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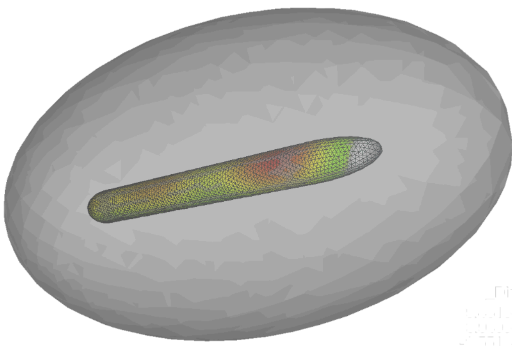

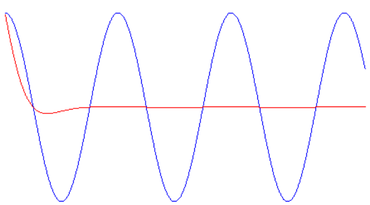

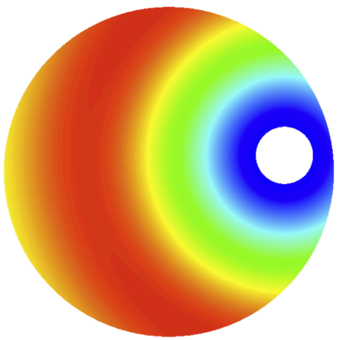

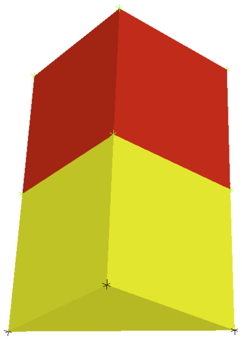

A comparison of perfectly matched layers and infinite elements for exterior Helmholtz problems

Gregory Bunting, Arun Prakash, Timothy Walsh

U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration

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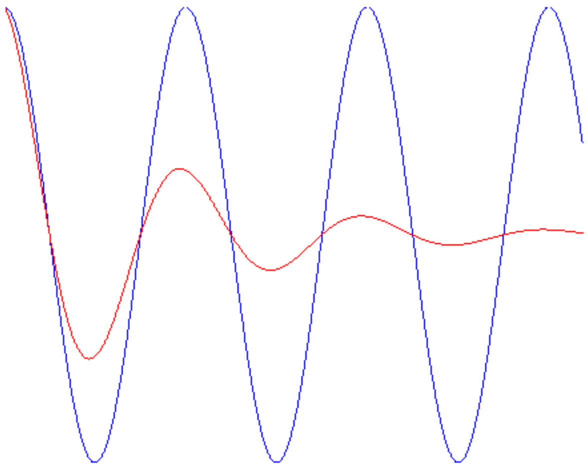
Outline

- Perfectly Matched Layers
  - Motivation
  - Gaps in PML Literature
  - Formulation
  - Results – PML Parameter Analysis
  - Conclusions
  - Future Work
  - Acknowledgements

Overview of PML

WTF4

- Undamped wave equation: e^{ikx}
  - this wave will propagate indefinitely in the x direction
- Complex Coordinate System:
  - $\tilde{x} = a(x) + ib(x)$
- Wave Equation becomes:
  - $e^{ik\tilde{x}} = e^{i(-ka(x)+ikb(x))} = e^{-kb(x)}e^{ika(x)}$
  - Damped Wave Equation



Slide 3

WTF4 I would just set a(x) = x

Walsh, Timothy Francis, 7/24/2014

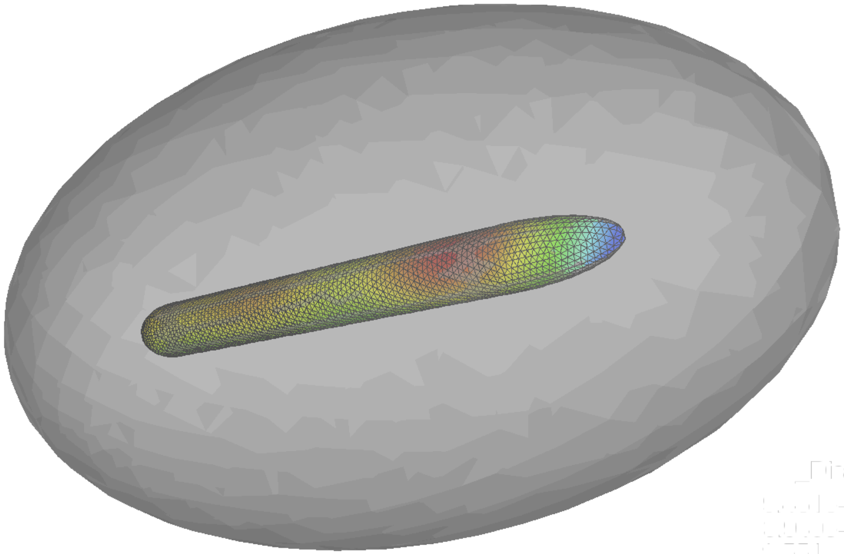
Motivation

- PML exhibits zero reflection coefficient at all angles of incidence and all frequencies (on the continuous level)
  - This is not true for absorbing BC and infinite elements

- Once we discretize the problem, that property is lost – but it can be recovered as mesh converges to continuous solution
- Thus PML converts absorbing boundary condition error into discretization error.

Motivation

- Why do we want PML?
  - Ship in Water
  - Reentry vehicles in air
  - Other unbounded domains



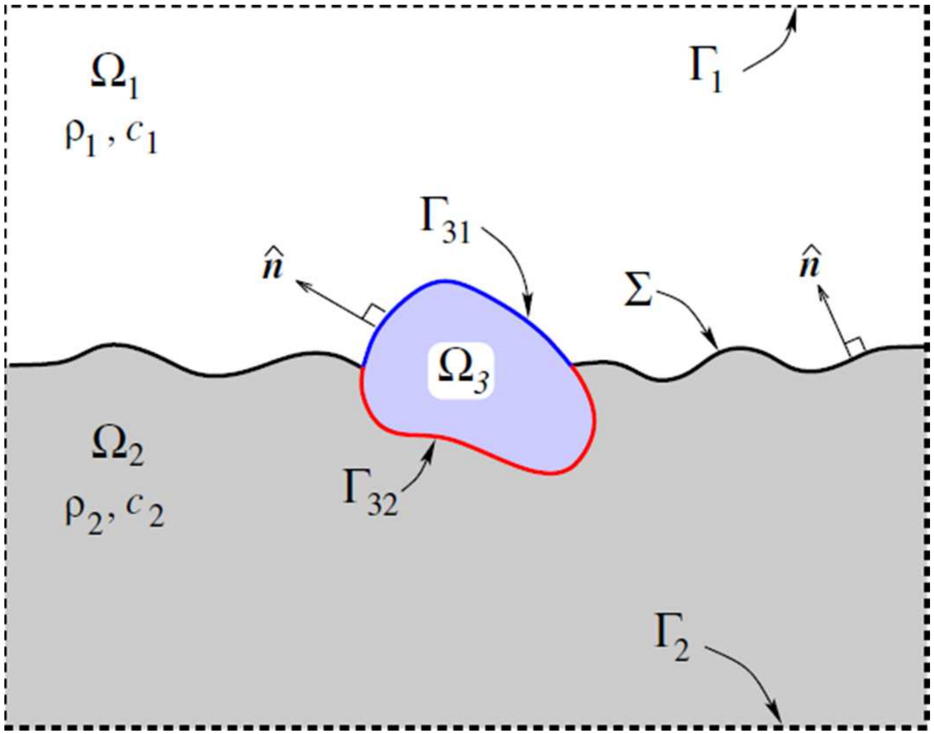
- RTHS
  - Nuclear reactor in soil (earthquake)
  - Skyscraper
  - Heterogenous Soil – classical approaches are not viable

WTF5

Infinite Elements

- Infinite elements solve many of the same problems
- Infinite elements cannot handle some types of problems
  - Non-homogenous domains
  - Explicit Time Integration (singular mass matrix)

Partially submerged mine



Shirron 2006

Slide 6

WTF5 add some pictures (buried mine), earthquake FEM model, etc

Walsh, Timothy Francis, 7/24/2014

Advantages of PML

- Heterogeneous Materials
- Layers of elements
- Explicit Time Integration

- Research Goals
  - Develop Ellipsoidal PML formulation and implement in Sierra-SD
  - Compare performance of PML and Infinite Elements in Sierra-SD
  - Evaluate performance of PML in a massively parallel environment

Gaps in PML Literature

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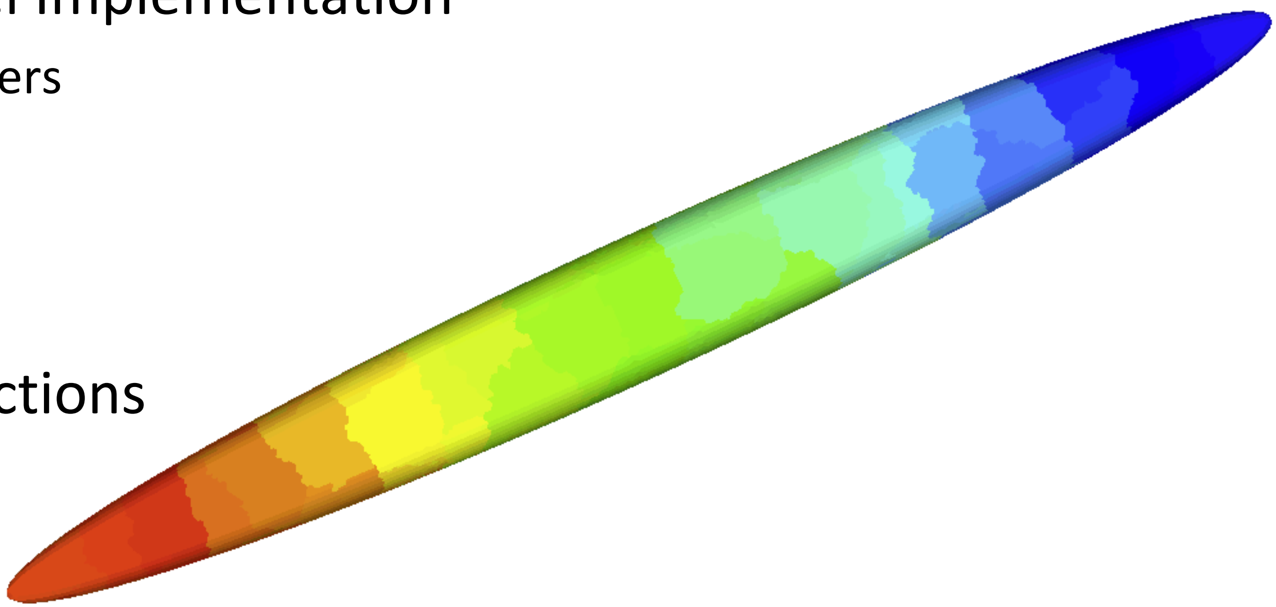
- Ellipsoidal Formulation
- Massively Parallel Implementation
  - Condition Numbers
  - Iteration Counts
  - Decomposition
- Types of loss functions
- PML Parameters



Slide 8

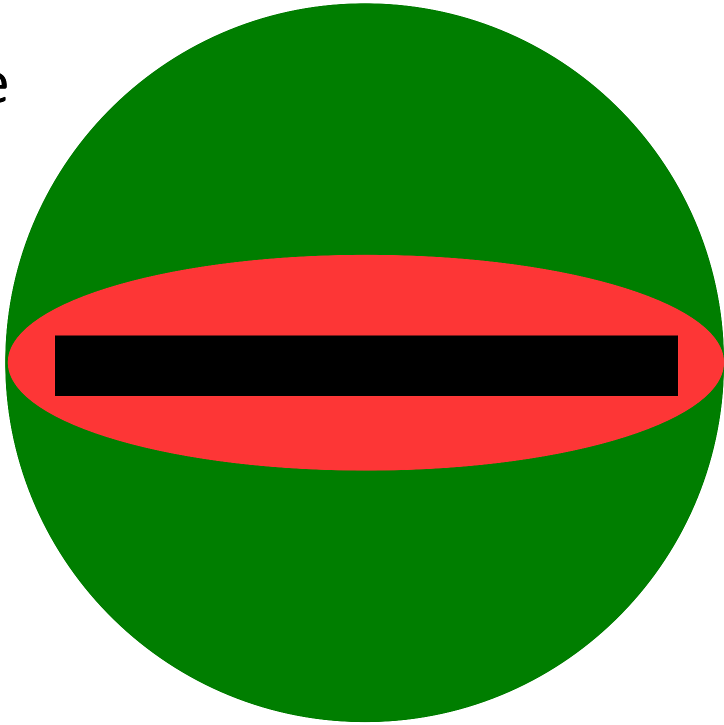
WTF10 ellipsoidal encompases both Spherical and Cartesian - existing approaches in the literature have to be either Spherical or Cartesian

Walsh, Timothy Francis, 7/24/2014

Ellipsoidal PML

We can inscribe even the most complex shapes inside of a minimal volume ellipsoid

- Sphere – Volume = $\frac{4}{3}\pi r^3$
- Ellipsoid – Volume = $\frac{4}{3}\pi a b c$
- Compare Volume of Ellipsoid to Sphere
- 10:1 aspect ratio ellipse 1% of Sphere
- 20:1 aspect ratio has 0.25% of Sphere



Slide 9

WTF9 I'd show a picture of a long skinny structure and say "we can enscribe any complex shape inside of an ellipse"
Walsh, Timothy Francis, 7/24/2014

PML Mathematics - Overview

- Cartesian PML
  - Typically done with multiple PML regions
- Rotated Cartesian PML
- Spherical PML
- Ellipsoidal – most general
  - Spherical is a special case of ellipsoidal formulation
  - Cartesian is a special case of ellipsoidal/spherical formulations

Exterior Acoustic Formulatoin

We wish to solve the Helmholtz equation on an exterior acoustic domain

Helmholtz equation

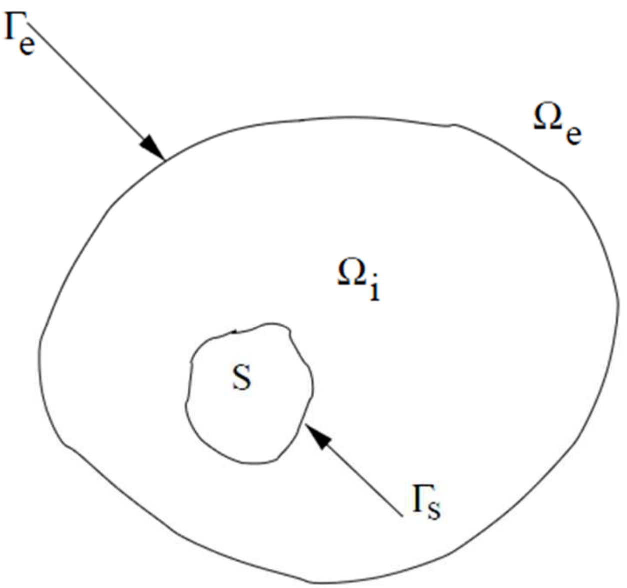
$$-\Delta p - k^2 p = 0$$

Sommerfeld condition

$$\frac{\partial p}{\partial n} + ikp \in L^2(\Omega_e)$$

Neumann loading condition

$$\frac{\partial p}{\partial n} = g(x,t)$$



Domains Ω_i and Ω_e and interface Γ for the exterior acoustic problem.

General Formulation for PML

Complex coordinate stretching $\tilde{x} = x - \frac{i}{\omega} \int_x^a \sigma(\xi) d\xi \quad a < x < \bar{a}$

Helmholtz equation over complex coordinates $-\tilde{\Delta} p - k^2 p = 0$

Weak form over complex coordinates

$$\int_{\tilde{\Omega}_I} \langle \tilde{\nabla} p, \tilde{\nabla} q \rangle - k^2 pq \; d\Omega_I = \int_{\tilde{\Gamma}_S} gqdS$$

Mapped weak form back to real coordinates

$$\int_{\Omega_I} \left[(\boldsymbol{J}^{-1} \nabla p) \cdot (\boldsymbol{J}^{-1} \nabla q) - k^2 pq \right] J(x, y, z) d\Omega_I = \int_{\Gamma_S} gqdS$$

Re-write as Helmholtz equation with variable coefficients

$$\int_{\Omega_I} \tilde{\boldsymbol{A}} \langle \nabla p, \nabla \bar{q} \rangle - k^2 \tilde{J} p \bar{q} \; d\Omega_I = \int_{\Gamma_S} g \bar{q} d\Gamma_S$$

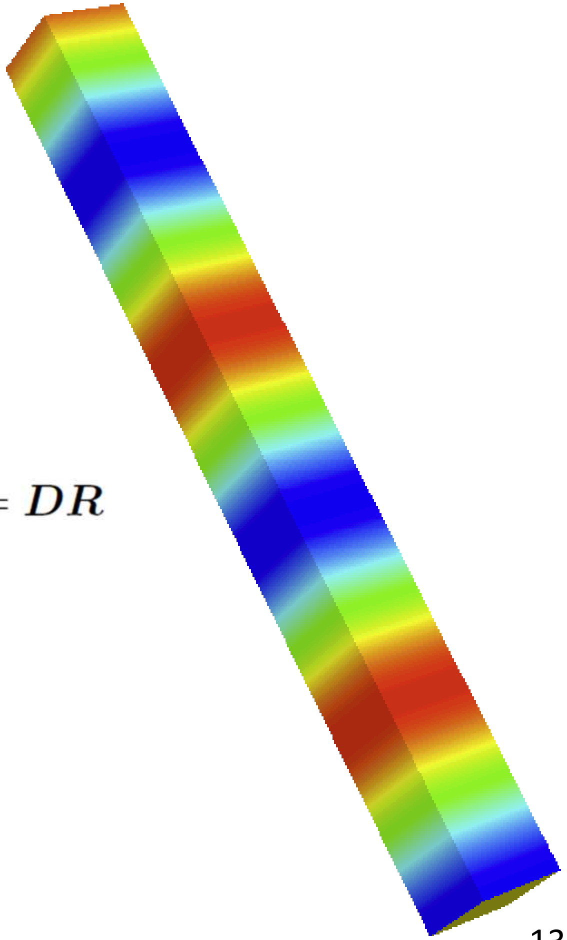
$$\tilde{\boldsymbol{A}} = \tilde{J} \tilde{\boldsymbol{J}}^{-1} \tilde{\boldsymbol{J}}^{-T}$$

Rotated Cartesian PML
1D Loss Function in 3D Domain

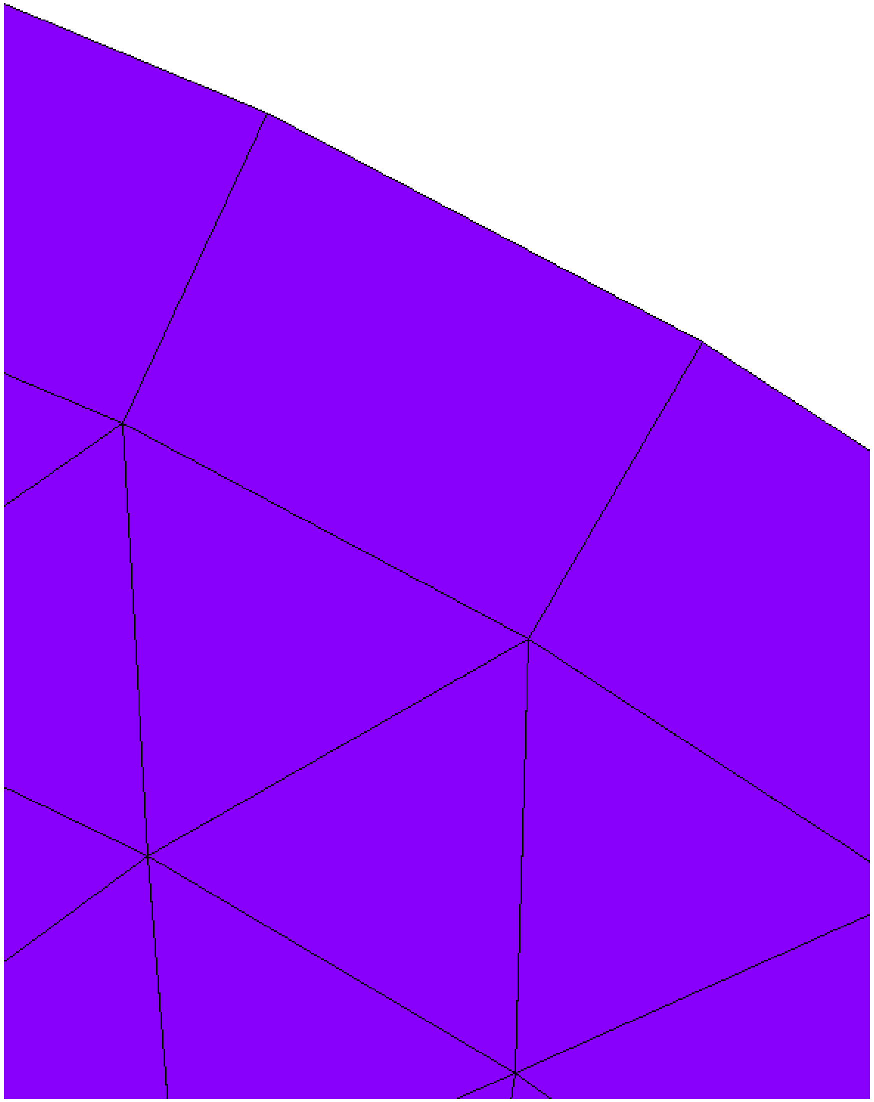
$$\gamma = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \frac{1}{\gamma_z} \end{bmatrix}$$

$$\boldsymbol{x}' = \boldsymbol{R}\boldsymbol{x}$$

$$\boldsymbol{J} = \frac{\partial(\tilde{x}, \tilde{y}, \tilde{z})}{\partial(x, y, z)} = \frac{\partial(\tilde{x}, \tilde{y}, \tilde{z})}{\partial(x' y', z')} \frac{\partial(x', y', z')}{\partial(x, y, z)} = \begin{bmatrix} \frac{1}{\gamma_x} & 0 & 0 \\ 0 & \frac{1}{\gamma_y} & 0 \\ 0 & 0 & \frac{1}{\gamma_z} \end{bmatrix} \boldsymbol{R} = \boldsymbol{D}\boldsymbol{R}$$



Cartesian PML Applied to Sphere



- Apply Rotated Cartesian PML to Each Outer Face of Sphere
- Good Results, but not Great
- Results converged with mesh, but slowly
- Use spherical formulation to account for “gaps” between the elements

Slide 14

WTF14 need a new title, but looks good

Walsh, Timothy Francis, 7/24/2014

Spherical PML - Demkowicz

Mapping between spherical and Cartesian coordinates

$$x = rsin(\phi)cos(\theta) \qquad \tilde{x} = \tilde{r}sin(\phi)cos(\theta)$$

$$y = rsin(\phi)sin(\theta) \qquad \tilde{y} = \tilde{r}sin(\phi)sin(\theta)$$

$$z = rcos(\phi) \qquad \tilde{z} = \tilde{r}cos(\phi)$$

The Jacobian follows directly

$$J = \frac{\partial(\tilde{x},\tilde{y},\tilde{z})}{\partial(x,y,z)} = \frac{\partial(\tilde{x},\tilde{y},\tilde{z})}{\partial(r,\phi,\theta)} \frac{\partial(x,y,z)}{\partial(r,\phi,\theta)}^{-1} = \begin{bmatrix} \tilde{r}' sin(\phi)cos(\theta) & \tilde{r}cos(\phi)cos(\theta) & -\tilde{r}sin(\phi)sin(\theta) \\ \tilde{r}' sin(\phi)sin(\theta) & \tilde{r}cos(\phi)sin(\theta) & \tilde{r}sin(\phi)cos(\theta) \\ \tilde{r}' cos(\phi) & -\tilde{r}sin(\phi) & 0 \end{bmatrix} \begin{bmatrix} sin(\phi)cos(\theta) & rcos(\phi)cos(\theta) & -rsin(\phi)sin(\theta) \\ sin(\phi)sin(\theta) & rcos(\phi)sin(\theta) & rsin(\phi)cos(\theta) \\ cos(\phi) & -rsin(\phi) & 0 \end{bmatrix}^{-1}$$

Ellipsoidal PML

Mapping between ellipsoidal and Cartesian coordinates

$$x = \sqrt{r^2 - f^2} sin(\phi) cos(\theta)$$
$$y = \sqrt{r^2 - f^2} sin(\phi) sin(\theta)$$
$$z = r cos(\phi)$$

$$\tilde{x} = \sqrt{\tilde{r}^2 - f^2} sin(\phi) cos(\theta)$$
$$\tilde{y} = \sqrt{\tilde{r}^2 - f^2} sin(\phi) sin(\theta)$$
$$\tilde{z} = \tilde{r} cos(\phi)$$

The Jacobian follows directly

$$J = \frac{\partial(\tilde{x},\tilde{y},\tilde{z})}{\partial(x,y,z)} = \frac{\partial(\tilde{x},\tilde{y},\tilde{z})}{\partial(r,\phi,\theta)} \frac{\partial(x,y,z)}{\partial(r,\phi,\theta)}^{-1}$$

$$= \begin{bmatrix} \frac{\tilde{r}\tilde{r}'}{\sqrt{\tilde{r}^2-f^2}} sin(\phi)cos(\theta) & \sqrt{\tilde{r}^2 - f^2} cos(\phi)cos(\theta) & -\sqrt{\tilde{r}^2 - f^2} sin(\phi)sin(\theta) \\ \frac{\tilde{r}\tilde{r}'}{\sqrt{\tilde{r}^2-f^2}} sin(\phi)sin(\theta) & \sqrt{\tilde{r}^2 - f^2} cos(\phi)sin(\theta) & \sqrt{\tilde{r}^2 - f^2} sin(\phi)cos(\theta) \\ \frac{\tilde{r}\tilde{r}'}{\sqrt{\tilde{r}^2-f^2}} cos(\phi) & -\sqrt{\tilde{r}^2 - f^2} sin(\phi) & 0 \end{bmatrix}$$

$$\begin{bmatrix} \frac{r}{\sqrt{r^2-f^2}} sin(\phi)cos(\theta) & \sqrt{r^2 - f^2} cos(\phi)cos(\theta) & -\sqrt{r^2 - f^2} sin(\phi)sin(\theta) \\ \frac{r}{\sqrt{r^2-f^2}} sin(\phi)sin(\theta) & \sqrt{r^2 - f^2} cos(\phi)sin(\theta) & \sqrt{r^2 - f^2} sin(\phi)cos(\theta) \\ \frac{r}{\sqrt{r^2-f^2}} cos(\phi) & -\sqrt{r^2 - f^2} sin(\phi) & 0 \end{bmatrix}^{-1}$$

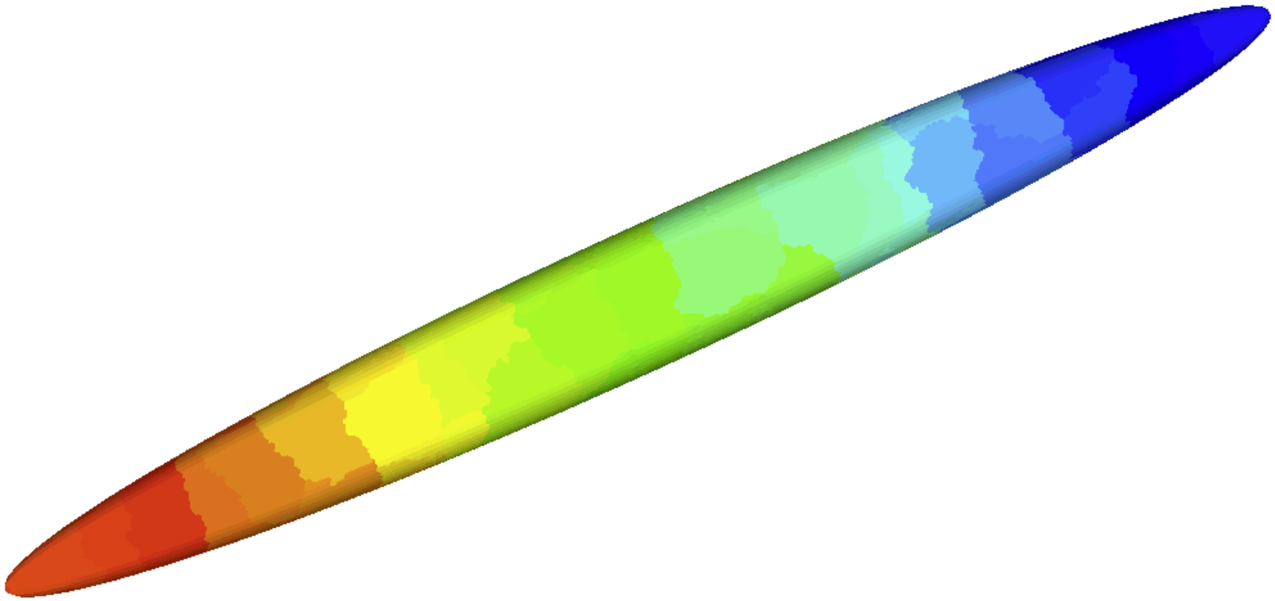
Slide 16

WTF17 I'd put a picture in here

Walsh, Timothy Francis, 7/24/2014

Parallel

- Modify communication maps
- Reused technology for infinite elements
- PML Can unbalance decomposition – boundaries are expensive

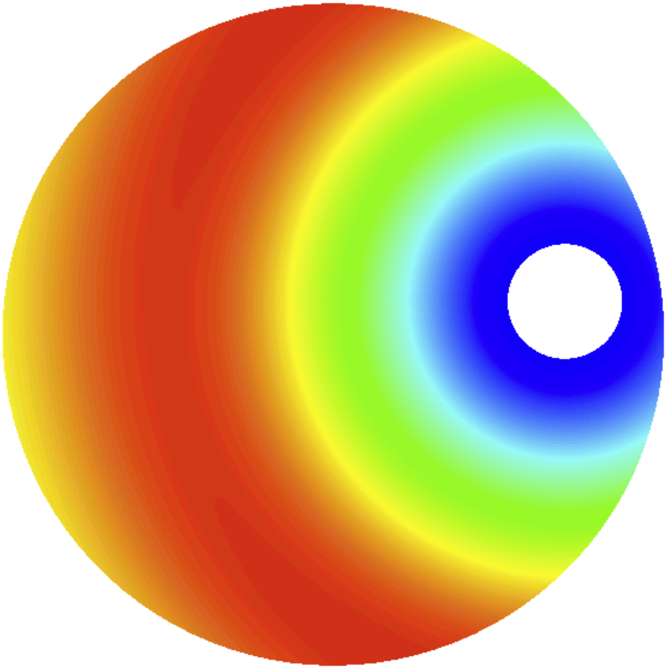


Slide 17

WTF19 need a picture here for virtual nodes/elements
Walsh, Timothy Francis, 7/24/2014

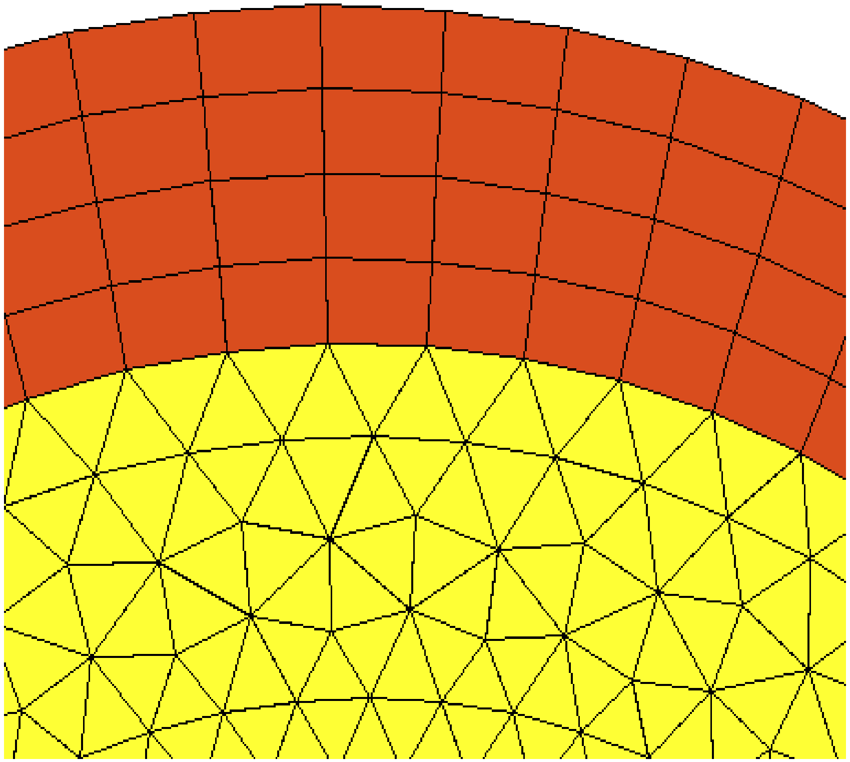
Results – Pressure on an offset Spherical Surface (Non Symmetric Domain)

- Acoustic velocity applied to inner sphere
- Solution is spherically symmetric about loading surface
- Compared to exact solution
- Solution obtained using GDSW Helmholtz Solver



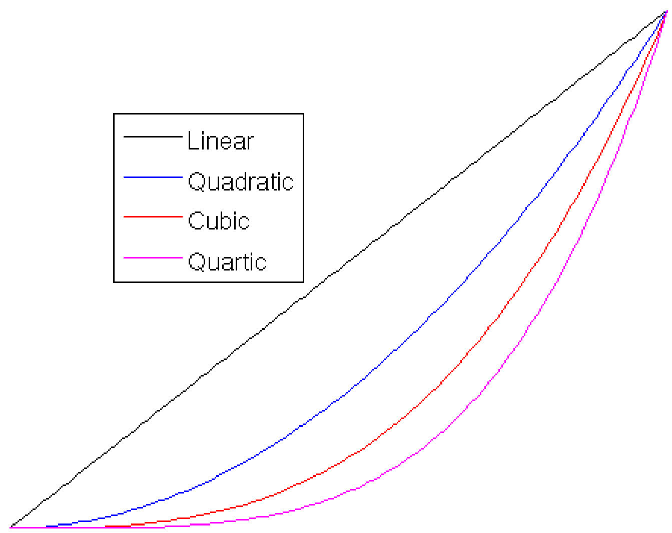
Loss Functions

- PML Inner Boundary can create reflections
  - Something we are specifically trying to avoid
  - How do we pick loss functions to get the best solution?

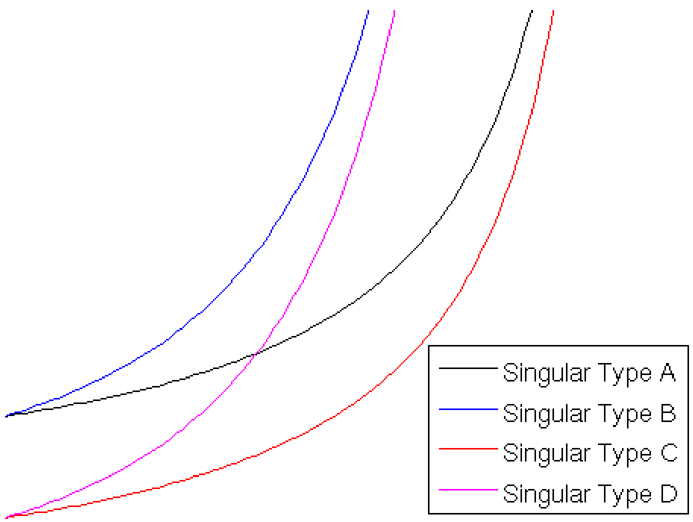


Types of Loss Functions

Polynomial



Singular



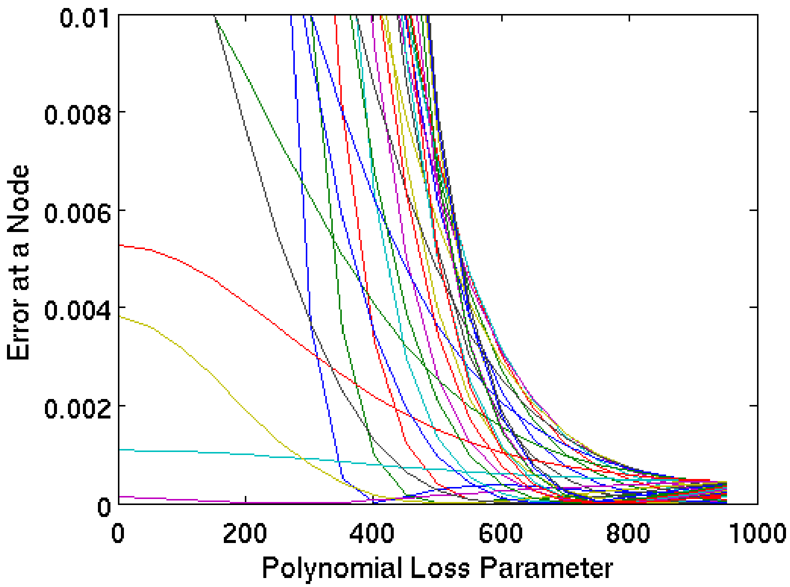
Types of Loss Functions Limitations in PML Literature

- Many PML papers include little to no numerical results
- Papers discussing loss functions tend to find that theirs is the best
- PML results are often shown for only one frequency
  - We want loss parameters that can be used for frequency sweeps

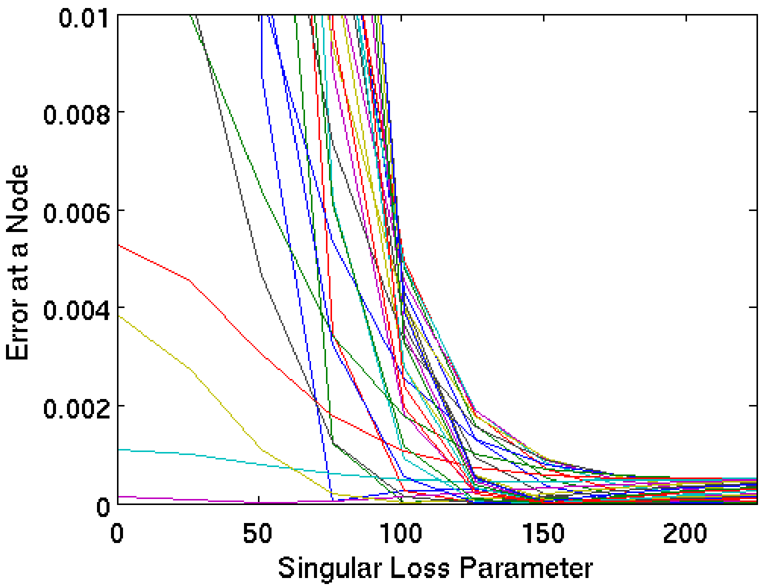
Results – Parameter Study – Loss Parameters

- Each color represents another frequency
  - Different frequencies have different discretization errors

Polynomial

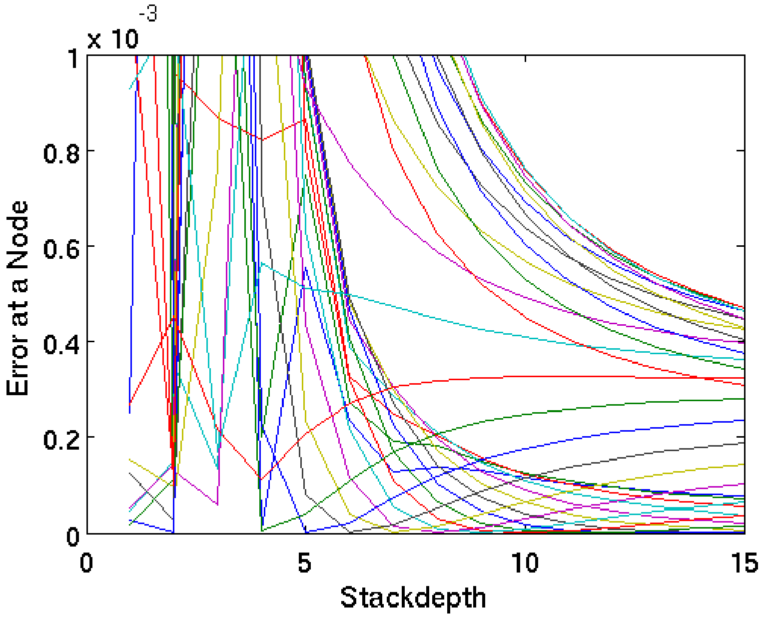


Singular

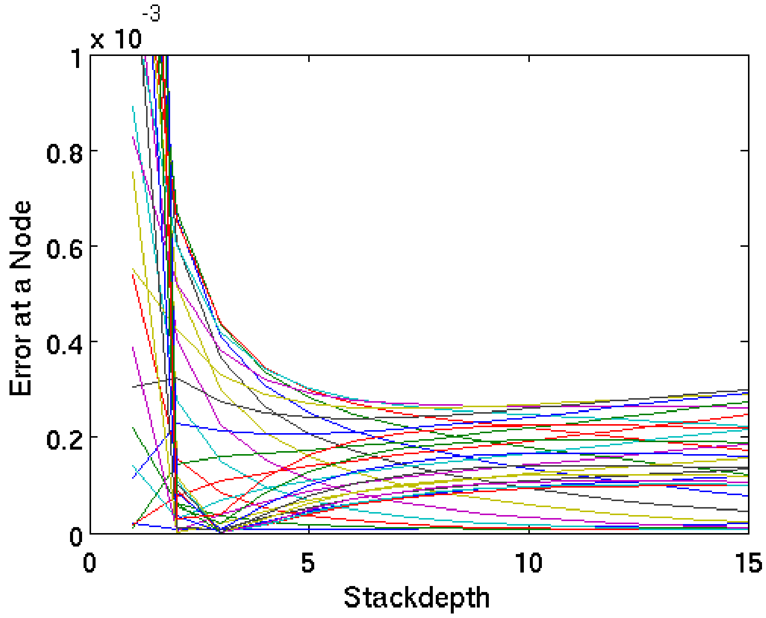


Results – Parameter Study – Stackdepth with Thickness = 2

Polynomial



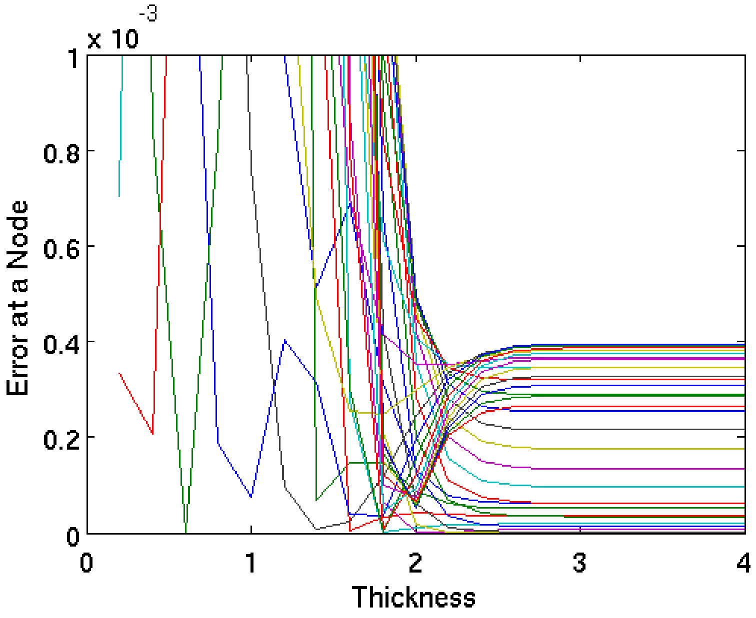
Singular



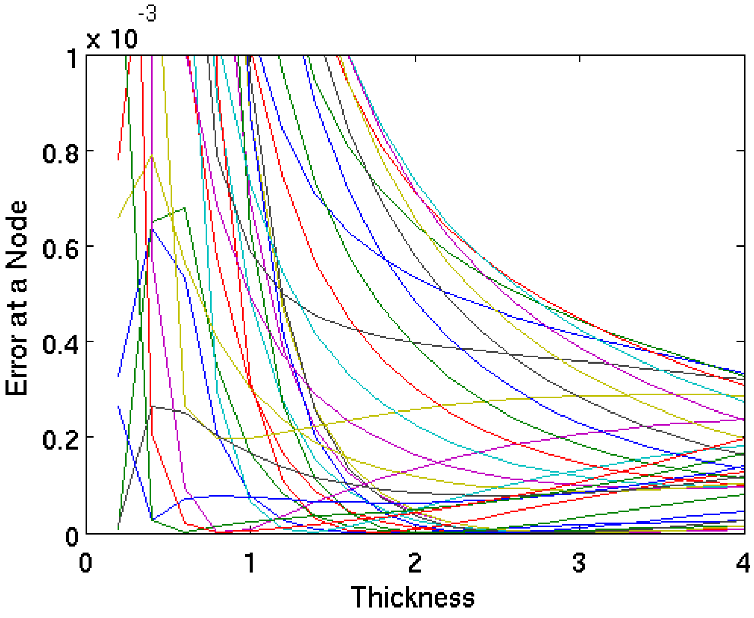
Results – Parameter Study Thickness, Stackdepth

- Increased thickness with constant element size

Polynomial



Singular



Results - Formulations

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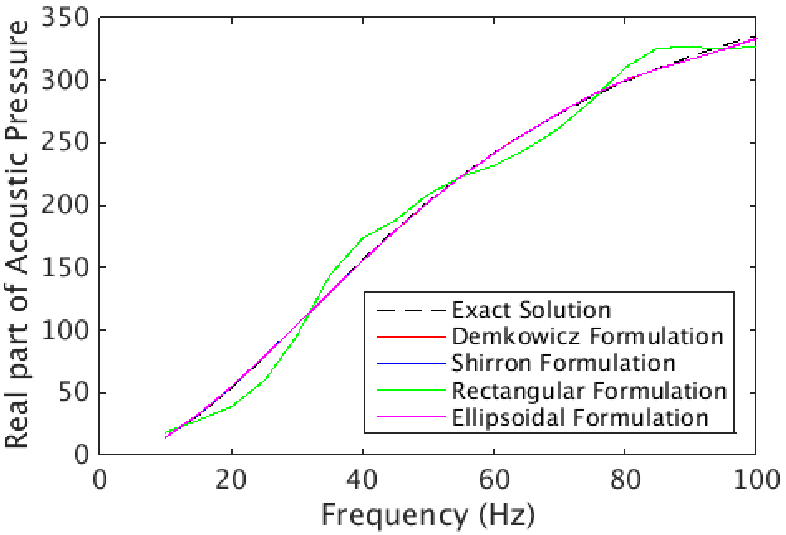
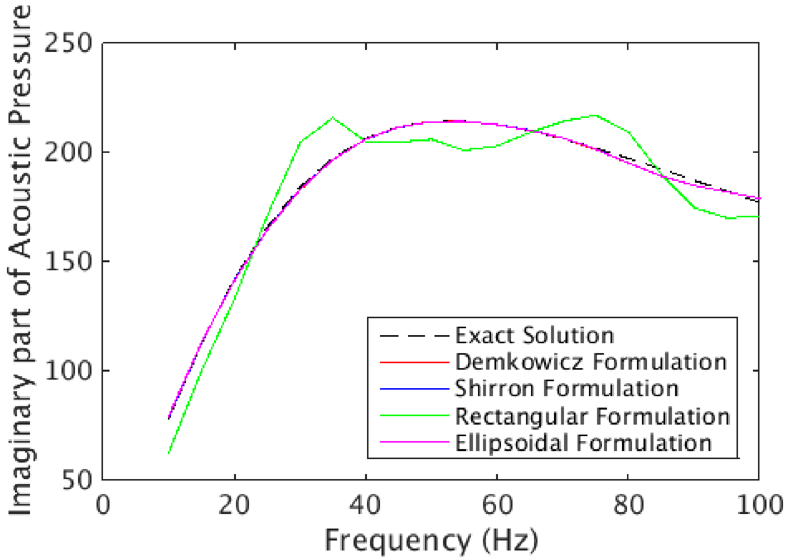
Real

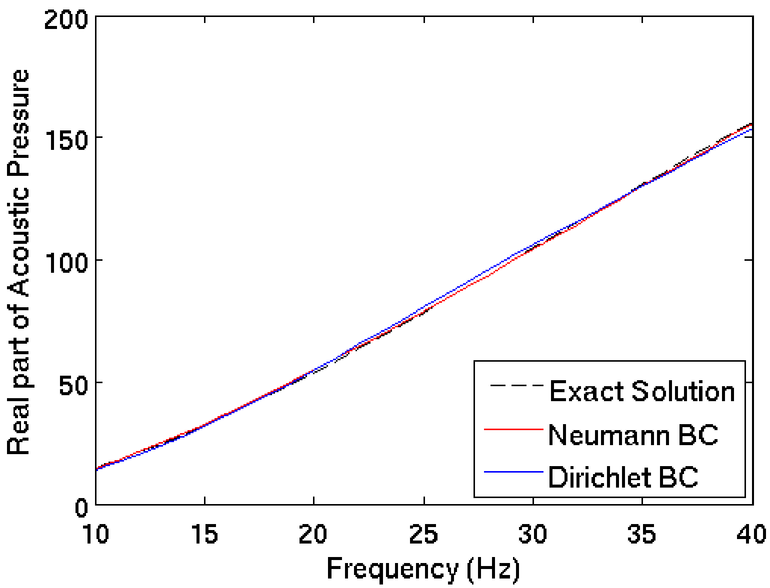


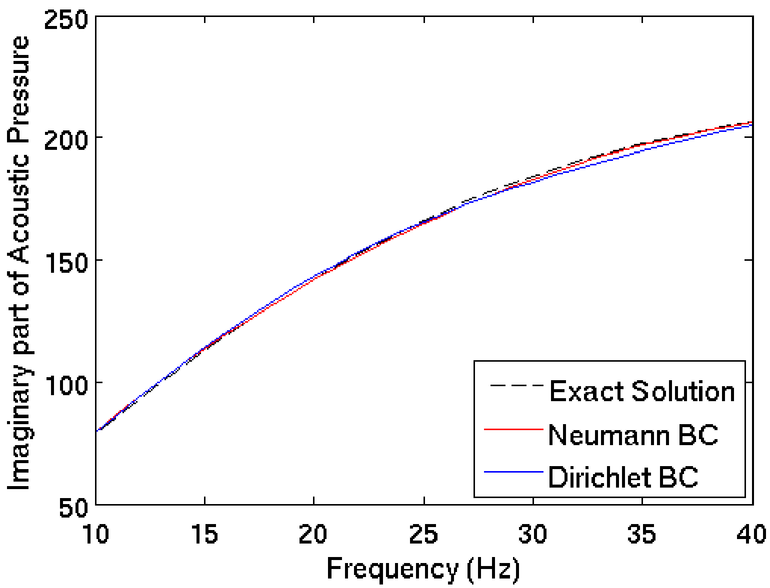
Imaginary



PML Theory – Neumann vs Dirichlet

- Expect Same Results
- Numerical Differences
- Neither is clearly better
- Do these have an effect on solve time?

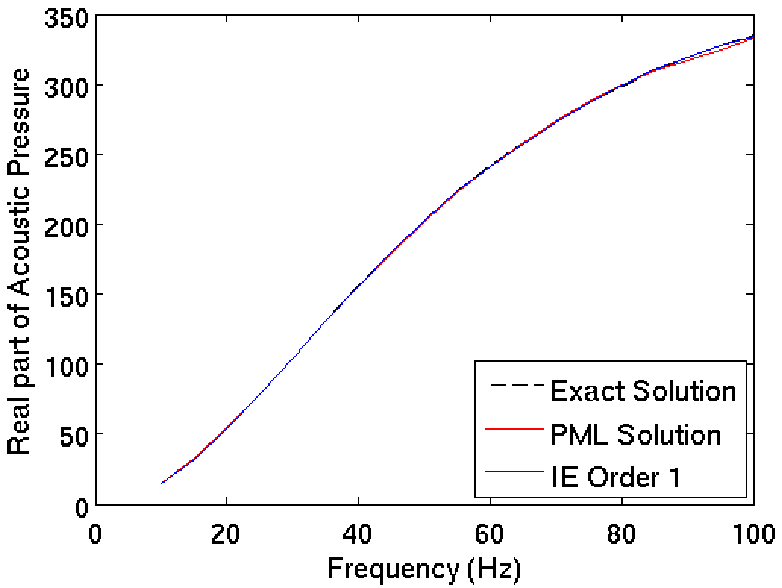




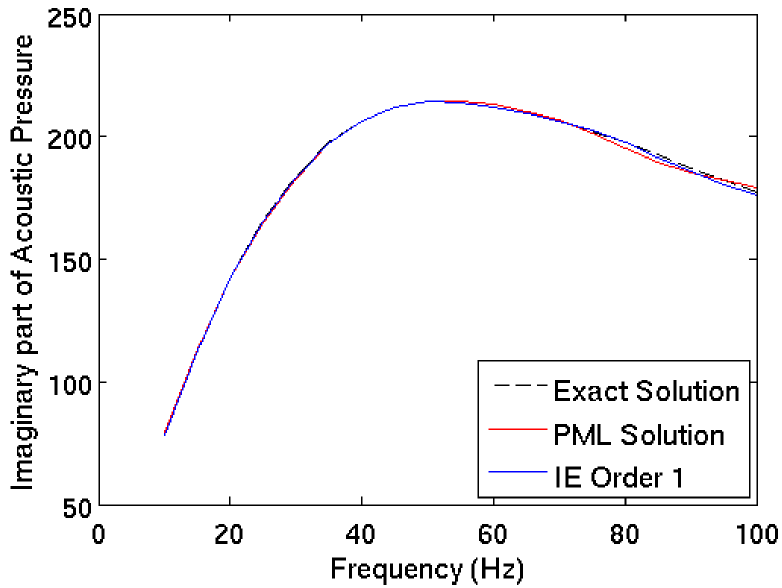
Comparison to Infinite Elements

- Results for sphere problem

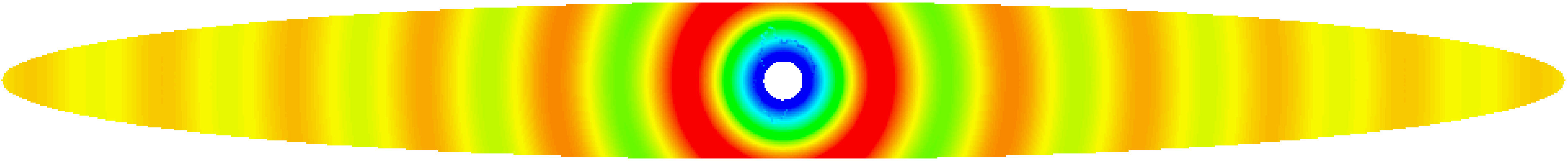
Real



Imaginary

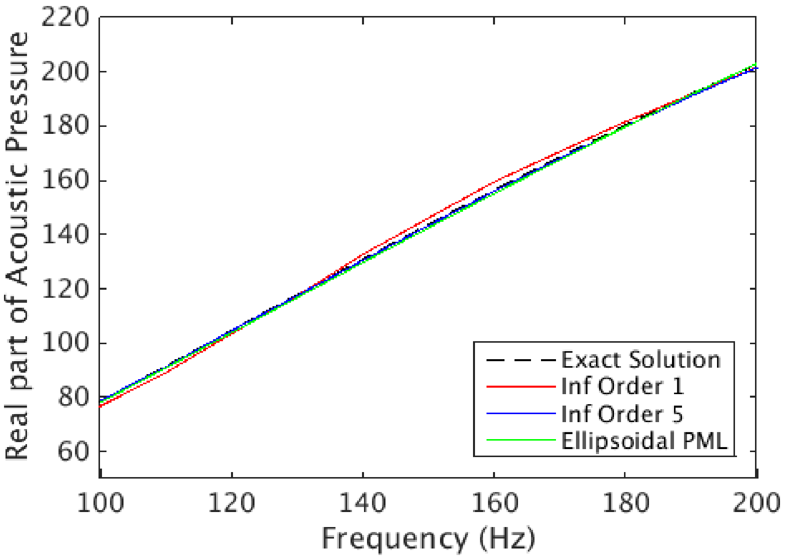


Comparison to Infinite Elements

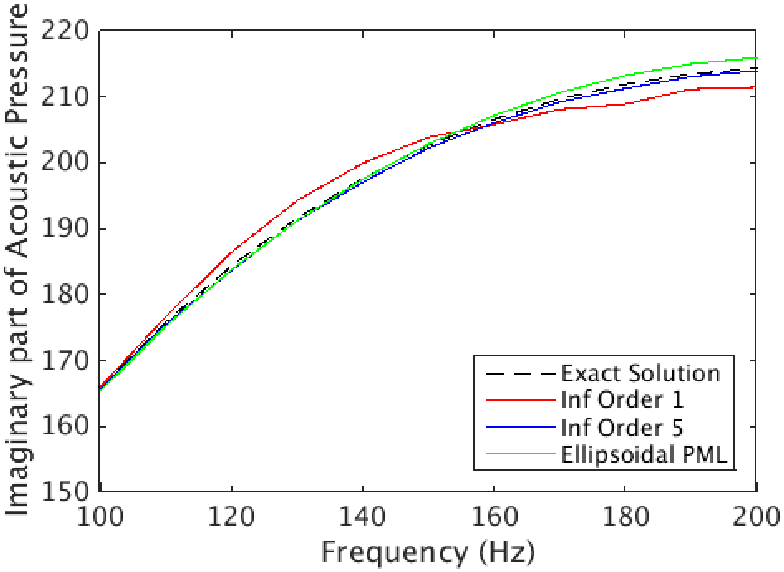


- Results for ellipse problem

Real



Imaginary



Conclusions

- We have one formulation that encompasses Ellipsoidal, Spherical, Cartesian, and rotated Cartesian
- Our results verify the literature for the spherical and Cartesian problems
- Our results on ellipsoidal are pending
- For structural acoustic problems, we recommend using the same PML parameters as the pure acoustic problem

Future Work

- Repeat analysis for ellipsoidal formulation
- Compare computational costs on massively parallel problems
- Time domain problems
- Surface waves

Acknowledgements

- Advisor – Arun Prakash
- Mentor – Tim Walsh
- Manager – Joe Jung
- Team - SierraSD

WTF20

Implementation – Use of Salinas Damping Matrix

$$Kp - \omega^2 Mp = f$$

$$\begin{aligned} K - \omega^2 M &= \Re\left[K - \omega^2 M\right] + i\Im\left[K - \omega^2 M\right] \\ &= \Re\left[K - \omega^2 M\right] + \frac{i\omega\Im\left[K - \omega^2 M\right]}{\omega} \\ &= \Re\left[K - \omega^2 M\right] + i\omega C \end{aligned}$$

$$C = \Im\frac{K - \omega^2 M}{\omega}$$

Slide 32

WTF20 may not be needed

Walsh, Timothy Francis, 7/24/2014

Implementation in Sierra-SD – Input Parser

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Perfectly Matched Layers

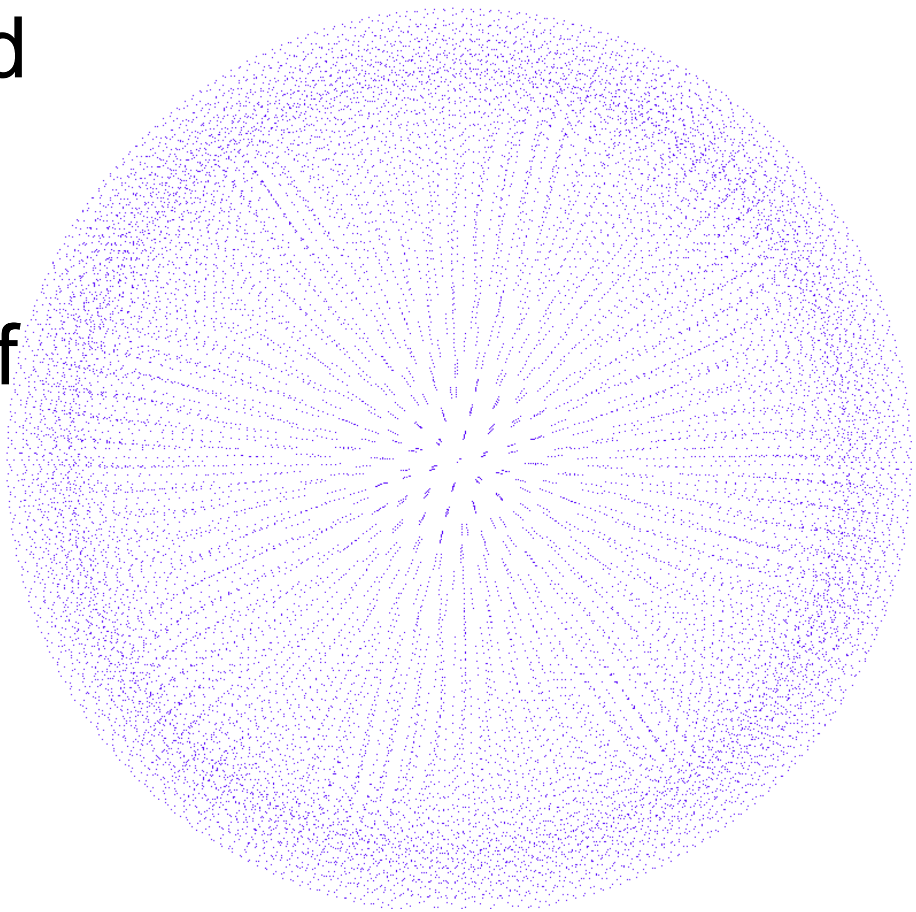
```
BOUNDARY
  sideset 2
    pml_element
    stack_depth 5
    ellipsoid_dimensions 5 5 5
    source_origin 0 0 0
    pml_thickness 1
    loss_function = polynomial
    loss_params = 0 960 960 960
    pmlDirichlet
END
```

Infinite Elements

```
BOUNDARY
  sideset 2
    infinite_element
    order = 3
    ellipsoid_dimensions 5 5 5
    source_origin 0 0 0
    neglect_mass yes
END
```

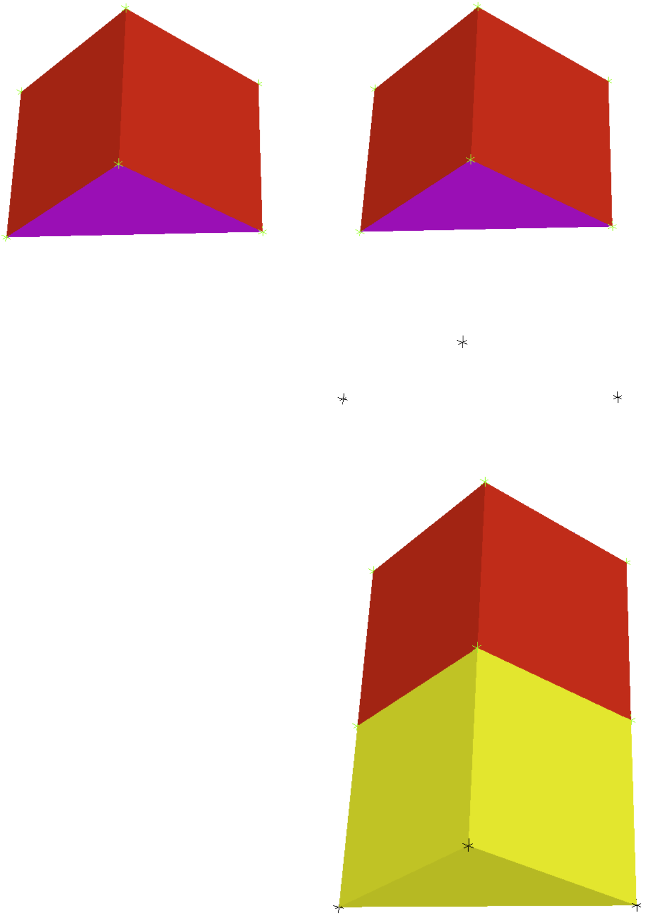
Implementation in Salinas – Virtual Nodes

- Nodes are meshed from original boundary nodes normal to center of sphere (or foci of ellipse)



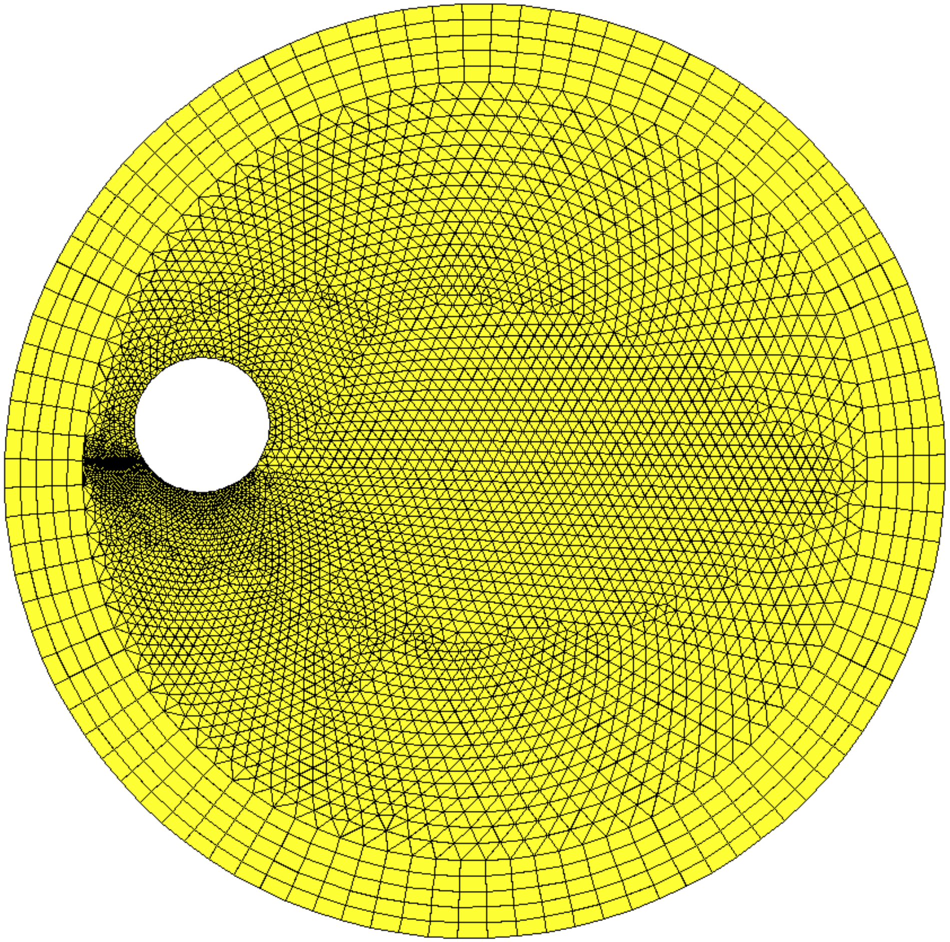
Implementation in Salinas – Virtual Meshing

- Elements are added to the nodes
- Each element knows it's location in the PML stack



Implementation in Salinas – Virtual Elements

- Wedge Elements are meshed out from tetmesh
- Hexes are not supported



Slide 36

WTF25 I would combine slides 18 and 20

Walsh, Timothy Francis, 7/24/2014