Boundary Perturbation Methods for Interface Reconstruction

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Collaborators and References

Collaborators on this project:

- Alison Malcolm (Earth Sciences, MIT)
- Zheng Fang (UIC)

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- DOE (DE–SC0001549)

References:

- Malcolm & DPN, "A Boundary Perturbation Method for Recovering Interface Shapes in Layered Media," *Inverse Problems*, 27 (2011).
- Malcolm & DPN, "Operator Expansions and Constrained Quadratic Optimization for Interface Reconstruction: Impenetrable Acoustic Media," *submitted*.

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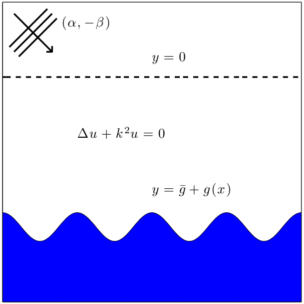
The Objective: What We Would Like to Do

- We would like to model the earth as a three–dimensional, layered media with a general crust–atmosphere interface.
- We would like to accommodate "illumination" of this structure by incident waves either from below (e.g., earthquakes) or at the surface.
- From (many) such measurements we would like to determine properties of the structure, e.g.
  - Wave speeds in each layer,
  - Thickness of each layer,
  - Interface shapes between each layer.

What We Can Do: Single–Layered Acoustic Media



- Simplify to two dimensions.
- Simplify to the Helmholtz equation.
- Simplify to a single layer with *known* velocity.
- Measure at $y = 0$.
- Suppose that the interface has shape $y = \bar{g} + g(x)$.
- Seek the interface depth: $\bar{g}$.
- Seek the interface shape: $g(x)$.

Numerical Methods

- A variety of numerical methods have been brought to bear on this problem.
- Finite Differences: Easy to implement, but expensive (volumetric) and awkward for complicated geometries.
- Finite Elements: More involved to implement but accommodate complicated geometries. However, also expensive (volumetric).
- Integral Equations: Efficient (surface) but require subtle quadratures near singularities.
- IE methods also give rise to dense, non–SPD, linear systems requiring sophisticated iterative methods (e.g., GMRES accelerated by Fast Multipole Method).
- Boundary Perturbation Methods (BPM): Fast (surface) methods which require neither special quadrature rules nor the solution of dense linear systems.
- Idea: Apply a BPM to layered media.

Previous Work (Sample)

- Moczo, Robertsson, Eisner, "The finite-difference time-domain method for modeling of seismic wave propagation," *Adv. Geophys.* 48 (2007).
- Komatitsch and Tromp, "Spectral-element simulations of global seismic wave propagation," *Geophys. J. Inter.* 149 (2002).
- Bouchon, "A review of the discrete wavenumber method," *J. Pure Appl. Geophys.* 160 (2003).
- Bruno and Reitich, "Numerical solution of diffraction problems: A method of variation of boundaries," *J. Opt. Soc. Am. A* 10 (1993).
- Milder, "An improved formalism for wave scattering from rough surfaces," *J. Acoust. Soc. Am.* 89 (1991).
- Ito and Reitich, "A high–order perturbation approach to profile reconstruction," *Inverse Problems* 15 (1999).

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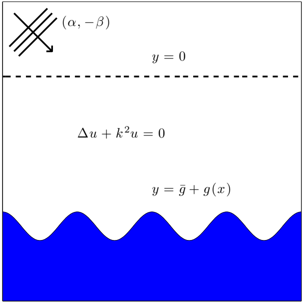
Periodic Gratings



- Consider a d–periodic grating shaped by $y = \bar{g} + g(x)$,

$$g(x + d) = g(x),$$

defining the region

$$\Omega := \{y > \bar{g} + g(x)\}.$$

- We suppose $\bar{g} < 0$, $\bar{g} + |g|_{L^\infty} < 0$, and make “observations” at $y = 0$.
- This is filled by with a constant–density acoustic medium with velocity c.

Plane–Wave Scattering

- We begin with the Forward Problem: We "illuminate" our structure from above with a downward propagating plane–wave
$$\bar{u}^i(x,y,t) = e^{i(\alpha x - \beta y - i\omega t)} =: u^i(x,y)e^{-i\omega t}.$$
- Solving for the reduced field, u, the well–known "time–harmonic" governing equations for a sound–soft material are
$$\begin{aligned} &\Delta u + k^2 u = 0 && \text{in } \Omega \\ &\mathcal{P}\{u\} = 0 && y \to \infty \\ &u = \zeta && z = \bar{g} + g(x) \\ &u(x+d,y) = e^{i\alpha d}u(x,y), && \end{aligned}$$
where:
  - $\alpha^2 + \beta^2 = k^2$ and $k = \omega/c$.
  - $\mathcal{P}$ is the outgoing (upward) propagating operator,
  - the Dirichlet data is:
$$\zeta(x) = -u^i(x, \bar{g} + g(x)) = -e^{i(\alpha x - \beta(\bar{g} + g(x)))}.$$

Boundary Formulation: Unknown

- We aim towards a Boundary Perturbation approach to the forward problem of determining the scattered field u given known structure (α, β, $\bar{g}$, and g).
- We begin by formulating on the boundary, and thus define

$$U(x) := u(x, \bar{g} + g(x)),$$

the "Dirichlet trace" of the function u.
- Quite simply, the governing equation is now

$$U = \zeta.$$

- The unknown U may be useful for the forward problem where $\bar{g}$ and $g(x)$ are known, however, it is useless for the inverse problem as this is data we cannot measure!

The Dirichlet–Propagator Operator (DPO)

- With the inverse problem in mind we pose a new "far field" unknown

$$\tilde{u}(x) := u(x, 0).$$

- By solving the Helmholtz equation we can recover $\tilde{u}$ from U and denote this by P, the "Dirichlet–Propagator Operator" (DPO):

$$P = P(\bar{g}, g) : U \to \tilde{u}.$$

- Our governing equations become

$$\tilde{u} = P[U], \quad U = \zeta,$$

or, more simply,

$$\tilde{u} = P[\zeta].$$

Boundary Perturbation Method

If $g = \varepsilon f$ then P and ζ are analytic in ε, e.g.,

$$P(\varepsilon) = \sum_{n \geq 0} P_n \varepsilon^n, \quad \zeta(x;\varepsilon) = \sum_{n \geq 0} \zeta_n(x) \varepsilon^n,$$

it can be shown that $\tilde{u}$ is also analytic in ε so:

$$\tilde{u}(x;\varepsilon) = \sum_{n=0}^{\infty} \tilde{u}_n(x) \varepsilon^n.$$

Inserting these forms into our governing equation gives:

$$\sum_{n=0}^{\infty} \tilde{u}_n \varepsilon^n = \sum_{n=0}^{\infty} P_n \varepsilon^n \left[\sum_{m=0}^{\infty} \zeta_m \varepsilon^m \right].$$

At order zero we find $\tilde{u}_0 = P_0[\zeta_0]$.

Boundary Perturbation Method: Higher Orders

- At order $n > 0$ we recover:

$$\tilde{u}_n = \sum_{m=0}^{n} P_{n-m}[\zeta_m].$$

- The ζ_n can be found via Taylor expansions.
- We compute the DNO P by "Operator Expansions" (Milder, 1991; Craig & Sulem, 1993).
- This gives, at order zero,

$$P_0\,[\xi] = e^{-i\bar{g}\beta_D}\xi := \sum_{p=-\infty}^{\infty} e^{-i\bar{g}\beta_p}\hat{\xi}_p.$$

- For $n > 0$

$$P_n(f)\,[\xi] = -\sum_{m=0}^{n-1} P_m(f)\left[F_{n-m}(i\beta_D)^{n-m}\xi\right].$$

Boundary Perturbation Method: Forward Problem

- Recall that in our BP framework we need to solve

$$\tilde{u}_n = \sum_{m=0}^{n} P_{n-m}[\zeta_m].$$

  The right–hand side can now be evaluated using our OE formulas and the Fourier coefficients of $\tilde{u}$ recovered from these.
- Numerical Method: In brief, the OE method is a Fourier Collocation/Taylor method enhanced by Padé summation.
- We approximate the far–field, $\tilde{u}$, by

$$\tilde{u} \approx \tilde{u}^{N_x,N} = \sum_{n=0}^{N} \sum_{p=-N_x/2}^{N_x/2-1} e^{i\alpha_p x} \varepsilon^n \tilde{u}_{p,n}.$$

- Convolution products are computed via the FFT.

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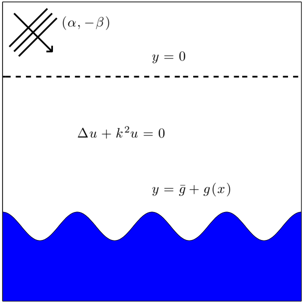
Nontrivial Analytic Profile



- Consider the analytic interface with Fourier coefficients

$$\hat{f}_p = \begin{cases} \frac{1}{2}(2\rho)^{(|p|-1)/(M-1)} & p \neq 0 \\ 0 & p = 0 \end{cases}.$$

- We note that f has mean zero, f is "cosine–like" as

$$\hat{f}_1 = \hat{f}_{-1} = 1/2,$$

and $\hat{f}_M = \hat{f}_{-M} = \rho$.

- At left we plot this profile with $M = 10$, $\rho = 10^{-16}$, and scaled by a factor $\varepsilon = 0.01$.

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Physical and Numerical Parameters

- We now present results of a numerical experiment with a one–layer structure.
- We choose a $d = 2\pi$–periodic interface at mean level $\bar{g} = -1.5$, shaped by $g(x) = \varepsilon f(x)$.
- This grating is illuminated by incident radiation specified by $\alpha = 0$, $\beta = 5.5$.
- We will select $(\varepsilon, M) = (0.1, 30)$.
- We choose numerical parameters $N_x = 128$ and $N_{max} = 12$.
- We compute the “energy defect”:

$$\delta := 1 - \sum_{p \in \mathcal{U}} e_p := 1 - \sum_{p \in \mathcal{U}} \frac{\beta_p}{\beta} |\tilde{u}_p|^2 .$$

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Convergence: Results ($(\varepsilon, M) = (0.1, 30)$)

Energy defect versus number of Taylor series terms retained in a simulation of scattering by a singly layered structure. Numerical parameters were $N_x = 128$ and $N_{max} = 12$ for $(\varepsilon, M) = (0.1, 30)$.

N	δ (Taylor)	δ (Padé)
2	0.01196	0.1572
4	0.0002475	0.0003088
6	2.806×10^{-6}	3.08×10^{-6}
8	2.045×10^{-8}	8.376×10^{-9}
10	1.079×10^{-10}	9.633×10^{-12}
12	4.38×10^{-13}	4.294×10^{-13}

The Inverse Problem

- We now have an algorithm for the "forward problem": Given incident radiation (α, β) and an interface shape $\bar{g} + g(x)$, determine the scattered (far field) data, $\tilde{u}(x) := u(x, 0)$, from

$$\tilde{u} = P(g)[U(x; g)] = P(g)[\zeta(x; g)].$$

- Question: If we know far–field data, can we recover $\bar{g}$ and $g(x)$? (For brevity assume we have $\bar{g}$)
- Typically gather the "efficiencies"

$$e_p := (\beta_p/\beta) \left|\tilde{u}_p\right|^2, \quad p \in \mathcal{U},$$

so we are asking for a *little* more.

- As with the forward problem, we adopt a Boundary Perturbation philosophy for the inverse problem.

Linear Approximation (LA): Formula for g

- Write our equation with linear term explicit

$$\tilde{u} = P_0[\zeta_0] + \{P_1(\cdot)[\zeta_0] + P_0[\zeta_1(\cdot)]\}[g] + \mathcal{O}(g^2)$$

- Defining the function, b, and operator, M,

$$b := P_0[\zeta_0], \quad M := \{P_1(\cdot)[\zeta_0] + P_0[\zeta_1(\cdot)]\},$$

and truncating at linear order we find $\tilde{u} = b + Mg$.

- Setting $\tilde{u} = \eta$ we can solve for g via

$$g = M^{-1}[\eta - b].$$

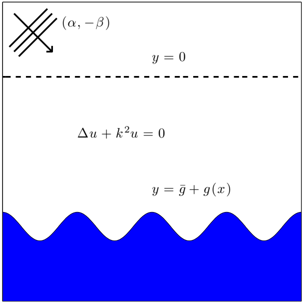
- Ill–Posedness: The ill–posedness of this problem is displayed by M^{-1}. It is not difficult to see that

$$M = P_0\left[-g(i\gamma_D)\zeta_0 + \zeta_1(\cdot)\right]$$

so that M^{-1} involves P_0^{-1}, a terrible operator:

$$P_0^{-1}[\xi] = \sum_p e^{i\beta_p \bar{g}} \hat{\xi}_p e^{i\alpha_p x}$$

Numerical Experiments: Inverse Problem



- Consider a 2π–periodic, singly layered medium with interface at $\bar{g} = -1.5$ and deviation $g = \varepsilon f$:

$$\hat{f}_p = \begin{cases} \frac{1}{2}(2\rho)^{(|p|-1)/(M-1)} & p \neq 0 \\ 0 & p = 0 \end{cases}$$

  with $\rho = 10^{-16}$.
- Plane–wave illumination with $(\alpha, \beta) = (0, 5.5)$.
- Investigate the performance of this "Linear Approximation" (LA) for $(\varepsilon, M) = (0.01, 10)$.

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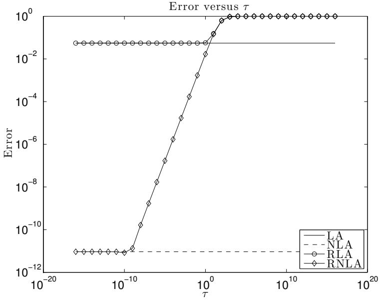
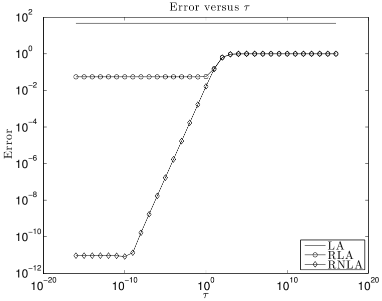
Results: LA $(\varepsilon, M) = (0.01, 10)$ $[N_x = 32]$



- Consider the analytic profile f with $(\varepsilon, M) = (0.01, 10)$.
- Plot of relative L^{∞} error in reconstructed solution (compared to exact solution) for LA algorithm.

Results: LA $(\varepsilon, M) = (0.01, 10)$ $[N_x = 128]$



- Consider the analytic profile f with $(\varepsilon, M) = (0.01, 10)$.
- Plot of relative L^∞ error in reconstructed solution (compared to exact solution) for LA algorithm.

Nonlinear Approximation (NLA): Iteration for g

- Write our equation with order N_i term explicit

$$\tilde{u} = P_0[\zeta_0] + \{P_1(\cdot)[\zeta_0] + P_0[\zeta_1(\cdot)]\}[g] + R(g) + \mathcal{O}(g^{N_i+1}),$$

where

$$R(g) := \sum_{n=2}^{N_i} \sum_{m=0}^{n} P_m(g)[\zeta_{n-m}(x; g)].$$

- Recalling our definitions for b and M, and truncating at order N_i we find $\tilde{u} = b + Mg + R(g)$.
- Once again, setting $\tilde{u} = \eta$ we can solve for g via

$$g = M^{-1}[\eta - b - R(g)].$$

- To solve this “Nonlinear Approximation” (NLA) we set up the iteration

$$g^{(k+1)} = M^{-1}[\eta - b - R(g^{(k)})],$$

using $g^{(0)} = M^{-1}[\eta - b]$.

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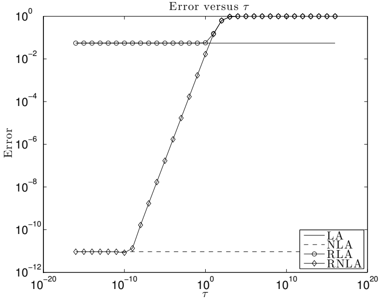
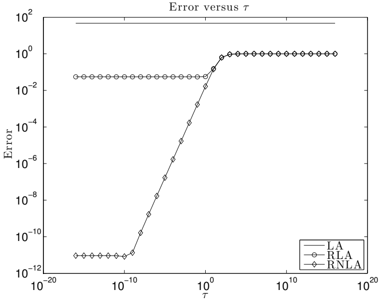
Results: LA, NLA $(\varepsilon, M) = (0.01, 10)$ $[N_x = 32]$



- Consider the analytic profile f with $(\varepsilon, M) = (0.01, 10)$.
- Plot of relative L^∞ error in reconstructed solution (compared to exact solution) for LA, NLA algorithms.

Results: LA, NLA $(\varepsilon, M) = (0.01, 10)$ $[N_x = 128]$



- Consider the analytic profile f with $(\varepsilon, M) = (0.01, 10)$.
- Plot of relative L^∞ error in reconstructed solution (compared to exact solution) for LA, NLA algorithms.

The Inverse Problem: Regularization

- While the direct method above is elegant and computationally efficient, it is evidently problematic due to ill–conditioning.
- We propose to regularize the problem by relaxing the demand that we match the far–field pattern exactly.
- For this we consider the quadratic form

$$\tilde{q}(\tilde{u}, g) := (1/2) \|\tilde{u} - \eta\|_{L^2}^2 + (\tau/2) \|g\|_{H^1}^2 .$$

- We do not change the class of minimizers by subtracting off a constant (in this case $(1/2) \|\eta\|_{L^2}^2$) so we focus on

$$\begin{aligned} q(\tilde{u}, g) &:= (1/2) \|\tilde{u} - \eta\|_{L^2}^2 - (1/2) \|\eta\|_{L^2}^2 + (\tau/2) \|g\|_{H^1}^2 \\ &= (1/2) \langle \tilde{u}, \tilde{u} \rangle - \langle \eta, \tilde{u} \rangle + (\tau/2) (\langle g, g \rangle + \langle \partial_x g, \partial_x g \rangle) . \end{aligned}$$

Constrained Minimization

- Integrating by parts gives

$$q(\tilde{u}, g) = (1/2) \langle \tilde{u}, \tilde{u} \rangle - \langle \eta, \tilde{u} \rangle + (\tau/2) \left\langle g, (1 - \partial_x^2) g \right\rangle$$

which we write as $q(X) = (1/2) \langle X, QX \rangle - \langle c, X \rangle$, where

$$X := \begin{pmatrix} \tilde{u} \\ g \end{pmatrix}, \quad Q := \begin{pmatrix} I & 0 \\ 0 & \tau(1 - \partial_x^2) \end{pmatrix}, \quad c := \begin{pmatrix} \eta \\ 0 \end{pmatrix}.$$

- We constrain this with $B(X) = 0$ where

$$B(X) := B(\tilde{u}, g) = \tilde{u} - P(g)[\zeta(g)].$$

- With our BP philosophy in mind we record that

$$B(\tilde{u}, \varepsilon f) = \tilde{u} - \sum_{n=0}^{\infty} \sum_{m=0}^{n} P_m(f)[\zeta_{n-m}(f)] \varepsilon^n$$

and that, to first order,

$$B(X) \approx B^{(1)}(X) = \tilde{u} - P_0[\zeta_0] - \{P_1(\cdot)[\zeta_0] + P_0[\zeta_1(\cdot)]\} g.$$

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Inverse Problem: Regularized Linear Approx (RLA)

- We approximate solutions of the inverse problem by solving the linearly constrained quadratic optimization problem

$$\min_{X} q(X) = \min_{X} (1/2) \langle X, QX \rangle + \langle c, X \rangle , \quad AX - b = 0,$$

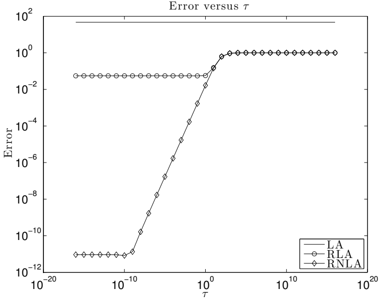
where

$$A = \begin{pmatrix} I & -M \end{pmatrix}, \quad M = P_1(\cdot)[\zeta_0] + P_0[\zeta_1(\cdot)], \quad b = P_0[\zeta_0].$$

- After simplifying we find the "Regularized Linear Approx" (RLA)

$$y = b, \quad z = K^{-1} M^{*}[\eta - b], \quad \lambda = \tilde{u} - \eta.$$

Results: LA, NLA, RLA $(\varepsilon, M) = (0.01, 10)$ $[N_x = 128]$



- Consider the analytic profile f with $(\varepsilon, M) = (0.01, 10)$.
- Plot of relative L^{∞} error in reconstructed solution (compared to exact solution) versus the regularization parameter τ for LA, NLA, RLA algorithms.

Inverse Problem: Regularized Nonlin Approx (RNLA)

- We now approximate solutions of the inverse problem by solving the nonlinearly constrained quadratic optimization problem

$$\min_X q(X) = \min_X (1/2) \langle X, QX \rangle + \langle c, X \rangle , \quad B(X) = 0,$$

where

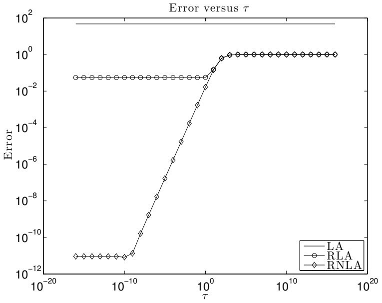
$$B(X) = AX - b - R(X), \quad R(X) := \sum_{n=2}^{N_i} \sum_{m=0}^{n} P_m(g)[\zeta_{n-m}(g)].$$

- Mimicking the Null Space Method, we attempt the iterative scheme ("Regularized Nonlinear Approximation"–RNLA)

$$y^{(k+1)} = b + R(X^{(k)}), \quad z^{(k+1)} = K^{-1} M^* [\eta - b - R(X^{(k)})]$$
$$\lambda^{(k+1)} = \tilde{u}^{(k+1)} - \eta.$$

- We start with $X^{(0)}$ generated by the RLA.

Results: LA, NLA, RLA, RNLA $(\varepsilon, M) = (0.01, 10)$ $[N_x = 128]$



- Consider the analytic profile f with $(\varepsilon, M) = (0.01, 10)$.
- Plot of relative L^∞ error in reconstructed solution (compared to exact solution) versus the regularization parameter τ for LA, NLA, RLA, RNLA algorithms.

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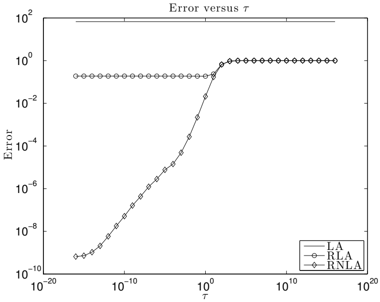
Results: LA, NLA, RLA, RNLA $(\varepsilon, M) = (0.03, 20)$ $[N_x = 128]$



- Consider the analytic profile f with $(\varepsilon, M) = (0.03, 20)$.
- Plot of relative L^∞ error in reconstructed solution (compared to exact solution) versus the regularization parameter τ for LA, NLA, RLA, RNLA algorithms.

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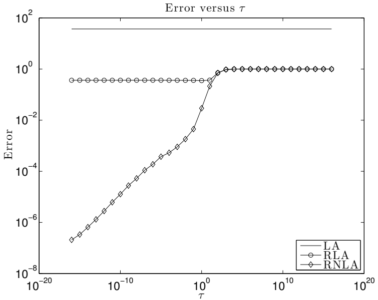
Results: LA, NLA, RLA, RNLA $(\varepsilon, M) = (0.05, 30)$ $[N_x = 128]$



- Consider the analytic profile f with $(\varepsilon, M) = (0.05, 30)$.
- Plot of relative L^{∞} error in reconstructed solution (compared to exact solution) versus the regularization parameter τ for LA, NLA, RLA, RNLA algorithms.

Summary

- Layered–media scattering is an idealized model of acoustic propagation in the earth.
- We have generalized the fast and accurate Operator Expansions approach of Milder (1991) to produce far field data. More importantly, we have further expanded the method (not discussed today [DPN 2011]) to the multi–layer case.
- We have also shown how this OE formulation can be used to address the inverse problem of identifying internal boundary shapes given surface measurements.
- Future Directions: The method needs to be expanded in several directions: Three dimensions, multiple layers, full equations of elasticity, . . .