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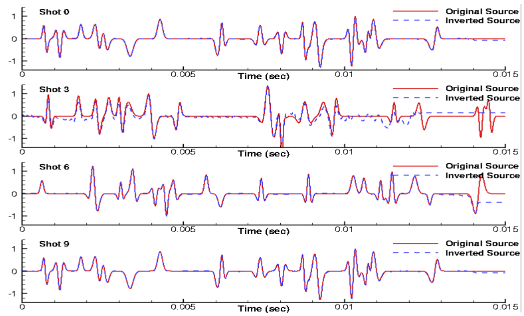

Large-Scale Optimization for Non-Invasive Testing with Discontinuous Galerkin Methods

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Sandia National Laboratories

Exceptional service in the national interest

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Non-Invasive Testing

- … determine the characteristics engineering systems without disassembling or damaging them.
- Source Inversion
  - Interested in mimicing operational conditions within an experimental setup to test conditions throughout the system
  - Direct Field Acoustic Testing – DFAT
    - Acoustic testing of aerospace structures
    - Use an array of acoustic drivers
- Material inversion
  - Characterize material properties
  - Aging, cracks
  - Miss-assembly
  - DFAT and ultrasonic testing

Direct Field Acoustic Testing

http://en.wikipedia.org/wiki/Direct_Field_Acoustic_Testing

Constrained Optimization Problem

$$\min_{\mathbf{\Phi}} J(\mathbf{U}, \mathbf{\Phi}) \equiv \frac{1}{2} \sum_{s=1}^{N_s} \sum_{r=1}^{N_r} \int_{\mathsf{Q}} \xi_{s,r}(\mathbf{x}) \, \left\| \mathsf{R} \left(\mathbf{U}_s - \hat{\mathbf{U}}_s \right) \right\|^2 \, d\mathsf{Q} + \frac{\beta}{2} \int_{\Omega} \left\| \mathsf{R} \left(\mathbf{\Phi} \right) \right\|^2 \, d\Omega$$

- Subject to the acoustic wave equation

$$\frac{\partial p}{\partial t} + \kappa \frac{\partial v_i}{\partial x_i} = -\frac{1}{3} \frac{\partial m_{ii}^{iso}}{\partial t} \quad \text{in } \Omega \times (0, T]$$

$$\rho \frac{\partial v_i}{\partial t} + \frac{\partial p}{\partial x_i} = f_i + \frac{\partial m_{ij}^{dev}}{\partial x_j} \quad \text{in } \Omega \times (0, T]$$

$$p(\mathbf{x}, 0) = 0 \quad \text{for } \mathbf{x} \in \Omega$$

$$v_i(\mathbf{x}, 0) = 0 \quad \text{for } \mathbf{x} \in \Omega$$

$$\mathbf{U} = (p, v_i)^T$$

$$\kappa = \rho c^2 - \text{bulk modulus}$$

$$\rho = \text{mass density}$$

$$c = \text{wave speed}$$

$$f_i = \text{force density}$$

$$m_{ij} = m_{ij}^{iso} + m_{ij}^{dev} - \text{moment density tensor}$$

$$m_{ij}^{iso} \equiv \frac{1}{3} m_{kk} \delta_{ij}$$

$$\Omega = \text{computational domain}$$

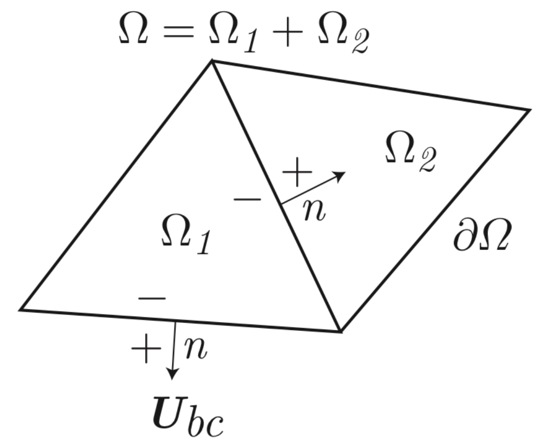
$$T = \text{time horizon}$$

$$\xi_{s,r} = \text{receiver spatial kernel for shot } s$$

$$\mathsf{R} = \text{selection operator}$$

$$\mathbf{\Phi} = \text{optimization parameters}$$

Discontinuous Galerkin



Strong form:

$$\mathbf{U}_{,t} + \mathbf{F}_{i,i} = \mathbf{S}, \quad \text{in } \Omega$$

$$\mathbf{U}(x,0) = \mathbf{U}_0(x) \quad \text{at } t = 0$$

and appropriate boundary conditions on $\partial\Omega$.

Partition Ω into N subdomains Ω_e.

$$\int_{\Omega_e} \left(\mathbf{W}^T\mathbf{U}_{,t} - \mathbf{W}^T_{,i}\mathbf{F}_i\right) d\Omega + \int_{\partial\Omega_e} \mathbf{W}^T\mathbf{F}_n \, d\Gamma = \int_{\Omega_e} \mathbf{W}^T\mathbf{S} \, d\Omega$$

Introduce numerical fluxes $\mathbf{F}_n(\mathbf{U}) \rightarrow \hat{\mathbf{F}}_n(\mathbf{U}^-, \mathbf{U}^+)$ and sum over all elements

$$\sum_{e=1}^{N_e} \int_{\Omega_e} \left(\mathbf{W}^T\mathbf{U}_{,t} - \mathbf{W}^T_{,i}\mathbf{F}_i - \mathbf{W}^T\mathbf{S}\right) d\Omega + \int_{\partial\Omega_e} \mathbf{W}^T\hat{\mathbf{F}}_n \, d\Gamma = 0$$

$$\sum_{e=1}^{N_e} \int_{\Omega_e} \left(\mathbf{W}^T\mathbf{U}_{,t} + \mathbf{W}^T\mathbf{F}_{i,i} - \mathbf{W}^T\mathbf{S}\right) d\Omega + \int_{\partial\Omega_e} \mathbf{W}^T \left(\hat{\mathbf{F}}_n - \mathbf{F}_n\right) \, d\Gamma = 0$$

for all $\boldsymbol{W} \in \mathcal{V}$.

DGM Software

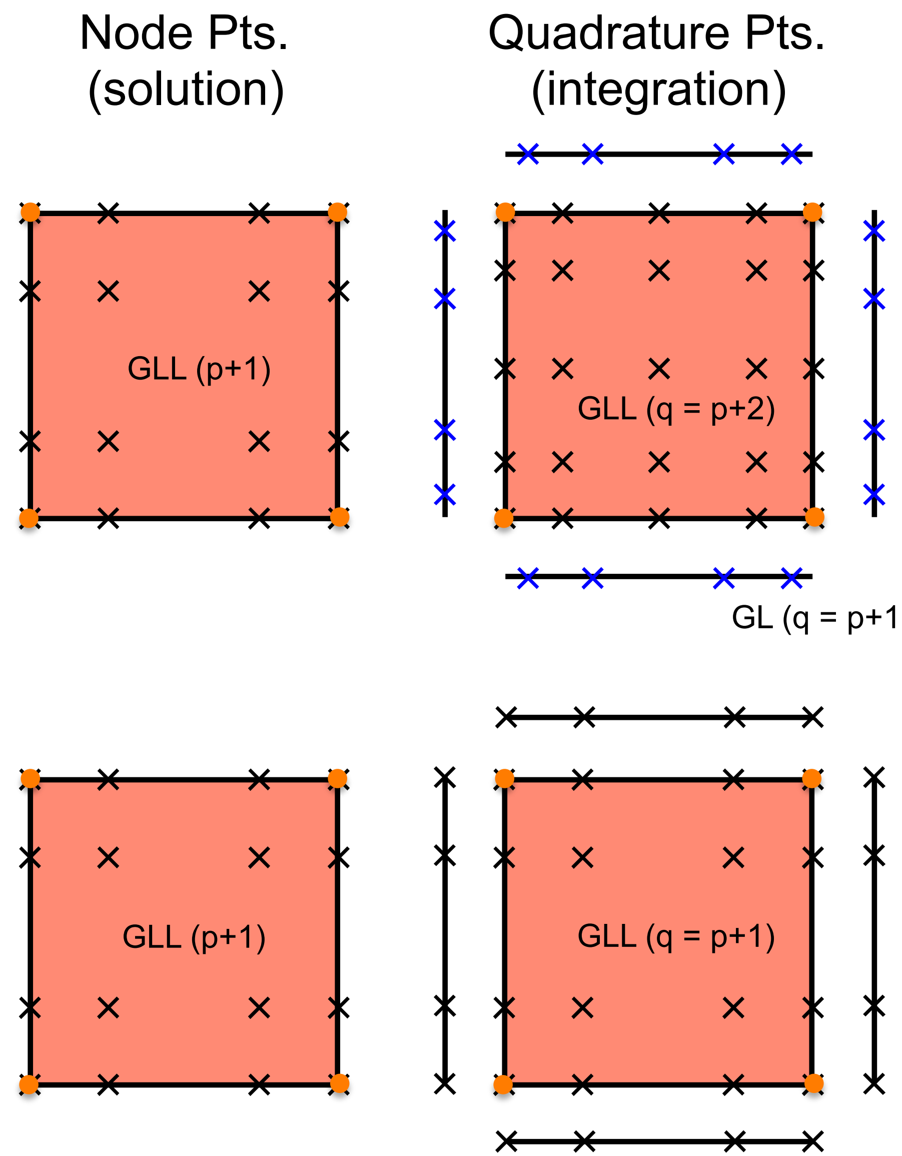
- Variety of physics
  - In- & compressible Euler, compressible Navier-Stokes (with LES)
  - Darcy, Helmholtz, Wave equation
- High-order DG on unstructured meshes (low dispersion)
  - Modal elements: Line, Quad, Tri, Hex
  - Nodal elements: Line, Quad, Tri, Hex, Tet
  - Spectral Elements: Line, Quad, Hex
  - Curved elements and hybrid meshes
  - Variable-order polynomial representation (For both solution and media)
  - Local polynomial and mesh refinement
  - Various flux functions (Lax-Friedrichs, Steger-Warming, Riemann)
- Range of explicit and implicit time integrators
  - Forward & Backward Euler, Trapezoidal, 4^{th} Order Runge-Kutta (low dispersion)
- Designed for adjoint-based optimization
  - ROL, PEOpt, Dakota, MOOCHO, Aristos
  - Steady-state and transient with check pointing

Modal vs. Nodal vs. Spectral

	Modal (Karniadakis & Sherwin, 2005, Collis, 2002)	**Nodal** (Hesthaven & Warburton, 2000; Kaser & Dumbser, 2006, 2008)	**Spectral** (Karniadakis & Sherwin, 2005)
Elements	Line, Tri,Quad, Hex	Line, Tri, Quad, Hex, Tet	Line, Quad, Hex
DoFs	coefficients of polynomial bases	nodes of the Lagrange polynomials	GLL nodes
Interpolation	transform/Lagrange	Lagrange	Lagrange sampled at Legendre zeros
Mass term integration	constant for affine elements, Gauss quadrature for non-affine	orthogonal bases – exact integration for affine elements, Gauss quadrature for non-affine	diagonal for affine and non-affine elements
Volume Integration	Gauss-Lobatto quadrature Q≥P+2; exact integration	orthogonal bases – exact analytic	Gauss-Lobatto quadrature, Q=P+1
Surface integration/ Flux data	interpolate on face, Gauss quadrature Qedg=P+1	data is native to face – no interpolation- exact integration	no interpolation for constant P, face interpolation for non-const. P
Media	variable within element	constant within element	variable within element
Element Jacobian	variable within element	constant over element	variable within element
Non-linear terms	increase number of quadrature points GLL	filter or use quadrature	filter high modes (de-alias)

Modal and Spectral Elements

- Modal (more accurate)
  - Uses Legendre basis (modes)
  - Uses quadrature for all integrals
  - Can exactly integrate higher-order polynomial products by increasing quadrature ($q \geq p+2$)
  - Requires interpolation from nodes to quad pts.
  - For affine elements, mass matrix is constant and easily inverted and stored.
  - For non-affine elements, mass matrix is dense and needs inverting every time step and stage.
- In Common
  - Uses tensor-products of orthogonal polynomials
  - Support spatially variable polynomial order
  - Variable media, nonlinearities, & non-affine elements produce higher-order polynomial products
- Spectral (less accurate; less expensive)
  - Uses Lagrange basis on optimal node distributions
  - Under integrates higher-order polynomial products because of fixed quadrature ($q = p+1$)
  - May need to resort to modal or inexact quadrature + filtering for higher-order polynomial products
  - No interpolation required.
  - For affine & non-affine elements, mass matrix is diagonal and easily inverted.



× - Gauss-Labatto-Legendre (GLL); × - Gauss-Legendre (GL)

Numerical Fluxes

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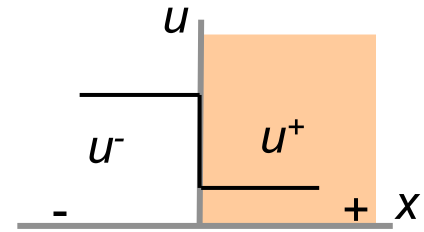
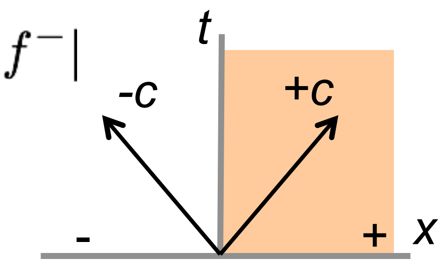


- Riemann Flux (Exact flux)
  - Conversative form $u_{,t} + f_{,x} = 0$ not $u_{,t} + c\,u_{,x} = 0$
  - Rankine-Hugoniot Jump Conditions $c|u^+ - u^-| = |f^+ - f^-|$
  - Entropy Conditions



- Flux, flux Jacobian, and eigenvalues are

$$\boldsymbol{F}_n = (\boldsymbol{A}_n \boldsymbol{U}) \qquad \boldsymbol{A}_i \equiv \frac{\partial \boldsymbol{F}_i}{\partial \boldsymbol{U}}$$

$$\begin{aligned} \boldsymbol{\Lambda} &= \quad diag\{\lambda_1, ..., \lambda_N\} \\ &= \quad diag\{eigen(\boldsymbol{A}_n)\} \end{aligned}$$

- Lax-Friedrich Flux

$$\hat{\boldsymbol{F}}_n(\boldsymbol{U}^-, \boldsymbol{U}^+) = \frac{1}{2}\left[\boldsymbol{F}_n^- + \boldsymbol{F}_n^+ + \xi\left(\boldsymbol{U}^- - \boldsymbol{U}^+\right)\right] \qquad \xi = \max|\lambda_i|$$

- Steger-Warming Flux (Flux-Vector Splitting)

$$\boldsymbol{A}_n = \boldsymbol{A}^+ + \boldsymbol{A}^- = \boldsymbol{T}\boldsymbol{\Lambda}^+\boldsymbol{T}^{-1} + \boldsymbol{T}\boldsymbol{\Lambda}^-\boldsymbol{T}^{-1} \qquad \boldsymbol{\Lambda}^\pm = \left(\boldsymbol{\Lambda} \pm |\boldsymbol{\Lambda}|\right)/2$$

$$\hat{\boldsymbol{F}}_n = \frac{1}{2}\left[\boldsymbol{A}_n^- \boldsymbol{U}^- + \boldsymbol{A}_n^- \boldsymbol{U}^+ + |\boldsymbol{A}_n|\left(\boldsymbol{U}^- - \boldsymbol{U}^+\right)\right] \qquad |\boldsymbol{A}| = \boldsymbol{T}\,|\boldsymbol{\Lambda}|\,\boldsymbol{T}^{-1}$$

Optimization Software

- Rapid Optimization Library (ROL)
  - Release within Trilinos in October 2014
  - Rewrite and consolidation of existing tools
    - PEOpt, Aristos, Moocho, Optipack
  - Lead developers: Drew Kouri (primary) and Denis Ridzal
  - Unconstrained optimization
    - Gradient descent, quasi-Newton, nonlinear CG, inexact Newton (FD Hessvecs), with line searches and trust regions.
  - Inequality constraints
    - Box constraints using projected gradient and projected Newton methods

ROL: Methods – FD Hessvecs

$$\min_z J(z)$$

- Goal: Obtain near quadratic convergence from Newton-CG with finite difference Hessian-times-a-vector
  - Set $H(z,v,t) = \left[\nabla J(z+tv) - \nabla J(z)\right]/t$
  - Apply inexact CG to Newton system: $H(z_k, s, t) = -\nabla J(z_k)$
  - At j^{th} iteration of inexact CG require:

    $$\|H(z_k, v_j, t_j) - \nabla^2 J(z_k) v_j\| \leq c_m \varepsilon_k / \|r_{j-1}\|$$

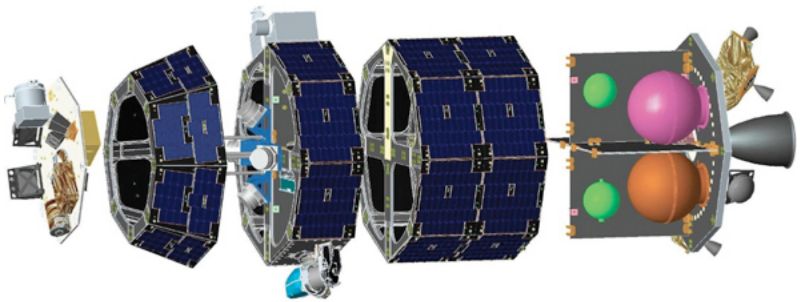
    - Constant depending on max # CG iterations, c_m
    - Previous inexact G residual, ε_k
    - Tolerance governed by inexact Newton's method, r_{j-1}

ROL: Methods – FD Hessvecs

- Convergence
  - Standard assumptions for Newton's
    - If $\nabla^2 J(z)$ is Lipschitz then $\|H(z,v,t) - \nabla^2 J(z)v\| = \mathcal{O}(t)$
  - Error between inexact and true CG residuals is ε_k
    - Simoncini and Szyld 2002
  - Inexact Newton's Methods: Can satisfy Krylov tolerances which ensure superlinear or quadratic convergence.
- Notes
  - FD Hessvecs require an additional gradient computation per CG iteration
  - $t_j = \varepsilon_k / (\|v_j\| \|r_{j-1}\|)$ works well in practice.
  - Use line search to globalize new step.

Mock Satellite

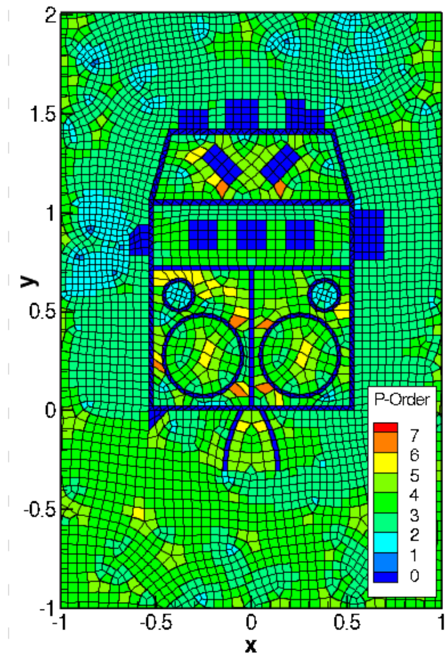
- Modeling structure after
  - NASA Ames Lunar Atmosphere Dust and Environment Explorer (LADEE)
  - Crude 2D representation to demonstrate capabilities



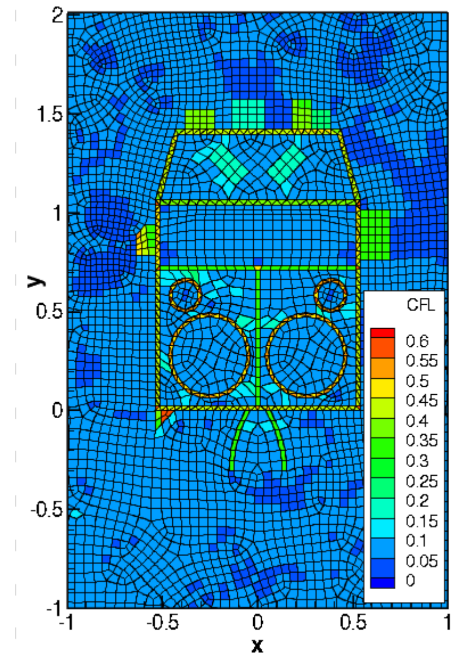
http://machinedesign.com/cad/software-lets-spacecraft-carry-heavier-loads

Mesh

Polynomial Order

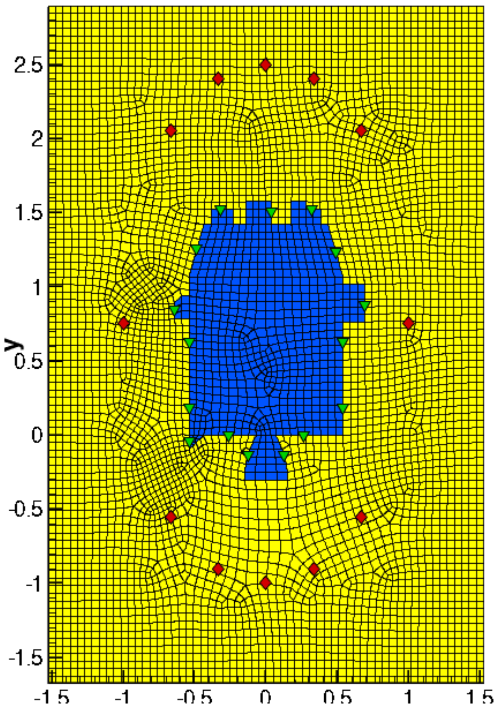


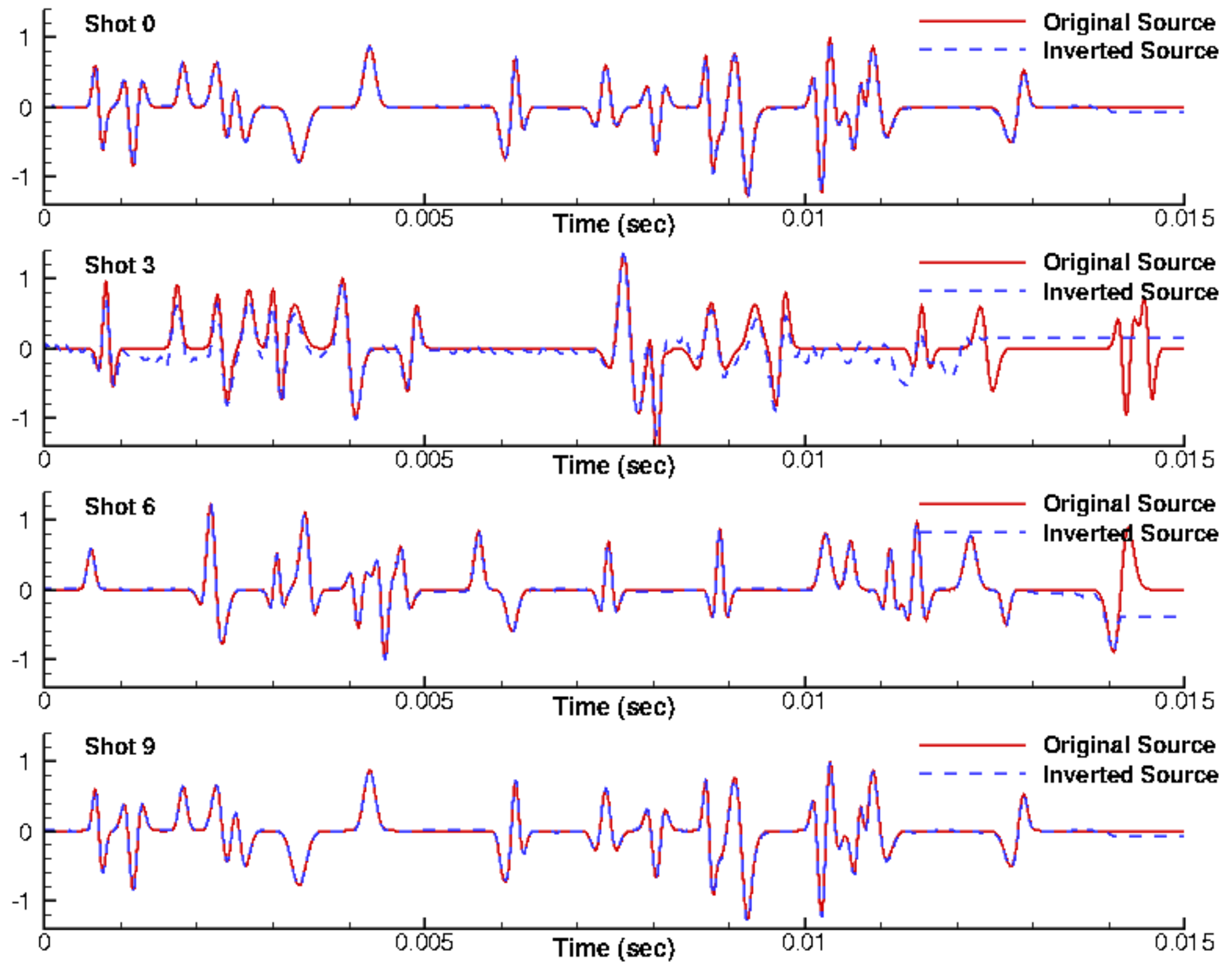
CFL



2D Source Inversion

- 12 sources
- Inversion crime
- Supershot





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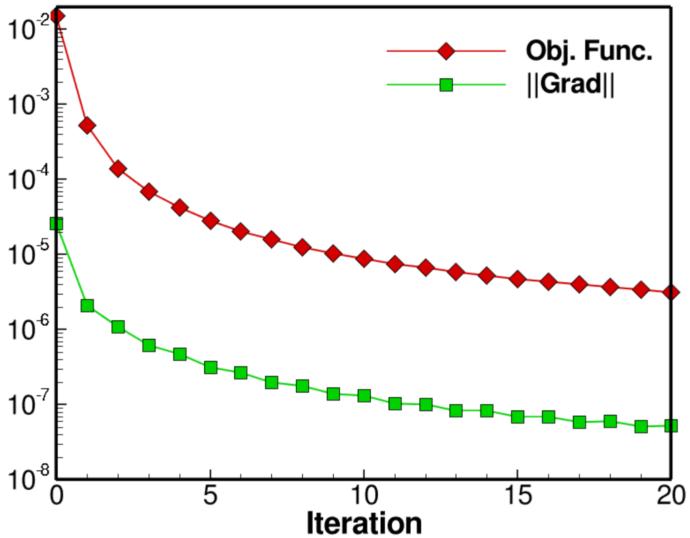
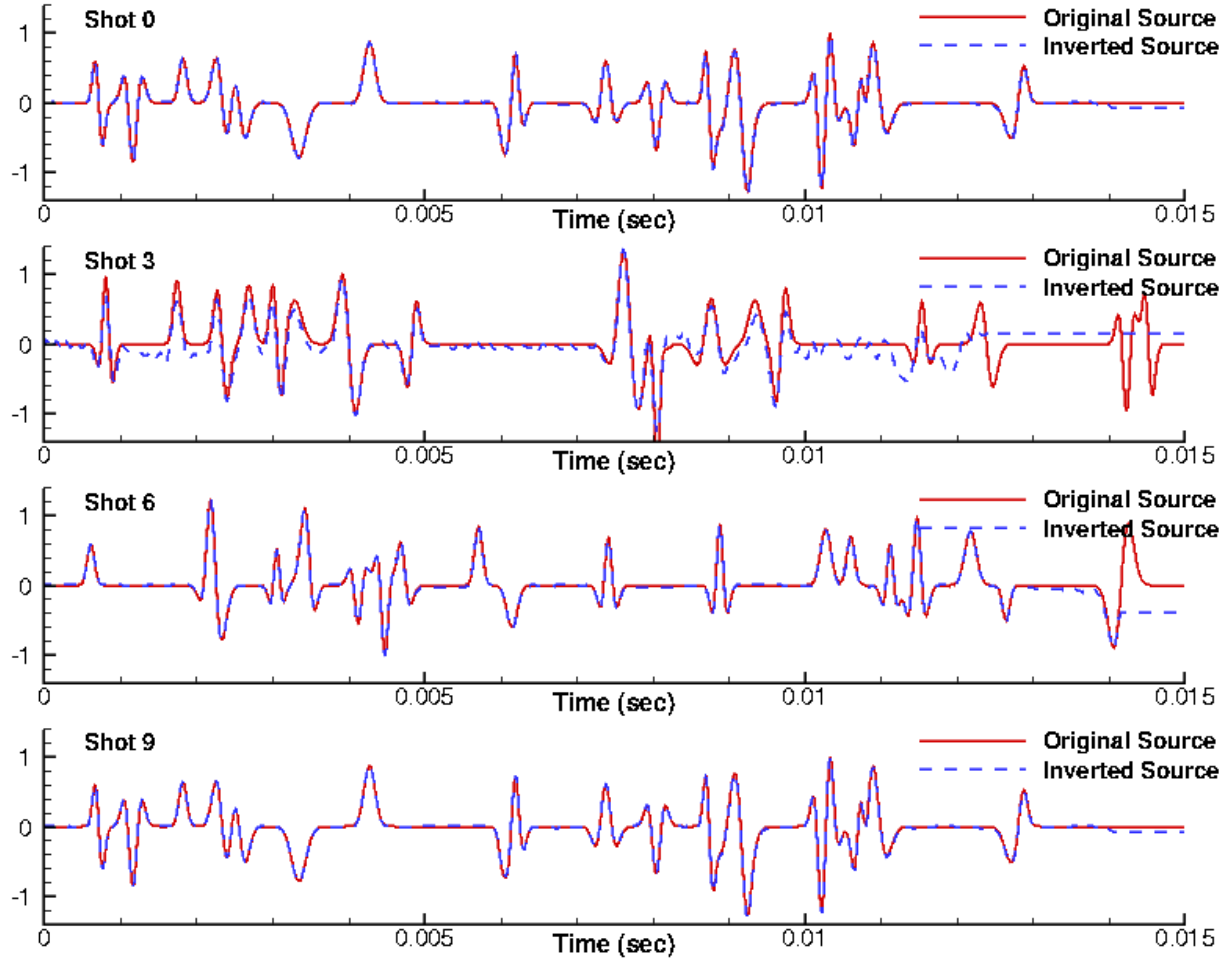
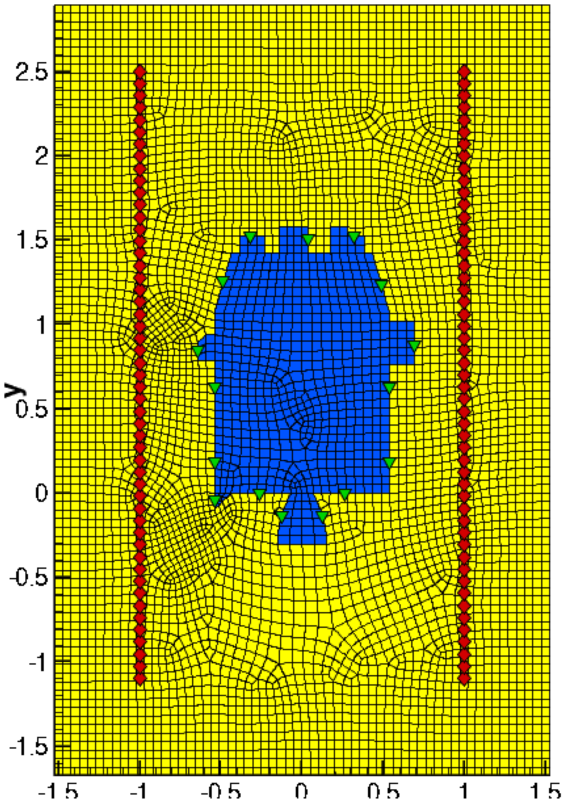
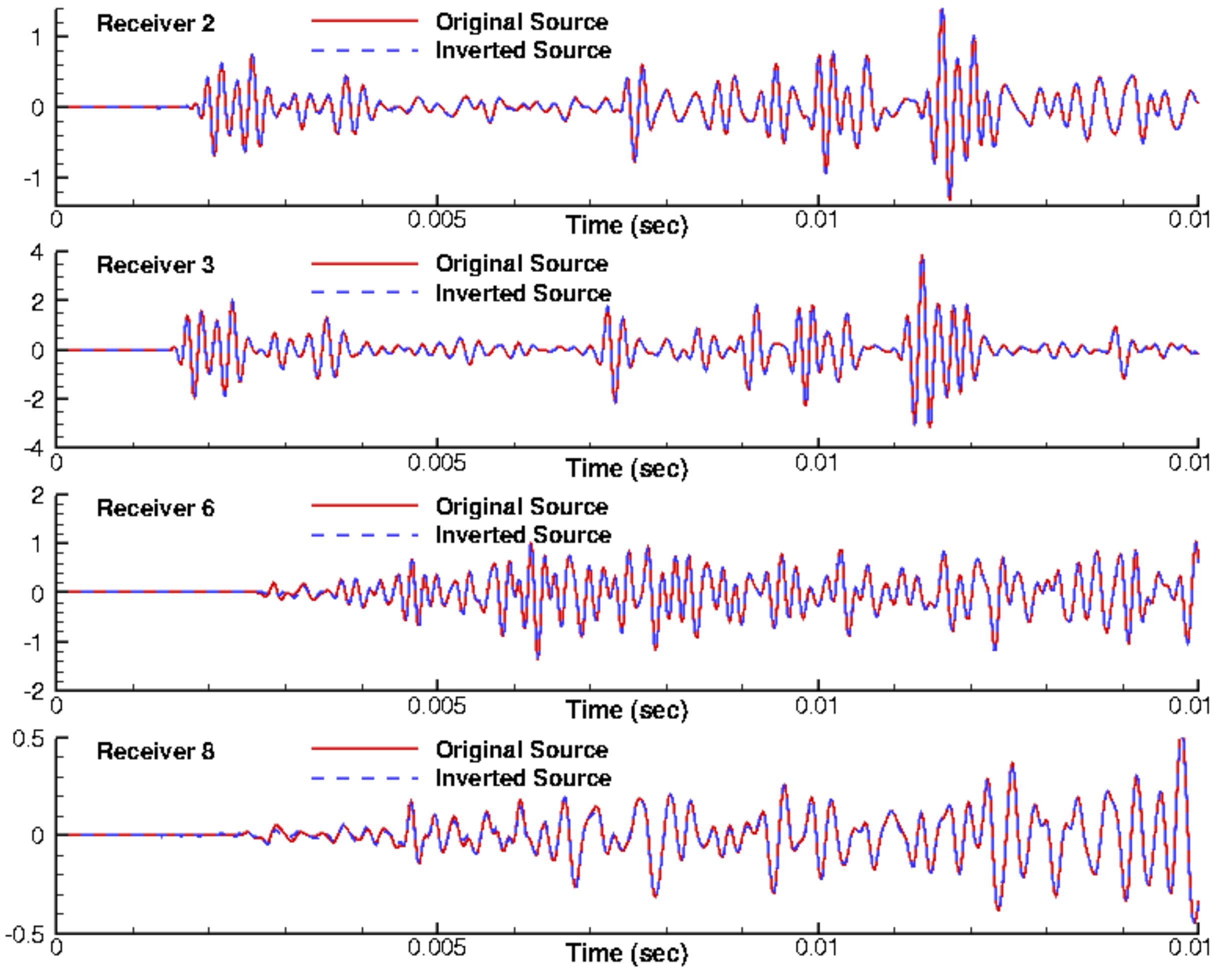




2D Source Inversion

- 102 sources
- Supershot





2D Source Inversion

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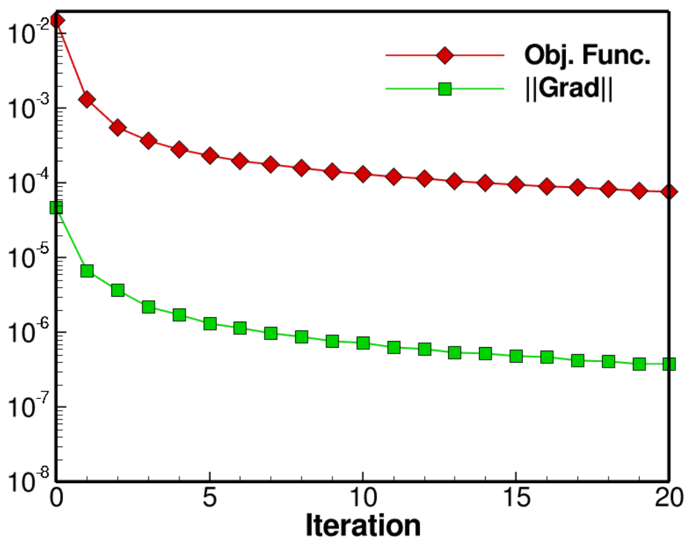
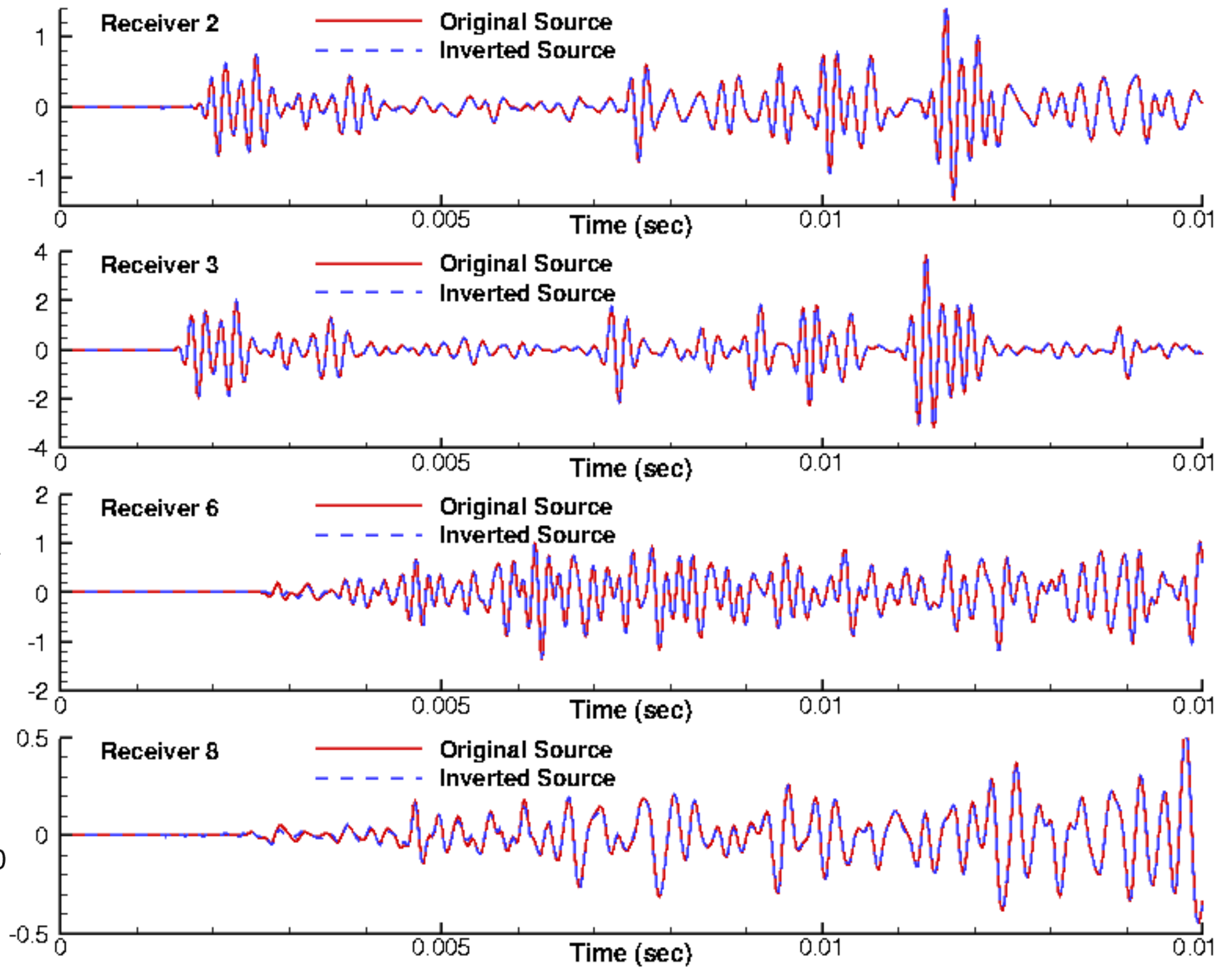
- Supershot





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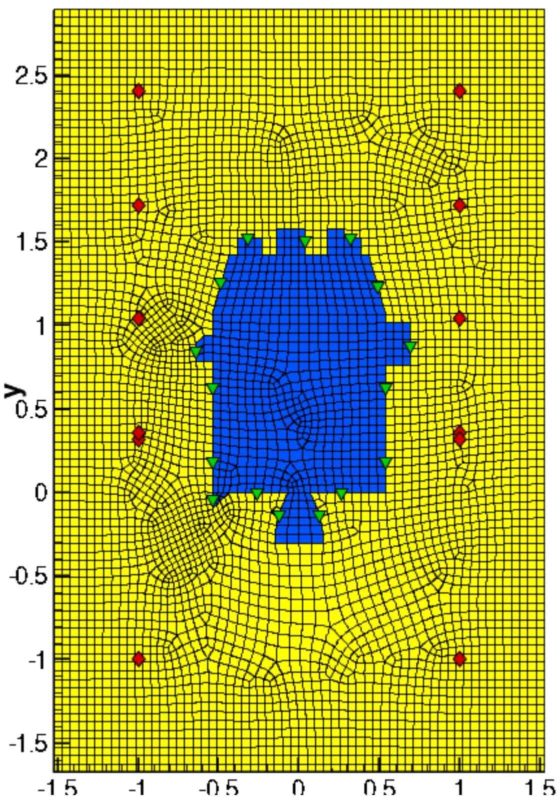

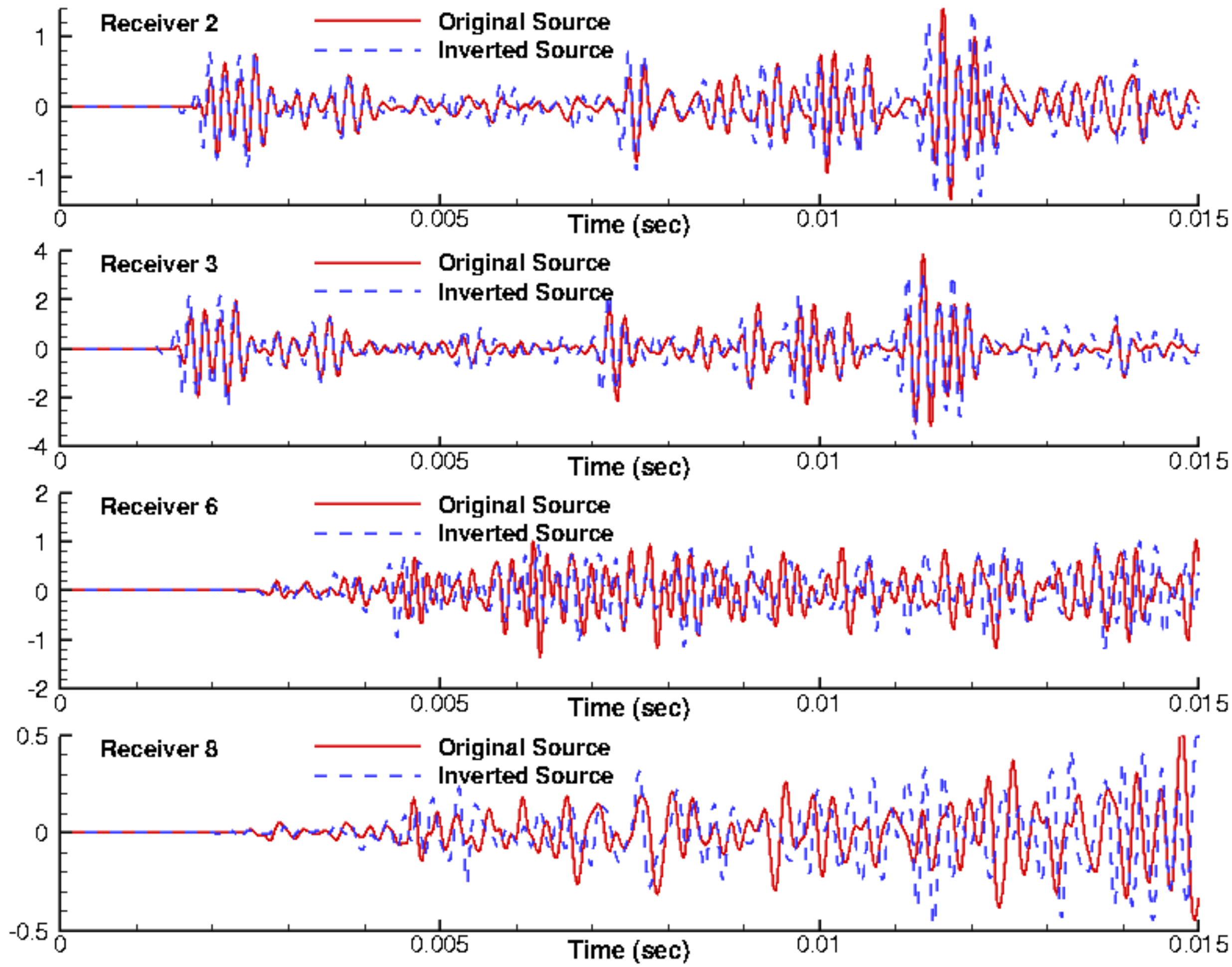

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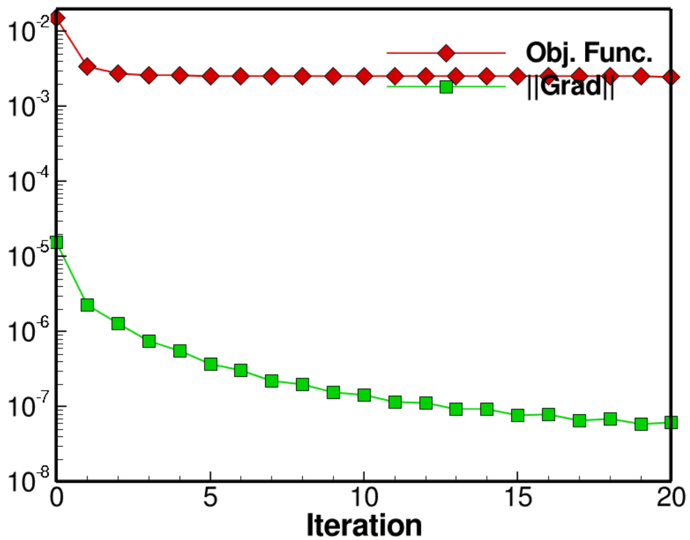
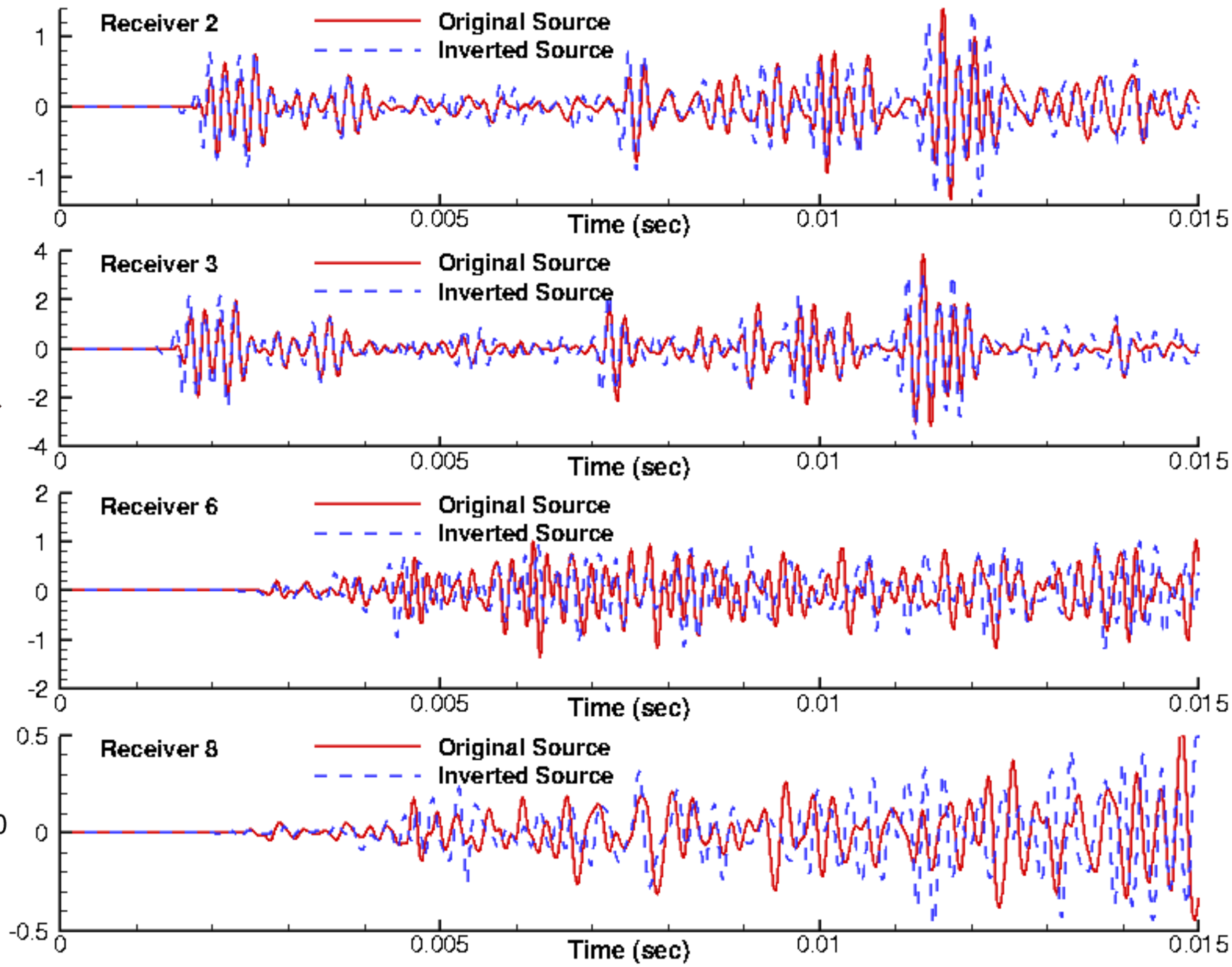
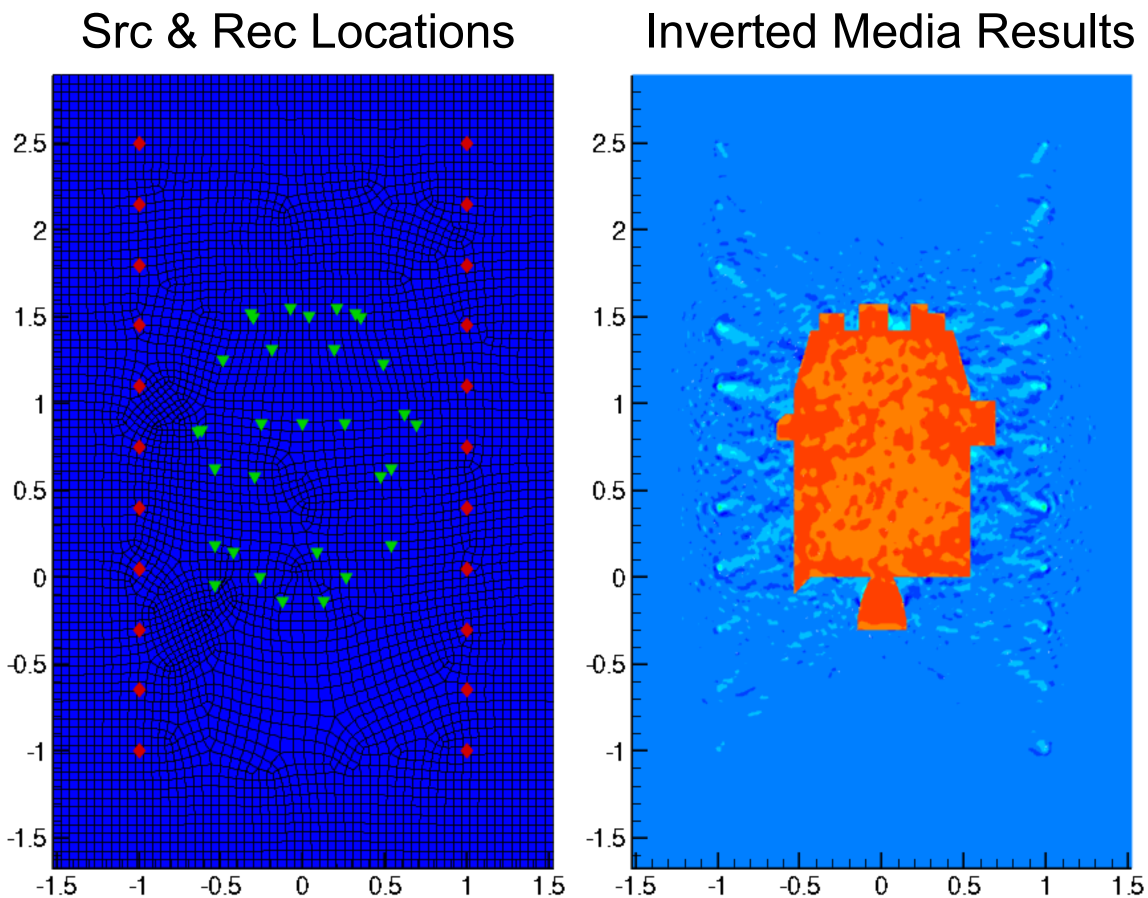




2D Material Inversion

- 22 individual sources
- 31 receivers
  - 16 on surface
  - 15 on the interior
- Sim time T = 0.015 sec.
- Constant p = 4
- Absorbing BCs
- After 11 iterations



Summary

- Demonstration of DG inversion for non-invasive testing
  - Low dispersion properties allows coarser mesh
  - Variable p-order mesh allows matching order to wavelengths for every element size
  - 2D hybrid mesh using triangles and quadrilaterals
- Source inversion to mimic launch conditions
  - Open question whether there is enough speakers
- Material inversion
  - Initial work promising