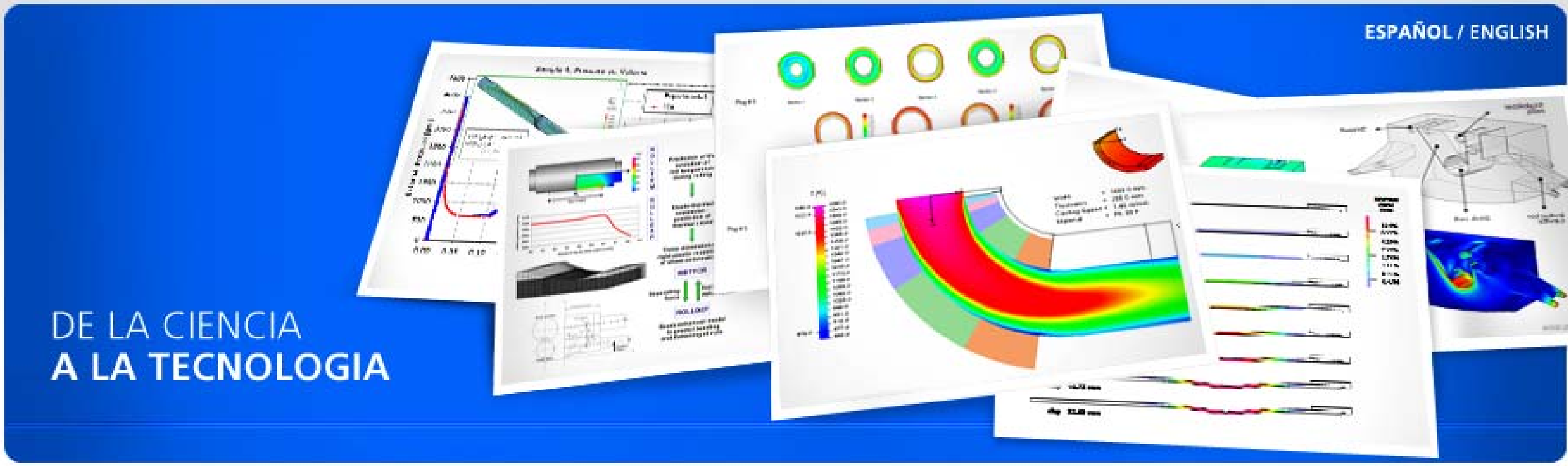
SIM&TEC

Simulación y Tecnología

Simulation and Technology



FEM in Heat Transfer
Part 4

Marcela B. Goldschmit

CONTENTS

Part 1

- Introduction to heat transfer
- Heat transfer equations
- Non-dimensional numbers
- The finite element method in heat transfer
- Boundary conditions: natural convection, forced convection
- Boundary conditions: radiation, boiling
- Examples on conduction-convection heat transfer problems

Part 2

- Boundary conditions: review
- Boundary conditions: condensation
- Time integration
- Non-linear equations: Picard method, Newton-Raphson method, BFGS
- Examples on transitory thermal problems

CONTENTS

Inverse Problems

What are inverse problems ?

Are they useful ?

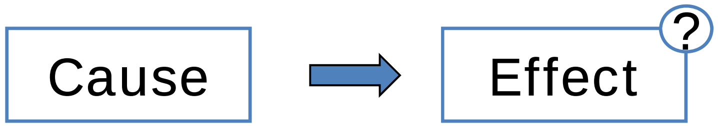
General statement of an inverse problem

Regularization methods

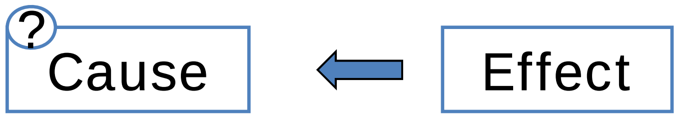
Inverse problems in engineering

What are inverse problem? Are they useful?

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



The solution of an **inverse problem** involves determining unknown causes based on observations of their effects.

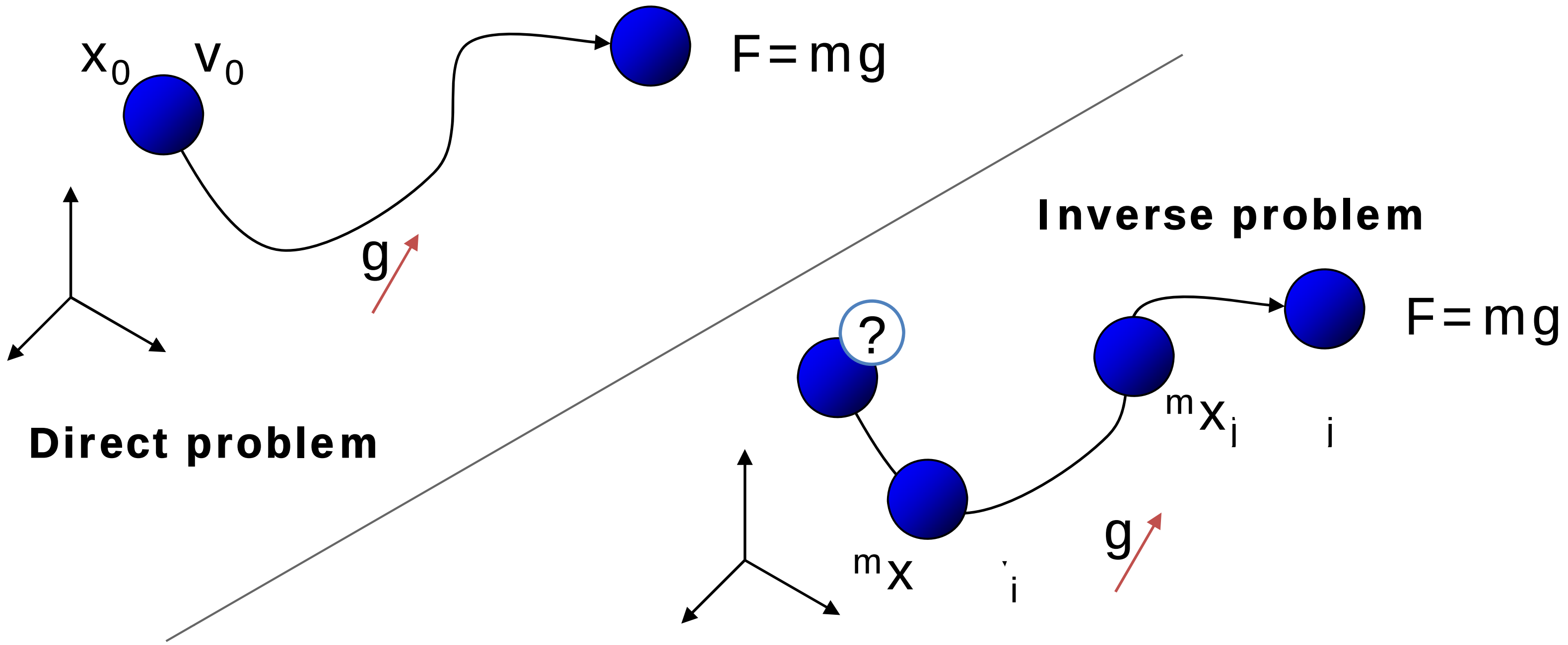


Prof. Oleg Mikailivitch Alifanor proponent of Inverse Methods: “Solution of an inverse problem entails determining unknown causes based on observation of their effects. This is in contrast to the corresponding direct problem, whose solution involves finding effects based on a complete description of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



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

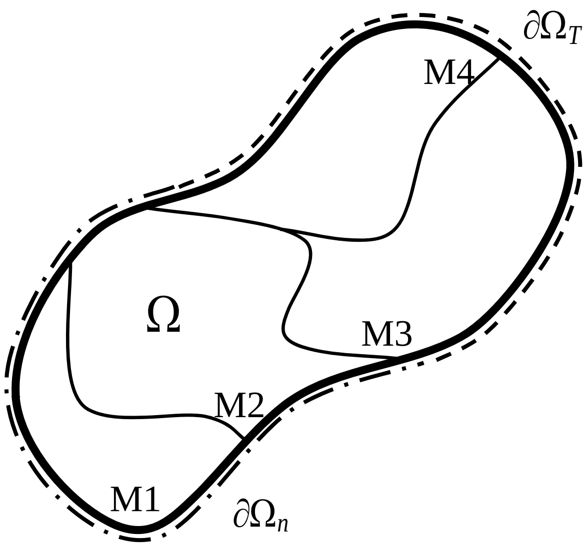
Backward or retrospective problem: the initial conditions are to be found.

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

$$\nabla \cdot (k \nabla T) = 0 \qquad \forall \mathbf{x} \in \Omega$$

- BC

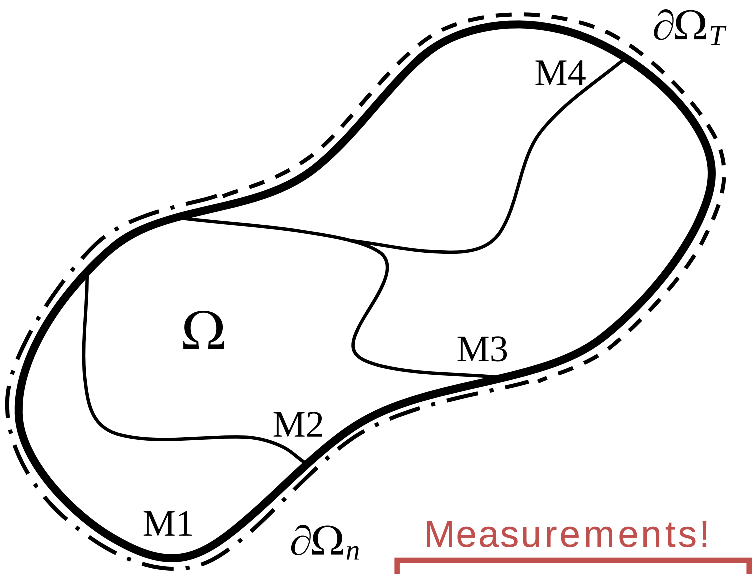
$$T = T_w \qquad \forall \mathbf{x} \in \partial\Omega_T$$

$$-k \, \nabla T \cdot \mathbf{n} = q_w \qquad \forall \mathbf{x} \in \partial\Omega_q$$

$$-k \, \nabla T \cdot \mathbf{n} = h \, (T - T_\infty) \qquad \forall \mathbf{x} \in \partial\Omega_c$$

General statement of an inverse problem

Definition of an inverse problem



Measurements!

T_i^{Obs} at $\mathbf{x}_i^{Obs}$

- PDE

Parameter identification — Inverse geometry problem

$$\nabla \cdot (k \nabla T) = 0 \qquad \forall \mathbf{x} \in \Omega$$

- BC

Boundary inverse problem

$$T = T_w \qquad \forall \mathbf{x} \in \partial\Omega_T$$

$$-k\, \nabla T \cdot \mathbf{n} = q_w \qquad \forall \mathbf{x} \in \partial\Omega_q$$

$$-k\, \nabla T \cdot \mathbf{n} = h\,(T - T_\infty) \qquad \forall \mathbf{x} \in \partial\Omega_c$$

Parameter identification

General statement of an inverse problem

Well-posed problems and ill-posed problems

- A solution exists for all admissible data *solvability condition*
- The solution is unique *uniqueness condition*
- The solution depends continuously on the data *stability condition*

well-posed problems

- 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) → Regularization methods!

ill-posed problems

General statement of an inverse problem

Well-posed problems and ill-posed problems

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

- Inverse problem

1) Given $\mathbf{A}$ and $\mathbf{y}$, find $\mathbf{x}$ $\quad \mathbf{y} \xrightarrow{\mathbf{A}^{-1}} \mathbf{x}$

2) Given $\mathbf{x}$ and $\mathbf{y}$, find $\mathbf{A}$

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

If $\mathbf{y} \notin I_{\mathbf{A}}$ (measurement uncertainties) → $\mathbf{x}_0 = \arg\min_{\mathbf{x}} \|\mathbf{Ax} - \mathbf{y}\|$

In finite-dimensional subspaces → the solution is stable

In infinite-dimensional subspaces → 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 $\mathbf{y}^{obs}$ (noisy measurements)

- Least squares minimization $\mathbf{x} = (\mathbf{A}^T\mathbf{A})^{-1} \cdot \mathbf{A}^T\mathbf{y}^{obs}$ → Unstable !!
- Tikhonov regularization $\mathbf{x}^{sn} = (\mathbf{A}^T\mathbf{A} + \alpha\mathbf{I})^{-1} \cdot \mathbf{A}^T\mathbf{y}^{obs}$

Regularization parameter (α)

$$\mathbf{x}^{sn} = \arg \min_{\mathbf{x}} \|\mathbf{A}\mathbf{x} - \mathbf{y}^{obs}\|^2 + \alpha\|\mathbf{x}\|^2$$

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

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

Sensitivity matrix
Partial derivatives of the data with respect to the unknowns.

But the iteration is unstable !!

Regularization methods

Nonlinear inverse problems

1) The Landweber's method

$$\mathbf{x}^{Iter+1} = \mathbf{x}^{Iter} + \omega\, \mathbf{I} \cdot \left[\mathbf{DT}^{T}_{(\mathbf{x}^{Iter})} \left(\mathbf{T}^{Obs} - \mathbf{T}_{(\mathbf{x}^{Iter})} \right) \right]$$

Relaxation parameter

2) The Levenberg-Marquardt method

$$\mathbf{x}^{Iter+1} = \mathbf{x}^{Iter} + \left[\mathbf{DT}^{T}_{(\mathbf{x}^{Iter})}\, \mathbf{DT}_{(\mathbf{x}^{Iter})} + \alpha_{Iter}\, \mathbf{I} \right]^{-1} \cdot \left[\mathbf{DT}^{T}_{(\mathbf{x}^{Iter})} \left(\mathbf{T}^{Obs} - \mathbf{T}_{(\mathbf{x}^{Iter})} \right) \right]$$

Regularization parameter

3) The iteratively regularized Gauss-Newton method

$$\mathbf{x}^{Iter+1} = \mathbf{x}^{Iter} + \left[\mathbf{DT}^{T}_{(\mathbf{x}^{Iter})}\, \mathbf{DT}_{(\mathbf{x}^{Iter})} + \alpha_{Iter}\, \mathbf{L}^{T}\, \mathbf{L} \right]^{-1} \cdot \left[\mathbf{DT}^{T}_{(\mathbf{x}^{Iter})} \left(\mathbf{T}^{Obs} - \mathbf{T}_{(\mathbf{x}^{Iter})} \right) + \alpha_{Iter}\, \mathbf{L}^{T}\, \mathbf{L} \left(\mathbf{x}^{\triangle} - \mathbf{x}^{Iter} \right) \right]$$

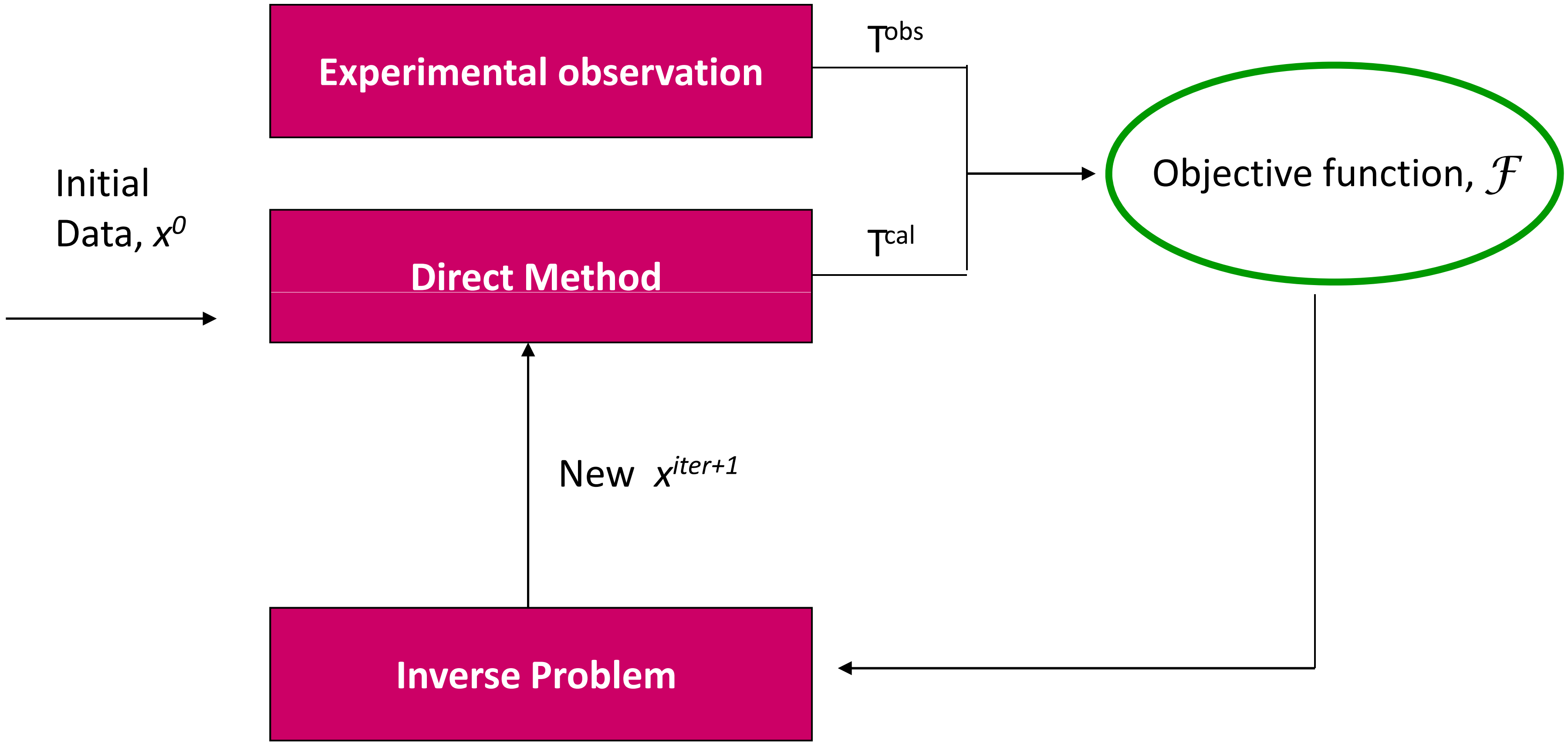
Regularization matrix
Differential operators

Regularization methods

Nonlinear inverse problems – The must-do list

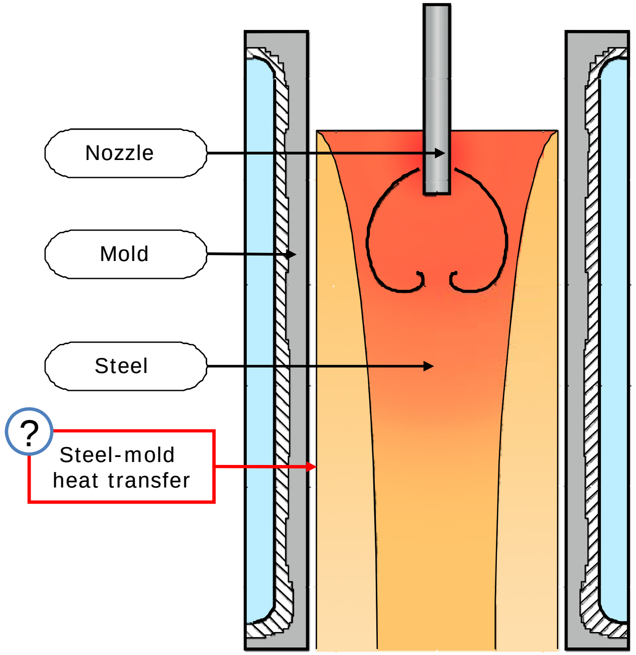
a) Identify the observations, its location and noise level.
b) Identify the unknowns and parametrize them in order to consider finite-dimensional subspaces.
c) State the direct problem and solve it (F.E.M.).
d) State the inverse problem … we usually deal with nonlinear inverse problems.
e) Decide how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

Inverse problems in engineering



Inverse problems in engineering

Continuous casting steel-mold heat transfer



Copper mold model

- PDE: $$\nabla \cdot [\mathbf{k}_m \nabla T_m] = 0 \qquad \forall \mathbf{x} \in \Omega_m$$
- BC:

$$-\mathbf{k}_m \nabla T_m \cdot \mathbf{n} = h_w(T_m - T_w) \quad \forall \mathbf{x} \in \partial\Omega_c^w$$

$$-\mathbf{k}_m \nabla T_m \cdot \mathbf{n} = h_s(T_m - T_s) \quad \forall \mathbf{x} \in \partial\Omega^s$$

$$\mathbf{k}_m \nabla T_m \cdot \mathbf{n} = 0 \quad \forall \mathbf{x} \in \partial\Omega_q^a$$

Steel solidification model

- PDE:

$$\rho_s \dot{\mathcal{H}}_s - \nabla \cdot (\mathbf{k}_s \nabla T_s^*) = 0 \qquad \forall (\mathbf{x}, t) \in \Omega_s \times (t_m^i, t_m^o)$$

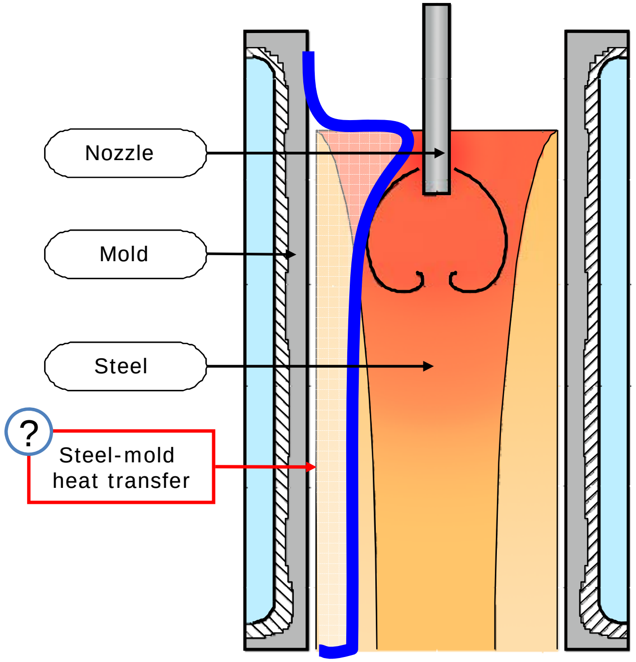
- BC:

$$T_s^* = T_{cast} \qquad \forall \mathbf{x} \in \Omega_s,\ t = t_m^i$$

$$-\mathbf{k}_s \nabla T_s^* \cdot \mathbf{n} = h_s^*(T_s^* - T_m^*) \qquad \forall (\mathbf{x}, t) \in \partial\Omega_s \times (t_m^i, t_m^o)$$

Inverse problems in engineering

Continuous casting steel-mold heat transfer



Observations:

Measurement	Observed variable
T_i^{obs}	T_i^{obs}
G_w^{obs} ΔT_w^{obs}	$Q_w^{obs} = G_w^{obs} c_w \Delta T_w^{obs}$
	--

$$n_{coef} \gg n_{tc} + 1$$

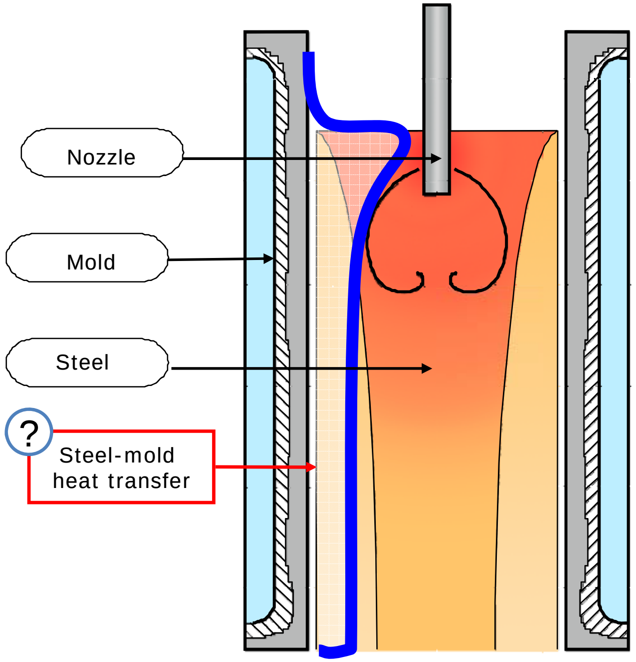
Measurement	Observed variable	A priori information
T_i^{obs}	T_i^{obs}	--
G_w^{obs} ΔT_w^{obs}	$Q_w^{obs} = G_w^{obs} c_w \Delta T_w^{obs}$	--
h_{level}^{obs}	--	Local maximum
--	--	Smooth function

Useful a priori information:

- maximum at meniscus
- smooth function

Inverse problems in engineering

Continuous casting steel-mold heat transfer



Statement of the inverse problem:

$$\min \quad \frac{1}{2}\|\mathbf{x}\|^2 + \varepsilon\, \mathcal{J}^{apriori}$$

$$\text{subject to} \quad \mathbf{A}\mathbf{x} - \mathbf{b} = \mathbf{0}$$

$$g_i \leq 0 \qquad i = 1, n_{level},$$

The system is underdetermined and does not have an unique solution

Measurements are imposed

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

$$\mathcal{J}^{apriori} = \frac{1}{2}\|\mathbf{L}_{max}(\mathbf{h}_s^0 + \mathbf{x})\|^2 + \frac{1}{2}\|\mathbf{L}_{smooth}(\mathbf{h}_s^0 + \mathbf{x})\|^2$$

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

$$\left[\mathbf{K}_{cond} + \mathbf{K}_{w} + \sum_{k=1}^{n_{coef}} \mathrm{h}_{s,k}\,\mathbf{K}_{s,k}\right]\mathbf{T}_{m} - \mathbf{K}_{w}\mathbf{T}_{w} - \left[\sum_{k=1}^{n_{coef}} \mathrm{h}_{s,k}\,\mathbf{K}_{s,k}\right]\mathbf{T}_{s} = \mathbf{0}$$

Sensitivity equations

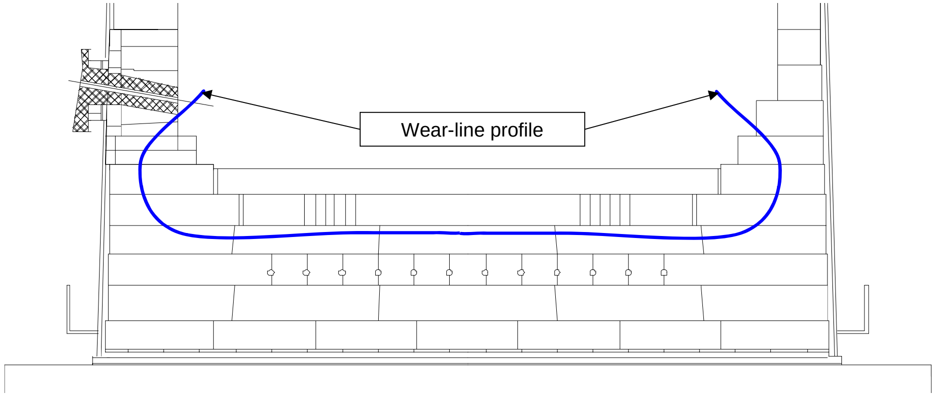
$$\left[\mathbf{K}_{cond} + \mathbf{K}_{w} + \sum_{k=1}^{n_{coef}} \mathrm{h}_{s,k}\,\mathbf{K}_{s,k}\right]\frac{\partial \mathbf{T}_{m}}{\partial \mathrm{h}_{s,j}} - \left[\sum_{k=1}^{n_{coef}} \delta_{j,k}\,\mathbf{K}_{s,k}\right](\mathbf{T}_{s} - \mathbf{T}_{m}) = \mathbf{0}$$

Are used in the sensitivity matrix

Inverse problems in engineering

Estimation of the blast furnace hearth wear profile

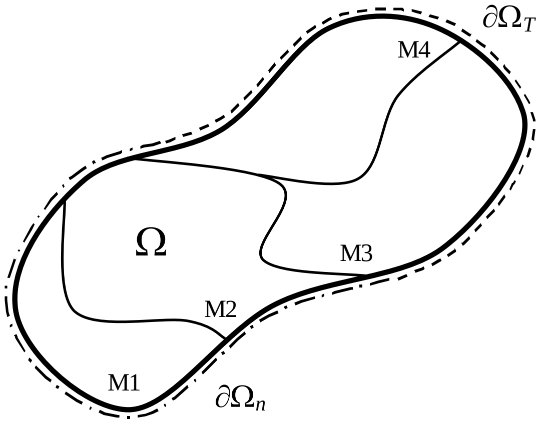
The 1150°C isotherm represents a potential limit on the penetration of liquid into the hearth wall porosity (1150°C is the eutectic temperature of carbon saturated iron).

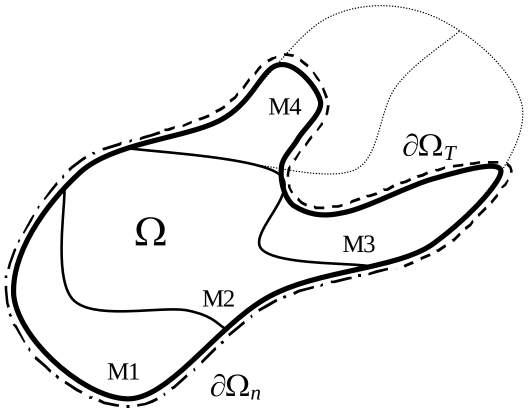


The location of the 1150°C isotherm is estimated solving a non-linear inverse heat transfer problem, where the observations are temperature measurements and the unknown is the geometry.

Inverse problems in engineering

Estimation of the blast furnace hearth wear profile





$\partial\Omega_n$ Fixed boundary, where natural boundary conditions are applied.

$\partial\Omega_T$ 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 $\mathbf{p}^* = \arg \min_{\mathbf{p}\in\mathbb{R}^{n_p}} \mathcal{F}_{(\mathbf{p})}$

where $\mathcal{F}_{(\mathbf{p})} = \frac{1}{2} \| \mathbf{T}_{(\mathbf{p})} - \mathbf{T}^{OBS} \|^2$

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:

$$ {}^{GN}\mathbf{p}^{Iter+1} = \mathbf{p}^{Iter} + \left[\mathbf{DT}^{T}_{(\mathbf{p}^{Iter})}\, \mathbf{DT}_{(\mathbf{p}^{Iter})} + \alpha_{Iter}\, \mathbf{L}^{T}\, \mathbf{L} \right]^{-1} \cdot \left[\mathbf{DT}^{T}_{(\mathbf{p}^{Iter})}\, \Delta\mathbf{T}^{OBS}_{(\mathbf{p}^{Iter})} + \alpha_{Iter}\, \mathbf{L}^{T}\, \mathbf{L}\, (\mathbf{p}^{\triangle} - \mathbf{p}^{Iter}) \right] $$

where:

$\mathbf{DT}_{(\mathbf{p})}$ Sensitivity matrix *(partial derivatives of the temperature with respect to the set of geometry parameters)*

$\mathbf{L}$ Regularization matrix *(a discrete form of some differential operator)*

$\mathbf{p}^{\triangle}$ *A priori* suitable approximation of the unknown set of parameters

The problem is highly non-linear: $\mathbf{p}^{Iter+1} = \mathbf{p}^{Iter} + \beta^{Iter} \left({}^{GN}\mathbf{p}^{Iter+1} - \mathbf{p}^{Iter} \right)$

[*] Bakushinskii, *Comput. Maths Math. Phys.*, 1992.

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

$$\left.\frac{\partial T}{\partial p_j}\right|_{(\mathbf{x},\mathbf{p})} \approx \frac{\tilde{T}\left(\mathbf{x},\{p_1,\ldots,p_j+\Delta p_j,\ldots,p_{np}\}\right) - \tilde{T}\left(\mathbf{x},\{p_1,\ldots,p_j,\ldots,p_{np}\}\right)}{\Delta p_j}$$

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

$$\left.\frac{\partial T}{\partial p_j}\right|_{(\mathbf{x},\mathbf{p})} \approx \mathbf{N}_{(\mathbf{x})} \left.\frac{\partial \mathbf{T}}{\partial p_j}\right|_{(\mathbf{p})}^{FEM}$$

Are used in the sensitivity matrix

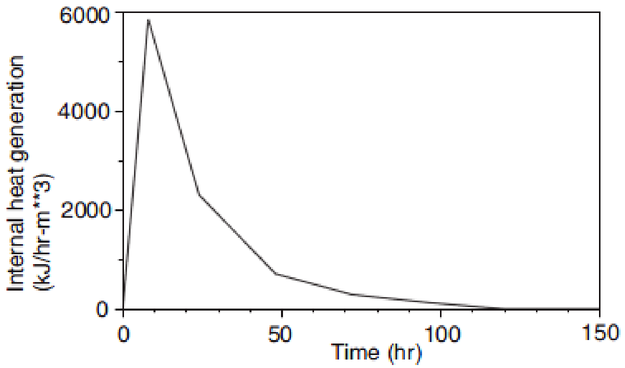
Summary

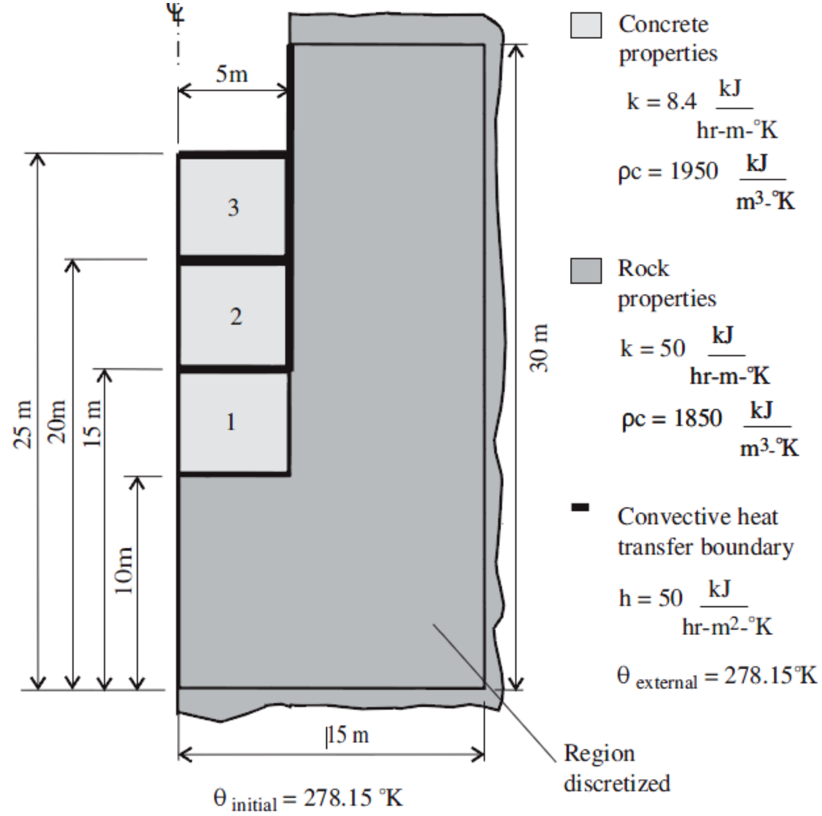
Nonlinear inverse problems – The must-do list

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 monotically decreasing sequence) and the regularization matrixes.
g) Decide the convergence criterion / stopping rule
(the discrepancy principle).
h) Think about useful *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 atmoshpere. 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 -20ºC, calculate how much time is it necessary to solidify a 1m x 1m x 1m block of 20ºC water. All points in the block must be at most at -5ºC after solidifying.