CERFACS-Toulouse

# A Framework for the Simulation of Multiphysics Problems Based on a hp Fourier-Finite-Element Method


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# overview

1. Motivation and Objectives: Joint Multiphysics Inversion
2. Simulation of Forward Problems
   - Parallel Self-Adaptive Goal-Oriented $hp$-Finite Element Method
   - Electromagnetic Applications
   - Sonic Applications
3. Inversion Library (Work in Progress)
   - $h$-Adaptive Newton's Method
   - Implementation
4. Conclusions and Future Work

# motivation and objectives

## Seismic Measurements

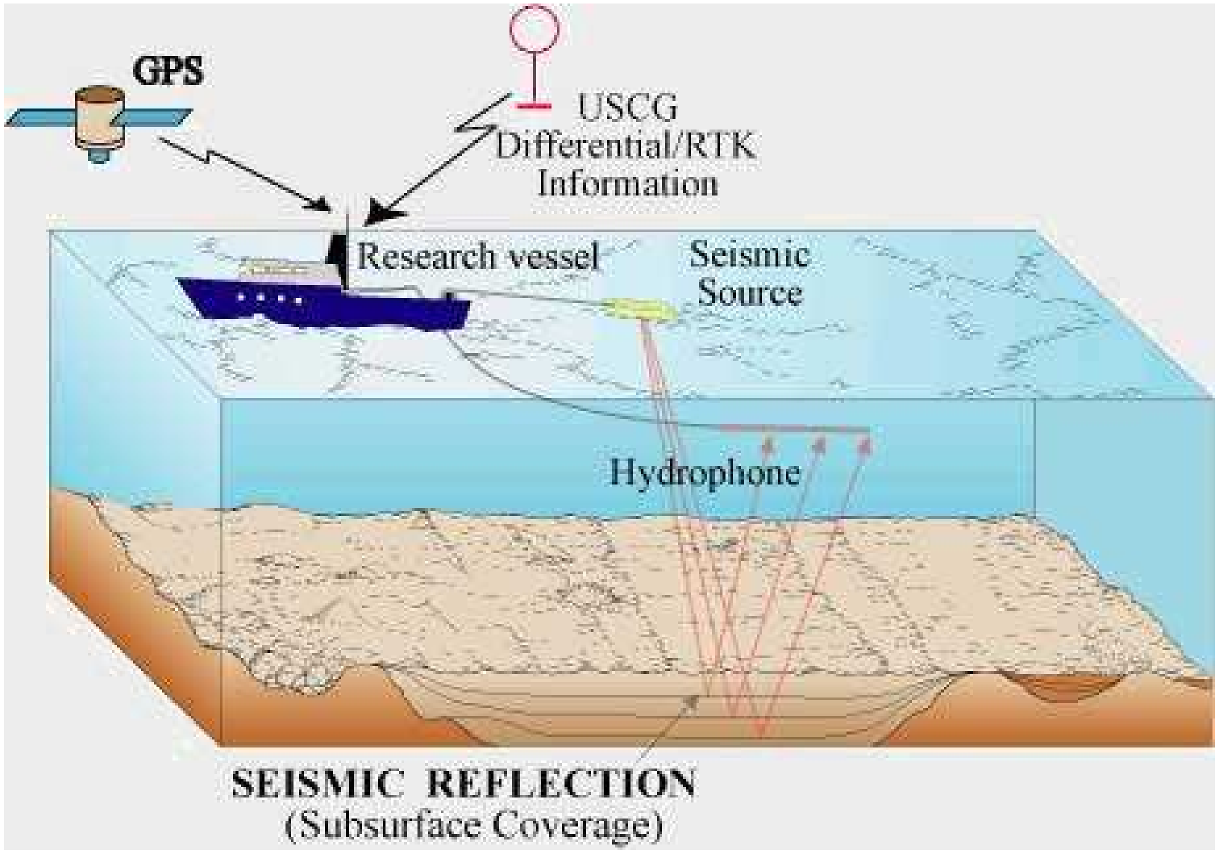



*Figure from the USGS Science Center for Coastal and Marine Geology*

# motivation and objectives

## Marine Controlled-Source Electromagnetics (CSEM)

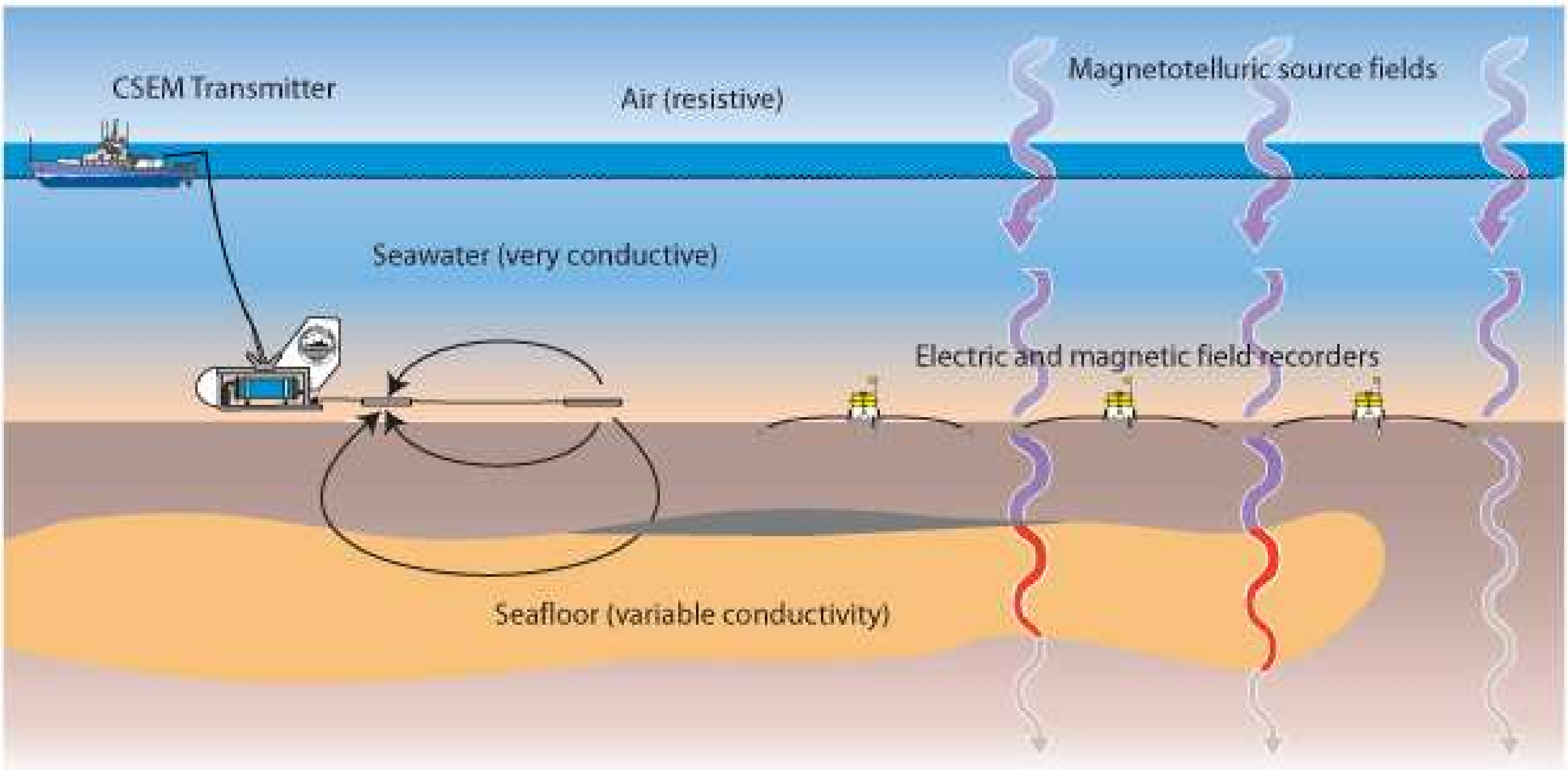
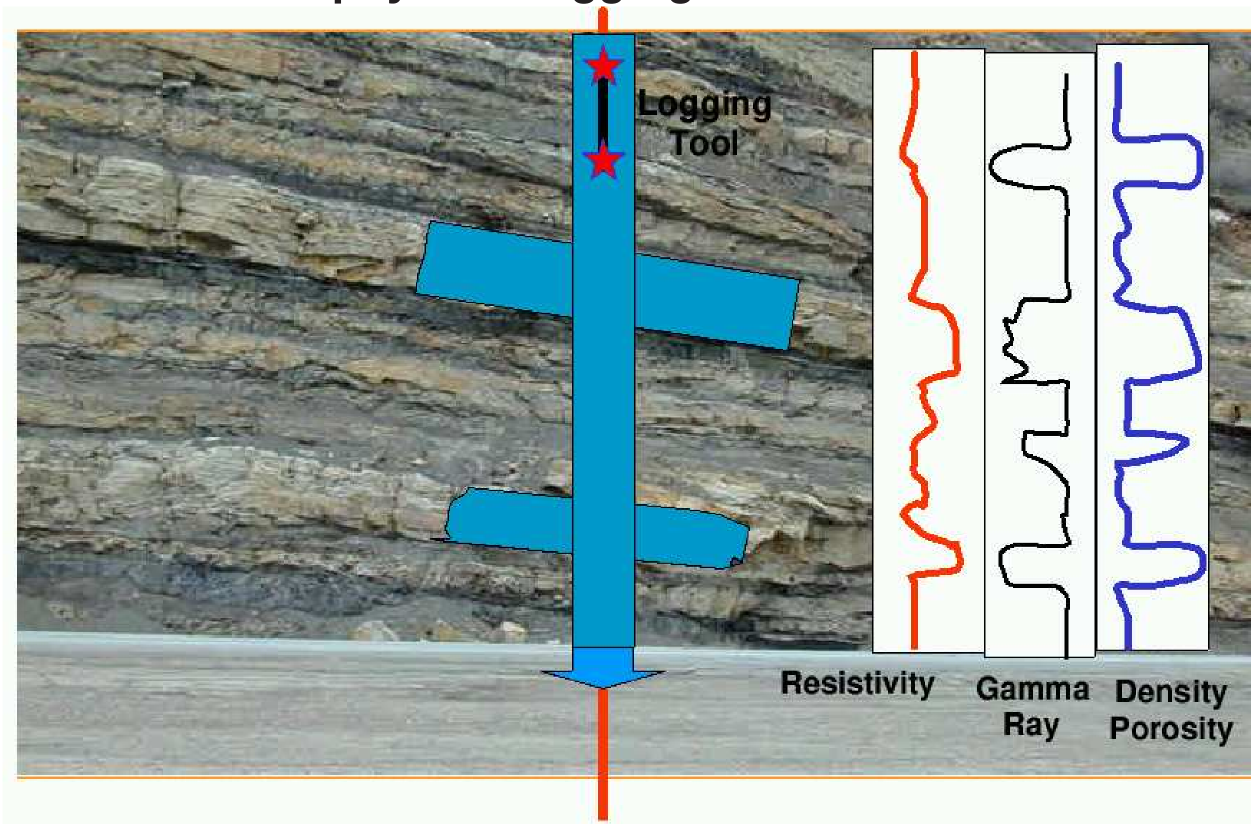



*Figure from the UCSD Institute of Oceanography*

# motivation and objectives

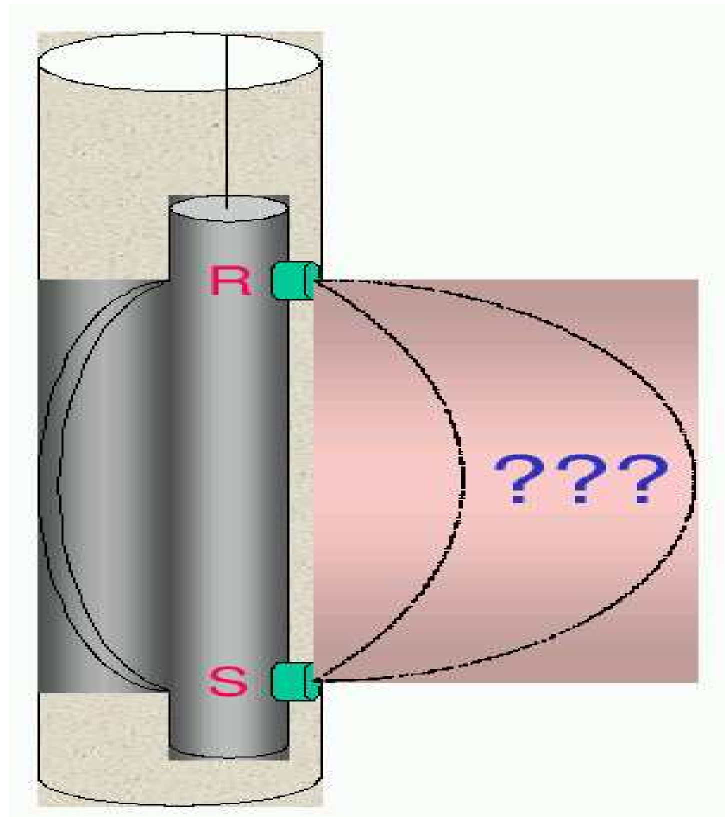
## Multiphysics Logging Measurements




**OBJECTIVES: To determine payzones (porosity), amount of oil/gas (saturation), and ability to extract oil/gas (permeability).**

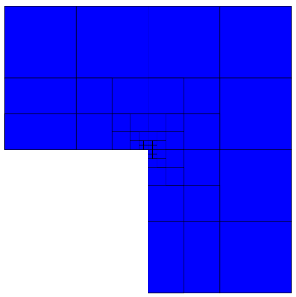
# motivation and objectives

**Main Objective: To Solve a Multiphysics Inverse Problem**



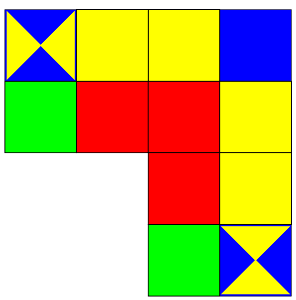

**Software to solve the DIRECT problem is essential in order to solve the INVERSE problem.**

# simulation of forward problems (hp-fem)



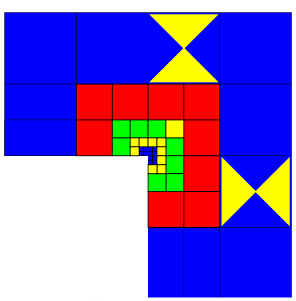
## The $h$-Finite Element Method

1. Convergence limited by the polynomial degree, and large material contrasts.
2. Optimal $h$-grids do NOT converge exponentially in real applications.
3. They may “lock” (100$\%$ error).



## The $p$-Finite Element Method

1. Exponential convergence feasible for analytical (“nice”) solutions.
2. Optimal *p*-grids do NOT converge exponentially in real applications.
3. If initial *h*-grid is not adequate, the *p*-method will fail miserably.



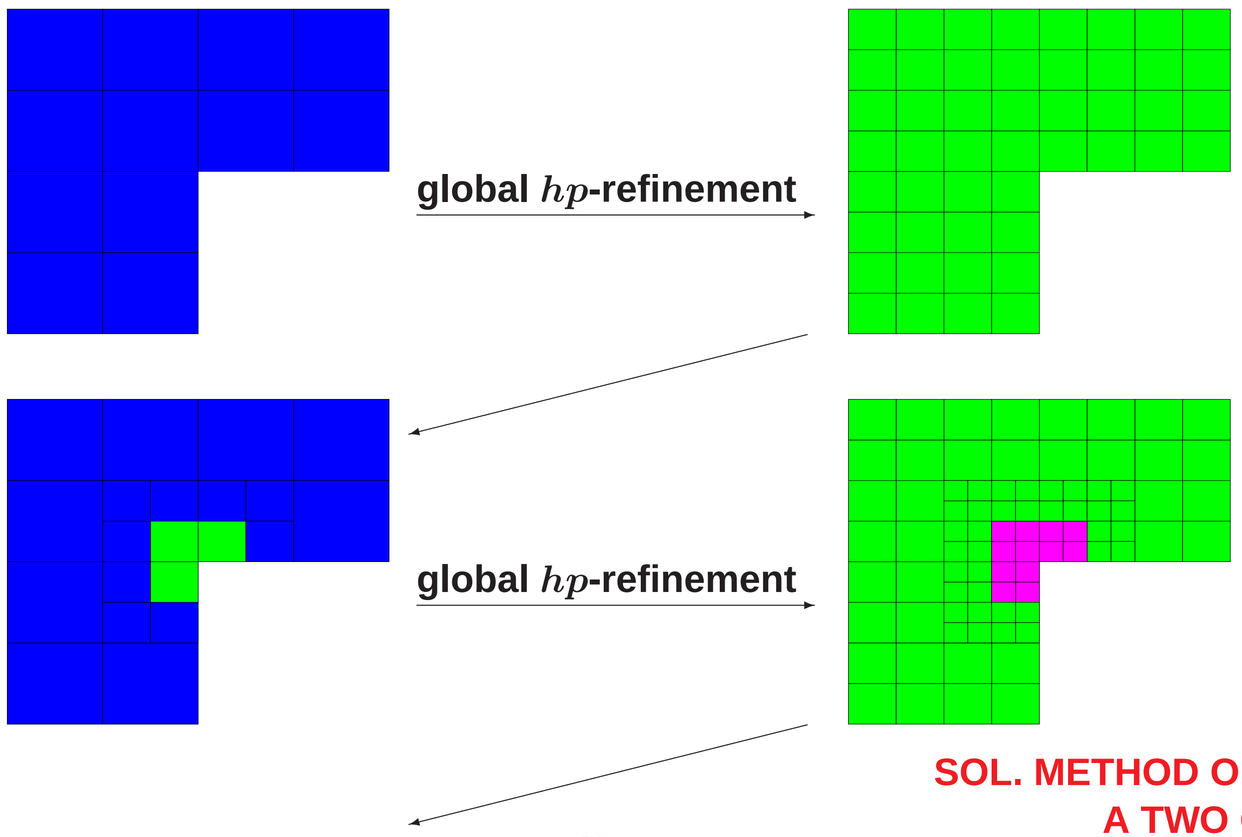
## The $hp$-Finite Element Method

1. Exponential convergence feasible for ALL solutions.
2. Optimal *hp*-grids DO converge exponentially in real applications.
3. If initial *hp*-grid is not adequate, results will still be great.

# simulation of forward problems (hp-fem)

**Energy norm based fully automatic *hp*-adaptive strategy**

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

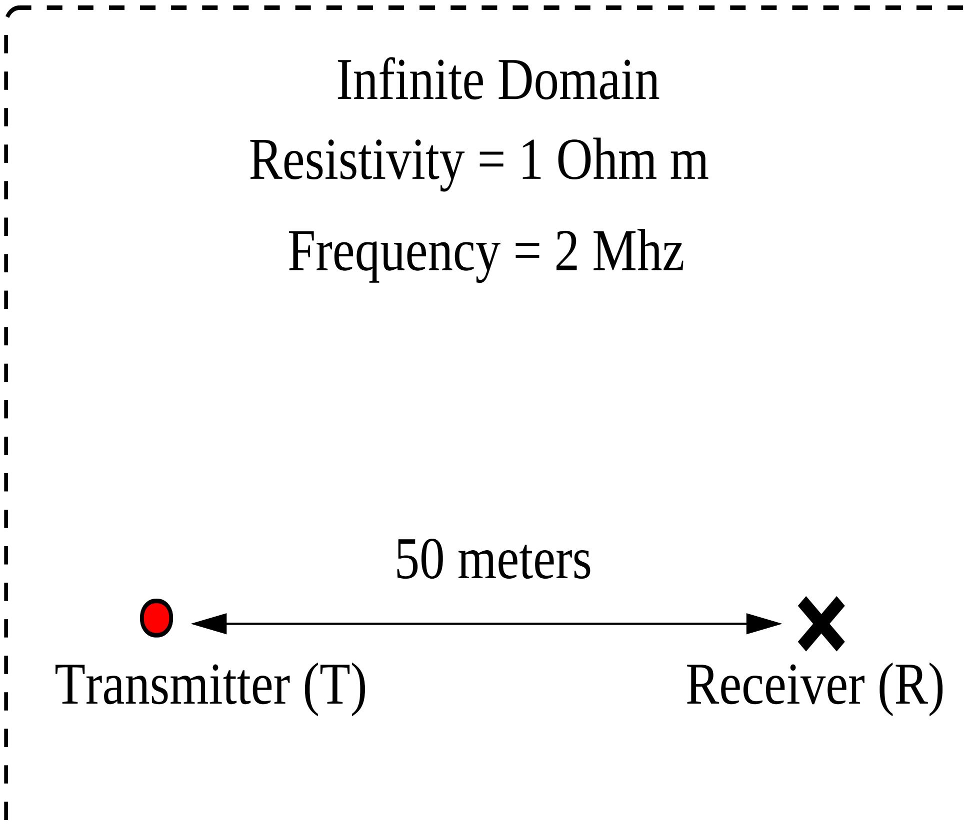



**SOL. METHOD ON FINE GRIDS:**
**A TWO GRID SOLVER**

# simulation of forward problems (hp-fem)

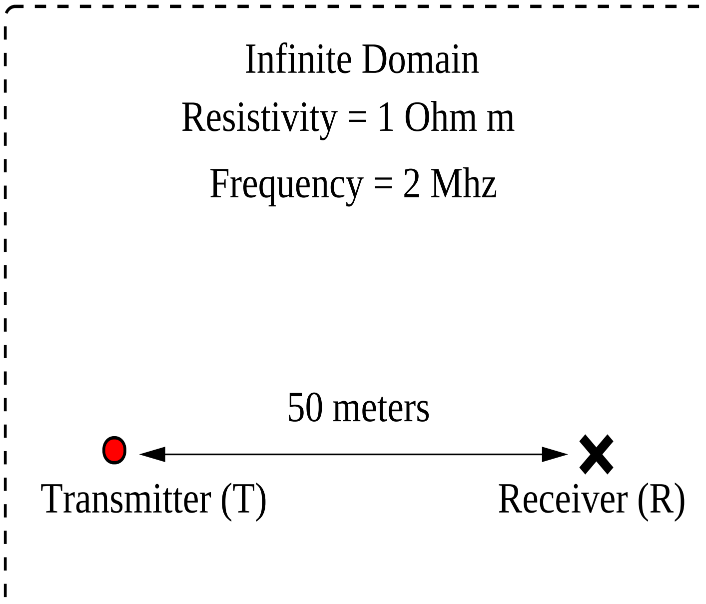
## Motivation (Goal-Oriented Adaptivity)

### Test Problem



# simulation of forward problems (hp-fem)

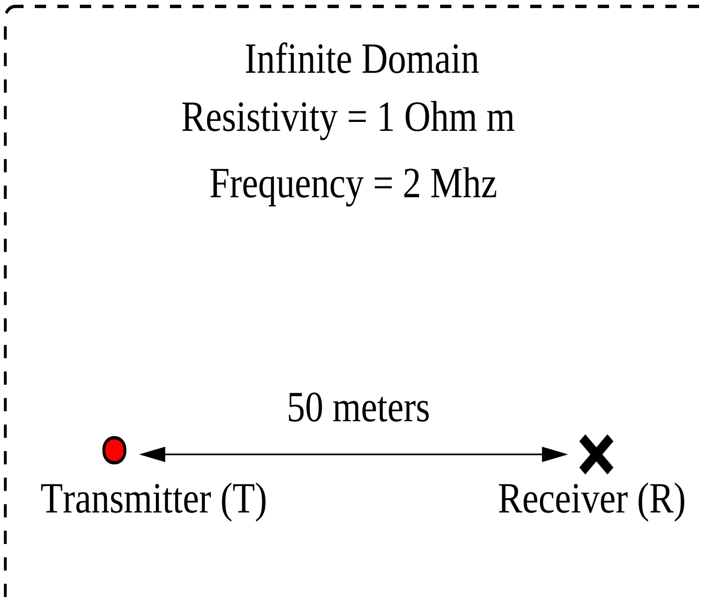
## Motivation (Goal-Oriented Adaptivity)




- **Solution decays exponentially.**
- $\frac{|E(T)|}{|E(R)|} \approx 10^{60}$
- **Results using energy-norm adaptivity:**
  - **Energy-norm error:** $0.001\%$
  - **Relative error in the quantity of interest** $> 10^{30}$ %.

# simulation of forward problems (hp-fem)

## Motivation (Goal-Oriented Adaptivity)

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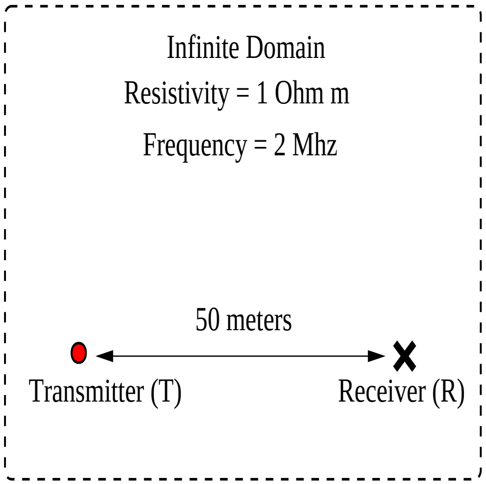
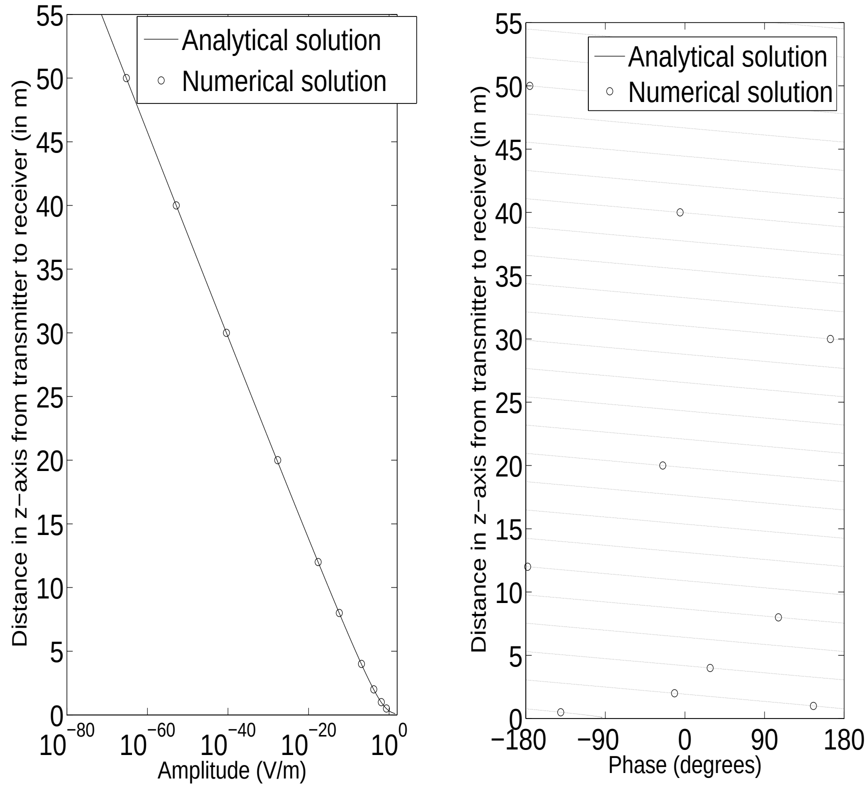
**Goal-oriented adaptivity is needed.** **Becker-Rannacher (1995,1996), Rannacher-Stuttmeier (1997), Cirak-Ramm (1998), Paraschivoiu-Patera (1998), Peraire-Patera (1998), Prudhomme-Oden (1999, 2001), Heuveline-Rannacher (2003), Solin-Demkowicz (2004).**

# simulation of forward problems (hp-fem)

## Motivation (Goal-Oriented Adaptivity)




**Goal-oriented adaptivity is needed**

# simulation of forward problems (hp-fem)

## Mathematical Formulation (Goal-Oriented Adaptivity)

We consider the following problem (in variational form):

$$\begin{cases} \text{Find } L(\Psi), \text{ where } \Psi \in V \text{ such that :} \\ b(\Psi, \xi) = f(\xi) \quad \forall \xi \in V \;. \end{cases}$$

We define residual $r_e(\xi) = b(e, \xi)$. We seek for solution $G$ of:

$$\begin{cases} \text{Find } G \in V'' \sim V \text{ such that :} \\ G(r_e) = L(e) \;. \end{cases}$$

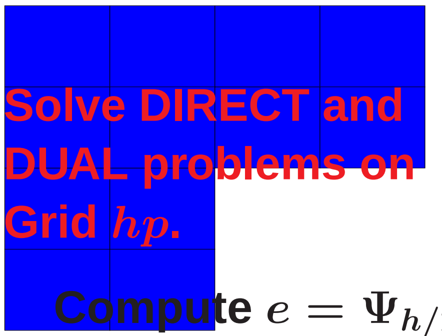
This is necessarily solved if we find the solution of the *dual* problem:

$$\begin{cases} \text{Find } G \in V \text{ such that :} \\ b(\Psi, G) = L(\Psi) \quad \forall \Psi \in V \;. \end{cases}$$

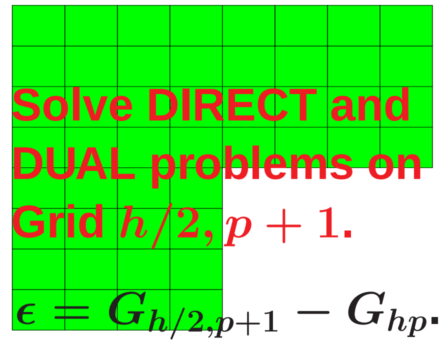
Notice that $L(e) = b(e, G)$.

# simulation of forward problems (hp-fem)

## Algorithm for Goal-Oriented Adaptivity



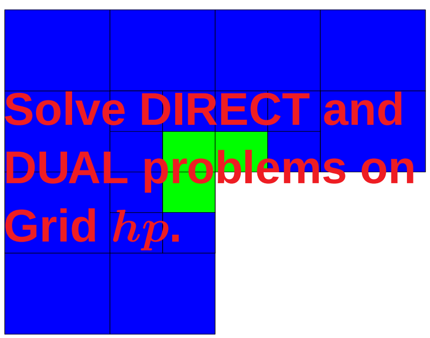

$\longrightarrow$



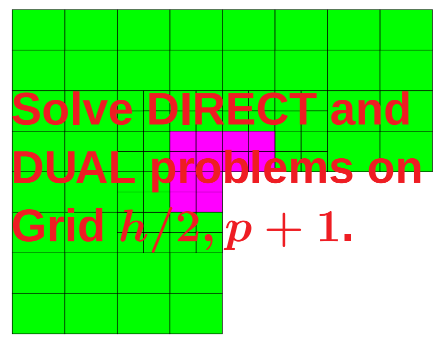

Compute $e = \Psi_{h/2,p+1} - \Psi_{hp}$, and $\epsilon = G_{h/2,p+1} - G_{hp}$.

Represent the error as: $|L(e)| = |b(e, \epsilon)| \leq \sum_K |b_K(e, \epsilon)|$.

Apply the fully automatic $hp$-adaptive algorithm.



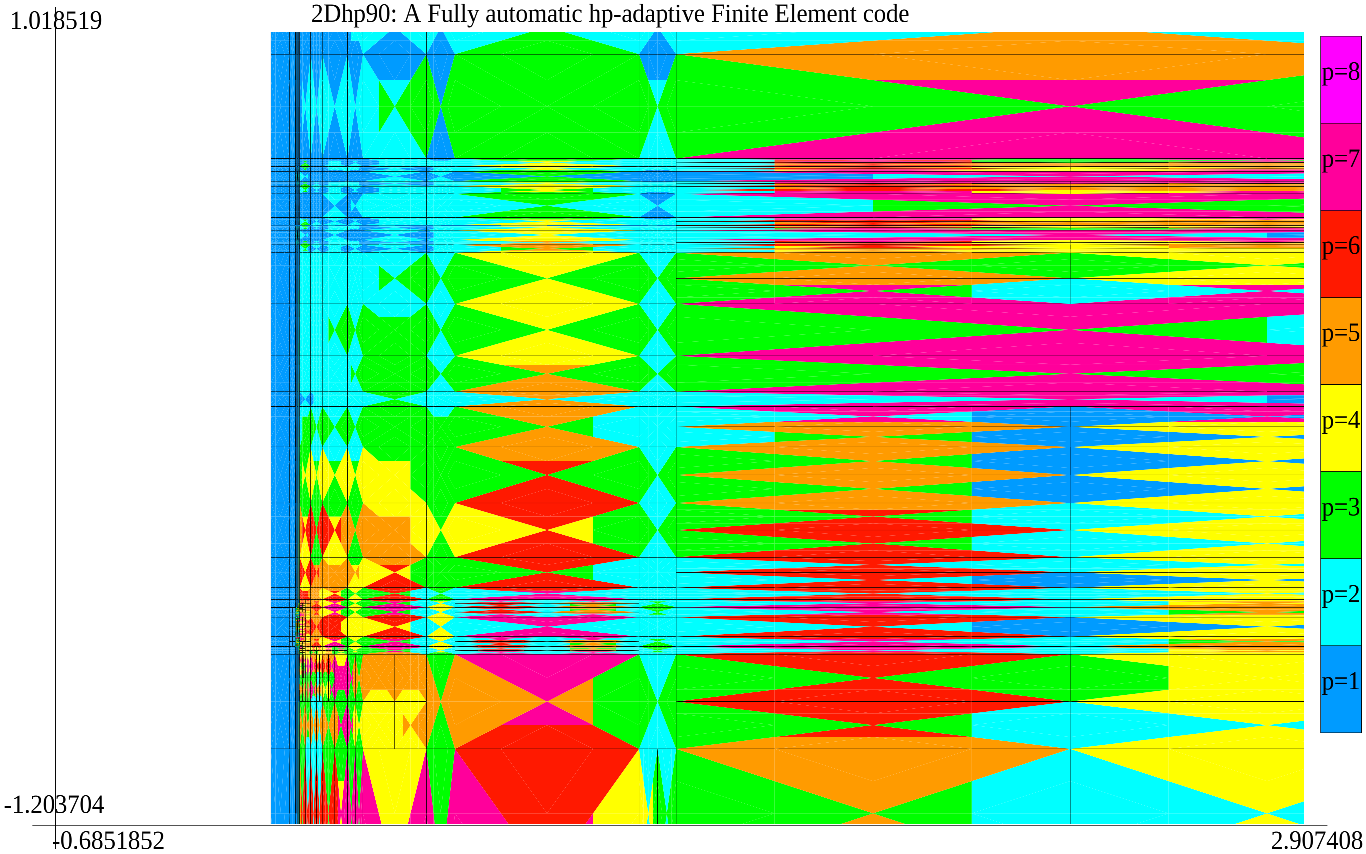

$\longrightarrow$



# simulation of forward problems (hp-fem)

## Axisymmetric Logging-While-Drilling (LWD) Simulation

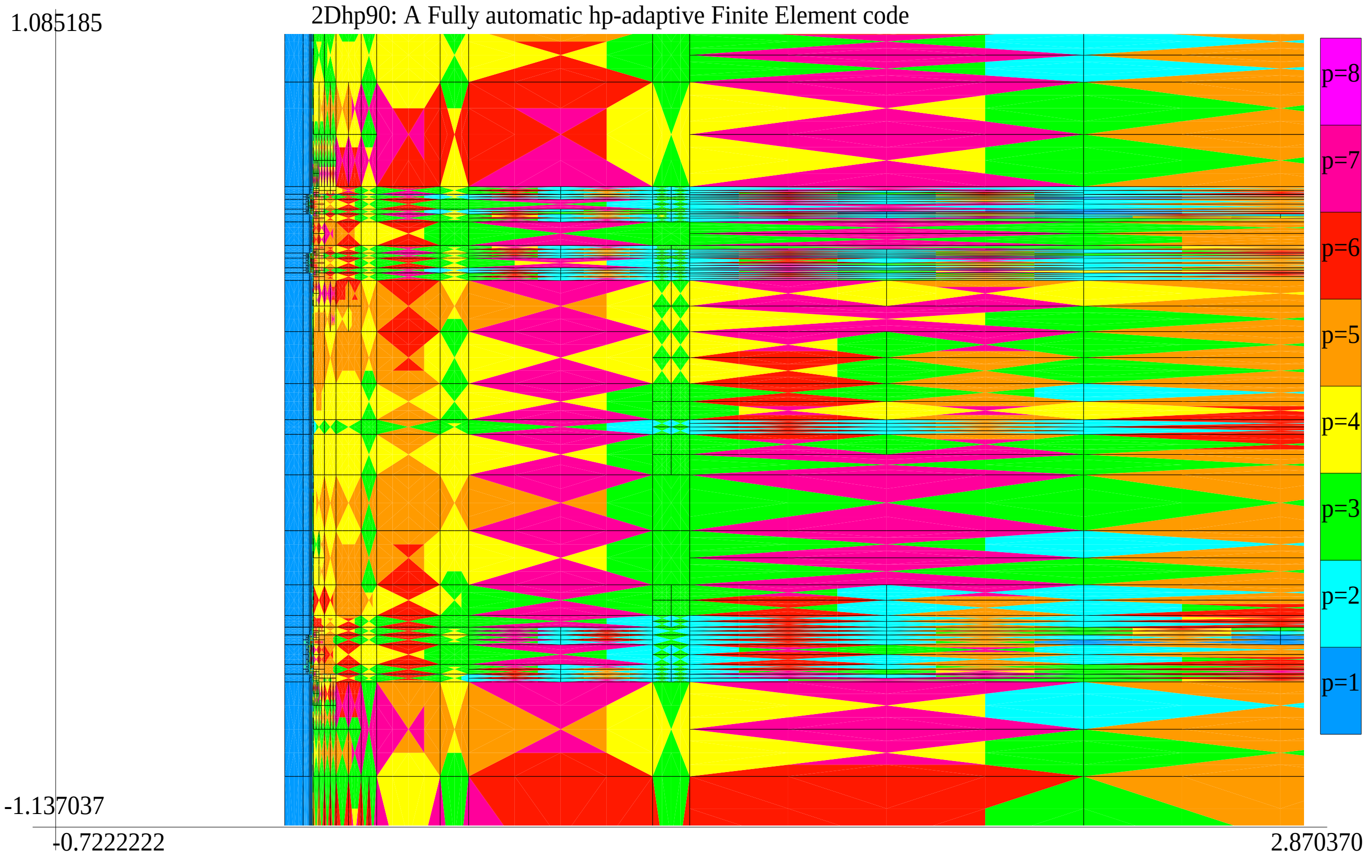
## ENERGY-NORM HP-ADAPTIVITY



# simulation of forward problems (hp-fem)

## Axisymmetric Logging-While-Drilling (LWD) Simulation

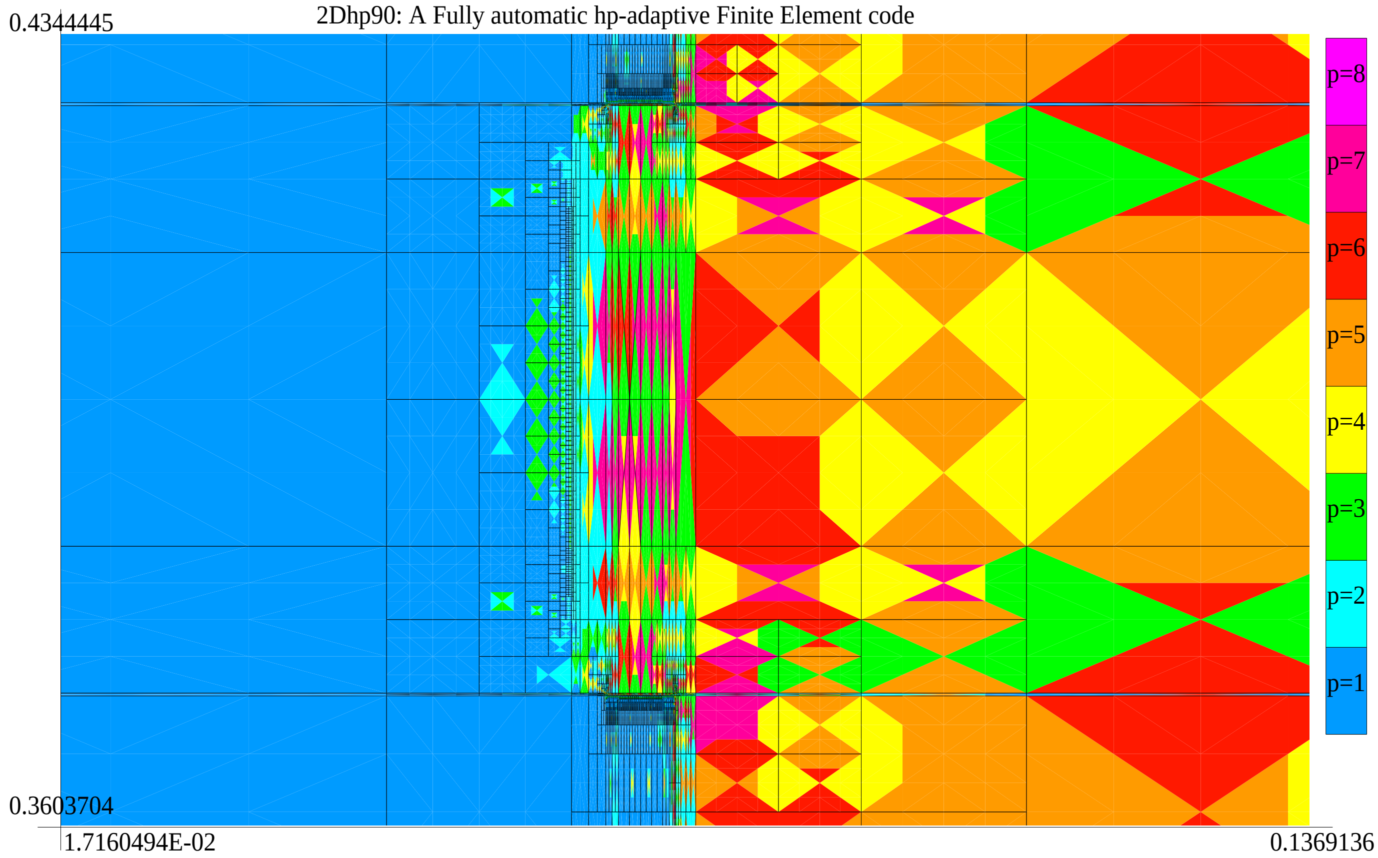
## GOAL-ORIENTED HP-ADAPTIVITY (Quadrilateral Elements)



# simulation of forward problems (hp-fem)

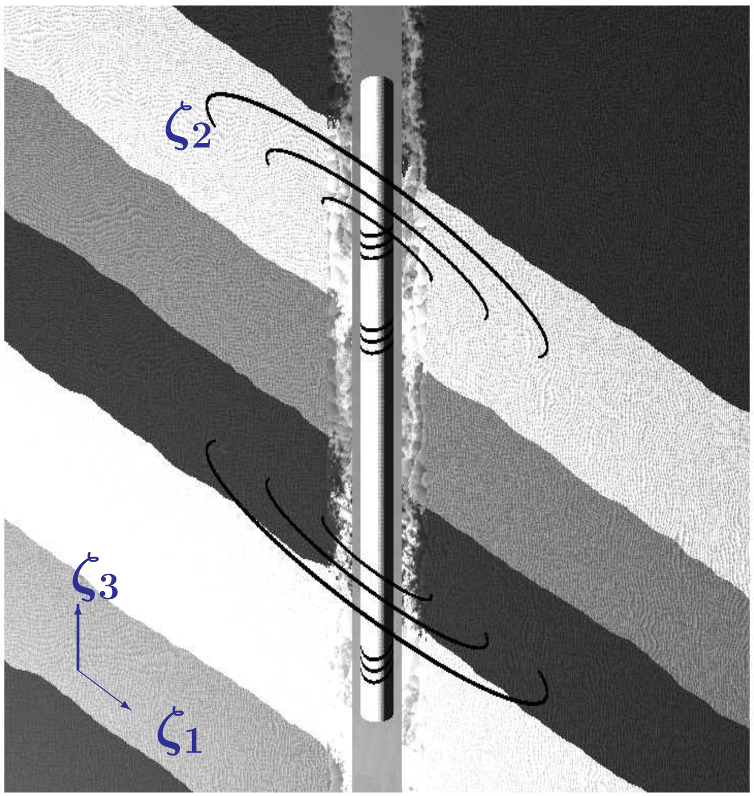
## Axisymmetric Logging-While-Drilling (LWD) Simulation

## GOAL-ORIENTED HP-ADAPTIVITY (Zoom towards first receiver)



# simulation of forward problems (hp-fem)

## Non-Orthogonal System of Coordinates




## Fourier Series Expansion in $\zeta_2$

**DC Problems:** $-\nabla \sigma \nabla u = f$

$$u(\zeta_1, \zeta_2, \zeta_3) = \sum_{l=-\infty}^{l=\infty} u_l(\zeta_1, \zeta_3) e^{jl\zeta_2}$$

$$\sigma(\zeta_1, \zeta_2, \zeta_3) = \sum_{m=-\infty}^{m=\infty} \sigma_m(\zeta_1, \zeta_3) e^{jm\zeta_2}$$

$$f(\zeta_1, \zeta_2, \zeta_3) = \sum_{n=-\infty}^{n=\infty} f_n(\zeta_1, \zeta_3) e^{jn\zeta_2}$$

**Fourier modes $e^{jl\zeta_2}$ are orthogonal high-order basis functions that are (almost) invariant with respect to the gradient operator.**

# simulation of forward problems (hp-fem)

## De Rham diagram

**De Rham diagram is critical to the theory of FE discretizations of multi-physics problems.**

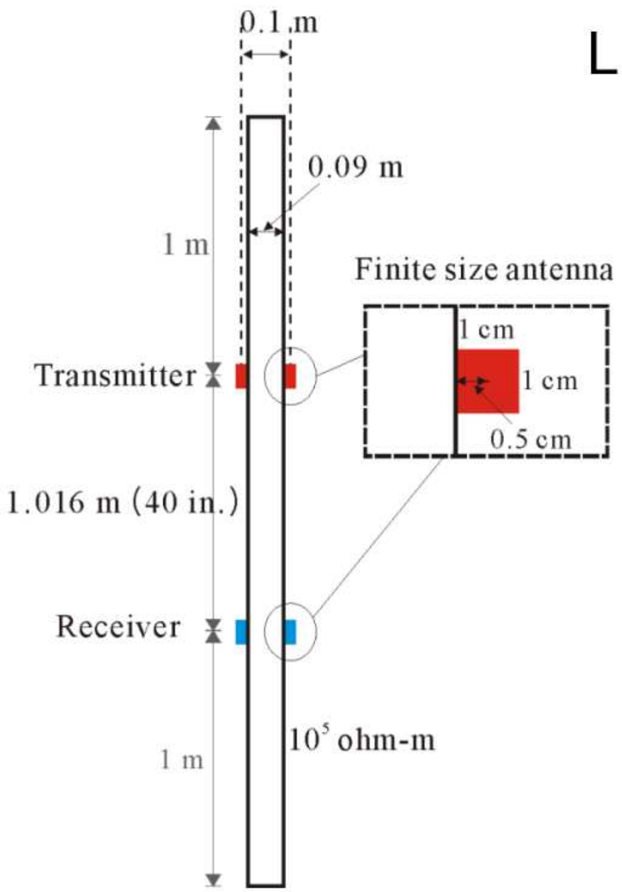
$$\begin{array}{ccccccccccc}
\mathbb{R} & \longrightarrow & W & \xrightarrow{\nabla} & Q & \xrightarrow{\nabla\times} & V & \xrightarrow{\nabla\circ} & L^2 & \longrightarrow & 0 \\
\downarrow id & & \downarrow \Pi & & \downarrow \Pi^{curl} & & \downarrow \Pi^{div} & & \downarrow P & & \\
\mathbb{R} & \longrightarrow & W^p & \xrightarrow{\nabla} & Q^p & \xrightarrow{\nabla\times} & V^p & \xrightarrow{\nabla\circ} & W^{p-1} & \longrightarrow & 0\,.
\end{array}$$

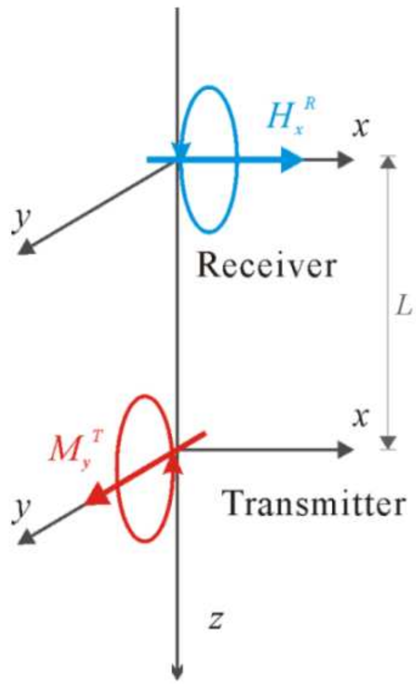
**This diagram relates two exact sequences of spaces, on both continuous and discrete levels, and corresponding interpolation operators.**

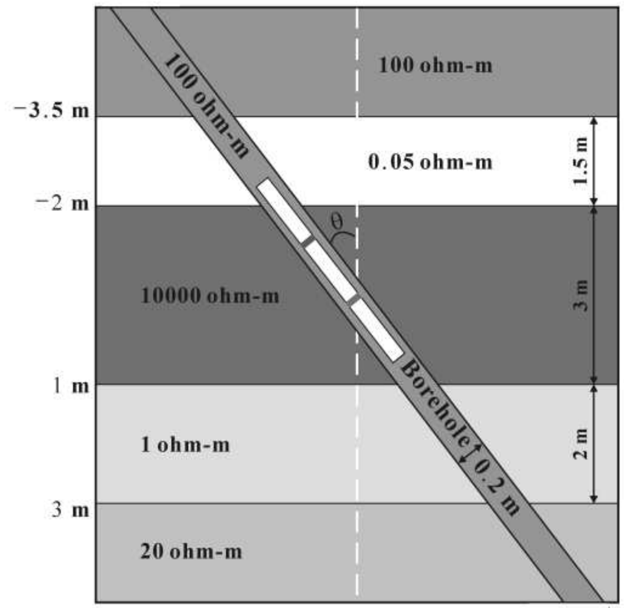
# simulation of forward problems (hp-fem)

## Tri-Axial Induction Tool

L=40 in, Frequency=20 kHz

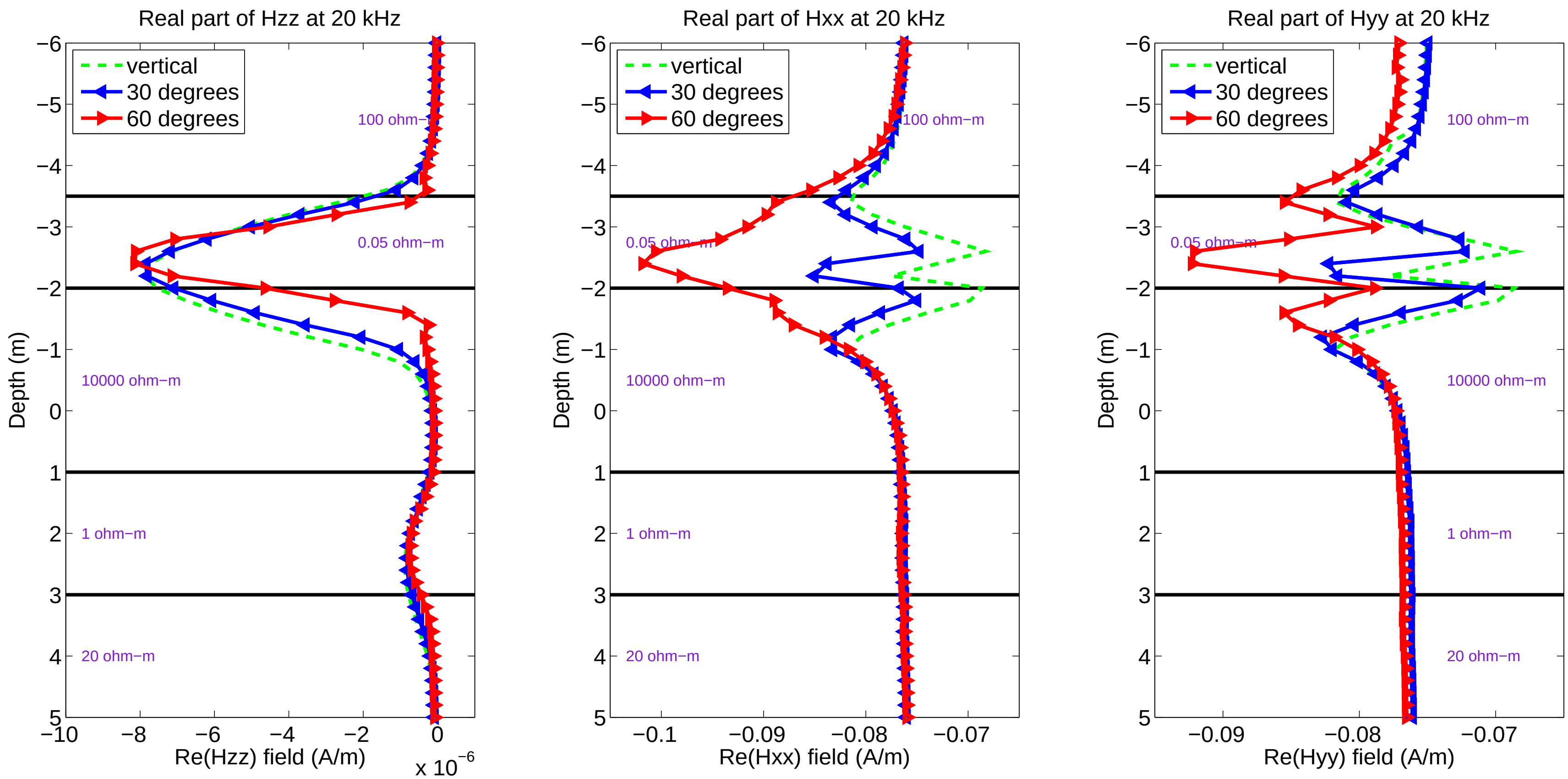


# simulation of forward problems (hp-fem)

## Tri-Axial Induction Tools in Deviated Wells (0, 30, and 60 degrees)




**Triaxial tools are more sensitive to dip angle effects**

# simulation of forward problems (hp-fem)

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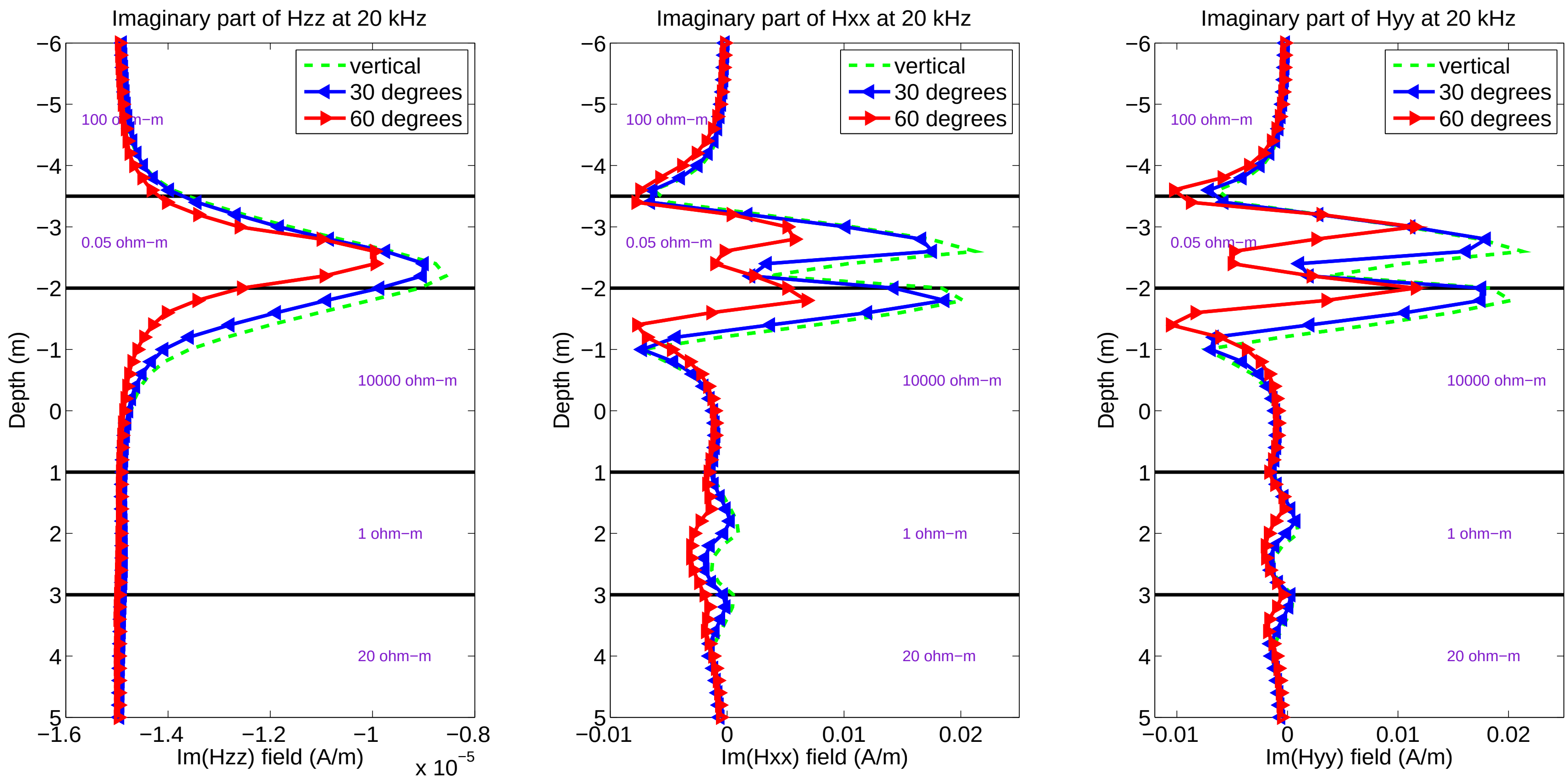
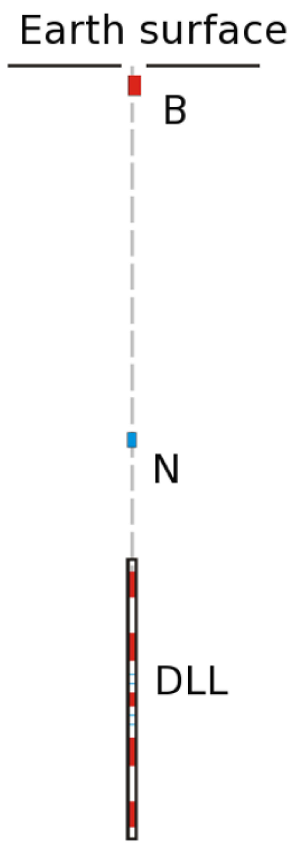
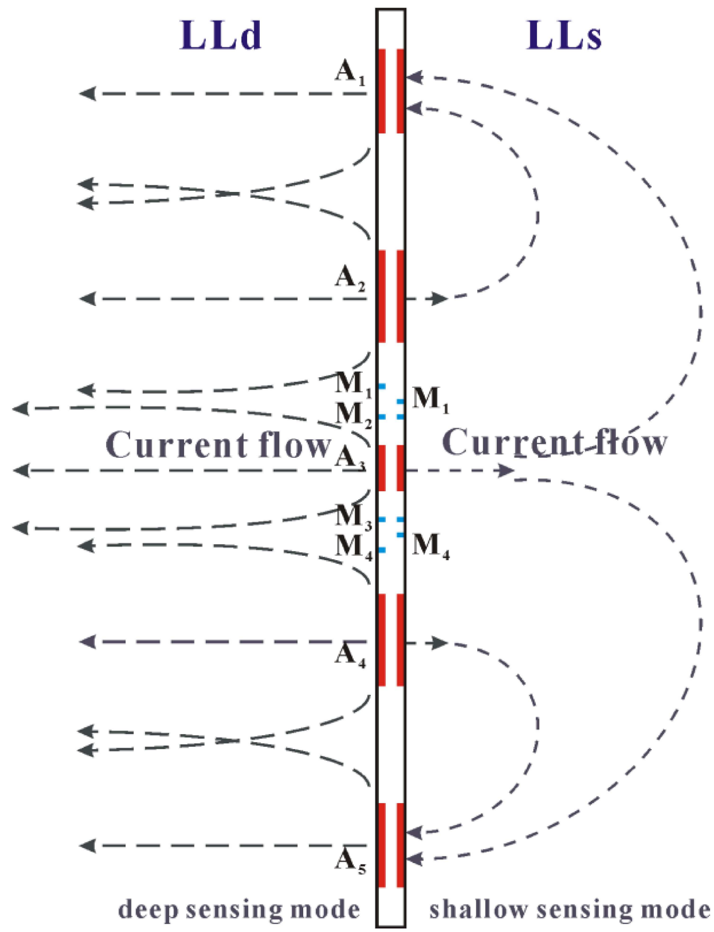


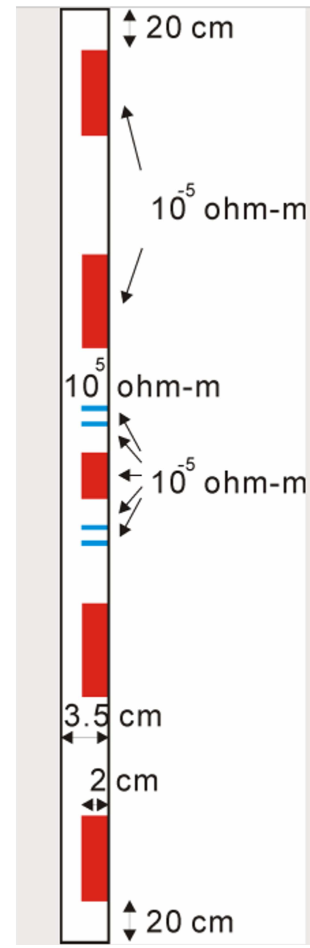

**Triaxial tools are more sensitive to dip angle effects**

# simulation of forward problems (hp-fem)

## DLL Tool

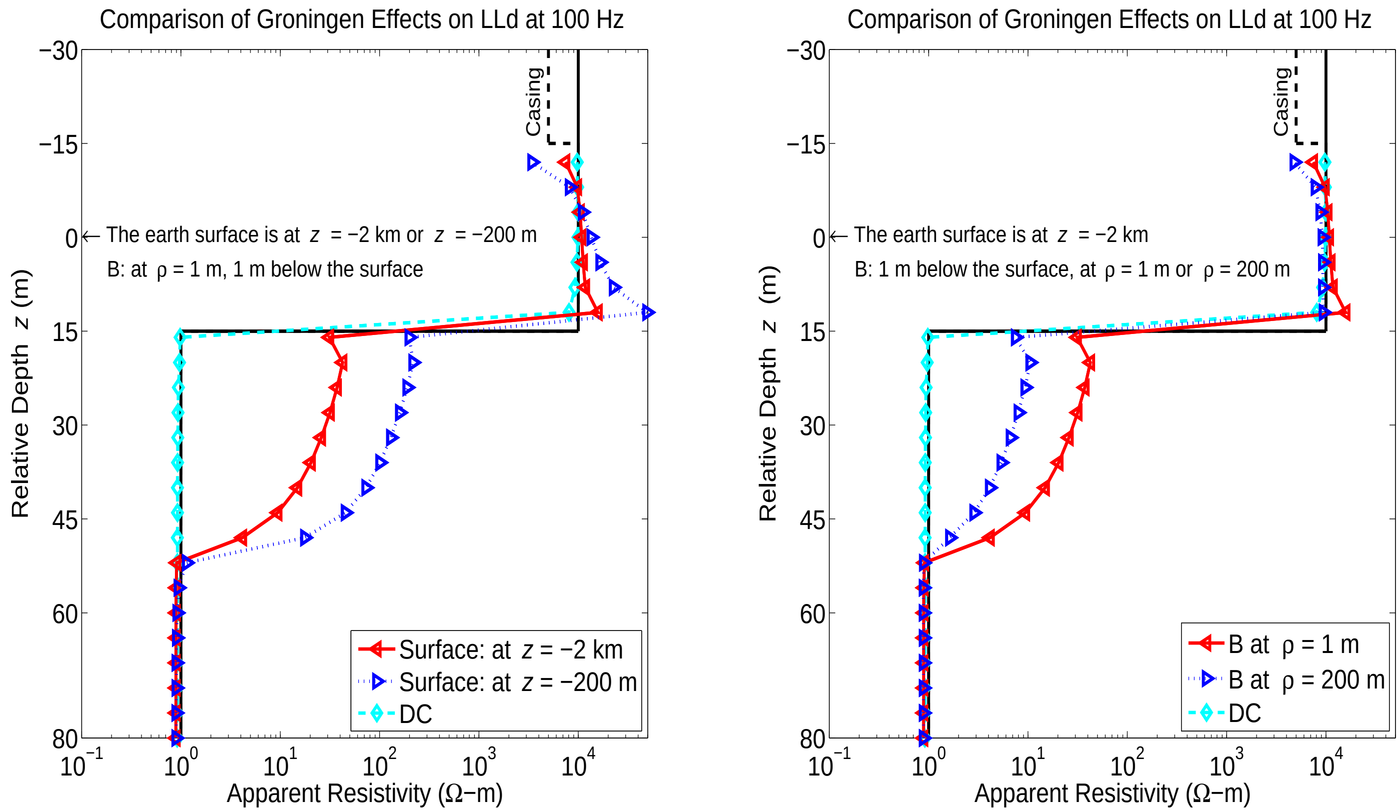


# simulation of forward problems (hp-fem)

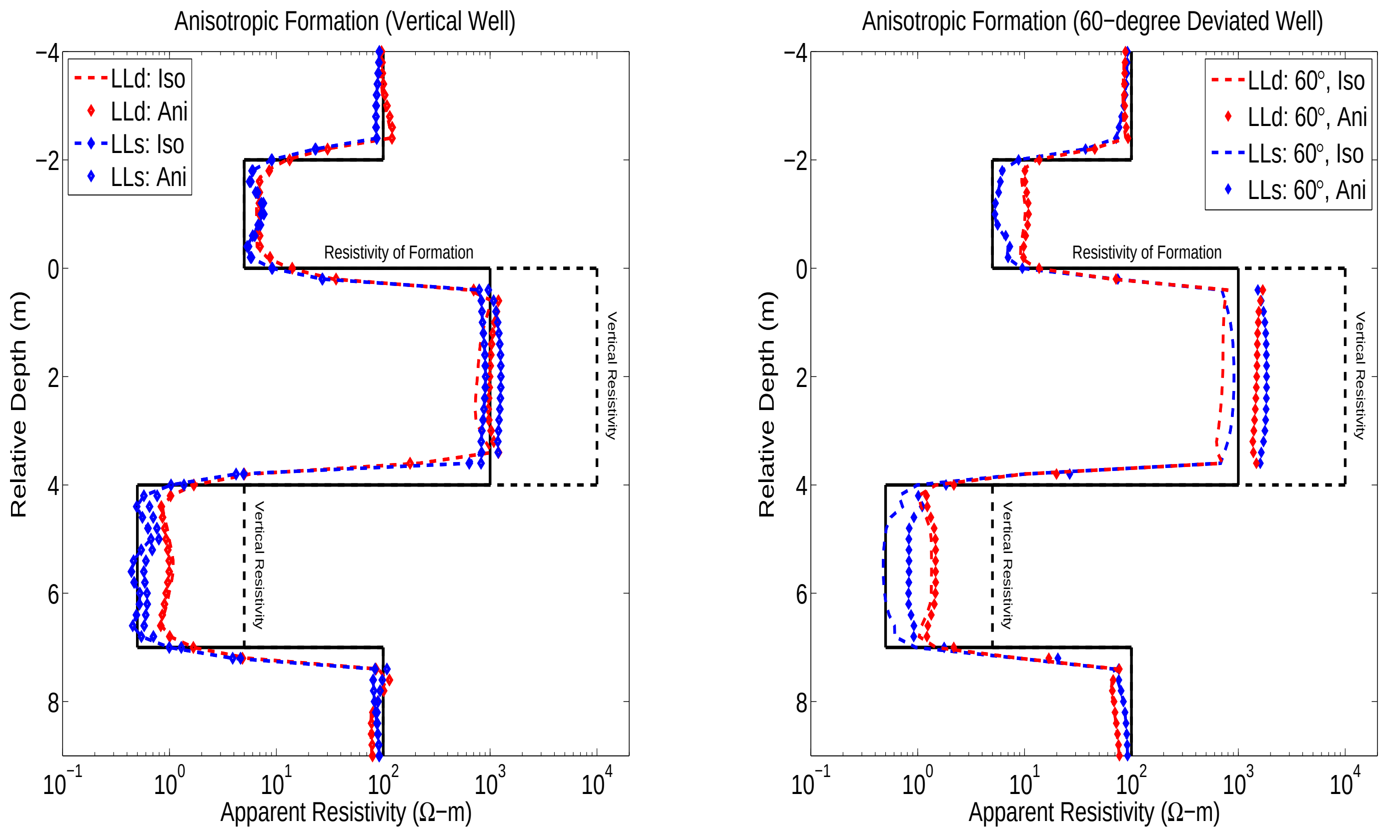
## Groningen Effect




**As we place the current return electrode B farther from the logging instrument, the Groningen effect diminishes**

# simulation of forward problems (hp-fem)

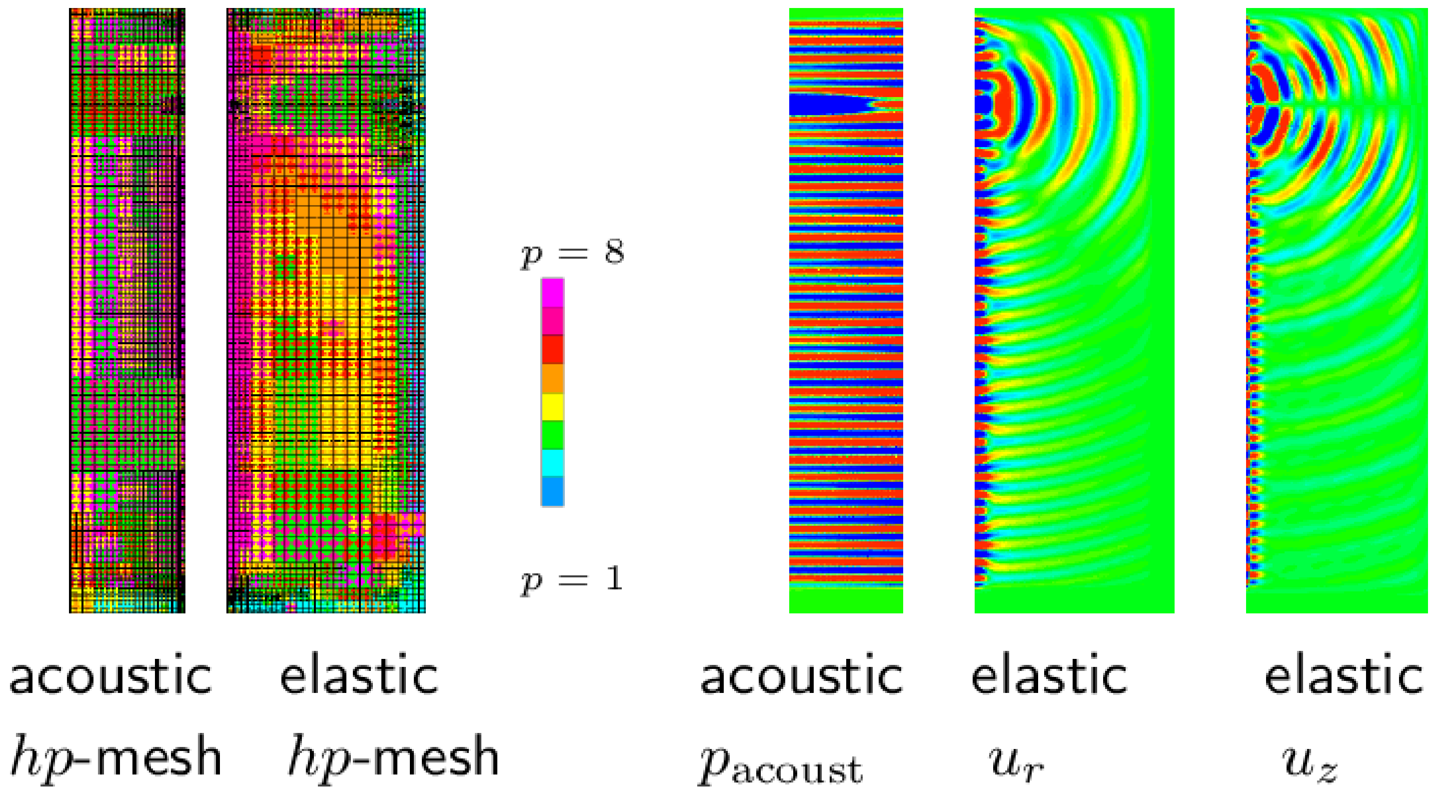
## DC DLL in Deviated Wells




**Anisotropy is better identified when using deviated wells**

# simulation of forward problems (hp-fem)

**Final $hp$-grid and solution**




**8 KHz, acoustics, open borehole setting (no logging instrument).**

# new library for inverse problems

## Variational Formulation (DC)

**Notation:**

$$B(u, v; \sigma) =< \nabla v, \sigma \nabla u >_{L^2(\Omega)} \qquad \textbf{(bilinear } u, v\textbf{)}$$

$$F_i(v) =< v, f_i >_{L^2(\Omega)} + < v, g_i >_{L^2(\partial\Omega)} \qquad \textbf{(linear } v\textbf{)}$$

$$L_i(u) =< l_i, u >_{L^2(\Omega)} + < h_i, u >_{L^2(\partial\Omega)} \qquad \textbf{(linear } u\textbf{)}$$

**Direct Problem (homogeneous Dirichlet BC's):**

$$\begin{cases} \text{Find } \hat{u}_i \in \text{V such that :} \\ B(\hat{u}_i, v; \sigma) = F_i(v) \quad \forall v \in V \end{cases}$$

**Dual (Adjoint) Problem:**

$$\begin{cases} \text{Find } \hat{v}_i \in \text{V such that :} \\ B(u, \hat{v}_i; \sigma) = L_i(u) \quad \forall u \in V \end{cases}$$

# new library for inverse problems

## Variational Formulation (AC)

**Notation:**

$$B(\mathrm{E},\mathrm{F};\sigma) = < \nabla\times\mathrm{F}, \mu^{-1}\nabla\times\mathrm{E} >_{L^2(\Omega)} - < \mathrm{F}, (\omega^2\epsilon - j\omega\sigma)\mathrm{E} >_{L^2(\Omega)}$$

$$F_i(\mathrm{F}) = -j\omega < \mathrm{F}, \mathrm{J}_i^{imp} >_{L^2(\Omega)} + j\omega < \mathrm{F}, \mathrm{J}_{S,i}^{imp} >_{L^2(\partial\Omega)}$$

$$L_i(\mathrm{E}) = < \mathrm{J}_i^{adj}, \mathrm{E} >_{L^2(\Omega)} + < \mathrm{J}_{S,i}^{adj}, \mathrm{E} >_{L^2(\partial\Omega)}$$

**Direct Problem (homogeneous Dirichlet BC's):**

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# new library for inverse problems

**Constrained Nonlinear Optimization Problem**

**Cost Functional:**

$$\begin{cases} \text{Find } \sigma > 0 \text{ such that it minimizes } C_\beta(\sigma)\text{, where :} \\ C_\beta(\sigma) = ||W_m(L(\hat{u}_\sigma) - M)||_{l_2}^2 + \beta||R(\sigma - \sigma_0)||_{L_2}^2 \,, \end{cases}$$

**where**

$M_i$ denotes the $i$-th measurement, $M = (M_1, ..., M_n)$

$L_i$ is the $i$-th quantity of interest, $L = (L_1, ..., L_n)$

$$||M||_{l_2}^2 = \sum_{i=1}^{n} M_i^2 \quad ; \quad ||R(\sigma - \sigma_0)||_{L_2}^2 = \int (R(\sigma - \sigma_0))^2$$

$\beta$ is the relaxation parameter, $\sigma_0$ is given, $W_m$ are weights

**Main objective (inversion problem): Find $\hat{\sigma} = \min_{\sigma > 0} C_\beta(\sigma)$**

# new library for inverse problems

**Solving a Constrained Nonlinear Optimization Problem**

**We select the following deterministic iterative method:**

$$\boldsymbol{\sigma}^{(n+1)} = \boldsymbol{\sigma}^{(n)} + \boldsymbol{\alpha}^{(n)} \boldsymbol{\delta\sigma}^{(n)}$$

- **How to find a search direction $\delta\sigma^{(n)}$ ?**
  - **We will employ a change of coordinates and a truncated Taylor's series expansion.**
- **How to determine the step size $\alpha^{(n)}$?**
  - **Either with a fixed size or using an approximation for computing $L(\boldsymbol{\sigma}^{(n)} + \boldsymbol{\alpha}^{(n)}\boldsymbol{\delta\sigma}^{(n)})$.**
- **How to guarantee that the nonlinear constraints will be satisfied?**
  - **Imposing the Karush-Kuhn-Tucker (KKT) conditions or with a penalization method, or via a change of variables.**

# new library for inverse problems

## Search Direction Method

**Change of coordinates:**

$$h(s) = \sigma \quad => \text{ Find } \hat{s} = \min_{h(s)>0} C_\beta(s)$$

**Taylor's series expansion:**

**A)** $C_\beta(s+\delta s) \approx C_\beta(s) + \delta s \nabla C_\beta(s) + 0.5 \delta s^2 H_{C_\beta}(s)$

**B)** $L(s+\delta s) \approx L(s) + \delta s \nabla L(s)\ ,\ R(s+\delta s) = R(s) + \delta s \nabla R(s)$

**Expansion A) leads to the Newton-Raphson method.**

**Expansion B) leads to the Gauss-Newton method.**

**Expansion A) with $H_{C_\beta} = I$ leads to the steepest descent method.**

**Higher-order expansions require from higher-order derivatives.**

# new library for inverse problems

## Computation of Jacobian Matrix

**Using the Fréchet Derivative:**

$$\frac{\partial L_i(\hat{u}_i)}{\partial s_j} = B\left(\frac{\partial \hat{u}_i}{\partial s_j}, \hat{v}_i, h(s)\right) + B\left(\hat{u}_i, \frac{\partial \hat{v}_i}{\partial s_j}, h(s)\right) + B\left(\hat{u}_i, \hat{v}_i, \frac{\partial h(s)}{\partial s_j}\right)$$

$$\|$$

$$L_i\left(\frac{\partial \hat{u}_i}{\partial s_j}\right) = B\left(\frac{\partial \hat{u}_i}{\partial s_j}, \hat{v}_i, h(s)\right)$$

$$\|$$

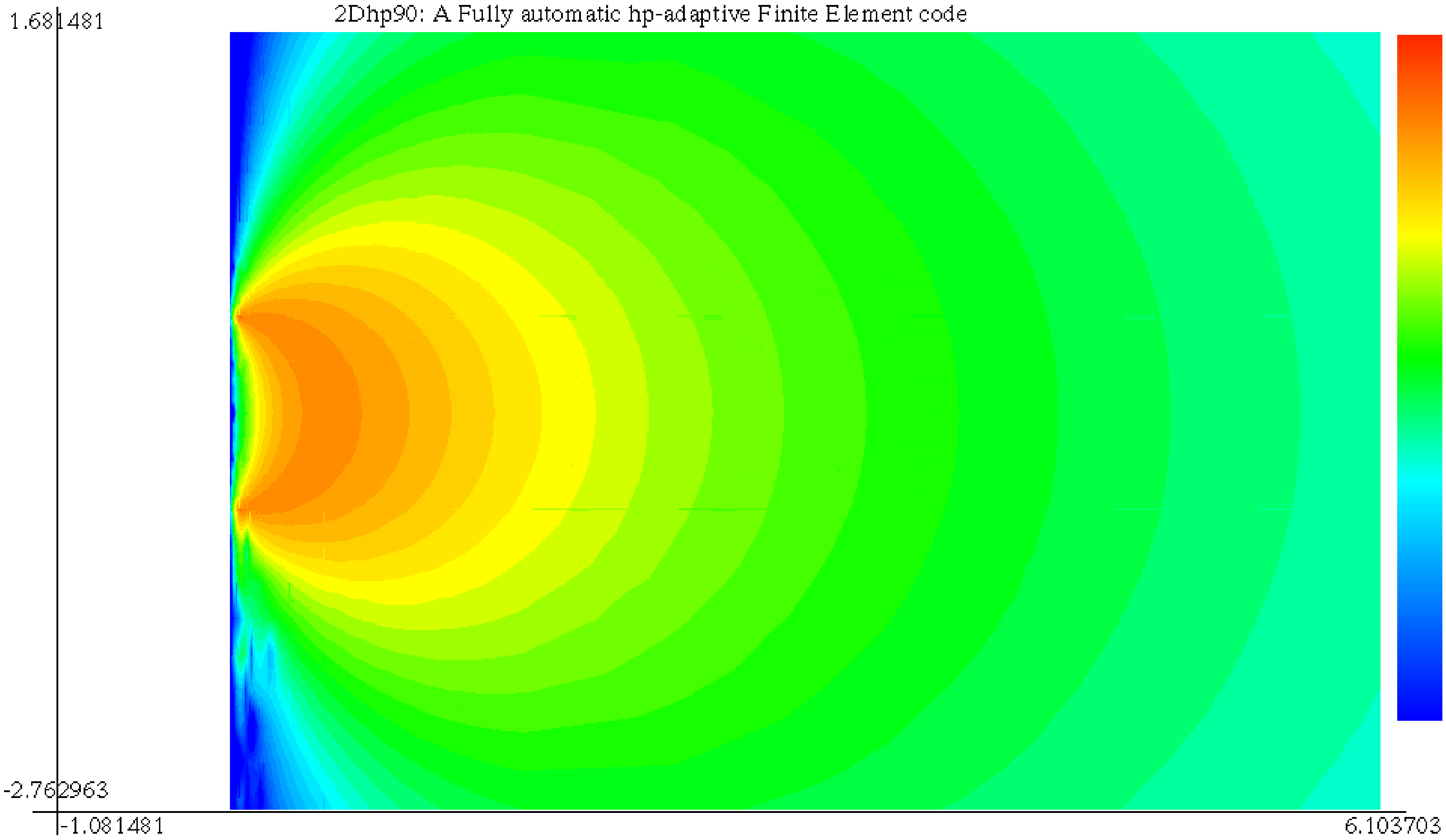
$$F_i\left(\frac{\partial \hat{v}_i}{\partial s_j}\right) = B\left(\hat{u}_i, \frac{\partial \hat{v}_i}{\partial s_j}, h(s)\right)$$

**Therefore, we conclude:**

**Jacobian Matrix** $= \frac{\partial L_i(\hat{u}_i)}{\partial s_j} = -B\left(\hat{u}_i, \hat{v}_i, \frac{\partial h(s)}{\partial s_j}\right)$

# new library for inverse problems

## Jacobian Function: One TX, one RX



# new library for inverse problems

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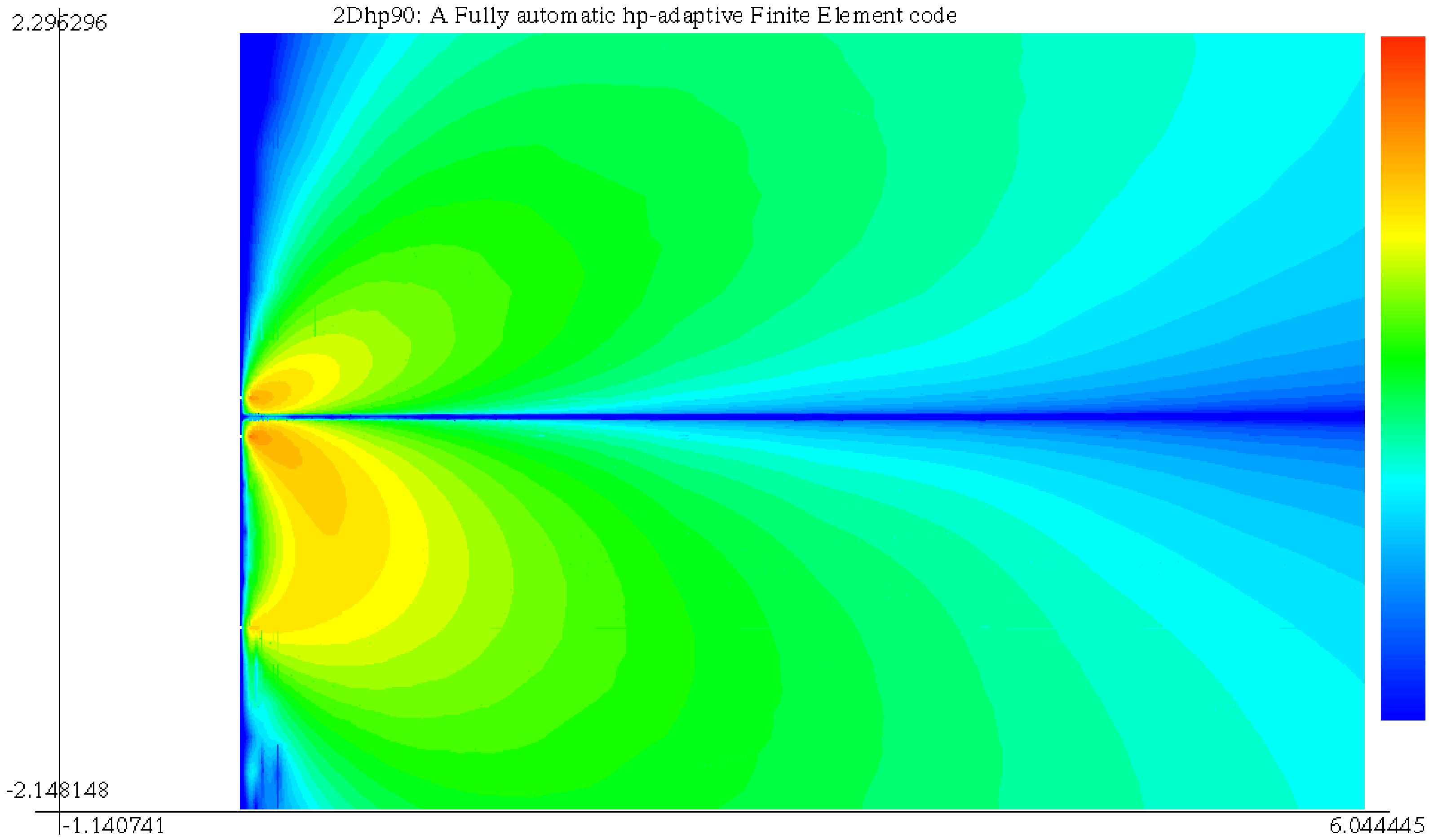

# new library for inverse problems

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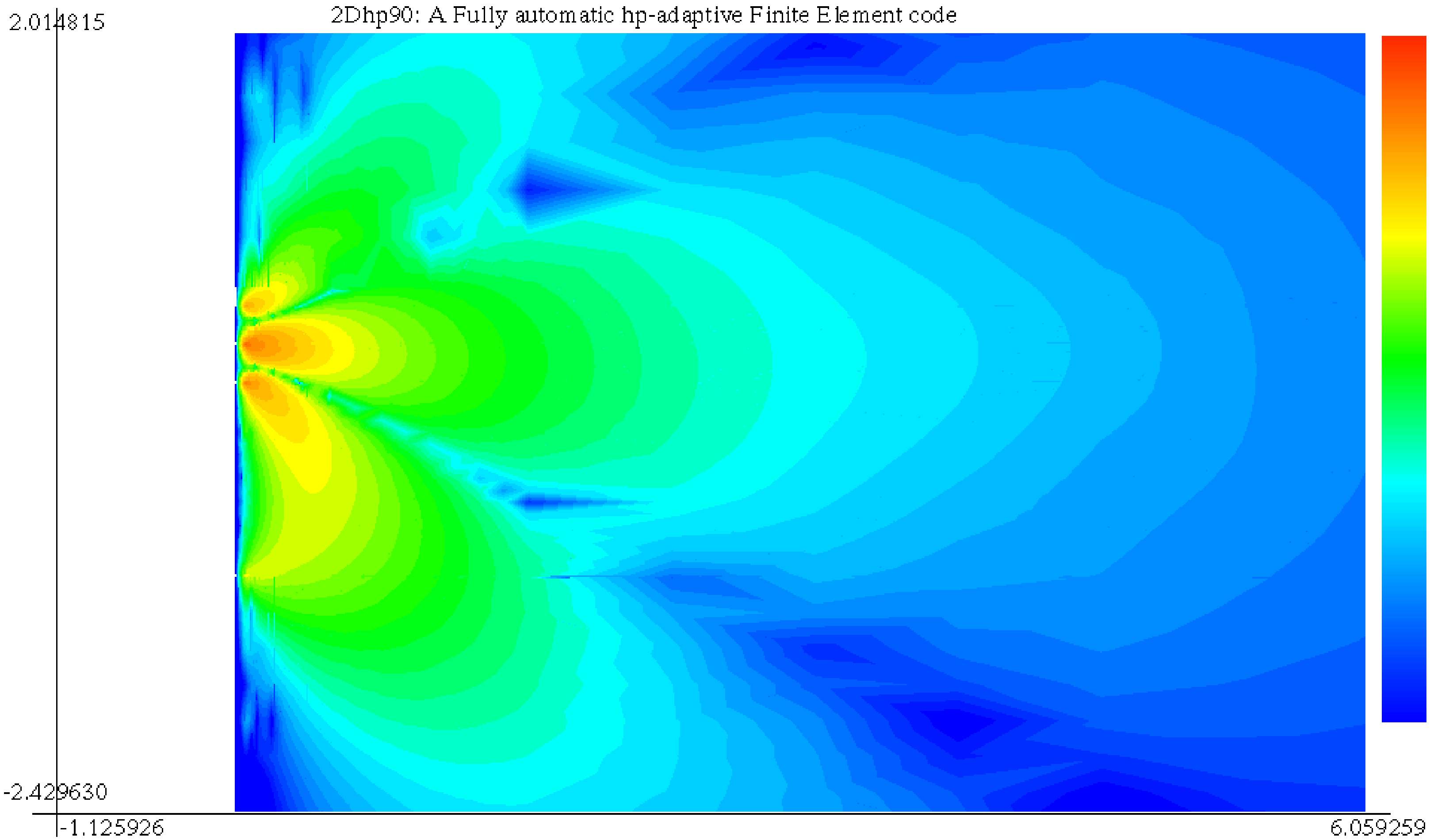


# new library for inverse problems

## Computation of Hessian Matrix

**Following a similar argument as for the Jacobian matrix, we obtain:**

$$\frac{\partial^2 L_i(\hat{u}_i)}{\partial s_j \partial s_k} = -B\left(\frac{\partial \hat{u}_i}{\partial s_j}, \hat{v}_i, \frac{\partial h(s)}{\partial s_k}\right) - B\left(\hat{u}_i, \frac{\partial \hat{v}_i}{\partial s_j}, \frac{\partial h(s)}{\partial s_k}\right) - B\left(\hat{u}_i, \hat{v}_i, \frac{\partial^2 h(s)}{\partial s_j \partial s_k}\right)$$

**How do we compute $\frac{\partial \hat{u}_i}{\partial s_j}$ and $\frac{\partial \hat{v}_i}{\partial s_j}$?**

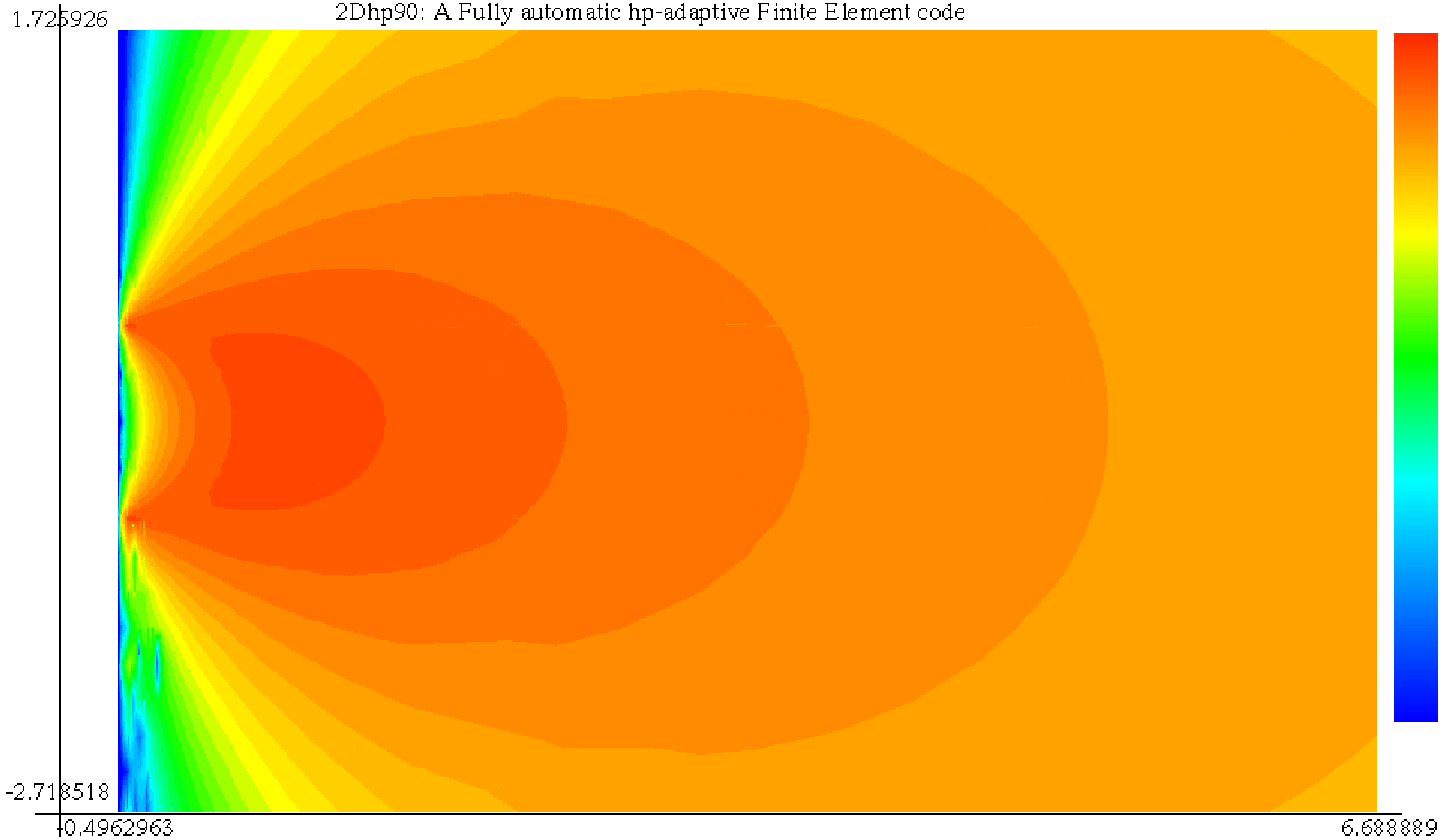
**Find** $\frac{\partial \hat{u}_i}{\partial s_j}$ **such that :** $B\left(\frac{\partial \hat{u}_i}{\partial s_j}, v_i, h(s)\right) = -B\left(\hat{u}_i, v_i, \frac{\partial h(s)}{\partial s_j}\right) \quad \forall v_i$

**Find** $\frac{\partial \hat{v}_i}{\partial s_j}$ **such that :** $B\left(\frac{\partial \hat{v}_i}{\partial s_j}, u_i, h(s)\right) = -B\left(\hat{v}_i, u_i, \frac{\partial h(s)}{\partial s_j}\right) \quad \forall u_i$

**We can compute the Hessian matrix EXACTLY by just solving our original problem for different right-hand-sides, and performing additional integrations.**

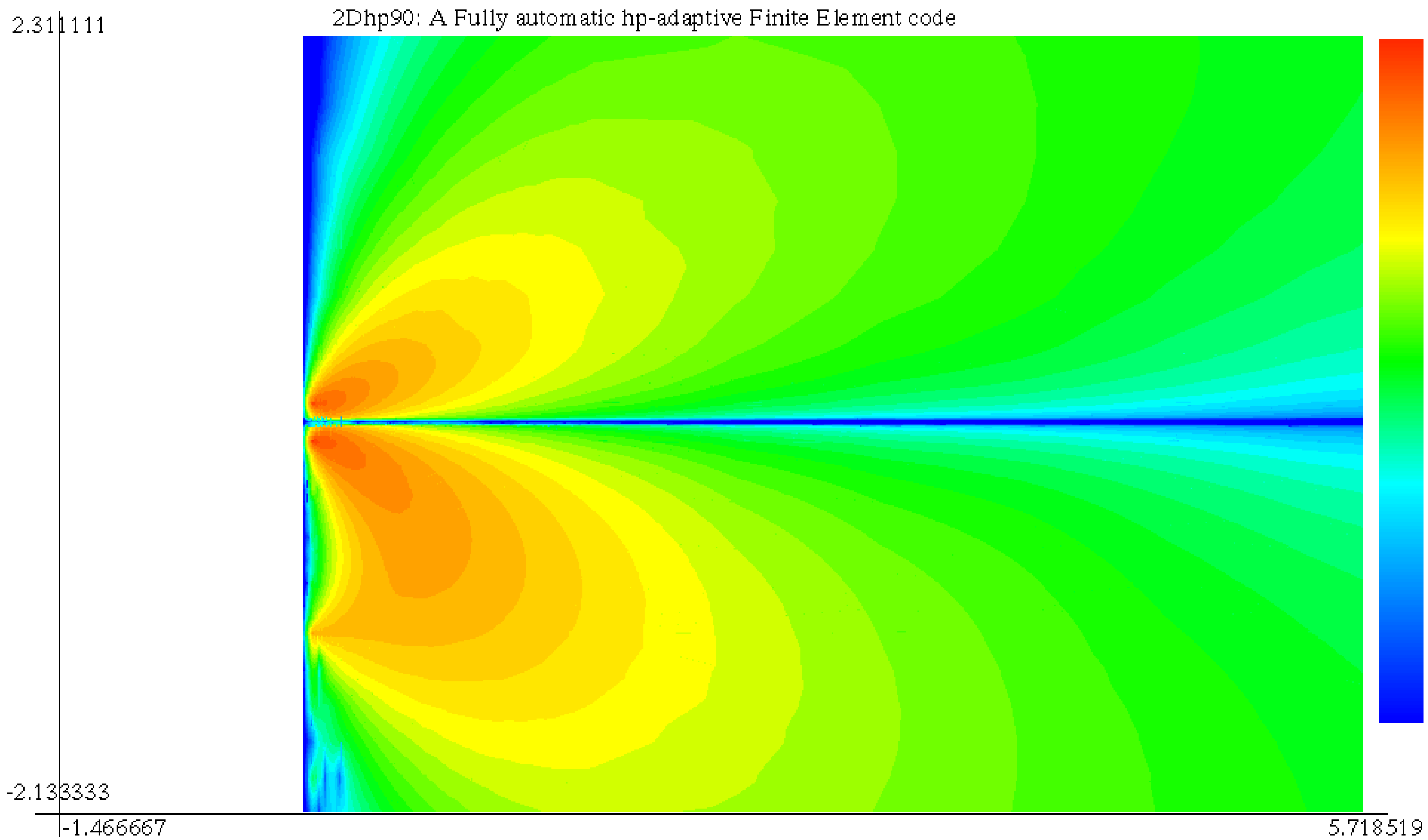
# new library for inverse problems

## Hessian Function: One TX, one RX



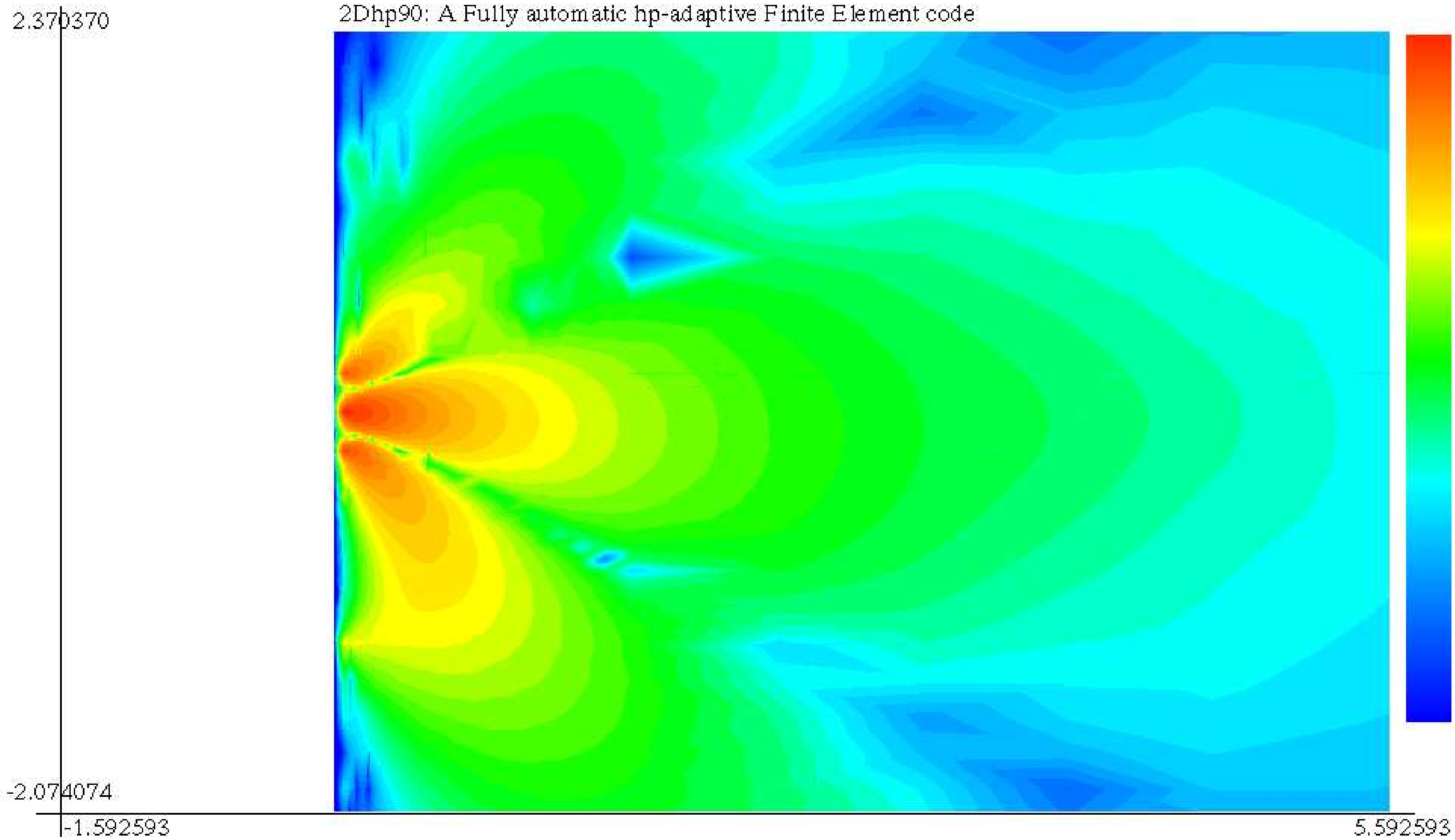
# new library for inverse problems

## Hessian Function: One TX, two RXs



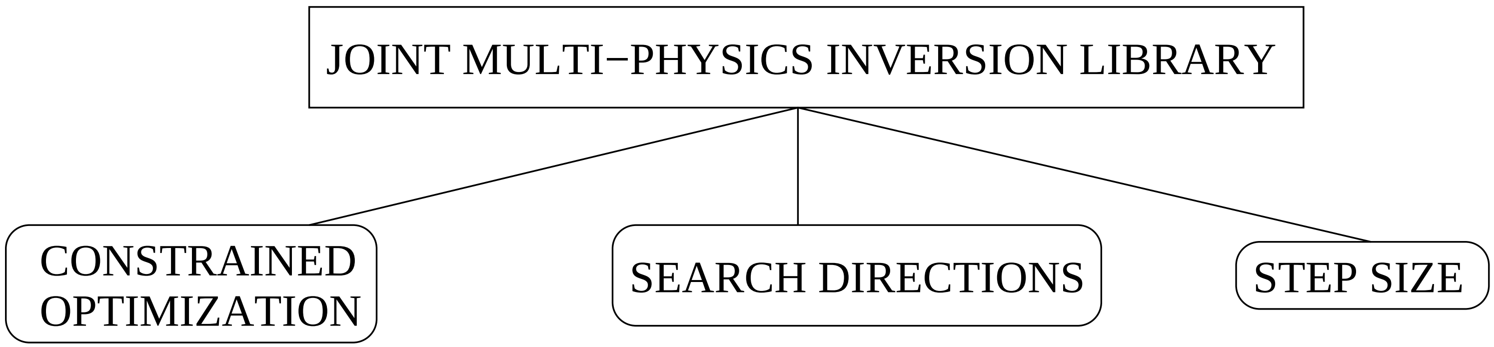
# new library for inverse problems

## Hessian Function: One TX, three RXs



# new library for inverse problems

## Algorithms implemented within the inverse library




1. KKT− Conditions
2. Penalization Method
3. Change of coordinates

1. Steepest Descent
2. Gauss−Newton
3. Newton−Raphson

1. Uniform step−size
2. Variable step−size (multiple algorithms)

**The inverse library is composed of multiple algorithms for imposing constraints, and finding search directions and corresponding step sizes.**

**Jacobian and Hessian matrices are computed exactly by simply solving the dual (adjoint) formulation and performing additional integrations.**

**The inverse library is compatible with multi-physics problems.**

# conclusions

- We have described an efficient numerical method for solving PDE's based on a self-adaptive goal-oriented $hp$ refinement strategy.
- We are developing a multiphysics version of the code.
- We are building a new module for the resolution of inverse problems.
- Our main objective is to create a software infrastructure enabling solution of challenging multiphysics inverse problems with applications to geophysics (hydrocarbon detection and monitoring, etc.), aeronautics and medicine.
- To achieve this objective, we need Ph.D. students, post-doctoral fellows, experienced researchers, and collaborators in different areas (inversion, solvers, etc).