# Towards Combining Interval and Probabilistic Uncertainty in Finite Element Methods

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# 1. Uncertainty in FEM: Probabilistic Approach

- *Traditional approach to FEM:* we know the *exact* equations and the *exact* values of the parameters $x_i$ of these equations.
- *In practice:* we only know the *approximate* values of the corresponding parameters.
- *Question:* estimate how the uncertainty in the parameters of the system can affect the result $y$ of applying the FEM techniques.
- *Probabilistic approach – assumption:* we know the exact *probability* distributions of all $x_i$.
- *Probabilistic approach – algorithm:* e.g., use Monte-Carlo simulations.

## 2. Uncertainty in FEM: Interval Approach and Remaining Problem

- *Interval approach – assumption:* sometimes, we only know the lower bounds $\underline{x}_i$ and the upper bounds $\overline{x}_i$ on $x_i$.
- *Example:* the probabilities of different values of Young modulus may depend on the manufacturing process.
- *Interval approach – objective:* find the interval

$$[\widetilde{y} - \Delta, \widetilde{y} + \Delta]$$

  that contains $y$.
- *Interval approach – algorithms:* presented in talks by Muhanna, Nakao, Neumaier, Pownuk.

## 3. Uncertainty in FEM: Remaining Problem

- *In practice:* we sometimes have *both* interval and probabilistic uncertainty.
- *Example:*
  - for manufacturing-related parameters, we may only know intervals of possible values;
  - for weather-related parameters, we also know the probabilities of different values (e.g., from the weather records).
- *Objective:* for different $p \in [0, 1]$, find the value $\Delta(p)$ that bound $\Delta y$ with probability $p$.

## 4. General Algorithm

- *Problem – reminder:*
  - for some $x_i$, we know intervals $[\underline{x}_i, \overline{x}_i]$;
  - for some $x_j$, we know the probability distribution;
  - we want to find the value $\Delta(p)$ that bound $\Delta y$ with probability $p$.
- *Algorithm:*
  - use Monte-Carlo techniques to simulate parameters $x_j$ with known probability distributions;
  - for each such simulation, use interval FEM techniques to get an upper bound $\Delta$ for $|y - \widetilde{y}|$;
  - after several simulations, we get the resulting bounds distribution;
  - from this distribution, we can find the desired bound $\Delta(p)$.

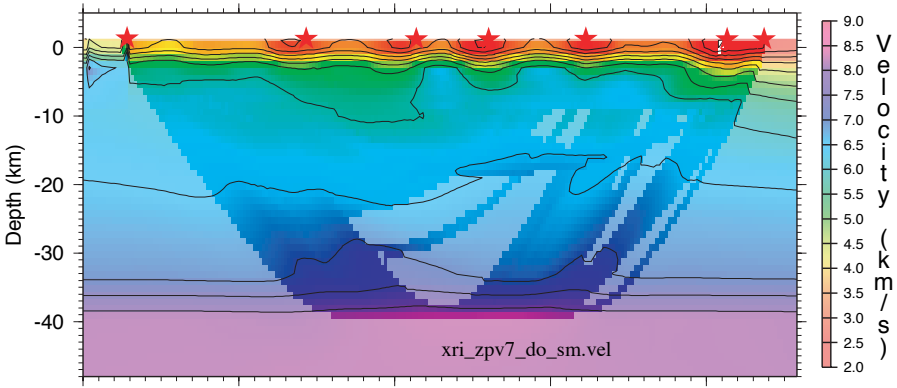
## 5. Case Study: Determining Earth Structure

- *Importance:* civilization greatly depends on the things we extract from the Earth: oil, gas, water.
- *Need* is growing, so we must find new resources.
- *Problem:* most easy-to-access mineral resources have been discovered.
- *Example:* new oil fields are at large depths, under water, in remote areas – so drilling is very expensive.
- *Objective:* predict resources before we invest in drilling.
- *How:* we know what structures are promising.
- *Example:* oil and gas concentrate near the top of (natural) underground domal structures.
- *Conclusion:* to find mineral resources, we must determine the structure at different depths $z$ at different locations $(x, y)$.

# 6. Data that We Can Use to Determine the Earth Structure

- *Available measurement results:* those obtained without drilling boreholes.
- *Examples:*
  - gravity and magnetic measurements;
  - travel-times $t_i$ of seismic ways through the earth.
- *Need for active seismic data:*
  - passive data from earthquakes are rare;
  - to get more information, we make explosions, and measure how the resulting seismic waves propagate.
- *Resulting seismic inverse problem:*
  - we know the travel times $t_i$;
  - we want to reconstruct velocities at different depths.

# Hole Tomography Smashed Masked Velocity Models



## 7. Seismic Inverse Problem: Towards Mathematical Formulation

- *General description:* wave equation with unknown $v(x)$.
- *Difficulty:* due to noise, we only know $t_i$.
- *Ray approximation:* a seismic wave follows the shortest path $t = \int \frac{d\ell}{v} \to \min$; Eikonal equation $|\nabla t| = \frac{1}{v}$.
- *Discontinuity:* $v$ is only piece-wise continuous; Snell's law describes the transition $\frac{\sin(\varphi)}{v} = \frac{\sin(\varphi')}{v'}$.
- *Ill-posed problem:* a change in $v$ outside paths does not affect observed travel-times $t_i$; hence, many drastically different $v(x)$ are consistent with observations.
- *Current solution:*
  - start with a meaningful first approximation;
  - use physically motivated iterations.

## 8. Seismic Inverse Problem: FEM Approach

- $v(x) = v_j$ is constant within each element $j$.
- *We know:* travel-times $t_i$ between known points $A_i$, $B_i$.
- *We want to find:* velocities $v_j$ for which $t_i = t_i(v) \stackrel{\text{def}}{=} \min \sum_j \frac{\ell_{ij}}{v_j}$, where:
  - min is taken over all paths between $A_i$ and $B_i$, and
  - $\ell_{ij}$ is the length of the part of $i$-th path within element $j$.
- *Shortest path:* straight inside each element, Snell's law on each border.
- *Simplification:* use slownesses $s_j \stackrel{\text{def}}{=} \frac{1}{v_j}$; $t_i = \sum_j \ell_{ij} \cdot s_j$.
- *Problem:* system is under-determined.

# 9. Existing Algorithm for the Seismic Inverse Problem: General Description

- *The most widely used:* John Hole's iterative algorithm.
- *Starting point:* reasonable initial slownesses $s_j^{(0)}$.
- *Starting an iteration:* we use current (approximate) slownesses $s_j^{(k)}$ to:
  - find the shortest paths and
  - compute the corr. travel-times $t_i = \sum_j \ell_{ij} \cdot s_j^{(k)}$.
- *Fact:* measured travel-times $\widetilde{t}_i$ are somewhat different: $\Delta t_i \stackrel{\text{def}}{=} \widetilde{t}_i - t_i \neq 0$.
- *On each iteration:*
  - we find $\Delta s_j$ for which $\sum_j \ell_{ij} \cdot (s_j + \Delta s_j) = \widetilde{t}_i$;
  - we take $s_j^{(k+1)} = s_j^{(k)} + \Delta s_j$.

## 10. Algorithm for the Inverse Problem: Details

- *Objective (reminder):* find $\Delta s_j$ s.t. $\sum \ell_{ij} \cdot \Delta s_j = \Delta t_i$.
- *Simplest case:* one path.
- *Specifics:* under-determined system: 1 equation, many unknowns $\Delta s_j$.
- *Idea:* no reason for $\Delta s_j$ to be different: $\Delta s_j \approx \Delta s_{j'}$.
- *Formalization:* minimize $\sum\limits_{j,j'} (\Delta s_j - \Delta s_{j'})^2$ under the constraint $\sum \ell_{ij} \cdot \Delta s_j = \Delta t_i$.
- *Solution:* $\Delta s_j = \dfrac{\Delta t_i}{L_i}$ for all $j$, where $L_i = \sum\limits_j \ell_{ij}$.
- *Realistic case:* several paths; we have $\Delta s_{ij}$ for different paths $i$.
- *Idea:* least squares $\sum\limits_i (\Delta s_j - \Delta s_{ij})^2 \to \min$.
- *Solution:* $\Delta s_j$ is the average of $\Delta s_{ij}$.

## 11. Successes, Limitations, Need for Prior Knowledge

- *Successes:* the algorithm usually leads to reasonable geophysical models.
- *Limitations:* often, the resulting velocity model is not geophysically meaningful.
- *Example:* resulting velocities outside of the range of reasonable velocities at this depth.
- *What is currently done:* trying different initial models (hacking).
- *Problem with this approach:* there is no algorithm for selecting a good starting model; often, dozens of tries are needed – and each try requires hours of computations.
- *It is desirable:* to incorporate the expert knowledge into the algorithm for solving the inverse problem.

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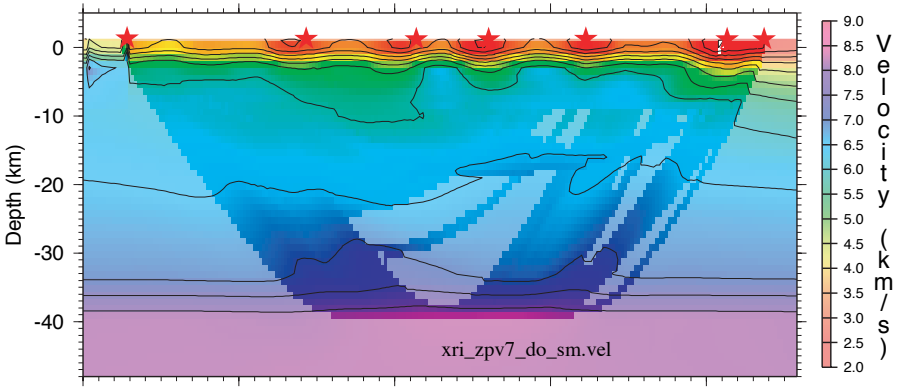

## 12. Case of Interval Prior Knowledge

- *Additional information:* an interval $[\underline{s}_j, \overline{s}_j]$ that contains the (unknown) actual value $s_j$.
- *Problem:* for $\Delta s_{ij} = \dfrac{\Delta t_i}{L_i}$, we may have $s_j^{(k)} + \Delta s_{ij} \notin [\underline{s}_j, \overline{s}_j]$.
- *Idea:* as $s_j^{(k+1)}$, take the value from $[\underline{s}_j, \overline{s}_j]$ which is the closest to $s_j^{(k)} + \Delta s_{ij}$, i.e., cut off at $\overline{s}_j$ (or at $\underline{s}_j$).
- *Problem:* since we decreased $\Delta s_{ij}$, we have a remaining discrepancy $\Delta t_i' \stackrel{\text{def}}{=} \Delta t_i - \sum\limits_j \ell_{ij} \cdot \Delta s_{ij}$.
- *Solution:* repeat the same process for $\Delta t_i'$, etc.
- *Problem:* many iterations instead of one – increase in computation time.
- *Our result:* a new linear time algorithm that computes the final result of these additional iterations.

# 13. A New Linear-Time Algorithm

- At each iteration, we have three sets:
  - $J^- = \{j : \text{we know} \Delta s_{ij} = \overline{\Delta}_j \stackrel{\text{def}}{=} \overline{s}_j - s_j^{(k)}\}$;
  - $J^+ = \{j : \text{we know} \Delta s_{ij} < \overline{\Delta}_j\}$,
  - $J = -(J^- \cup J^+)$.

  and quantities $A^- \stackrel{\text{def}}{=} \sum\limits_{j \in J^-} \ell_{ij} \cdot \overline{\Delta}_j$ and $\mathcal{L}^+ \stackrel{\text{def}}{=} \sum\limits_{j \in J^+} \ell_{ij}$.
- We start with $J^- = J^+ = \emptyset$ and $J = \{1, \ldots, c\}$.
- At each iteration:
  - we compute the median $m$ of the set $J$ (median in terms of sorting by $\overline{\Delta}_j$);
  - then, by analyzing the elements of the undecided set $J$ one by one, we divide them into subsets

$$P^- \stackrel{\text{def}}{=} \{j : \overline{\Delta}_j \le \overline{\Delta}_m\}, \quad P^+ \stackrel{\text{def}}{=} \{j : \overline{\Delta}_j > \overline{\Delta}_m\}.$$

## 14. A New Linear-Time Algorithm (cont-d)

- we compute $a^- \stackrel{\text{def}}{=} A^- + \sum\limits_{j \in P^-} \ell_{ij} \cdot \overline{\Delta}_j$ and $\ell^+ \stackrel{\text{def}}{=} \mathcal{L}^+ + \sum\limits_{j \in P^+} \ell_{ij}$;
- then, we compute $\Delta s = \dfrac{\Delta_i - a^-}{\ell^+}$; also, among all the values from $P^+$, we select the smallest value, which we will denote by $\overline{\Delta}_{(p+1)}$;
- if $\Delta s > \overline{\Delta}_{(p+1)}$, then we replace $J^-$ with $J^- \cup P^-$, $A^-$ with $a^-$, and $J$ with $P^+$;
- if $\Delta s \le \overline{\Delta}_m$, then we replace $J^+$ with $J^+ \cup P^+$, $\mathcal{L}^+$ with $\ell^+$, and $J$ with $P^-$;
- finally, if $\overline{\Delta}_m < \Delta s \le \overline{\Delta}_{(p+1)}$, then we replace $J^-$ with $J^- \cup P^-$, $J^+$ with $J^+ \cup P^+$, and $J$ with $\emptyset$.

- Iterations continue until $J = \emptyset$.
- Return $\Delta s_{ij} = \overline{\Delta}_j$ when $\overline{\Delta}_j \le \overline{\Delta}_m$, else $\Delta s_{ij} = \Delta s$.

## 15. Case of Probabilistic Prior Knowledge

- *Description:* from prior observations, we know $\widetilde{s}_j \approx s_j$, and we know the st. dev. $\sigma_j$ of this value.
- *Minimize:* $\sum\limits_{j,j'}(\Delta s_{ij} - \Delta s_{ij'})^2$ s.t. $\sum\limits_{j=1}^{c} \ell_{ij} \cdot \Delta s_{ij} = \Delta t_i$ and

$$\frac{1}{n} \cdot \sum_{j=1}^{c} \frac{((s_j^{(k)} + \Delta s_{ij}) - \widetilde{s}_j)^2}{\sigma_j^2} = 1.$$

- *Solution* (Lagrange multipliers): $\overline{\Delta s} \stackrel{\text{def}}{=} \dfrac{1}{n} \cdot \sum\limits_{j=1}^{c} \Delta s_{ij}$,

$$\frac{2}{n} \cdot \Delta s_{ij} - \frac{2}{n} \cdot \overline{\Delta s} + \lambda \cdot \ell_{ij} + \frac{2\mu}{n \cdot \sigma_j^2} \cdot (s_j^{(k)} + \Delta s_{ij} - \widetilde{s}_j) = 0.$$

- *Fact:* $\Delta s_{ij}$ is an explicit function of $\lambda$, $\mu$, $\overline{\Delta s}$.
- *Algorithm:* solve 3 non-linear equations (above one + 2 constraints) with unknowns $\lambda$, $\mu$, $\overline{\Delta s}$.

# 16. Combination of Different Types of Prior Knowledge

- *Need:* we often have both:
  - prior measurement results – i.e., *probabilistic* knowledge, and
  - expert estimates – i.e., *interval* knowledge.
- *Minimize:* $\sum\limits_{j,j'}(\Delta s_{ij} - \Delta s_{ij'})^2$ s.t. $\sum\limits_{j=1}^{c} \ell_{ij} \cdot \Delta s_{ij} = \Delta t_i$,

$$\frac{1}{n} \cdot \sum_{j=1}^{c} \frac{((s_j^{(k)} + \Delta s_{ij}) - \widetilde{s}_j)^2}{\sigma_j^2} \le 1,$$

  and $\underline{s}_j \le s_j^{(k)} + \Delta s_{ij} \le \overline{s}_j$.
- *Idea:* we minimize a convex function under convex constraints; efficient algorithms are known.

## 17. Combination of Different Types of Prior Knowledge: Algorithm

- *Idea* – method of alternating projections:
  - first, add a correction that satisfy the first constraint,
  - then, the additional correction that satisfies the second constraint,
  - etc.
- *Specifics:*
  - first, add equal values $\Delta s_{ij}$ to minimize $\Delta t_i$;
  - restrict the values to the nearest points from $[\underline{s}_j, \overline{s}_j]$,
  - find the extra corrections that satisfy the probabilistic constraint,
  - repeat until converges.

## 18. Effects of Discretization: Technique

- *Worst-case bound:* $\infty$.
- *Geophysical approach – "checkerboard" method:*
  - add a doubly periodic function $\Delta v(x)$ to the solution $v(x)$;
  - compute corresponding $t'_i$;
  - reconstruct $v'(x)$ from $t'_i$;
  - compare $v'(x)$ with $v(x) + \Delta v(x)$.
- *Conclusion:*
  - For small-step $\Delta v(x)$, we will not see the difference – hence details of this size in $v(x)$ are not reliable.
  - If for some step $h$, we see the difference, this means that details of size $h$ are more reliable.

# 19. Effects of Discretization: Mathematical Results

- *Problem:* how to select functions $\Delta v_i(x)$?
- *Idea:* we want a shift-invariant process.
- *Analysis:* in linear approximation, what matters is the linear hull of the functions $\Delta v_i(x)$.
- *First result:* for bounded $\Delta v_i(x)$, we get

$$\Delta v_i(x_1, x_2) = \sin(a_1 \cdot x_1 + b_1) \cdot \sin(a_2 \cdot x_2 + b_2).$$

- *Alternative formulation:* we require that the family of functions $\{\Delta v_i(x)\}$ is optimal w.r.t. a shift-invariant optimality criterion.
- *Second result:* for each such criterion, we get the same functions

$$\Delta v_i(x_1, x_2) = \sin(a_1 \cdot x_1 + b_1) \cdot \sin(a_2 \cdot x_2 + b_2).$$

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