DE LA CIENCIA A LA TECNOLOGÍA
FEM in Heat Transfer
Part 4

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Inverse Problems

What are inverse problems?
Are they useful?
General statement of an inverse problem
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What are inverse problem? Are they useful?

The solution of a **direct problem** involves finding effects based on a complete description of their causes.

<table>
<thead>
<tr>
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<th>Effect</th>
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The solution of an **inverse problem** involves determining unknown causes based on observations of their effects.

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**Prof. Oleg Mikailivitch Alifanor** proponent of Inverse Methods: “Solution of an inverse problem entails determining unknown causes based on observation of their effects. This is in contrast to the corresponding direct problem, whose solution involves finding effects based on a complete description of their causes”
What are inverse problem? Are they useful?

A simple illustration in particle dynamics

A motion of a mass in a gravitational field depends completely on the initial position and velocity of the object.

Direct problem

Inverse problem
What are inverse problem? Are they useful?

Inverse problems in engineering

• Parameter identification (e.g. Physical properties of materials)
• NDT (e.g. Detection of voids and cracks)
• Boundary inverse problems
• Retrospective problems (e.g. Backward evolution)
• Inverse Scattering and Tomography (e.g. Medical engineering)
• Image processing (e.g. Image deblurring and denoising)
• Product development (e.g. Shape optimization in acoustics, aerodynamics, electromagnetism)
• Process optimization (e.g. Continuous casting cooling strategy)
What are inverse problem? Are they useful?

Class of inverse problems

**Backward or retrospective problem:** the initial conditions are to be found.

**Coefficient inverse problem:** a coefficient in a governing equation is to be found.

**Boundary inverse problem:** some missing information at the boundary of a domain is to be found.
General statement of an inverse problem

Definition of a general direct problem

- PDE
  \[ \nabla \cdot (k \nabla T) = 0 \quad \forall x \in \Omega \]

- BC
  \[ T = T_w \quad \forall x \in \partial \Omega_T \]
  \[ -k \nabla T \cdot \mathbf{n} = q_w \quad \forall x \in \partial \Omega_q \]
  \[ -k \nabla T \cdot \mathbf{n} = h (T - T_\infty) \quad \forall x \in \partial \Omega_c \]
General statement of an inverse problem

Definition of an inverse problem

- **PDE**
  \[ \nabla \cdot (k \nabla T) = 0 \]
  \( \forall x \in \Omega \)

- **BC**
  \[ T = T_w \]
  \( \forall x \in \partial\Omega_T \)
  \[ -k \nabla T \cdot n = q_w \]
  \( \forall x \in \partial\Omega_q \)
  \[ -k \nabla T \cdot n = h (T - T_\infty) \]
  \( \forall x \in \partial\Omega_c \)

Measurements!

\[ T^\text{Obs}_i \text{ at } x^\text{Obs}_i \]

Inverse geometry problem
General statement of an inverse problem

Well-posed problems and ill-posed problems

- A solution exists for all admissible data \textit{solvability condition}
- The solution is unique \textit{uniqueness condition}
- The solution depends continuously on the data \textit{stability condition}

- If one of these properties does not hold
  - Solvability condition can usually be enforced by relaxing the notion of a solution.
  - Uniqueness condition is considered to be much more serious. Non-uniqueness is usually introduced by the need for discretization.
  - Stability condition is usually violated (small observation perturbations can lead to big errors in the solution) \rightarrow \text{Regularization methods!}
General statement of an inverse problem

Well-posed problems and ill-posed problems

- Direct problem
  \[ \mathbf{x} \xrightarrow{A} \mathbf{y} \quad A\mathbf{x} = \mathbf{y} \quad A \in \mathbb{R}^{m \times n}, \mathbf{x} \in \mathbb{R}^{n}, \mathbf{y} \in \mathbb{R}^{m} \]

- Inverse problem
  1) Given \( A \) and \( \mathbf{y} \), find \( \mathbf{x} \)
  \[ \mathbf{y} \xrightarrow{A^{-1}} \mathbf{x} \]
  2) Given \( \mathbf{x} \) and \( \mathbf{y} \), find \( A \)

If \( m < n \) and \( \mathbf{y} \in I_{A} \) (imagen de A) \( \rightarrow \) Infinite solutions

If \( \mathbf{y} \not\in I_{A} \) (measurement uncertainties) \( \rightarrow \) \( \mathbf{x}_{0} = \arg \min_{\mathbf{x}} \| A\mathbf{x} - \mathbf{y} \| \)

In finite-dimensional subspaces \( \rightarrow \) the solution is stable

In infinite-dimensional subspaces \( \rightarrow \) the solution is unstable

(when discretized, matrixes are ill-conditioned)
Regularization methods

The most active and stable period for development of solution methods and their application has been during the last 25-30 years.

Tikhonov Regularization Method

Given \( y^{obs} \) (noisy measurements)

- Least squares minimization \( x = (A^TA)^{-1} \cdot A^T y^{obs} \) \( \Rightarrow \) Unstable !!

- Tikhonov regularization \( x^{sn} = (A^TA + \alpha I)^{-1} \cdot A^T y^{obs} \)

\[
x^{sn} = \arg \min_x \|Ax - y^{obs}\|^2 + \alpha \|x\|^2
\]

Compromise between minimizing the residual norm, and keeping the “penalty term” small.
Regularization methods

Nonlinear inverse problems

Given $\mathcal{F}(\mathbf{x})$, a function defined by least-square error between the calculated and measured data:

$$\mathcal{F}(\mathbf{x}) = \frac{1}{2} \left\| \mathbf{T}(\mathbf{x}) - \mathbf{T}^{Obs} \right\|^2$$

... using the Gauss-Newton method for the minimization

$$\mathbf{x}^{Iter+1} = \mathbf{x}^{Iter} + \left[ DT^T_{(\mathbf{x}^{Iter})} DT_{(\mathbf{x}^{Iter})} \right]^{-1} \cdot \left[ DT^T_{(\mathbf{x}^{Iter})} \left( \mathbf{T}^{Obs} - \mathbf{T}^{(\mathbf{x}^{Iter})} \right) \right]$$

But the iteration is unstable !!
Regularization methods

Nonlinear inverse problems

1) The Landweber’s method

\[ x^{\text{Iter}+1} = x^{\text{Iter}} + \omega I \cdot \left[ DT_{(x^{\text{Iter}})}^T \left( T^{\text{Obs}} - T_{(x^{\text{Iter}})} \right) \right] \]

- Relaxation parameter

2) The Levenberg-Marquardt method

\[ x^{\text{Iter}+1} = x^{\text{Iter}} + \left[ DT_{(x^{\text{Iter}})}^T DT_{(x^{\text{Iter}})} + \alpha_{\text{Iter}} I \right]^{-1} \cdot \left[ DT_{(x^{\text{Iter}})}^T \left( T^{\text{Obs}} - T_{(x^{\text{Iter}})} \right) \right] \]

- Regularization parameter

3) The iteratively regularized Gauss-Newton method

\[ x^{\text{Iter}+1} = x^{\text{Iter}} + \left[ DT_{(x^{\text{Iter}})}^T DT_{(x^{\text{Iter}})} + \alpha_{\text{Iter}} L^T L \right]^{-1} \cdot \left[ DT_{(x^{\text{Iter}})}^T \left( T^{\text{Obs}} - T_{(x^{\text{Iter}})} \right) + \alpha_{\text{Iter}} L^T L (x^\Delta - x^{\text{Iter}}) \right] \]

- Regularization matrix
- Differential operators
Regularization methods

Nonlinear inverse problems - The must-do list

a) Identify the observations, its location and noise level.
b) Identify the unknowns and parametrize them in order to consider finite-dimensional subspaces.
c) State the direct problem and solve it (F.E.M.).
d) State the inverse problem ... we usually deal with nonlinear inverse problems.
e) Decide how to evaluate the sensitivity matrix:
   “discretize-then-differentiate” or “differentiate-then-discretize”
f) Determine the regularization parameter (a monotonically decreasing sequence) and the regularization matrixes.
g) Decide the convergence criterion / stopping rule (the discrepancy principle).
h) Think about useful \textit{a priori} information to enhance regularization.
Inverse problems in engineering

Experimental observation

Direct Method

Inverse Problem

Initial Data, $x^0$

New $x^{iter+1}$

Objective function, $F$

$T_{obs}$

$T_{cal}$
Inverse problems in engineering

Continuous casting steel-mold heat transfer

Copper mold model
- PDE: \( \nabla \cdot [k_m \nabla T_m] = 0 \quad \forall x \in \Omega_m \)
- BC:
  \(-k_m \nabla T_m \cdot n = h_w(T_m - T_w) \quad \forall x \in \partial \Omega_w^w \)
  \(-k_m \nabla T_m \cdot n = h_s(T_m - T_s) \quad \forall x \in \partial \Omega_s^s \)
  \(k_m \nabla T_m \cdot n = 0 \quad \forall x \in \partial \Omega_q^a \)

Steel solidification model
- PDE:
  \( \rho_s \dot{\mathcal{H}}_s - \nabla \cdot (k_s \nabla T_s^*) = 0 \quad \forall (x, t) \in \Omega_s \times (t_m^i, t_m^o) \)
- BC:
  \( T_s^* = T_{\text{cast}} \quad \forall x \in \Omega_s, \ t = t_m^i \)
  \(-k_s \nabla T_s^* \cdot n = h_s^*(T_s^* - T_m^*) \quad \forall (x, t) \in \partial \Omega_s \times (t_m^i, t_m^o) \)
Inverse problems in engineering
Continuous casting steel-mold heat transfer

Observations:

<table>
<thead>
<tr>
<th>Measurement</th>
<th>Observed variable</th>
<th>A priori information</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{i}^{obs}$</td>
<td>$T_{i}^{obs}$</td>
<td>--</td>
</tr>
<tr>
<td>$G_{w}^{obs}$</td>
<td>$Q_{w}^{obs} = G_{w}^{obs} c_{w} \Delta T_{w}^{obs}$</td>
<td>--</td>
</tr>
<tr>
<td>$\Delta T_{w}^{obs}$</td>
<td>$n_{coef} \gg n_{tc} + 1$</td>
<td>Local maximum</td>
</tr>
<tr>
<td>$h_{level}^{obs}$</td>
<td>--</td>
<td>Smooth function</td>
</tr>
</tbody>
</table>

Useful a priori information:
- maximum at meniscus
- smooth function
Inverse problems in engineering
Continuous casting steel-mold heat transfer

Statement of the inverse problem:

\[
\begin{align*}
\min & \quad \frac{1}{2} \| x \|_2^2 + \varepsilon J_{\text{apriori}} \\
\text{subject to} & \quad A x - b = 0 \\
& \quad g_i \leq 0 \quad i = 1, n_{\text{level}},
\end{align*}
\]

The system is underdetermined and does not have a unique solution.

Measurements are imposed.

A priori information is incorporated in order to cope with the non-uniqueness of the problem.

\[
J_{\text{apriori}} = \frac{1}{2} \| L_{\text{max}}(h_s^0 + x) \|_2^2 + \frac{1}{2} \| L_{\text{smooth}}(h_s^0 + x) \|_2^2
\]
Inverse problems in engineering

Continuous casting steel-mold heat transfer

From the must-do list ....

• Decide how to evaluate the sensitivity matrix: “discretize-then-differentiate” or “differentiate-then-discretize”

Direct problem

\[
\begin{bmatrix}
K_{cond} + K_w + \sum_{k=1}^{n_{coef}} h_{s,k} K_{s,k}
\end{bmatrix} T_m - K_w T_w - \left[ \sum_{k=1}^{n_{coef}} h_{s,k} K_{s,k} \right] T_s = 0
\]

Sensitivity equations

\[
\begin{bmatrix}
K_{cond} + K_w + \sum_{k=1}^{n_{coef}} h_{s,k} K_{s,k}
\end{bmatrix} \frac{\partial T_m}{\partial h_{s,j}} - \left[ \sum_{k=1}^{n_{coef}} \delta_{j,k} K_{s,k} \right] (T_s - T_m) = 0
\]

Are used in the sensitivity matrix
Inverse problems in engineering

Estimation of the blast furnace hearth wear profile

The 1150°C isotherm represents a potential limit on the penetration of liquid into the hearth wall porosity (1150°C is the eutectic temperature of carbon saturated iron).

The location of the 1150°C isotherm is estimated solving a non-linear inverse heat transfer problem, where the observations are temperature measurements and the unknown is the geometry.
Inverse problems in engineering

Estimation of the blast furnace hearth wear profile

\[ \bar{\Omega}_n \quad \text{Fixed boundary, where natural boundary conditions are applied.} \]

\[ \bar{\Omega}_T \quad \text{Unknown boundary, where a known temperature is applied.} \]

We consider our problem in finite-dimensional subspaces:

- \( n_p \) Number of parameters that describe the geometry
- \( n_{obs} \) Number of observations located inside

Non-linear inverse problem \( p^* = \arg \min_{p \in \mathbb{R}^{n_p}} F(p) \)

where \( F(p) = \frac{1}{2} \| T(p) - T^{OBS} \|_2^2 \)
Inverse problems in engineering

Estimation of the blast furnace hearth wear profile

In order to guarantee a stable solution the iteratively regularized Gauss-Newton method is applied:

\[
\text{GN} p_{\text{Iter}+1} = p_{\text{Iter}} + \left[ DT(p_{\text{Iter}}) DT(p_{\text{Iter}}) + \alpha_{\text{Iter}} L^T L \right]^{-1} \\
\cdot \left[ DT(p_{\text{Iter}}) \Delta T^{\text{OBS}}(p_{\text{Iter}}) + \alpha_{\text{Iter}} L^T L (p^\Delta - p_{\text{Iter}}) \right]
\]

where:

- \( DT(p) \) Sensitivity matrix (partial derivatives of the temperature with respect to the set of geometry parameters)
- \( L \) Regularization matrix (a discrete form of some differential operator)
- \( p^\Delta \) A priori suitable approximation of the unknown set of parameters

The problem is highly non-linear:

\[
p_{\text{Iter}+1} = p_{\text{Iter}} + \beta_{\text{Iter}} \left( \text{GN} p_{\text{Iter}+1} - p_{\text{Iter}} \right)
\]

Inverse problems in engineering

Estimation of the blast furnace hearth wear profile

From the must-do list ....

• Decide how to evaluate the sensitivity matrix:
  “discretize-then-differentiate” or “differentiate-then-discretize

By finite difference approximation

\[
\frac{\partial T}{\partial p_j} \bigg|_{(x,p)} \approx \frac{\tilde{T}(x,\{p_1,\ldots,p_j+\Delta p_j,\ldots,p_{np}\}) - \tilde{T}(x,\{p_1,\ldots,p_j,\ldots,p_{np}\})}{\Delta p_j}
\]

If we do it on each node and we use the same discretization support used for the temperature field:

\[
\frac{\partial T}{\partial p_j} \bigg|_{(x,p)} \approx N(x) \frac{\partial T}{\partial p_j}^{FEM} \bigg|_{(p)}
\]

Are used in the sensitivity matrix
Summary

Nonlinear inverse problems - The must-do list

a) Identify the observations, its location and noise level.
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h) Think about useful \textit{a priori} information to enhance regularization.
Examples on phase change problems

Phase Change and Element birth and death problem: During a twelve day period, concrete is added to a hole previously drilled into rock. At the beginning of each 4 day interval, a 5 meter depth of concrete is poured. As the concrete solidifies, internal heat is generated as the water and cement in the concrete react and this heat is conducted into the surrounding rock and convected to the surrounding atmosphere. Calculate the temperature distribution in the concrete and surrounding rock as a function of time. An axisymmetric analysis is appropriate here. There is a change in the concrete volume and heat transfer surface area as the concrete is added.
Examples on phase change problems

Exercise 2: Considering an environmental temperature of -20°C, calculate how much time is it necessary to solidify a 1m x 1m x 1m block of 20°C water. All points in the block must be at most at -5°C after solidifying.