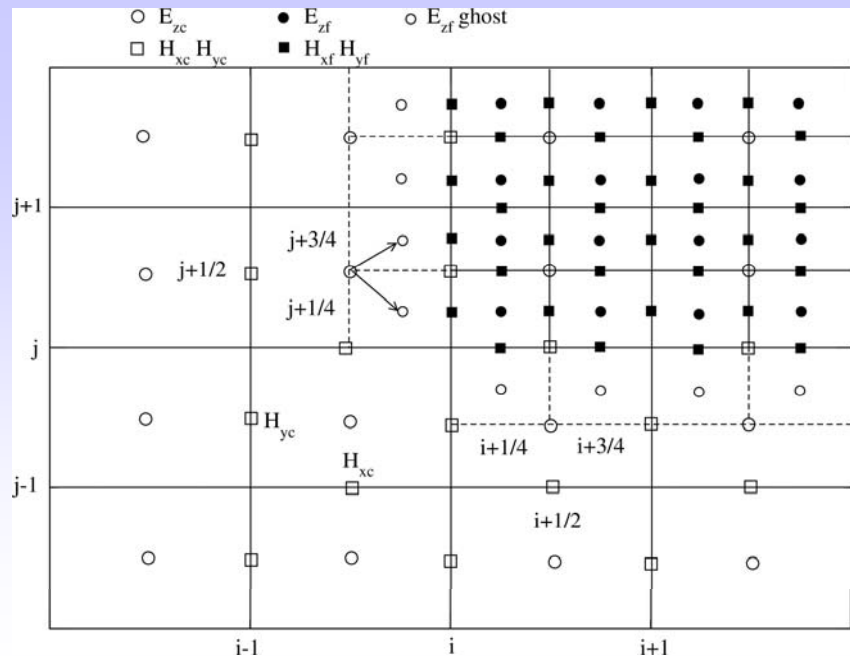
- A.R.Zakharian, M. Brio

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

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

$$H_{x,i+1/2,j}^{n+1/2} - H_{x,i+1/2,j}^{n-1/2} = -\frac{\Delta t}{\Delta y} \left(E_{z,i+1/2,j+1/2}^n - E_{z,i+1/2,j-1/2}^n \right)$$

$$H_{y,i+1/2,j}^{n+1/2} - H_{y,i+1/2,j}^{n-1/2} = \frac{\Delta t}{\Delta x} \left(E_{z,i+1/2,j+1/2}^n - E_{z,i-1/2,j+1/2}^n \right)$$

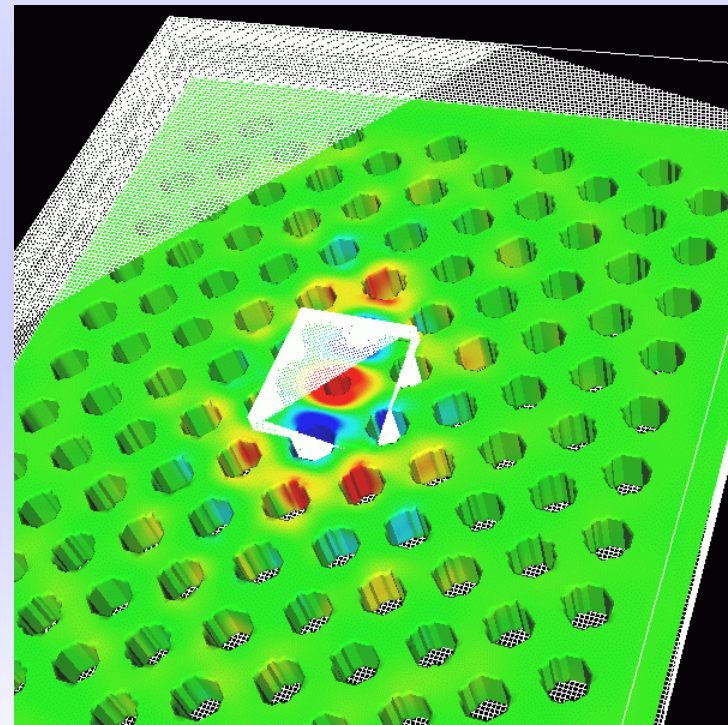
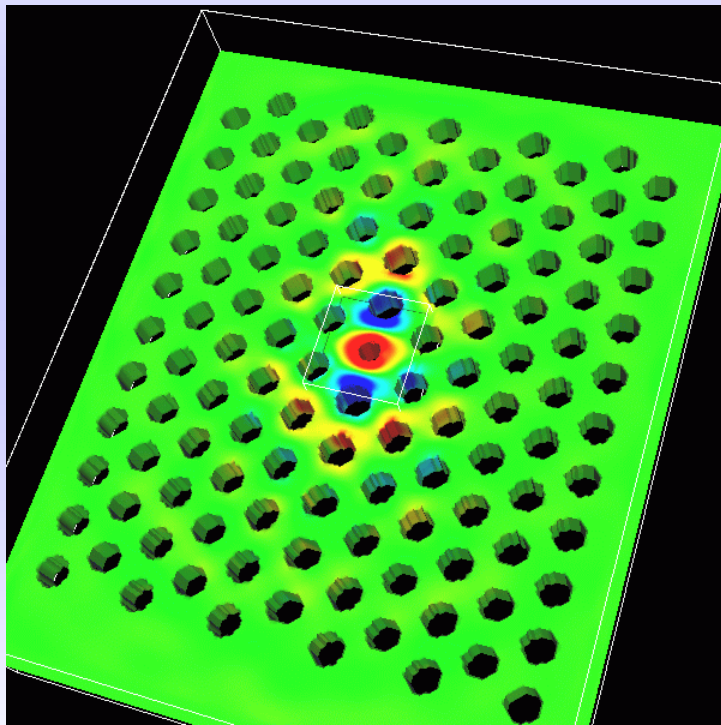


AMR refines the computational domain locally using nested rectangular grid patches. A standard FDTD update is applied to each patch.

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

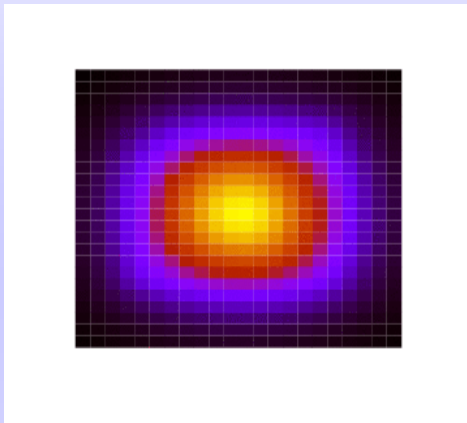


- confined defect mode of a 3D PBG lattice

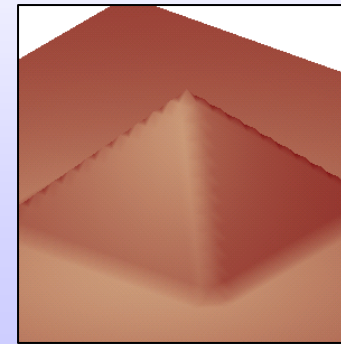
Resolving a QD in a PBG Lattice

-Jens Foerstner - experiment Gibbs et al.

QD Wavefunction

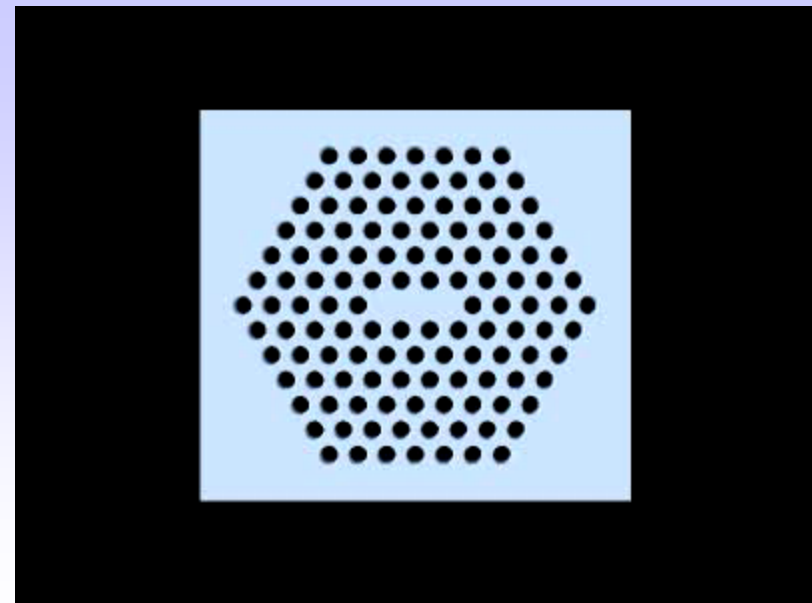
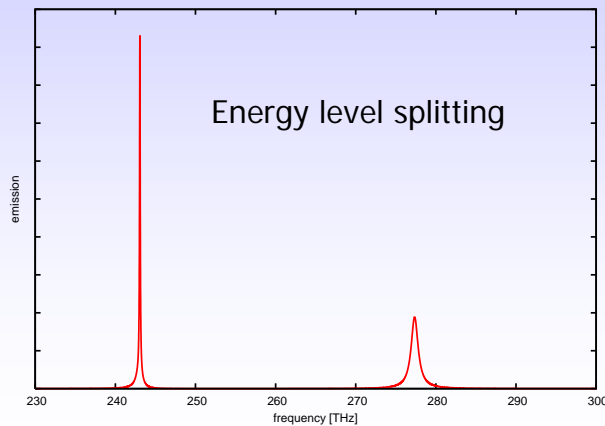


← 4-20 nm →



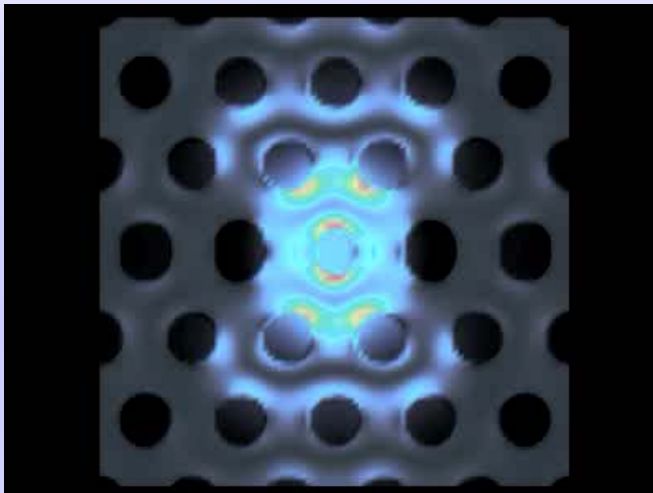
AMR Mesh

Coupling QD to High Q Defect Mode

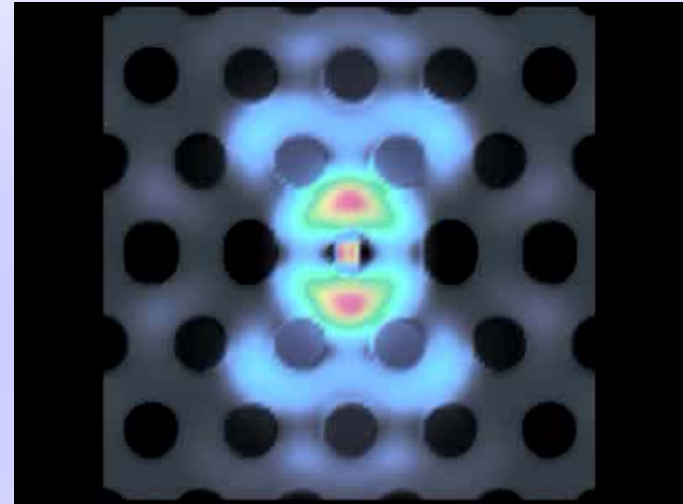


PBG+QD Confined/Radiating Modes

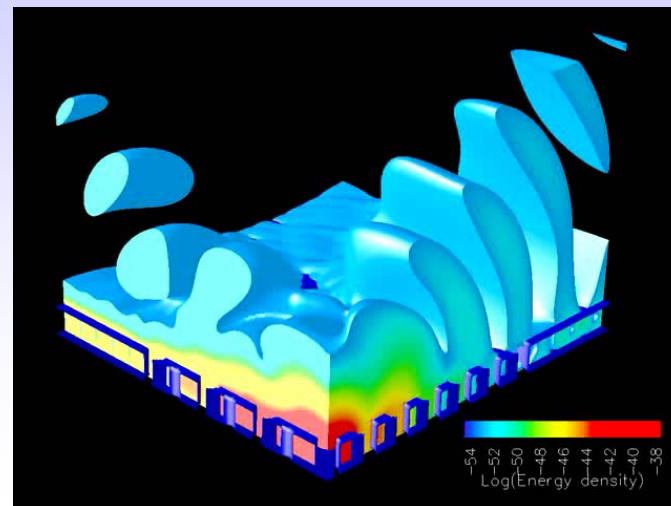
Bare PBG Mode from Top



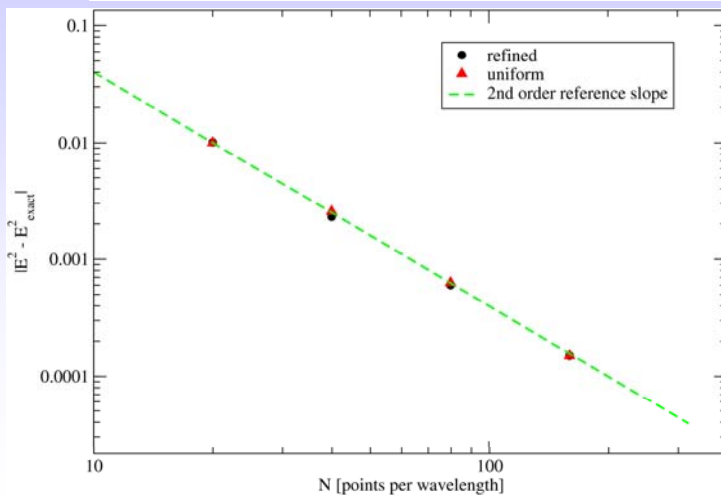
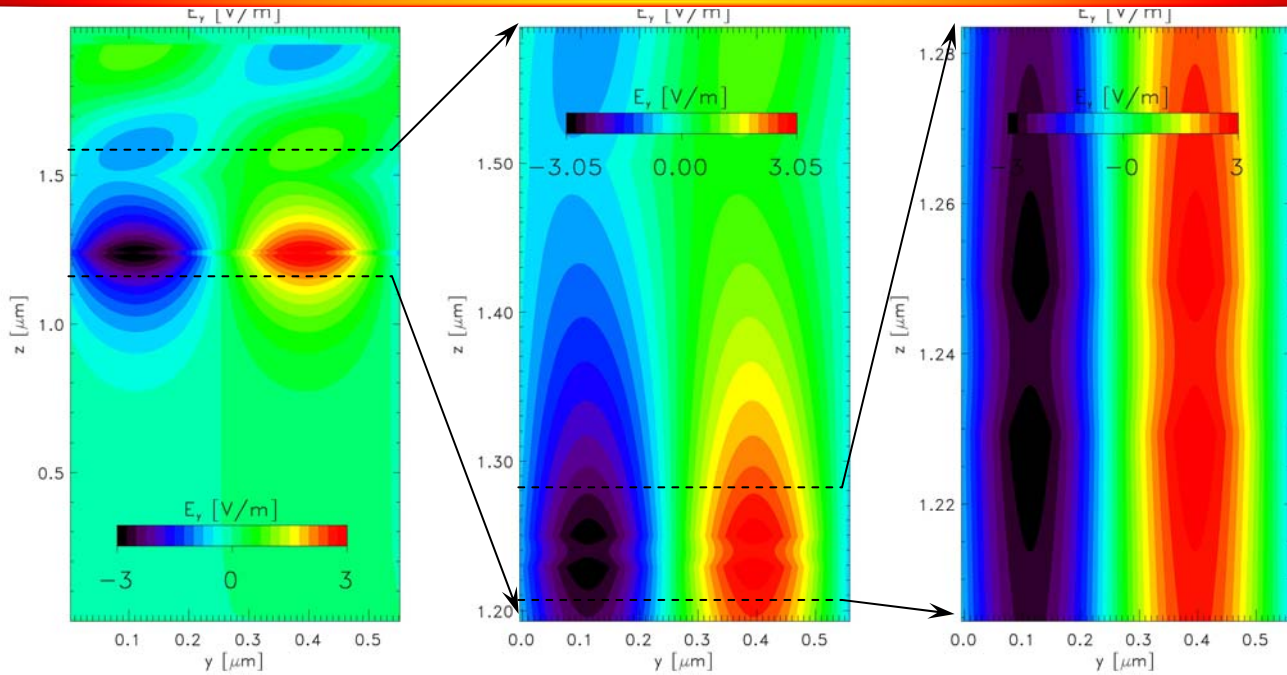
Coupled QD+PBG Energy Transfer



Radiating Pattern



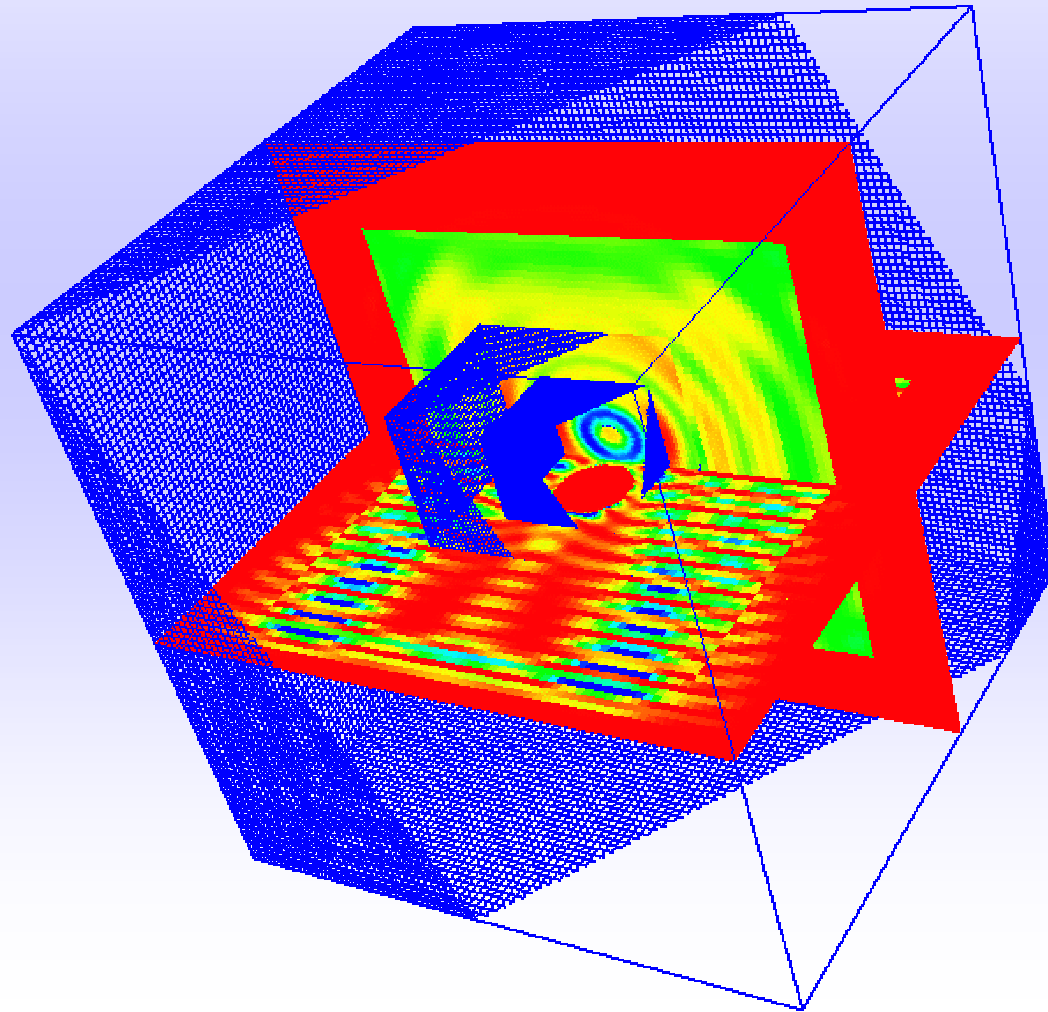
Nested 3-level AMR Resolves SP on 20nm Metal Film



z	Nlevels	Runtime ratio
2nm	2	2.3
1nm	3	8.1

Scattering from a metal Nanosphere

– 3 nested AMR Levels



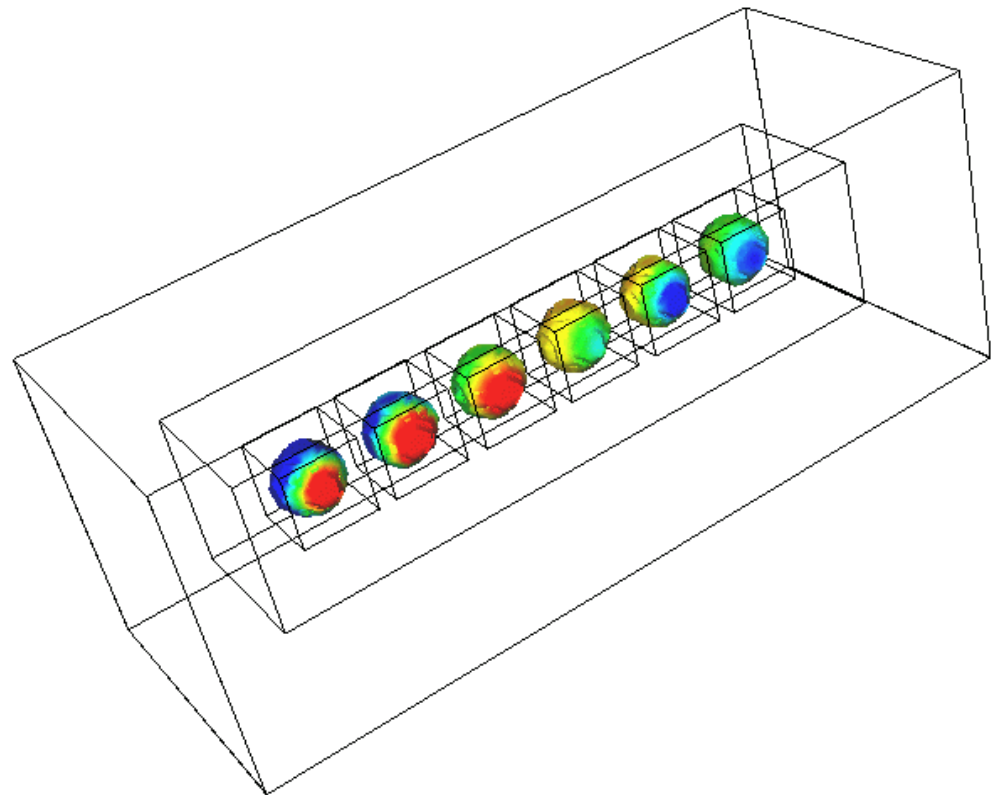
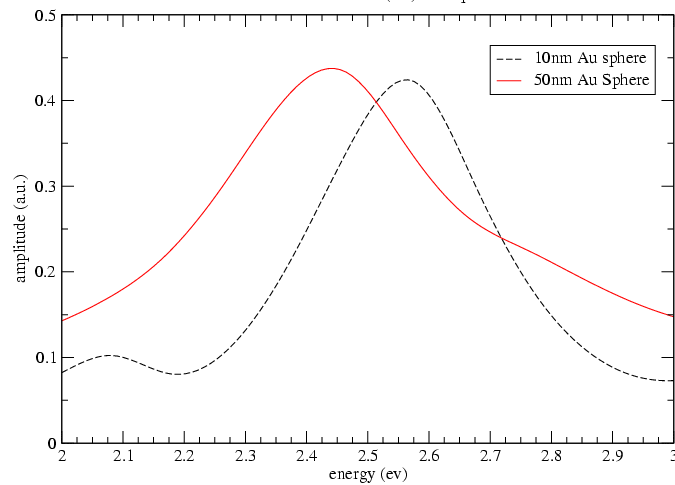
Nested AMR Mesh for a Plasmon Waveguide

- A.R. Zakharian, C. Dineen

- shows 3 levels of mesh refinement

Single particle plasmon resonance frequency

10nm and 50nm Gold (Au) nanospheres



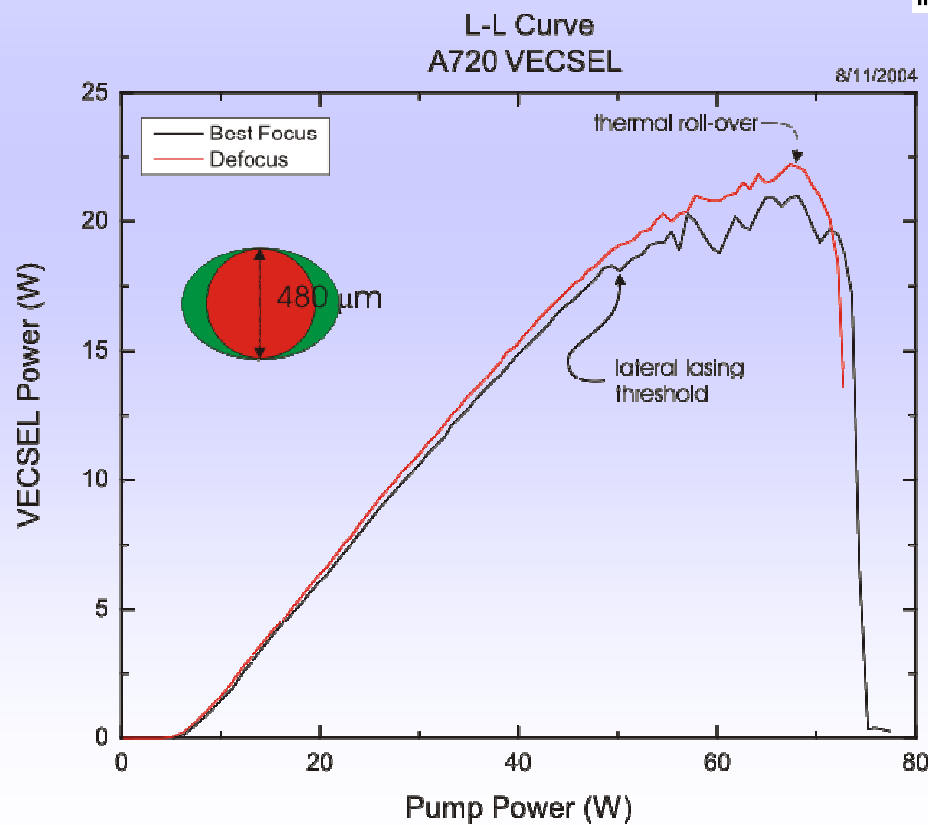
Summary

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)



Imaging Photoluminescence

