Scalable Simulation of Fiber Laser Model with DPG

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Minimum Residual and Least-Squares Finite Element Methods (MINRES/LS-5)

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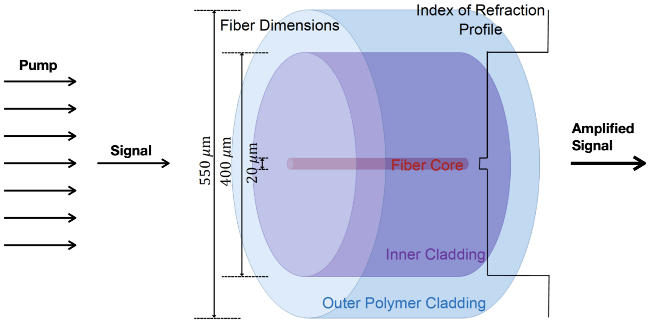
The University of Texas at Austin
Oden Institute for Computational Engineering and Sciences

Outline

Active Gain Fiber Amplifiers



Benefits:

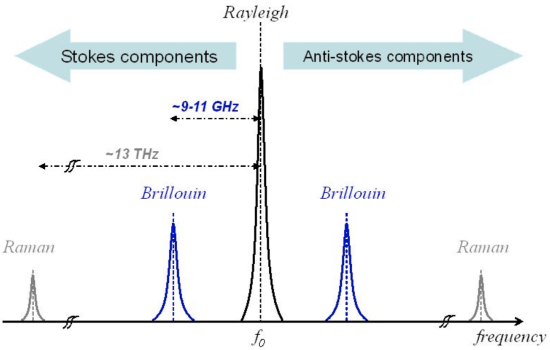
- Efficient
- Coherent output (beam combinable)
- Spatially compact

Weakly-guiding, continuous-wave, step-index fiber amplifier schematic[1]

[1] J. Grosek. "Coupled mode theory fiber amplifier model". Technical Report, AFRL. 2018

Motivation

- (Combinable) Power scaling in single-mode continuous-wave optical fiber amplifiers limited by onset of nonlinear effects at high optical intensities including:
  - **Stimulated Brillouin Scattering (SBS)** – Acoustic scattering of field by medium
  - **Stimulated Raman Scattering (SRS)** – Optical scattering of field by medium



Spontaneous scattering[2]

[2] W. Zou, X. Long, and J. Chen. "Brillouin scattering in optical fibers and its application to distributed sensors". In: *Advances in Optical Fiber Technology: Fundamental Optical Phenomena and Applications* (2015)

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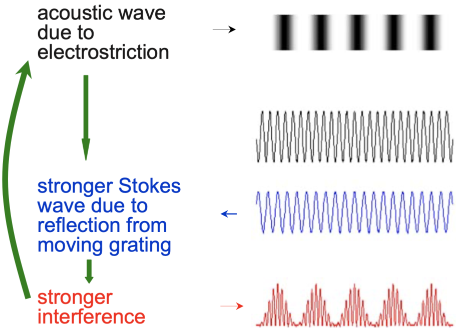
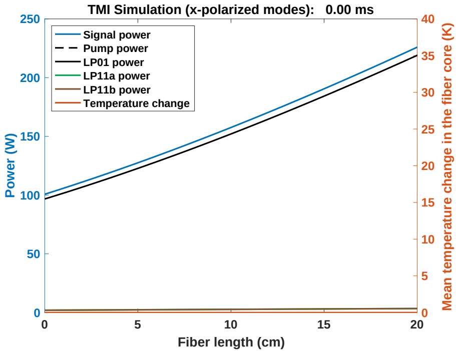


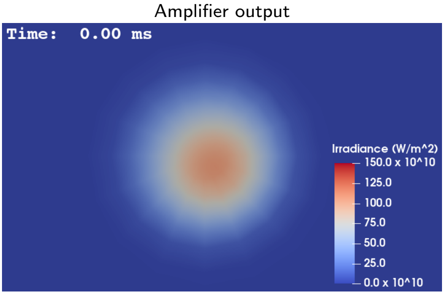
Stimulated Brillouin scattering[2]

[2] A. Kobyakov, M. Sauer, and D. Chowdhury. "Stimulated Brillouin scattering in optical fibers". In: *Advances in optics and photonics* 2.1 (2010), pp. 1–59

Motivation

- Large mode-area (LMA) fibers
  - Reduce optical intensity by increasing core size
  - Permit propagation of high-order modes
  - Susceptible to **transverse mode instability (TMI)** – Interference of modes causes unstable exchange of energy, severely degrading coherence

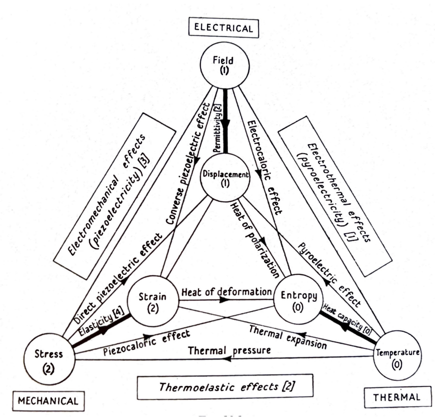




TMI simulation in a 20 cm long fiber using the vectorial Maxwell envelope model (2 kW pump)[3]

[3] Results from ongoing collaboration with S. Henneking (not yet published)

Motivation



Physical coupling effects in optical materials[4]

- Nonlinear effects caused by interaction of physical phenomena
- Phenomena span multiple timescales (optical >> elastic >> thermal)
- Simplified models often fail to predict high-power operation

Our approach:

- High-fidelity models
- Scalable computation

[4] J. F. Nye et al. *Physical properties of crystals: their representation by tensors and matrices.* Oxford University Press, 1985

Outline

Fiber Model

Maxwell Equations:

$$\nabla \times \boldsymbol{\mathcal{E}} = -\frac{\partial \boldsymbol{\mathcal{B}}}{\partial t} \qquad \nabla \cdot \boldsymbol{\mathcal{D}} = \rho_f$$

$$\nabla \times \boldsymbol{\mathcal{H}} = J_f + \frac{\partial \boldsymbol{\mathcal{D}}}{\partial t} \qquad \nabla \cdot \boldsymbol{\mathcal{B}} = 0$$

Constitutive Relations:

$$\boldsymbol{\mathcal{B}} = \mu_0 \boldsymbol{\mathcal{H}} + \boldsymbol{\mathcal{I}}$$

$$\boldsymbol{\mathcal{D}} = \epsilon_0 \boldsymbol{\mathcal{E}} + \boldsymbol{\mathcal{P}}$$

Symbol	Description
$\boldsymbol{\mathcal{E}}$	Electric field
$\boldsymbol{\mathcal{H}}$	Magnetic field
$\boldsymbol{\mathcal{D}}$	Electric flux density
$\boldsymbol{\mathcal{B}}$	Magnetic flux density
ϵ_0	Electric permittivity (vacuum)
μ_0	Magnetic permeability (vacuum)
J_f	(Free) Current density
ρ_f	(Free) Charge density
$\boldsymbol{\mathcal{P}}$	Induced electric polarization
$\boldsymbol{\mathcal{I}}$	Induced magnetic polarization

In silica glass:

- Magnetization $\boldsymbol{\mathcal{I}}$ is negligible
- Polarization $\boldsymbol{\mathcal{P}}$ is expanded in terms of susceptibilities χ^i as

$$\boldsymbol{\mathcal{P}} = \epsilon_0 \left(\chi^{(1)} \cdot \boldsymbol{\mathcal{E}} + \chi^{(2)} : \boldsymbol{\mathcal{E}} \otimes \boldsymbol{\mathcal{E}} + \chi^{(3)} \vdots \boldsymbol{\mathcal{E}} \otimes \boldsymbol{\mathcal{E}} \otimes \boldsymbol{\mathcal{E}} + \dots \right)$$

- Linearizing high-order susceptibilities, define relative permittivity $\boldsymbol{\varepsilon}_r = I + \chi^{(1)}$

Fiber Model

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In silica glass:

$$\boxed{\begin{array}{ll} \nabla \times \boldsymbol{\mathcal{E}} = -\mu_0 \dfrac{\partial \boldsymbol{\mathcal{H}}}{\partial t} & \nabla \cdot (\boldsymbol{\varepsilon}_r \boldsymbol{\mathcal{E}}) = 0 \\ \nabla \times \boldsymbol{\mathcal{H}} = \epsilon_0 \dfrac{\partial \boldsymbol{\varepsilon}_r \boldsymbol{\mathcal{E}}}{\partial t} & \nabla \cdot \boldsymbol{\mathcal{H}} = 0 \end{array}}$$

- **Time-Harmonic Maxwell Model**

  Making the time-harmonic ansatz:

$$\boldsymbol{\mathcal{E}}(x,y,z,t) = \Re\{\mathbf{E}(x,y,z)e^{i\omega t}\} \qquad \boldsymbol{\mathcal{H}}(x,y,z,t) = \Re\{\mathbf{H}(x,y,z)e^{i\omega t}\}$$

  the Maxwell model reduces to the time-harmonic Maxwell model:

$$\begin{cases} \nabla \times \mathbf{E} + i\omega\mu_0 \mathbf{H} = \mathbf{0} \\ \nabla \times \mathbf{H} - i\omega\epsilon_0 \boldsymbol{\varepsilon}_r \mathbf{E} = \mathbf{0} \end{cases} \tag{1}$$

- **Vectorial Envelope Maxwell Model**

  We can instead solve for an envelope of the field by making the ansatz

$$\mathbf{E}(x,y,z) = \mathsf{E}(x,y,z)e^{-ikz} \qquad \mathbf{H}(x,y,z) = \mathsf{H}(x,y,z)e^{-ikz}.$$

  Time-harmonic Maxwell system (1) becomes

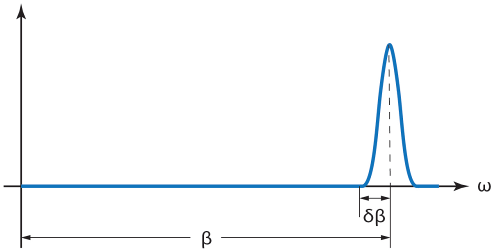
$$\begin{cases} \nabla \times \mathsf{E} - ik\mathbf{e_z} \times \mathsf{E} + i\omega\mu_0 \mathsf{H} = \mathbf{0} \\ \nabla \times \mathsf{H} - ik\mathbf{e_z} \times \mathsf{H} - i\omega\epsilon_0 \boldsymbol{\varepsilon}_r \mathsf{E} = \mathbf{0} \end{cases}$$

Vectorial Envelope Maxwell System

- **Vectorial Envelope Maxwell Model**

$$\begin{cases} \nabla \times \mathsf{E} - ik\mathbf{e_z} \times \mathsf{E} + i\omega\mu_0\mathsf{H} = \mathbf{0} \\ \nabla \times \mathsf{H} - ik\mathbf{e_z} \times \mathsf{H} - i\omega\epsilon_0\boldsymbol{\varepsilon}_r\mathsf{E} = \mathbf{0} \end{cases}$$

- Adds only additional linear terms; wave ansatz vanishes
- Suppose longitudinal frequency distributed as:



Choosing $k = \beta$ reduces longitudinal discretization requirements from $\mathcal{O}(\beta)$ to $\mathcal{O}(\delta\beta)$

We employ an ultraweak Discontinuous Petrov-Galerkin (DPG) discretization[5],

$$\left\{\begin{array}{lll} \mathsf{E},\mathsf{H} \in \left(L^2(\Omega_h)\right)^3, \;\; \hat{\mathsf{E}} \in \hat{U}_1, \;\; \hat{\mathsf{H}} \in \hat{U}_2 & & \\ (\mathsf{E}, \nabla_h \times \mathsf{F}) + \langle \mathbf{n} \times \hat{\mathsf{E}}, \mathsf{F}\rangle_{\Gamma_h} - ik(\mathbf{e_z} \times \mathsf{E}, \mathsf{F}) + i\omega\mu_0(\mathsf{H},\mathsf{F}) & = 0, & \mathsf{F} \in H(\mathsf{curl}, \Omega_h), \\ (\mathsf{H}, \nabla_h \times \mathsf{G}) + \langle \mathbf{n} \times \hat{\mathsf{H}}, \mathsf{G}\rangle_{\Gamma_h} - ik(\mathbf{e_z} \times \mathsf{H}, \mathsf{G}) - i\omega\epsilon_0(\boldsymbol{\varepsilon}_r \mathsf{E},\mathsf{G}) & = 0, & \mathsf{G} \in H(\mathsf{curl}, \Omega_h), \end{array}\right.$$

where trace spaces are defined

$$\hat{U}_1 := \left\{ \hat{\mathbf{u}} \in H^{-1/2}(\mathsf{curl}, \Gamma_h) \,:\, \mathbf{n} \times \hat{\mathbf{u}} = \mathbf{n} \times \mathsf{E}_0 \;\; \text{on} \;\; \Gamma_1 \right\},$$
$$\hat{U}_2 := \left\{ \hat{\mathbf{u}} \in H^{-1/2}(\mathsf{curl}, \Gamma_h) \,:\, \mathbf{n} \times \hat{\mathbf{u}} = \mathbf{n} \times \mathsf{E}_0 \;\; \text{on} \;\; \Gamma_2 \right\},$$

and discretized element-wise

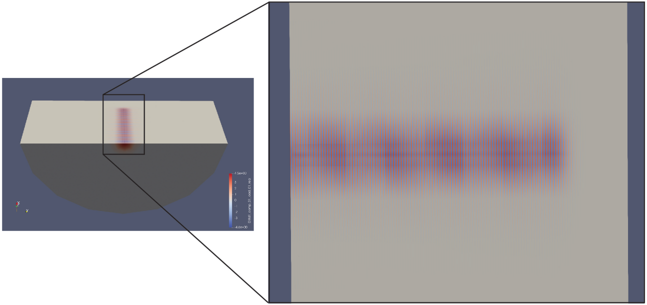
$$H^{-1/2}(\mathsf{curl}, \Gamma_h) := \left\{ \hat{\mathbf{u}} \in \prod_{K \in \Omega_h} H^{-1/2}(\mathsf{curl}, \partial K) : \exists \mathbf{u} \in H(\mathsf{curl}, \Omega) : \gamma_t\left(\mathbf{u}_K\right) = \hat{\mathbf{u}} \right\}.$$

We employ a weighted adjoint graph test norm:

$$||\mathfrak{v}||_V^2 := ||A^*\mathfrak{v}||^2 + \alpha^2 ||\mathfrak{v}||^2$$

[5] S. Henneking. “A scalable hp-adaptive finite element software with applications in fiber optics”. PhD thesis. The University of Texas at Austin, 2021

Example – Time Harmonic Maxwell Fiber Model

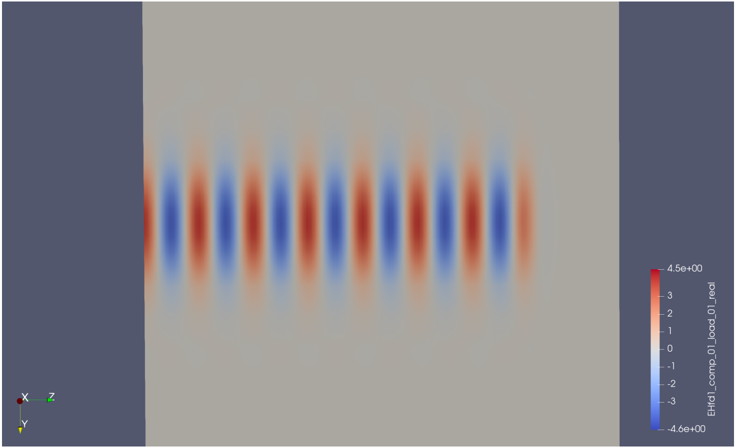


Real part of $\mathbf{E}_x$ (signal), 128 optical wavelengths

- UW-DPG discretization
- $\lambda = 1\,064$ nm
- $n_1 = 1.4512$
- $n_2 = 1.45$
- $r_{\text{core}} = 12.7\,\mu$m
- $r_{\text{core}} = 127\,\mu$m

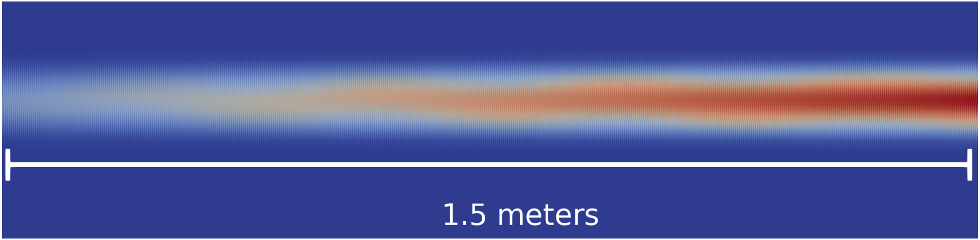
Example – Vectorial Envelope Maxwell Fiber Model

- Vectorial envelope Maxwell model with $k = 80$
- Fundamental mode has propagation constant $\beta \approx 86$
- Envelope has longitudinal wavenumber $\approx 86 - 80 = 6$



Real part of E$_x$ (signal)

Vectorial Envelope Fiber Model – Resolving All Length Scales



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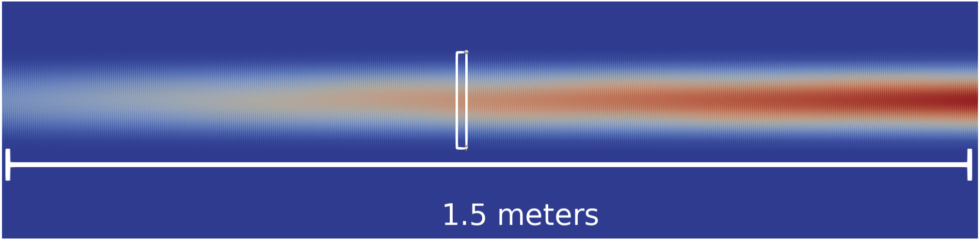

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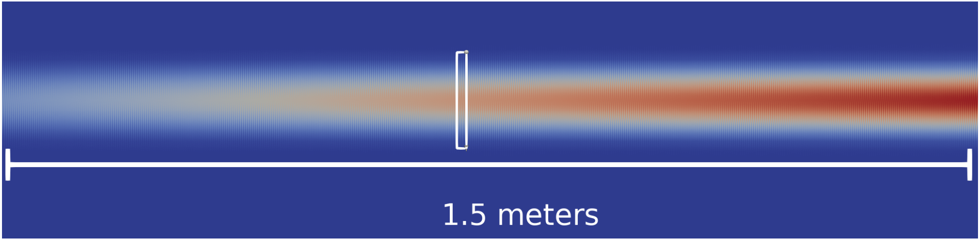

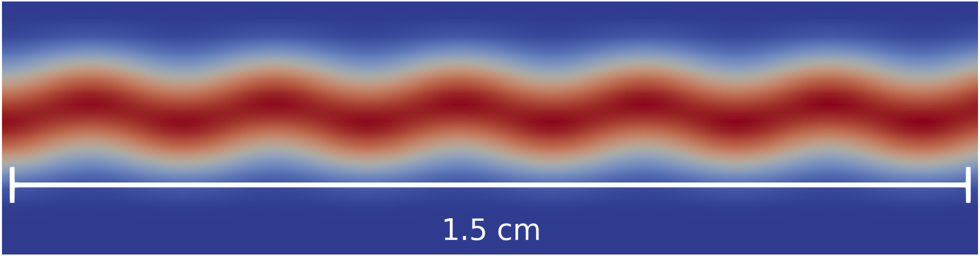

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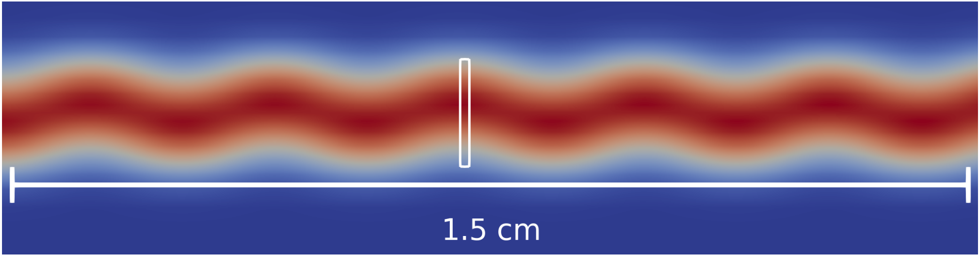

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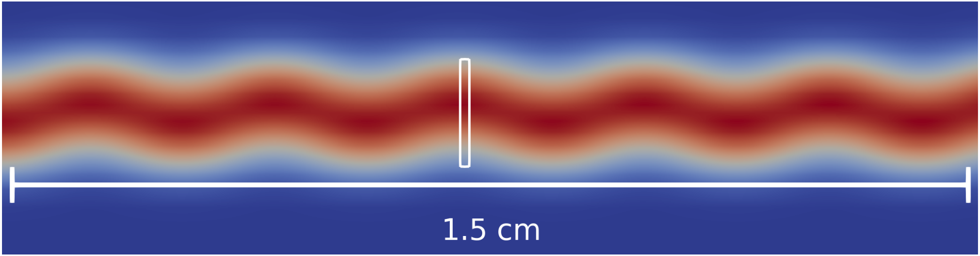

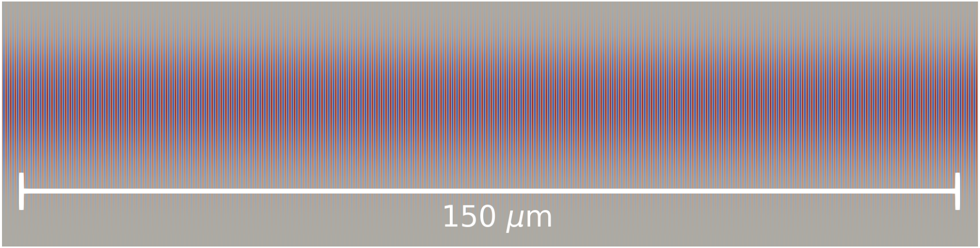

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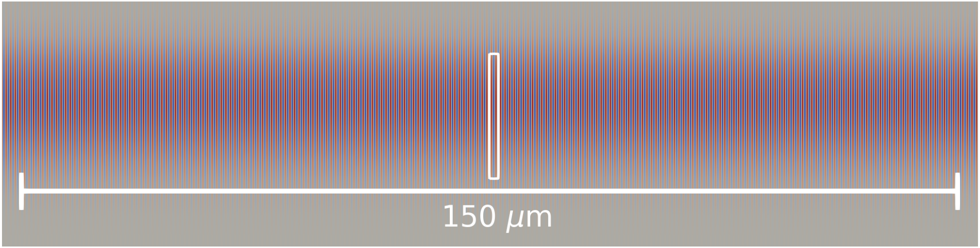

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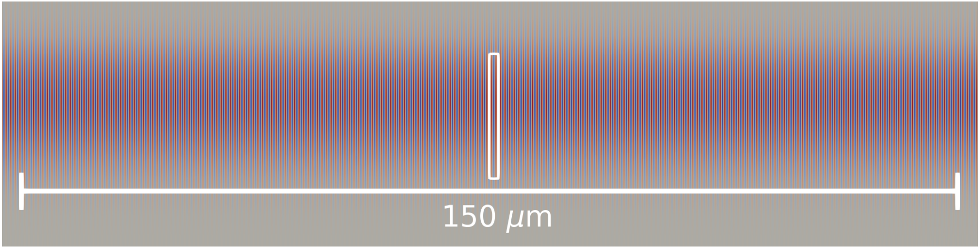
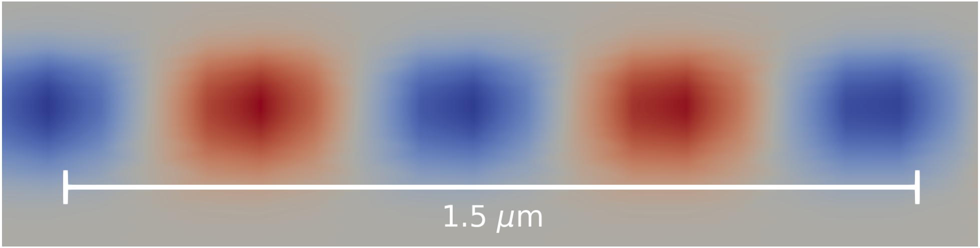
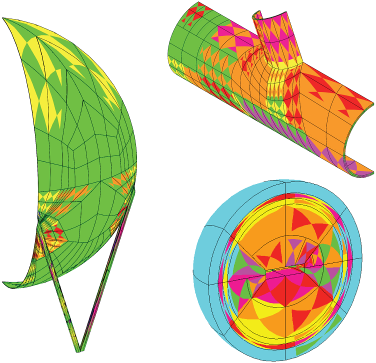




Outline



Scalable finite element software supporting:

- Elements of all shapes
- Isotropic/anisotropic hp refinements
- Exact-sequence energy spaces
- Conforming discretization of traces
- Interfaces for PETSc, Zoltan, MUMPS, etc.
- Advanced solvers

GitHub repository:

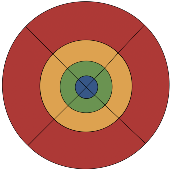
- hp3D software: https://github.com/Oden-EAG/hp3d

Preprint documents:

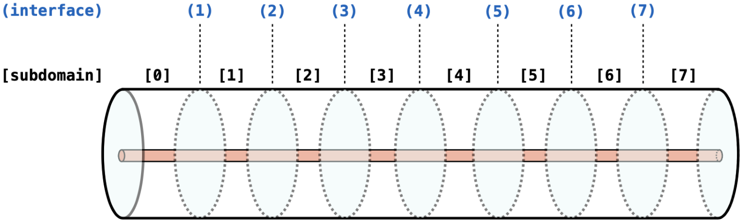
- hp3D user manual: https://github.com/Oden-EAG/hp3d_user_guide
- hp Book Vol. 3: *Computing with hp Finite Elements III. Parallel hp3D Code* (upon request)

Nested Dissection Solver

- Quasi-1D geometry enables $\mathcal{O}(N \log N)$ for longitudinal refinement
- $\mathcal{O}(N^2)$ for transverse refinement/general geometries
- Need different approach for problems including:
  - Complex cross-section fibers
  - Bending of optical fibers



Mesh cross-section



Nested dissection interface schematic

DPG Mulitgrid Solver

The DPG-MG solver[6] leverages three primary benefits of the DPG methodology:

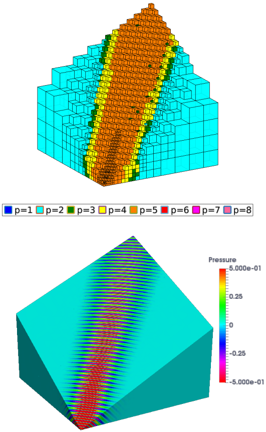
- Hermitian positive definite discrete systems $\rightarrow$ Multigrid preconditioned conjugate gradient
- Preasymptotic (mesh-independent) stability $\rightarrow$ Coarse initial meshes
- Error indicator $\rightarrow$ hp-adaptivity

Solution on each mesh needed only to sufficient accuracy to define the next mesh; optimal meshes produced with relatively few iterations and at little cost

[6] S. Petrides and L. Demkowicz. "An adaptive multigrid solver for DPG methods with applications in linear acoustics and electromagnetics". In: *Comput. Math. Appl.* 87 (2021), pp. 12–26

Distributed DPG Multigrid Solver

- Multilevel preconditioner for general DPG systems[7]
- Leverages hp-adaptive multilevel hierarchy
- Supports:
  - Meshes of all element shapes
  - Isotropic/anisotropic refinements
- Hybrid MPI/OpenMP scalable implementation
- Dynamic repartitioning and load balancing



hp-adaptive mesh (top) and solution (bottom) to 3D linear acoustic problem produced by DPG-MG solver.

[7] Discretized with exact-sequence energy spaces

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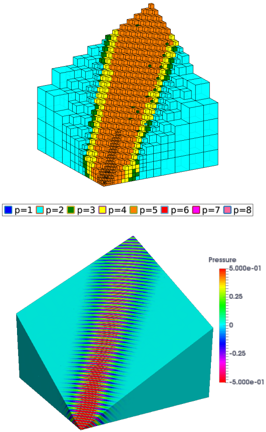
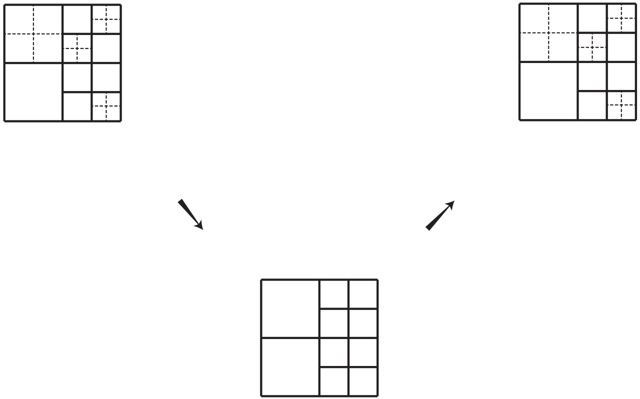


hp-adaptive mesh (top) and solution (bottom) to 3D linear acoustic problem produced by DPG-MG solver.

[7] Discretized with exact-sequence energy spaces

DPG-MG – V-cycle

- The DPG-MG solver operates on interface degrees-of-freedom (DoFs); new interface DoFs on h-refined elements don't have any natural coarse-grid representatives



DPG-MG – V-cycle

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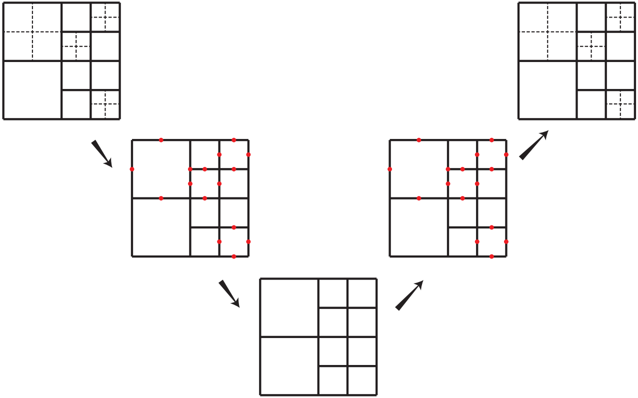
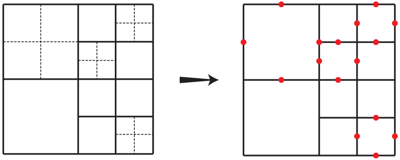
- **Macro** grid defined by statically condensing interface unknowns with no coarse representative



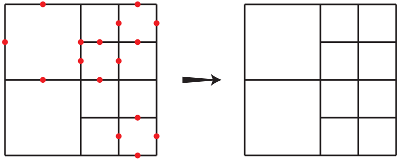
DPG-MG – Prolongation

Two stage prolongation:

1. **Fine** to **Macro** – Static condensation



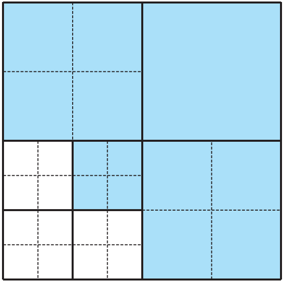
2. **Macro** to **Coarse** – Constrained approximation[8]



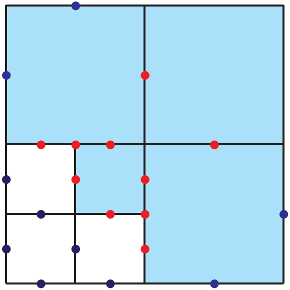
[8] L. Demkowicz. *Computing with hp Finite Elements. I. One- and Two-Dimensional Elliptic and Maxwell Problems.* Chapman & Hall/CRC Press, Taylor and Francis, 2006

DPG-MG – Smoothing

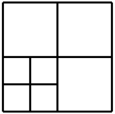
- Additive Schwarz (overlapping block Jacobi) smoother
- Smoothing blocks correspond to macro grid DoFs supported on coarse grid vertex patches



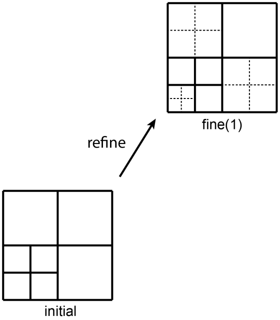
$\Rightarrow$



DPG-MG – Workflow


Initial

DPG-MG – Workflow



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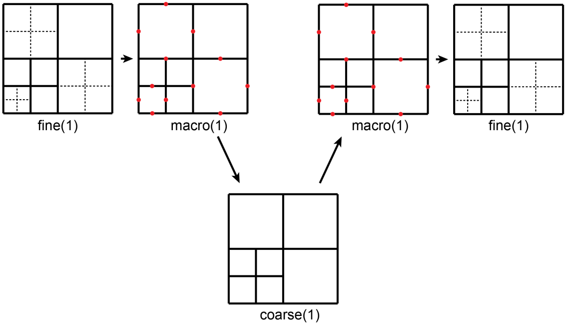

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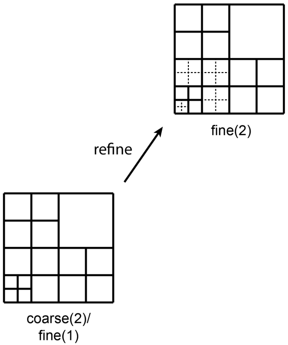

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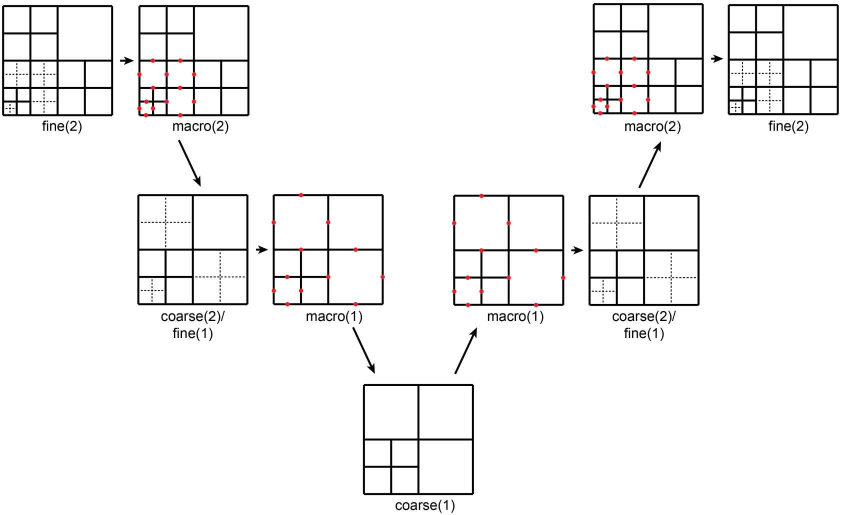
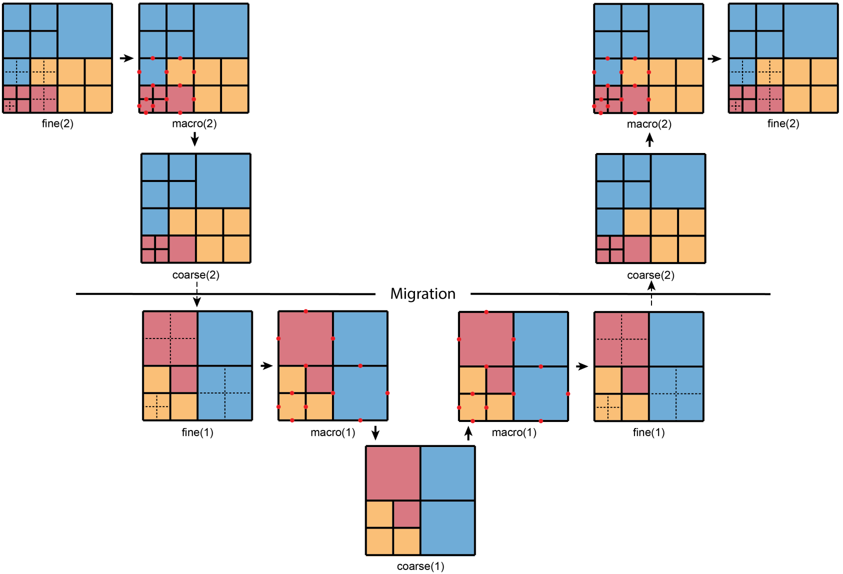


DPG-MG – Dynamic Repartitioning



Load Balancing

- **Macro assembly** and **PCG iteration** dominate computational cost
- These operations scale differently under h and p refinements
- In hp-adaptive scheme, both operations need to be balanced

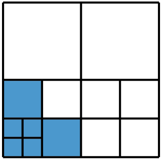
Table: Complexity of dominating operations in DPG-MG solver ($\mathcal{O}(\cdot)$)

	p-refinement	h-refinement
Macro Assembly		
Elem. Assembly	p^9	h^{-3}
Condense Macro	p^6	h^{-6}
PCG Iteration		
Smooth	p^4	h^{-6}
Matrix mult.	p^4	h^{-3}

Load Balancing

Two-step partitioning to balance cost of macro assembly and PCG iteration:

1. Repartition fine(i) to define coarse($i+1$)
   - Weighted graph-based partitioner
   - Weights account for macro-grid assembly only



Load Balancing

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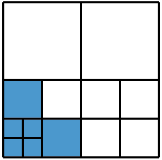
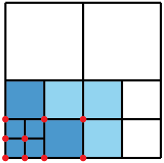


2. Partition smoothing patches
   - Patches in a single subdomain claimed
   - Patches shared by multiple subdomains partitioned (weighted partition balances smoothing cost)
   - Ghost elements appended to complete patches



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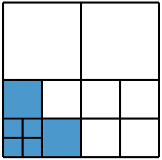

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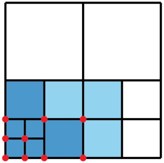
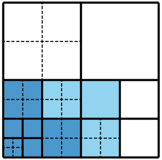


3. Execute refinements to define fine$(i+1)$



Example – Acoustic Beam

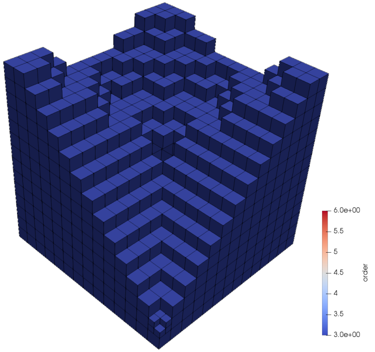
Ultraweak Acoustics:

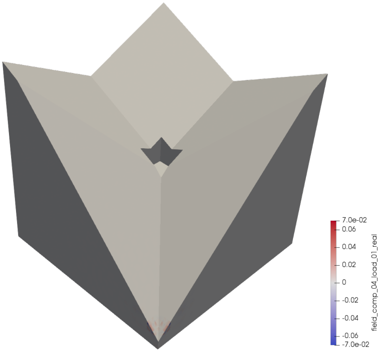
$$\begin{cases} (p,u) \in L^2(\Omega) \times (L^2(\Omega))^d \\ (\hat{p},\hat{u}_n) \in H^{\frac{1}{2}}(\Gamma_h) \times H^{-\frac{1}{2}}(\Gamma_h) \\ i\omega(p,q) + (u,\nabla_h q) + \langle \hat{u}_n, q\rangle_{\Gamma_h} = \langle u_0, q\rangle_{\Gamma_u} \qquad q \in H^1(\Omega_h) : q = 0 \text{ on } \Gamma_p \\ i\omega(u,v) + (p,\mathrm{div}_h v) + \langle \hat{p}, v_n\rangle_{\Gamma_h} = \langle p_0, v_n\rangle_{\Gamma_p} \qquad v \in H(\mathrm{div},\Omega_h) : v_n = 0 \text{ on } \Gamma_u \end{cases}$$

- Boundary conditions:
  - Impedence exterior boundary; manufactured gaussian beam data
  - Hard (Dirichlet) interior boundary
- Initial mesh:
  - 2736 hexahedral elements
  - Order $p = 3$
  - ca. 420 000 degrees-of-freedom (DoFs)
- Refinements:
  - Dörfler marking strategy (refinement factor $= 0.5$)
  - h-refinements until 2 elements/wavelength; then p-refinements[9]

[9] J. Melenk and S. Sauter. "Wavenumber explicit convergence analysis for Galerkin discretizations of the Helmholtz equation". In: *SIAM J. Numer. Anal.* 49.3 (2011), pp. 1210–1243

Example – Adaptive solution

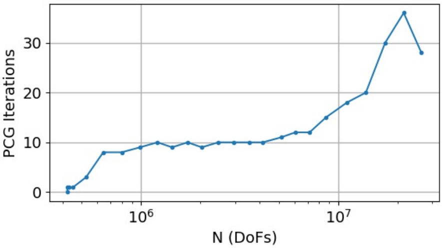




Cutaway of hp-adaptive mesh (left) and real part of acoustic pressure (right)

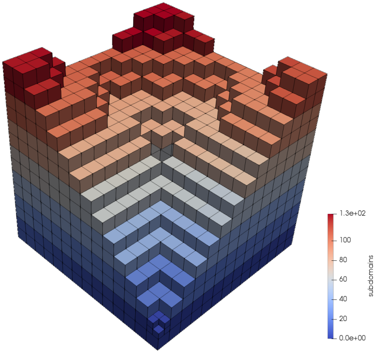
Example – PCG Iterations

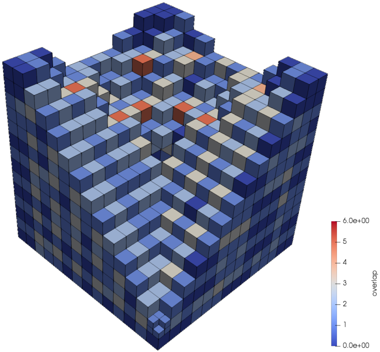
- Smoothing steps/level $= 10$
- Relaxation parameter $= 0.2$
- PCG iteration terminated when norm of relative discrete residual is smaller than 10^{-4}



Number of PGC iterations at each grid level

Example – Partition

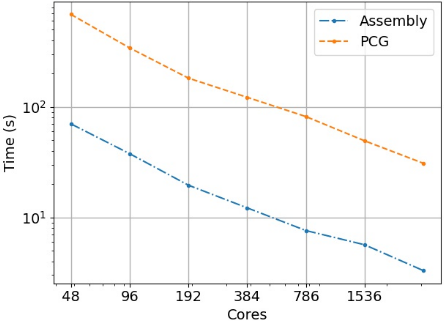


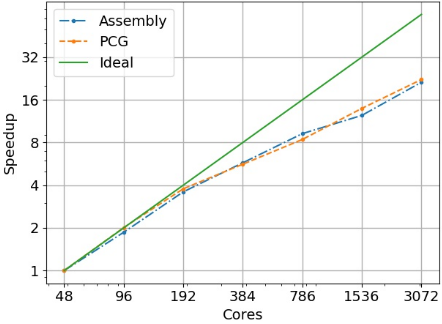


Cutaway illustrating mesh partition among 128 MPI processes (left), and redundant element computations due to ghosting (right)

Example – Strong Scaling

- Fine mesh: 20 adaptive refinements, 11 000 000 DoFs
- Resources:
  - Stampede2 – Texas Advanced Computing Center (TACC)
  - Intel Xeon Platinum 8160 (Skylake) processors; 12 cores / MPI process

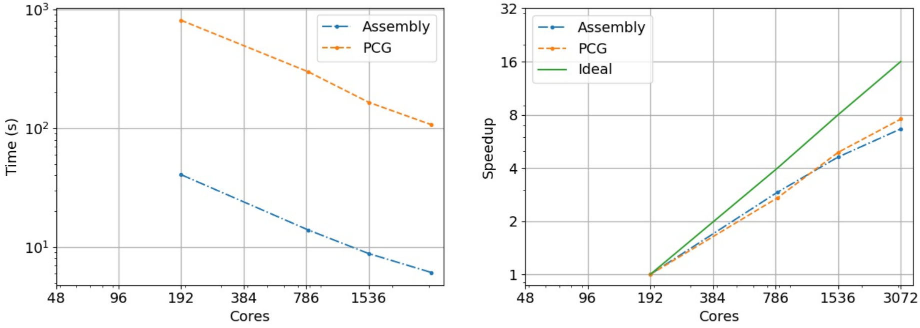




Strong scaling for ultraweak acoustic problem

Example – Strong Scaling

- Fine mesh: 25 adaptive refinements, 27 000 000 DoFs
- Resources:
  - Stampede2 – Texas Advanced Computing Center (TACC)
  - Intel Xeon Platinum 8160 (Skylake) processors; 12 cores / MPI process



Strong scaling for ultraweak acoustic problem

Ongoing and Future Work

Fiber model

- Simulation of loss and polarization-dependent nonlinearities in bent optical fibers
- Simulation of pulsed optical fiber lasers

Distributed DPG-MG solver

- Anisotropic refinements
- Block Gauss-Seidel smoothing
- Mixed precision

Open-source code and hp FE book volume III

- Open-sourcing of the hp3D codebase under a BSD-4 license.
- Publishing the third volume of the hp FE book series.[a,b]

[a] L. Demkowicz. *Computing with hp Finite Elements. I. One- and Two-Dimensional Elliptic and Maxwell Problems.* Chapman & Hall/CRC Press, Taylor and Francis, 2006

[b] L. Demkowicz et al. *Computing with hp Finite Elements. II. Frontiers: Three-Dimensional Elliptic and Maxwell Problems with Applications.* Chapman & Hall/CRC, 2007