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A Novel Finite-Element Formulation Applied to Wave Propagation in Optically Large Structures

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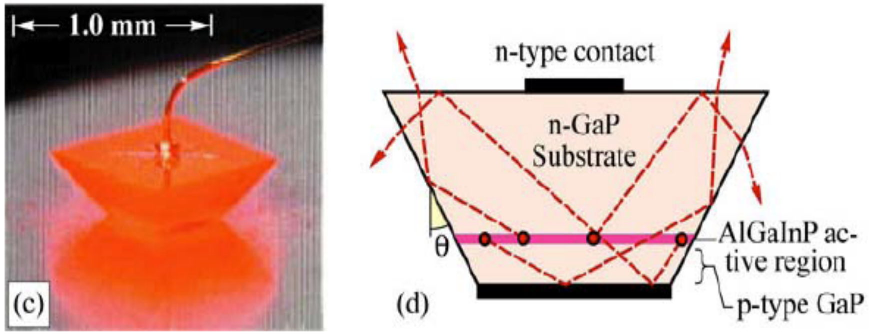
Motivation

- Challenge: Optical Simulation of large (1000s xλ) optoelectronic devices (LEDs, BA Lasers)
- Usually two different approaches
  - FEM/FDTD
    - **Accurate**
    - **Considers wave nature**
    - **Computationally expensive**
  - Ray Tracing
    - **Fast**
    - **Not necessarily robust**
    - **Loss of wave nature**

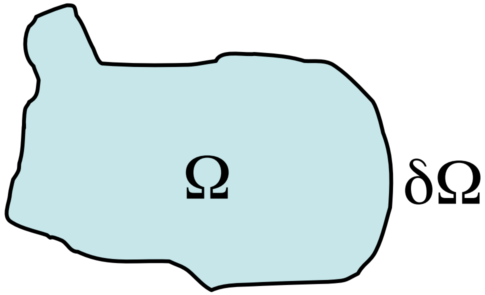


Krames et al., 1999

Ultra-Weak Variational Formulation*

- Discontinuous Galerkin FE-Method for inhomogeneous Helmholtz equation

$$\Delta u + \omega^2 u = -f \text{ in } \Omega$$
$$\frac{\partial u}{\partial \mathbf{n}} + i\omega u = 0 \text{ on } \partial\Omega$$



- UWVF Solves problem on the boundaries of the domain
- Base functions η satisfy homogeneous Helmholtz equation on each patch but may be discontinuous across boundaries
- Linear equation system to be solved with GMRES

*: Huttunen et al. J Comp Phys 223, 2007

Variational Formulation

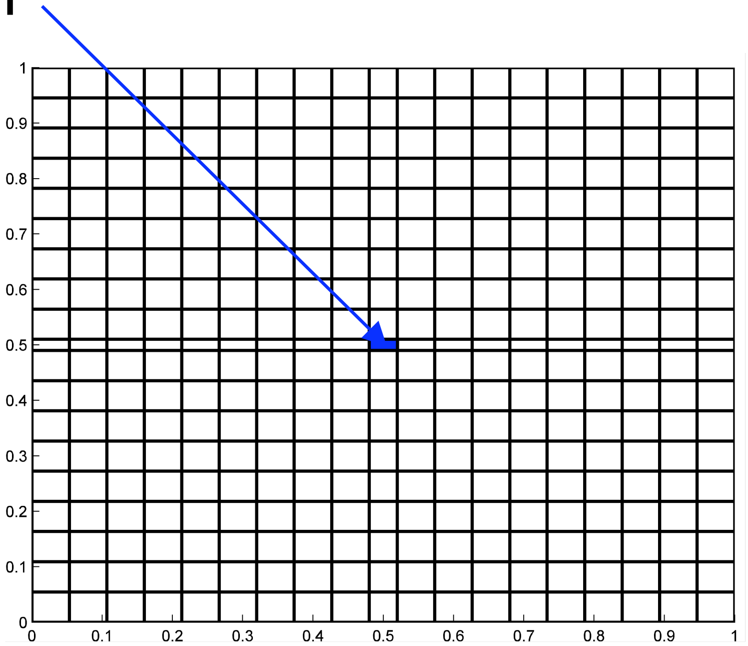
$$\sum_{k} \int_{\partial\Omega_k} x_k \overline{\left(\frac{-\partial\eta_k}{\partial\mathbf{n}} + i\omega\eta_k\right)} ds - \sum_{k,j} \int_{\Sigma_{kj}} x_j \overline{\left(\frac{\partial\eta_k}{\partial\mathbf{n}} + i\omega\eta_k\right)} ds = -2i\omega \sum_{k} \int_{\partial\Omega_k} f\overline{\eta_k}\, d\Omega, \quad \forall\eta \in H$$

$$\eta_k = \eta|_{\Omega_k}, \quad \Delta\eta_k + \omega^2\eta_k = 0 \text{ on } \Omega_k \qquad\qquad x_k := \left.\frac{-\partial u}{\partial\mathbf{n}} + i\omega u\right|_{\partial\Omega_k}$$

- Special choice of base functions
  → only boundary integrals on LHS
  → here: plane waves, #angles user choice
- Solution in source regions requires additional “traditional” FEM calculations
- Known numerical issue: ill-conditioning

Benchmark Example

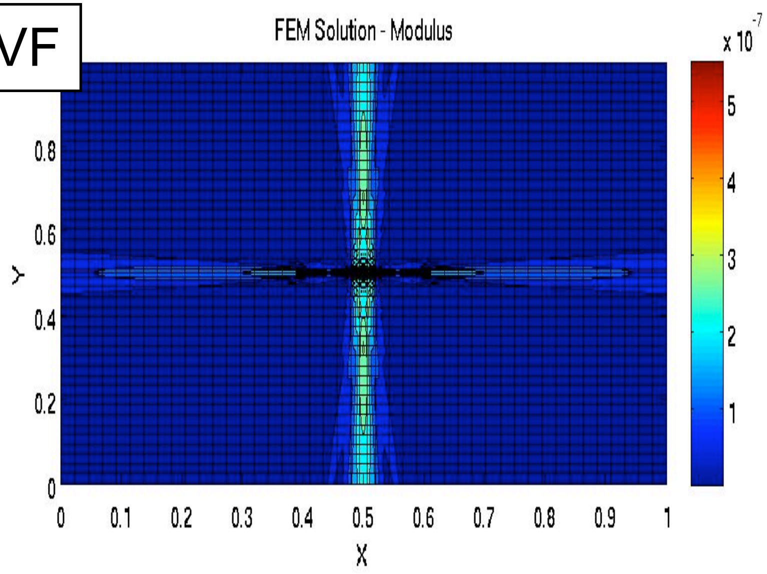
- Problem dimension: 1’000λ × 1’000λ
- Source region in center of domain
- UWVF (ca. 50xλ)
  - 1.4 million DoF
  - 543 million non-zero matrix entries
- FEM (λ/25)
  - 625 million DoF
  - 5625 million non-zero matrix entries



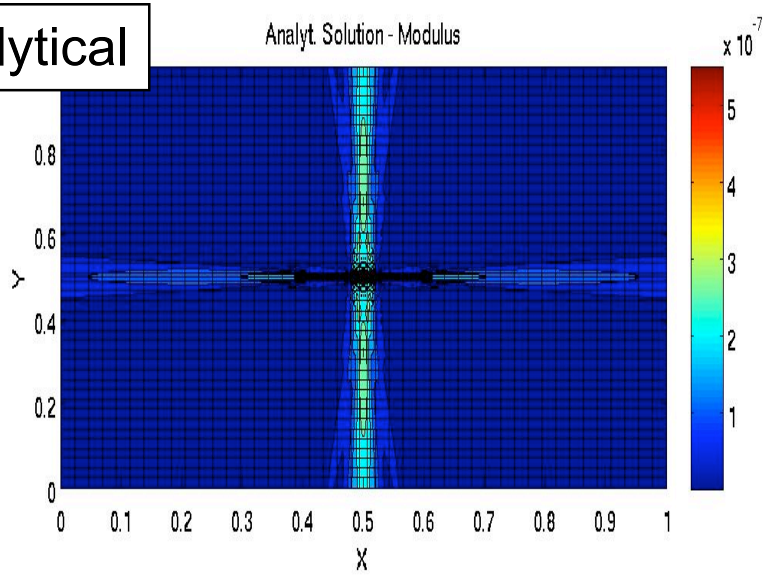
Solution $(1000\lambda)^2$

- 35.6 Gbyte memory
- 25min. (8 processors)
- Relative Error < 1.5%
- Standard FEM not applicable

UWVF

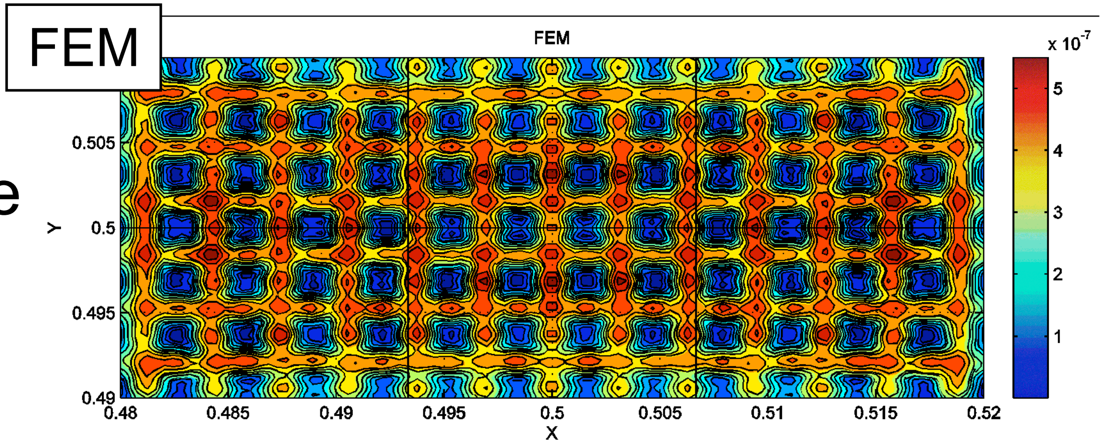


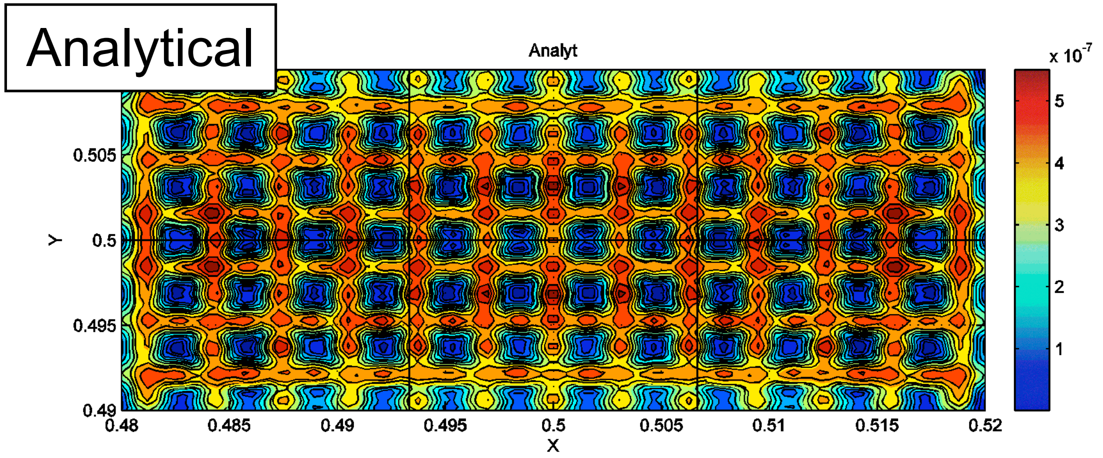
Analytical



Accuracy in the Source Region

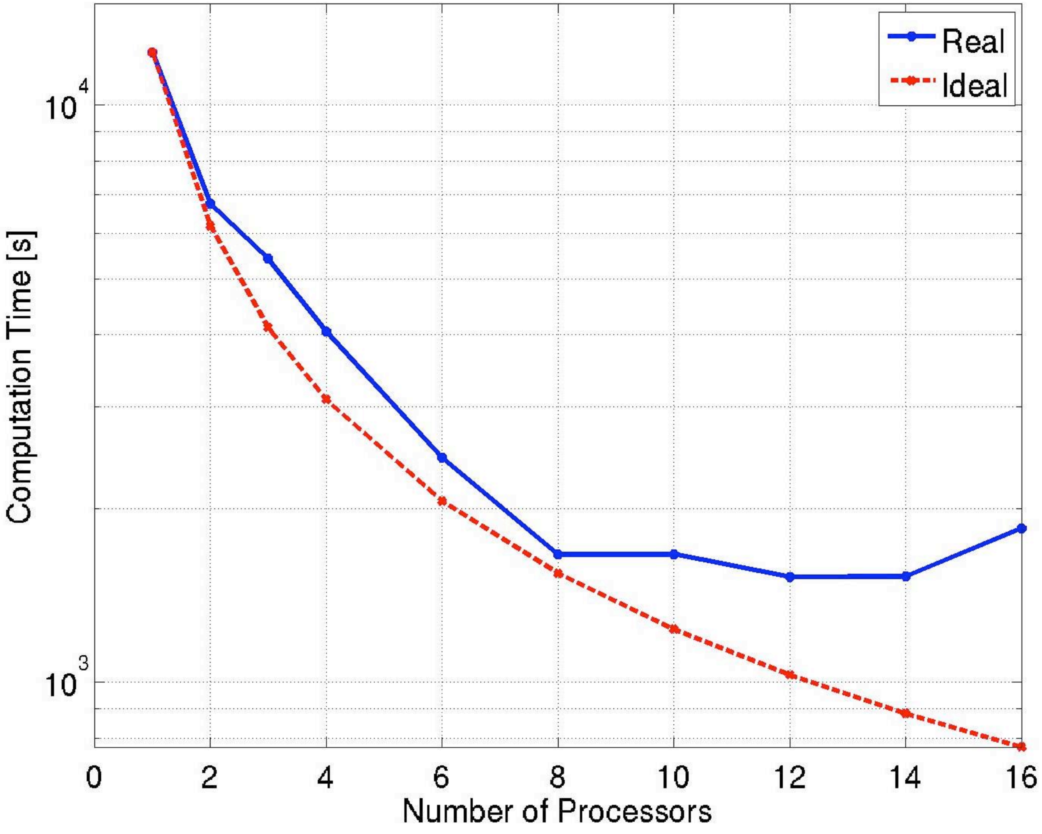
- Standard FEM for active region (spont. Emission sources)
- Typically small for OE devices
- Relative Error < 1.5%





Performance 1: Parallelization

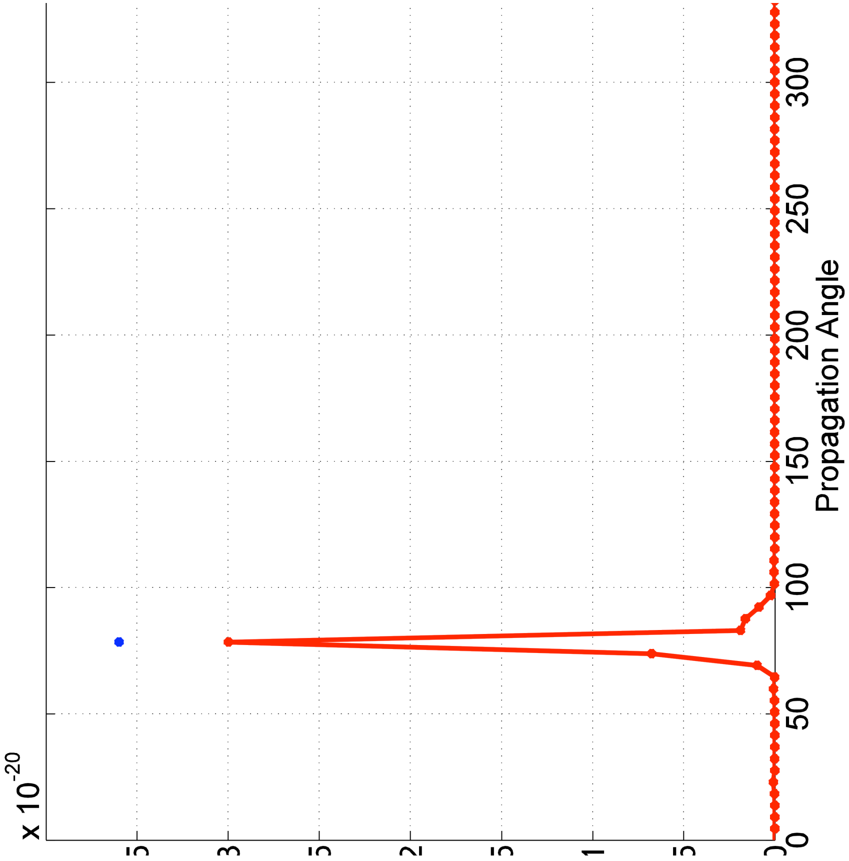
- PETSc Solver*: computation time ~ 1/n up to 8 processors.



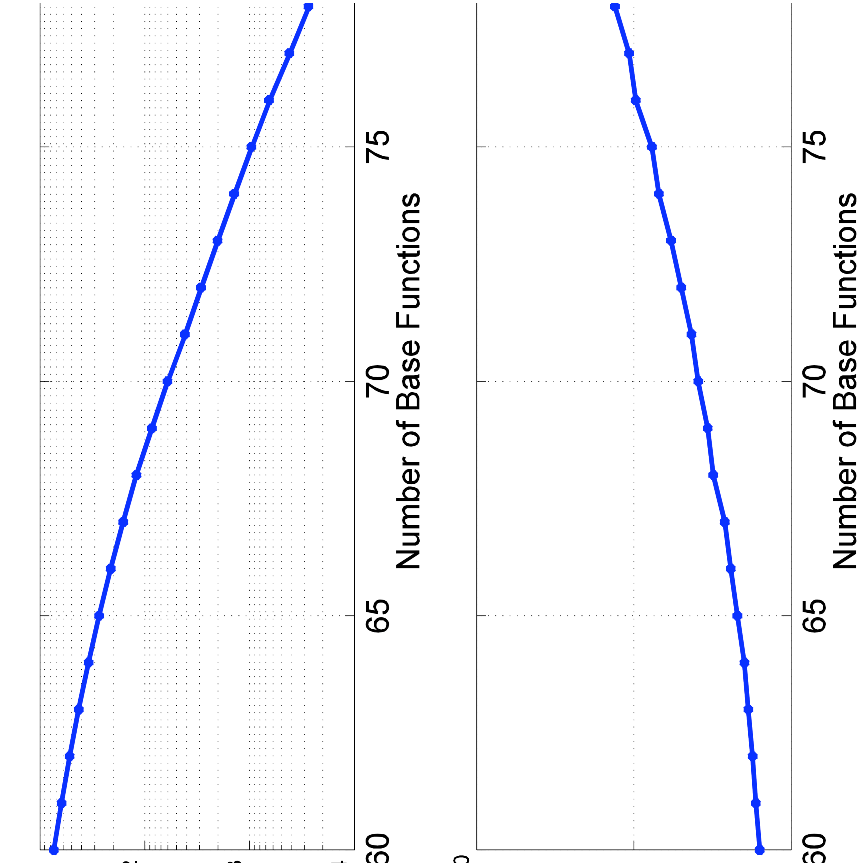
*: www.mcs.anl.gov/petsc

Performance 2: Information Reduction

- Accuracy of solution:
  - Discretization
  - #Angles for base function
- In many cases: only one dominant direction of propagation
- Memory reduction from 36GB to 17GB with same rel. error for $(1000\lambda)^2$ example.
- A priori or a posteriori

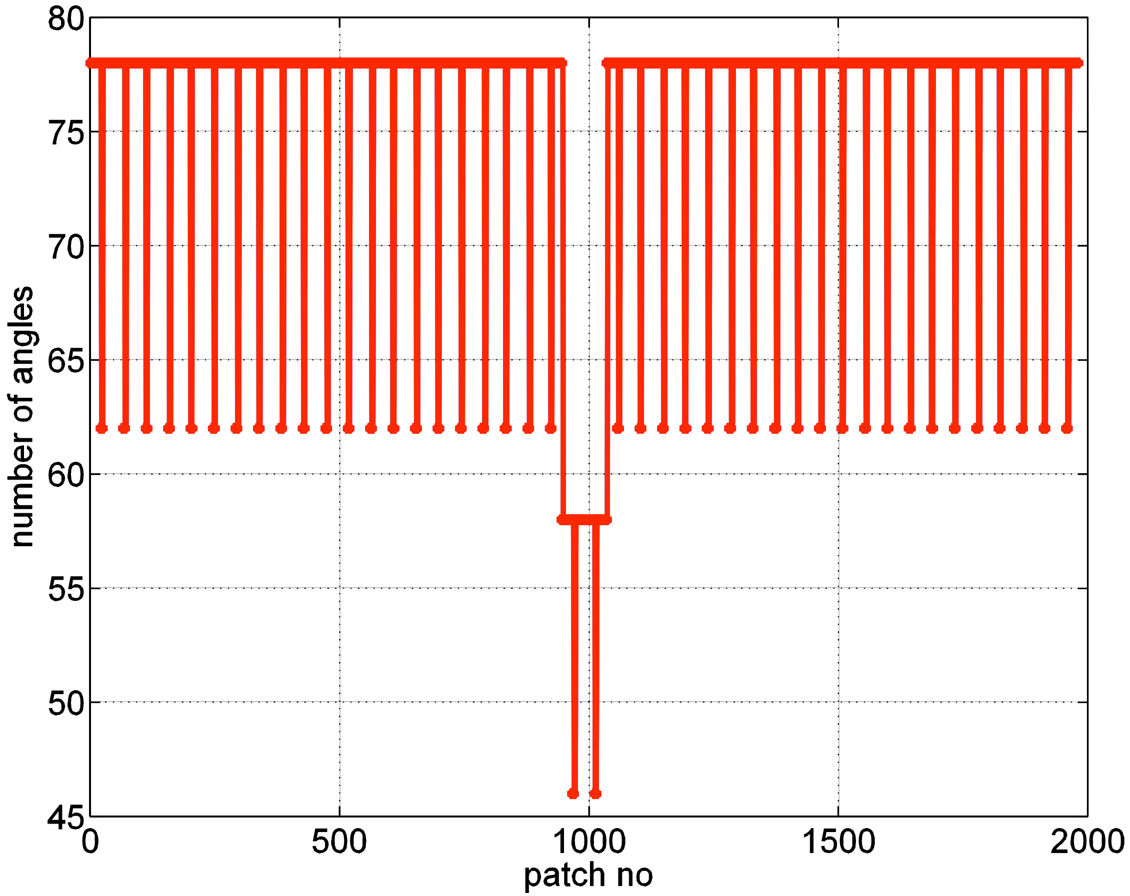


Known Issue of UWVF—Matrix Condition



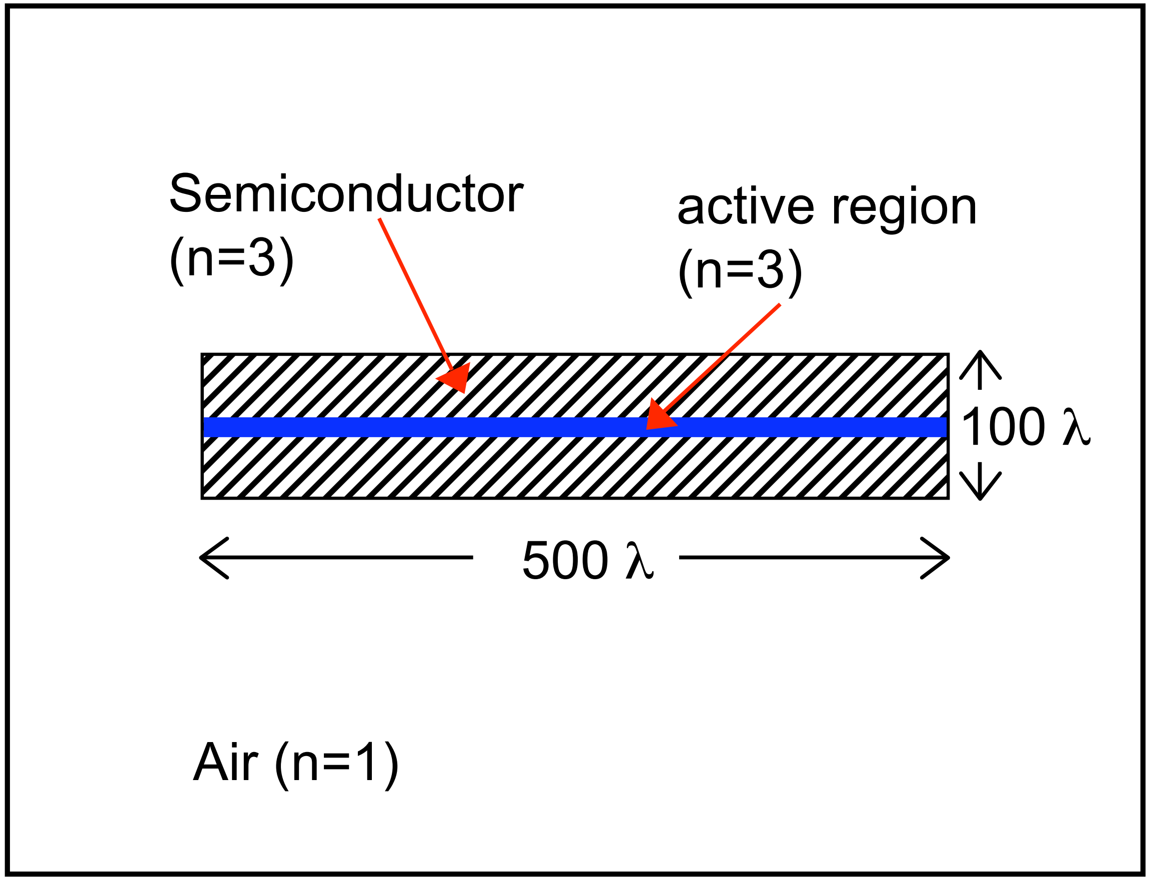
With increasing accuracy the matrix condition also increases.

Strategy to Control Matrix Condition



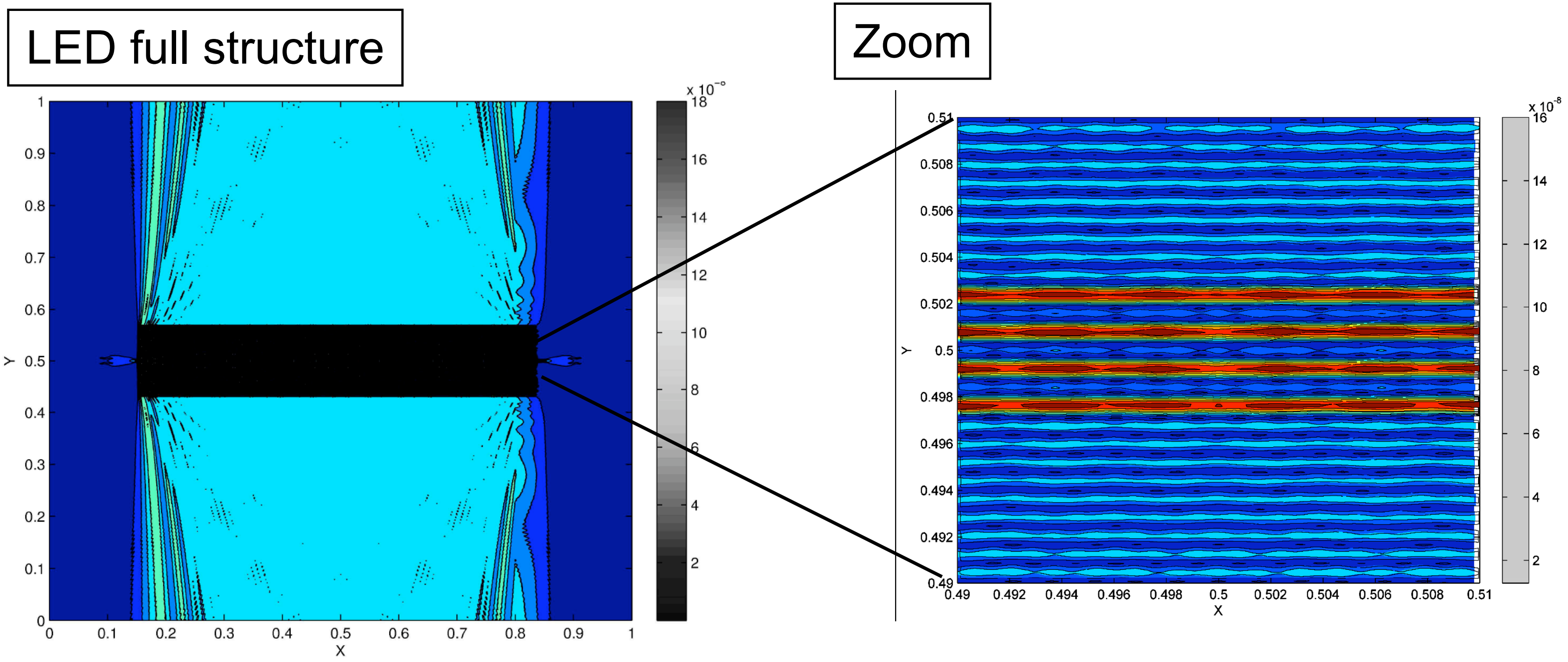
Dynamically adjust the number of base functions on each patch.

Simulation Example: ‘LED’ Simulation (I)



LED-like structure with large active region emitting into free space.

Extended Features: LED Simulation (II)

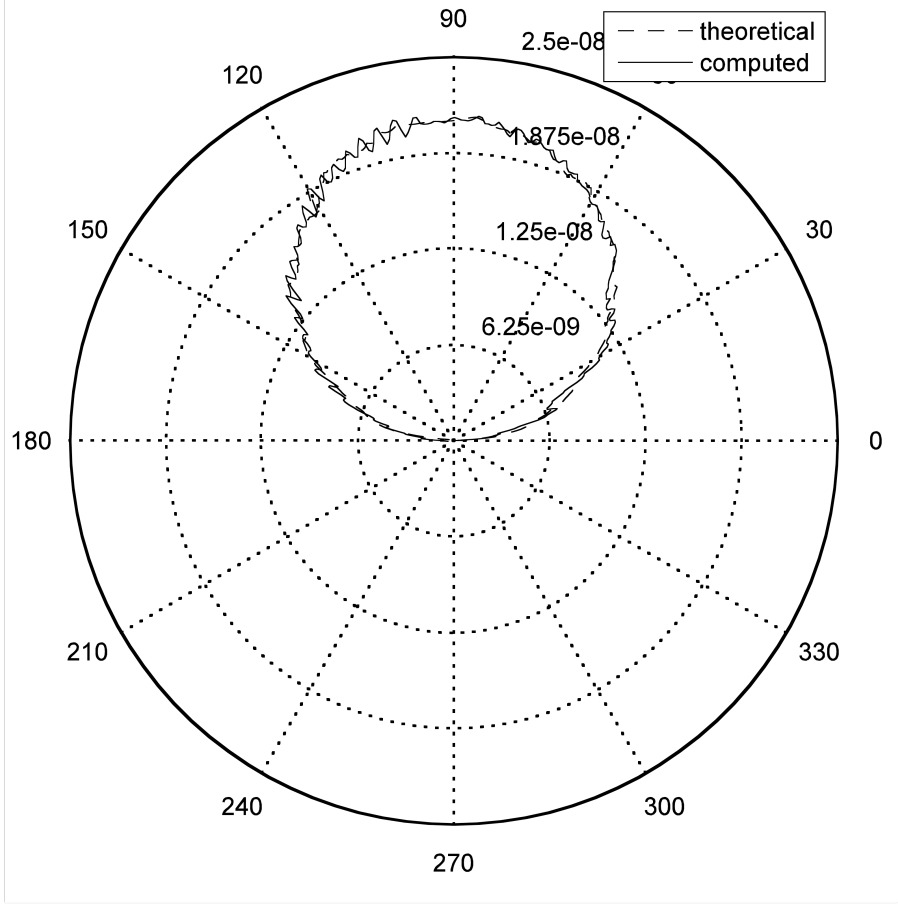


LED full structure

Zoom

- Inside semiconductor: standing wave pattern, waveguide effects.

Extended Features: LED Simulation (III)



Computed and predicted radiation pattern match very well.

Conclusion and Outlook

- The UWVF as efficient strategy for solving the inhomogeneous Helmholtz equation on ‘optically large’ domains
- Two independent ways to reduce computation time
  - Parallelization
  - Information reduction
- Formalism applicable to LED-like structures
- Outlook: transition to 3-D domains, vectorial electromagnetics