Ph.D. Dissertation Defense

Integration of hp-Adaptivity with a Two Grid Solver: Applications to Electromagnetics.

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April 2, 2004

Computational and Applied Mathematics (CAM) Program

Institute for Computational Engineering and Sciences (ICES)
The University of Texas at Austin

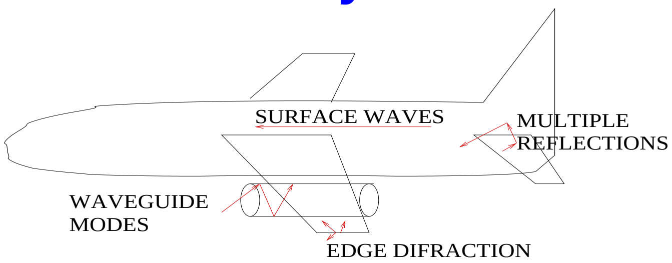
Supported by the Continuing Education Fellowship and a Teaching Assistantship from the University of Texas at Austin, and a U.S. Air Force Grant

OVERVIEW

1. Overview.
2. Motivation.
3. The Fully Automatic *hp*-Adaptive Strategy.
4. Summary of Previously Presented Work
   - A Two Grid Solver for 2D and 3D Electrostatics.
   - A Two Grid Solver for 2D Electrodynamics.
5. A Two Grid Solver for 3D Electrodynamics.
6. Accomplishments of the Dissertation.
7. Limitations and Future Work.
8. Conclusions.

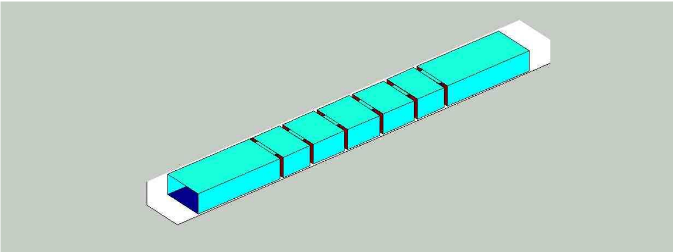
MOTIVATION

Radar Cross Section (RCS) Analysis



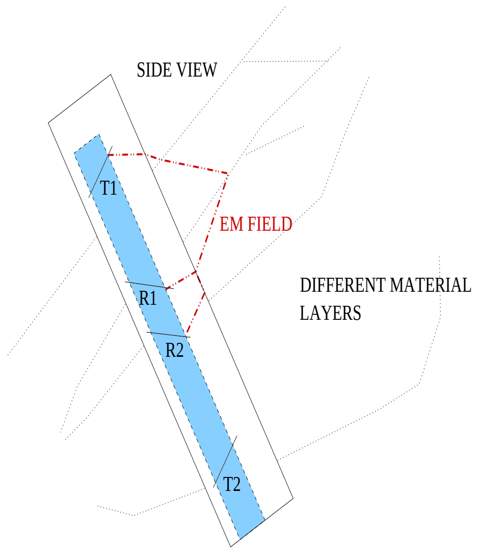
Goal: Determine the RCS of a plane.

Waveguide Design



Goal: Determine electric field intensity at the ports.

Modeling of a Logging While Drilling (LWD) electromagnetic measuring device



Goal: Determine EM field at the receiver antennas.

MAXWELL'S EQUATIONS (FREQUENCY DOMAIN)

Variational formulation

The reduced wave equation in Ω,

$$\nabla \times \left(\frac{1}{\mu} \nabla \times E \right) - (\omega^2 \epsilon - j\omega\sigma) E = -j\omega J^{imp} \,,$$

A variational formulation:

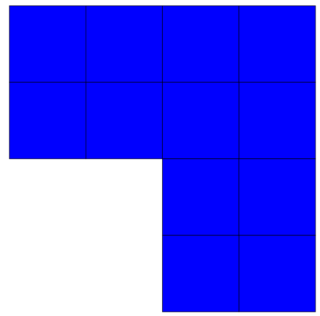
$$\begin{cases} \text{Find } \mathrm{E} \in H_D(\mathrm{curl};\Omega) \text{ such that} \\ \displaystyle\int_\Omega \frac{1}{\mu} (\nabla \times \mathrm{E}) \cdot (\nabla \times \bar{F}) dx - \int_\Omega (\omega^2 \epsilon - j\omega\sigma) E \cdot \bar{\mathrm{F}} dx = \\ \qquad -j\omega \left\{ \displaystyle\int_\Omega J^{imp} \cdot \bar{F} dx + \int_{\Gamma_2} J_S^{imp} \cdot \bar{F} dS \right\} \quad \text{for all } F \in H_D(\mathrm{curl};\Omega) \,. \end{cases}$$

A stabilized variational formulation (using *a Lagrange multiplier*):

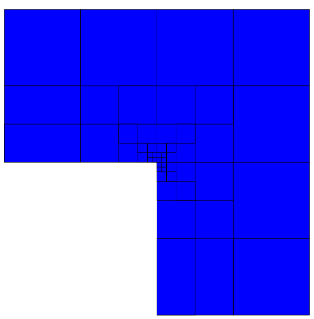
$$\begin{cases} \text{Find } E \in H_D(\mathrm{curl};\Omega), p \in H_D^1(\Omega) \text{ such that} \\ \displaystyle\int_\Omega \frac{1}{\mu} (\nabla \times E)(\nabla \times \bar{F}) dx - \int_\Omega (\omega^2 \epsilon - j\omega\sigma) E \cdot \bar{F} dx - \int_\Omega (\omega^2 \epsilon - j\omega\sigma) \nabla p \cdot \bar{F} dx = \\ \qquad -j\omega \left\{ \displaystyle\int_\Omega J^{imp} \cdot \bar{F} dx + \int_{\Gamma_2} J_S^{imp} \cdot \bar{F} dS \right\} \quad \forall F \in H_D(\mathrm{curl};\Omega) \\ \displaystyle -\int_\Omega (\omega\epsilon - j\sigma) E \cdot \nabla \bar{q} \, dx = -j \left\{ \int_\Omega J^{imp} \cdot \nabla \bar{q} \, dx + \int_{\Gamma_2} J_S^{imp} \cdot \nabla \bar{q} dS \right\} \quad \forall q \in H_D^1(\Omega) \,. \end{cases}$$

HP-FINITE ELEMENTS

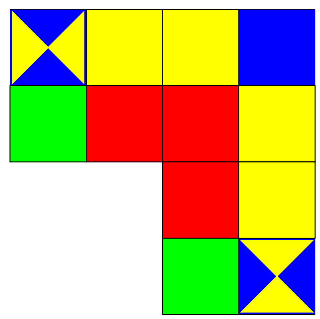
Different refinement strategies for finite elements:



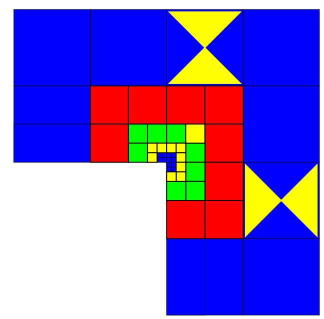
Given initial grid



***h*-refined grid**



***p*-refined grid**

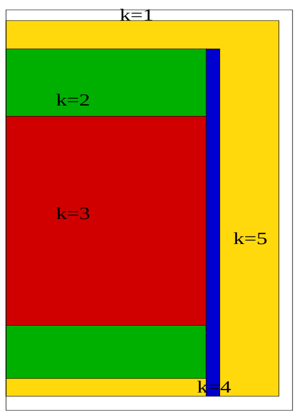


***hp*-refined grid**

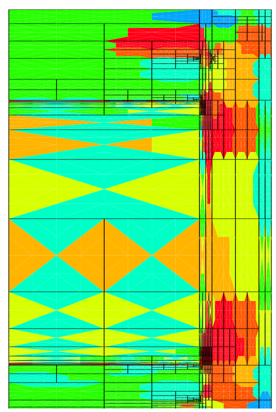
THE FULLY AUTOMATIC *HP*-ADAPTIVE STRATEGY

Convergence comparison: orthotropic heat conduction problem

Geometry



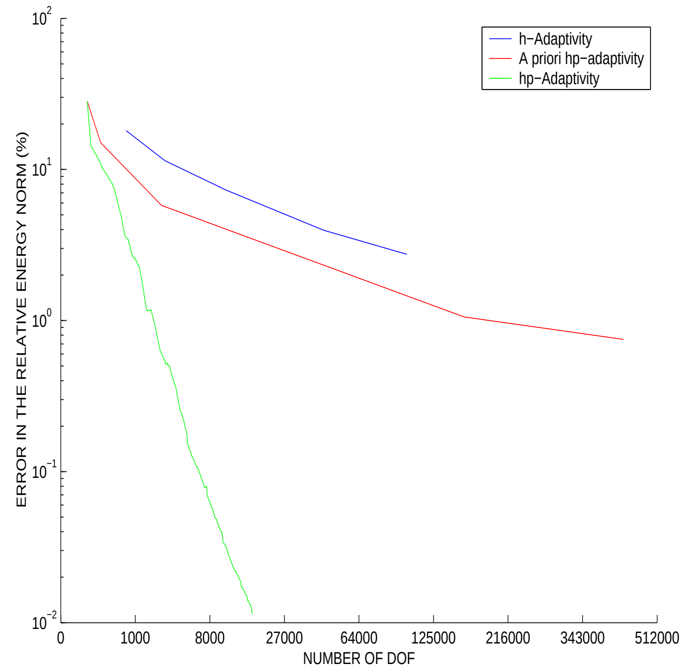
Final hp-grid



Equation: $\nabla(\mathrm{K}\nabla u) = f^{(k)}$

$$\mathrm{K} = \mathrm{K}^{(k)} = \begin{bmatrix} K_x^{(k)} & 0 \\ 0 & K_y^{(k)} \end{bmatrix}$$

$$K_x^{(k)} = (25,\ 7,\ 5,\ 0.2,\ 0.05)$$
$$K_y^{(k)} = (25,\ 0.8,\ 0.0001,\ 0.2,\ 0.05)$$

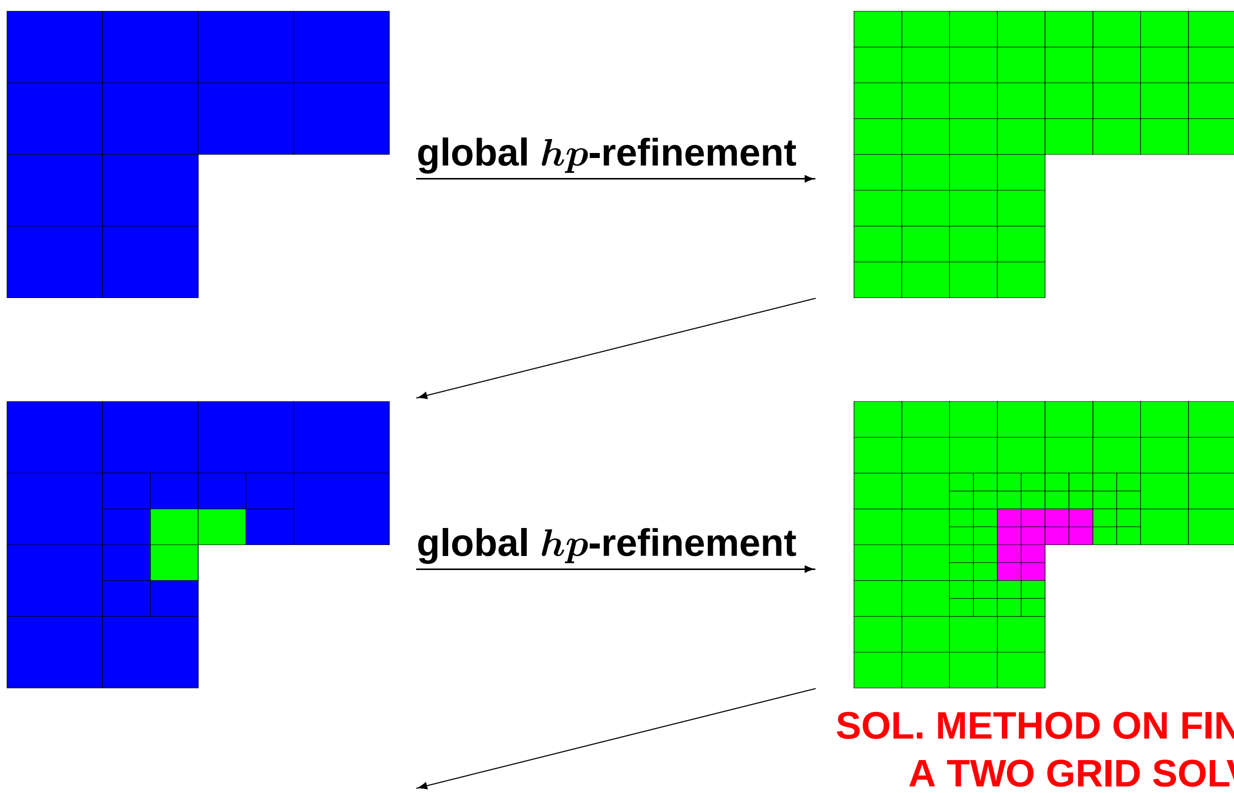


Automatic hp-adaptivity: 2K d.o.f.
***A priori* hp-adaptivity: 500K d.o.f.**
Automatic h-adaptivity: $>$5000K d.o.f.

THE FULLY AUTOMATIC *HP*-ADAPTIVE STRATEGY

Fully automatic *hp*-adaptive strategy

Coarse grids (hp) **Fine grids** ($h/2, p+1$)



SOL. METHOD ON FINE GRIDS: A TWO GRID SOLVER

A TWO GRID SOLVER FOR ELECTROSTATICS

We seek x such that $Ax = b$. Consider the following iterative scheme:

$$\begin{aligned} r^{(n+1)} &= [I - \alpha^{(n)} AS] r^{(n)} \\ x^{(n+1)} &= x^{(n)} + \alpha^{(n)} S r^{(n)} \end{aligned}$$

where S is a matrix, and $\alpha^{(n)}$ is a relaxation parameter. $\alpha^{(n)}$ *optimal* if:

$$\alpha^{(n)} = \arg\ \min \parallel x^{(n+1)} - x \parallel_A = \frac{(A^{-1} r^{(n)}, S r^{(n)})_A}{(S r^{(n)}, S r^{(n)})_A}$$

Then, we define our two grid solver as:

1 iteration with $S = S_F = \sum A_i^{-1}$ $+$

1 iteration with $S = S_C = P_C A_C^{-1} R_C$

A TWO GRID SOLVER FOR ELECTROSTATICS

Previously Presented Numerical and Theoretical Studies

- **Convergence analysis.**
- Importance of the choice of shape functions.
- Importance of the relaxation parameter.
- Selection of patches for the block Jacobi smoother.
- Effect of averaging.
- Error estimation.
- Smoothing vs two grid solver.
- Efficiency of the two grid solver.
- Guiding hp-adaptivity with a partially converged fine grid solution.

Error Reduction

$$\frac{\| e^{(n+1)} \|_A^2}{\| e^{(n)} \|_A^2} \leq \sup_e [1 - \frac{| (e, (P_C + S_F A)e)_A |^2}{\| e \|_A^2 \| S_F A e \|_A^2}]$$
$$\leq C < 1$$

Error reduction constant is independent of h and may depend logarithmically upon p.

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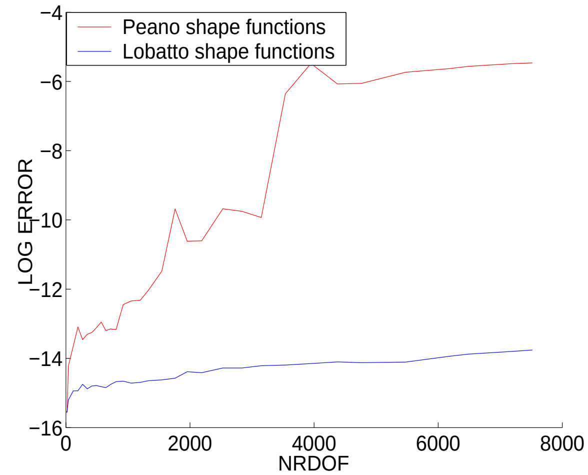
Different Sets of Shape Functions



L-shape domain problem. Difference between solutions obtained by two direct solvers using different sets of shape functions.

Selection of shape functions is important, and it affects conditioning.

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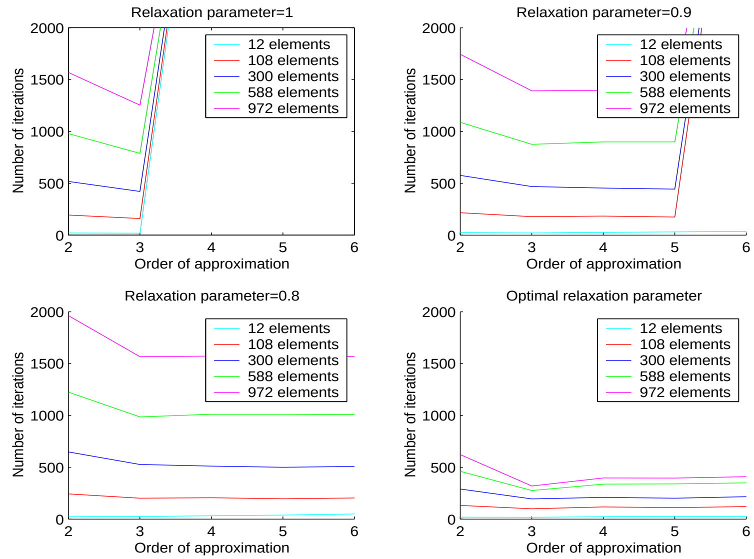
Optimal Relaxation Parameter



The optimal relaxation guarantees:

1. **convergence, and**
2. **faster convergence than with any fixed relaxation parameter.**

A TWO GRID SOLVER FOR ELECTROSTATICS

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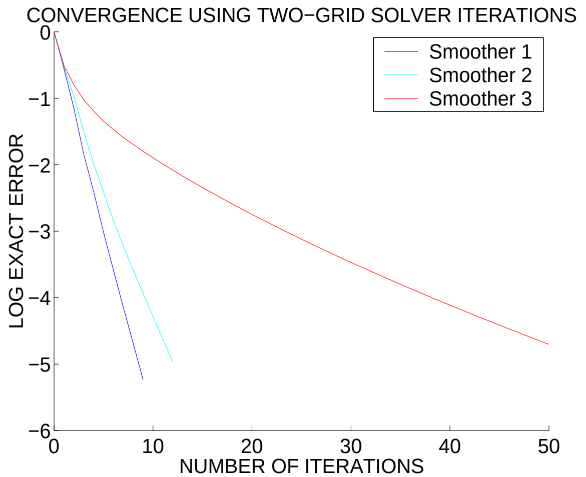
Different Block Jacobi Smoothers



Block Jacobi smoother corresponding to span of basis functions associated to an element stiffness matrix is **more efficient** than standard block Jacobi smoothers, **especially in the preasymptotic regime.**

A TWO GRID SOLVER FOR ELECTROSTATICS

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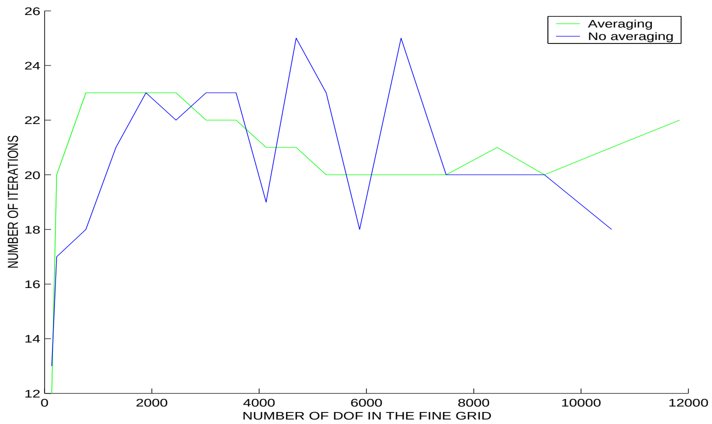
Averaging Operator



Number of iterations required by the two grid solver with and without an averaging operator.

It is NOT useful to include an averaging operator in the overlapping block Jacobi smoother formulation.

A TWO GRID SOLVER FOR ELECTROSTATICS

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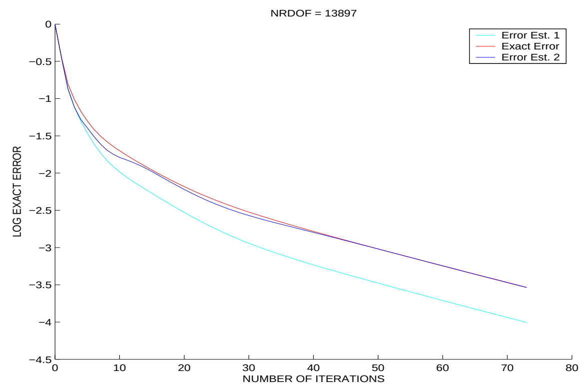
Error Estimation

$$\frac{\| e^{(n)} \|_A}{\| e^{(0)} \|_A} = \frac{\| A^{-1} r^{(n)} \|_A}{\| A^{-1} r^{(0)} \|_A} \approx \frac{\| \alpha^{(n)} S_F r^{(n)} \|_A}{\| \alpha^{(0)} S_F r^{(0)} \|_A} * C(n)$$



Exact error vs error estimate I vs error estimate II.

An accurate error estimator was designed and implemented.

A TWO GRID SOLVER FOR ELECTROSTATICS

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Smoothing vs Two Grid Solver iterations

Example	Nr of dof	1 - 1	3 - 1	Only Smoothing
L-shape	1889	13 /11	14 /12	34 /14
L-shape	11837	12 /9	13 /10	18 /13
Shock	2821	5 /6	6 /6	478 /295
Shock	12093	8 /7	9 /7	326 /9
Shock	34389	12 /9	13 /10	18 /12

Number of iterations needed for relative EXACT ERROR / ERROR ESTIMATE $\leq$ 0.01.

Both convergence properties AND error estimation degenerates if only smoothing iterations are used.

A TWO GRID SOLVER FOR ELECTROSTATICS

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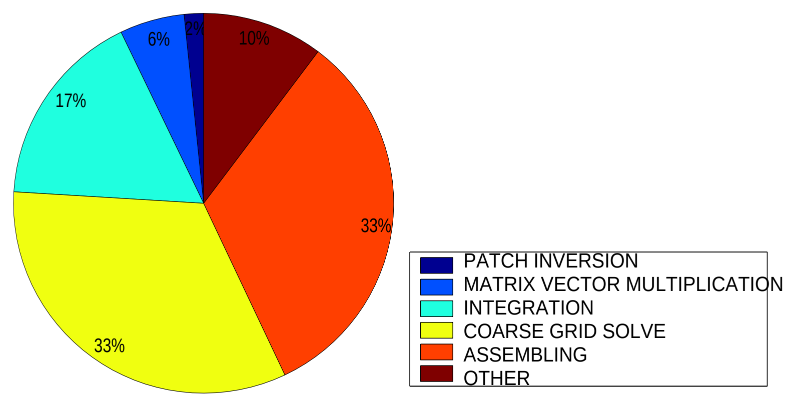
Efficiency for 3D problems

Speed = Coarse grid solve $+\mathcal{O}(p^9 N)$



2.15 millions unknowns, $p = 2$. Total solve time: $\approx$ 8 minutes

The two grid algorithm solves more than 2 million unknowns (with p=2) in only 8 minutes.

A TWO GRID SOLVER FOR ELECTROSTATICS

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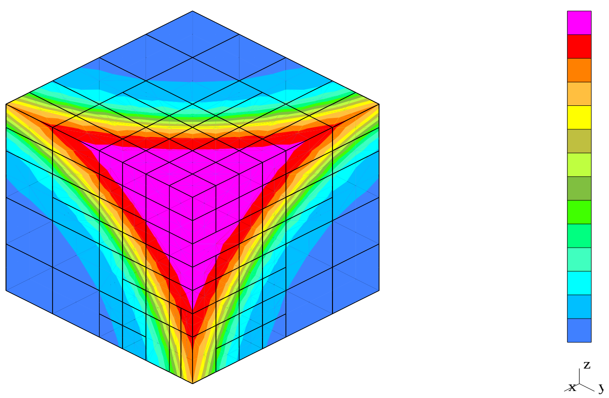
Guiding hp-refinements

It is possible to guide hp-refinements with partially converged solutions, requiring only about ten two grid solver iterations per grid.

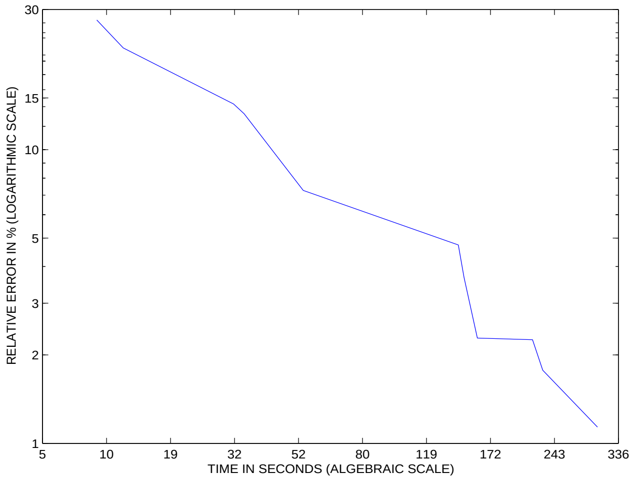
A TWO GRID SOLVER FOR ELECTROSTATICS

Integration of the fully automatic hp-adaptive strategy with the two grid solver

3D shock like solution example

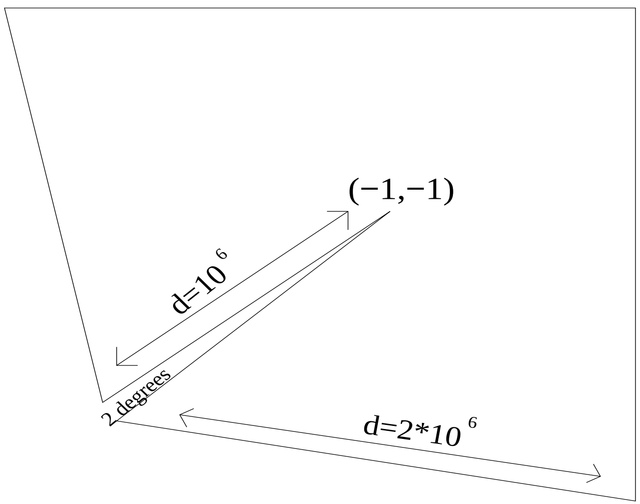


Scales: ERROR VS TIME.

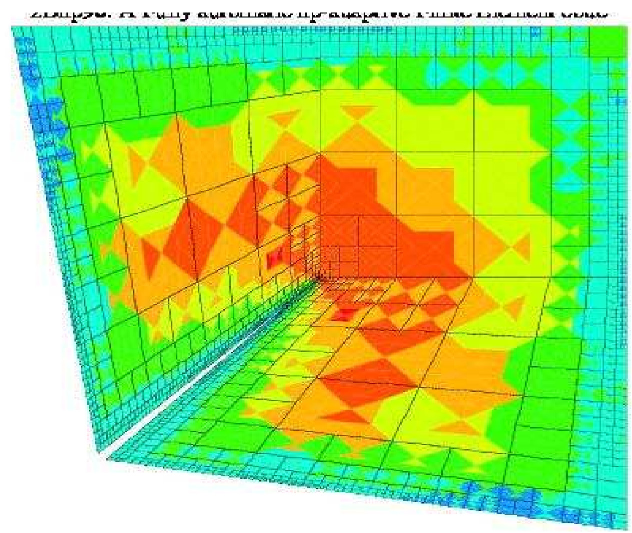


A TWO GRID SOLVER FOR ELECTROSTATICS

Edge diffraction example(Baker-Hughes): Electrostatics



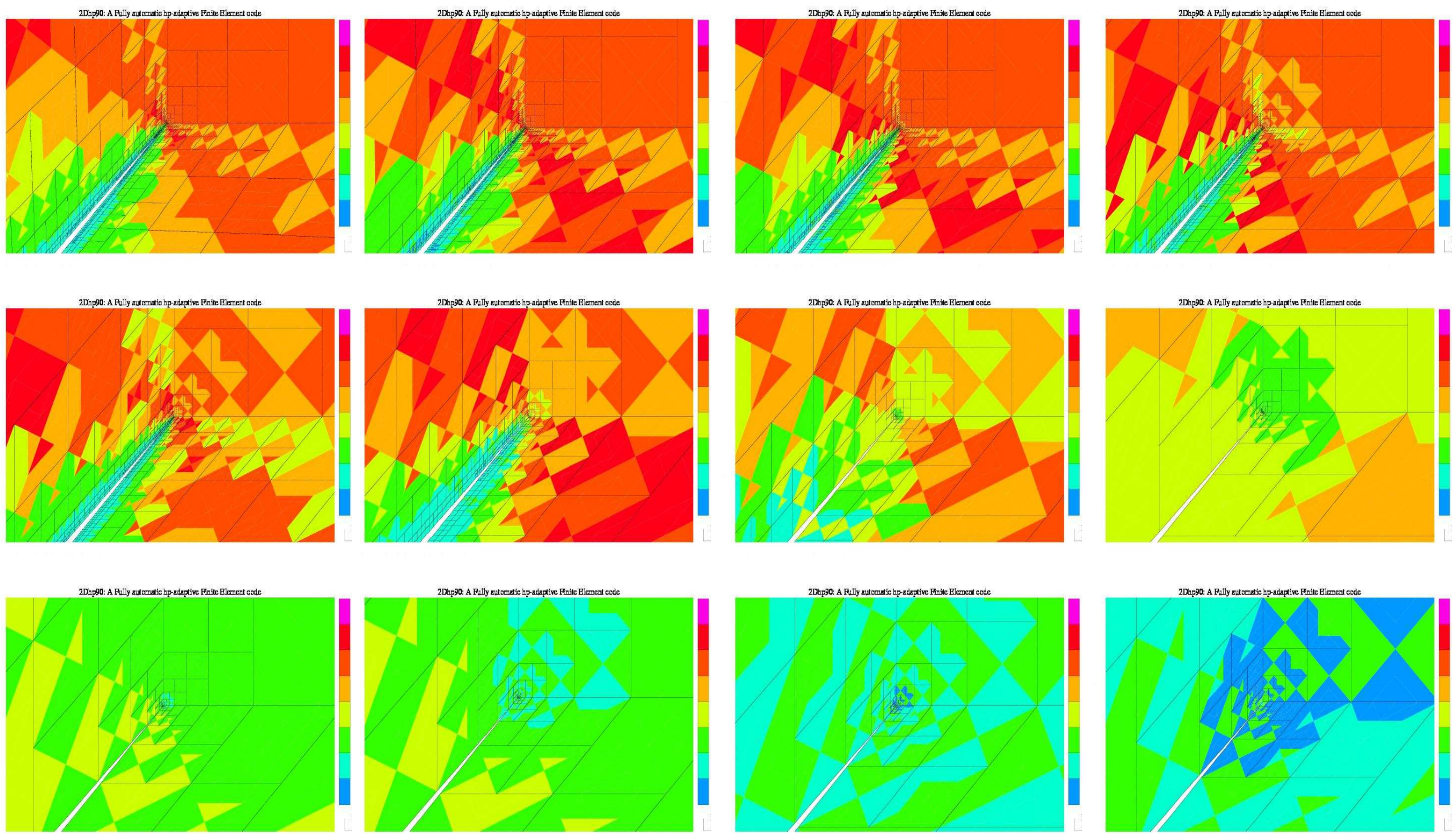
Dirichlet Boundary Conditions
u(boundary)=−ln r, r=sqrt (x*x+y*y)



Final hp-grid

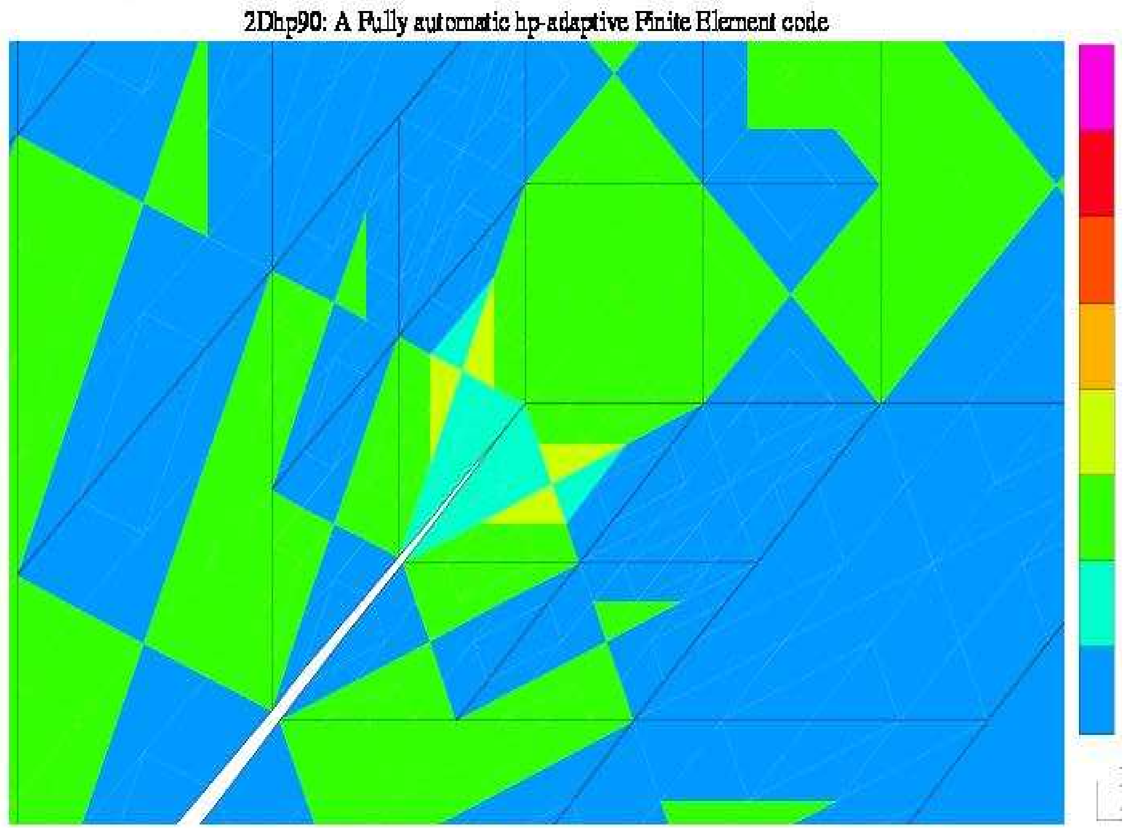
A TWO GRID SOLVER FOR ELECTROSTATICS

Edge diffraction example: final hp grid



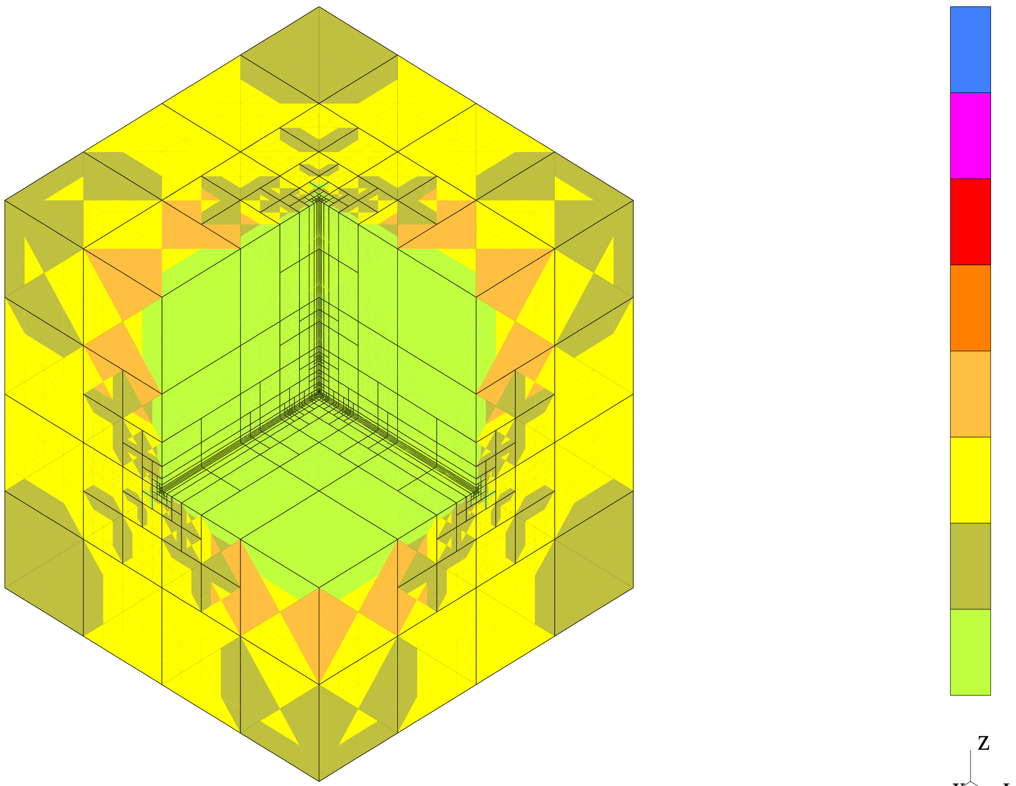
A TWO GRID SOLVER FOR ELECTROSTATICS

Edge diffraction example: final hp grid, zoom = 10^{13}



A TWO GRID SOLVER FOR ELECTROSTATICS

Fickera problem. Final hp-grid.



A TWO GRID SOLVER FOR ELECTRODYNAMICS

To solve iteratively $\boxed{\nabla \times \nabla \times \mathrm{E} - k^2\mathrm{E} = \mathrm{J}}$ has two difficulties

Indefiniteness

1) Consider the auxiliary problem:

$$\nabla \times \nabla \times \mathrm{E} + k^2\mathrm{E} = \mathrm{J}$$

2) Apply the following result (Cai and Widlund).

Theorem. If the coarse grid is fine enough, then: Convergence properties of the two grid solvers associated to the original and auxiliary problems are equal up to a constant times h.

Ker(curl) is large

1) Consider the following hp-FE spaces:

$$\mathrm{M} \subset H(\mathrm{curl}), W \subset H^1$$

2) Notice that: $Ker(\nabla \times \mathrm{M}) = \nabla \mathrm{W}$

3) Hiptmair: $M = \sum_e M_e + \sum_v \nabla W_v$

4) Arnold: $M = \sum_v M_v$

A TWO GRID SOLVER FOR ELECTRODYNAMICS

We seek x such that $Ax = b$. Consider the following iterative scheme:

$$\boldsymbol{r}^{(n+1)} = [\boldsymbol{I} - \boldsymbol{\alpha}^{(n)}\boldsymbol{AS}]\boldsymbol{r}^{(n)}$$
$$\boldsymbol{x}^{(n+1)} = \boldsymbol{x}^{(n)} + \boldsymbol{\alpha}^{(n)}\boldsymbol{S}\boldsymbol{r}^{(n)}$$

where S is a matrix, and $\alpha^{(n)}$ is a relaxation parameter. $\alpha^{(n)}$ *optimal* if:

$$\boldsymbol{\alpha}^{(n)} = \arg\ \min \parallel \boldsymbol{x}^{(n+1)} - \boldsymbol{x} \parallel_B = \frac{(\boldsymbol{A}^{-1}\boldsymbol{r}^{(n)}, \boldsymbol{S}\boldsymbol{r}^{(n)})_B}{(\boldsymbol{S}\boldsymbol{r}^{(n)}, \boldsymbol{S}\boldsymbol{r}^{(n)})_B}$$ **(NOT COMPUTABLE)**

Then, we define our two grid solver for electrodynamic problems as:

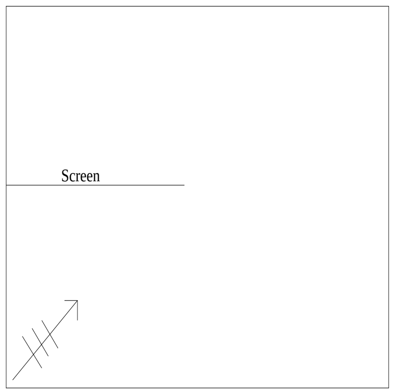
1 iteration with $S = S_F = \sum A_i^{-1}$ $+$

1 iteration with $S = S_\nabla = \sum G_i^{-1}$ $+$

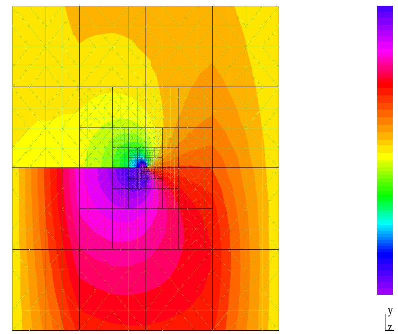
1 iteration with $S = S_C = P_C A_C^{-1} R_C$

A TWO GRID SOLVER FOR ELECTRODYNAMICS

Plane wave incident into a screen (diffraction problem)

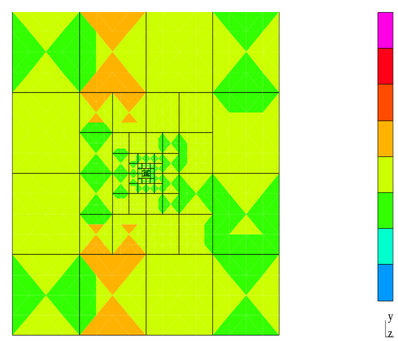


Geometry



Second component of electric field

Convergence history
(tolerance error= 0.1 %)

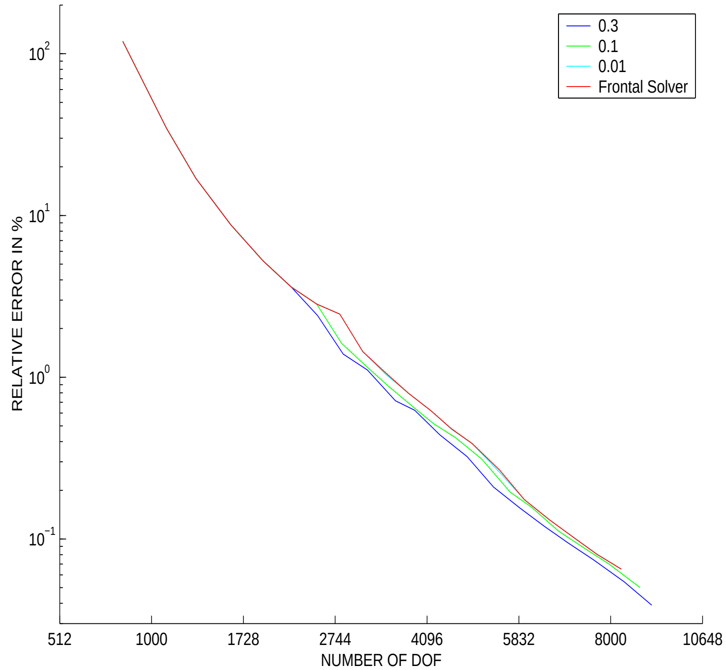


final hp grid

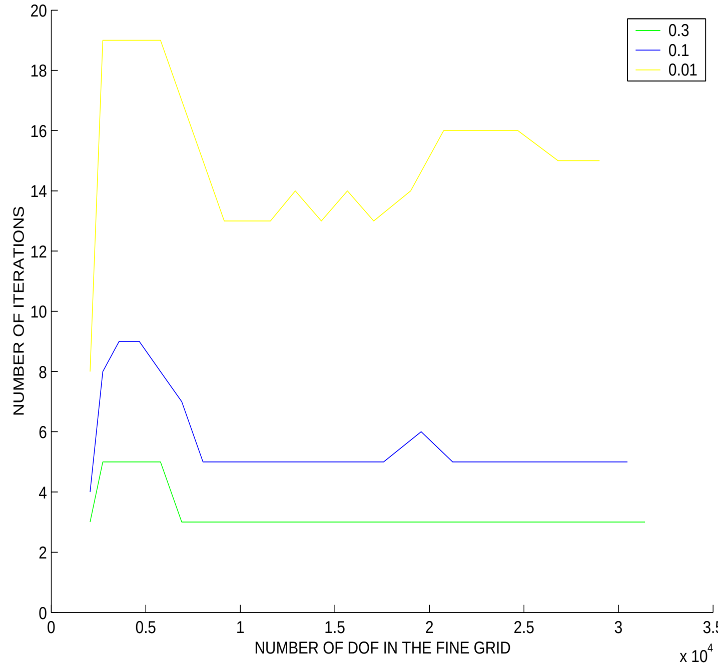
A TWO GRID SOLVER FOR ELECTRODYNAMICS

Guiding automatic hp-refinements

Diffraction problem. Guiding hp-refinements with a partially converged solution.



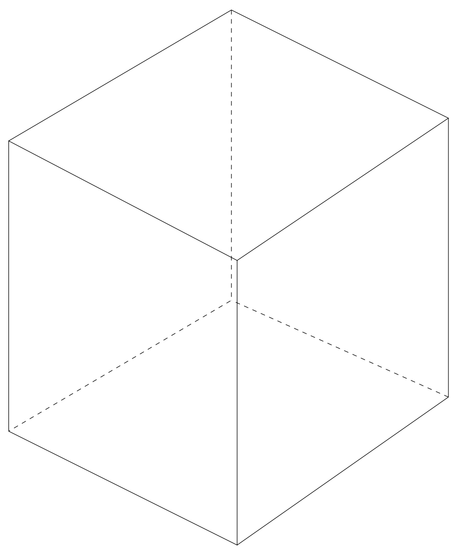
Discretization error



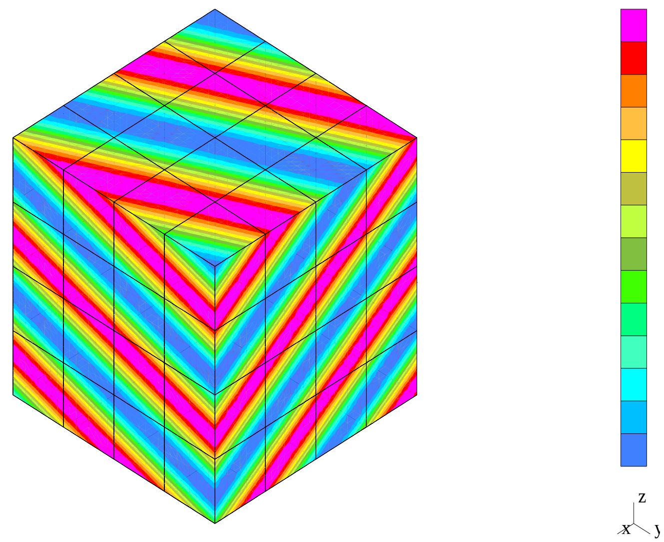
Number of iterations

A TWO GRID SOLVER FOR ELECTRODYNAMICS

3D EM Model Problem



Maxwell's equations
Boundary Conditions: Dirichlet, Cauchy

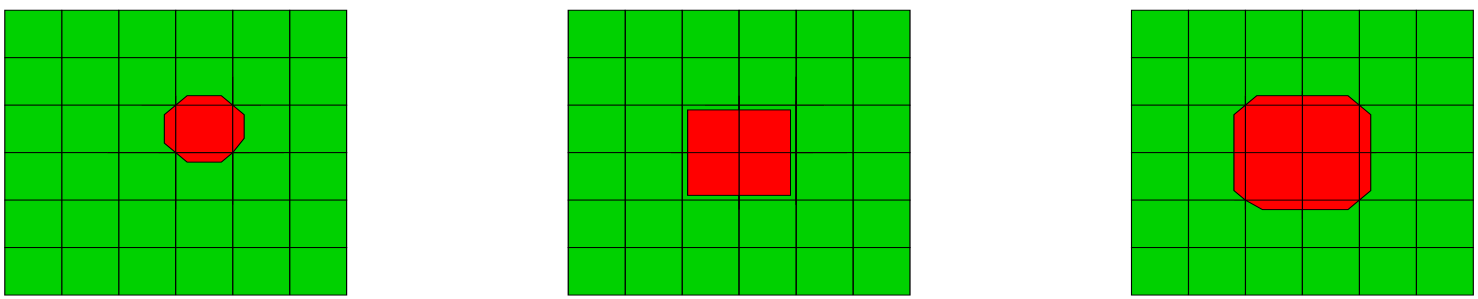


Solution: Plane wave

A TWO GRID SOLVER FOR ELECTRODYNAMICS

Selection of patches (for block Jacobi smoother)

Three examples of patches (blocks) for the Block Jacobi smoother:

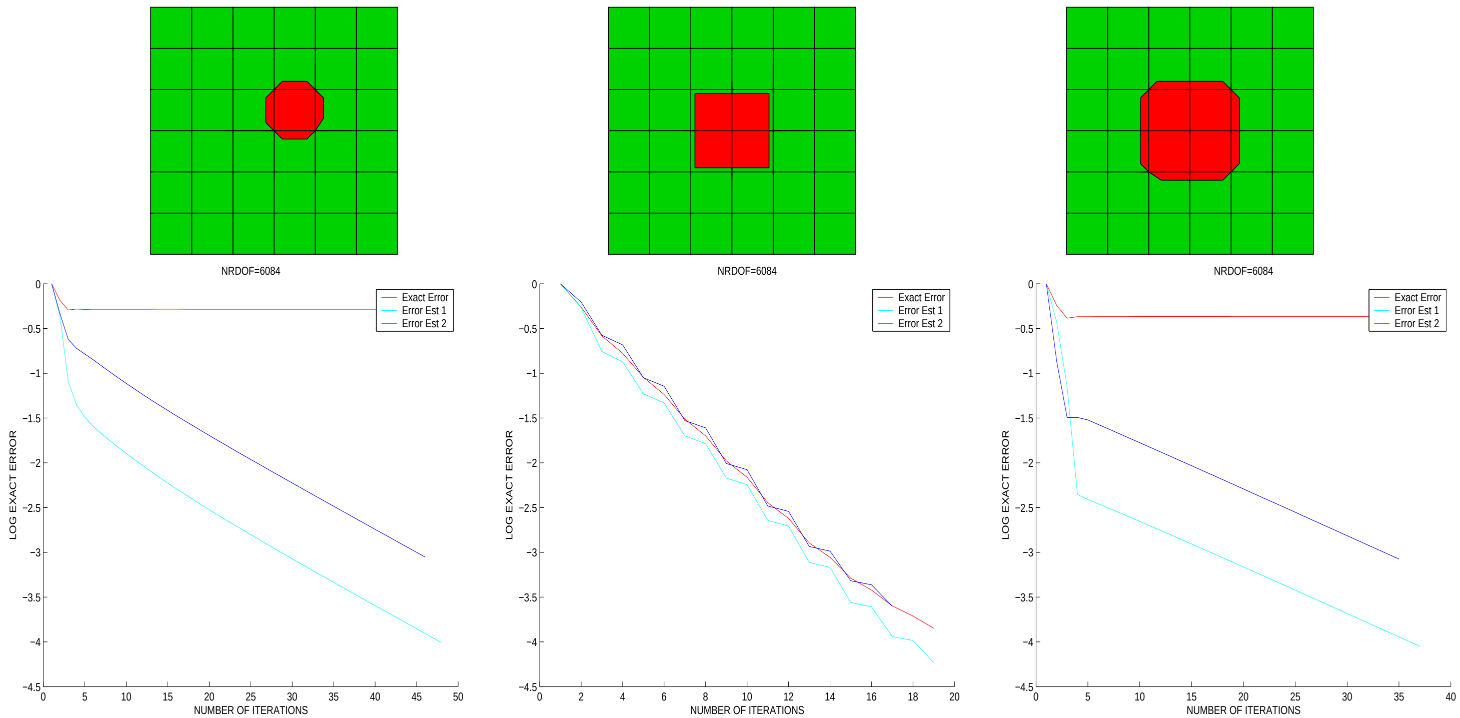


Example 1: span of basis functions corresponding to an element stiffness matrix.
Example 2: span of basis functions with support contained in the support of a fine grid vertex node basis function.
Example 3: span of basis functions corresponding to element stiffness matrices for all elements adjacent to a vertex.

A TWO GRID SOLVER FOR ELECTRODYNAMICS

Performance of different smoothers

3D EM Model Problem



ONLY SMOOTHER 2 CONVERGES

A two grid solver for discretization of Maxwell's equations using hp-FE

Both Arnold and Hiptmair algorithms are based on Helmholtz decomposition

$$\boxed{\boldsymbol{H}_D(\mathrm{curl};\Omega) = (\boldsymbol{Ker}(\mathrm{curl})) \oplus (\boldsymbol{Ker}(\mathrm{curl}))^{\perp}}$$

Arnold vs Hiptmair

1. **In 3D, Arnold's approach is approximately:**
   - **4 times more expensive in terms of memory and CPU time needed for a matrix-vector multiplication than Hiptmair's approach, and**
   - **500 times more expensive in terms of CPU time needed for construction of the block Jacobi smoother than the one needed for construction of each of the two Hiptmair's smoothers.**
2. **Hiptmair algorithm involves a more complex implementation, and requires implementation of the discrete embedding of gradients of potentials into $\boldsymbol{H}(\mathrm{curl})$.**

THE MAIN ACCOMPLISHMENT

Design,
implementation,
theoretical study,
and numerical study

of an efficient two grid solver,
integrated with the automatic hp-adaptive strategy,
suitable for highly nonuniform hp-grids,
for solution of general electromagnetic problems
in the frequency domain.

LIMITATIONS AND FUTURE WORK

Limitations of the numerical technique for real world EM applications

Limitation I

Size of the fine grid problem may be about 30 times larger than size of the corresponding coarse grid problem.

Limitation II

For wave propagation problems, convergence of the two grid solver is only guaranteed if the coarse grid is fine enough.

Limitation III

For a number of electromagnetic applications, a refinement strategy based on minimization of the energy norm is inadequate.

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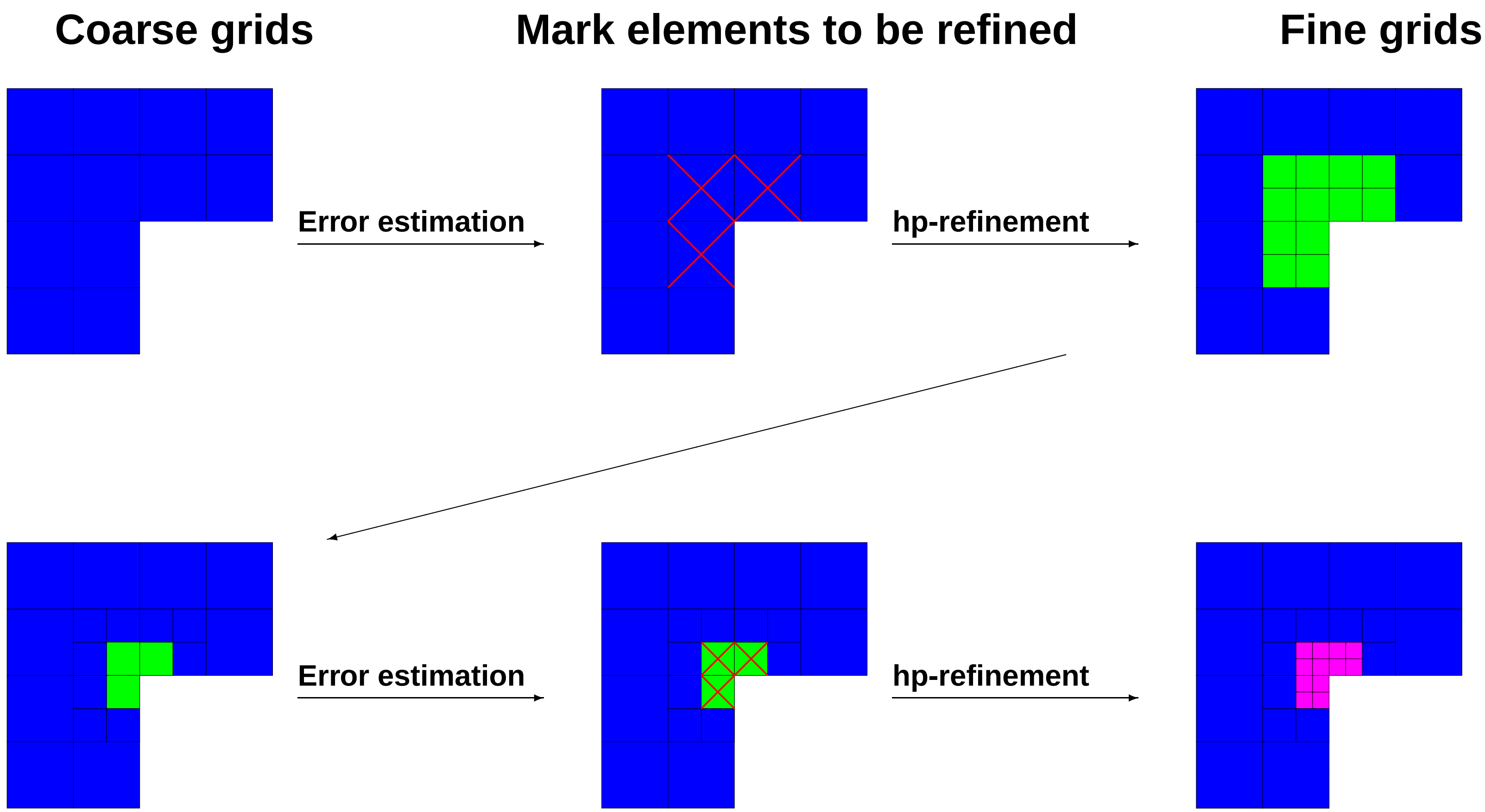

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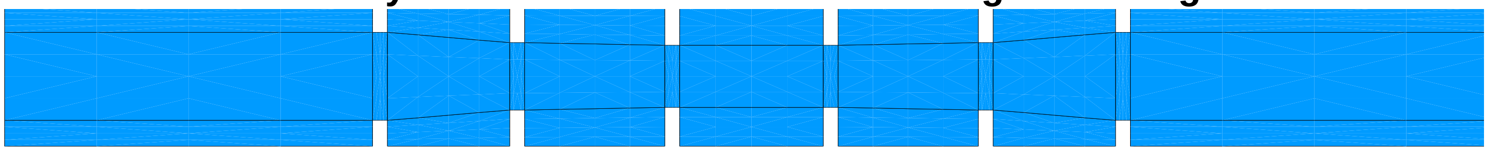
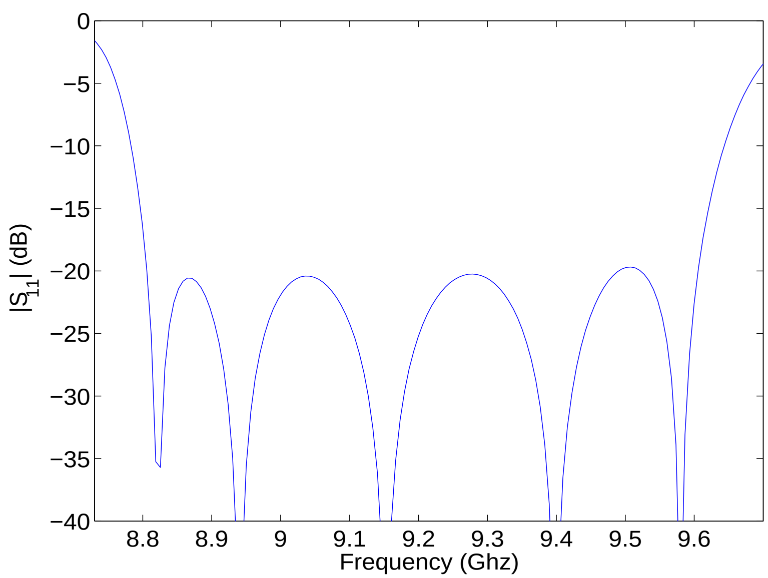
Geometry of a cross section of the rectangular waveguide





Return loss of the waveguide structure

H-plane six resonant iris filter.

Dominant mode (source): $TE_{10}-$**mode.**

Dimensions $\approx 20 \times 2 \times 1$ **cm.**

Operating Frequency $\approx 8.8 - 9.6$ **Ghz**

Cutoff frequency ≈ 6.56 **Ghz**

LIMITATIONS AND FUTURE WORK

For wave propagation problems, convergence of the two grid solver is only guaranteed if the coarse grid is fine enough.

Does convergence (or not) of the two grid solver depends upon h and/or p? How?

Convergence of the two grid solver	$p = 1$	$p = 2$	$p = 3$	$p = 4$
Nr. of elements per $\lambda = 7, 13$	YES	YES	YES	YES
Nr. of elements per $\lambda = 7, 11$	NO	NO	NO	YES
Nr. of elements per $\lambda = 6, 13$	NO	NO	NO	NO

Convergence (or not) of the two grid solver is (almost) insensitive to p-enrichment.

We need about 10-12 elements per wavelength on the coarse grid to guarantee convergence of the two grid solver

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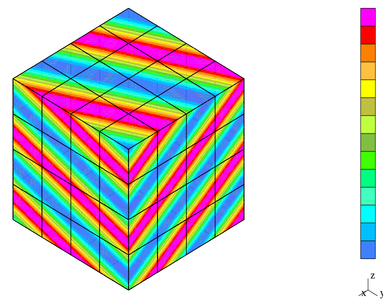

- **Length of main diagonal of the cube varying from 1 to 50 wavelengths.**
- **Stopping criterion: relative energy norm error below 5%.**

Nr. of λ vs p		p=1	p=2	p=3	p=4	p=5
1	λ/h	20	3	2	1	1
	D.O.F.	40K	946	1033	308	548
2	λ/h		3	1.5	1	1
	D.O.F.	($>$300K)	6427	2764	2226	4109
4	λ/h			1.25	1	0.75
	D.O.F.	($>$2300K)	($>$82K)	12K	14K	12K
8	λ/h					0.625
	D.O.F.	($>$20M)	($>$650K)	($>$167K)	($>$71K)	51K
50	λ/h					
	D.O.F.	($>$5000M)	($>$122M)	($>$25M)	($>$14M)	($>$9.5M)

Large p (with only few elements per wavelength) is needed to solve problems with domain size larger than 5-10 wavelengths.

LIMITATIONS AND FUTURE WORK

For wave propagation problems, convergence of the two grid solver is only guaranteed if the coarse grid is fine enough.

Summary

- **We need 10-12 elements per wavelength (on the coarse grid) to guarantee convergence of the two grid solver.**
- **If domain size is larger than 5-10 wavelengths, then elements with large p are needed.**

Conclusion

- **A multigrid with less restrictive conditions over the coarse grid is needed. Otherwise, multigrid algorithms will only be useful for problems with domain size up to 5 wavelengths.**

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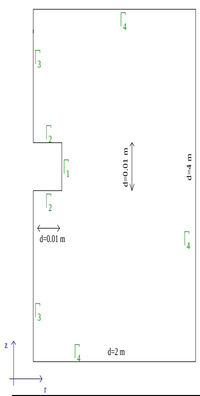


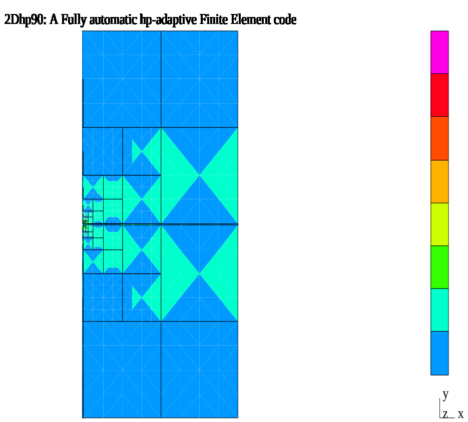
Reduced Wave Equation: $\nabla \times \left(\frac{1}{\mu}\nabla \times E\right) - (\omega^2\epsilon - j\omega\sigma)E = -j\omega J^{imp}$

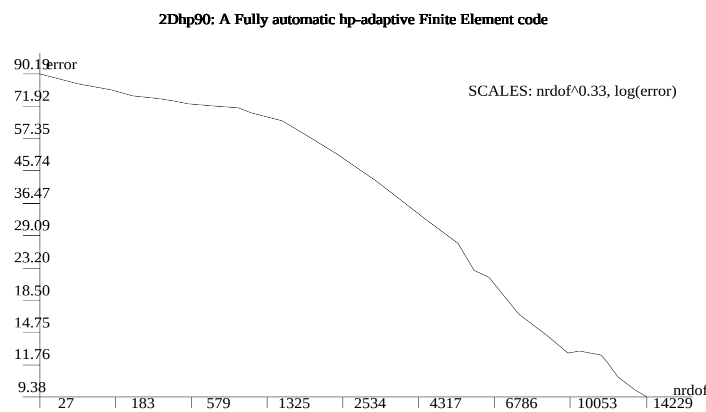
Boundary Conditions (BC):

Dirichlet BC at a PEC surface: $n \times E = 0 \;\; on \;\; \Gamma_2 \cup \Gamma_4$

Neumann BC's:

$$n \times \frac{1}{\mu}\nabla \times E = -j\omega \;\; on \;\; \Gamma_1 \quad ; \quad n \times \frac{1}{\mu}\nabla \times E = 0 \;\; on \;\; \Gamma_3$$





LIMITATIONS AND FUTURE WORK

For a number of electromagnetic applications, a refinement strategy based on minimization of the energy norm is inadequate

Optimization is based on minimization of the ENERGY NORM of the error, given by:

$$\| error \|^2 = \int | error |^2 + \int | \nabla \times error |^2$$

Interpretation of results:

- **The grid is optimal for the selected refinement criteria,**
- **but our refinement criteria is inadequate for our pourposes.**

We need an hp goal-oriented refinement strategy

LIMITATIONS AND FUTURE WORK

Future Work

- **Error estimators for wave propagation problems**
- **A multigrid method for wave propagation problems that overcomes the restriction on the maximum coarse grid element size.**
- **A fully automatic goal-oriented hp-adaptive algorithm.**
  1. Supported by L. Tabarovski (Baker-Hughes), C. Torres-Verdin, and L. Demkowicz.
  2. Starting date: April 5, 2004.
  3. Expected completion date of the 2D version: May 31, 2005.
  4. Expected completion date of the 3D version: May 31, 2006.

CONCLUSIONS AND FUTURE WORK

- For electromagnetic problems it is possible to guide optimal hp-refinements with partially converged solutions only.

- By combining the fully automatic hp-adaptive algorithm with the two grid solver, it is possible to obtain accurate solutions for a variety of electromagnetic problems.

- There is a conflict between large p (required to control dispersion error) and small h (needed to guarantee convergence of multigrid methods) for problems with high frequency.

- For a variety of electromagnetic applications, a goal-oriented hp-algorithm is needed.