

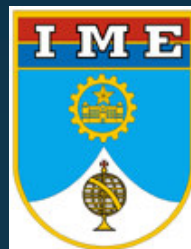
OPTIMIZATION PROBLEMS IN HEAT TRANSFER

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Optimization Problems

- **Introduction**

- Basic Concepts

- **Deterministic Methods**

- Steepest Descent Method
- Conjugate Gradient Method
- Newton-Raphson Method
- Quasi-Newton Methods

- **Evolutionary and Stochastic Methods**

- Genetic Algorithms
- Differential Evolution
- Particle Swarm
- Simulated Annealing

- **Hybrid Methods**

- Examples

Introduction

Inverse Problems



- Tries to find an unknown parameter or function
- Ill-posed

Minimization Problems



- Tries to find the best configuration of a problem

Introduction

Objective Function $\rightarrow U(\mathbf{x}); \mathbf{x}=\{x_1, x_2, \dots, x_N\}$

Equality Constraints $\rightarrow G(\mathbf{x})=C_1$

Inequality Constraints $\rightarrow H(\mathbf{x}) \leq C_2$

Deterministic Methods

→ **Steepest-Descent** Method:

Iterative process:

$$\mathbf{x}^{k+1} = \mathbf{x}^k + \alpha^k \mathbf{d}^k$$

$$\mathbf{d}^k = -\nabla U(\mathbf{x}^k)$$

where:

\mathbf{x} is the vector of parameters to be optimized

α is the search-step size

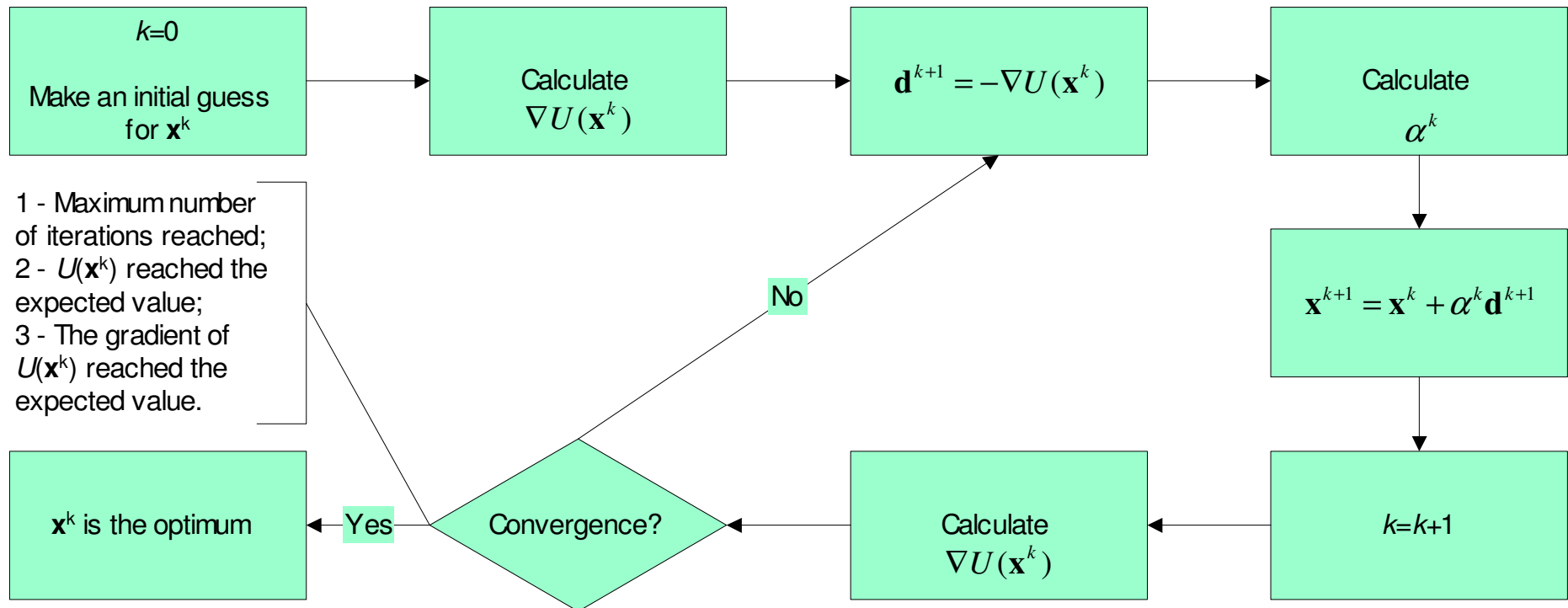
\mathbf{d} is the direction of descent

U is the objective function

k is the iteration number

Deterministic Methods

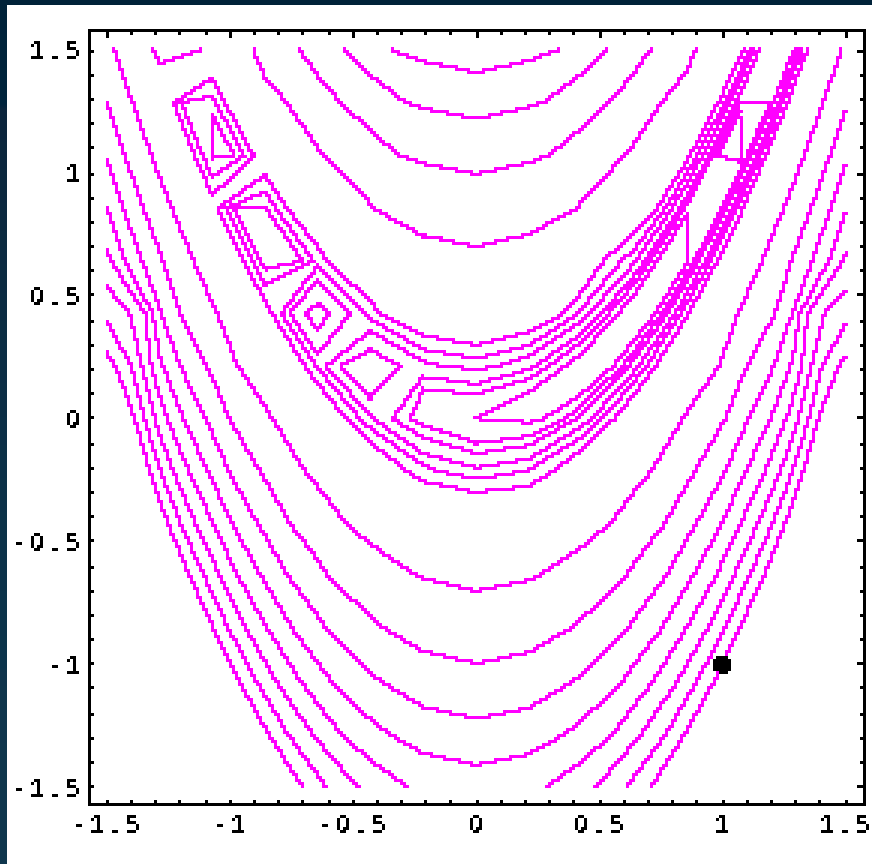
→ **Steepest-Descent** Method:



Deterministic Methods

→ Steepest-Descent Method:

SLOW!!!!!!



Deterministic Methods

→ **Conjugate Gradient** Method:

Iterative process:

$$\mathbf{x}^{k+1} = \mathbf{x}^k + \alpha^k \mathbf{d}^k$$

$$\mathbf{d}^k = -\nabla U(\mathbf{x}^k) + \gamma^k \mathbf{d}^{k-1}$$

where:

\mathbf{x} is the vector of parameters to be optimized

α is the search-step size

\mathbf{d} is the direction of descent

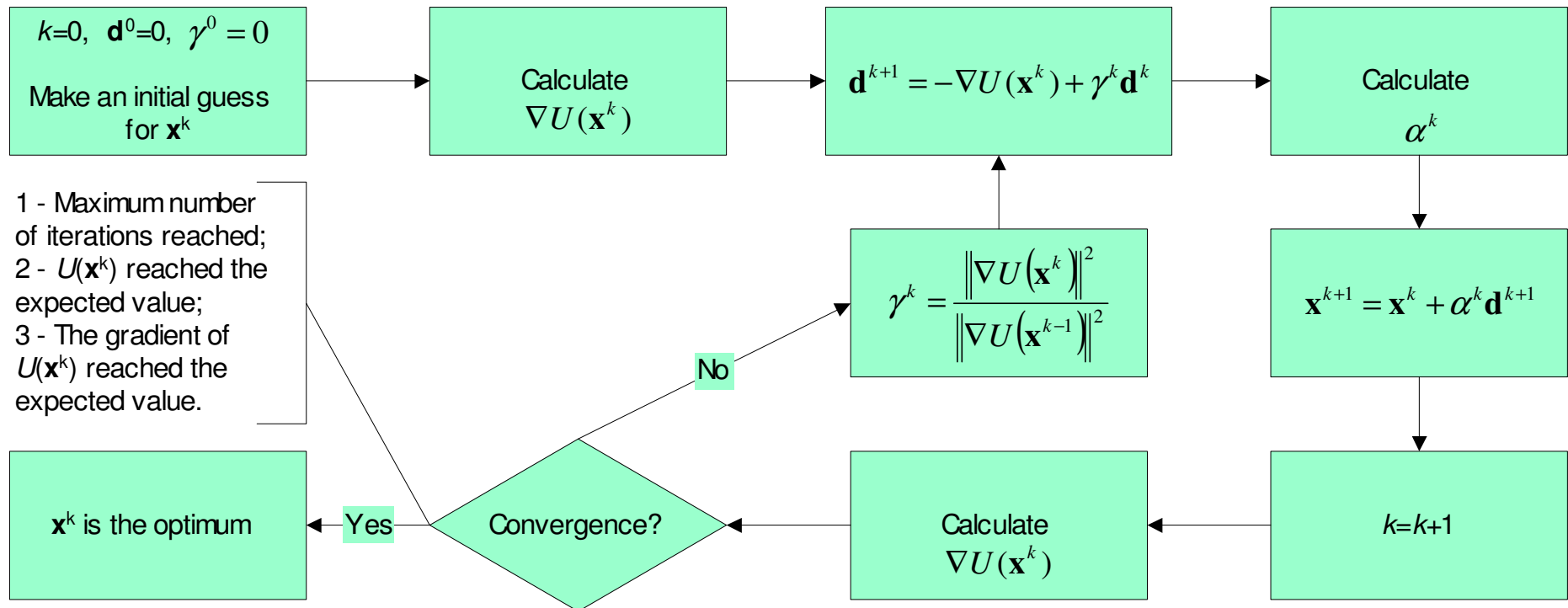
U is the objective function

k is the iteration number

γ is the conjugation coefficient

Deterministic Methods

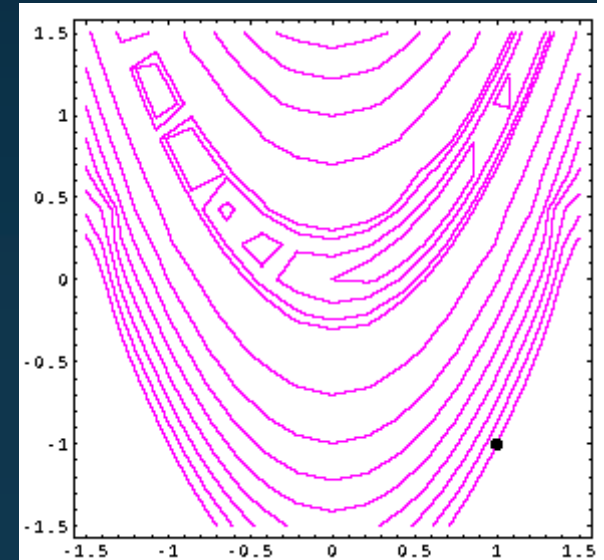
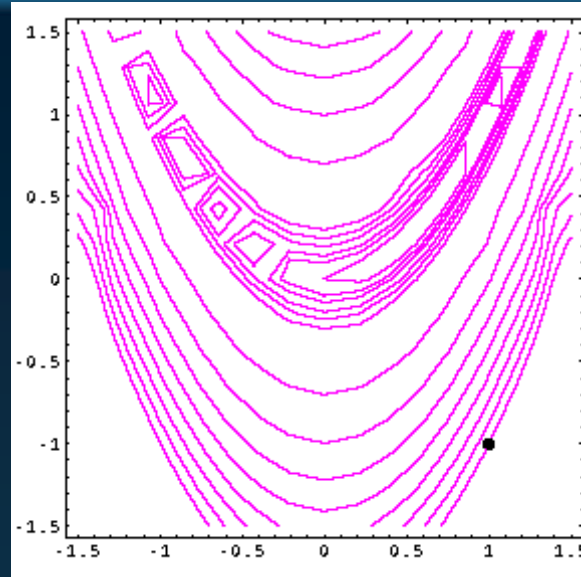
→ Conjugate Gradient Method:



Deterministic Methods

→ Conjugate Gradient Method:

**Faster than the
Steepest-Descent!**



Deterministic Methods

→ **Newton** Method:

Iterative process:

$$\mathbf{x}^{k+1} = \mathbf{x}^k + \alpha^k \mathbf{d}^k$$

$$\mathbf{d}^k = -\mathbf{H}^k \nabla U(\mathbf{x}^k)$$

where:

\mathbf{x} is the vector of parameters to be optimized

α is the search-step size

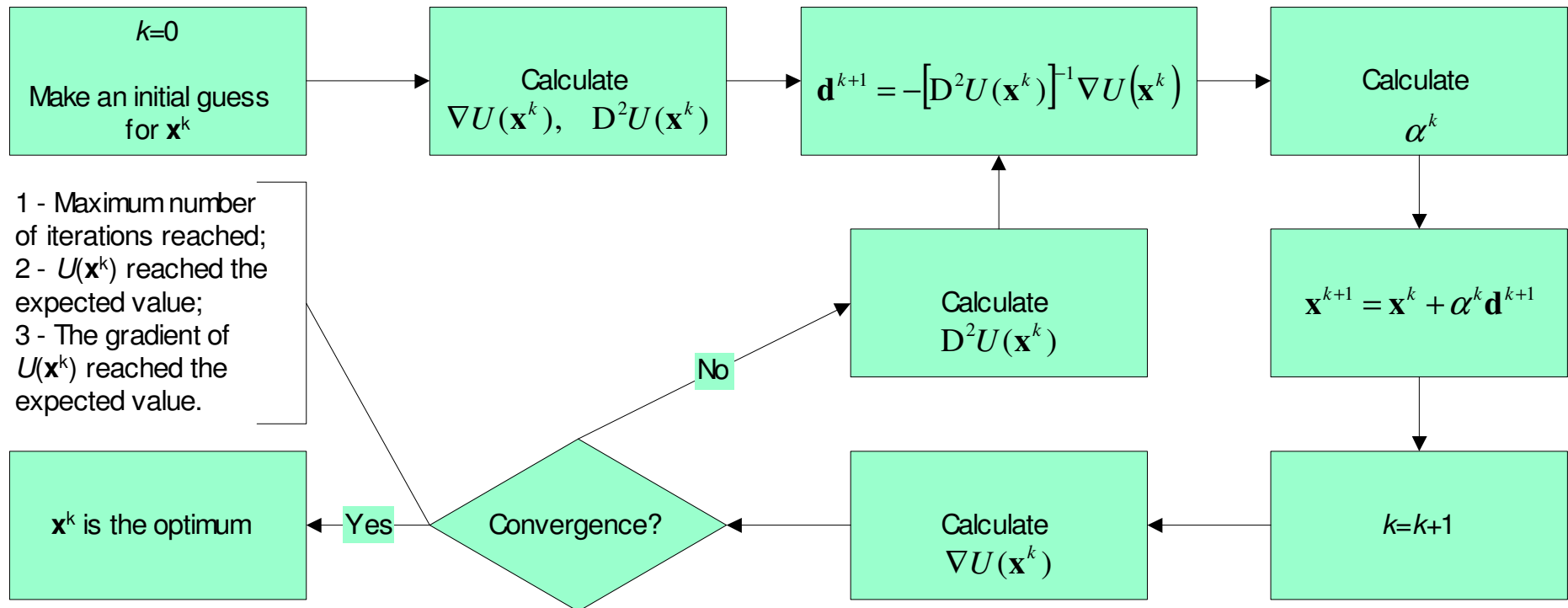
\mathbf{H} is the matrix of 2nd order derivatives – Expensive in terms of computational cost!

U is the objective function

k is the iteration number

Deterministic Methods

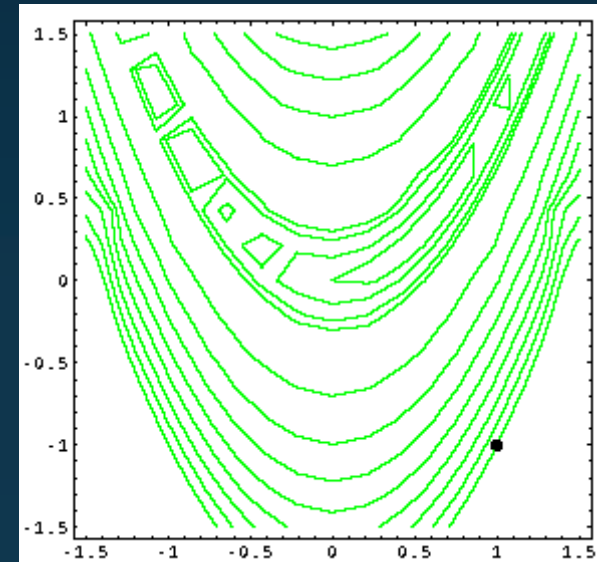
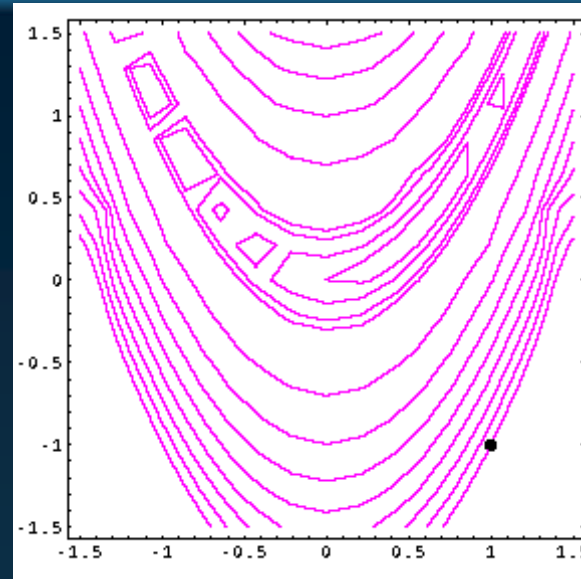
→ **Newton** Method:



Deterministic Methods

→ **Newton** Method:

**Faster than the
Conjugate Gradient!**



Deterministic Methods

→ BFGS (Broyden-Fletcher-Goldfarb-Shanno) Method:

- Quasi-Newton method, similar to the DFP method, but less dependent on the search-step size choice.
- Uses an iterative approximation for the Hessian

$$\mathbf{H}^k = \mathbf{H}^{k-1} + \mathbf{M}^{k-1} + \mathbf{N}^{k-1}$$

where

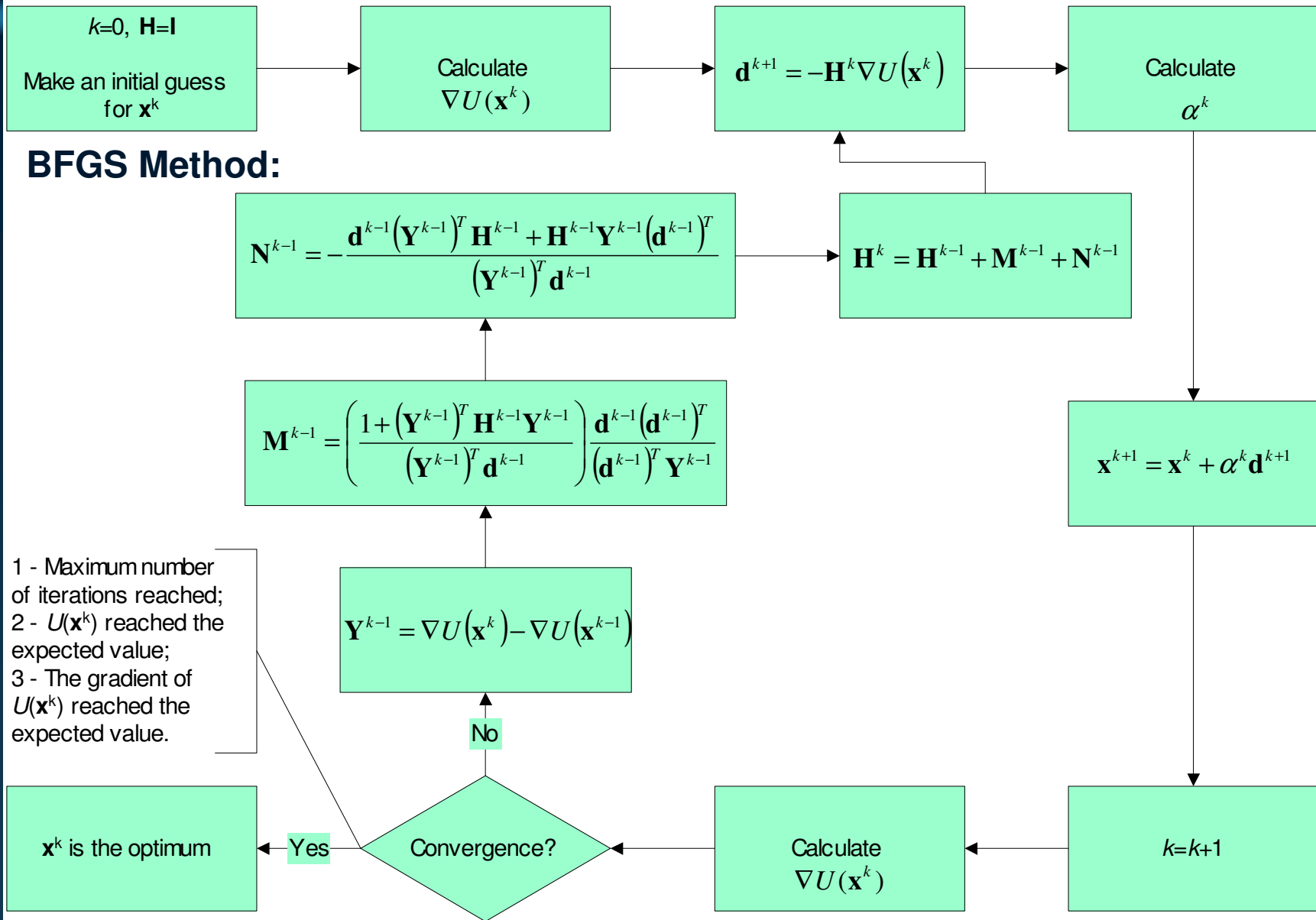
$$\mathbf{M}^{k-1} = \left(\frac{1 + (\mathbf{Y}^{k-1})^T \mathbf{H}^{k-1} \mathbf{Y}^{k-1}}{(\mathbf{Y}^{k-1})^T \mathbf{d}^{k-1}} \right) \frac{\mathbf{d}^{k-1} (\mathbf{d}^{k-1})^T}{(\mathbf{d}^{k-1})^T \mathbf{Y}^{k-1}}$$

$$\mathbf{N}^{k-1} = - \frac{\mathbf{d}^{k-1} (\mathbf{Y}^{k-1})^T \mathbf{H}^{k-1} + \mathbf{H}^{k-1} \mathbf{Y}^{k-1} (\mathbf{d}^{k-1})^T}{(\mathbf{Y}^{k-1})^T \mathbf{d}^{k-1}}$$

$$\mathbf{Y}^{k-1} = \nabla U(\mathbf{x}^k) - \nabla U(\mathbf{x}^{k-1})$$

Deterministic Methods

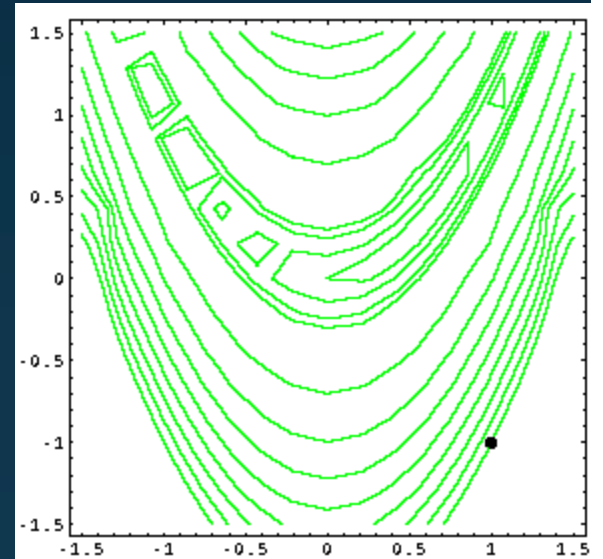
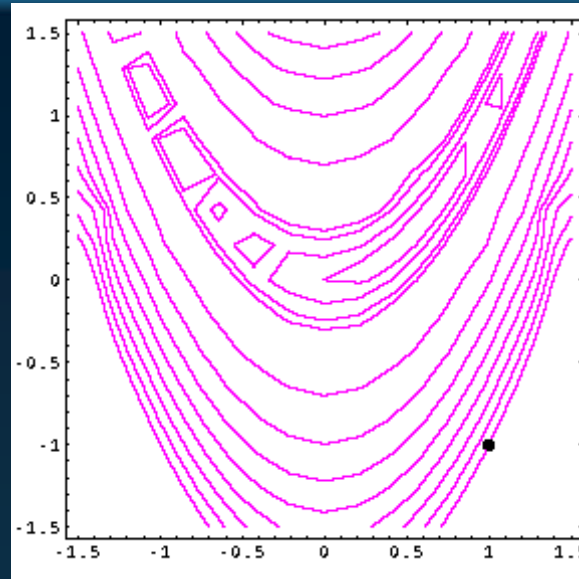
→ BFGS Method:



Deterministic Methods

→ **BFGS** Method:

**Faster than the
Conjugate Gradient!**



Evolutionary and Stochastic Methods

→ GA (Genetic Algorithm) and DE (Differential Evolution) Methods:

→ Based on Darwin's model for natural selection of species.

- Members of a certain population matches and have children. Those children are a combination of the parents' chromosomes.
- The strongest members of the population will have more chances to survive under a certain environment.
- The combination of the chromosomes is called crossover.
- Mutations can occur. They can be good or bad mutations.

Evolutionary and Stochastic Methods

→ DE Method:

- Alternative to the Genetic Algorithm method.
- Proposed in 1995 by Kenneth Price and Rainer Storn from Berkeley.

→ The method initializes with a random generated random matrix \mathbf{P} which contains N vector parameters \mathbf{x}

→ From the initial population matrix, generations are created until the best generation (optimum) is found.

Evolutionary and Stochastic Methods

→ **DE** Method:

→ The next generation is created as:

$$\mathbf{x}_i^{k+1} = \delta_1 \mathbf{x}_i^k + \delta_2 [\alpha + F(\beta - \gamma)]$$

1st parent

2nd parent

Mutation included

where


α , β and γ are three randomly chosen members of the population matrix **P**.

F is a weighting function which defines the **mutation** ($0.5 < F < 1$).

k is the generation counter.

δ_1 and δ_2 are delta Dirac functions that defines the **crossover**.

If $U(\mathbf{x}^{k+1}) < U(\mathbf{x}^k)$  \mathbf{x}^{k+1} replaces \mathbf{x}^k in the population matrix **P**

If $U(\mathbf{x}^{k+1}) > U(\mathbf{x}^k)$  \mathbf{x}^k is kept in the population matrix **P** and \mathbf{x}^{k+1} is discarded

Evolutionary and Stochastic Methods

→ **DE** Method:

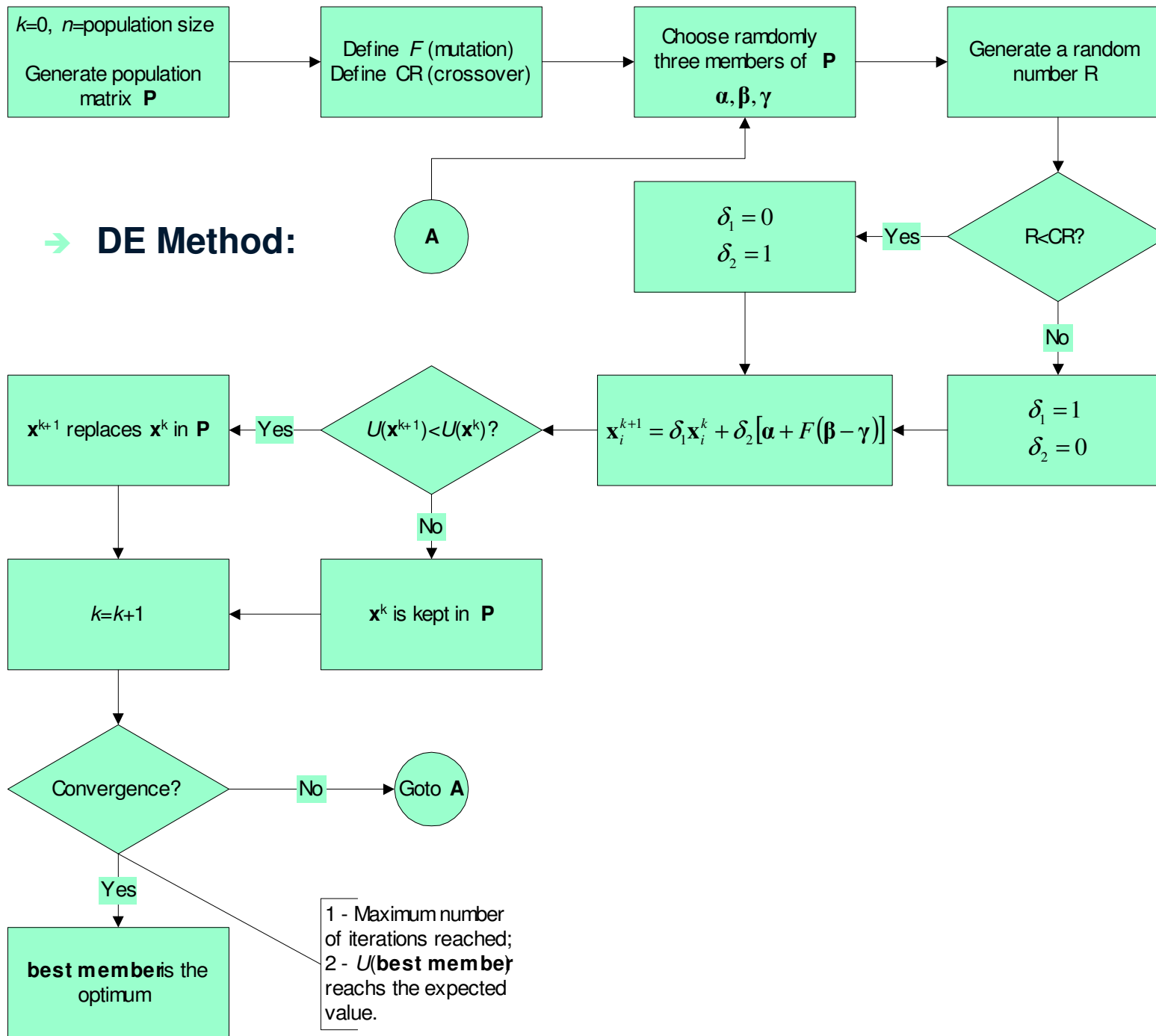
→ The crossover is obtained as:

$$\mathbf{x}_i^{k+1} = \delta_1 \mathbf{x}_i^k + \delta_2 [\mathbf{a} + F(\mathbf{b} - \mathbf{c})]$$

$$\delta_1 = \begin{cases} 0, & \text{if } R < CR \\ 1, & \text{if } R > CR \end{cases}$$

$$\delta_2 = \begin{cases} 1, & \text{if } R < CR \\ 0, & \text{if } R > CR \end{cases}$$

- R is a random number with uniform distribution between 0 and 1
- CR is the crossover factor ($0.5 < CR < 1$)



Evolutionary and Stochastic Methods

→ SA (Simulated Annealing) Method:

→ Based on thermodynamics and solidification process of liquids and metals.

Slow cooling → Pure crystal is formed with minimum energy state.

Fast cooling
“quenched” → Polycrystalline or amorphous state is formed with higher energy.

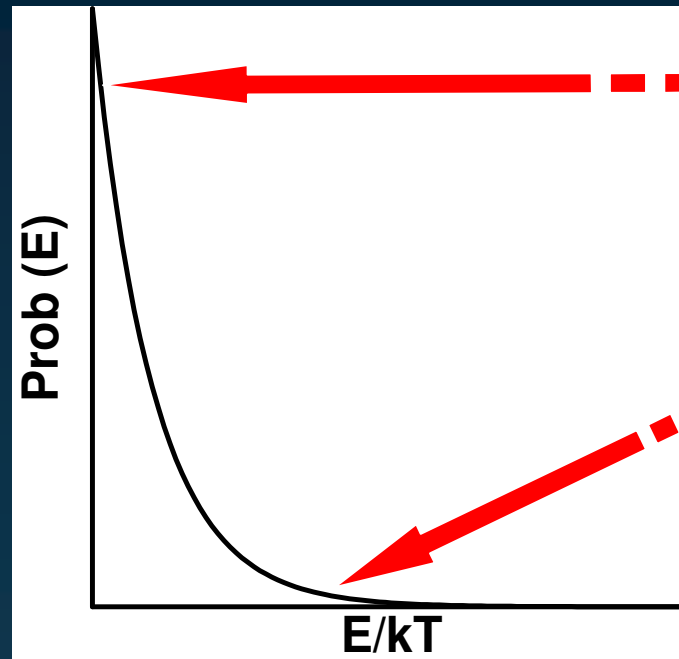
→ Gradient methods → “Fast cooling”. They can lead to a local minima.

Evolutionary and Stochastic Methods

→ SA Method:

→ Boltzmann probability distribution:

$$\text{Prob}(E) \approx \exp\left(-\frac{E}{kT}\right)$$



High temperature

High Probability of high energy state

Low temperature

Small Probability of high energy state

→ The method can move uphill as well as downhill depending on the probability of high energy states.

Evolutionary and Stochastic Methods

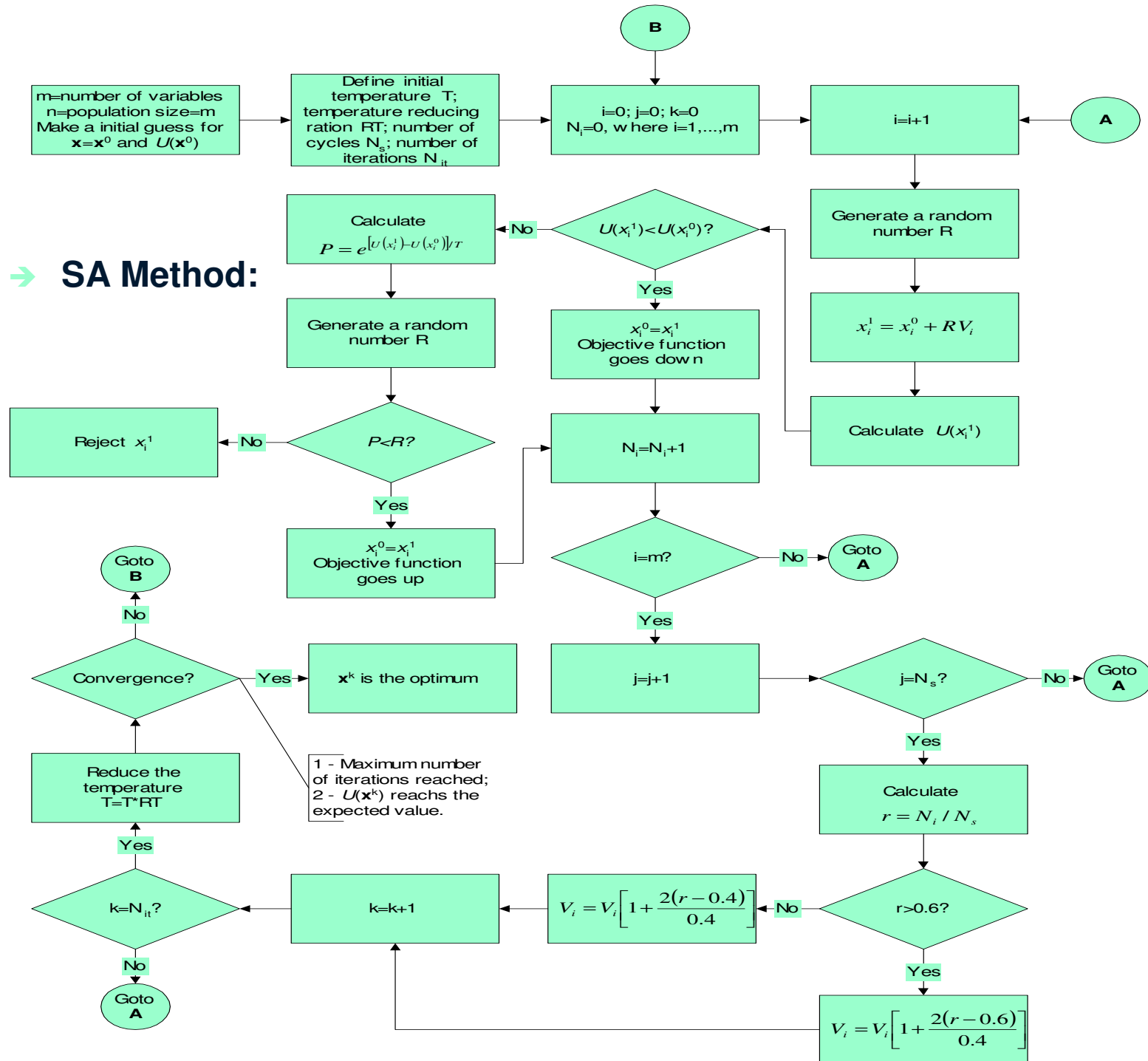
→ SA Method:

→ Iterative process is presented in the following papers:

- Corana, A., Marchesi, M., Martini, C. e Ridella, S., “Minimizing Multimodal Functions of Continuous Variables with the ‘Simulated Annealing Algorithm’”, *ACM Transactions on Mathematical Software*, vol. 13, pp. 262-280, 1987.
- Goffe, W. L., Ferrier, G. D. e Rogers, J., “Global Optimization of Statistical Functions with Simulated Annealing”, *Journal of Econometrics*, vol. 60, pp. 65-99, 1994.

→ Excessive number of objective function evaluations!!!

→ SA Method:



Evolutionary and Stochastic Methods

→ PS (Particle Swarm) method:

- Created in 1995 by an Electric Engineer (Russel Eberhart) and a Social-Psychologist (James Kennedy) as an alternative to Genetic Algorithm.
- Based on the social behavior of various species (including humans).
- Balances the individuality and sociability of individuals in order to find a optimum.

↑ Individuality

↑ Chances to find alternatives places
↓ Convergence

↑ Sociability

↑ Learning process among the individuals
↓ Chances to find alternatives places. Individuals can find a local minima

Evolutionary and Stochastic Methods

→ **PS** method:

→ Update process

$$\begin{aligned}\mathbf{x}_i^{k+1} &= \mathbf{x}_i^k + \mathbf{v}_i^{k+1} \\ \mathbf{v}_i^{k+1} &= \alpha \mathbf{v}_i^k + \beta \mathbf{r}_{1i} (\mathbf{p}_i - \mathbf{x}_i^k) + \beta \mathbf{r}_{2i} (\mathbf{p}_g - \mathbf{x}_i^k)\end{aligned}$$

Individuality

Sociability

where

\mathbf{x}_i is i-th individual of the vector of parameters

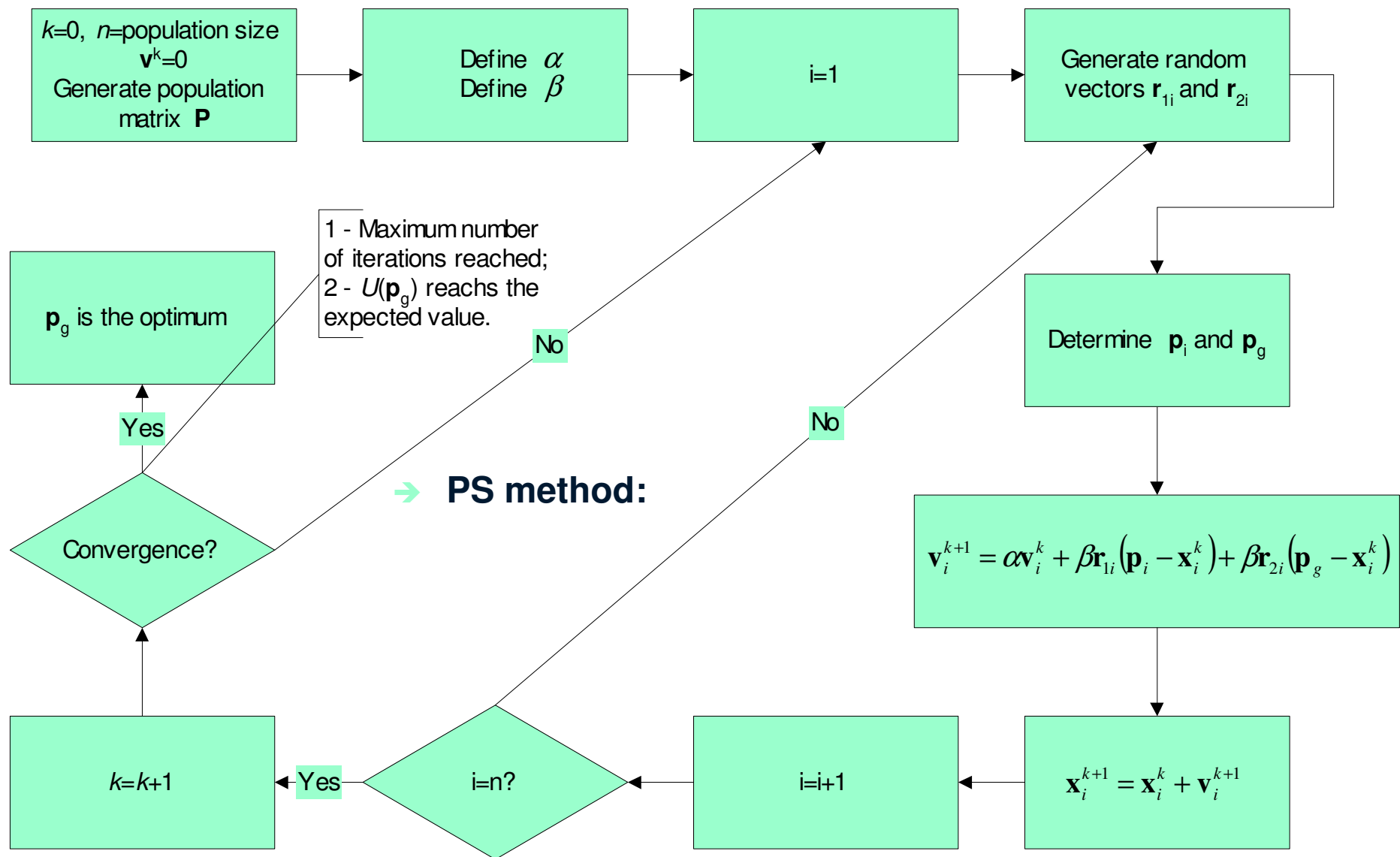
\mathbf{r}_{1i} and \mathbf{r}_{2i} are random numbers with uniform distribution between 0 and 1

\mathbf{p}_i is the best value found for the vector \mathbf{x}_i

\mathbf{p}_g is the best value found for the entire population

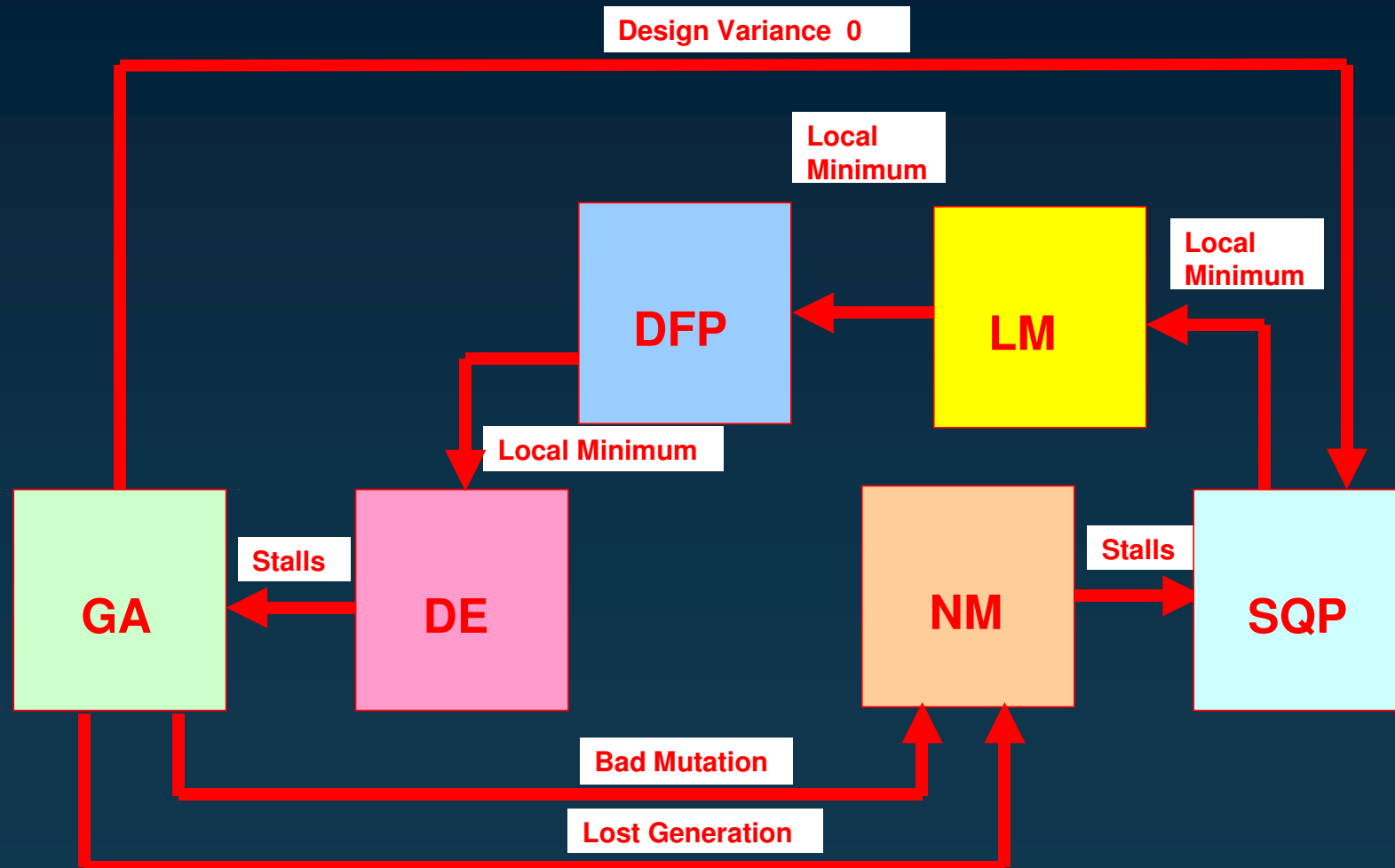
$0 < \alpha < 1; 1 < \beta < 2$

Evolutionary and Stochastic Methods



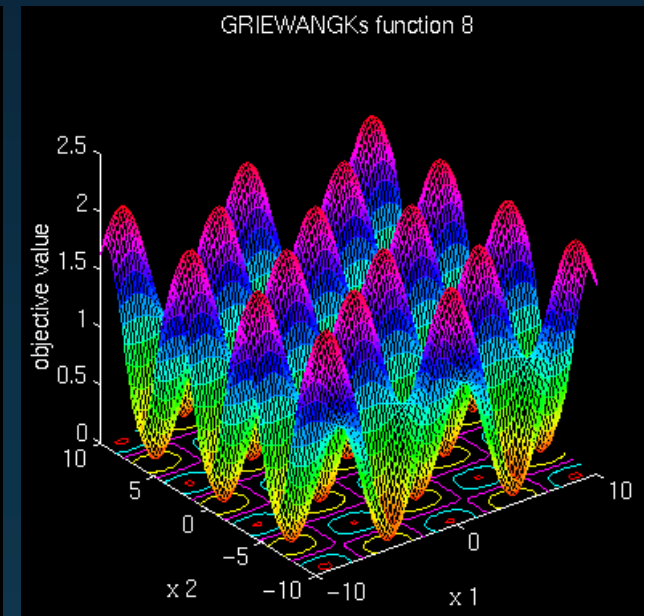
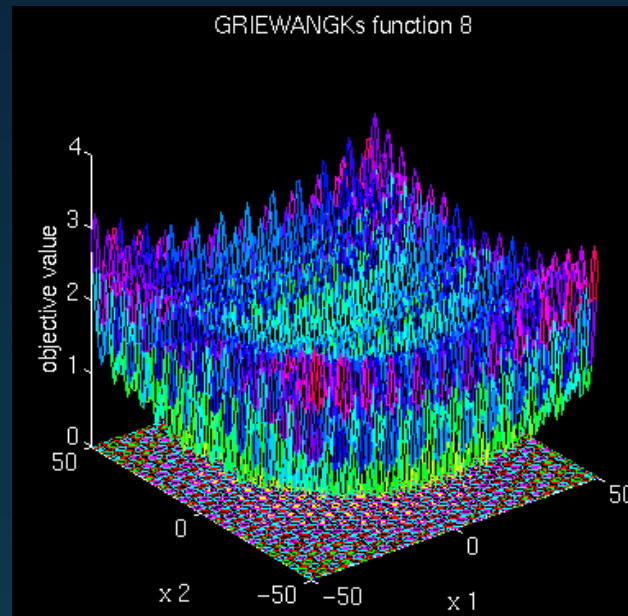
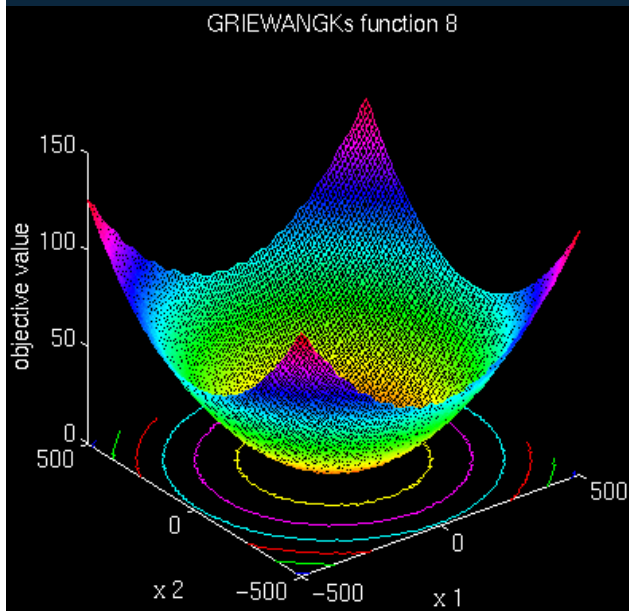
Hybrid Methods

→ Hybrid optimizer – version 1 (Martin, Colaço and Dulikravich)



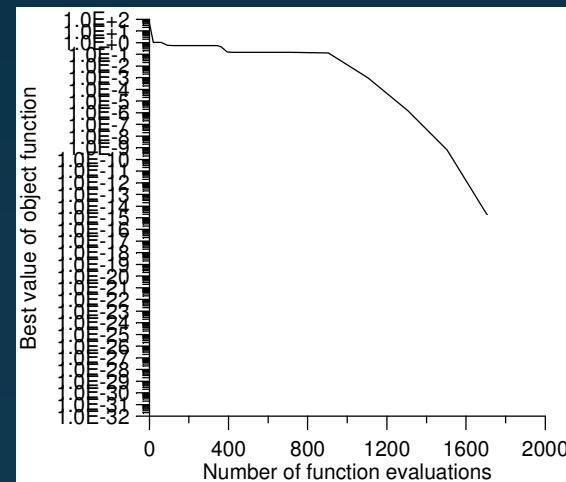
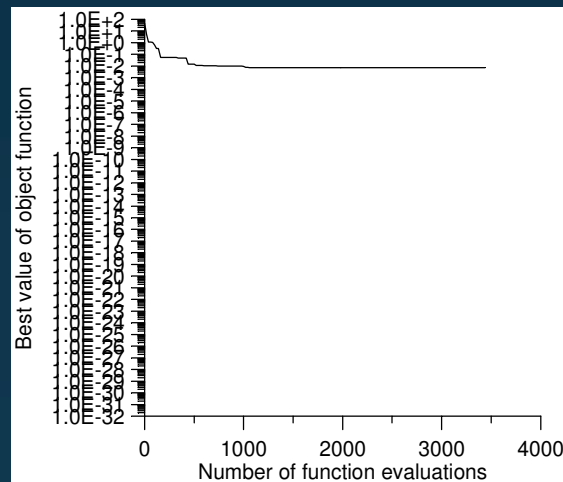
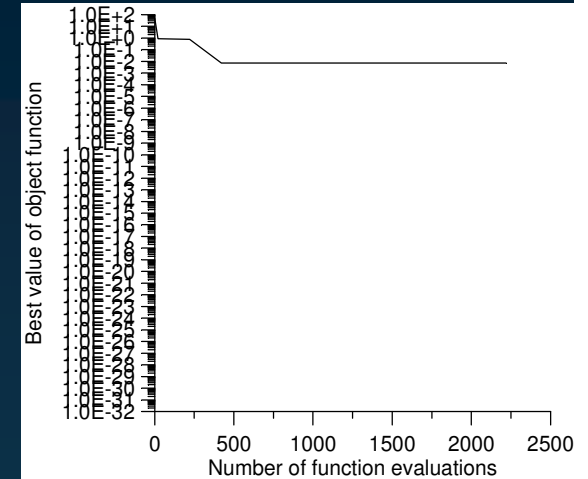
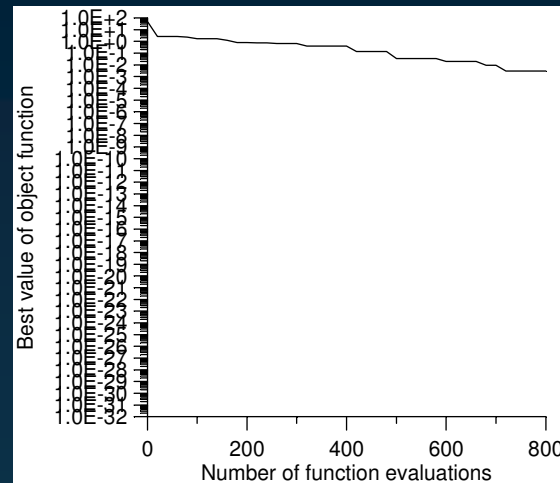
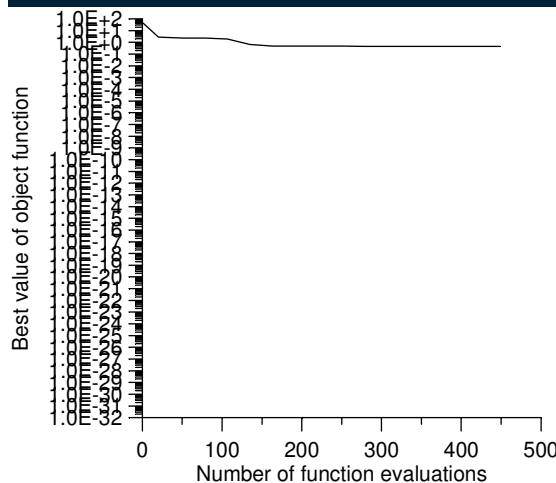
Example 1 - Griewangk's function

→ Multiple local minima



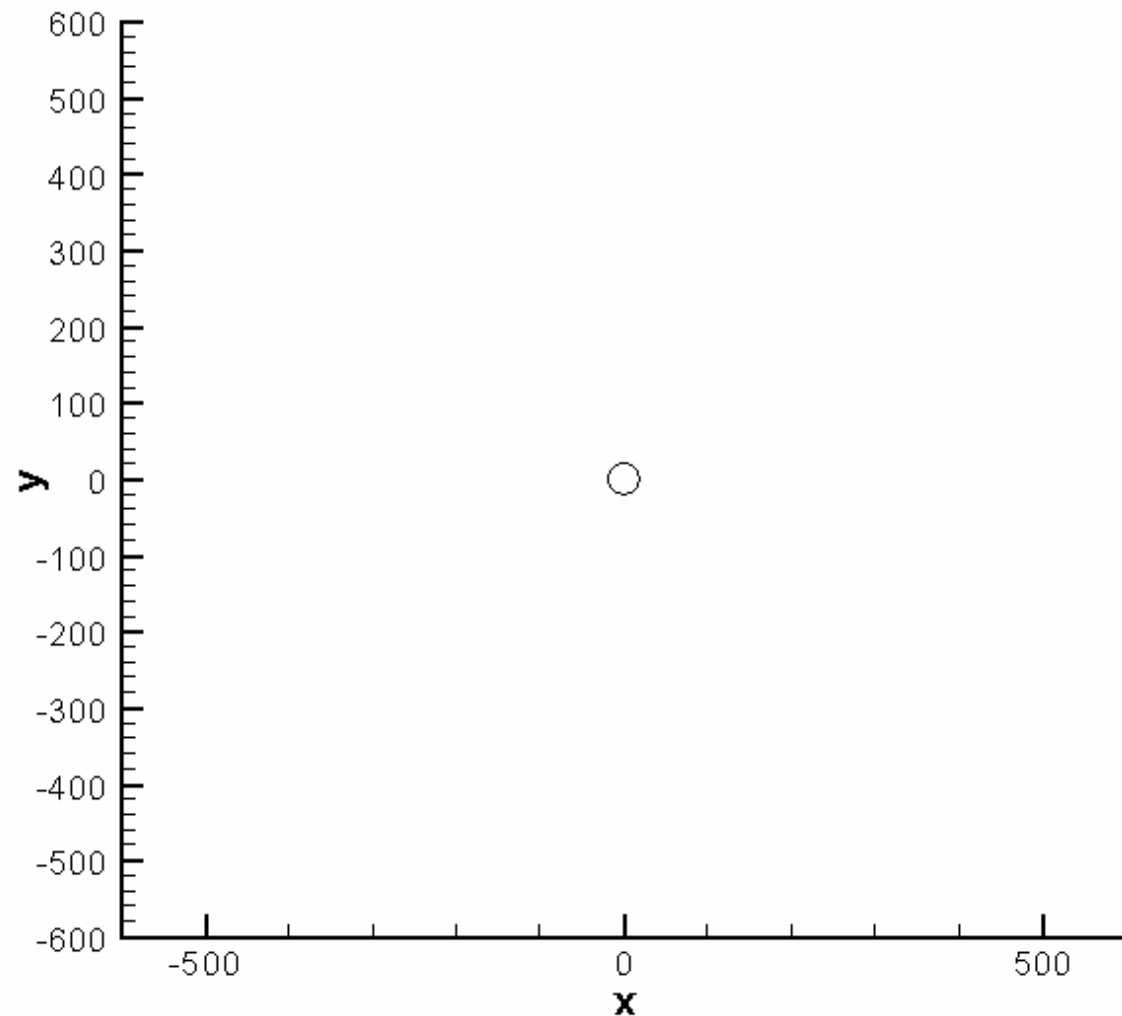
Example 1 - Griewangk's function

→ Comparison: BFGS, DE, SA, PS, Hybrid



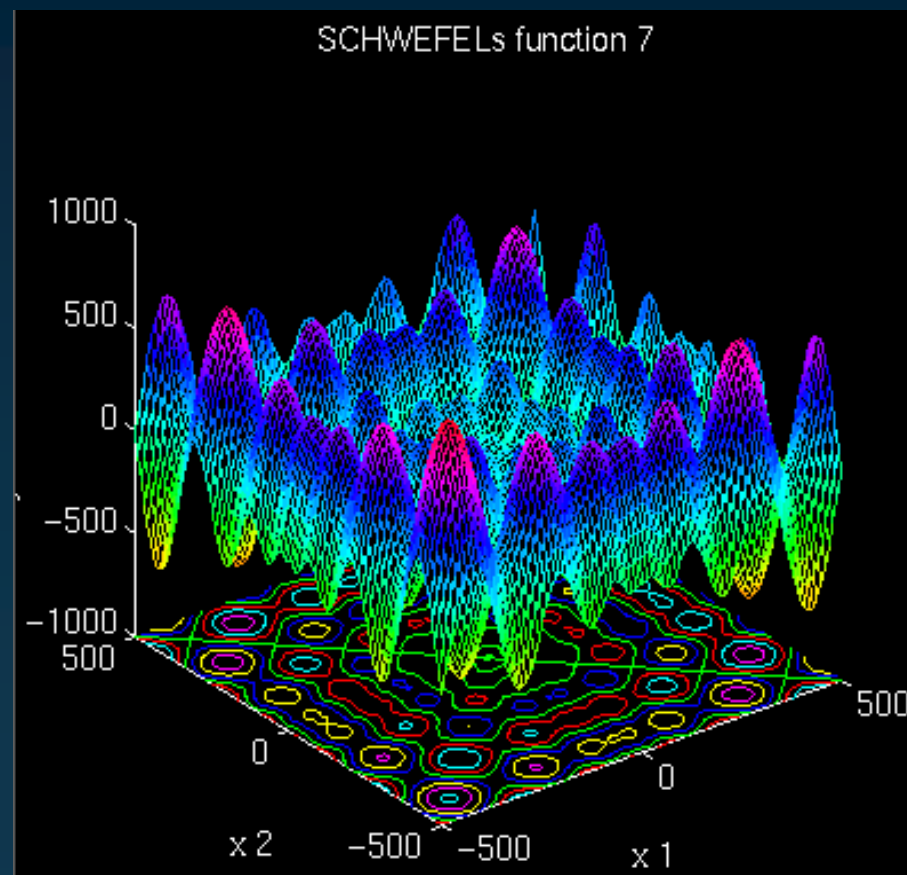
Example 1 - Griewangk's function

→ Particles' history



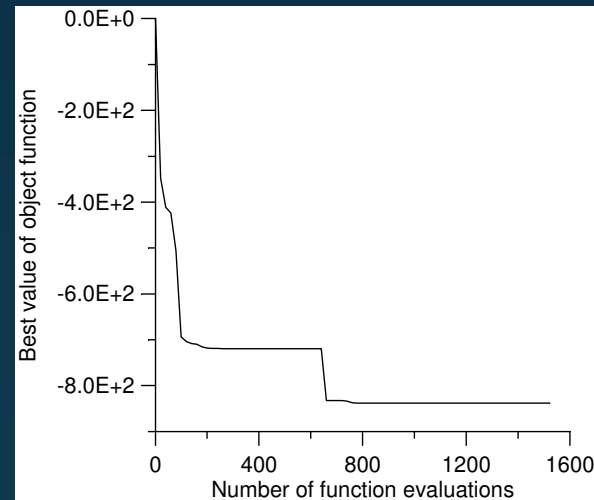
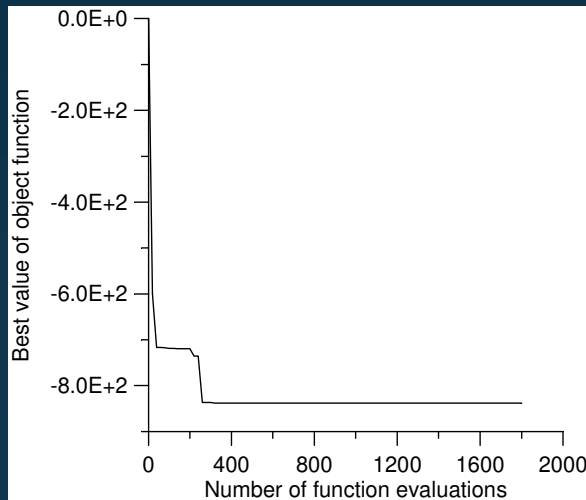
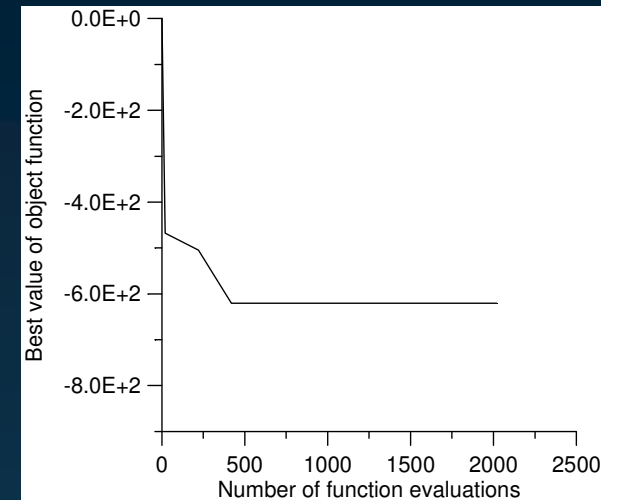
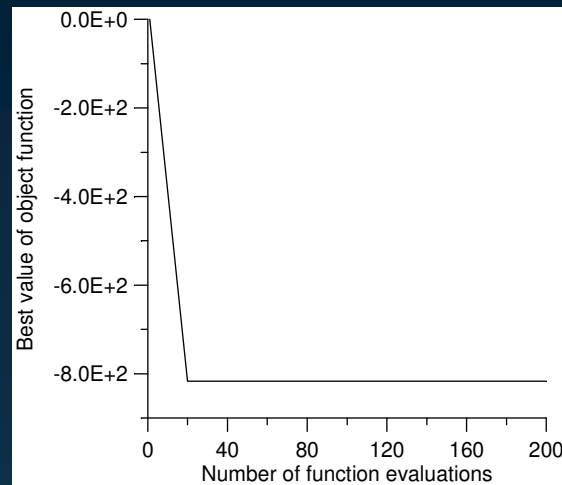
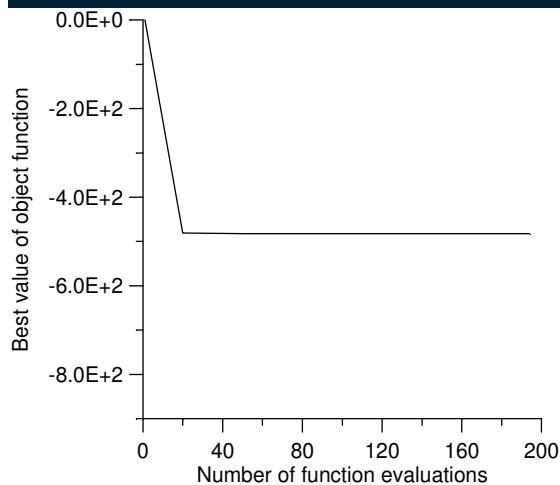
Example 2 - Schwefel's function

→ Multiple local minima



Example 2 - Schwefel's function

→ Comparison: BFGS, DE, SA, PS, Hybrid



Example 3

→ Comparison of two solution techniques for the inverse problem of simultaneously estimating the spatial variations of diffusion coefficients and source terms

- Conjugate Gradient Method with Adjoint Problem
- Tikhonov's Regularization with Hybrid Optimizer

$$C(\mathbf{r}) \frac{\partial U(\mathbf{r}, t)}{\partial t} = \nabla \cdot [D(\mathbf{r}) \nabla U] + \mu(\mathbf{r}) U$$

$$\frac{\partial U}{\partial t} = \frac{\partial}{\partial x} \left(D(x) \frac{\partial U}{\partial x} \right) + \mu(x) U \quad \text{in } 0 < x < 1, \text{ for } t > 0$$

$$\frac{\partial U}{\partial x} = 0 \quad \text{at } x = 0 \quad \text{for } t > 0$$

$$D(x) \frac{\partial U}{\partial x} = 1 \quad \text{at } x = 1 \quad \text{for } t > 0$$

$$U = 0 \quad \text{for } t = 0 \quad \text{in } 0 < x < 1$$

Example 3

DIRECT PROBLEM

Known:

$D(x)$ and $\mu(x)$



Determine:

$U(x,t)$

INVERSE PROBLEM

Known:

Measurements of $U(x,t)$



Simultaneously Estimate:

$D(x)$ and $\mu(x)$

Example 3

TEST-CASE

Heat Conduction – Steel

$$l^* = 0.050 \text{ m}$$

$$t_f^* = 60 \text{ s}$$

50 measurements per sensor

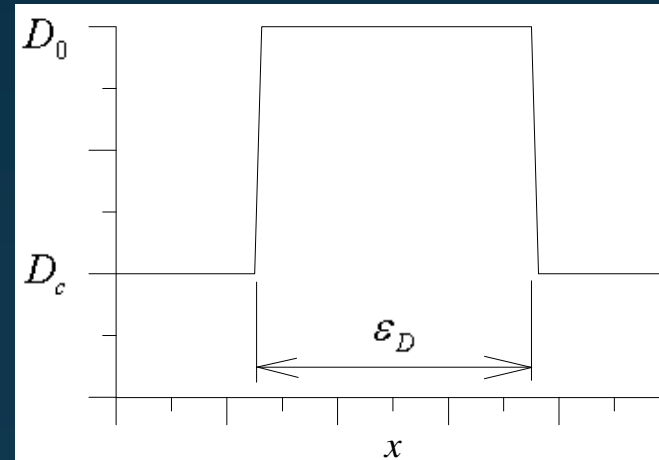
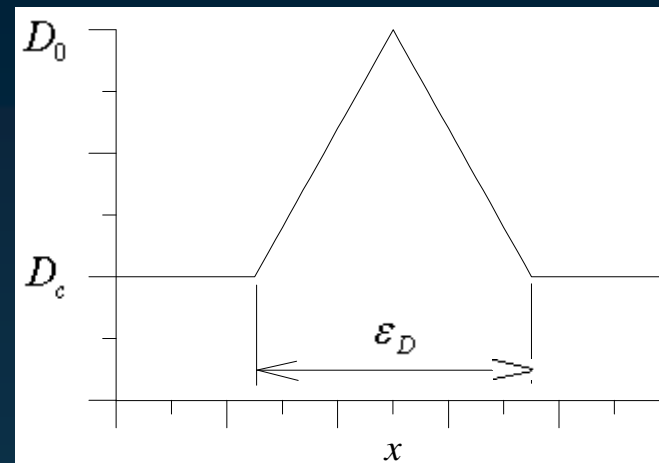
Simulated measurements

$$\rho = 7833 \text{ kg/m}^3$$

$$D_c = 54 \text{ W/m}^\circ\text{C}$$

$$c_p = 465 \text{ J/kg}^\circ\text{C}$$

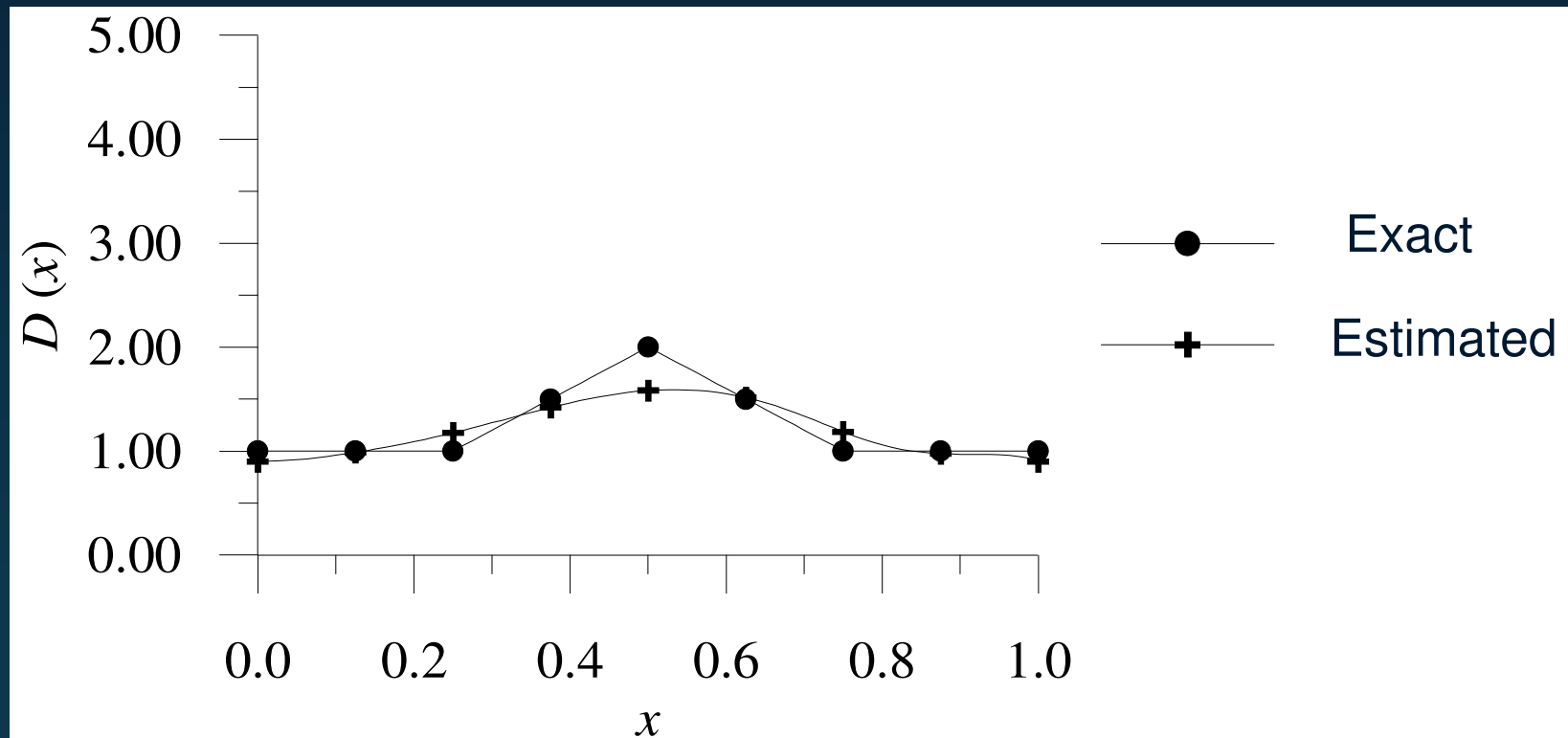
$$\mu_c^* = 10^5 \text{ W/m}^3^\circ\text{C}$$



Example 3

RESULTS - CGM Estimation of $D(x)$ for Known $\mu(x)$

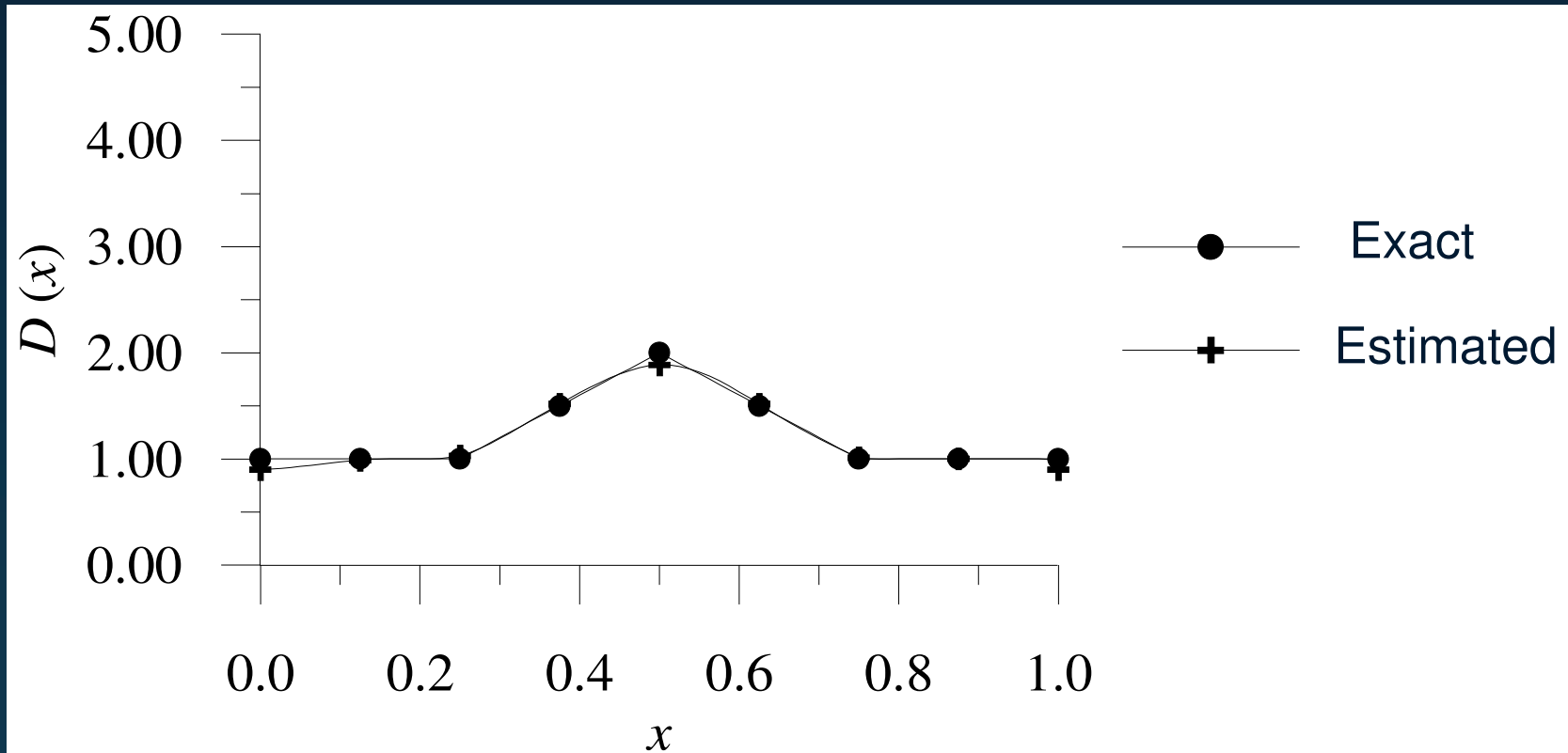
2 Non-intrusive sensors – Errorless measurements



Example 3

RESULTS - CGM Estimation of $D(x)$ for Known $\mu(x)$

10 Sensors – Errorless measurements

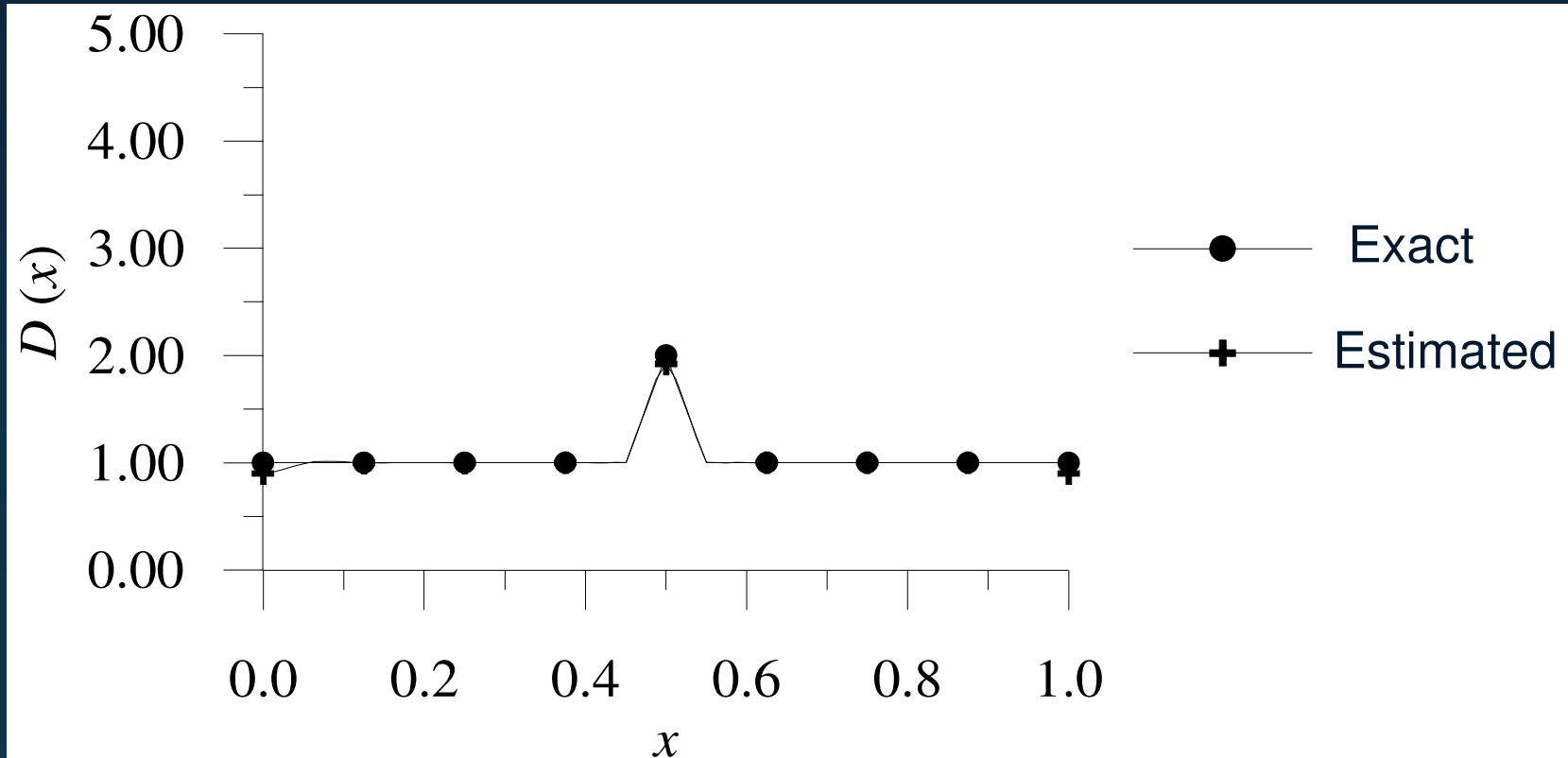


Example 3

RESULTS - CGM

Estimation of $D(x)$ for Known $\mu(x)$

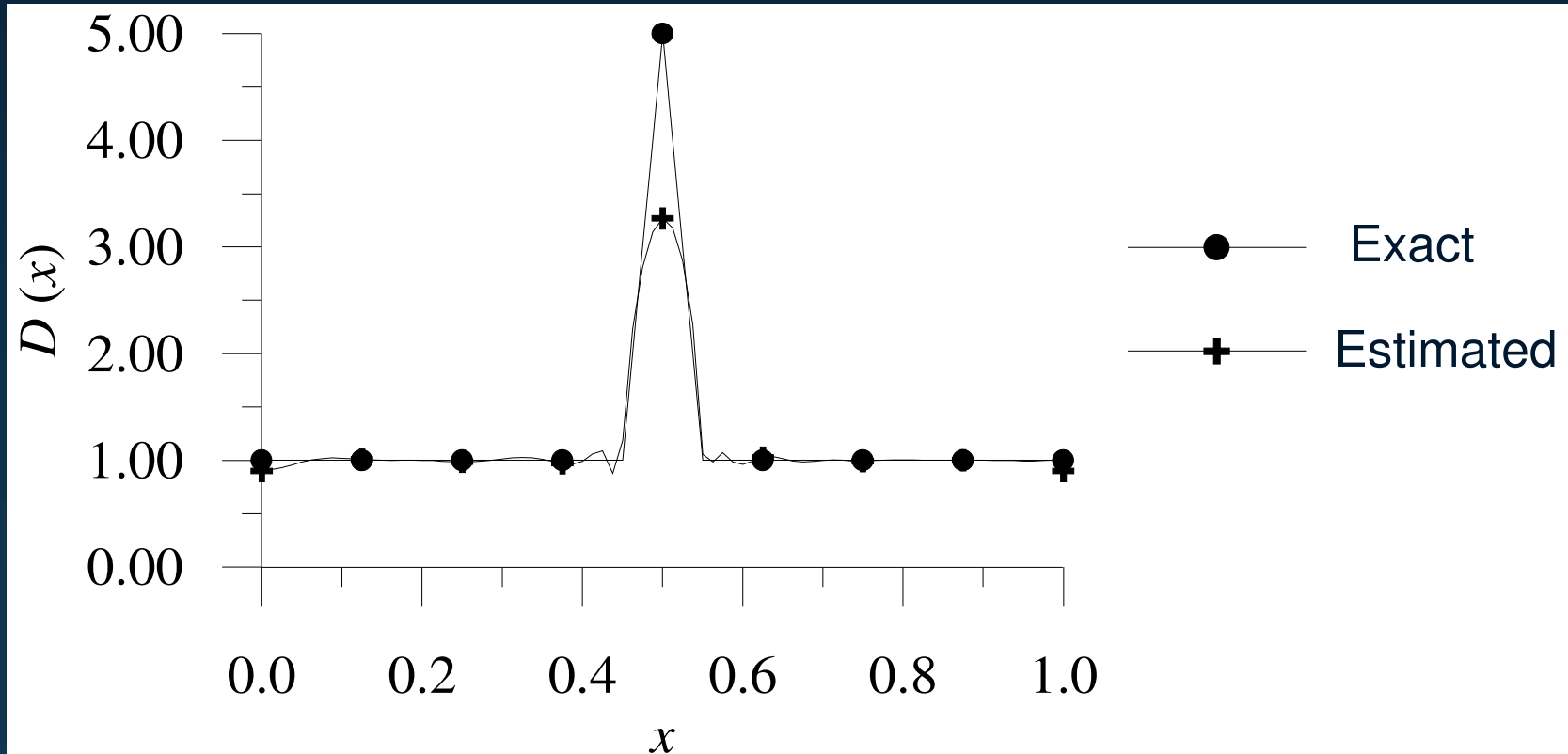
80 Sensors – Errorless measurements



Example 3

RESULTS - CGM Estimation of $D(x)$ for Known $\mu(x)$

80 Sensors – Errorless measurements

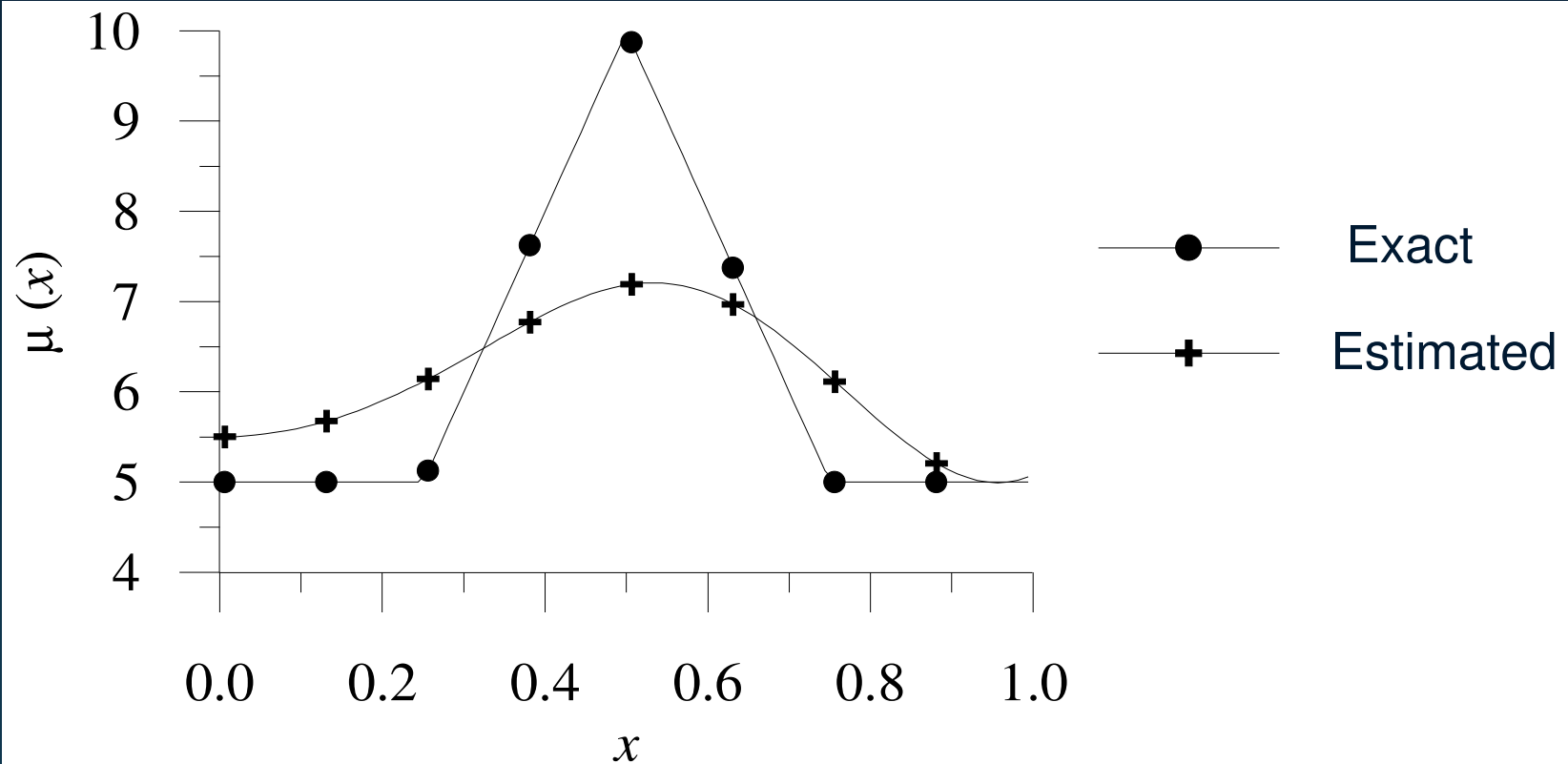


Example 3

RESULTS - CGM

Estimation of $\mu(x)$ for Known $D(x)$

2 Non-intrusive sensors – Errorless measurements

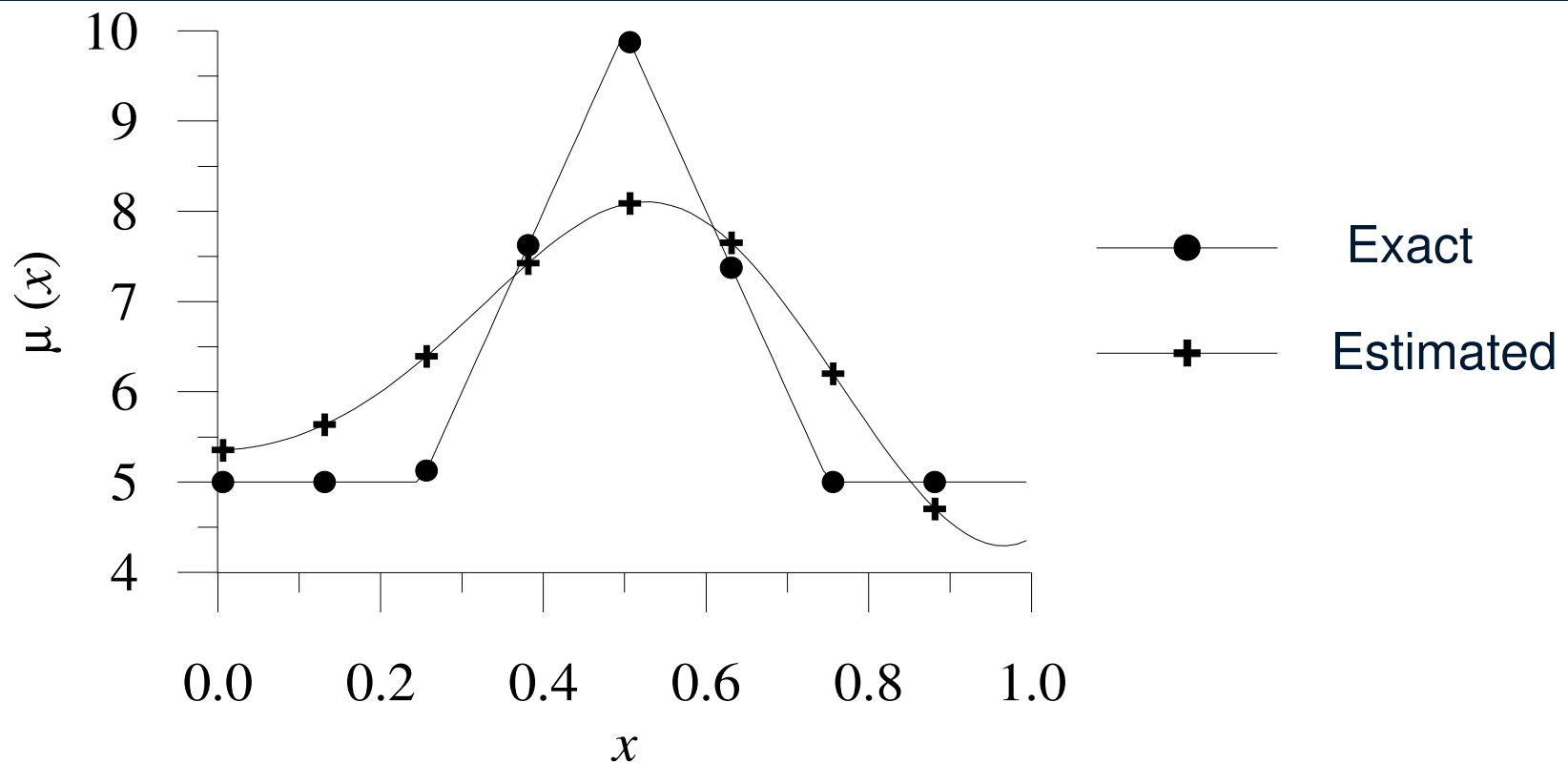


Example 3

RESULTS - CGM

Estimation of $\mu(x)$ for Known $D(x)$

10 Sensors – Errorless measurements

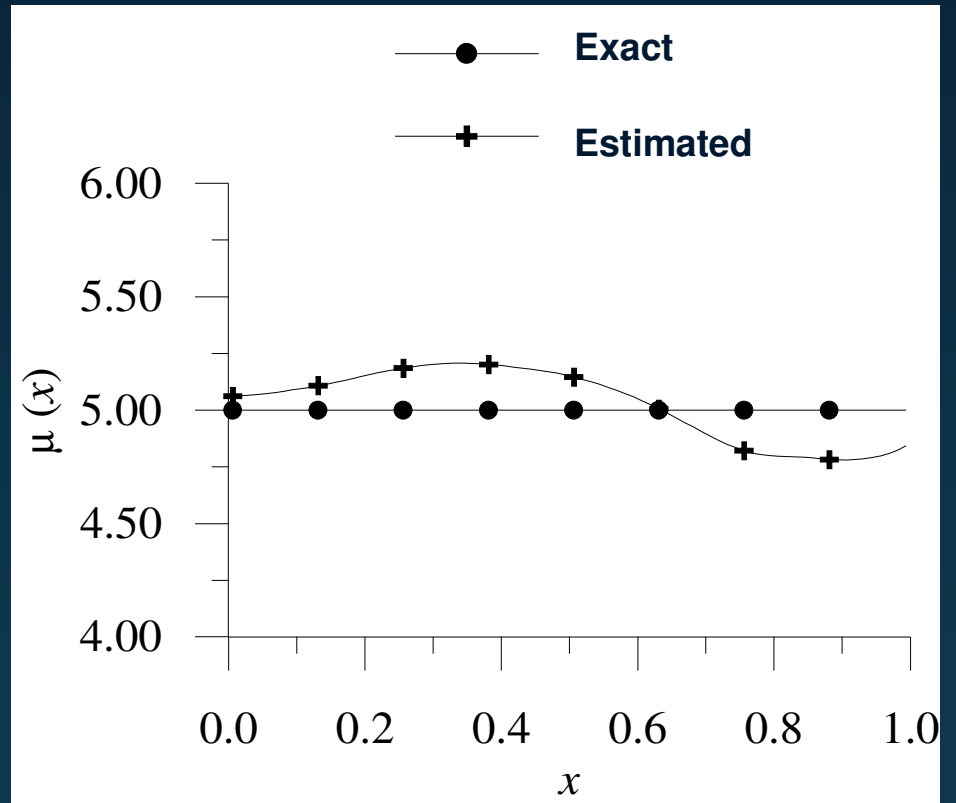
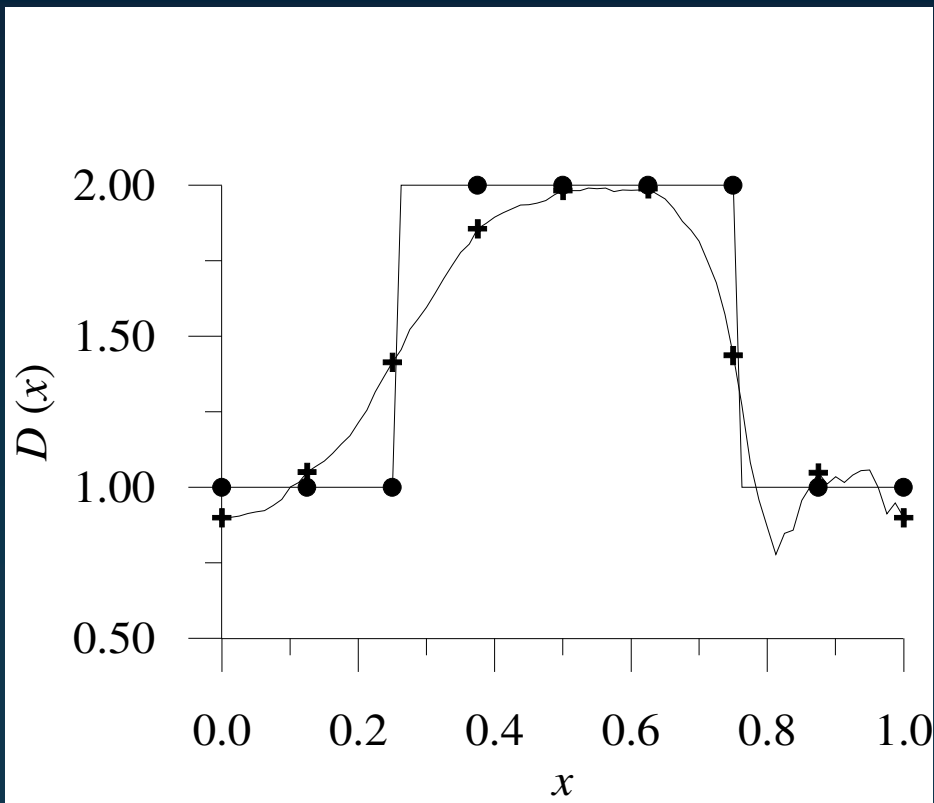


Example 3

RESULTS - CGM

Simultaneous estimation of $\mu(x)$ and $D(x)$

2 Non-intrusive sensors – Measurements with $\sigma = 0.01$ Y_{max}

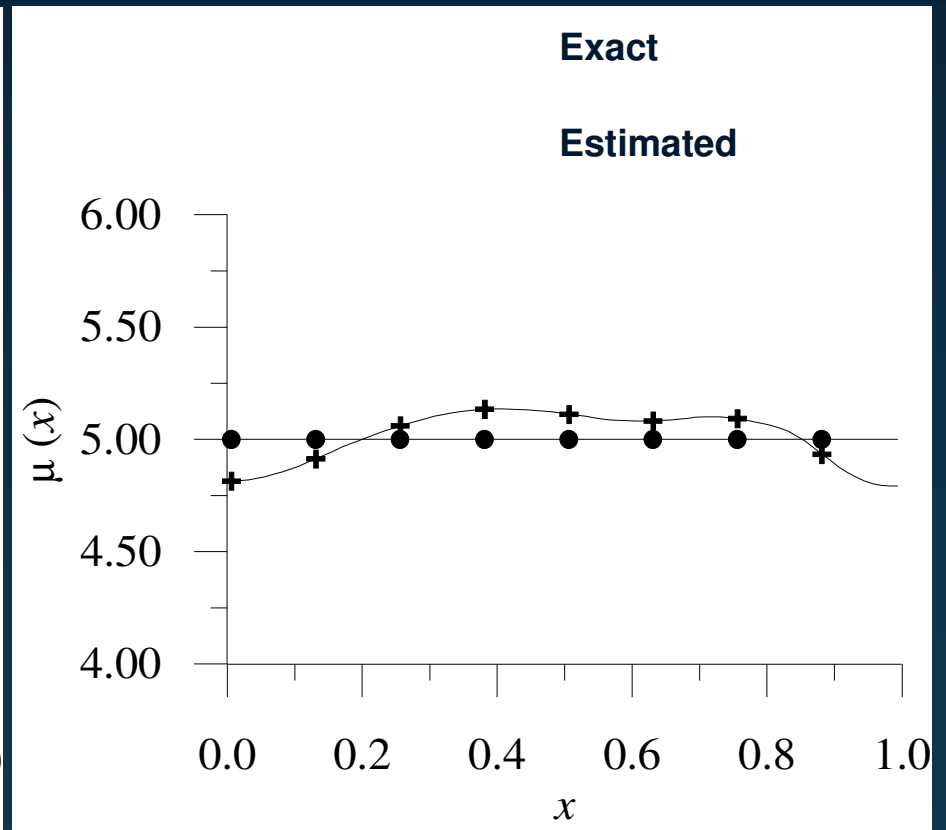
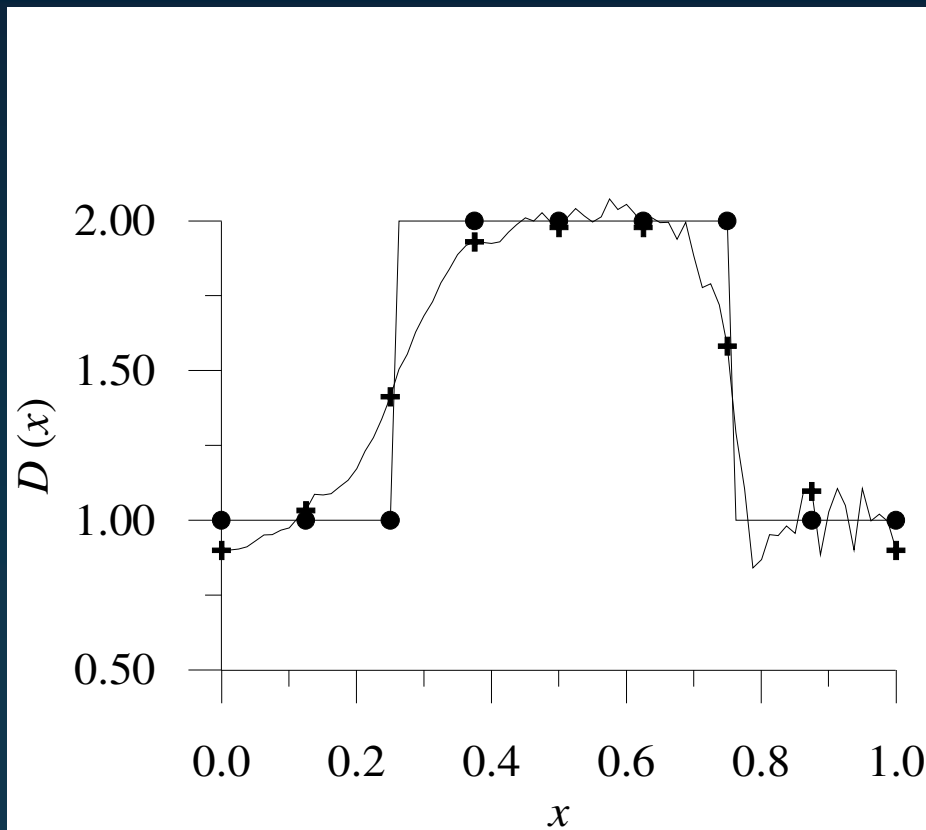


Example 3

RESULTS - CGM

Simultaneous estimation of $\mu(x)$ and $D(x)$

10 Sensors – Measurements with $\sigma = 0.01$ Y_{max}

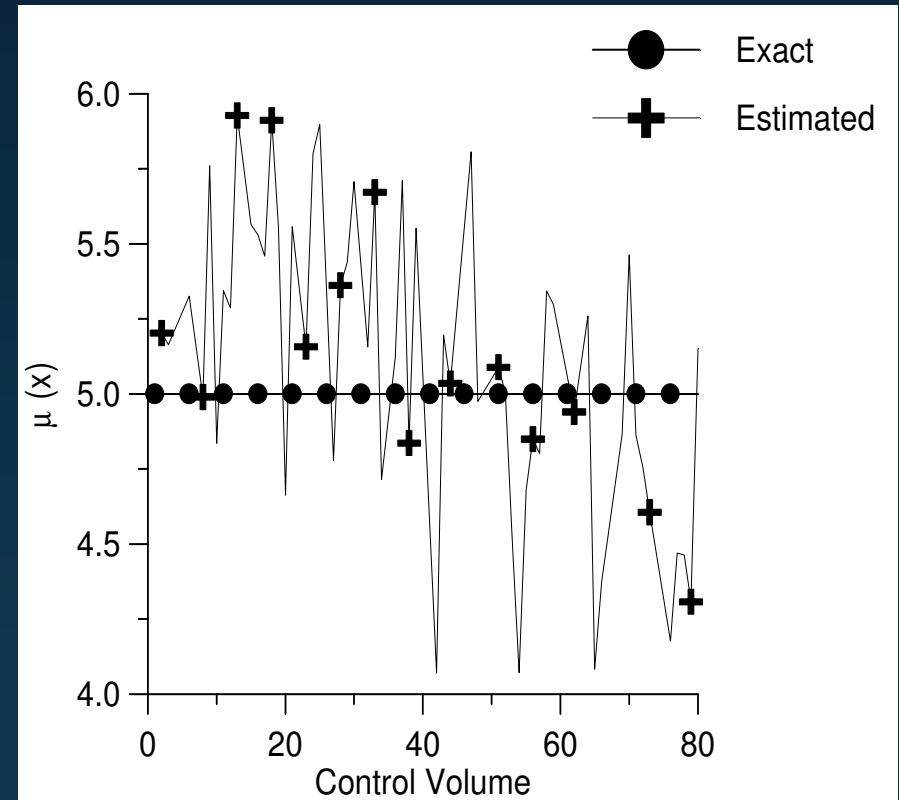
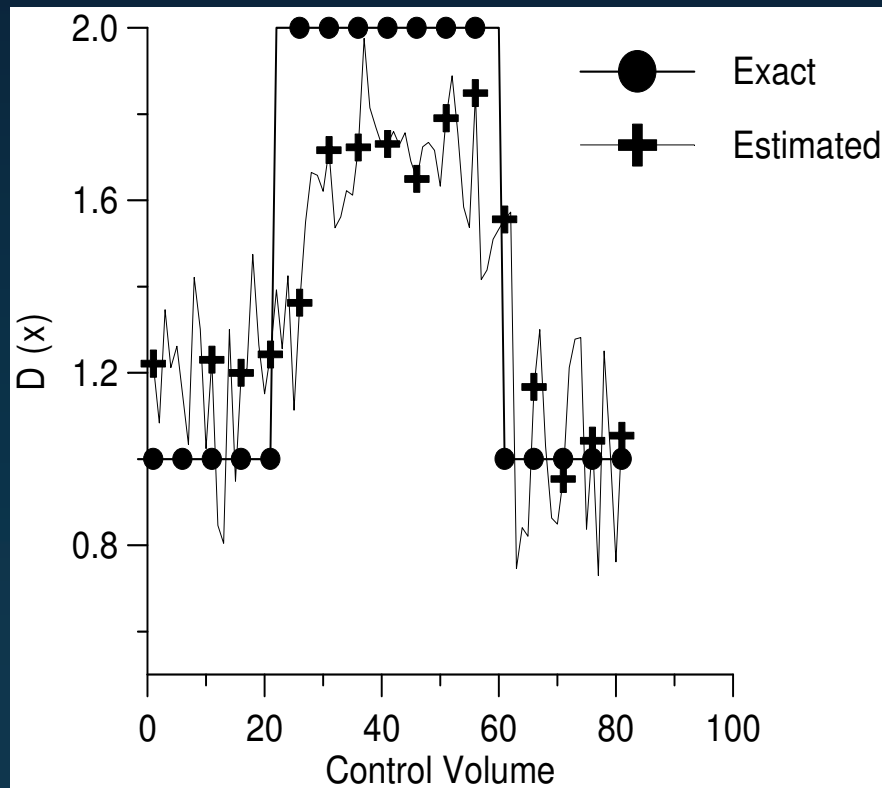


Example 3

RESULTS - TIKHONOV

Simultaneous estimation of $\mu(x)$ and $D(x)$

10 Sensors – Measurements with $\sigma = 0.01$ $Y_{max} - \alpha_1 = 0$

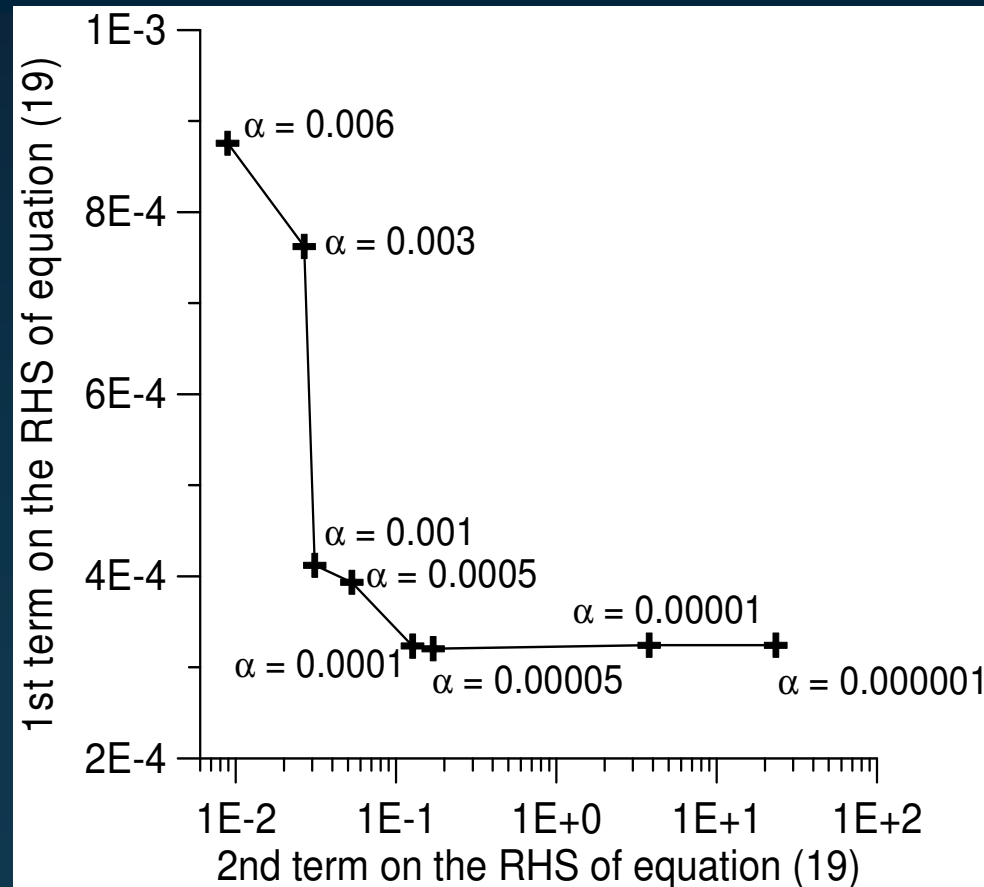


Example 3

RESULTS - TIKHONOV

Simultaneous estimation of $\mu(x)$ and $D(x)$

10 Sensors – Measurements with $\sigma = 0.01$ Y_{max}

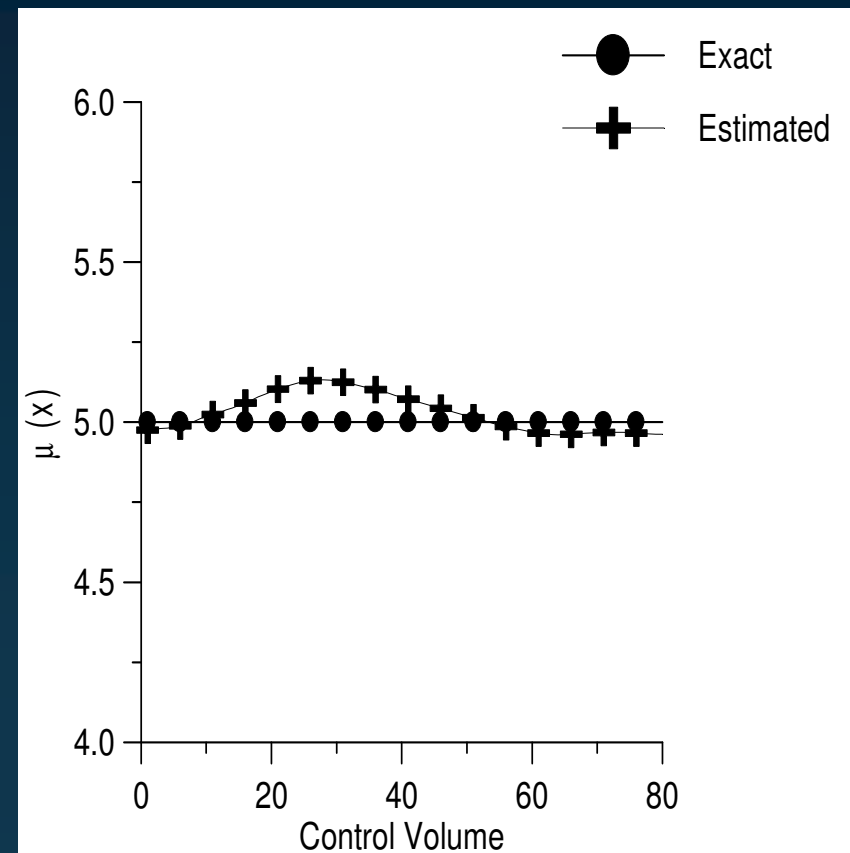
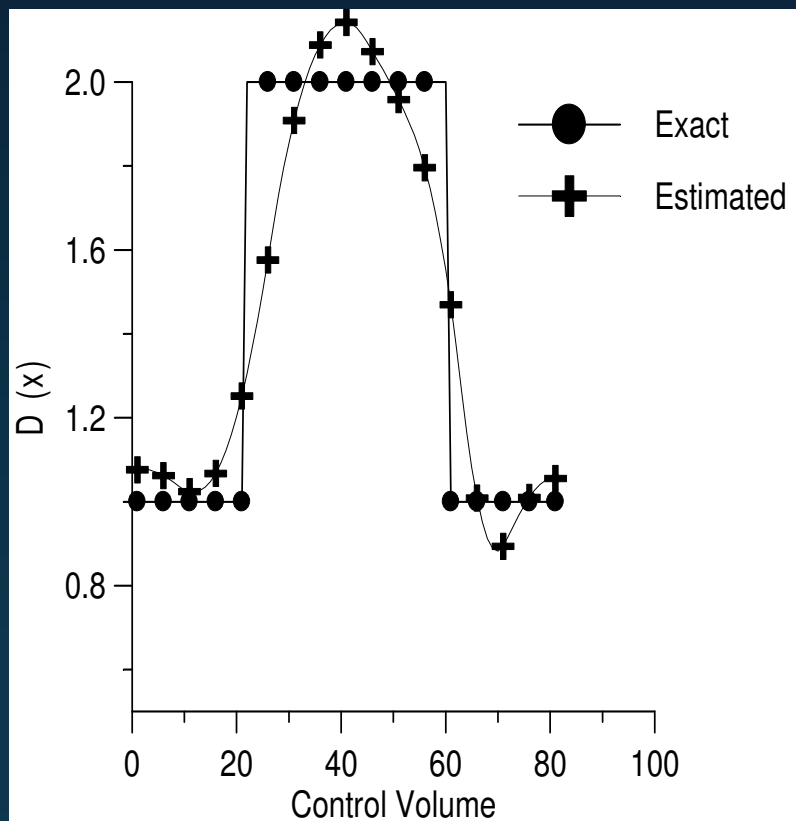


Example 3

RESULTS - TIKHONOV

Simultaneous estimation of $\mu(x)$ and $D(x)$

10 Sensors – Measurements with $\sigma = 0.01$ $Y_{max} - \alpha_1 = 0.0001$

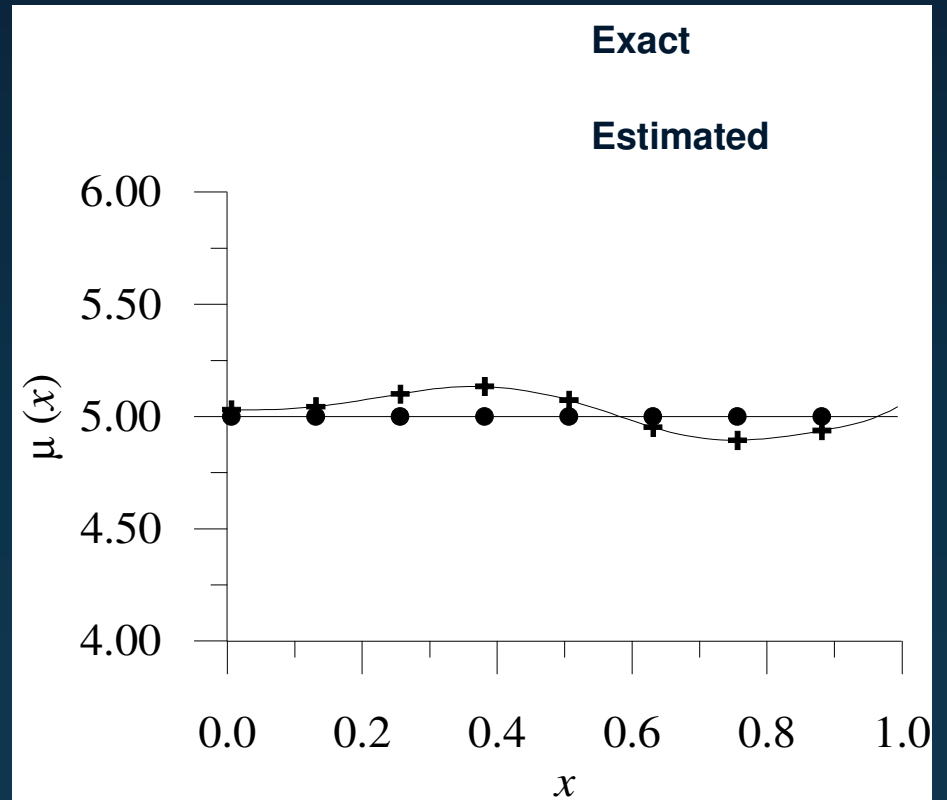
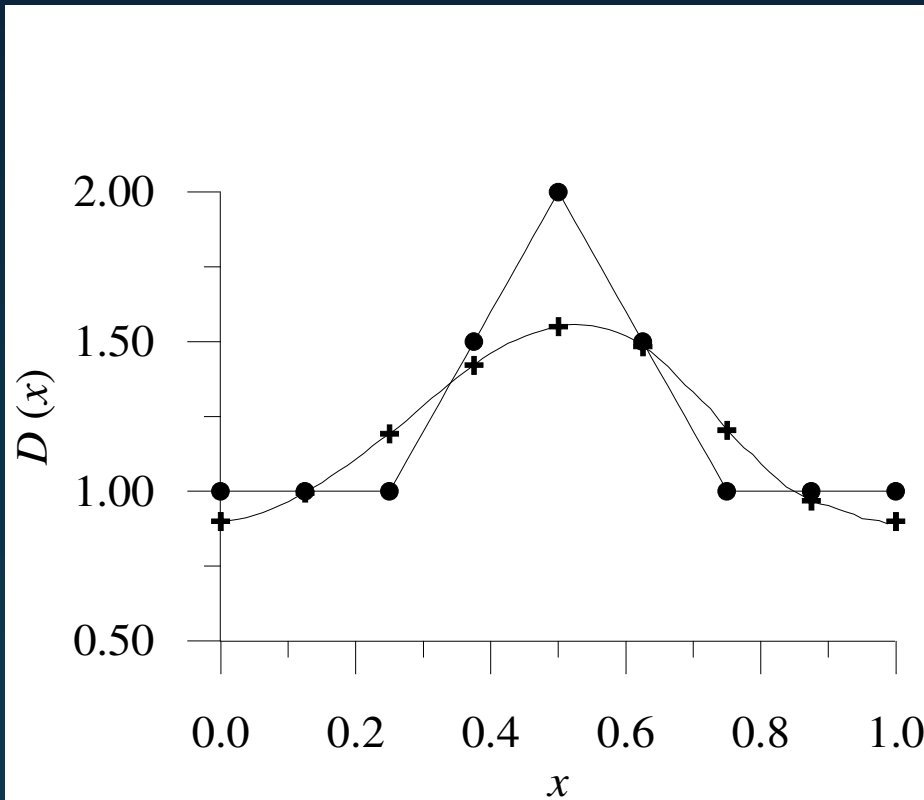


Example 3

RESULTS - CGM

Simultaneous estimation of $\mu(x)$ and $D(x)$

2 Non-intrusive sensors – Measurements with $\sigma = 0.01$ Y_{max}

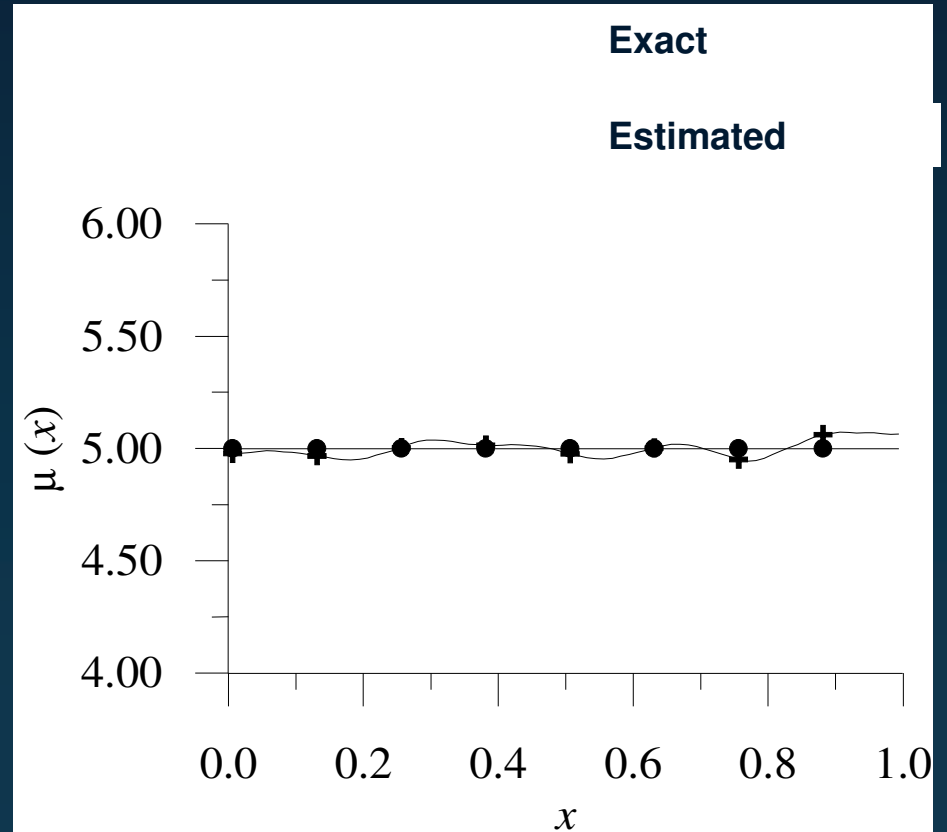
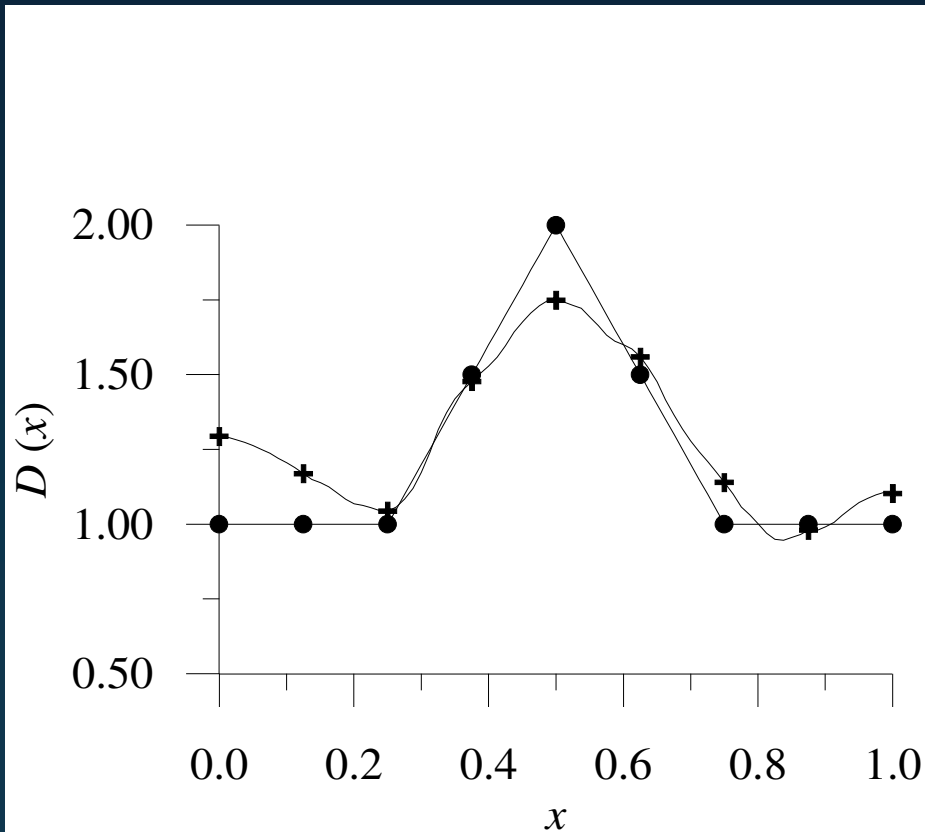


Example 3

RESULTS - TIKHONOV

Simultaneous estimation of $\mu(x)$ and $D(x)$

2 Non-intrusive sensors – Measurements with $\sigma = 0.01$ Y_{max}

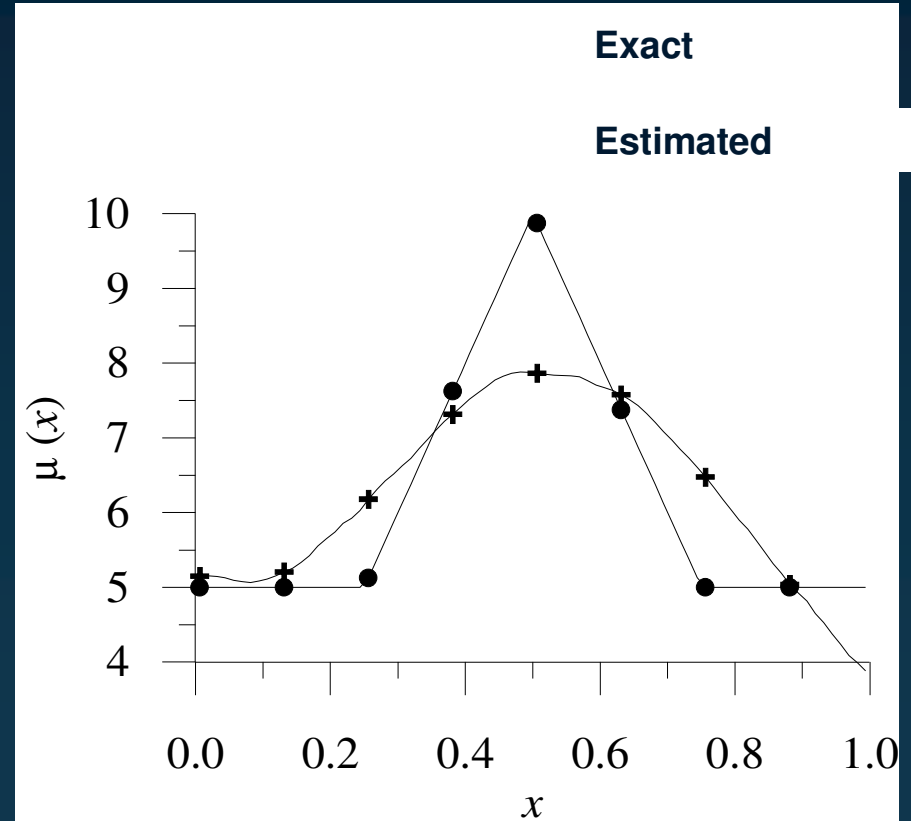
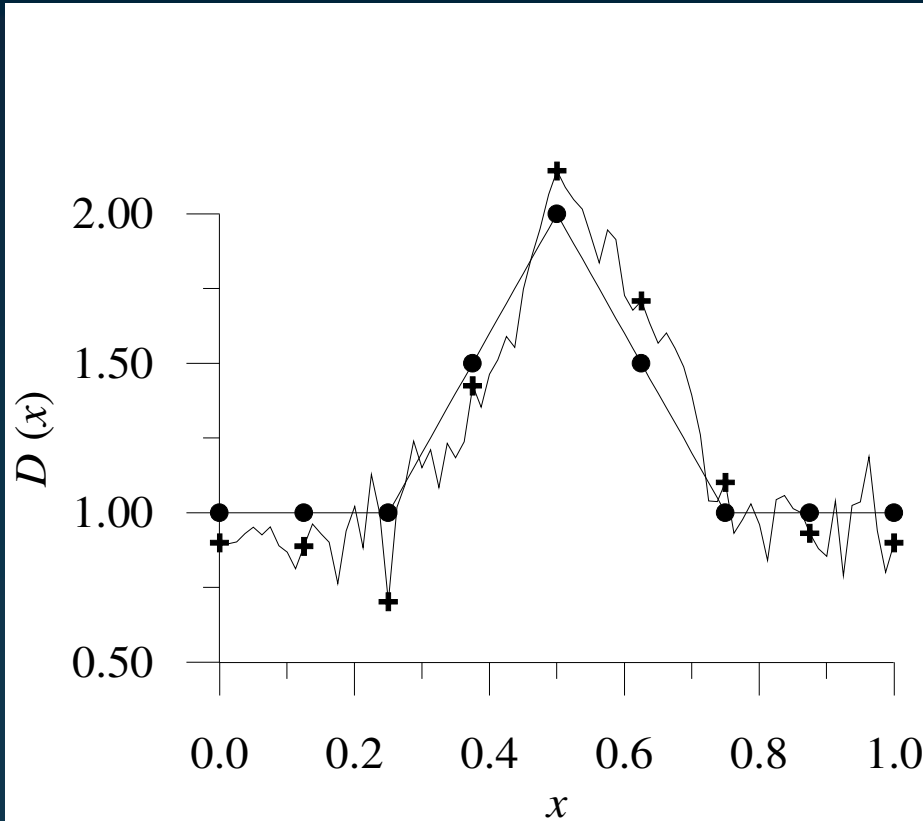


Example 3

RESULTS - CGM

Simultaneous estimation of $\mu(x)$ and $D(x)$

50 Sensors – Measurements with $\sigma = 0.01$ Y_{max}

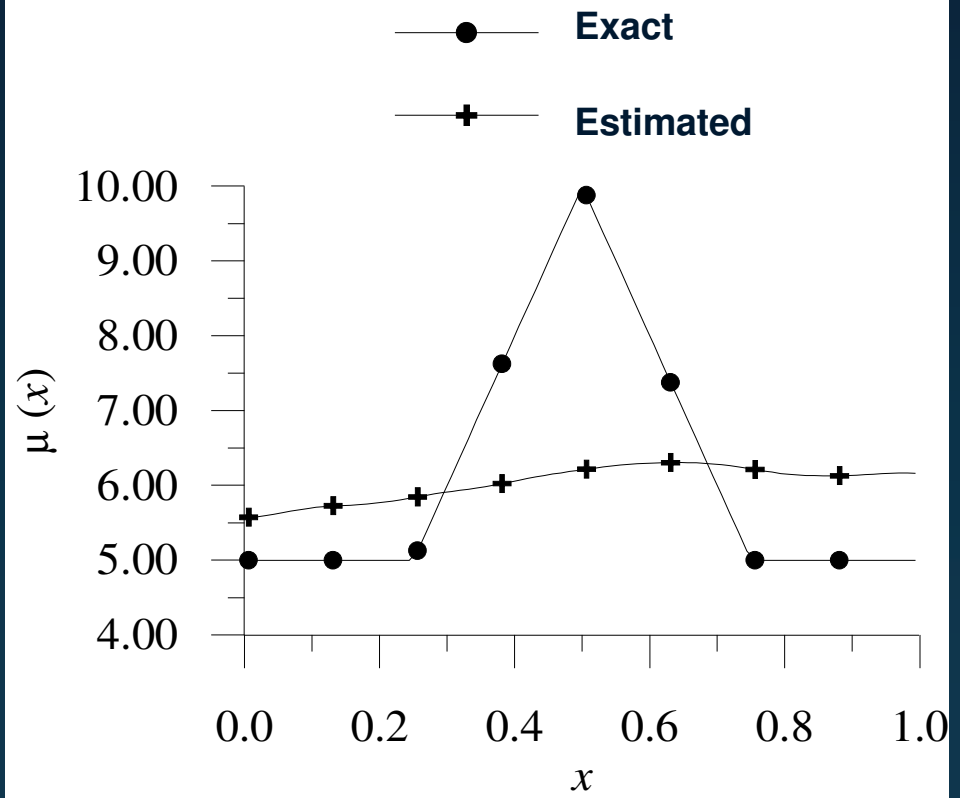
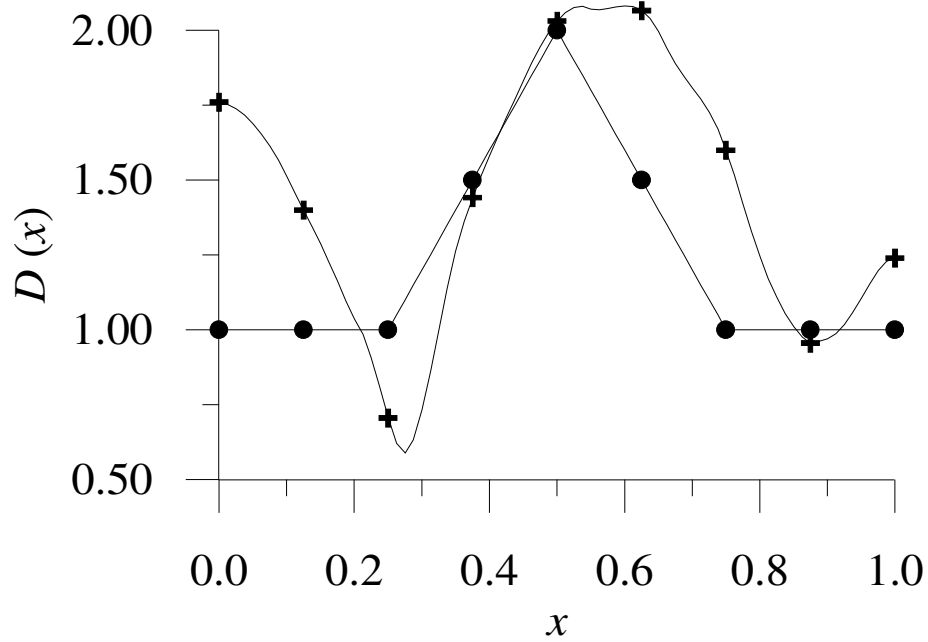


Example 3

RESULTS - TIKHONOV

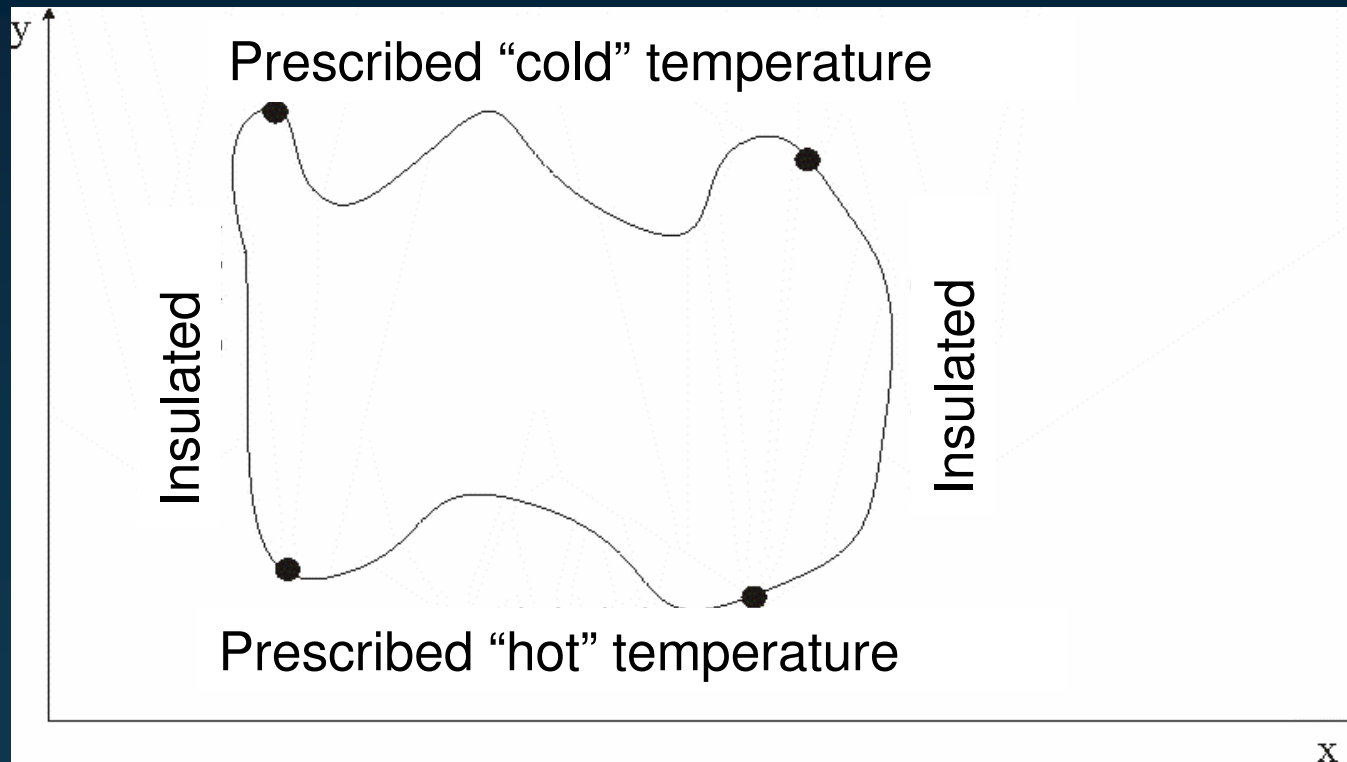
Simultaneous estimation of $\mu(x)$ and $D(x)$

50 Sensors – Measurements with $\sigma = 0.01$ Y_{max}



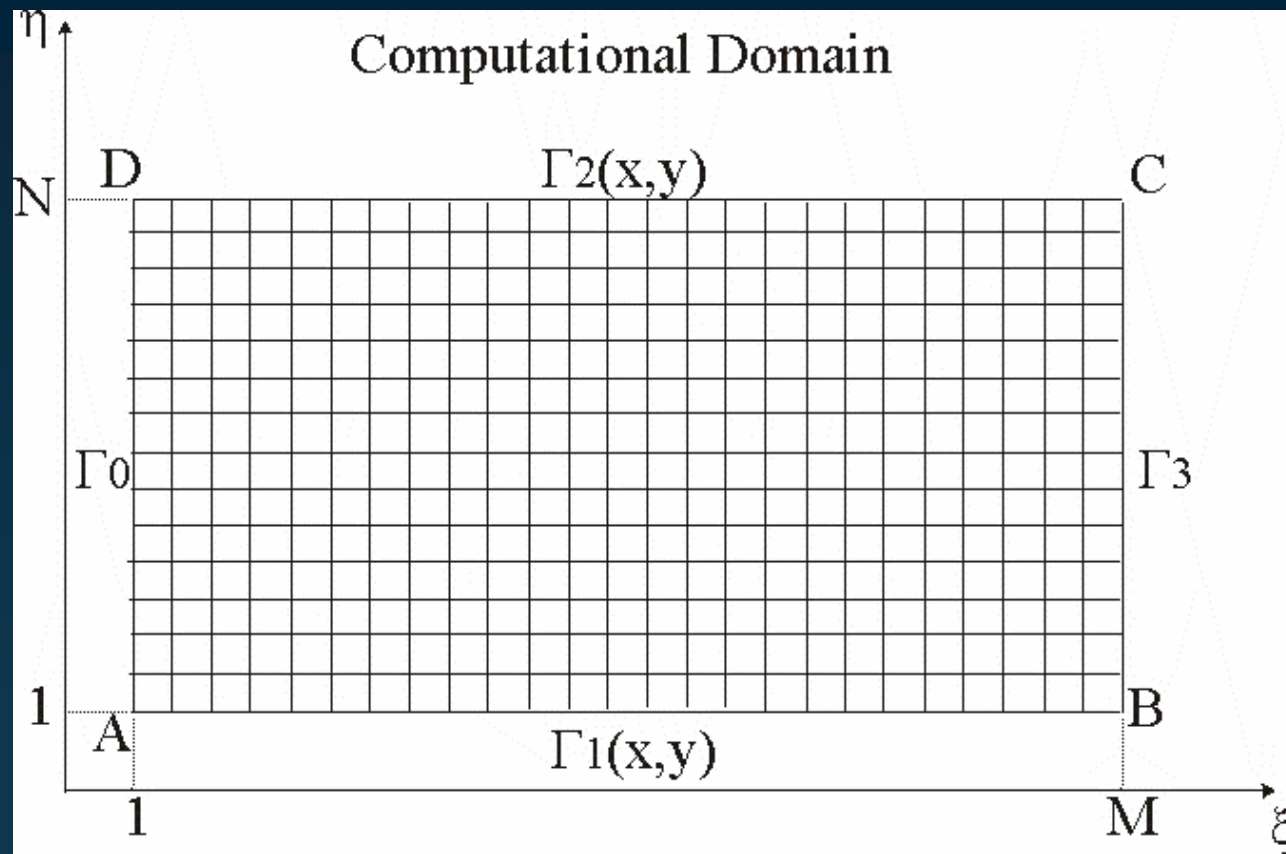
Example - EMHD Problem

→ Geometry in the cartesian coordinate system (x,y)



Example - EMHD Problem

→ Geometry in the “computational” coordinate system (ξ, η)



Example - EMHD Problem

→ Motivations:

- Control the natural convection phenomena by using electric or magnetic fields.
- Control the solidification process in order to produce materials with less thermal stresses.
- Produce materials with pre-specified thermal properties.
- Control the concentration of micro-fibers in solidifying composites.

Example - EMHD Problem

→ Two problems:

- **Magnetohydrodynamic:** Fluid flow under the influence of magnetic fields without electric charged particles.
- **Electrohydrodynamic:** Fluid flow under the influence of electric fields with electric charged particles and neglectable magnetic field.

Magnetohydrodynamic

Direct Problem - MHD

→ Conservation equations in the Cartesian coordinate system (x,y)

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} = S$$

where

$$Q = \lambda \phi$$

$$E = \lambda u \phi^* - \Gamma \frac{\partial \phi^{***}}{\partial x}$$

$$F = \lambda v \phi^{**} - \Gamma \frac{\partial \phi^{***}}{\partial y}$$

Conservation of	λ	ϕ	ϕ^*	ϕ^{**}	ϕ^{***}	Γ	S
Mass	ρ	1	1	1	1	0	0
Species	ρ	C	C	C	C	D	$\nabla \cdot [f_s \rho_s D_s \nabla (C_s - C)] + \nabla \cdot [f_l \rho_l D_l \nabla (C_l - C)]$
x-momentum	ρ	u	u	u	u	μ	$-\frac{\partial P}{\partial x} - \frac{B_y}{\mu_m} \left[\frac{\partial B_y}{\partial x} - \frac{\partial B_x}{\partial y} \right]$
y-momentum	ρ	v	v	v	v	μ	$-\frac{\partial p}{\partial y} - \rho g [1 - \beta(T - T_0) - \beta_s(C - C_0)] + \frac{B_y}{\mu_m} \left[\frac{\partial B_y}{\partial x} - \frac{\partial B_x}{\partial y} \right]$
Energy	ρ	h	h	h	T	k	$\frac{C_p}{\sigma \mu_m^2} \left[\frac{\partial B_y}{\partial x} - \frac{\partial B_x}{\partial y} \right]^2$
Magnetic x-flux	1	B_x	0	B_x	B_x	$\frac{1}{\mu_m \sigma}$	$\frac{\partial (u B_y)}{\partial y}$
Magnetic y-flux	1	B_y	B_y	0	B_y	$\frac{1}{\mu_m \sigma}$	$\frac{\partial (v B_x)}{\partial x}$

Direct Problem - MHD

→ Conservation of **mass, momentum, species and energy** in the “computational” coordinate system (ξ, η)

$$\frac{\partial(J\rho\phi)}{\partial t} + \frac{\partial(\tilde{U}\rho\phi)}{\partial \xi} + \frac{\partial(\tilde{V}\rho\phi)}{\partial \eta} =$$

$$\frac{\partial}{\partial \xi} \left\{ \mathcal{L}^\phi \left[a \frac{\partial \phi^{***}}{\partial \xi} + d \frac{\partial \phi^{***}}{\partial \eta} \right] \right\} + \frac{\partial}{\partial \eta} \left\{ \mathcal{L}^\phi \left[d \frac{\partial \phi^{***}}{\partial \xi} + b \frac{\partial \phi^{***}}{\partial \eta} \right] \right\} + JS$$

where

$$\tilde{U} = J(u\xi_x + v\xi_y)$$

$$\tilde{V} = J(u\eta_x + v\eta_y)$$

$$a = \xi_x^2 + \xi_y^2$$

$$b = \eta_x^2 + \eta_y^2$$

$$d = \xi_x \eta_x + \xi_y \eta_y$$

$$\xi_x = \frac{y_\eta}{J}$$

$$\xi_y = -\frac{x_\eta}{J}$$

$$\eta_x = -\frac{y_\xi}{J}$$

$$\eta_y = \frac{x_\xi}{J}$$

$$J = x_\xi y_\eta - x_\eta y_\xi$$

Conservation of	λ	ϕ	ϕ^*	ϕ^{**}	ϕ^{***}	Γ	S
Mass	ρ	1	1	1	1	0	0
x-momentum	ρ	u	u	u	u	μ	$-\frac{\partial P}{\partial x} - \frac{B_y}{\mu_m} \left[\frac{\partial B_y}{\partial x} - \frac{\partial B_x}{\partial y} \right]$
y-momentum	ρ	v	v	v	v	μ	$-\frac{\partial P}{\partial y} - \rho g[1 - \beta(T - T_0)] + \frac{B_y}{\mu_m} \left[\frac{\partial B_y}{\partial x} - \frac{\partial B_x}{\partial y} \right]$
Energy	ρ	h	h	h	T	K	$\frac{C_P}{\sigma \mu_m^2} \left[\frac{\partial B_y}{\partial x} - \frac{\partial B_x}{\partial y} \right]^2$

Direct Problem - MHD

- Conservation of **magnetic flux in x-direction** in the “computational” coordinate system (ξ, η)

$$\frac{\partial(J\rho\phi)}{\partial t} + \frac{\partial(\tilde{U}_{Bx}\rho\phi)}{\partial \xi} + \frac{\partial(\tilde{V}_{Bx}\rho\phi)}{\partial \eta} =$$

$$\frac{\partial}{\partial \xi} \left\{ \Pi^\phi \left[a \frac{\partial \phi^{***}}{\partial \xi} + d \frac{\partial \phi^{***}}{\partial \eta} \right] \right\} + \frac{\partial}{\partial \eta} \left\{ \Pi^\phi \left[d \frac{\partial \phi^{***}}{\partial \xi} + b \frac{\partial \phi^{***}}{\partial \eta} \right] \right\} + JS$$

where

$$\tilde{U}_{By} = J(0\xi_x + \nu\xi_y)$$

$$\tilde{V}_{By} = J(0\eta_x + \nu\eta_y)$$

$$a = \xi_x^2 + \xi_y^2$$

$$b = \eta_x^2 + \eta_y^2$$

$$d = \xi_x\eta_x + \xi_y\eta_y$$

$$\xi_x = \frac{y_\eta}{J}$$

$$\xi_y = -\frac{x_\eta}{J}$$

$$\eta_x = -\frac{y_\xi}{J}$$

$$\eta_y = \frac{x_\xi}{J}$$

$$J = x_\xi y_\eta - x_\eta y_\xi$$

Conservation of	λ	ϕ	ϕ^*	ϕ^{**}	ϕ^{***}	Γ	S
Magnetic flux in x-direction	1	B_x	0	B_x	B_x	$\frac{1}{\mu_m \sigma}$	$\frac{\partial(uB_y)}{\partial y}$

Direct Problem - MHD

- Conservation of **magnetic flux in y-direction** in the “computational” coordinate system (ξ, η)

$$\frac{\partial(J\rho\phi)}{\partial t} + \frac{\partial(\tilde{U}_{By}\rho\phi)}{\partial \xi} + \frac{\partial(\tilde{V}_{By}\rho\phi)}{\partial \eta} =$$

$$\frac{\partial}{\partial \xi} \left\{ \mathcal{L}^\phi \left[a \frac{\partial \phi^{***}}{\partial \xi} + d \frac{\partial \phi^{***}}{\partial \eta} \right] \right\} + \frac{\partial}{\partial \eta} \left\{ \mathcal{L}^\phi \left[d \frac{\partial \phi^{***}}{\partial \xi} + b \frac{\partial \phi^{***}}{\partial \eta} \right] \right\} + JS$$

where

$$\tilde{U}_{By} = J(u\xi_x + 0\xi_y)$$

$$\tilde{V}_{By} = J(u\eta_x + 0\eta_y)$$

$$a = \xi_x^2 + \xi_y^2$$

$$b = \eta_x^2 + \eta_y^2$$

$$d = \xi_x\eta_x + \xi_y\eta_y$$

$$\xi_x = \frac{y_\eta}{J}$$

$$\xi_y = -\frac{x_\eta}{J}$$

$$\eta_x = -\frac{y_\xi}{J}$$

$$\eta_y = \frac{x_\xi}{J}$$

$$J = x_\xi y_\eta - x_\eta y_\xi$$

Conservation of	λ	ϕ	ϕ^*	ϕ^{**}	ϕ^{***}	Γ	S
Magnetic flux in y-direction	1	B_y	B_y	0	B_y	$\frac{1}{\mu_m \sigma}$	$\frac{\partial(vB_x)}{\partial x}$

Direct Problem - MHD

→ Numerical method



- Finite Volumes (Implicit)

→ Linear system solver



- Bi-Conjugate gradient method (GMRES)

→ Interpolation function for the convective terms



- WUDS (Raithby and Torrance, 1974)

→ Pressure-velocity coupling



- SIMPLEC (Van Doormal and Raithby, 1984)

→ Phase-change model



- Enthalpy method (Voller et al, 1989)

Direct Problem - MHD

→ Finite Volume Method

- Control volume where the conservation equations are integrated

NW	N	NE
W	n w P e s	E
SW	S	SE

Direct Problem - MHD

→ Finite Volume Method – Integrated conservation equations

$$\begin{aligned}
 & \frac{(M_P \phi_P - M_P^0 \phi_P^0)}{\Delta t} + \dot{M}_e \phi_e - \dot{M}_w \phi_w + \dot{M}_n \phi_n - \dot{M}_s \phi_s = \\
 & = \left[D_{11} \frac{\partial \phi}{\partial \xi} + D_{12} \frac{\partial \phi}{\partial \eta} \right]_e - \left[D_{11} \frac{\partial \phi}{\partial \xi} + D_{12} \frac{\partial \phi}{\partial \eta} \right]_w + \\
 & + \left[D_{21} \frac{\partial \phi}{\partial \xi} + D_{22} \frac{\partial \phi}{\partial \eta} \right]_n - \left[D_{21} \frac{\partial \phi}{\partial \xi} + D_{22} \frac{\partial \phi}{\partial \eta} \right]_s + \\
 & + L[S^\phi J]_P \Delta V - L[P^\phi J]_P \Delta V
 \end{aligned}$$

where

$$M_P = \rho_P \Delta V J_P$$

$$M_P^0 = \rho_P^0 \Delta V J_P$$

$$\dot{M}_e = \rho \tilde{U}_e \Delta \eta$$

$$\dot{M}_w = \rho \tilde{U}_w \Delta \eta$$

$$\dot{M}_n = \rho \tilde{V}_n \Delta \xi$$

$$\dot{M}_s = \rho \tilde{V}_s \Delta \xi$$

$$D_{11} = \frac{\alpha_{11}}{J} \Gamma^\phi \Delta \eta$$

$$D_{12} = \frac{\alpha_{12}}{J} \Gamma^\phi \Delta \eta$$

$$D_{21} = \frac{\alpha_{21}}{J} \Gamma^\phi \Delta \xi$$

$$D_{22} = \frac{\alpha_{22}}{J} \Gamma^\phi \Delta \xi$$

$$\alpha_{11} = a J^2$$

$$\alpha_{12} = \alpha_{21} = d J^2$$

$$\alpha_{22} = b J^2$$

Direct Problem - MHD

→ WUDS interpolation scheme

$$\phi_e = \left(\frac{1}{2} + \bar{\alpha}_e \right) \phi_P + \left(\frac{1}{2} - \bar{\alpha}_e \right) \phi_E$$

$$\left. \frac{\partial \phi}{\partial \xi} \right|_e = \bar{\beta}_e \left(\frac{\phi_E - \phi_P}{\Delta \xi} \right)$$

where

$$\bar{\alpha} = \frac{r^2}{10 + 2r^2} \text{sign}(r)$$

$$\bar{\beta} = \frac{1 + 0.005r^2}{1 + 0.05r^2}$$

$$r = \frac{\dot{M}}{D}$$

Note that:

$\alpha=0; \beta=1 \Rightarrow$ Central differencing scheme

$\alpha=0.5; \beta=0 \Rightarrow$ Upwind scheme for $u > 0$

$\alpha= - 0.5; \beta=0 \Rightarrow$ Upwind scheme for $u < 0$

Direct Problem - MHD

→ WUDS interpolation scheme

$$\begin{aligned}
 A_e &= -\dot{M}_e \left(\frac{1}{2} - \bar{\alpha}_e \right) + \frac{D_{11e} \bar{\beta}_e}{\Delta \xi} + \frac{D_{21n} - D_{21s}}{4\Delta \xi} \\
 A_w &= \dot{M}_w \left(\frac{1}{2} + \bar{\alpha}_w \right) + \frac{D_{11w} \bar{\beta}_w}{\Delta \xi} + \frac{D_{21s} - D_{21n}}{4\Delta \xi} \\
 A_n &= -\dot{M}_n \left(\frac{1}{2} - \bar{\alpha}_n \right) + \frac{D_{22n} \bar{\beta}_n}{\Delta \eta} + \frac{D_{12e} - D_{12w}}{4\Delta \eta} \\
 A_s &= \dot{M}_s \left(\frac{1}{2} + \bar{\alpha}_s \right) + \frac{D_{22s} \bar{\beta}_s}{\Delta \eta} + \frac{D_{12w} - D_{12e}}{4\Delta \eta} \\
 A_{ne} &= \frac{D_{12e}}{4\Delta \eta} + \frac{D_{21n}}{4\Delta \xi} \\
 A_{se} &= -\frac{D_{12e}}{4\Delta \eta} - \frac{D_{21s}}{4\Delta \xi}
 \end{aligned}$$

$$\begin{aligned}
 A_{nw} &= -\frac{D_{12w}}{4\Delta \eta} - \frac{D_{21n}}{4\Delta \xi} \\
 A_{sw} &= \frac{D_{12w}}{4\Delta \eta} + \frac{D_{21s}}{4\Delta \xi} \\
 A_P &= \frac{M_P}{\Delta t} + \\
 &\quad + \dot{M}_e \left(\frac{1}{2} + \bar{\alpha}_e \right) - \dot{M}_w \left(\frac{1}{2} - \bar{\alpha}_w \right) + \\
 &\quad + \dot{M}_n \left(\frac{1}{2} + \bar{\alpha}_n \right) - \dot{M}_s \left(\frac{1}{2} - \bar{\alpha}_s \right) + \\
 &\quad + \frac{D_{11e} \bar{\beta}_e}{\Delta \xi} + \frac{D_{11w} \bar{\beta}_w}{\Delta \xi} + \frac{D_{22n} \bar{\beta}_n}{\Delta \eta} + \frac{D_{22s} \bar{\beta}_s}{\Delta \eta} \\
 B_P &= \frac{M_P^0 \phi_P^0}{\Delta t} + L[S^\phi J]_P \Delta V - L[P^\phi J]_P \Delta V
 \end{aligned}$$

$$\begin{aligned}
 A_P \phi_P &= A_e \phi_E + A_w \phi_W + A_n \phi_N + A_s \phi_S + \\
 &\quad + A_{ne} \phi_{NE} + A_{nw} \phi_{NW} + A_{se} \phi_{SE} + A_{sw} \phi_{SW} + B_P
 \end{aligned}$$



Solved by the GMRES method

Direct Problem - MHD

→ SIMPLEC

- The mass conservation equation and the momentum conservation equations are coupled through the pressure.
- SIMPLEC is one of the methodologies to deal with this problem which is known as pressure-velocity coupling.
- Others methods are SIMPLE, SIMPLER, PRIME, CELLS, etc
- SIMPLE means *Semi Implicit Linked Equations*
- SIMPLEC means *SIMPLE Consistent*

Direct Problem - MHD

→ Phase-Change Model – Energy equation:

$$\frac{\partial(\rho h)}{\partial t} + \frac{\partial(\rho h)}{\partial x} + \frac{\partial(\rho h)}{\partial y} = \frac{\partial}{\partial x} \left[K \frac{\partial T}{\partial x} \right] + \frac{\partial}{\partial y} \left[K \frac{\partial T}{\partial y} \right] + S$$

→ Enthalpy-Temperature relationships:

If $h < h_{\text{solid}}$:

$$T = \frac{h}{C_{Ps}}$$

If $h > h_{\text{liquid}}$:

$$T = \frac{h + T_s(C_{Pl} - C_{Ps}) - L}{C_{Pl}}$$

If $h_{\text{solid}} < h < h_{\text{liquid}}$:

$$T = \frac{h + [T_s(C_{Pl} - C_{Ps}) - L](1 - f)}{C_{Pl} + f(C_{Ps} - C_{Pl})}$$

→ Solid fraction (Scheil's model):

$$f = 1 - \left(\frac{T_s - T}{T_s - T_l} \right)^{1/(k-1)}$$

f and T equations are coupled

Direct Problem - MHD

→ Phase-Change Model

- Mixture Enthalpy-Temperature relationships

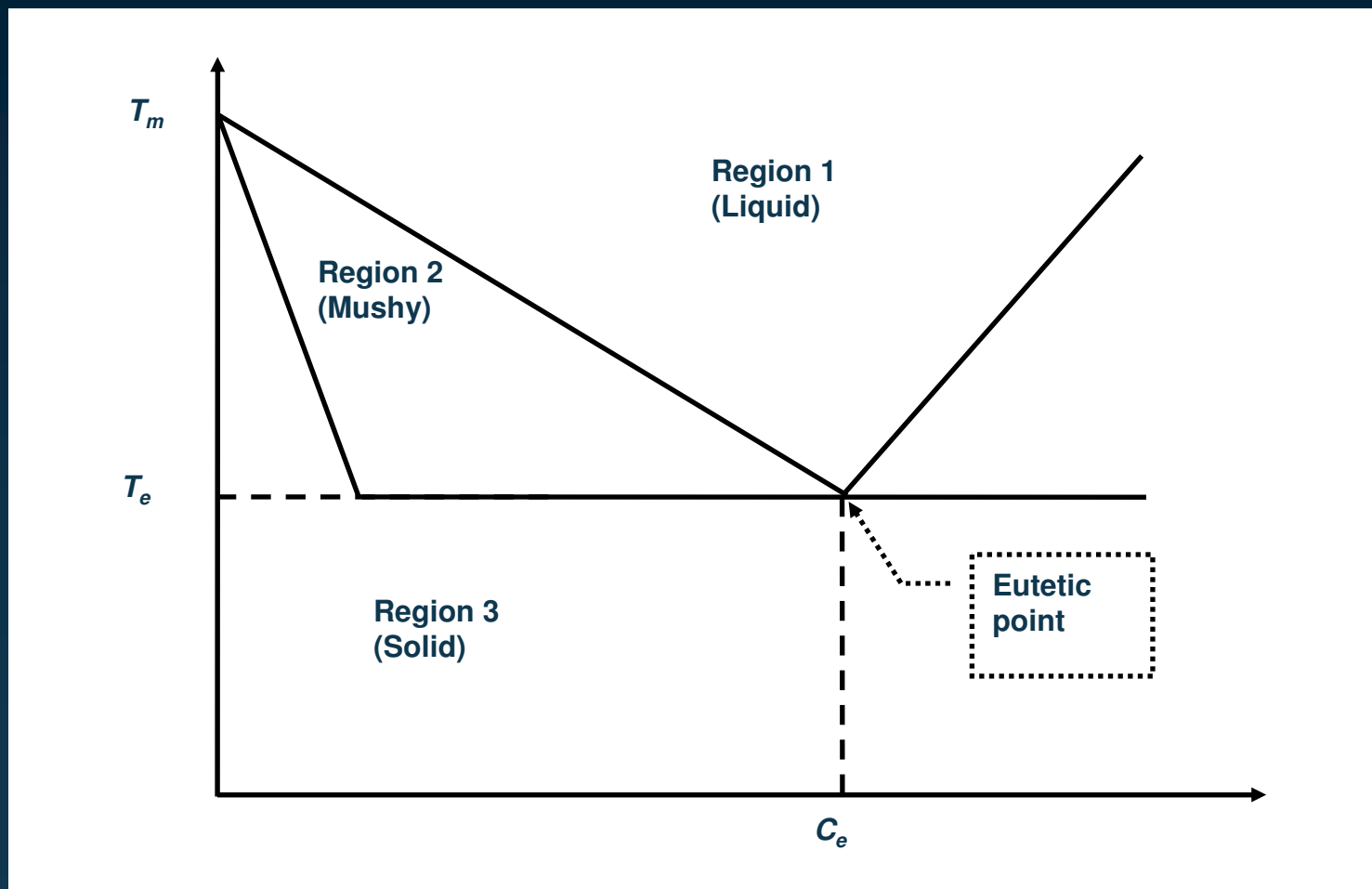
$$\frac{T - h + [T_s (C_{Pl} - C_{Ps}) - L] \left[\left(\frac{T_s - T}{T_s - T_l} \right)^{1/(k-1)} \right]}{C_{Pl} + \left[1 - \left(\frac{T_s - T}{T_s - T_l} \right)^{1/(k-1)} \right] (C_{Ps} - C_{Pl})} = 0$$



Solved by the secant
method

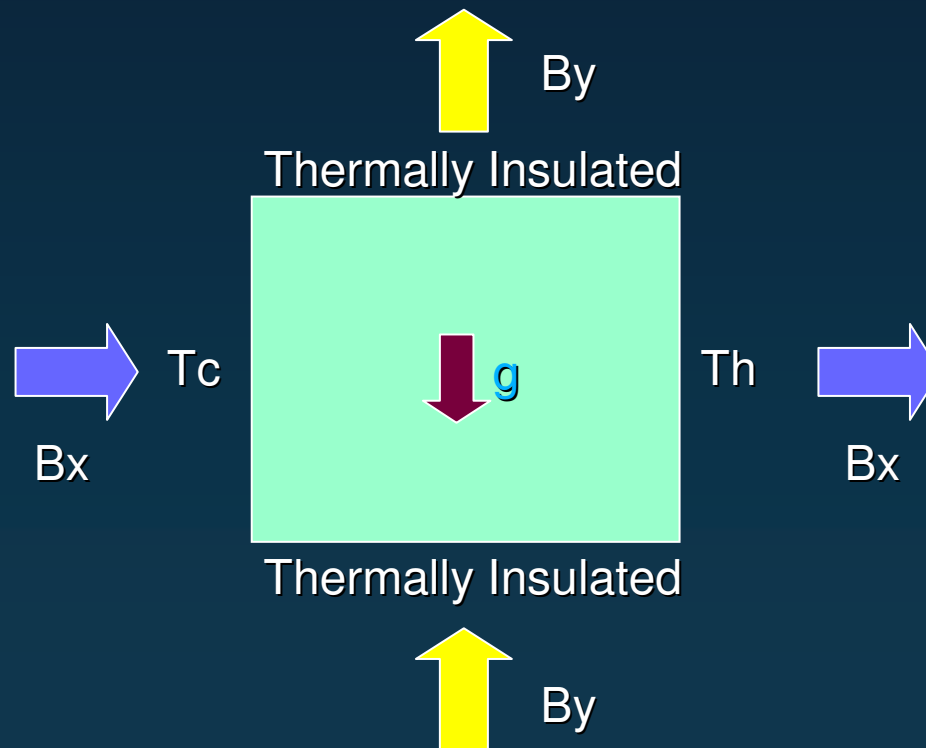
Direct Problem - MHD

→ Binary Diagram



MHD – Example 1

- **Optimization** of the magnetic boundary conditions in order to minimize the natural convection effects
- Test problem:



MHD – Example 1

→ Inverse Problem

→ The boundary conditions are parameterized as:

$$B(x_k) = \sum_{i=1}^M P_i C_i(x_k)$$

where:

$$C_i(x_k) = \cos\left[(i-1)\frac{\pi}{2}x_k\right] \quad \text{for } i = 1, 3, 5, \dots$$

$$C_i(x_k) = \cos\left[i\frac{\pi}{2}x_k\right] \quad \text{for } i = 2, 4, 6, \dots$$

MHD – Example 1

→ Inverse Problem

→ Two test cases: the physical parameters are:

$\rho_\ell = 2550 \text{ kg / m}^3$	$\rho_s = 2330 \text{ kg / m}^3$
$c_{p\ell} = 1059 \text{ J / kg K}$	$c_{ps} = 1038 \text{ J / kg K}$
$\kappa_\ell = 64 \text{ W / m K}$	$\kappa_s = 22 \text{ W / m K}$
$T_\ell = 1685 \text{ K}$	$T_s = 1681 \text{ K}$
$\sigma_\ell = 12.3 \times 10^5 \text{ 1 / } \Omega \text{ m}$	$\sigma_s = 4.3 \times 10^4 \text{ 1 / } \Omega \text{ m}$
$\mu_{v\ell} = 7.018 \times 10^{-4} \text{ kg / m s}$	$\mu = 7.022 \times 10^{-4} \text{ kg m / A}^2 \text{ s}^2$
$L = 1.803 \times 10^6 \text{ J / kg}$	$\alpha = 1.4 \times 10^{-4} \text{ 1 / K}$

Case 1 (small container)	Case 2 (large container)
$l_r = 0.01 \text{ m}$	$l_r = 0.02 \text{ m}$
$Re = 1000$	$Re = 1000$
$B_r = 0.1 \text{ T}$	$B_r = 0.1 \text{ T}$
$v_r = 2.7522 \times 10^{-2} \text{ m/s}$	$v_r = 1.3761 \times 10^{-2} \text{ m/s}$
$Pr = 1.1613 \times 10^{-2}$	$Pr = 1.1613 \times 10^{-2}$
$Gr = 1.8132 \times 10^5$	$Gr = 1.4506 \times 10^6$
$Ra = 2.1056 \times 10^3$	$Ra = 1.6845 \times 10^4$
$Fr = 8.7870 \times 10^{-2}$	$Fr = 3.1067 \times 10^{-2}$
$Ec = 7.1524 \times 10^{-8}$	$Ec = 1.7881 \times 10^{-8}$
$Ht = 4.1864 \times 10^1$	$Ht = 8.3729 \times 10^1$

MHD – Example 1

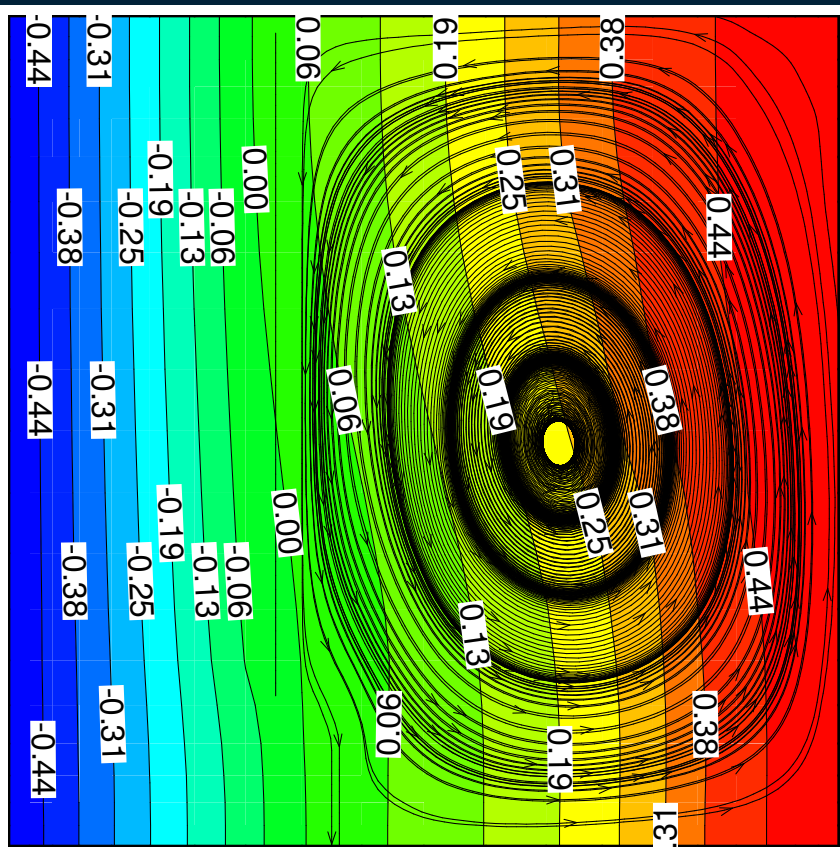
- Inverse Problem:
- Objective function

$$F = \left[\frac{1}{\# \text{liquid cells}} \sum_{i=1}^{\# \text{liquid cells}} \left(\frac{\partial T}{\partial y} \right)^2 \right]^{1/2}$$

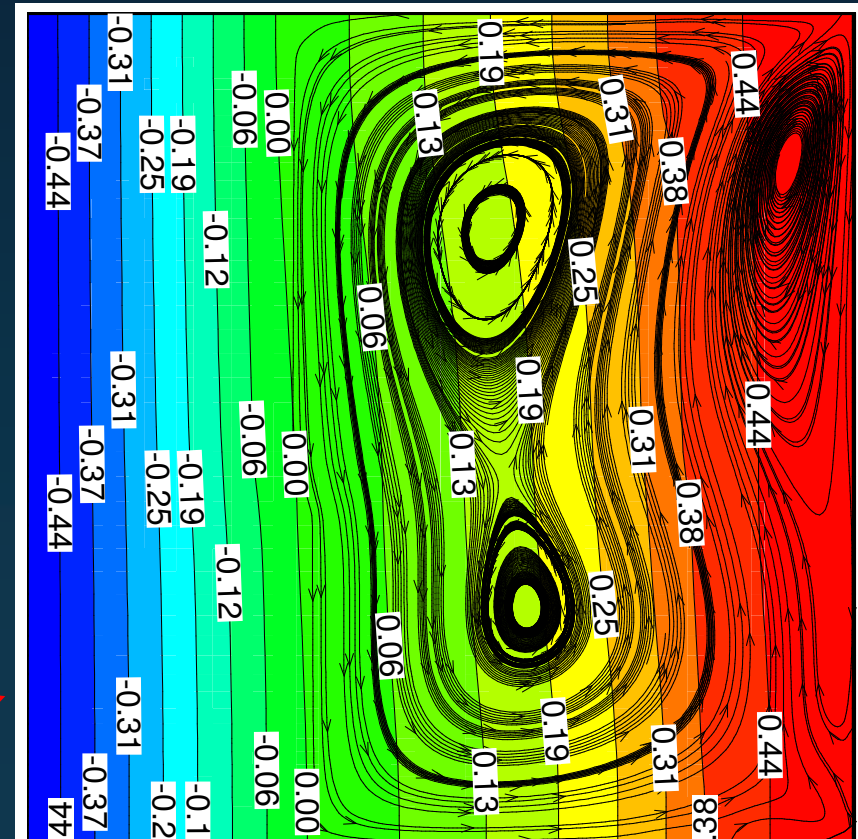
MHD – Example 1

→ Inverse Problem: Test case 1 (small container), 3 parameters per boundary

($Ra=2.1056 \times 10^3$)



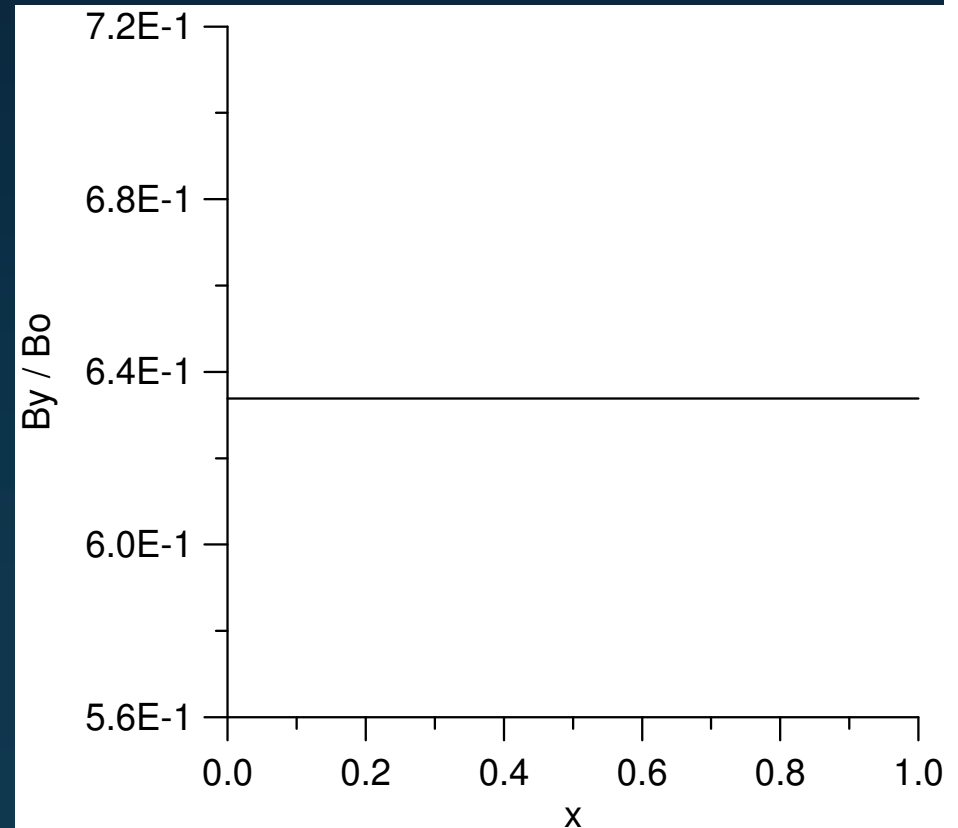
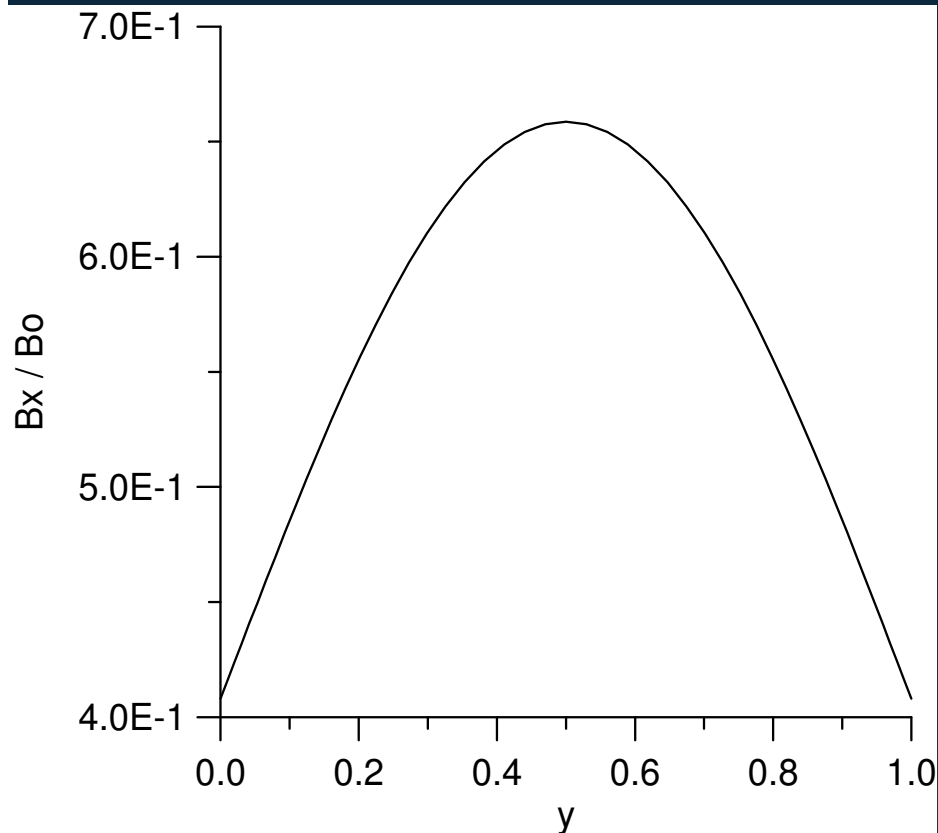
Without magnetic fields



With optimized magnetic fields

MHD – Example 1

- Inverse Problem: Test case 1 (small container), 3 parameters per boundary
- Optimized boundary conditions

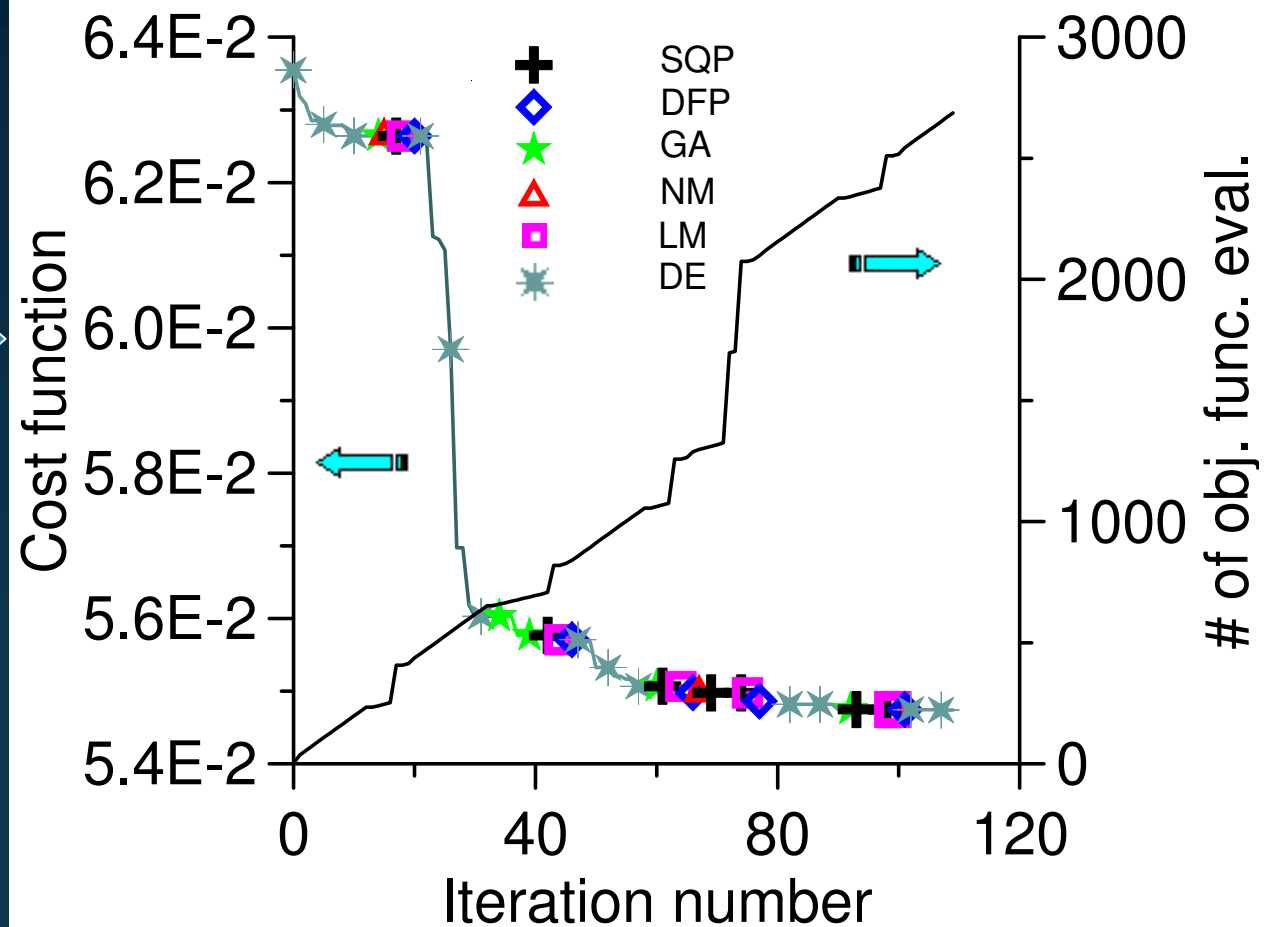


MHD – Example 1

→ Inverse Problem: Test case 1 (small container), 3 parameters per boundary

→ Convergence history

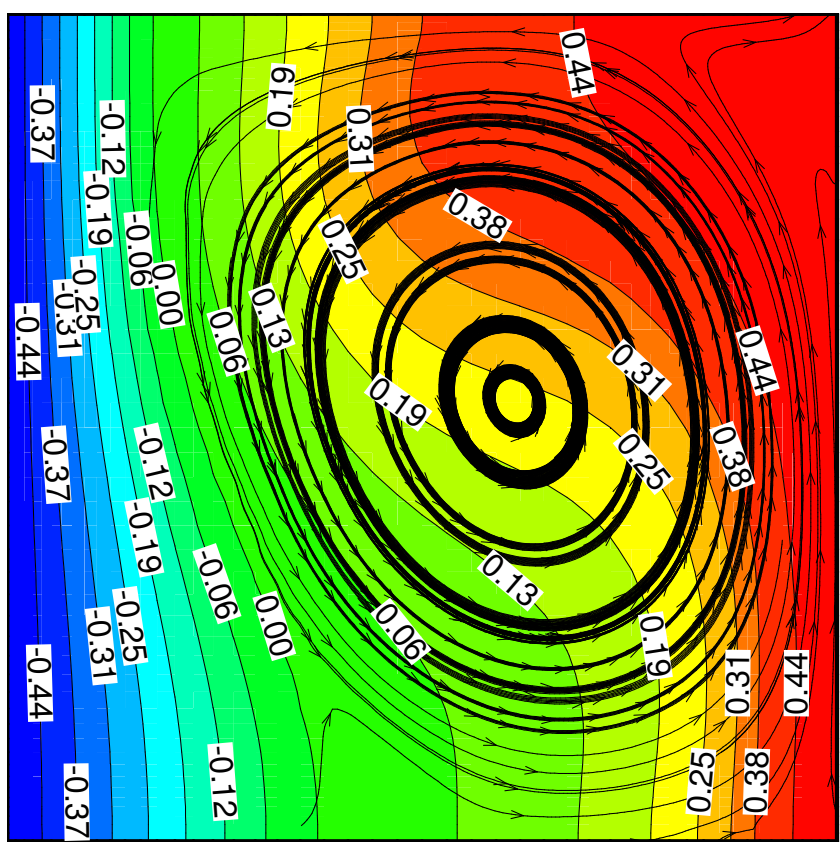
DE did almost all
the job



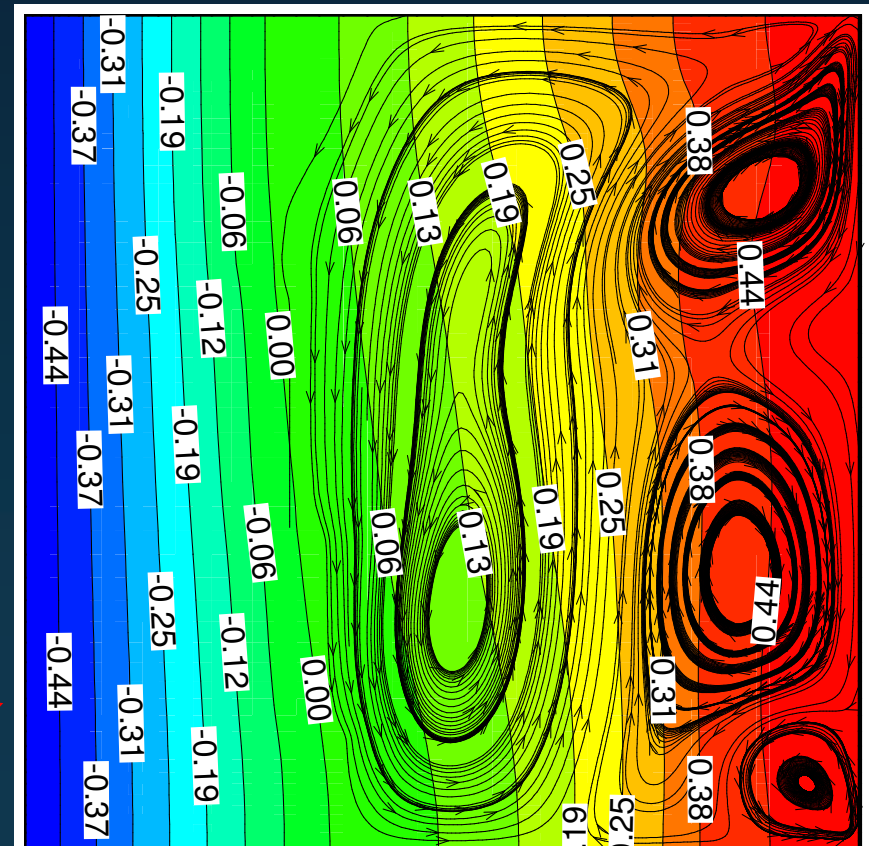
MHD – Example 1

→ **Inverse Problem:** Test case 2 (large container), 3 parameters per boundary

($Ra=1.6845 \times 10^4$)



Without magnetic fields

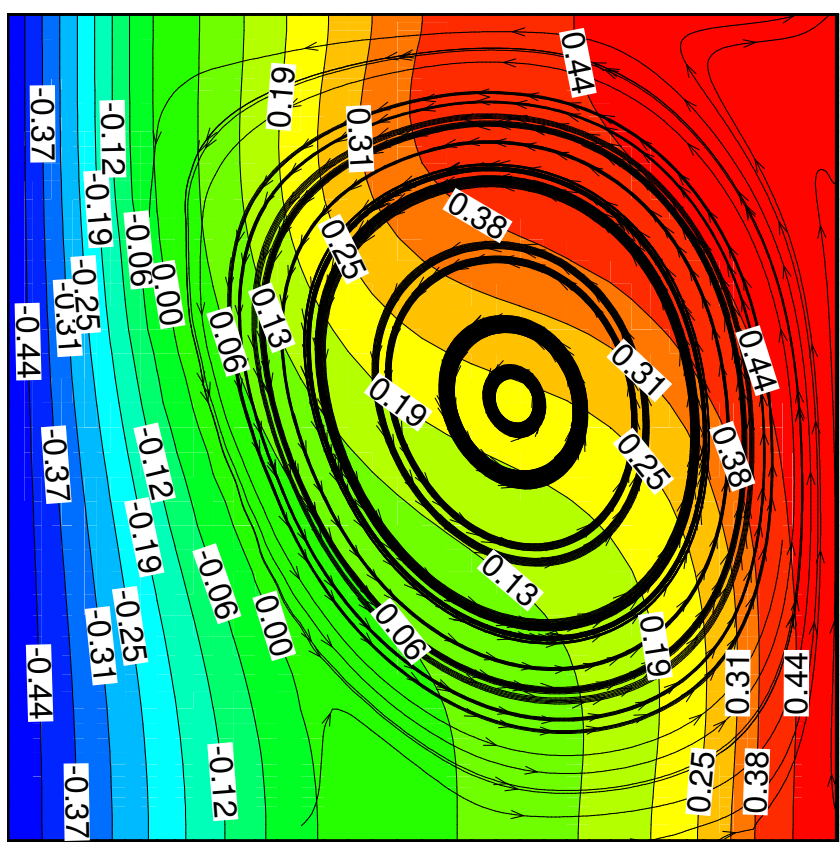


With optimized magnetic fields

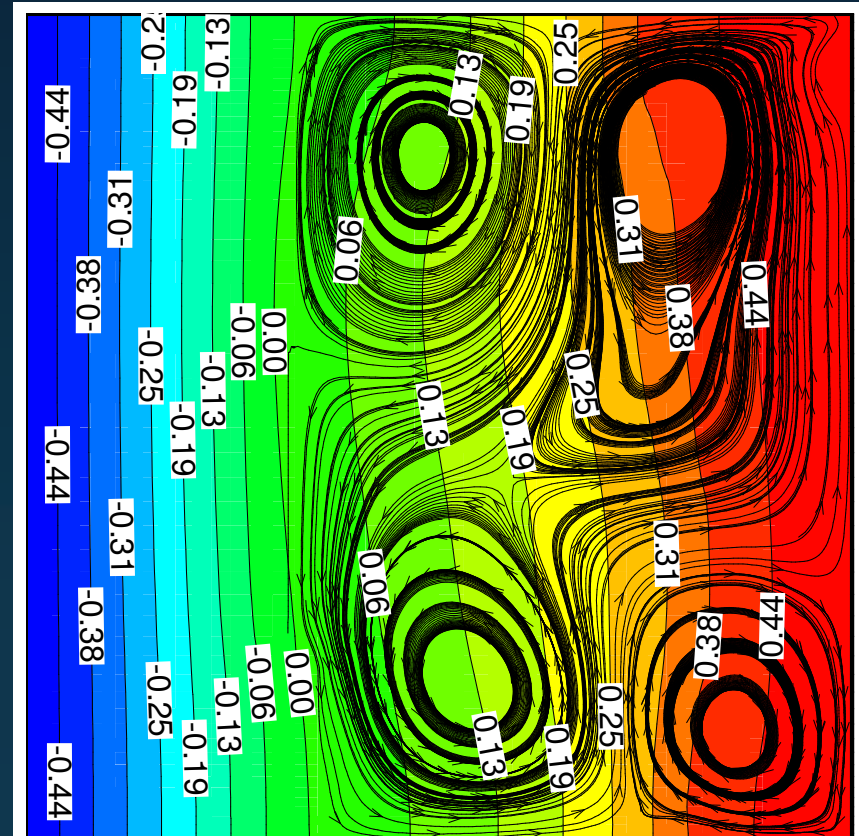
MHD – Example 1

→ **Inverse Problem:** Test case 2 (large container), 6 parameters per boundary

($Ra=1.6845 \times 10^4$)



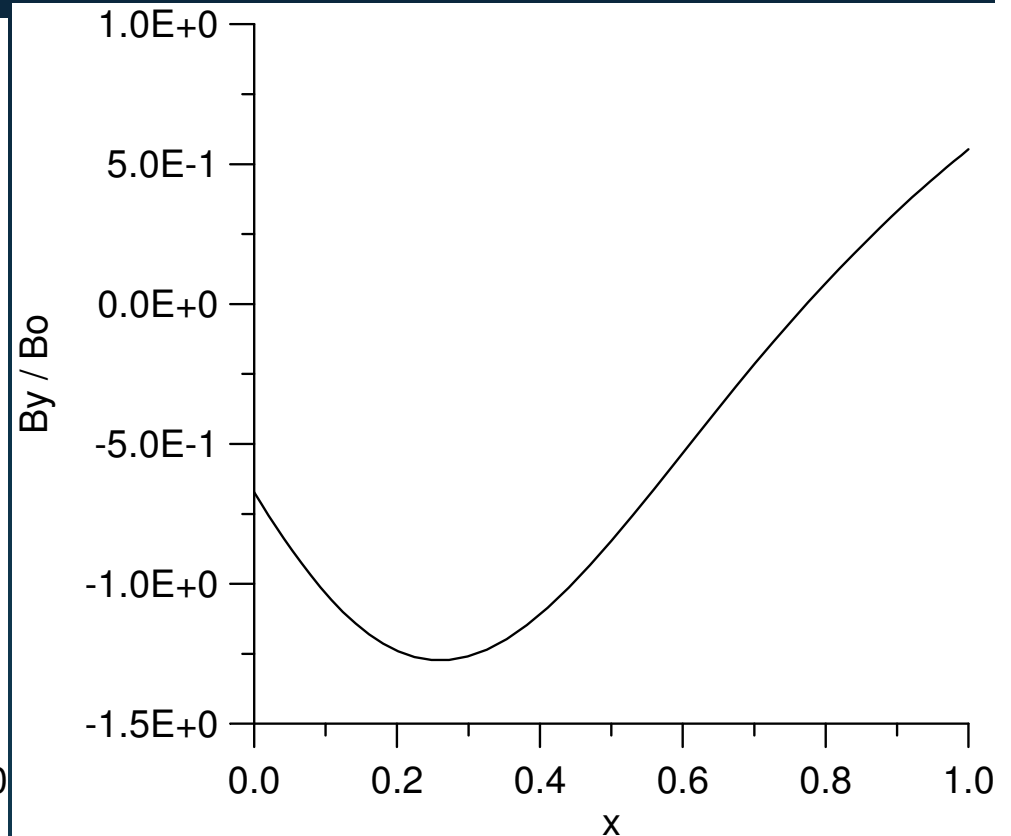
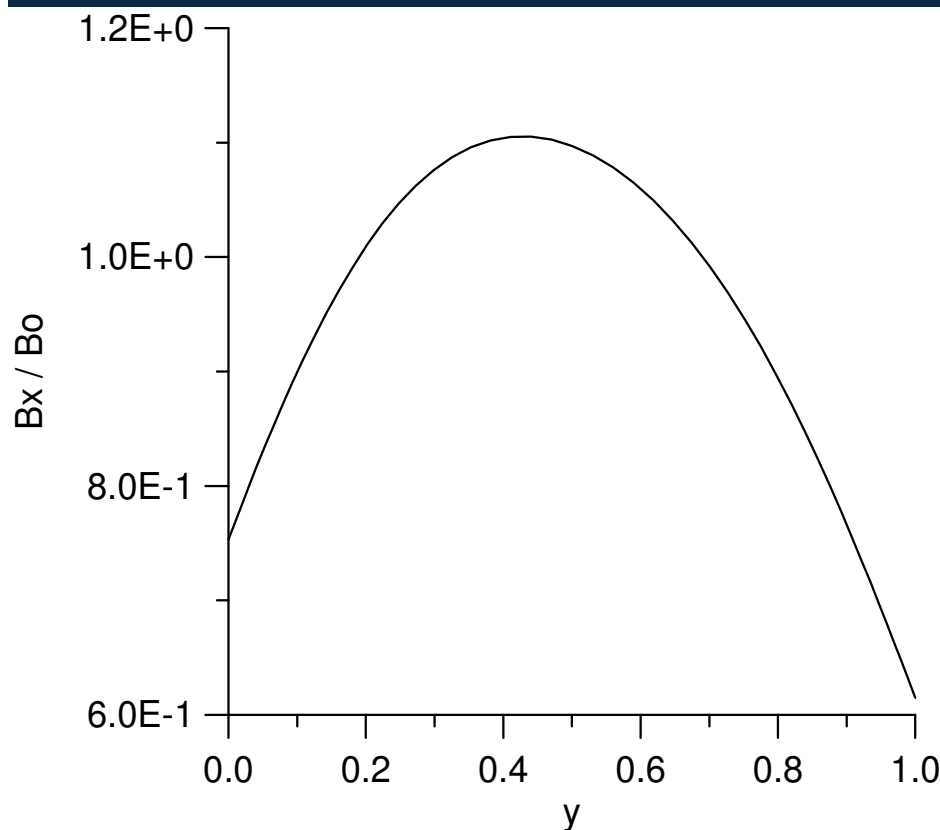
Without magnetic fields



With optimized magnetic fields

MHD – Example 1

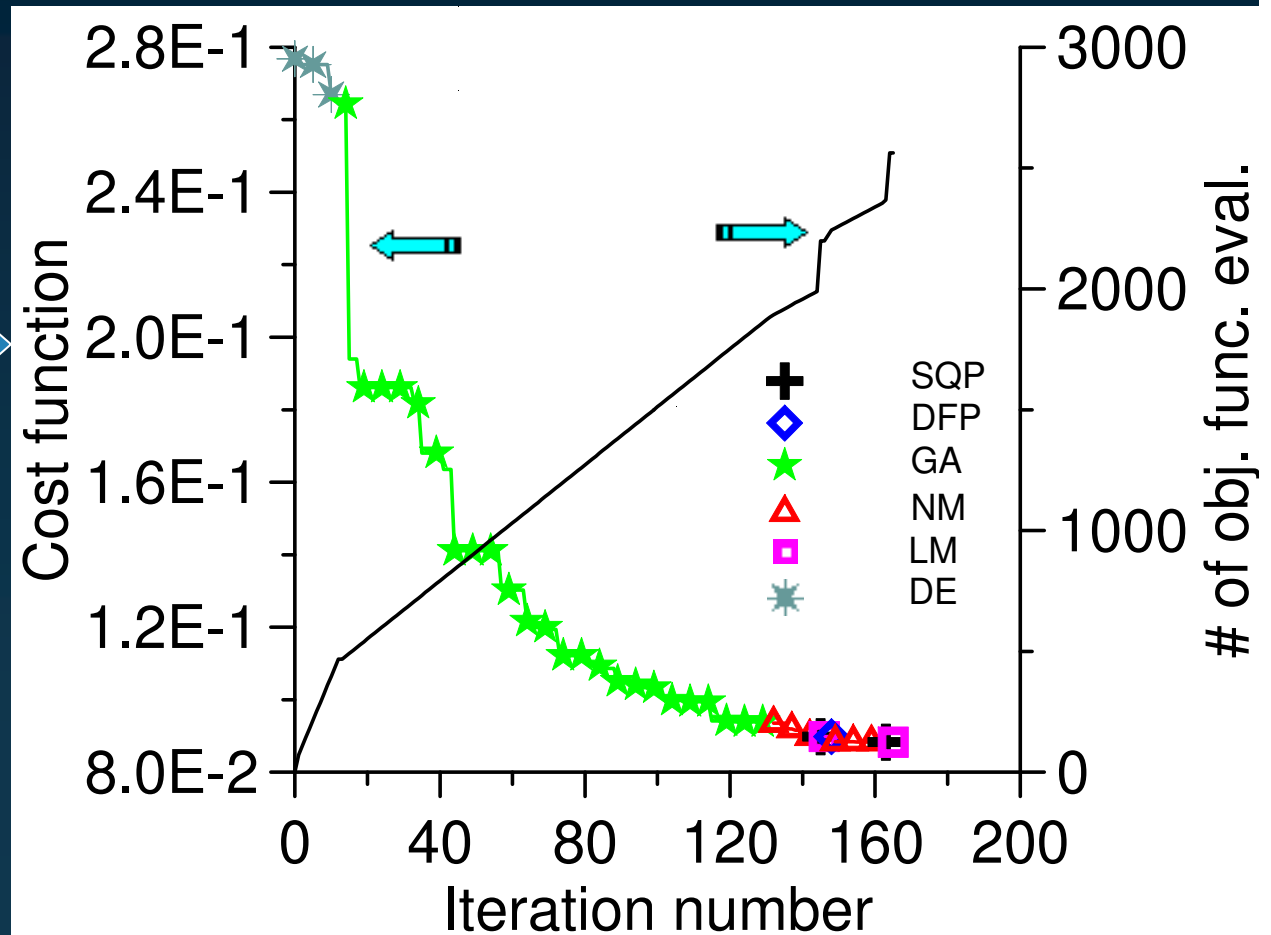
- Inverse Problem: Test case 2 (large container), 6 parameters per boundary
- Optimized boundary conditions



MHD – Example 1

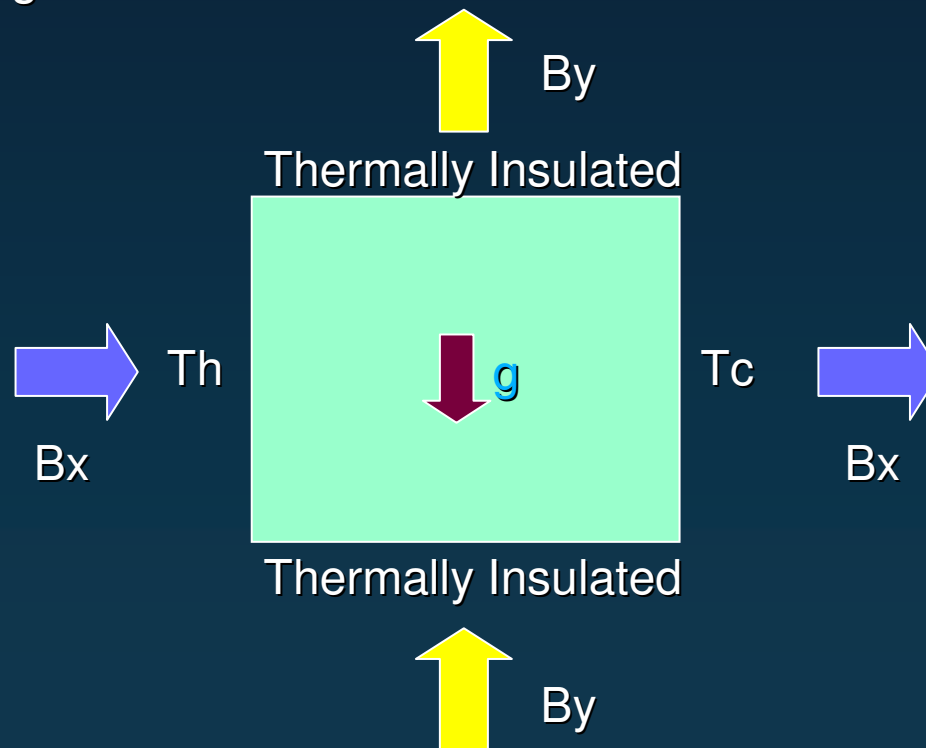
- Inverse Problem: Test case 2 (large container), 6 parameters per boundary
- Convergence history

GA did almost all
the job



MHD – Example 2

- **Optimization** of the magnetic boundary conditions in order to minimize the natural convection effects (*transient optimization*)
- Final time = 300 s
- Test problem:



MHD – Example 2

- Optimization Problem
- The boundary conditions are parameterized as B-Splines.
- NETLIB's subroutine GCVSPL, based on the cross-validation smoothing procedure, was used for the interpolation.
- Objective function:

$$F = \sqrt{\frac{1}{\#cells} \sum_{i=1}^{\#cells} \left(\frac{\partial T_i}{\partial y_i} \right)^2}$$

MHD – Example 2

→ Optimization Problem

→ Physical properties for silicon:

$$\begin{aligned}\rho_l &= 2550 \text{ kg m}^{-3} \\ k_l &= 64 \text{ W m}^{-1} \text{ K}^{-1} \\ C_{Pl} &= 1059 \text{ J kg}^{-1} \text{ K}^{-1} \\ \mu_l &= 0.0032634 \text{ kg m}^{-1} \text{ s}^{-1} \\ \sigma_l &= 12.3 \times 10^5 \text{ 1/m } \Omega \\ \beta &= 8.3 \times 10^{-4} \text{ K}^{-1} \\ \mu_m &= 1.2566 \times 10^{-5} \text{ T m A}^{-1}\end{aligned}$$

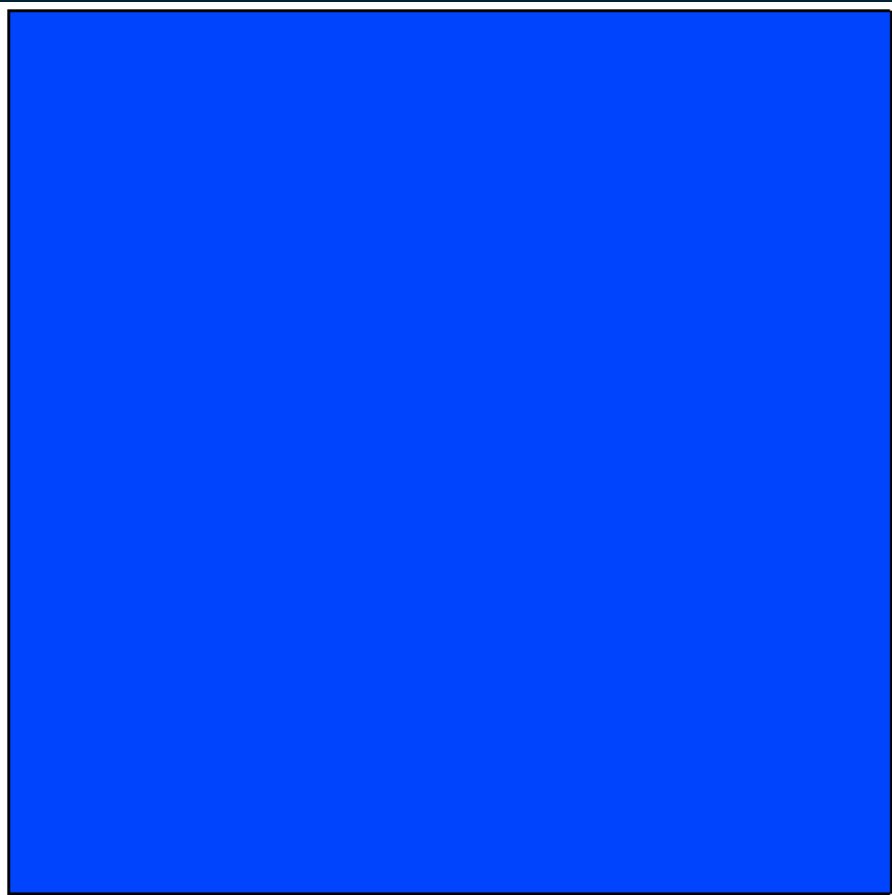
$$\begin{aligned}\rho_s &= 2330 \text{ kg m}^{-3} \\ k_s &= 22 \text{ W m}^{-1} \text{ K}^{-1} \\ C_{Ps} &= 1038 \text{ J kg}^{-1} \text{ K}^{-1} \\ \mu_s &= 1.0 \times 10^3 \text{ kg m}^{-1} \text{ s}^{-1} \\ \sigma_s &= 4.3 \times 10^4 \text{ 1/m } \Omega \\ g &= 9.81 \text{ m s}^{-2} \\ L &= 1.803 \times 10^6 \text{ J kg}^{-1} \\ \sigma_s &= 4.3 \times 10^4 \text{ 1/m } \Omega\end{aligned}$$

→ Test case without solidification → $H=0.15 \text{ m}$, $\Delta T=0.654351 \text{ K}$, $Ra=10^5$

→ Test case with solidification → $H=0.069624 \text{ m}$, $\Delta T=6.54351 \text{ K}$, $Ra=10^5$

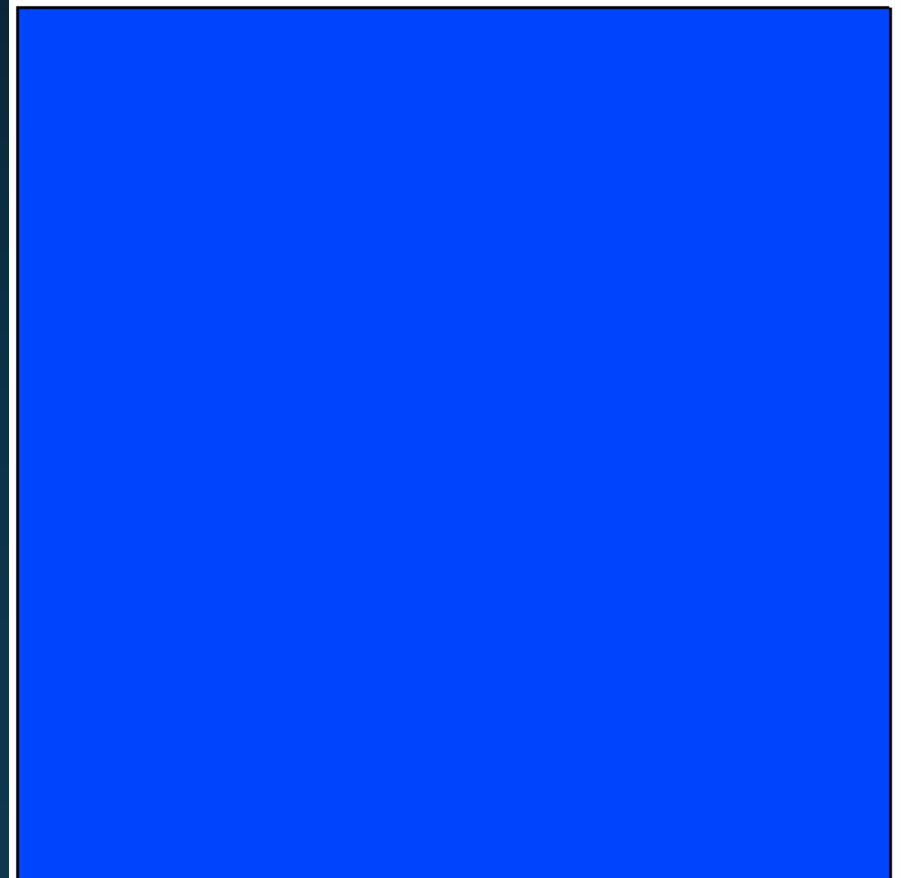
MHD – Example 2

→ Optimization Problem: Test case 1 (without solidification), 4 parameters per boundary



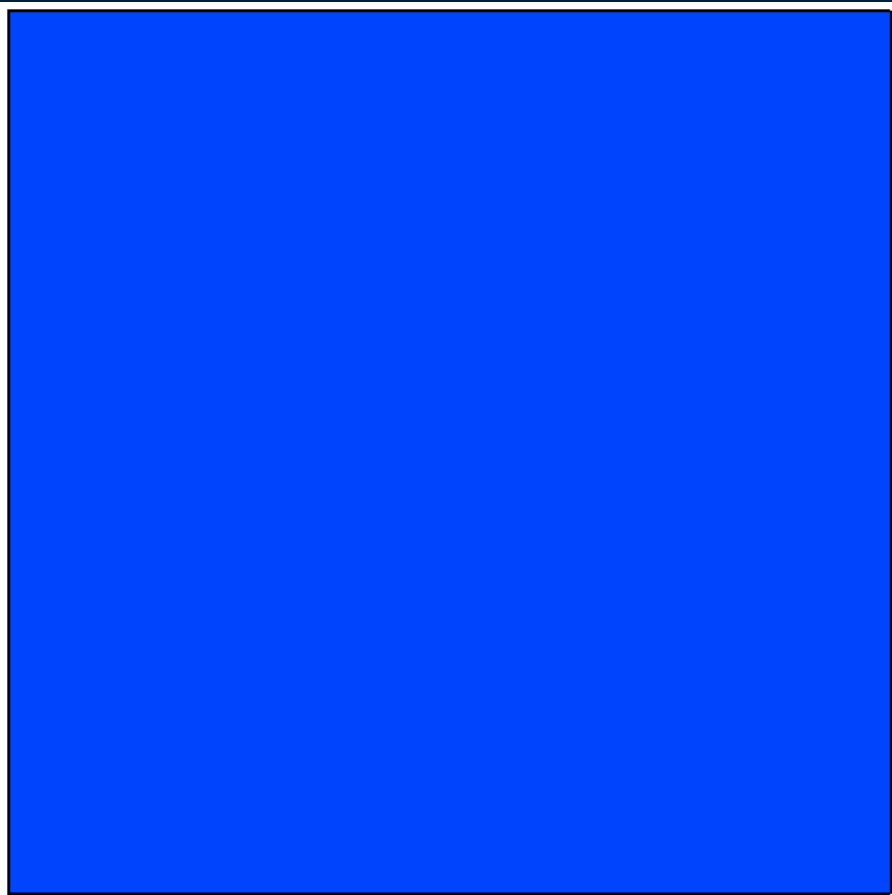
With optimized magnetic fields

Without magnetic fields

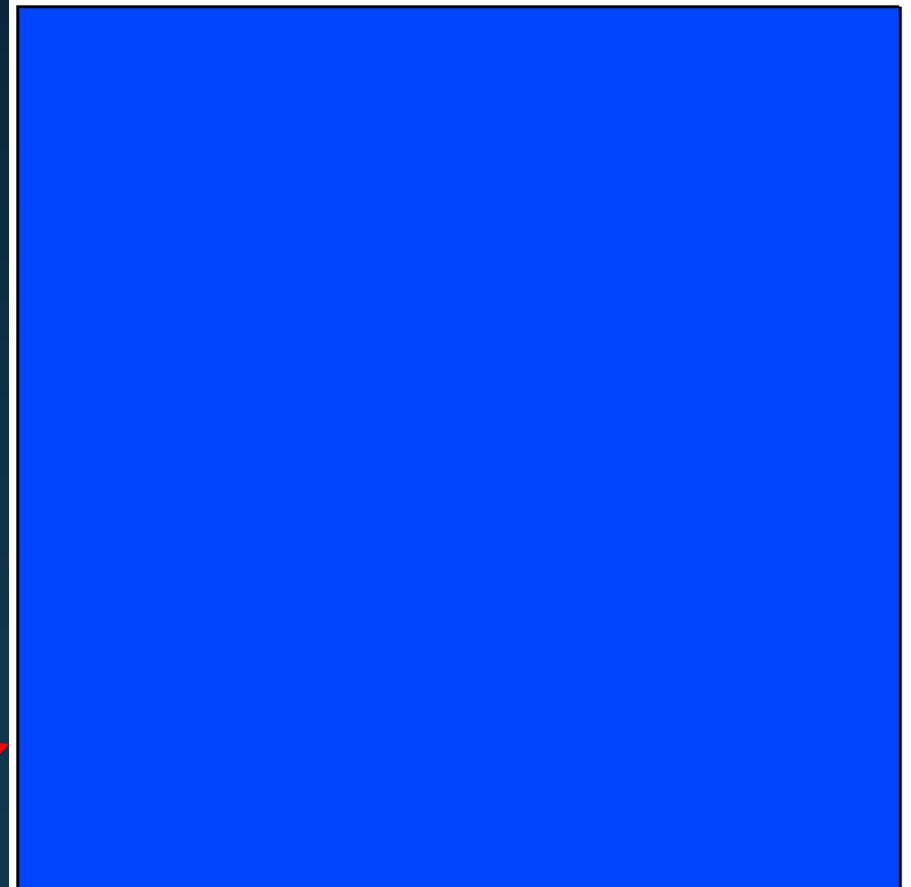


MHD – Example 2

→ Optimization Problem: Test case 1 (without solidification), 6 parameters per boundary



Without magnetic fields

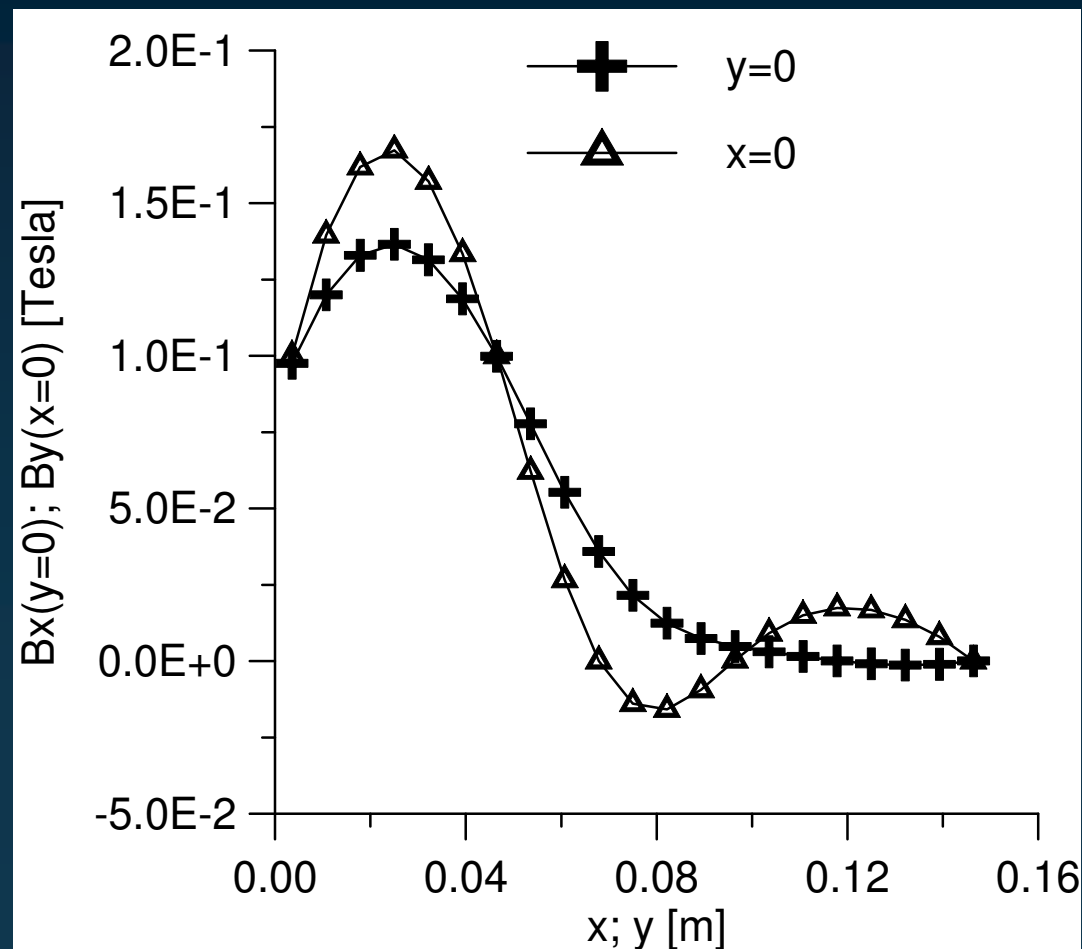


With optimized magnetic fields

MHD – Example 2

→ Optimization Problem: Test case 1 (without solidification), 6 parameters per boundary

Optimized boundary conditions

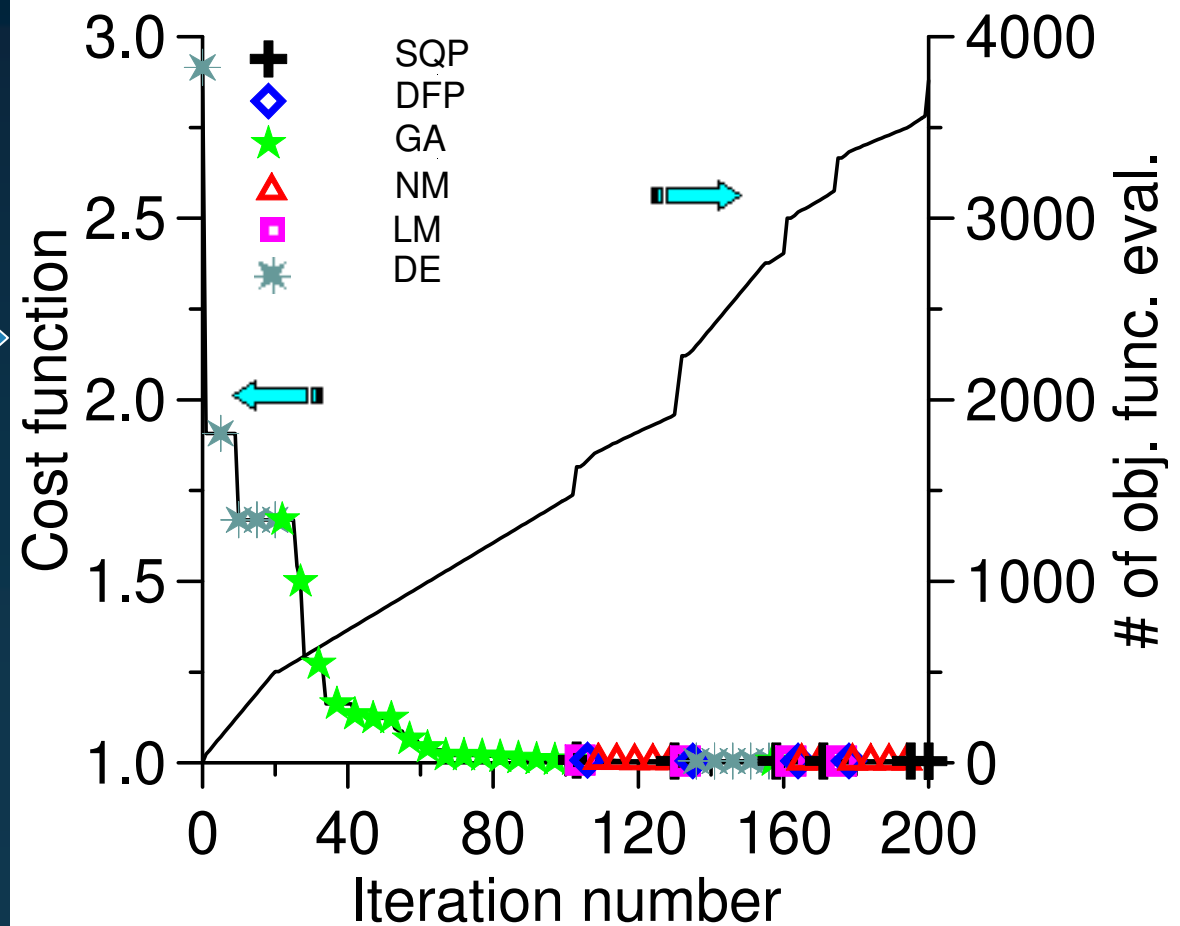


MHD – Example 2

→ Optimization Problem: Test case 1 (without solidification), 6 parameters per boundary

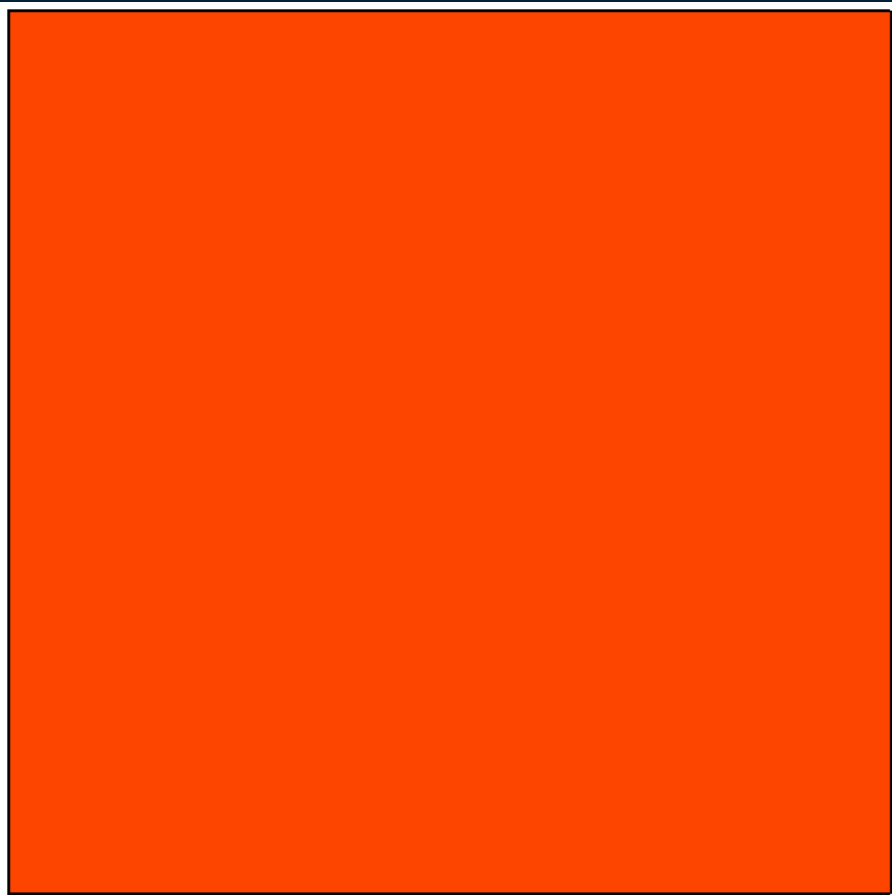
→ Convergence history

DE and GA did almost all the job



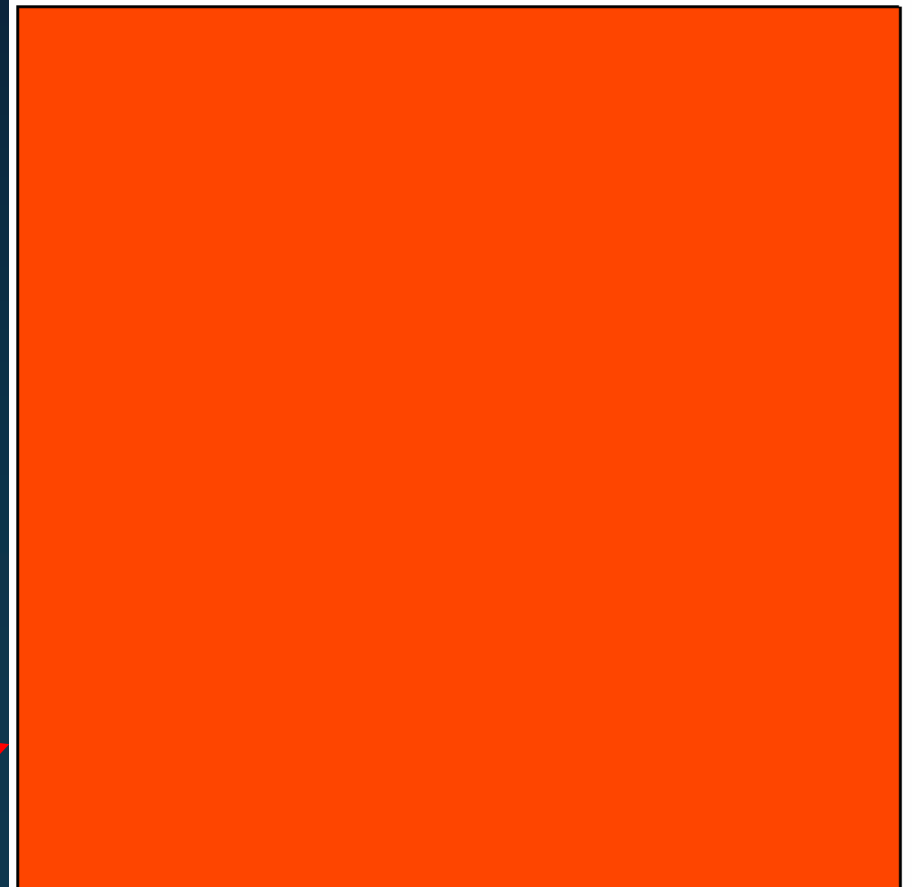
MHD – Example 2

→ Optimization Problem: Test case 2 (with solidification), 6 parameters per boundary



With optimized magnetic fields

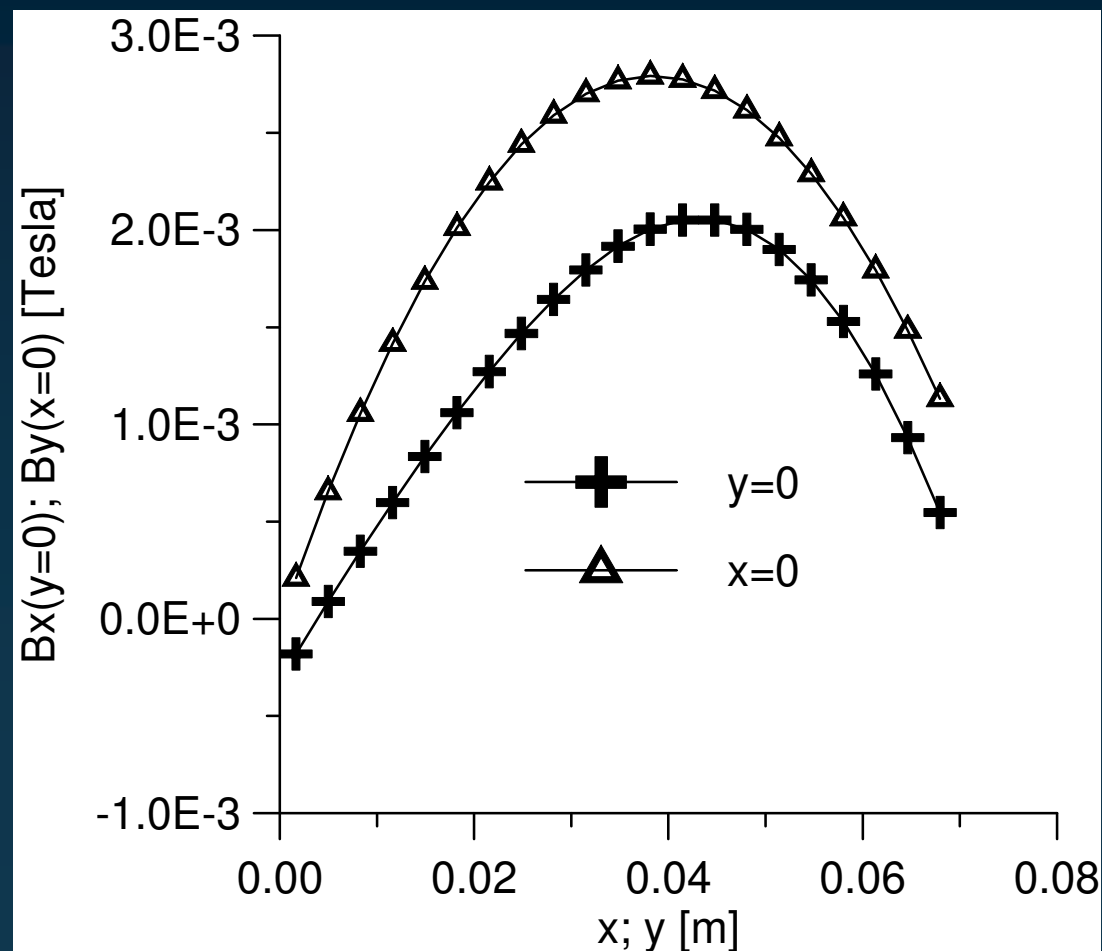
Without magnetic fields



MHD – Example 2

→ Optimization Problem: Test case 2 (with solidification), 6 parameters per boundary

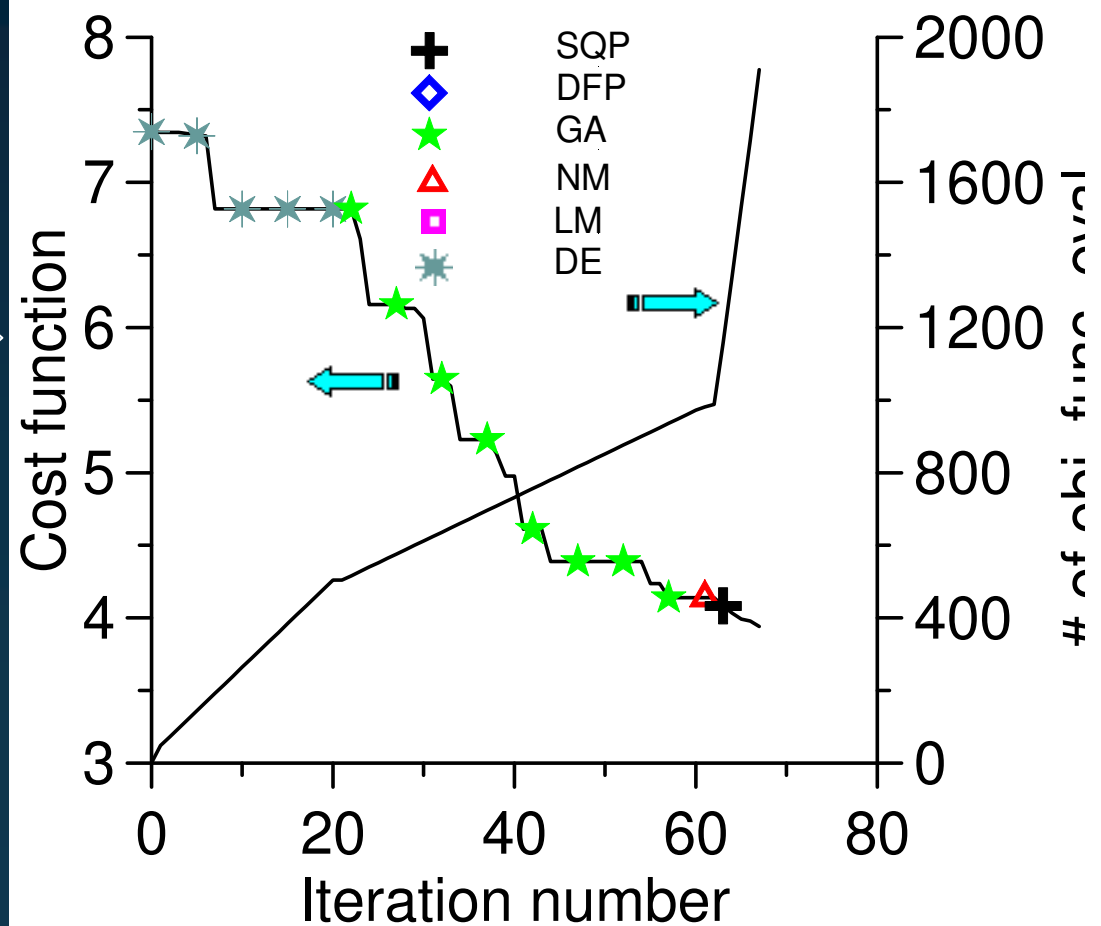
Optimized boundary conditions



MHD – Example 2

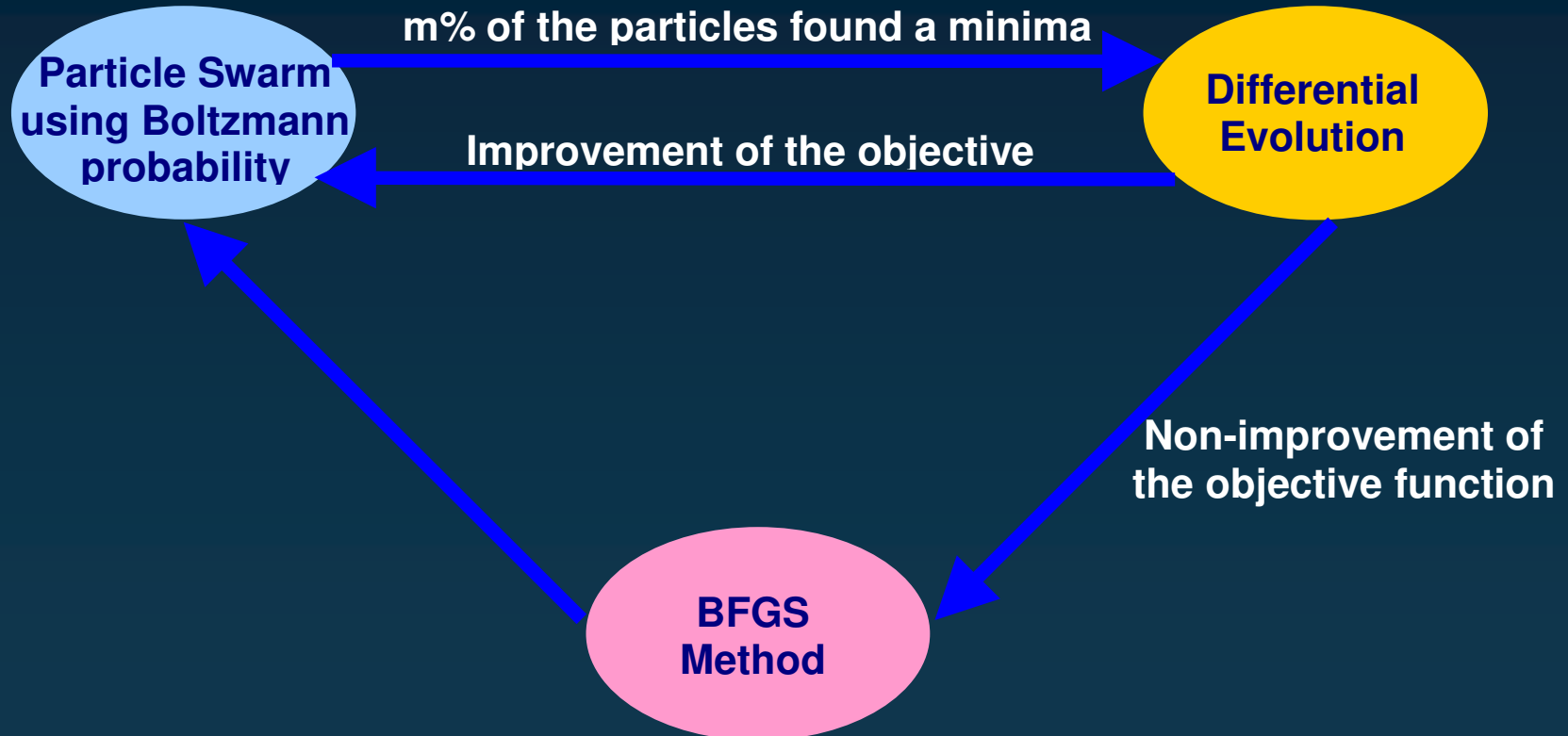
- Optimization Problem: Test case 2 (with solidification), 6 parameters per boundary
- Convergence history

DE and GA did almost all the job



Hybrid Methods

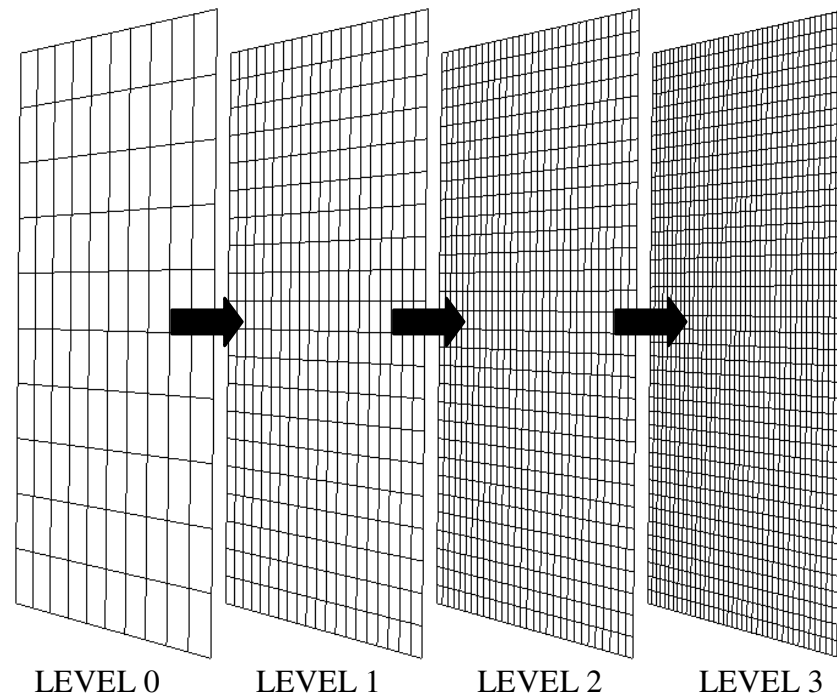
→ Hybrid optimizer – version 2 (Colaço and Dulikravich)



Hybrid Methods

→ Multilevel strategy

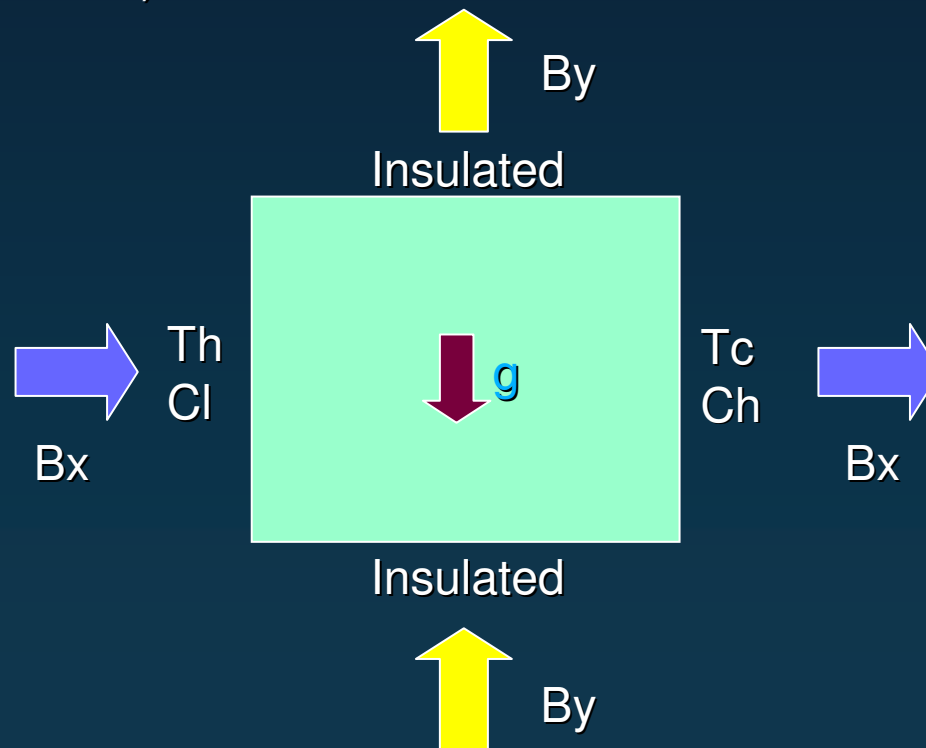
- Uses different grid sizes in order to speed-up the optimization task.



MHD – Example 3

- **Optimization** of the magnetic boundary conditions in order to minimize the natural convection effects in a fluid flow with a dispersed solute without solidification (multilevel optimization)

- Test problem:



MHD – Example 3

- Optimization Problem
- The boundary conditions are parameterized as B-Splines.
- NETLIB's subroutine GCVSPL, based on the cross-validation smoothing procedure, was used for the interpolation.
- Objective function:

$$F = \sqrt{\frac{1}{\#cells} \sum_{i=1}^{\#cells} \left(\frac{\partial C_i}{\partial y_i} \right)^2}$$

MHD – Example 3

→ Optimization Problem

→ Parameters for silicon:

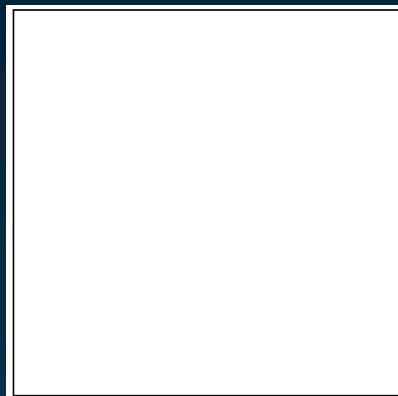
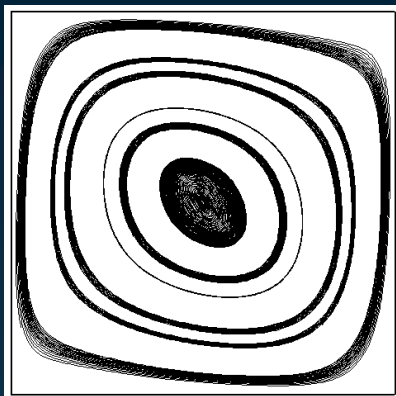
Grashoff number	Prandtl number
$Gr = \frac{g \beta \Delta T H^3}{\nu^2}$	$Pr = \frac{\nu}{\alpha}$
Solute Grashoff number	Schmidt number
$Gr_s = \frac{g \beta_s \Delta C H^3}{\nu^2}$	$Sc = \frac{\nu}{\alpha_s}$
Buoyancy ratio	Lewis number
$N = \frac{Gr_s}{Gr}$	$Le = \frac{\alpha_s}{\alpha}$

$$\begin{aligned}
 Gr &= 10^5 \\
 Pr &= 0.054 \\
 Le &= 2 \\
 Gr_s &= 5 \times 10^5 \\
 N &= 5.0 \\
 Sc &= 0.108
 \end{aligned}$$

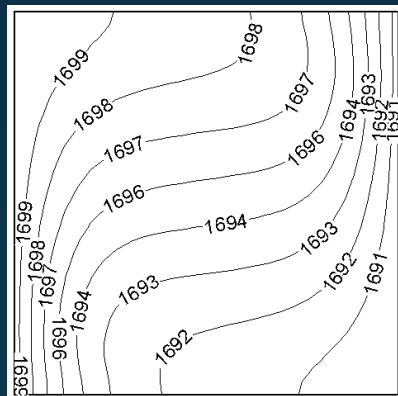
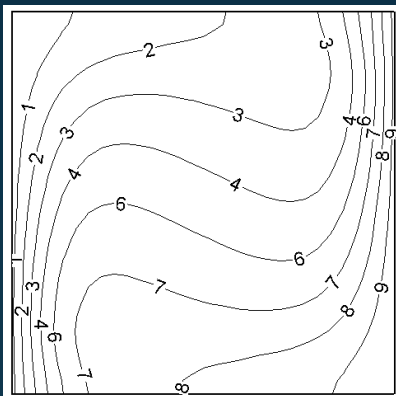
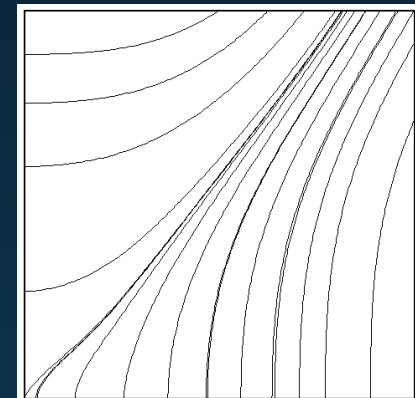
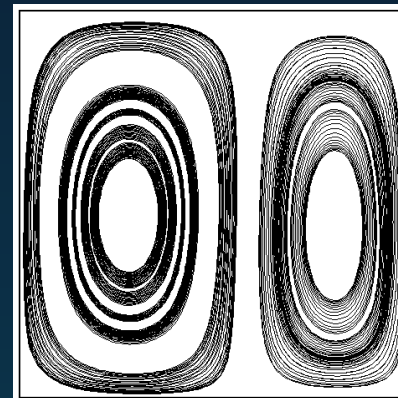
→ Test case without solidification → $H=23 \text{ m}, \Delta T=10 \text{ K}, \Delta T=10 \text{ kg / m}^3$

MHD – Example 3

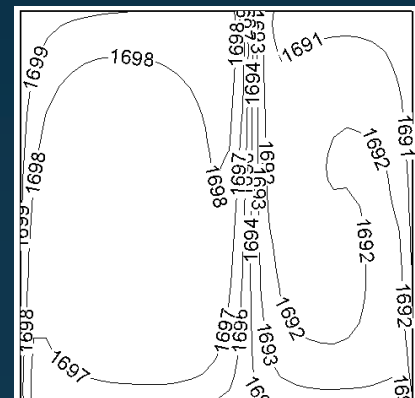
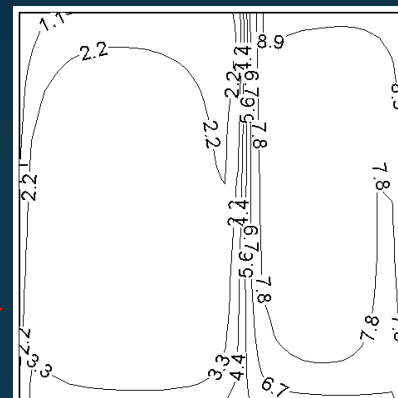
→ Optimization Problem: Test case 1 (single level optimization), 6 parameters/boundary



Without magnetic fields



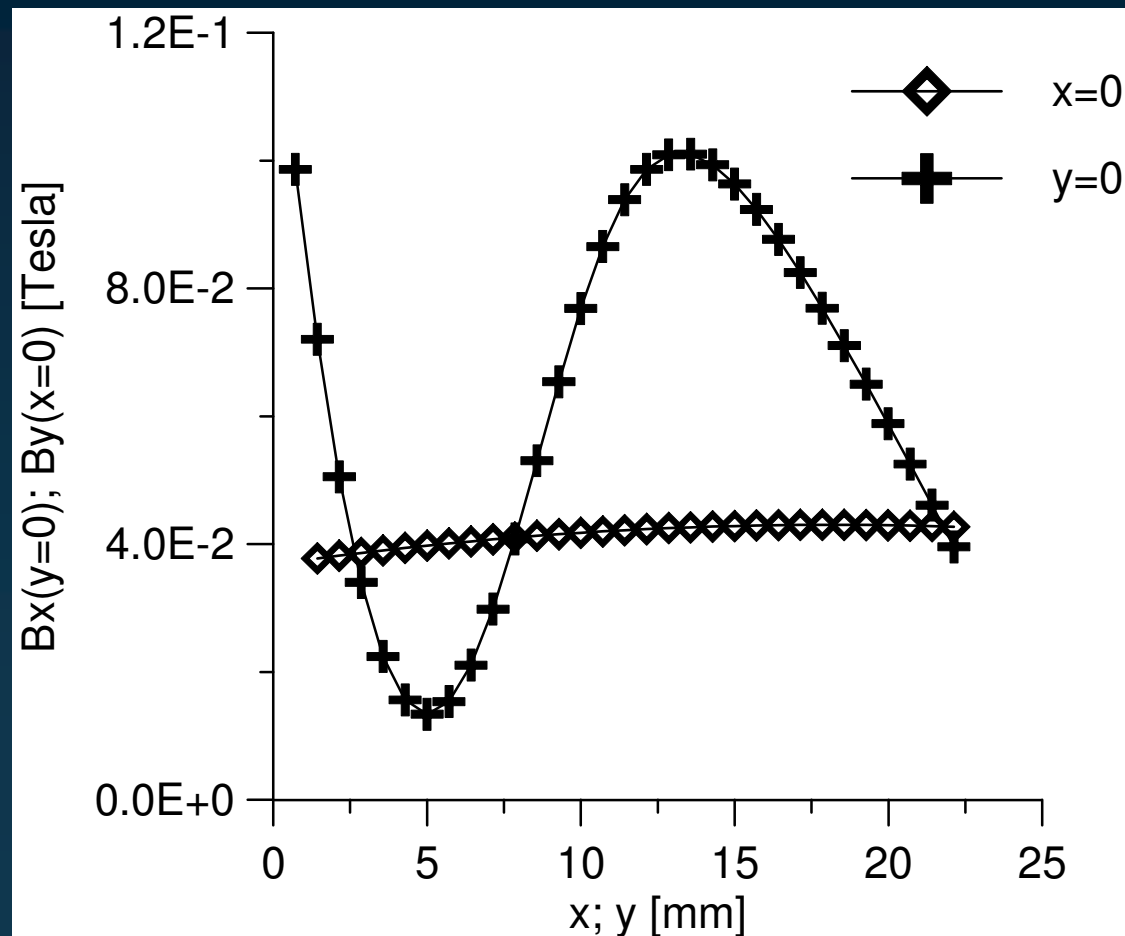
With optimized magnetic fields



MHD – Example 3

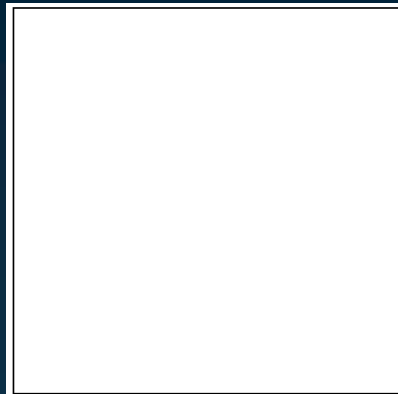
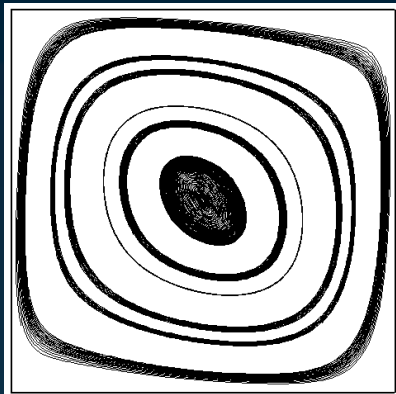
→ Optimization Problem: Test case 1 (single level optimization), 6 parameters/boundary

Optimized boundary conditions

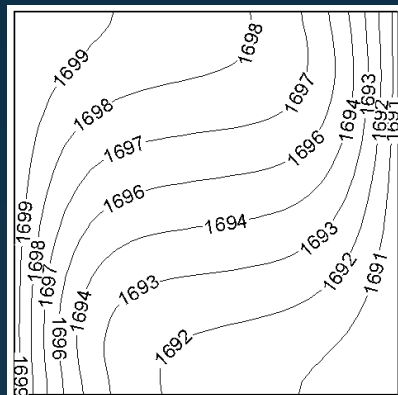
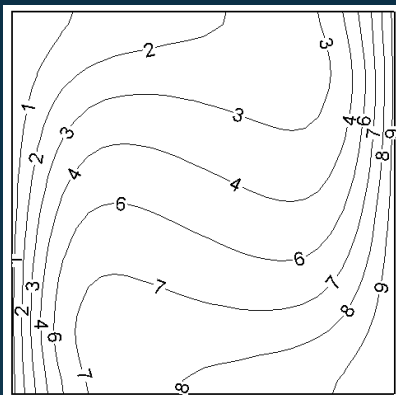
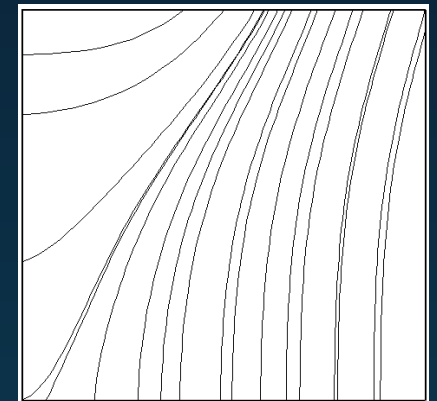
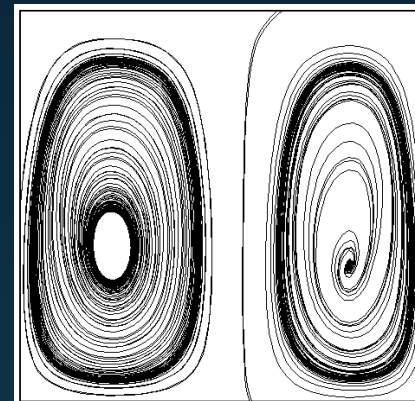


MHD – Example 3

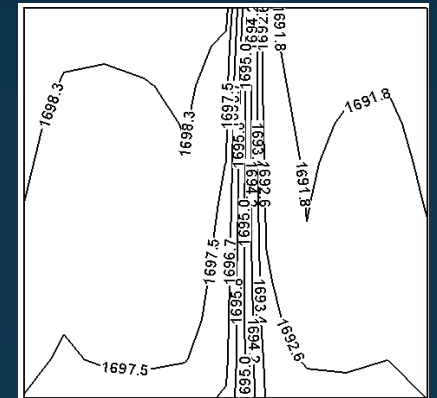
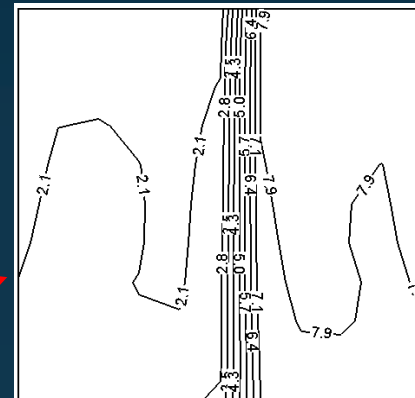
→ Optimization Problem: Test case 2 (multilevel optimization), 6 parameters/boundary



Without magnetic fields



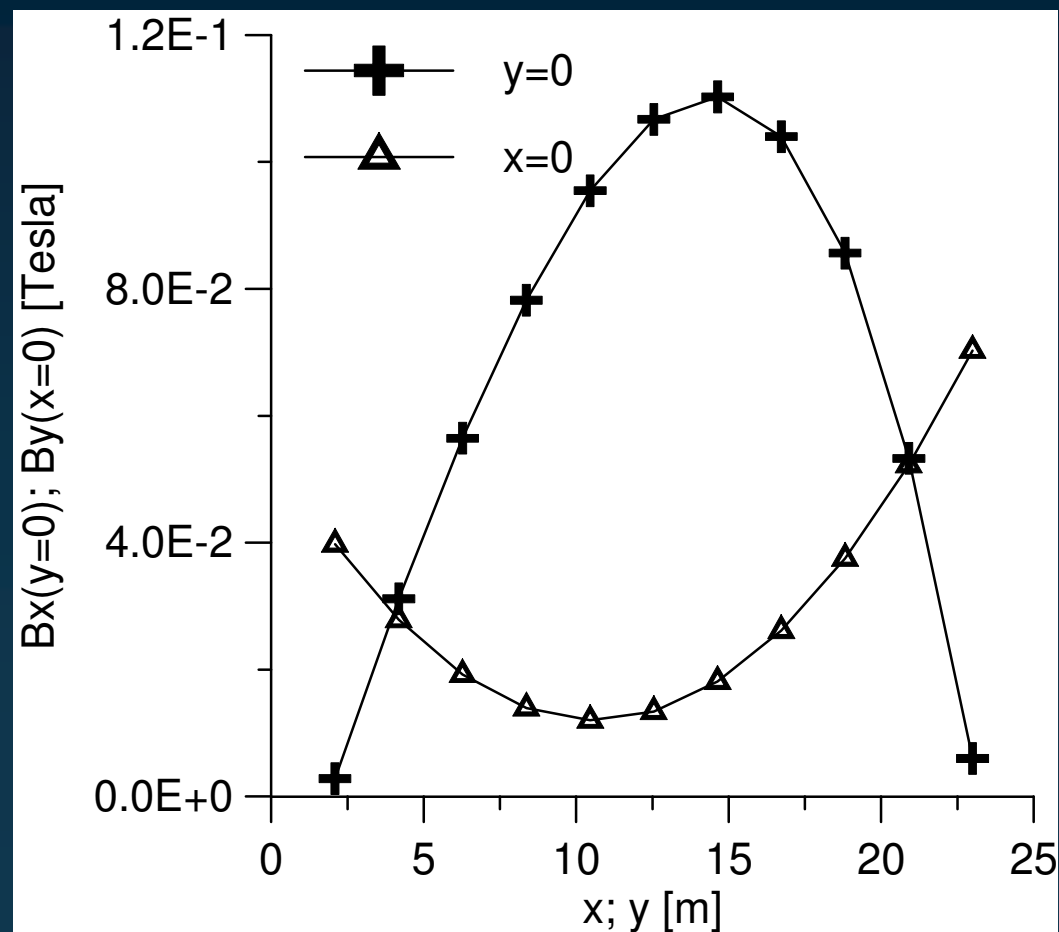
With optimized magnetic fields



MHD – Example 3

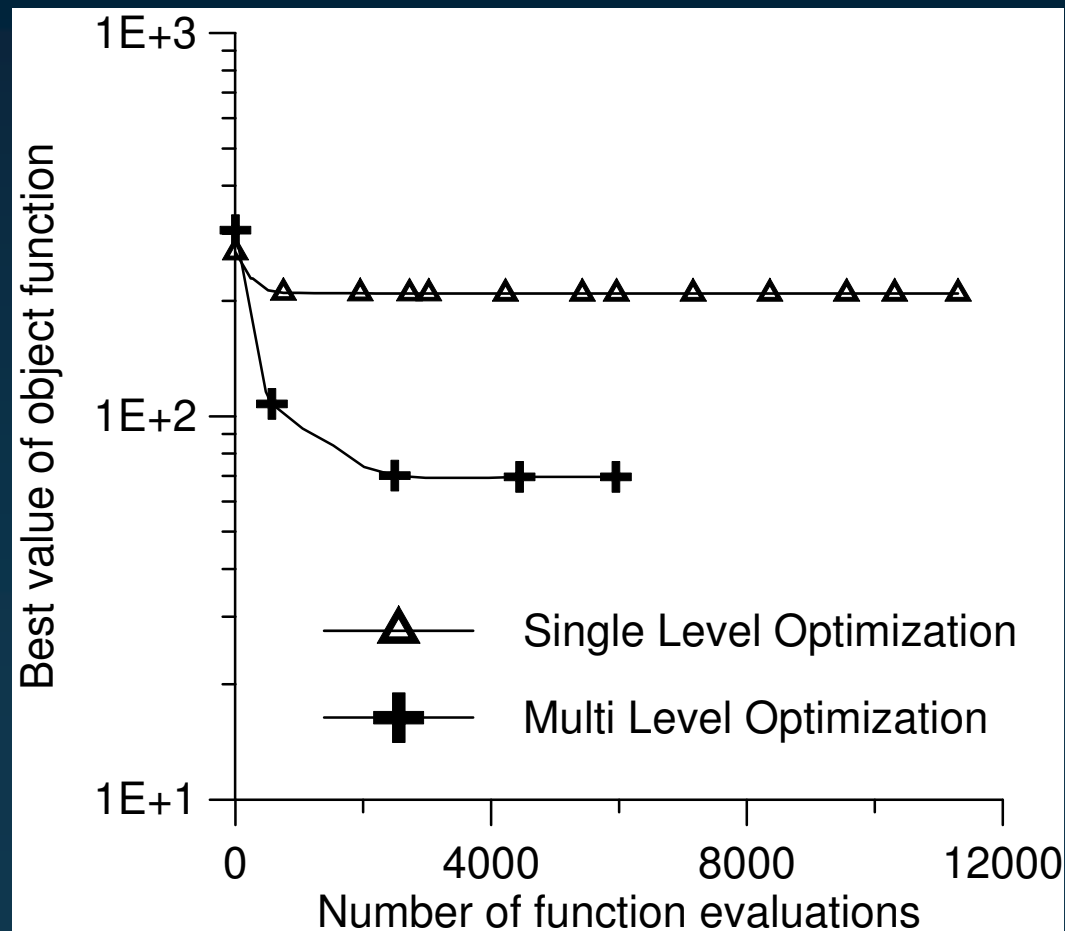
→ Optimization Problem: Test case 2 (multilevel optimization), 6 parameters/boundary

Optimized boundary conditions



MHD – Example 3

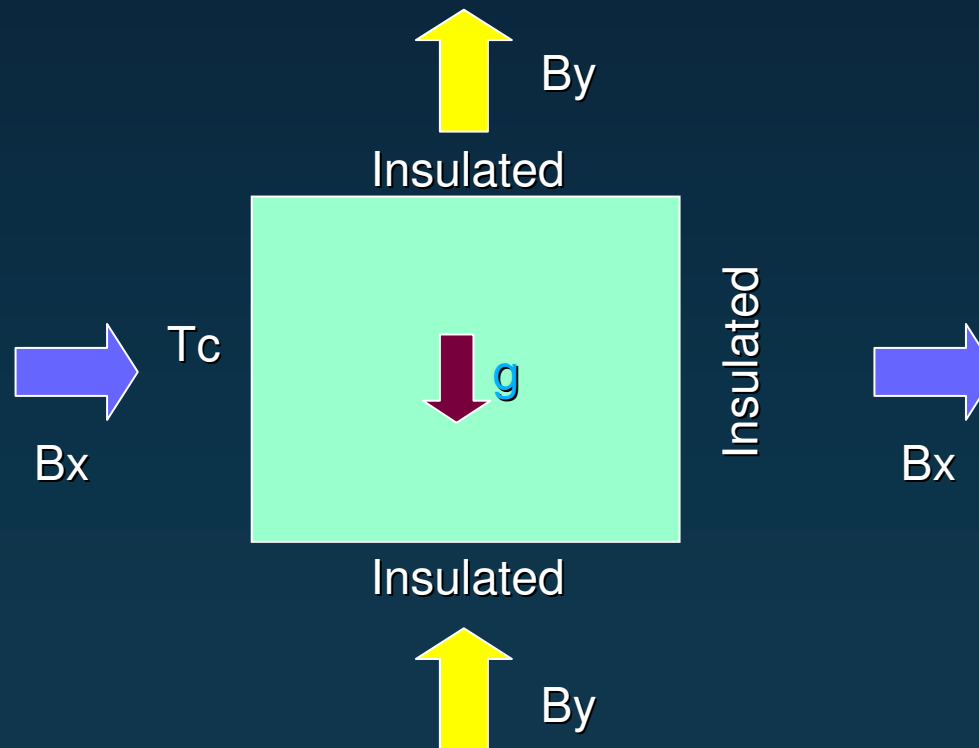
- Optimization Problem: Singlelevel versus Multilevel optimization
- Convergence history



MHD – Example 4

→ **Optimization** of the magnetic boundary conditions in order to minimize the natural convection effects in a fluid flow with a dispersed solute (**transient with phase change**)

→ Test problem:



MHD – Example 4

- Optimization Problem
- The boundary conditions are parameterized as B-Splines.
- NETLIB's subroutine GCVSPL, based on the cross-validation smoothing procedure, was used for the interpolation.
- Objective function:

$$F = \sqrt{\frac{1}{\#cells} \sum_{i=1}^{\#cells} \left(\frac{\partial C_i}{\partial y_i} \right)^2}$$

MHD – Example 4

→ Optimization Problem

→ Parameters for silicon:

$$\rho_l = 2550 \text{ kg m}^{-3}$$

$$C_{Pl} = 1059 \text{ J kg}^{-1} \text{ K}^{-1}$$

$$\sigma_l = 12.3 \times 10^5 \text{ 1/m } \Omega$$

$$D_l = 6.043 \times 10^{-9} \text{ kg m}^{-1} \text{ s}^{-1}$$

$$L = 1.8 \times 10^6 \text{ J/kg}$$

$$\rho_s = 2550 \text{ kg m}^{-3}$$

$$C_{Ps} = 1059 \text{ J kg}^{-1} \text{ K}^{-1}$$

$$\sigma_s = 4.3 \times 10^4 \text{ 1/m } \Omega$$

$$D_s = 0 \text{ kg m}^{-1} \text{ s}^{-1}$$

$$T_o = 1685.04 \text{ K}$$

$$k_l = 64 \text{ W m}^{-1} \text{ K}^{-1}$$

$$\mu_l = 0.0032634 \text{ kg m}^{-1} \text{ s}^{-1}$$

$$\beta = 1.4 \times 10^{-4} \text{ K}^{-1}$$

$$g = 9.81 \text{ m s}^{-2}$$

$$T_c = 1624.96 \text{ K}$$

$$k_s = 64 \text{ W m}^{-1} \text{ K}^{-1}$$

$$\mu_s = 326.34 \text{ kg m}^{-1} \text{ s}^{-1}$$

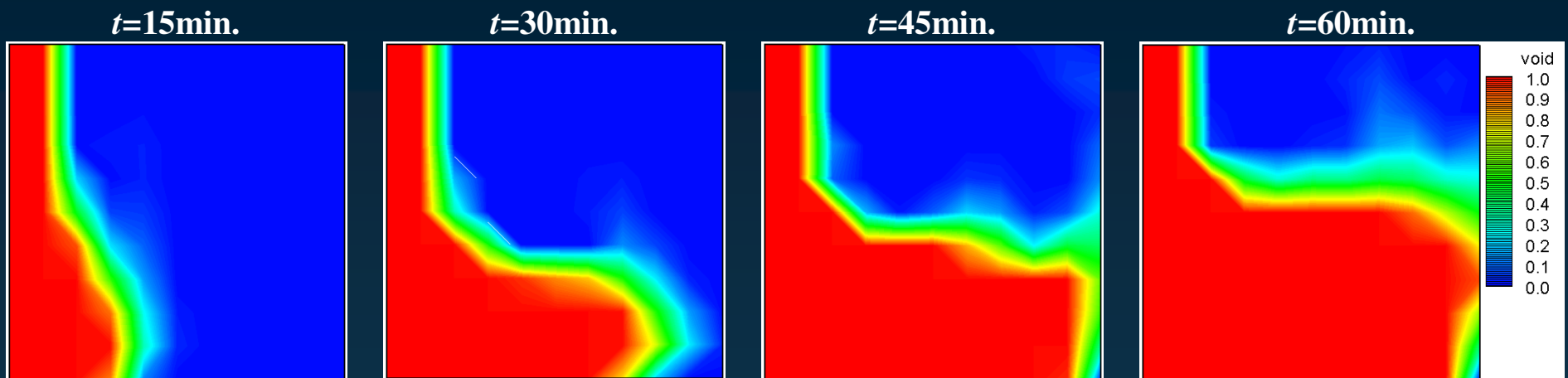
$$\beta_s = 0.0875$$

$$\mu_m = 1.2566 \times 10^{-5} \text{ T m A}^{-1}$$

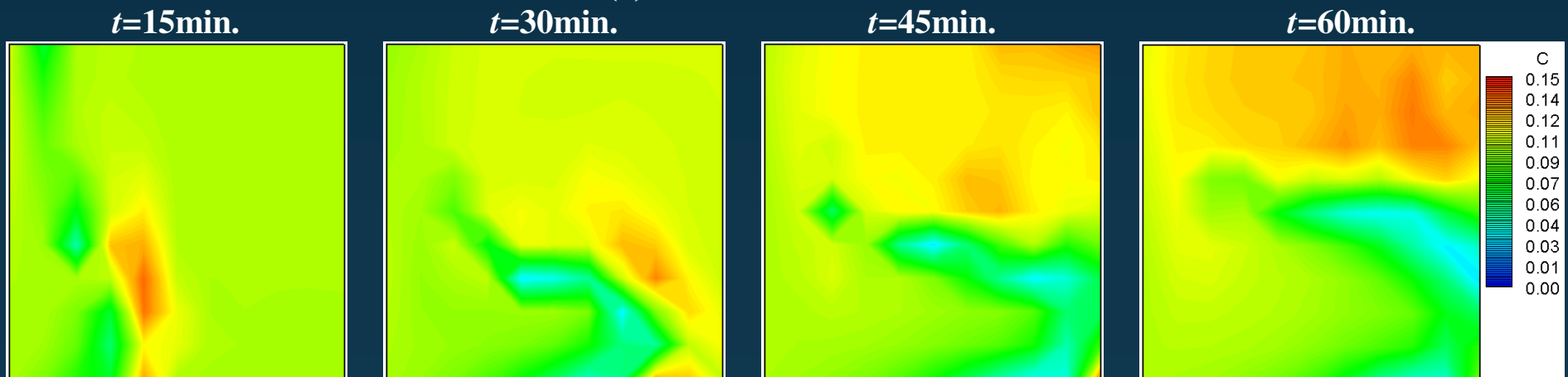
$$Co = 0.1 \text{ kg m}^{-3}$$

MHD – Example 4

→ Without Magnetic Fields



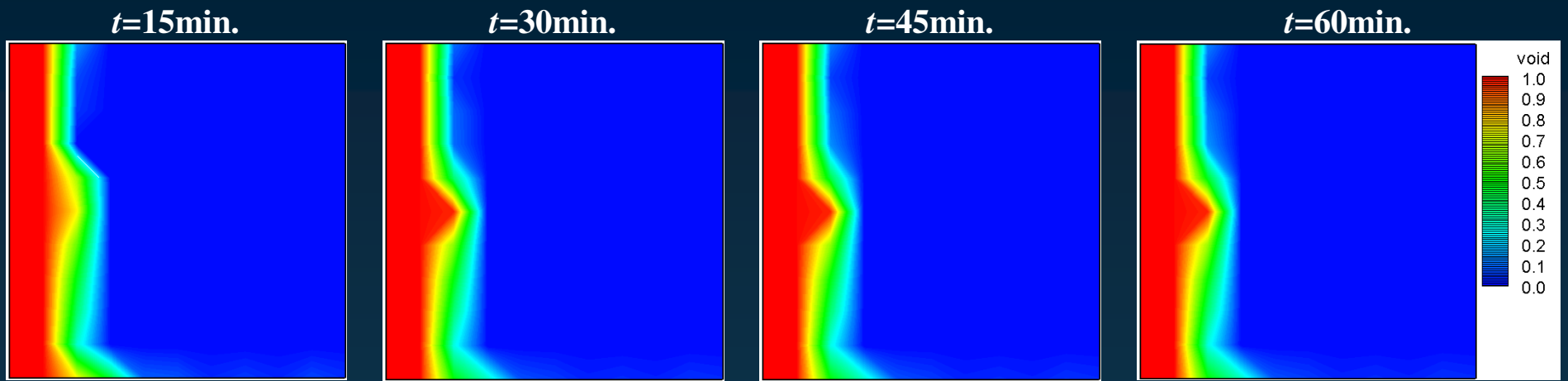
(a) iso-void fraction lines



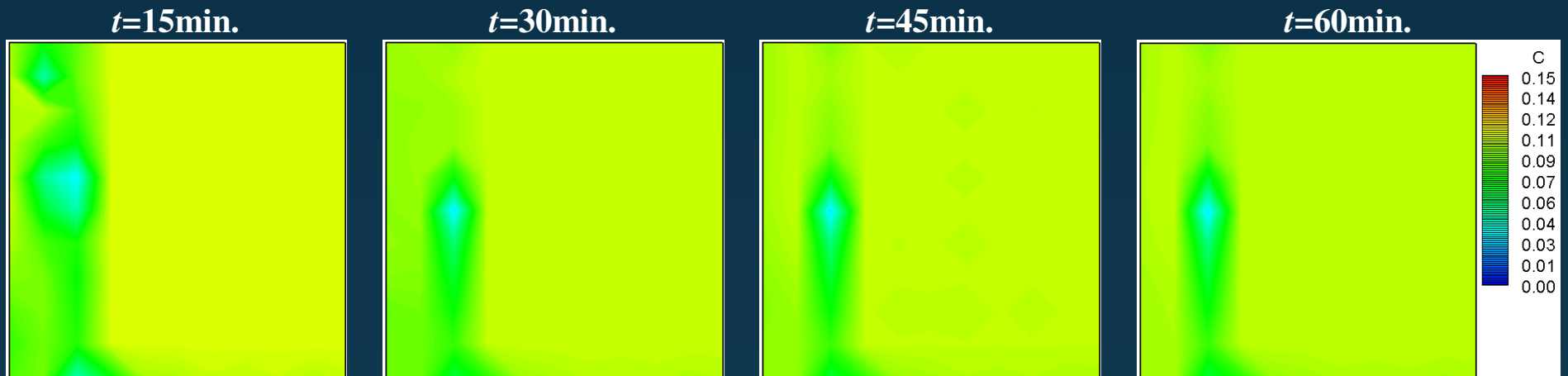
(b) iso-concentration lines

MHD – Example 4

→ With Optimized Magnetic Fields



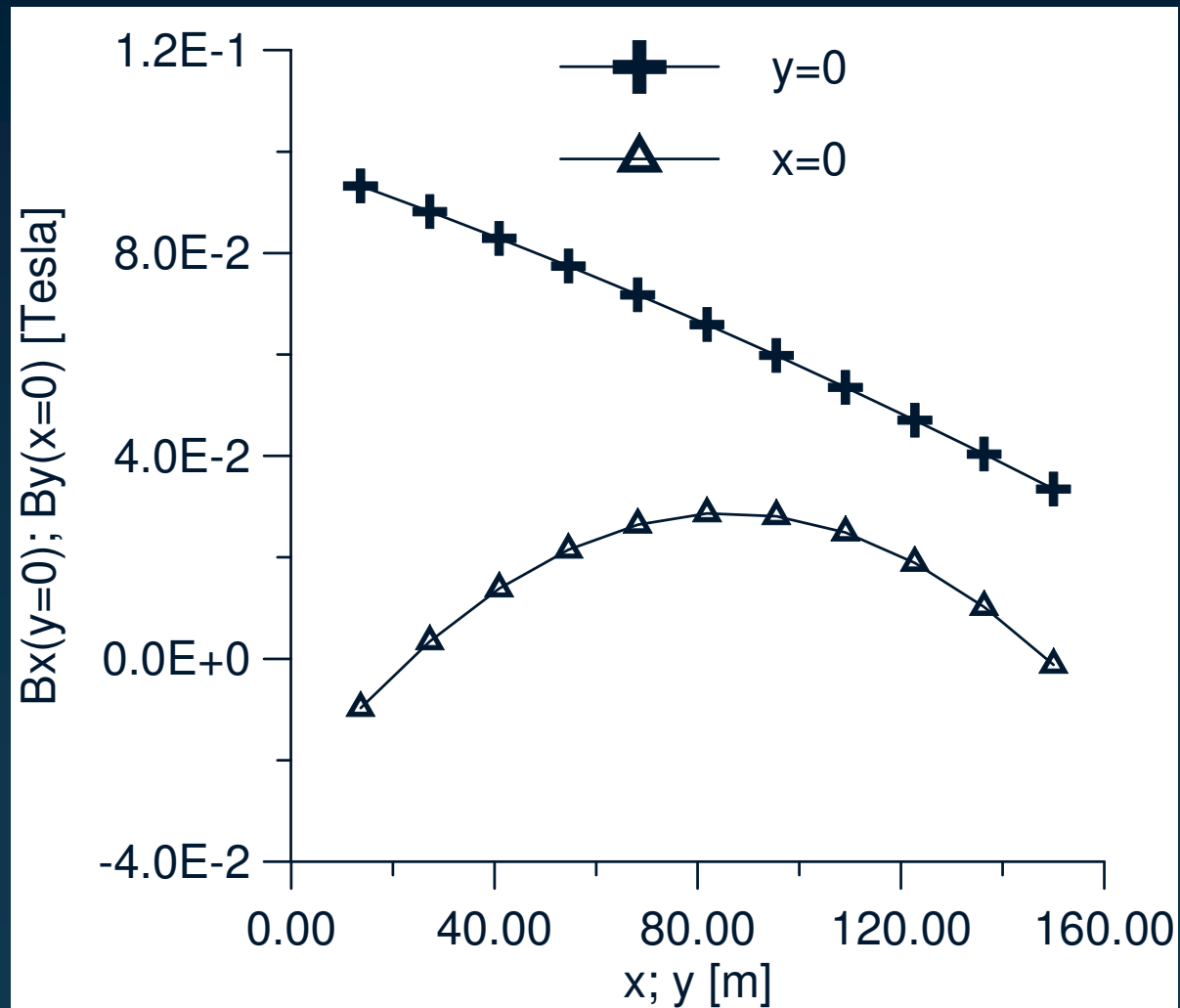
(a) iso-void fraction lines



(b) iso-concentration lines

MHD – Example 4

→ Optimized boundary conditions

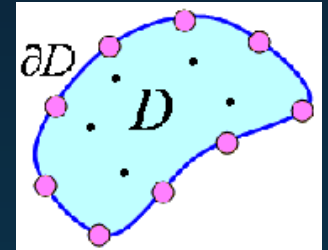


Radial Basis Function

- Can be classified as a “meshless method”.
- Can be used to generate an interpolation function or solve Partial Differential Equations.
- Original references:
 - Hardy, R.L., 1971, “Multiquadric Equations of Topography and Other Irregular Surfaces”, Journal of Geophysics Res., Vol. 176, pp. 1905-1915.
 - Kansa, E.J., 1990, “Multiquadrics – A Scattered Data Approximation Scheme with Applications to Computational Fluid Dynamics – II: Solutions to Parabolic, Hyperbolic and Elliptic Partial Differential Equations”, Comput. Math. Applic., Vol. 19, pp. 149-161.

Basic Theory

- Kansa's method (or asymmetric collocation) starts by building an approximation to the field of interest from the superposition of radial basis functions conveniently placed at points in the domain (and/or at the boundary).



- The unknowns (which are the coefficients of each RBF) are obtained from the (approximate) enforcement of the boundary conditions as well as the governing equations by means of collocation. Usually, this approximation only considers regular radial basis functions.

Basic Theory

→ The general equation for the RBF has the following form

$$s(x_i) = f(x_i) = \sum_{j=1}^N \alpha_j \phi(\|x_i - x_j\|) + \sum_{k=1}^M \beta_k p_k(x_i) + \beta_0$$

→ where $f(x_i)$ is known for a series of points x_i and $p_k(x_i)$ is one of the M terms of a given basis of polynomials. This approximation is solved for the α_j unknowns from the system of N linear equations, subject to the conditions (for the sake of uniqueness)

$$\sum_{j=1}^N \alpha_j p_k(x_j) = 0$$

$$\sum_{j=1}^N \alpha_j = 0$$

Basic Theory

→ Choices for the basis function

- Globally supported

- Multiquadrics

$$\phi(|x - x_j|) = \sqrt{(x - x_j)^2 + c_j^2}$$

- Gaussian

$$\phi(|x - x_j|) = e^{-c(x - x_j)^2}$$

- Polyharmonic splines

$$\phi(|x - x_j|) = \begin{cases} (x - x_j)^{2n} \log(x - x_j), & n \geq 1, \text{ in 2D,} \\ (x - x_j)^{2n-1}, & n \geq 1, \text{ in 3D.} \end{cases}$$

- etc

Basic Theory

→ Choices for the basis function

- Locally supported
 - Wendland forms

$$\text{W41: } \phi_i(x, y) = \left(\sqrt{(x-x_i)^2 + (y-y_i)^2} - 1 \right)_+^4 \left(1 + 4\sqrt{(x-x_i)^2 + (y-y_i)^2} \right)$$

$$\text{W42: } \phi_i(x, y) = \left(\sqrt{(x-x_i)^2 + (y-y_i)^2} - 1 \right)_+^6 \left\{ 3 + 18\sqrt{(x-x_i)^2 + (y-y_i)^2} + 35 \left[(x-x_i)^2 + (y-y_i)^2 \right] \right\}$$

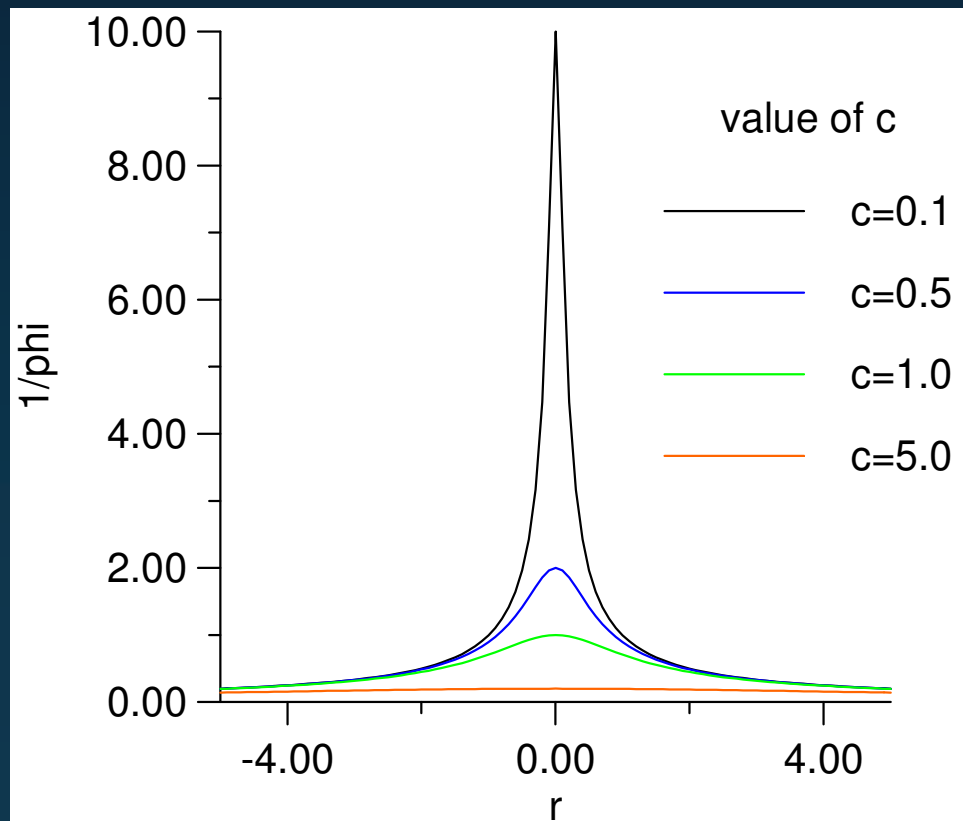
$$\text{W43: } \phi_i(x, y) = \left(\sqrt{(x-x_i)^2 + (y-y_i)^2} - 1 \right)_+^8 \left\{ 1 + 8\sqrt{(x-x_i)^2 + (y-y_i)^2} + 25 \left[(x-x_i)^2 + (y-y_i)^2 \right] + 32 \left[(x-x_i)^2 + (y-y_i)^2 \right]^{3/2} \right\}$$

Basic Theory

→ Multiquadrics

$$\phi(|x - x_j|) = \sqrt{(x - x_j)^2 + c_j^2}$$

- Depending on the choice of c , the function can be more or less smooth.



$$r = (x - x_j)$$

Generating Response Surfaces with RBFs

→ General Formulation

$$s(x_i) = f(x_i) = \sum_{j=1}^N \alpha_j \phi(|x_i - x_j|) + \sum_{k=1}^M \beta_k p_k(x_i) + \beta_0 \quad \sum_{j=1}^N \alpha_j p_k(x_j) = 0 \quad \sum_{j=1}^N \alpha_j = 0$$

→ The polynomial part of the expansion can be taken, for examples, as

$$p_k(x_i) = x_i^k$$

→ And the Multiquadrics can be used as basis functions

$$\phi(|x_i - x_j|) = \sqrt{(x_i - x_j)^2 + c_j^2}$$

Generating Response Surfaces with RBFs

→ Performance parameters

- R square

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} = 1 - \frac{MSE}{\text{variance}}$$

- While *MSE* (Mean Square Error) represents the departure of the metamodel from the real simulation model, the variance captures how irregular the problem is. *The larger the value of R Square, the more accurate the metamodel.*

Generating Response Surfaces with RBFs

→ Performance parameters

- RAAE

$$RAAE = \frac{\sum_{i=1}^n |y_i - \hat{y}_i|}{n * STD}$$

- where STD stands for standard deviation. The smaller the value of RAAE, the more accurate the metamodel.

Generating Response Surfaces with RBFs

→ Performance parameters

- RMAE

$$RMAE = \frac{\max(|y_1 - \hat{y}_1|, |y_2 - \hat{y}_2|, \dots, |y_n - \hat{y}_n|)}{STD}$$

- Large RMAE indicates large error in one region of the design space even though the overall accuracy indicated by R Square and RAAE can be very good. Therefore, a small RMAE is preferred; however, since this metric cannot show the overall performance in the design space, it is not as important as R Square and RAAE.

Generating Response Surfaces with RBFs

→ Some sample problems

Test function	Training points	Testing points	Minimum value of f	Maximum value of f	Standard deviation of f	Average value of f	Non-linearit
1	198	1000	-21.01	29.25	8.92	8.60	High
2	198		-1717.43	-539.36	187.40	-1146.82	Low
3	198		-1327241.16	-1.14	224561.73	-213124.84	High
4	198		258.78	4779.01	1002.27	2185.25	Low
5	459		7136.99	195608.81	27294.72	69060.73	Low
6	100		98.94	187.53	17.75	127.73	High
7	100		-0.26	0.26	0.15	0.00	High
8	100		-1.51	8.91	2.08	1.66	Low
9	125		2.15	146369.38	21527.31	10842.11	High
10	125		3.42	32.84	7.70	29.13	High
11	125		-40829.97	-40749.42	21.60	-40790.41	Low
12	100		-12.72	13.75	5.74	0.52	Low
13	100		-54.77	77.80	30.94	12.60	Low

Generating Response Surfaces with RBFs

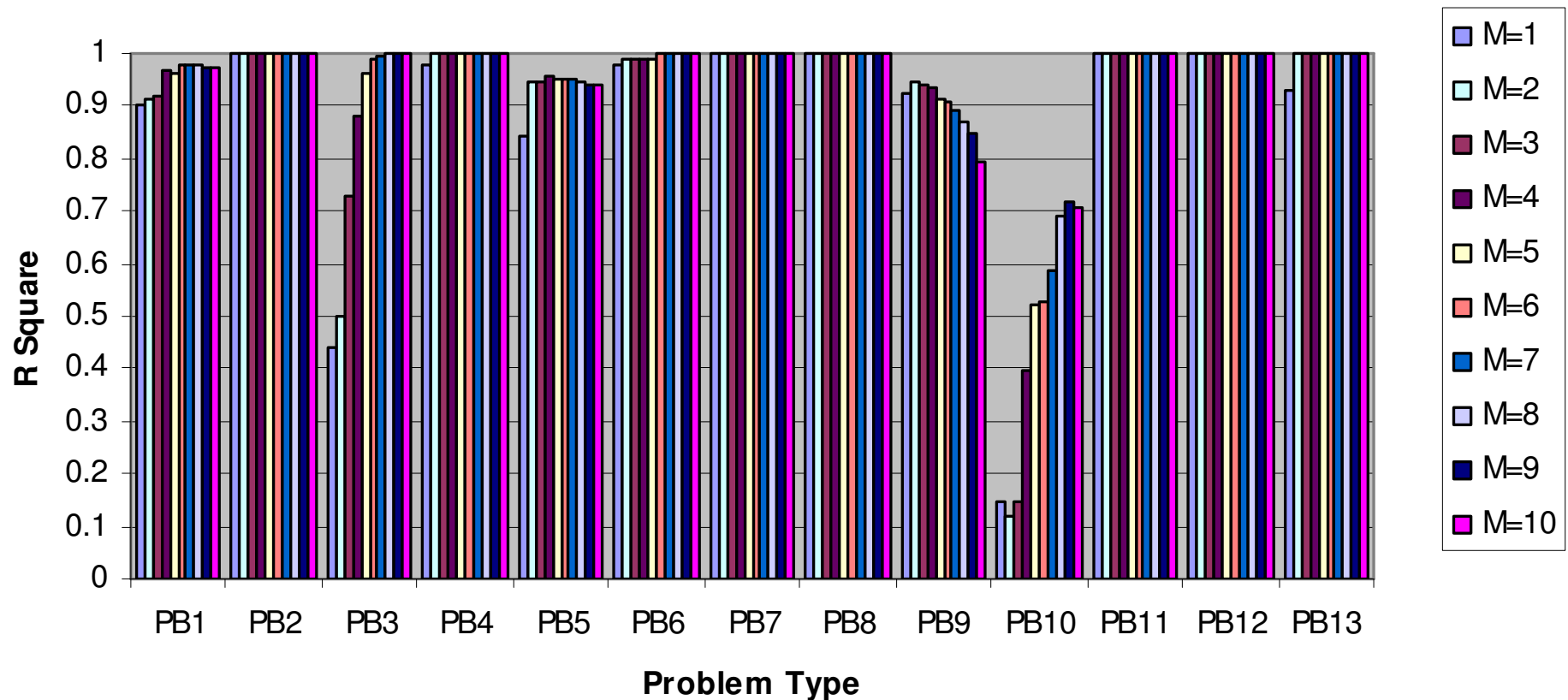
Number of training and testing points						Non Linearity
		Training			Testing	
PB #	# Vars	Scarce	Small	Large		
PB1	10	30	100	198	1000	High
PB2	10	30	100	198		Low
PB3	10	30	100	198		High
PB4	10	30	100	198		Low
PB5	16	48	160	459		Low
PB6	2	N/A	9	100		High
PB7	2		9	100		High
PB8	2		9	100		Low
PB9	3		27	125		High
PB10	3		27	125		High
PB11	3		27	125		Low
PB12	2		9	100		Low
PB13	2		9	100		Low

Generating Response Surfaces with RBFs

→ Large set of training points

$$s(x_i) = f(x_i) = \sum_{j=1}^N \alpha_j \phi(|x_i - x_j|) + \sum_{k=1}^M \beta_k p_k(x_i) + \beta_0$$

$$p_k(x_i) = x_i^k$$

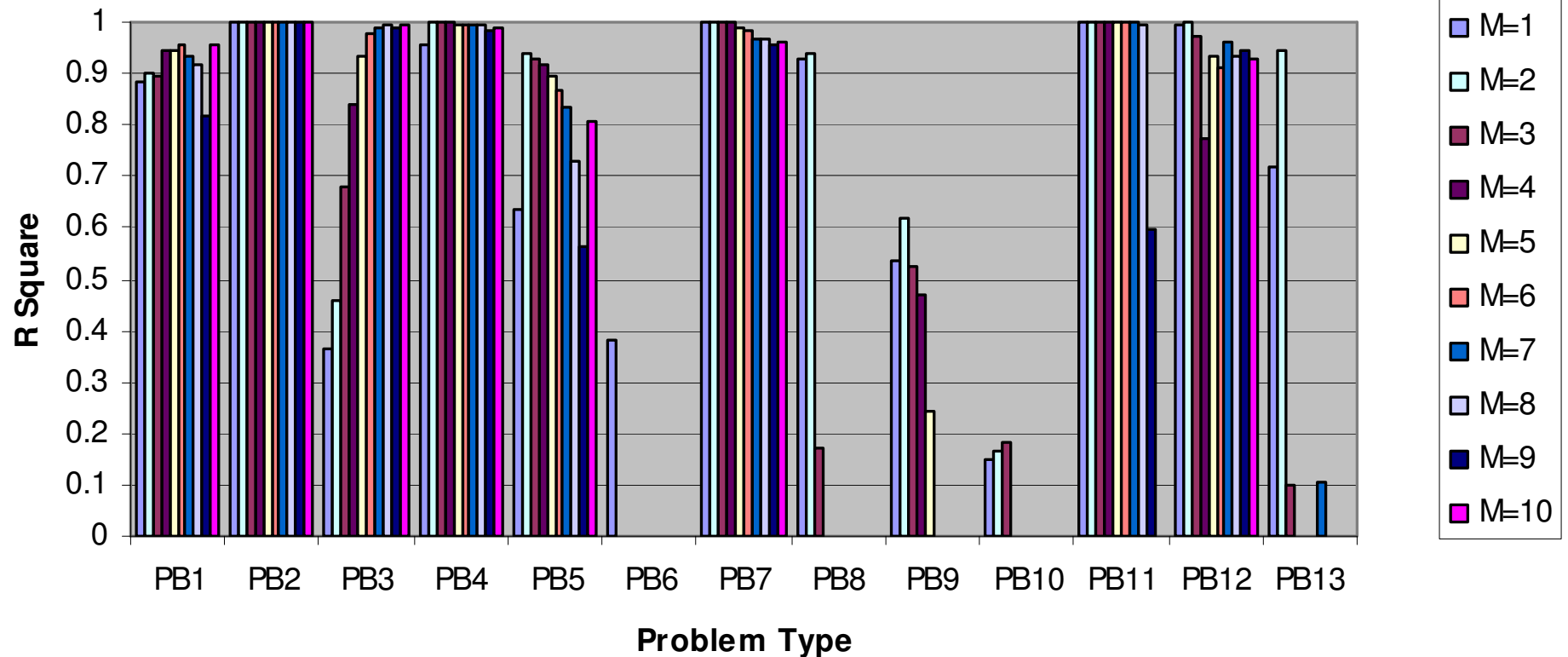


Generating Response Surfaces with RBFs

→ Small set of training points

$$s(x_i) = f(x_i) = \sum_{j=1}^N \alpha_j \phi(|x_i - x_j|) + \sum_{k=1}^M \beta_k p_k(x_i) + \beta_0$$

$$p_k(x_i) = x_i^k$$

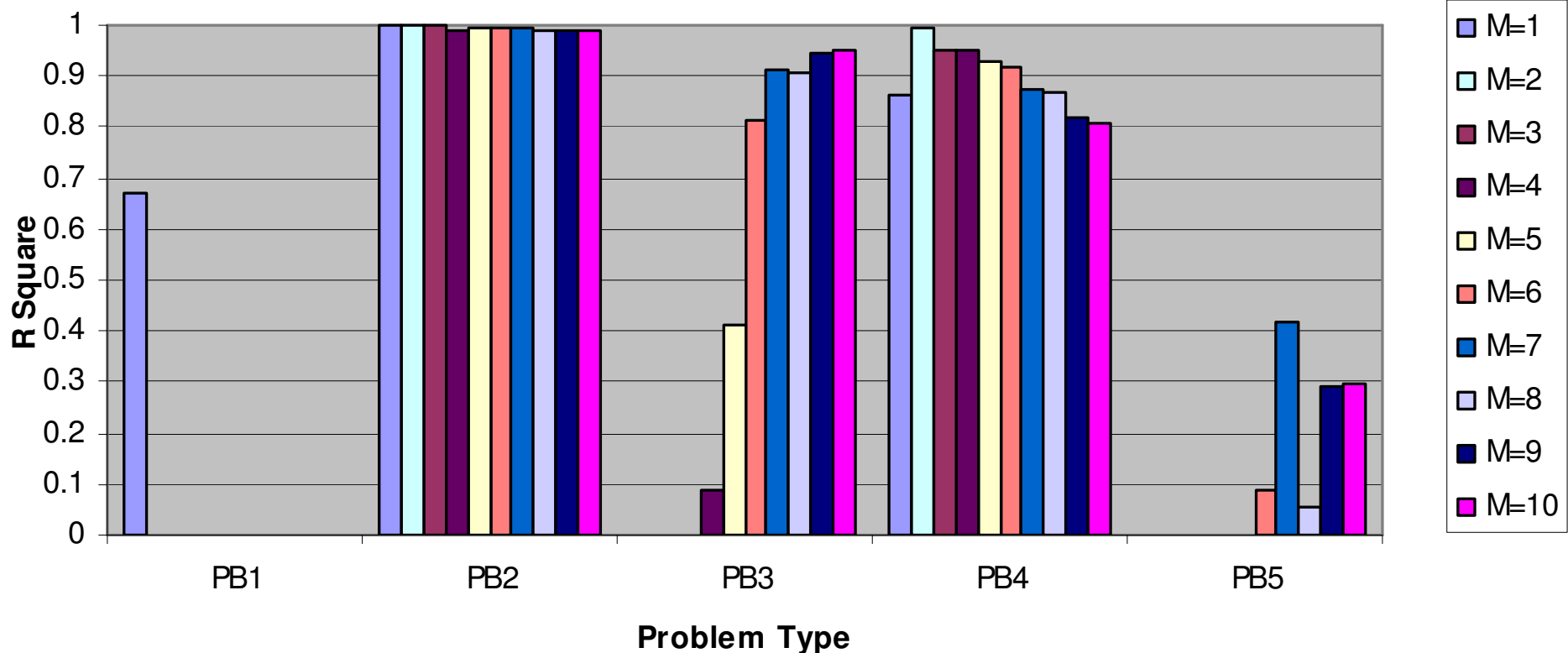


Generating Response Surfaces with RBFs

→ Scarce set of training points

$$s(x_i) = f(x_i) = \sum_{j=1}^N \alpha_j \phi(|x_i - x_j|) + \sum_{k=1}^M \beta_k p_k(x_i) + \beta_0$$

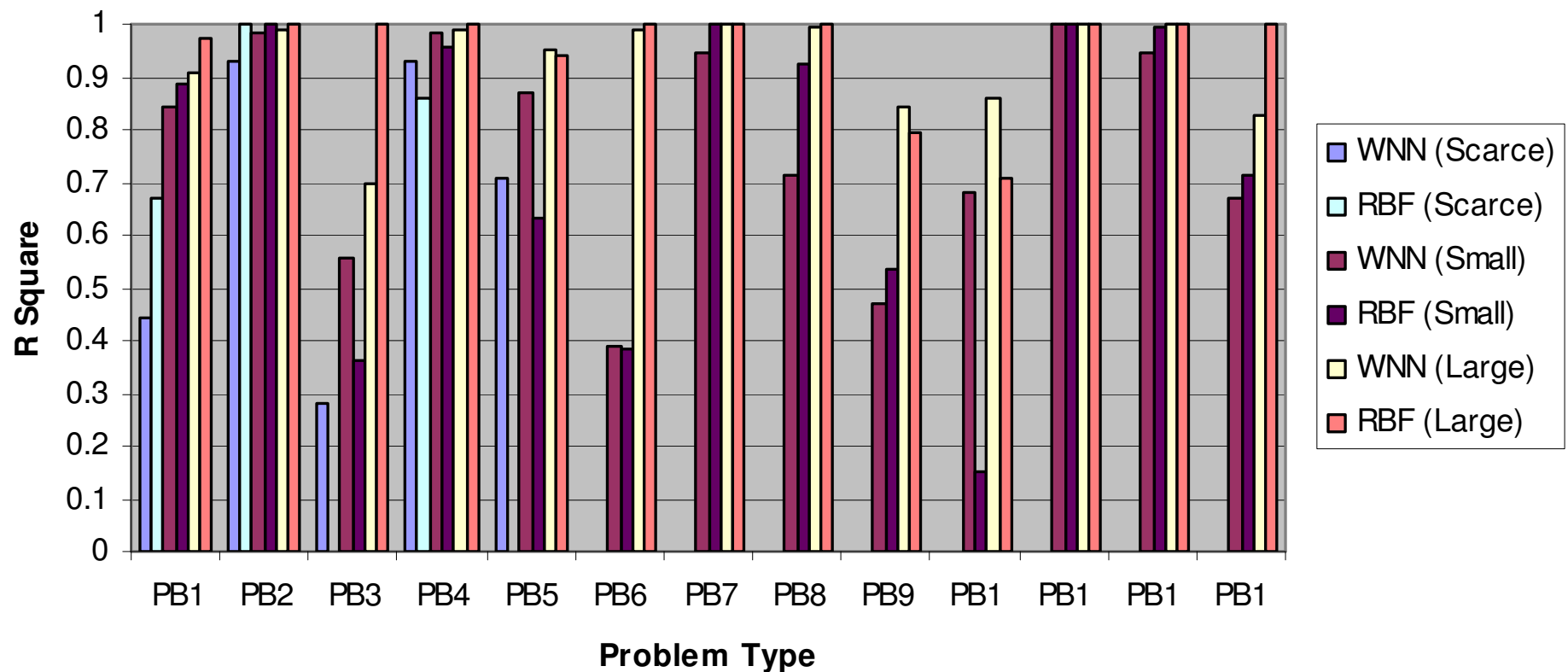
$$p_k(x_i) = x_i^k$$



Generating Response Surfaces with RBFs

→ Wavelets *versus* RBFs (R Square)

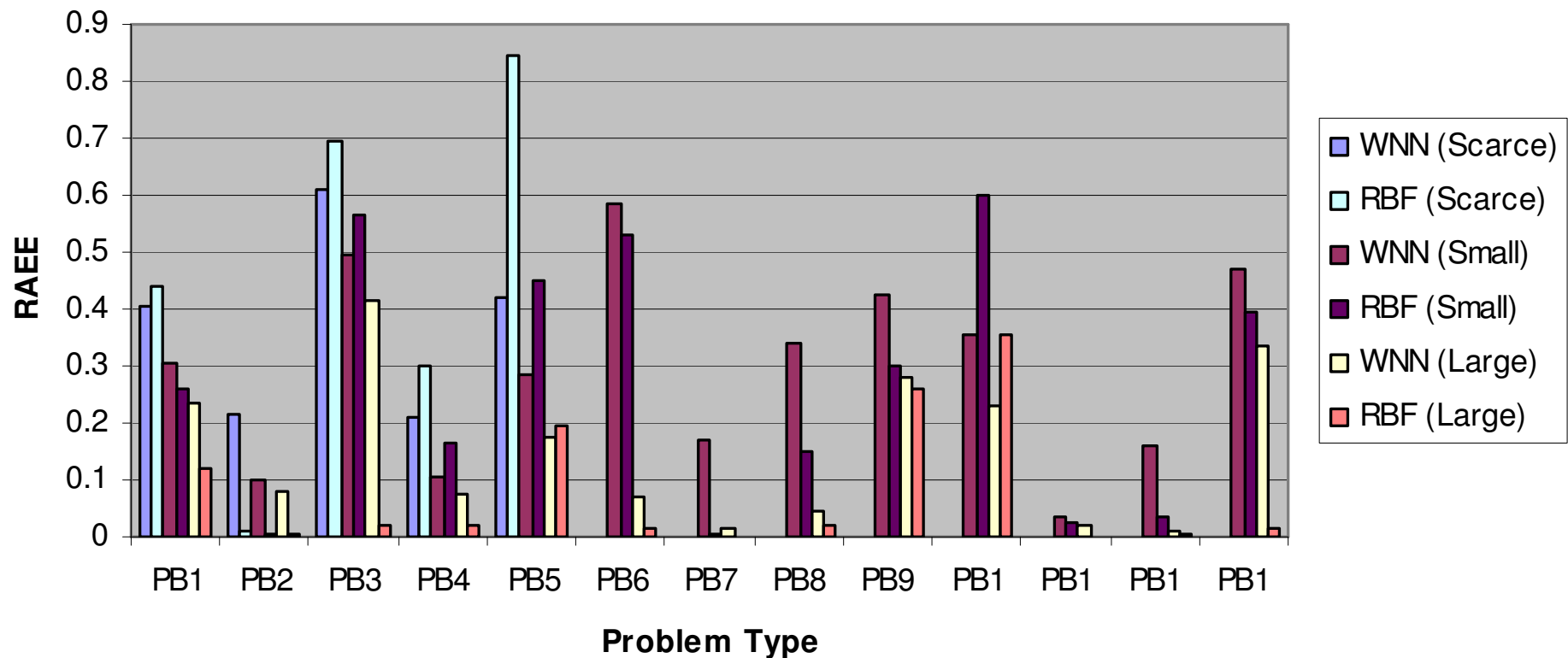
$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} = 1 - \frac{MSE}{\text{variance}}$$



Generating Response Surfaces with RBFs

→ Wavelets *versus* RBFs (RAEE)

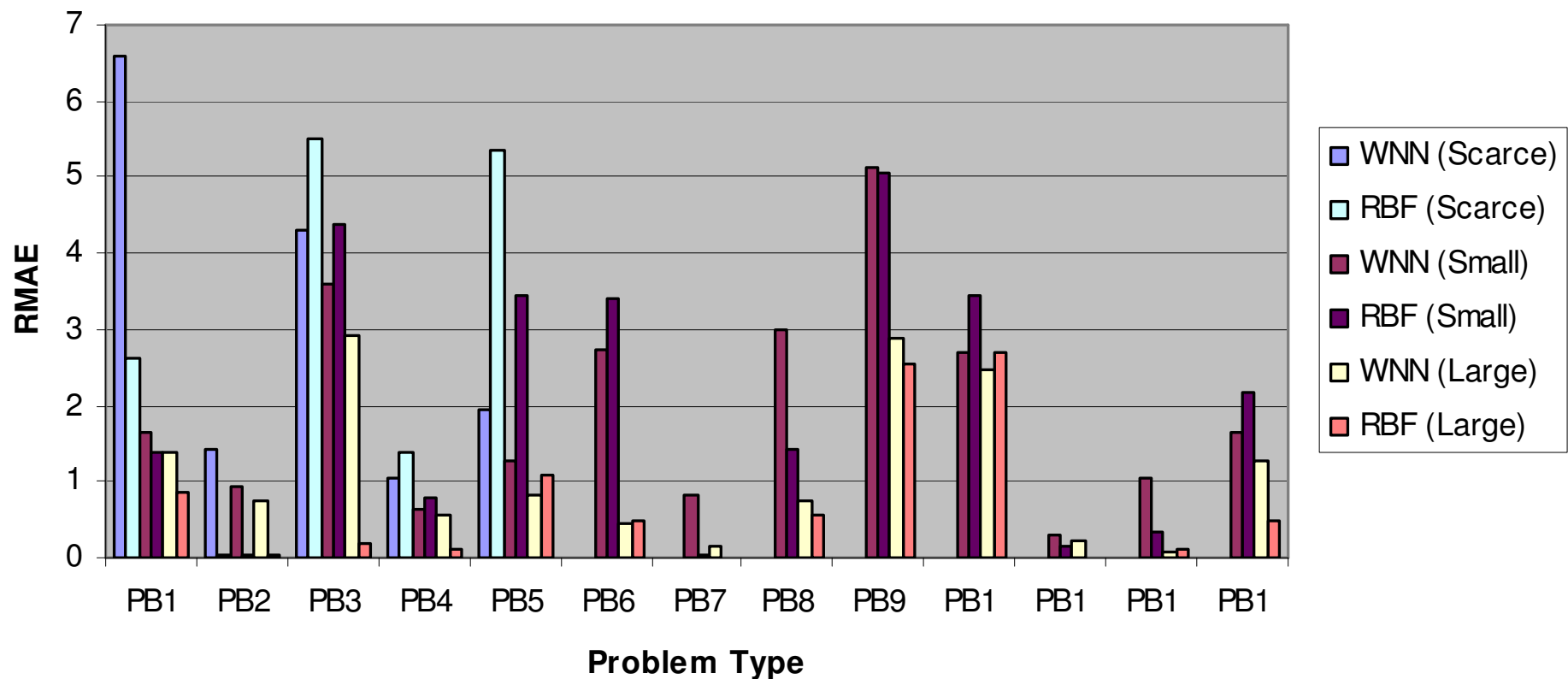
$$RAAE = \frac{\sum_{i=1}^n |y_i - \hat{y}_i|}{n * STD}$$



Generating Response Surfaces with RBFs

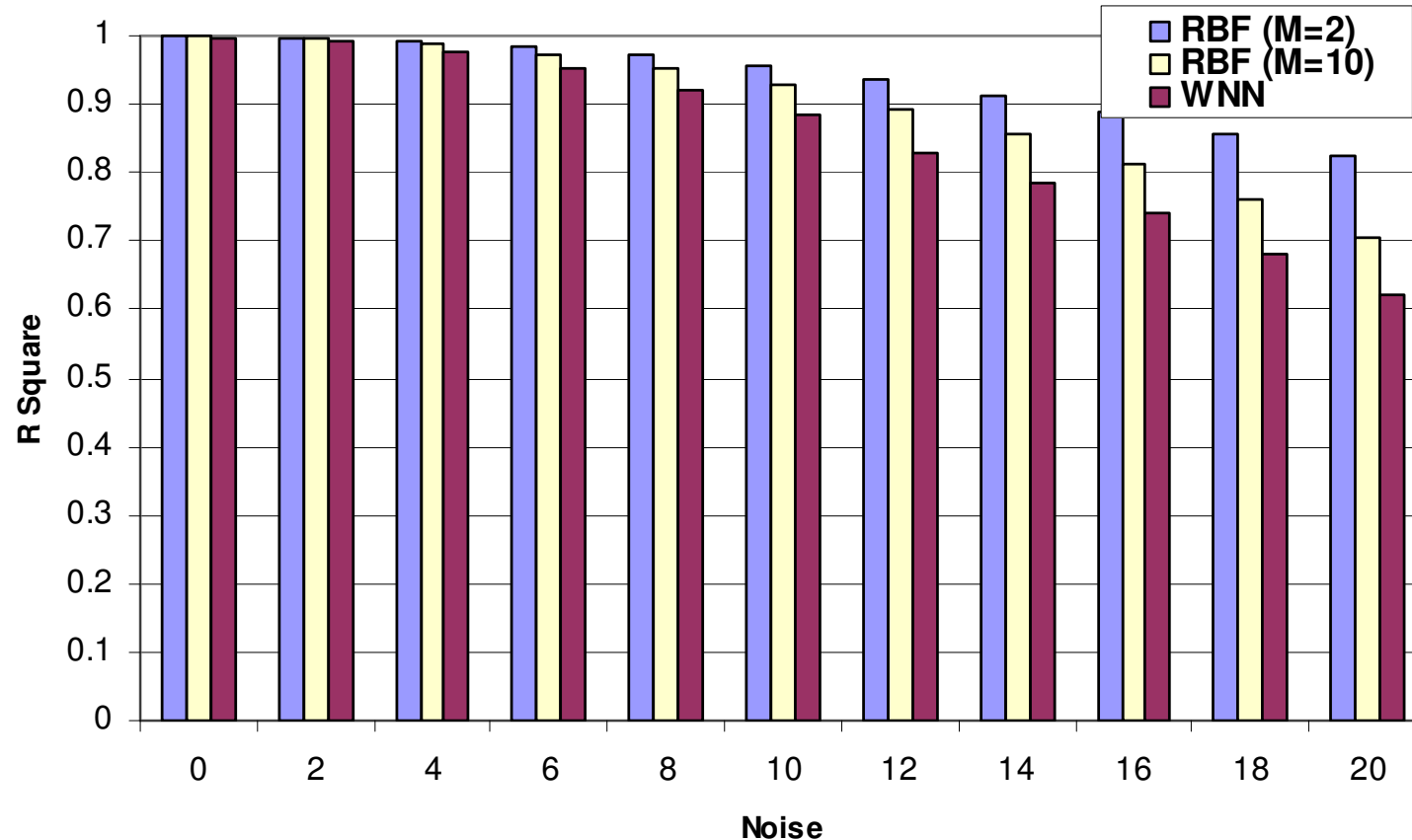
→ Wavelets *versus* RBFs (RMAE)

$$RMAE = \frac{\max(|y_1 - \hat{y}_1|, |y_2 - \hat{y}_2|, \dots, |y_n - \hat{y}_n|)}{STD}$$



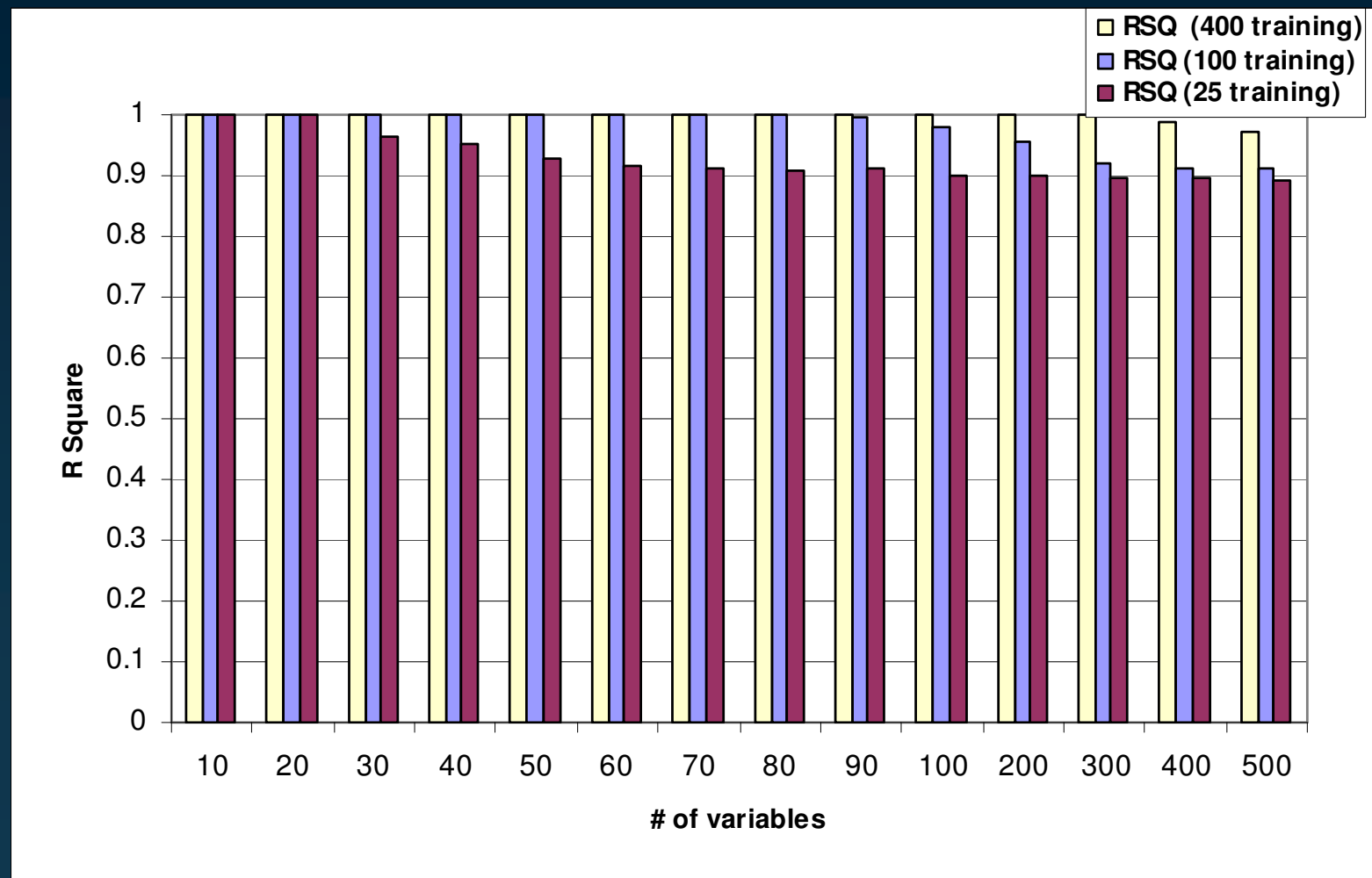
Generating Response Surfaces with RBFs

→ Wavelets *versus* RBFs (RSquare – PB#13 with NOISE)



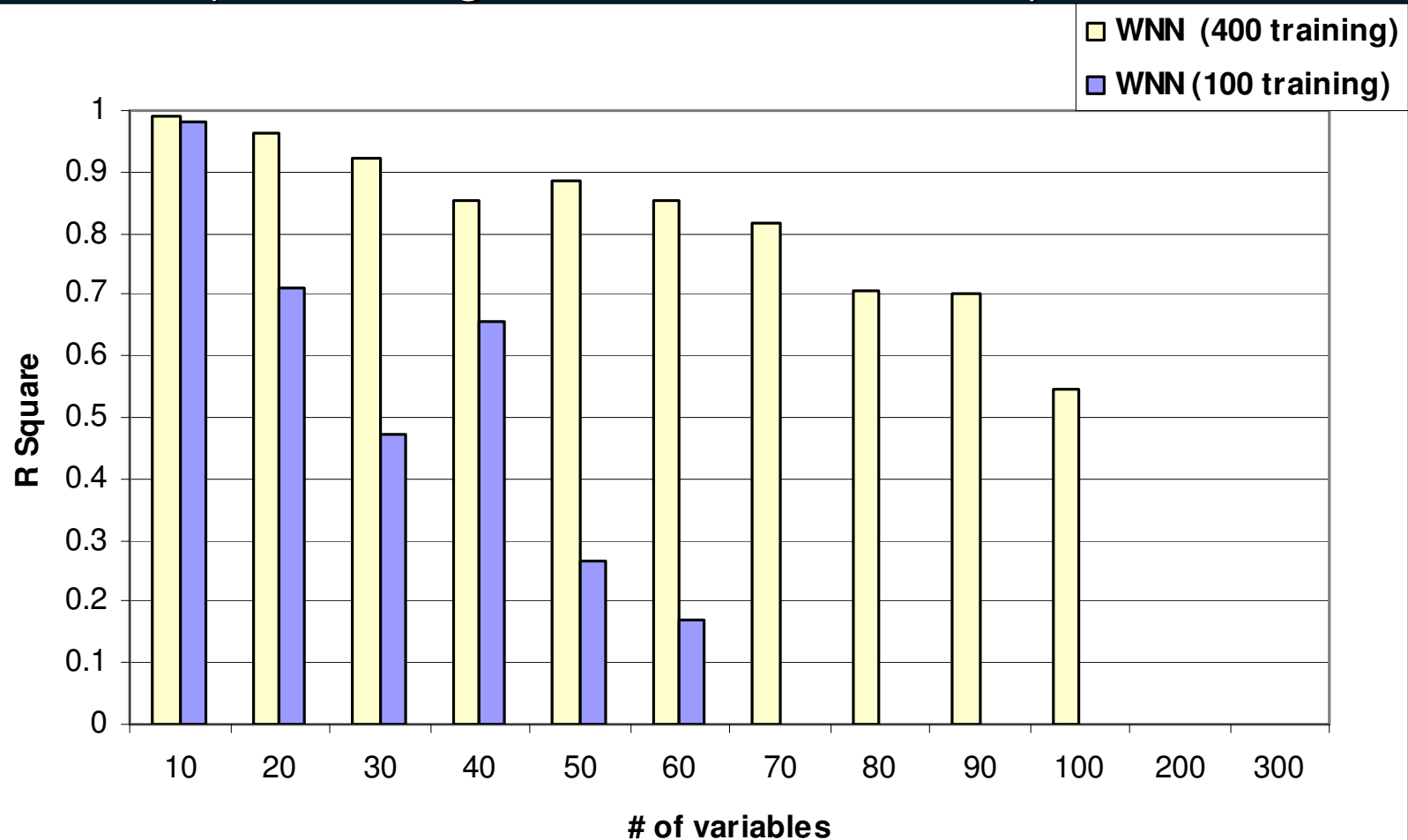
Generating Response Surfaces with RBFs

→ RBFs (PB#2 Large number of variables)



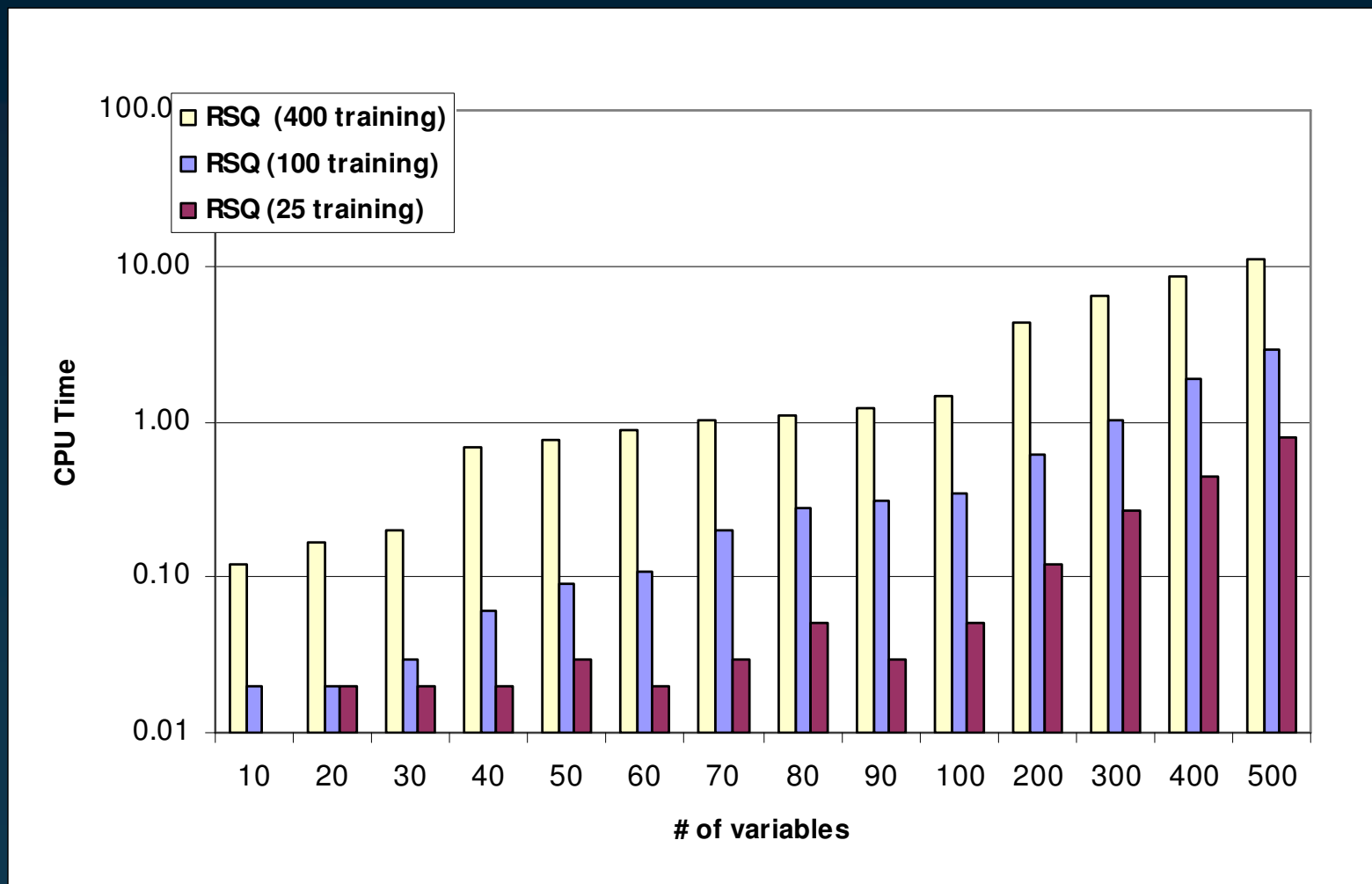
Generating Response Surfaces with RBFs

→ Wavelets (PB#2 Large number of variables)



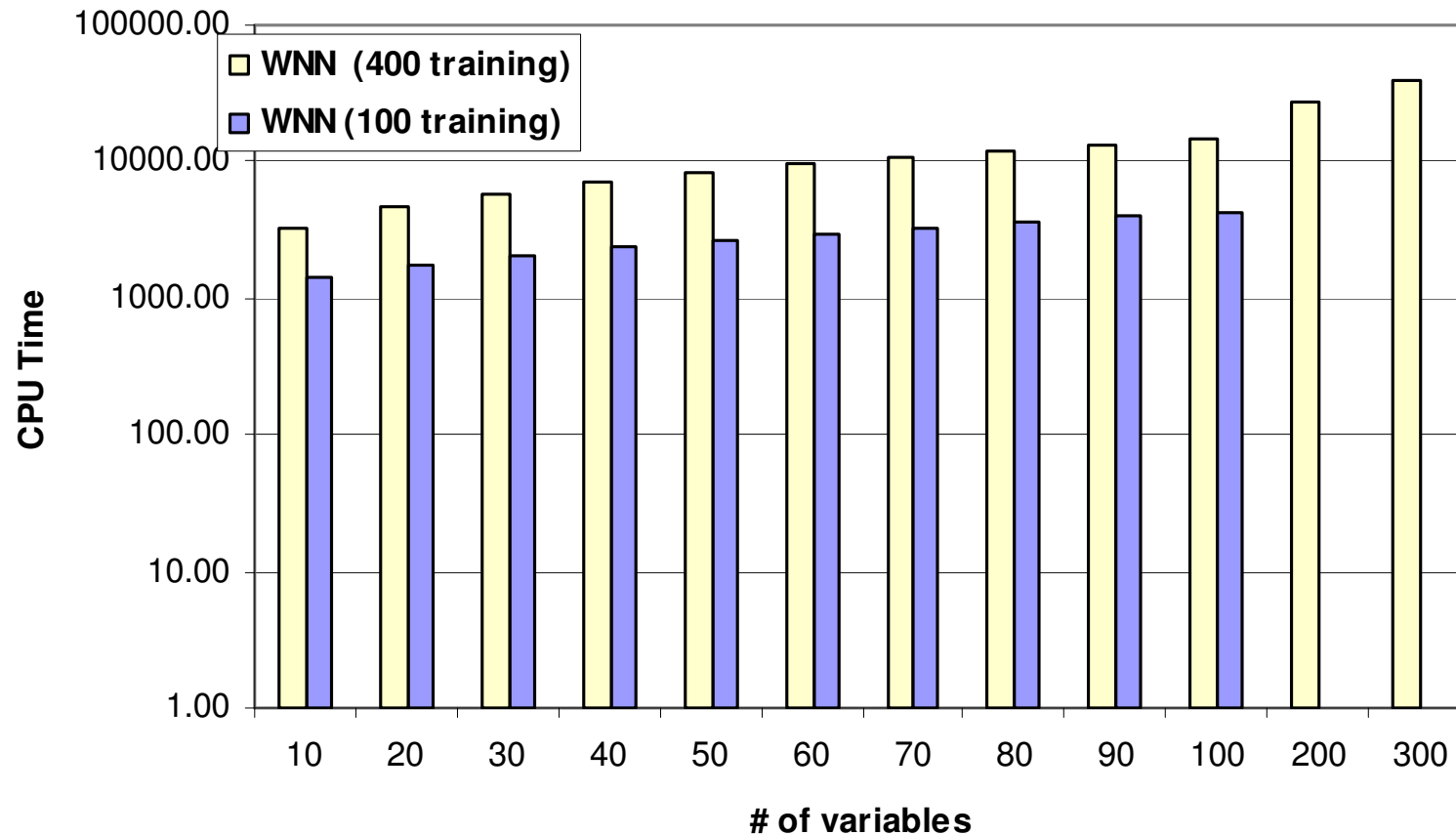
Generating Response Surfaces with RBFs

→ RBFs (PB#2 Large number of variables)



Generating Response Surfaces with RBFs

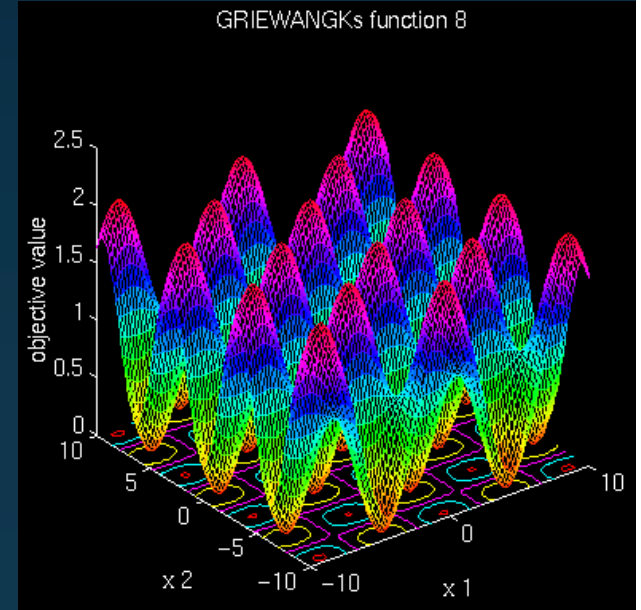
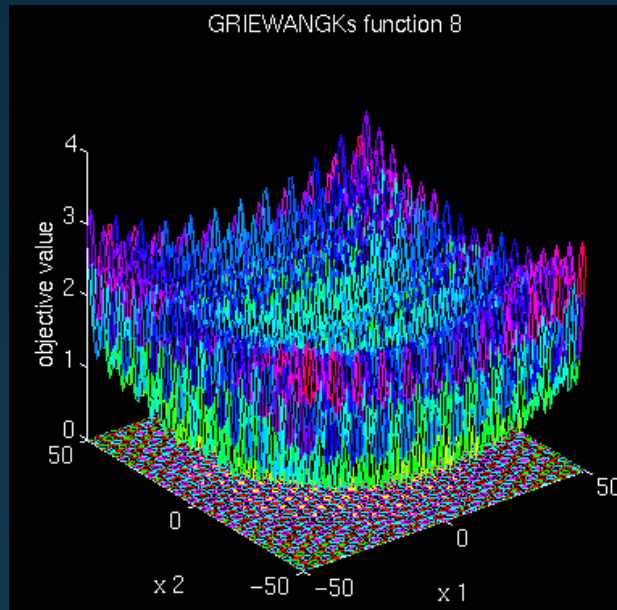
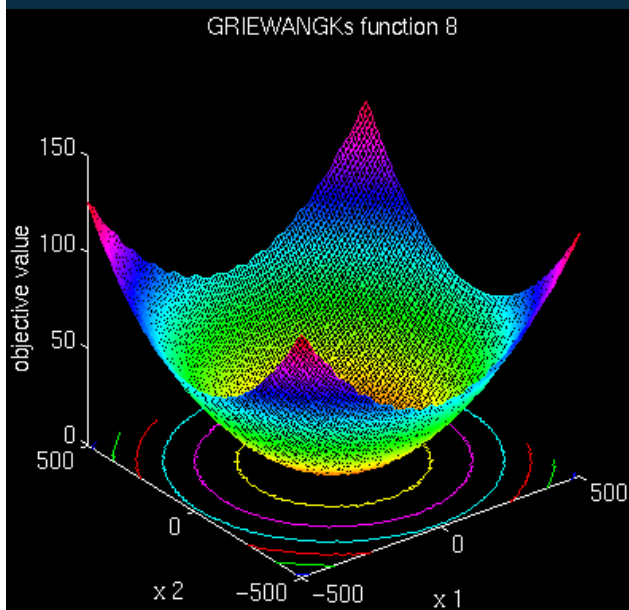
→ Wavelets (PB#2 Large number of variables)



Using RBFs as a MetaModel in Optimization

→ Sample test function (Griewangk's function)

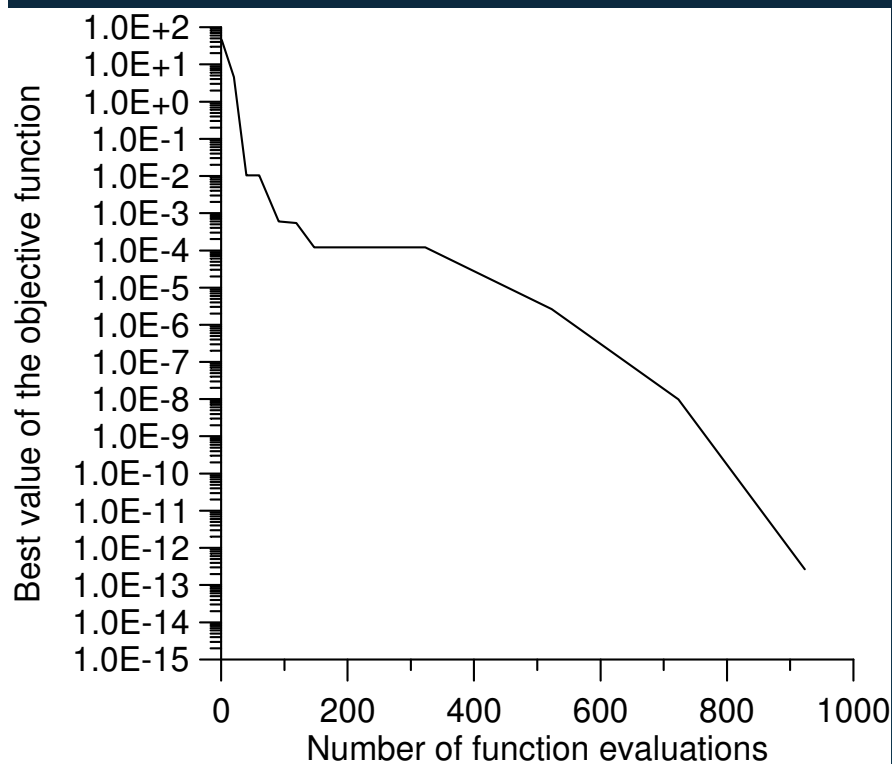
$$U = \sum_{i=1}^n \frac{x_i^2}{4000} - \prod_{i=1}^n \cos\left(\frac{x_i}{\sqrt{i}}\right) + 1$$
$$x \in [-600, 600]$$



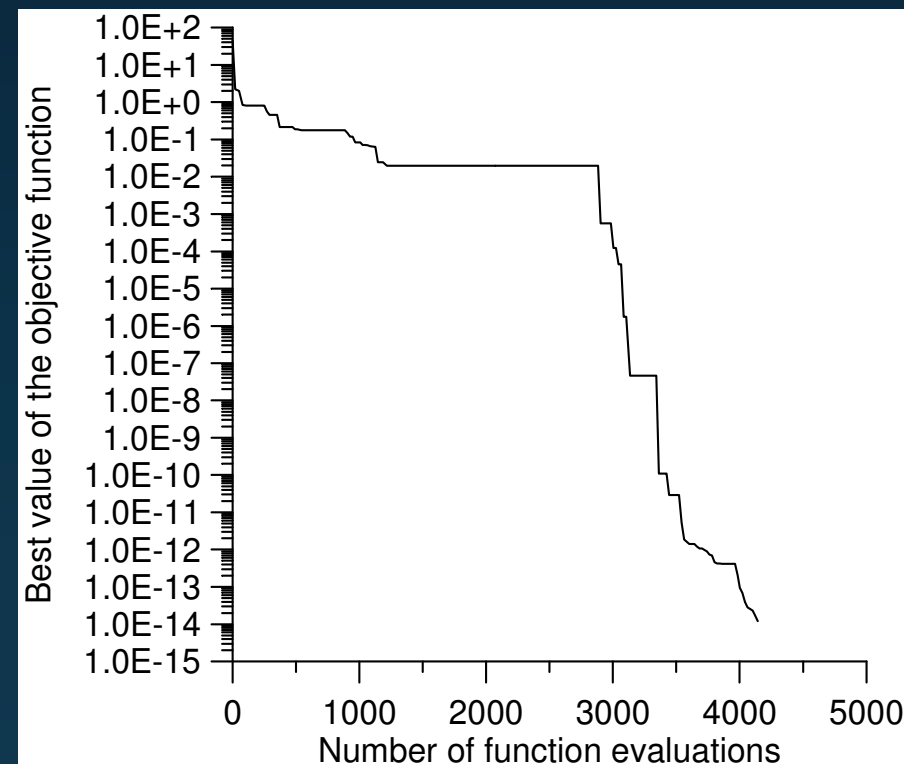
Using RBFs as a MetaModel in Optimization

→ Optimization history (Hybrid Code)

with RBFs



without RBFs



Summary of the results for the 295 test cases defined by Prof. Klaus Schittkowski

-K. Schittkowski (1987): More Test Examples for Nonlinear Programming, Lecture Notes in Economics and Mathematical Systems, Vol. 282, Springer

-W. Hock, K. Schittkowski (1981): Test Examples for Nonlinear Programming Codes, Lecture Notes in Economics and Mathematical Systems, Vol. 187, Springer

Scarce set – Number of training points = 3 times number of variables

Small set – Number of training points = 10 times number of variables

Medium set – Number of training points = 50 times number of variables

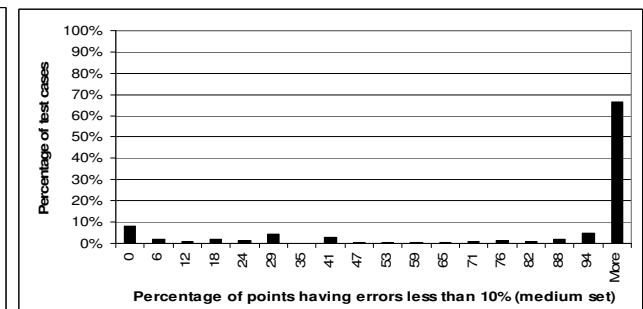
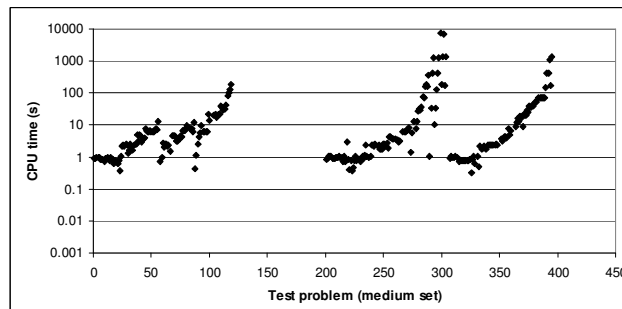
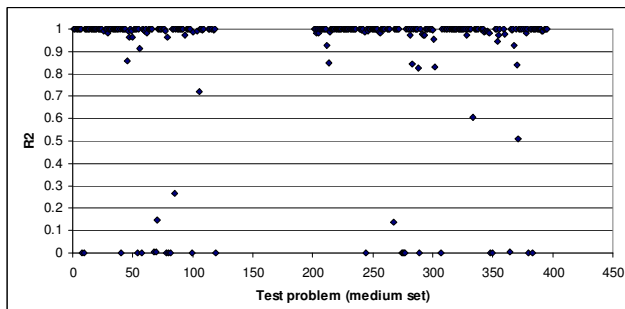
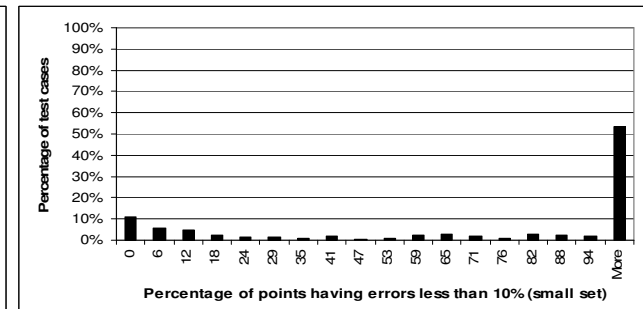
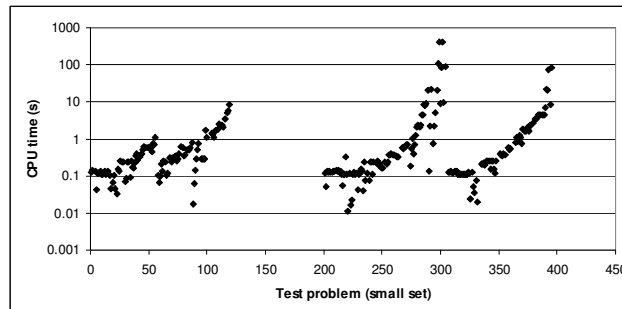
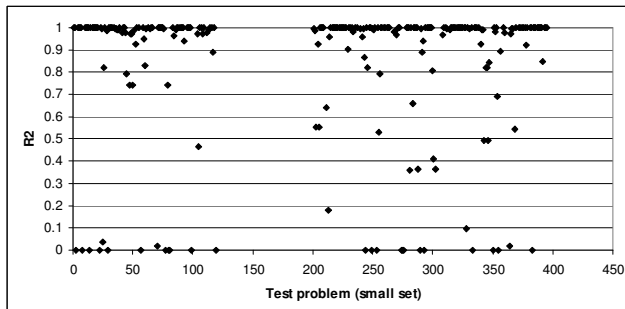
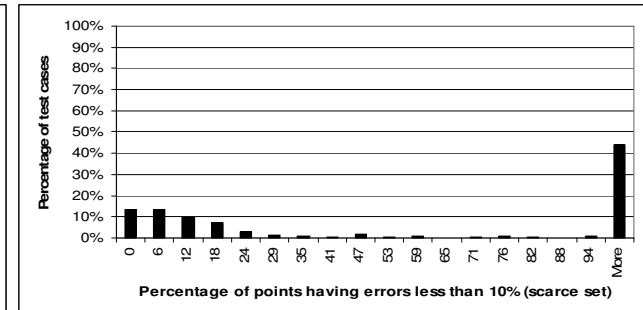
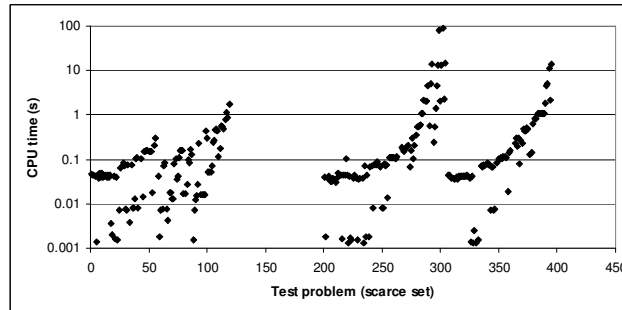
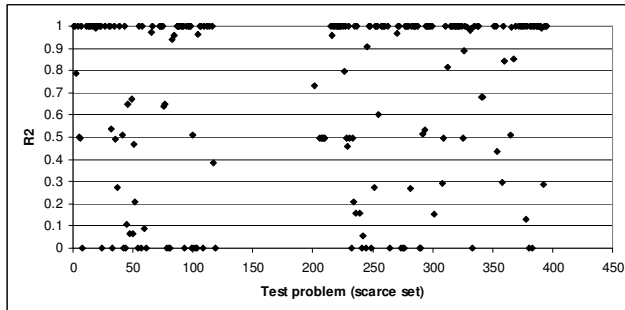
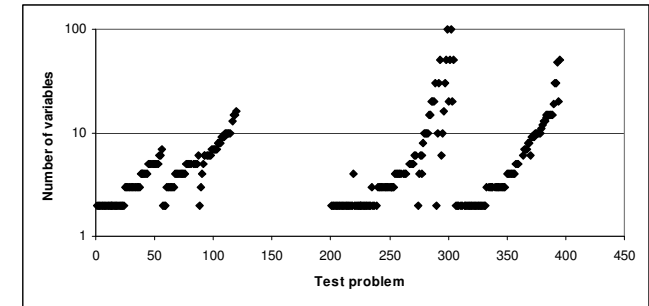
Number of testing points = 100 times number of training points

Polynomials up to order 6

Half of the training points used to validate the surface (cyclic)

Other preconditioning for the GMRES solver

4 Different RBFs used



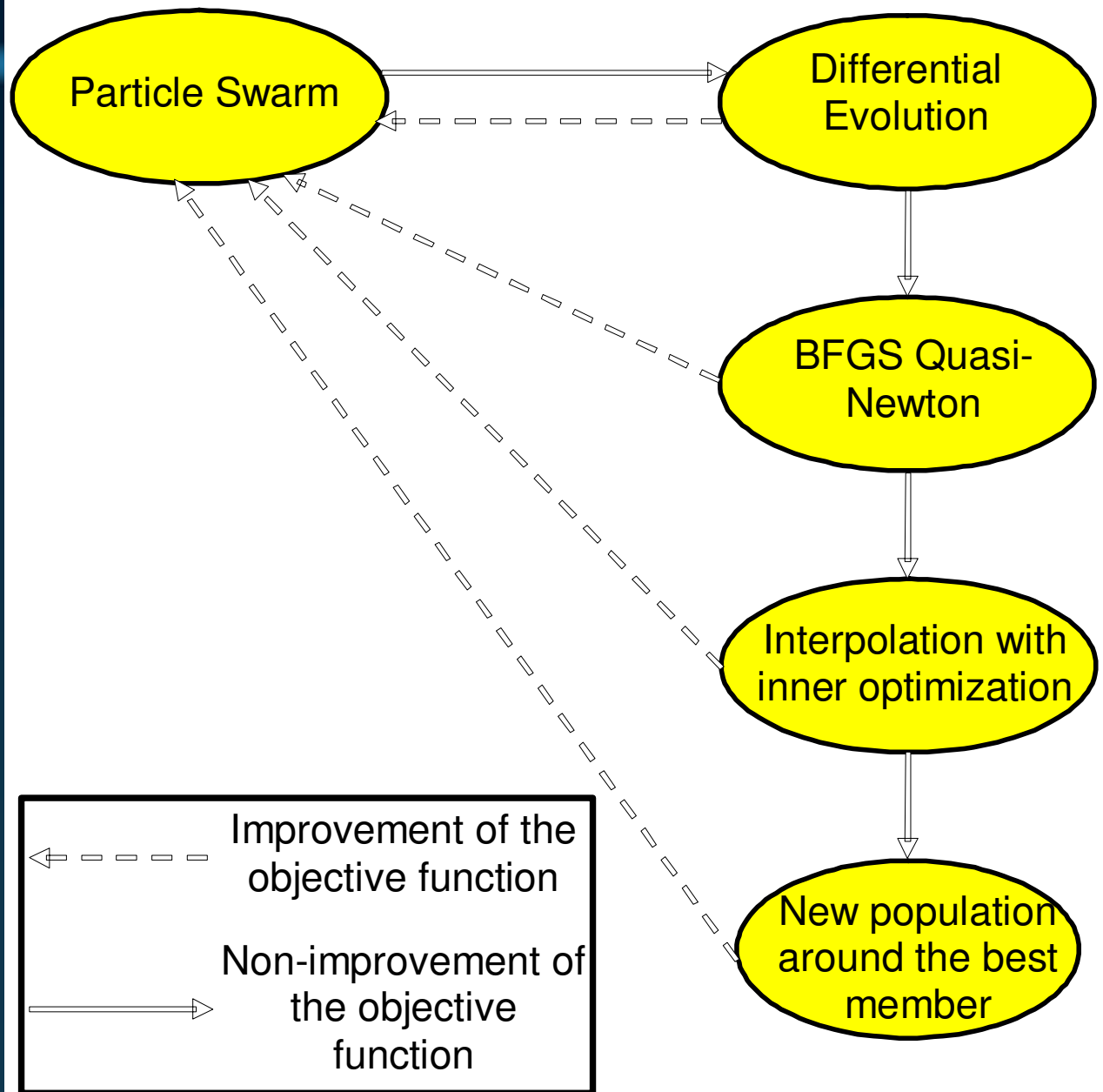
Hybrid Methods

→ Metamodel strategy

Colaço and Dulikravich

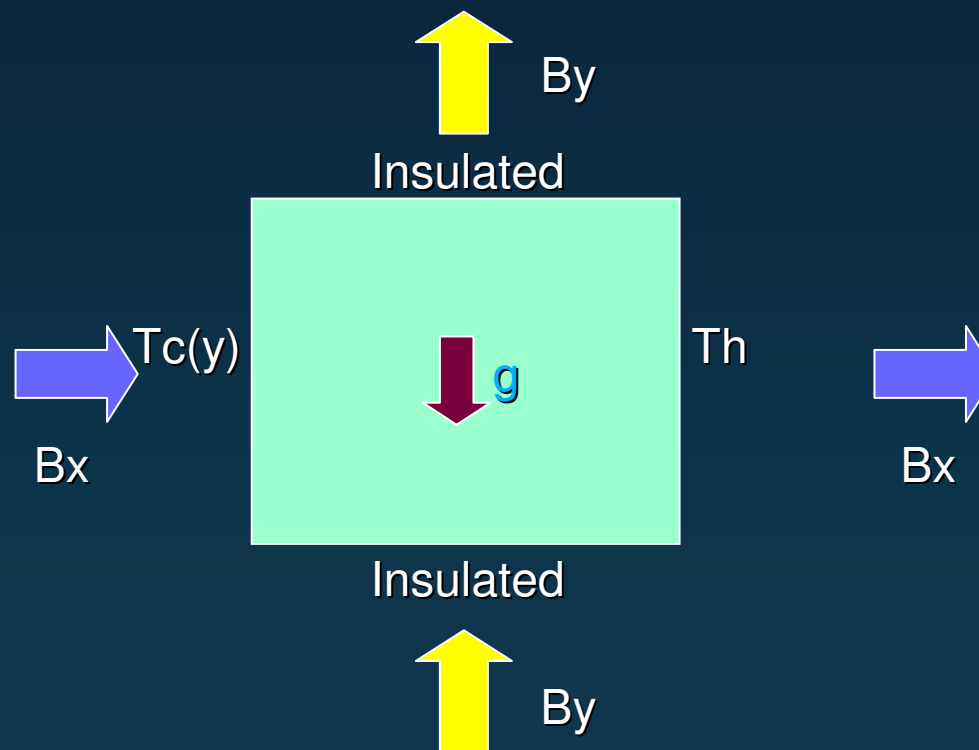
Hybrid Optimizer

version 3 – Nov. 2006



MHD – Example 5

- Optimization of the boundary conditions in order to minimize the natural convection effects (thermomagnetic optimization)
- Test problem:



MHD – Example 5

- Optimization Problem
- The boundary conditions are parameterized as B-Splines.
- NETLIB's subroutine GCVSPL, based on the cross-validation smoothing procedure, was used for the interpolation.
- Objective function:

$$F = \sqrt{\frac{1}{\# \text{liquid cells}} \sum_{i=1}^{\# \text{liquid cells}} \left(\frac{\partial C_i}{\partial y_i} \right)^2}$$

MHD – Example 5

→ Optimization Problem

→ Parameters for silicon:

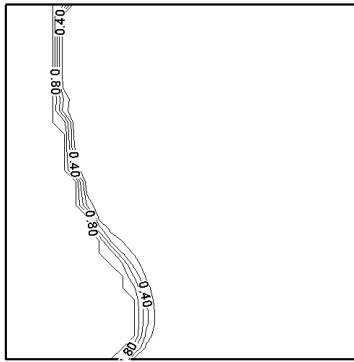
$\rho_l = 2550 \text{ kg m}^{-3}$	$\rho_s = 2550 \text{ kg m}^{-3}$
$C_{Pl} = 1059 \text{ J kg}^{-1} \text{ K}^{-1}$	$C_{Ps} = 1059 \text{ J kg}^{-1} \text{ K}^{-1}$
$\sigma_l = 12.3 \times 10^5 \text{ 1/m } \Omega$	$\sigma_s = 4.3 \times 10^4 \text{ 1/m } \Omega$
$D_l = 6.043 \times 10^{-9} \text{ kg m}^{-1} \text{ s}^{-1}$	$D_s = 0 \text{ kg m}^{-1} \text{ s}^{-1}$
$L = 1.8 \times 10^6 \text{ J kg}^{-1}$	$C_0 = 0.1 \text{ kg m}^{-3}$
$n = 0.3 \quad T_h = 1685.04 \text{ K} \quad 1620 \text{ K} < T_c < 1630 \text{ K}$	

$k_l = 64 \text{ W m}^{-1} \text{ K}^{-1}$	$k_s = 64 \text{ W m}^{-1} \text{ K}^{-1}$
$\mu_l = 0.0032634 \text{ kg m}^{-1} \text{ s}^{-1}$	$\mu_s = 326.34 \text{ kg m}^{-1} \text{ s}^{-1}$
$\beta = 1.4 \times 10^{-4} \text{ K}^{-1}$	$\beta_s = 0.0875$
$g = 9.81 \text{ m s}^{-2}$	$\mu_m = 1.2566 \times 10^{-5} \text{ T m A}^{-1}$
$Te = 1681 \text{ K}$	$C_e = 0.8 \text{ kg m}^{-3}$

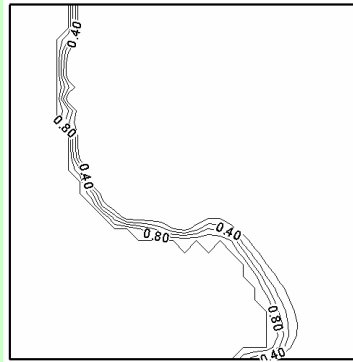
MHD – Example 5 (no magnetic fields)



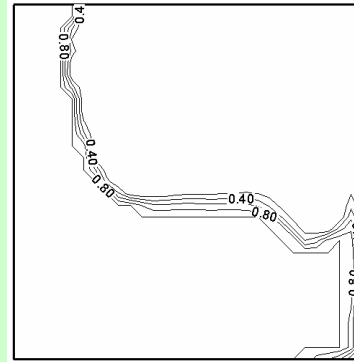
15 min



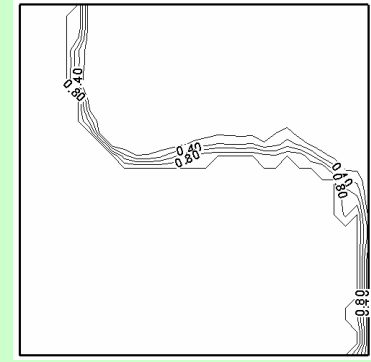
30 min



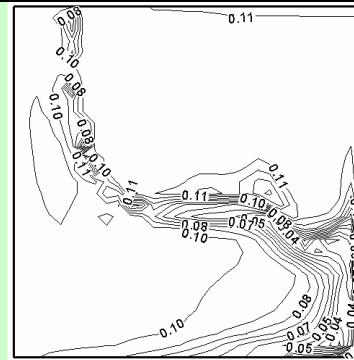
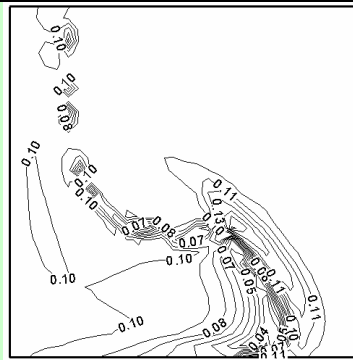
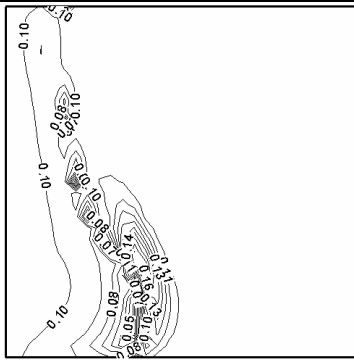
45 min



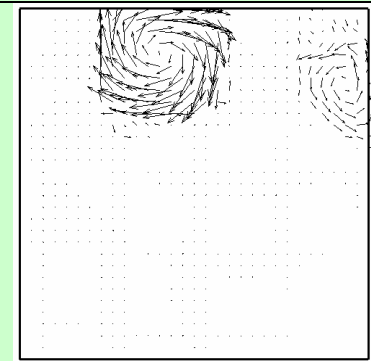
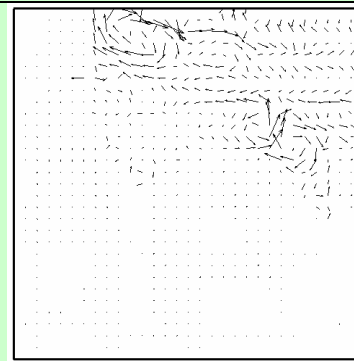
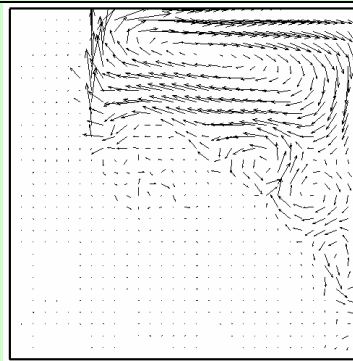
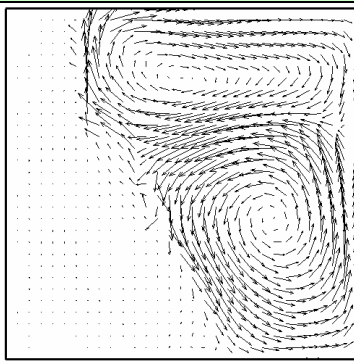
60 min



(a) Void fraction



(b) Concentration

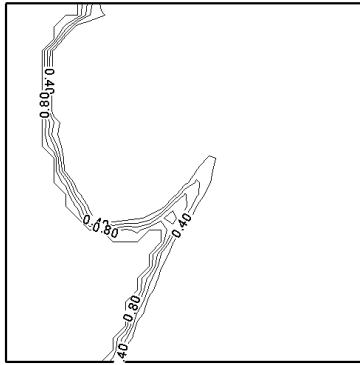


(c) Velocity vectors

MHD – Example 5 (optimized magnetic fields)



15 min



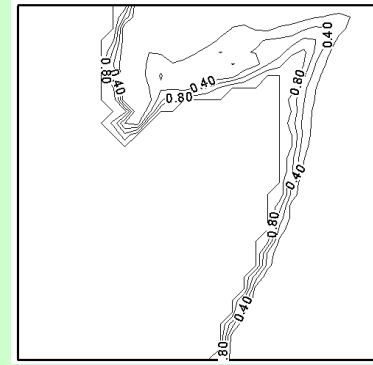
30 min



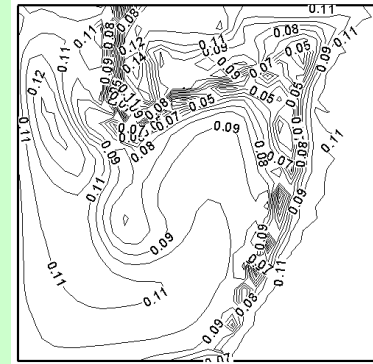
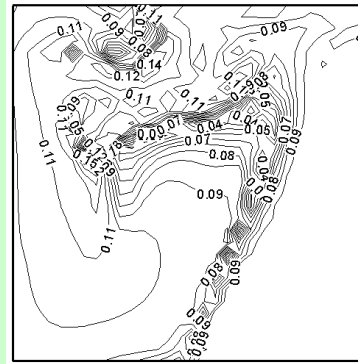
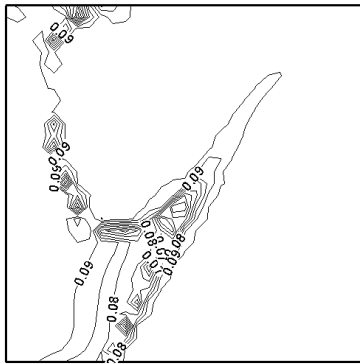
45 min



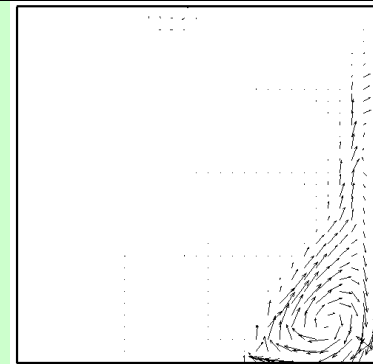
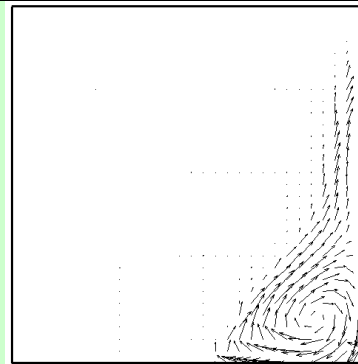
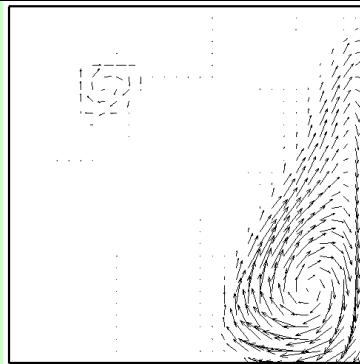
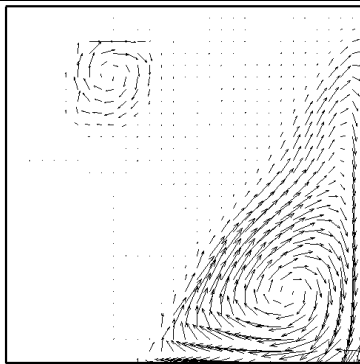
60 min



(a) void fraction



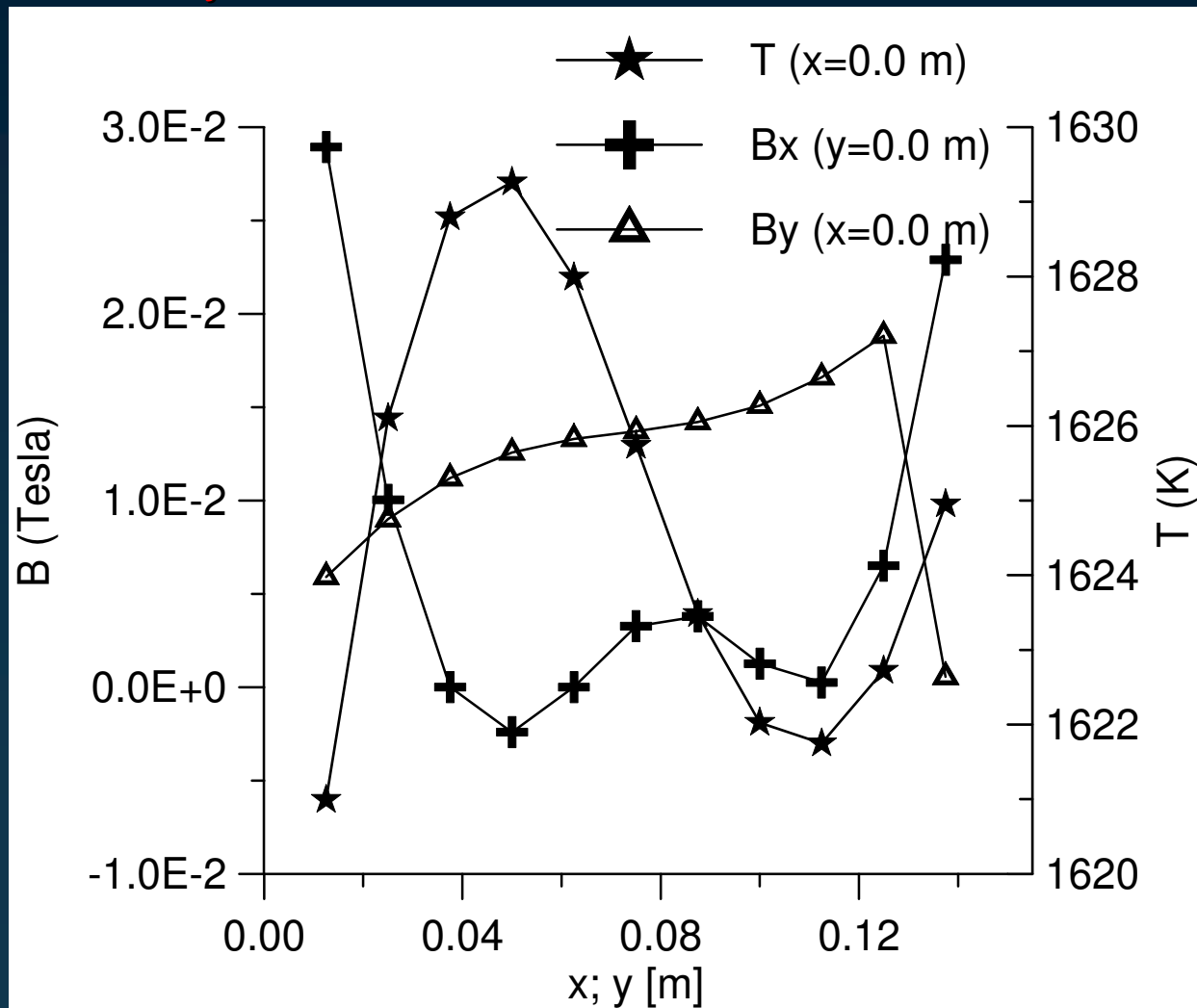
(b) Concentration



(c) Velocity vectors

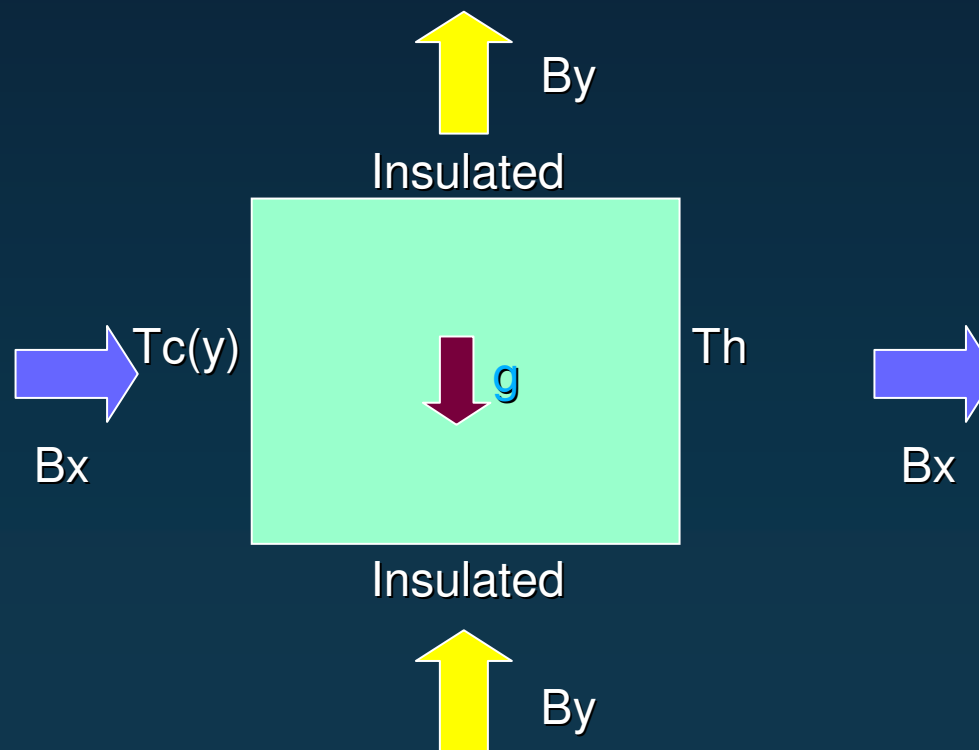
MHD – Example 5

→ Optimized boundary conditions



MHD – Example 6

- Optimization of the boundary conditions in order to minimize the natural convection effects (thermomagnetic multiobjective optimization)
- Test problem:



MHD – Example 6

- Optimization Problem
- The boundary conditions are parameterized as B-Splines.
- NETLIB's subroutine GCVSPL, based on the cross-validation smoothing procedure, was used for the interpolation.
- Objective function:

$$F = (\text{liquid area fraction})^2 + \sqrt{\frac{1}{\# \text{liquid cells}} \sum_{i=1}^{\# \text{liquid cells}} \left(\frac{\omega_i - \bar{\omega}_i}{\omega_{\max}} \right)^2}$$

MHD – Example 6

→ Optimization Problem

→ Parameters for silicon:

$\rho_l = 2550 \text{ kg m}^{-3}$	$\rho_s = 2550 \text{ kg m}^{-3}$
$C_{Pl} = 1059 \text{ J kg}^{-1} \text{ K}^{-1}$	$C_{Ps} = 1059 \text{ J kg}^{-1} \text{ K}^{-1}$
$\sigma_l = 12.3 \times 10^5 \text{ 1/m } \Omega$	$\sigma_s = 4.3 \times 10^4 \text{ 1/m } \Omega$
$D_l = 6.043 \times 10^{-9} \text{ kg m}^{-1} \text{ s}^{-1}$	$D_s = 0 \text{ kg m}^{-1} \text{ s}^{-1}$
$L = 1.8 \times 10^6 \text{ J kg}^{-1}$	$C_0 = 0.1 \text{ kg m}^{-3}$
$n = 0.3 \quad T_h = 1685.04 \text{ K} \quad 1620 \text{ K} < T_c < 1630 \text{ K}$	

$k_l = 64 \text{ W m}^{-1} \text{ K}^{-1}$	$k_s = 64 \text{ W m}^{-1} \text{ K}^{-1}$
$\mu_l = 0.0032634 \text{ kg m}^{-1} \text{ s}^{-1}$	$\mu_s = 326.34 \text{ kg m}^{-1} \text{ s}^{-1}$
$\beta = 1.4 \times 10^{-4} \text{ K}^{-1}$	$\beta_s = 0.0875$
$g = 9.81 \text{ m s}^{-2}$	$\mu_m = 1.2566 \times 10^{-5} \text{ T m A}^{-1}$
$Te = 1681 \text{ K}$	$C_e = 0.8 \text{ kg m}^{-3}$

MHD – Example 6 (no magnetic fields)

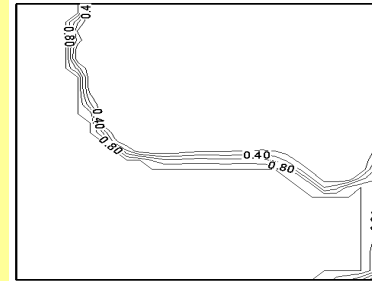
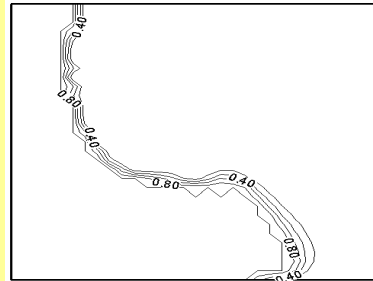
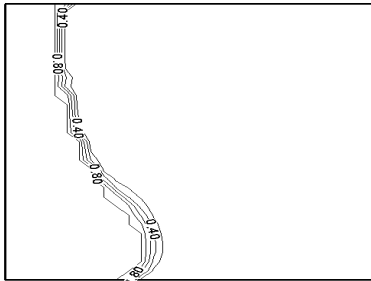


15 min

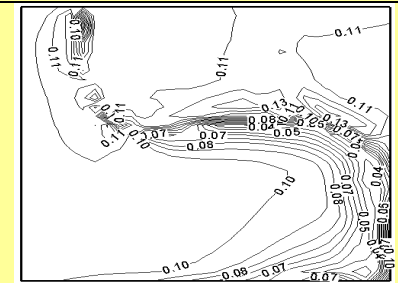
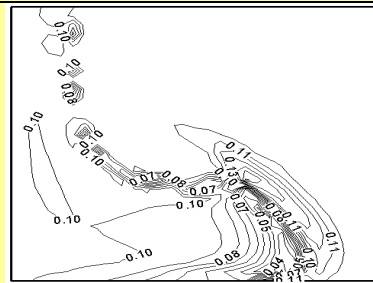
30 min

45 min

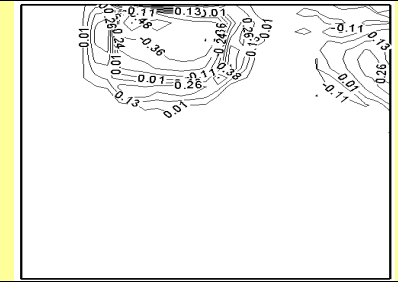
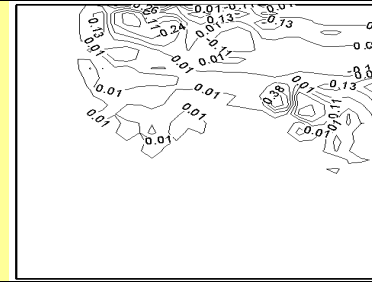
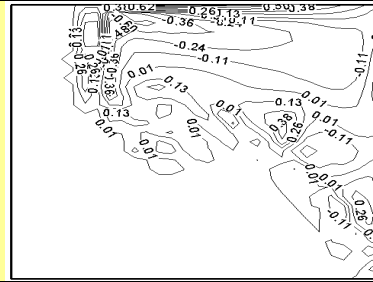
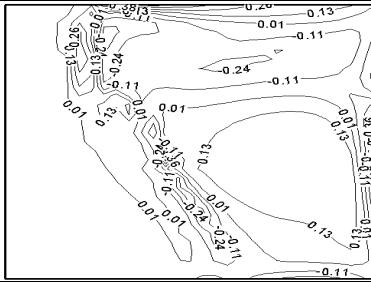
60 min



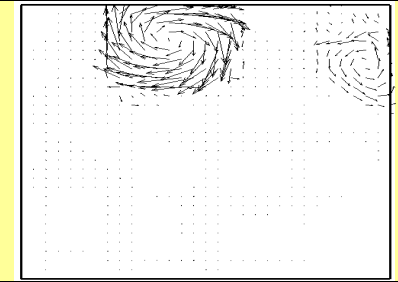
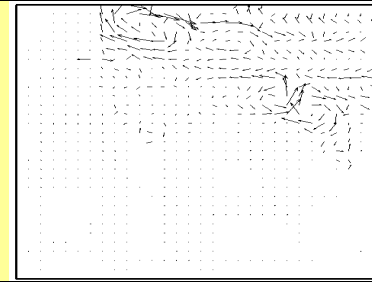
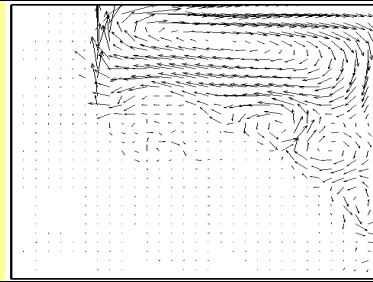
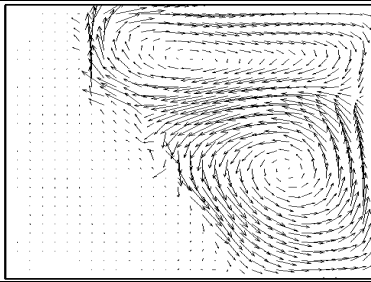
(a) Void fraction



(b) Concentration



(c) Vorticity

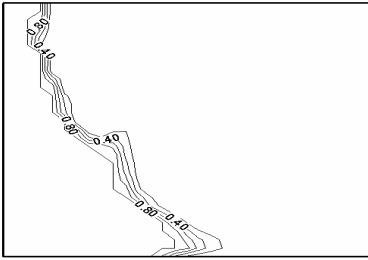


(e) Velocity vectors

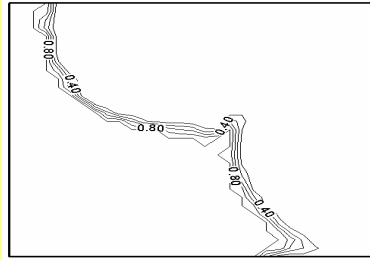
MHD – Example 6 (optimized magnetic fields)



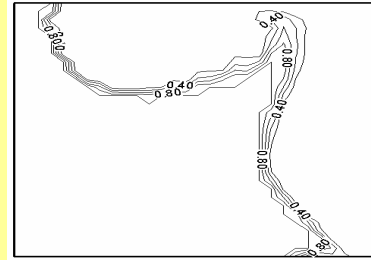
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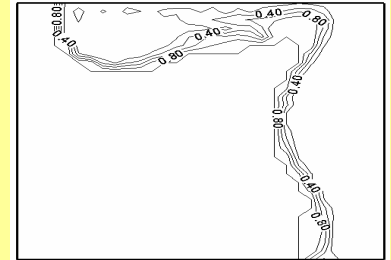
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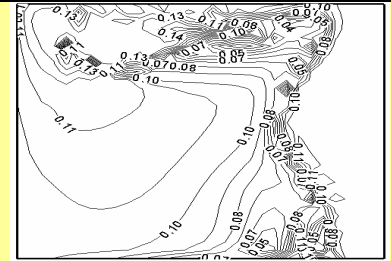
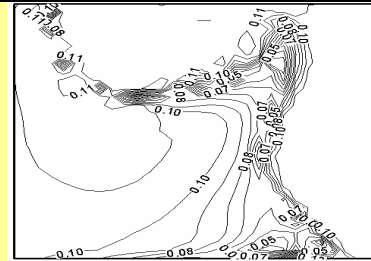
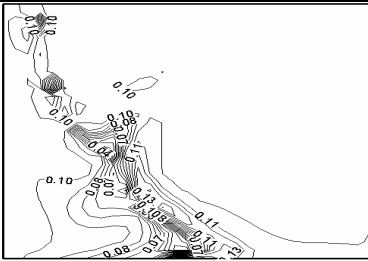
45 min



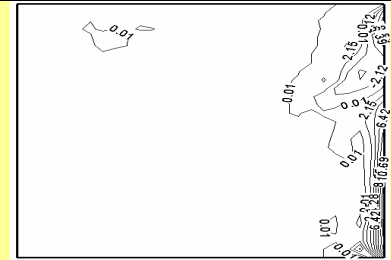
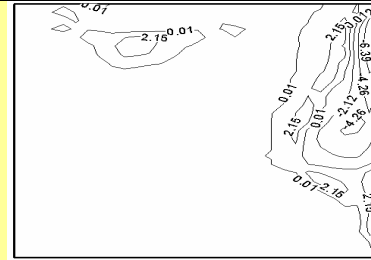
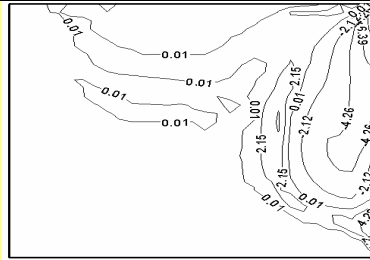
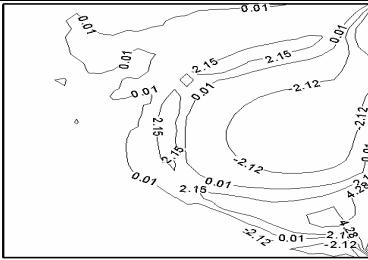
60 min



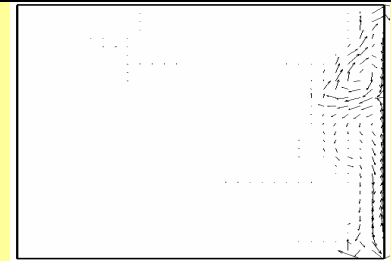
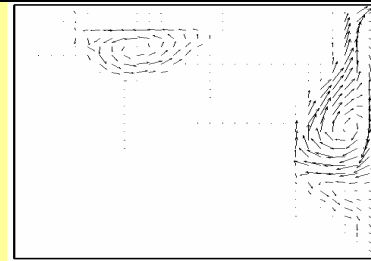
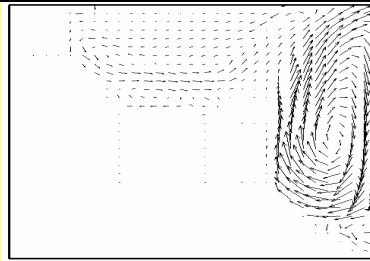
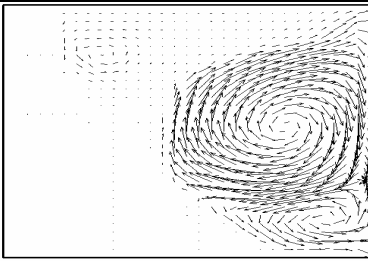
(a) Void fraction



(b) Concentration



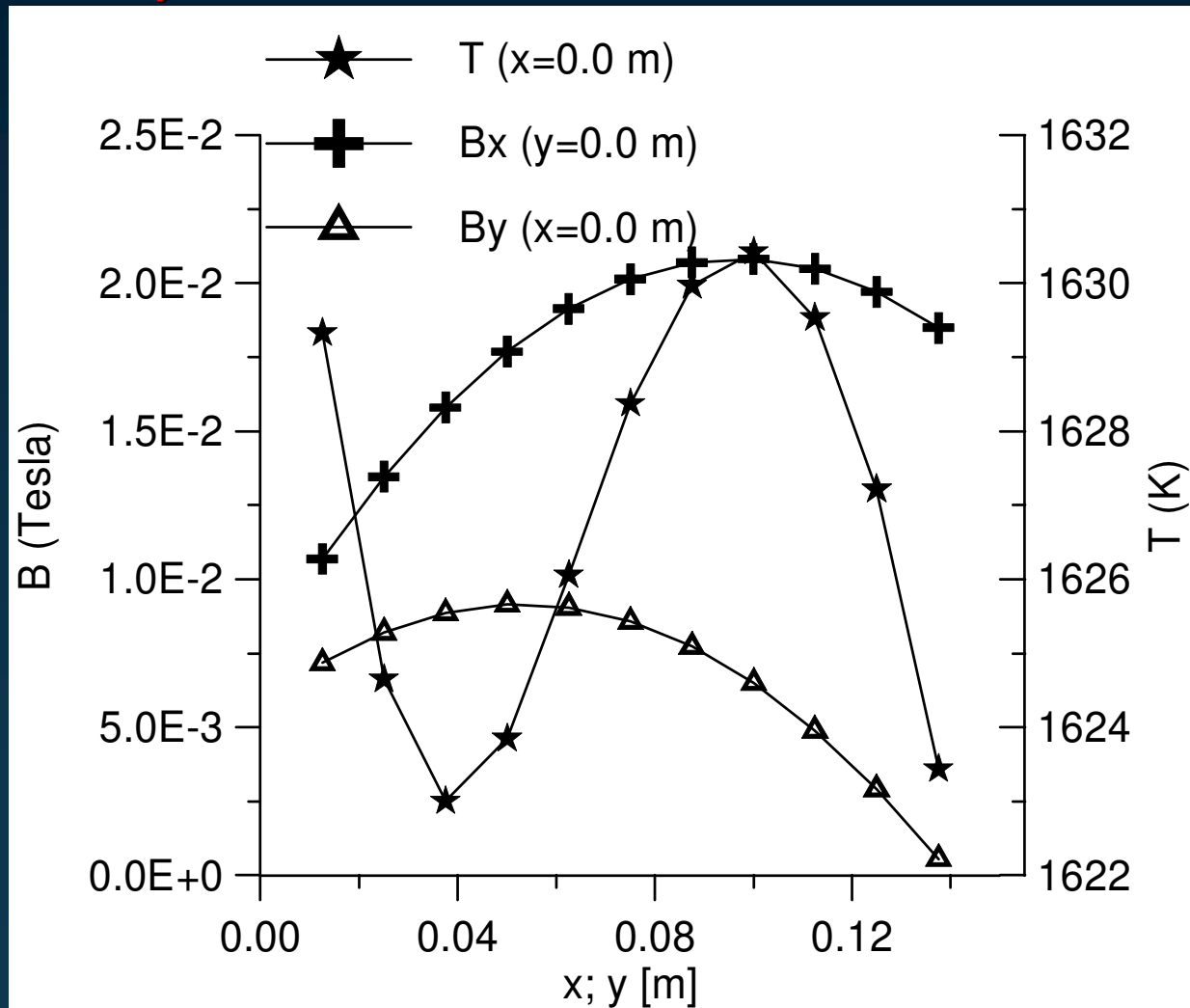
(c) Vorticity



(e) Velocity vectors

MHD – Example 6

→ Optimized boundary conditions



Electrohydrodynamic

Direct Problem - EHD

→ Conservation equations in the Cartesian coordinate system (x,y)

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} = S$$

where

$$Q = \lambda \phi$$

$$E = (\lambda u + \zeta E_x) \phi - \Gamma \frac{\partial \phi^*}{\partial x}$$

$$F = (\lambda v + \zeta E_y) \phi - \Gamma \frac{\partial \phi^*}{\partial y}$$

$$\mathbf{E} = -\nabla \phi$$

Conservation of	λ	ζ	ϕ	ϕ^*	Γ	S
Mass	ρ	0	1	1	0	0
x-momentum	ρ	0	u	u	μ	$-\frac{\partial P}{\partial x} + q_e E_x$
y-momentum	ρ	0	v	v	μ	$-\frac{\partial P}{\partial y} - \rho g[1 - \beta(T - T_0)] + q_e E_y$
Energy	ρ	0	h	T	K	$C_P \left[b(E_x^2 + E_y^2) + uE_x + vE_y - D_e \left(E_x \frac{\partial q_e}{\partial x} + E_y \frac{\partial q_e}{\partial y} \right) \right]$
Electric potential	0	0	0	ϕ	1	$-\frac{q_e}{\epsilon_0}$
Electric charged particles distribution	1	b	q_e	q_e	D_e	0

Direct Problem - EHD

- Conservation of **mass, momentum and energy** in the “computational” coordinate system (ξ, η)

$$\frac{\partial(J\rho\phi)}{\partial t} + \frac{\partial(\tilde{U}\rho\phi)}{\partial \xi} + \frac{\partial(\tilde{V}\rho\phi)}{\partial \eta} =$$

$$\frac{\partial}{\partial \xi} \left\{ \mathcal{M}^\phi \left[a \frac{\partial \phi^*}{\partial \xi} + d \frac{\partial \phi^*}{\partial \eta} \right] \right\} + \frac{\partial}{\partial \eta} \left\{ \mathcal{M}^\phi \left[d \frac{\partial \phi^*}{\partial \xi} + b \frac{\partial \phi^*}{\partial \eta} \right] \right\} + JS$$

where

$$a = \xi_x^2 + \xi_y^2$$

$$b = \eta_x^2 + \eta_y^2$$

$$d = \xi_x \eta_x + \xi_y \eta_y$$

$$\tilde{U} = J(u\xi_x + v\xi_y)$$

$$\tilde{V} = J(u\eta_x + v\eta_y)$$

$$\xi_x = \frac{y_\eta}{J}$$

$$\xi_y = -\frac{x_\eta}{J}$$

$$\eta_x = -\frac{y_\xi}{J}$$

$$\eta_y = \frac{x_\xi}{J}$$

$$J = x_\xi y_\eta - x_\eta y_\xi$$

Direct Problem - EHD

- Conservation of the **electric potential** in the “computational” coordinate system (ξ, η)

$$\frac{\partial}{\partial \xi} \left\{ J \Gamma^{\phi} \left[a \frac{\partial \phi^*}{\partial \xi} + d \frac{\partial \phi^*}{\partial \eta} \right] \right\} + \frac{\partial}{\partial \eta} \left\{ J \Gamma^{\phi} \left[d \frac{\partial \phi^*}{\partial \xi} + b \frac{\partial \phi^*}{\partial \eta} \right] \right\} + JS = 0$$

where

$$\begin{aligned} a &= \xi_x^2 + \xi_y^2 \\ b &= \eta_x^2 + \eta_y^2 \\ d &= \xi_x \eta_x + \xi_y \eta_y \end{aligned}$$

$$\begin{aligned} \xi_x &= \frac{y_{\eta}}{J} \\ \xi_y &= -\frac{x_{\eta}}{J} \\ \eta_x &= -\frac{y_{\xi}}{J} \\ \eta_y &= \frac{x_{\xi}}{J} \\ J &= x_{\xi} y_{\eta} - x_{\eta} y_{\xi} \end{aligned}$$

Direct Problem - EHD

- Conservation of the **electric charged particles distribution** in the “computational” coordinate system (ξ, η)

$$\frac{\partial(J\rho\phi)}{\partial t} + \frac{\partial(\tilde{U}\rho\phi)}{\partial \xi} + \frac{\partial(\tilde{V}\rho\phi)}{\partial \eta} =$$

$$\frac{\partial}{\partial \xi} \left\{ \mathcal{L}^\phi \left[a \frac{\partial \phi^*}{\partial \xi} + d \frac{\partial \phi^*}{\partial \eta} \right] \right\} + \frac{\partial}{\partial \eta} \left\{ \mathcal{L}^\phi \left[d \frac{\partial \phi^*}{\partial \xi} + b \frac{\partial \phi^*}{\partial \eta} \right] \right\} + JS$$

where

$$a = \xi_x^2 + \xi_y^2$$

$$b = \eta_x^2 + \eta_y^2$$

$$d = \xi_x \eta_x + \xi_y \eta_y$$

$$\tilde{U} = J[(u + bE_x)\xi_x + (v + bE_y)\xi_y]$$

$$\tilde{V} = J[(u + bE_x)\eta_x + (v + bE_y)\eta_y]$$

$$\xi_x = \frac{y_\eta}{J}$$

$$\xi_y = -\frac{x_\eta}{J}$$

$$\eta_x = -\frac{y_\xi}{J}$$

$$\eta_y = \frac{x_\xi}{J}$$

$$J = x_\xi y_\eta - x_\eta y_\xi$$

Direct Problem - EHD

→ Test-cases analyzed: Gallium Arsenide under natural convection

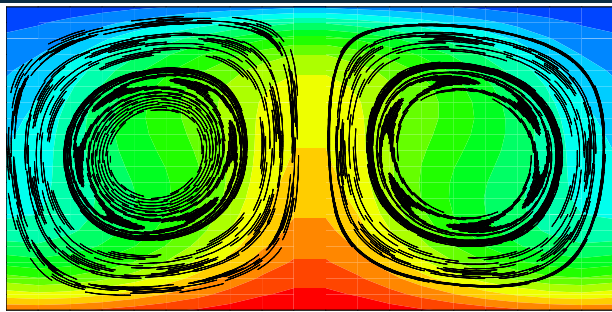
Property	Value
ρ_l	5710 kg/m ³
ρ_s	5196 kg/m ³
C_{Pl}	434 J/kg.K
C_{Ps}	416 J/kg.K
K_l	17.8 W/m.K
K_s	7 W/m.K
b_l	1 x 10 ⁻⁸ m ² /V
b_s	1 x 10 ⁻¹⁴ m ² /V
D_{el}	2.5 x 10 ⁻¹⁰ m ² /s
D_{es}	2.5 x 10 ⁻¹⁶ m ² /s

β_l	1.87 x 10 ⁻⁴ 1/K
β_s	1.87 x 10 ⁻⁴ 1/K
σ_l	8 x 10 ⁵ 1/W.m
σ_s	3 x 10 ⁴ 1/W.m
ϵ_0	8.854 x 10 ⁻¹² kg.m/s ² V ²
L	726,000 J/kg
μ_l	2.79 x 10 ⁻³ kg/m.s
μ_s	2.79 x 10 ² kg/m.s
T_l	1511.005 K
T_s	1511 K

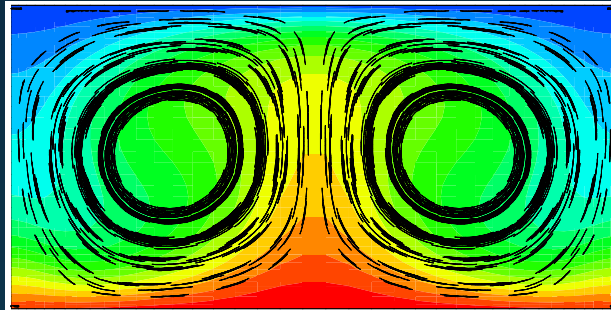
Direct Problem - EHD

→ Natural Convection without solidification ($Ra=1.9 \times 10^4$)

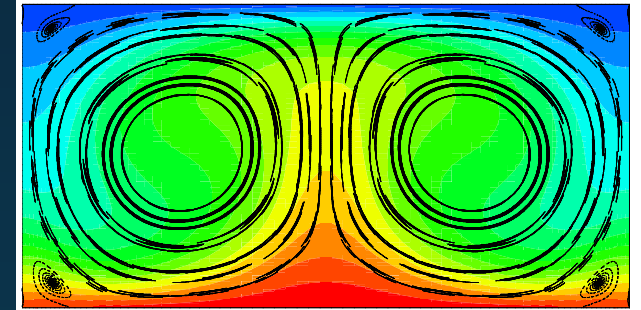
Grid 20x20 cells (9 min.)



Grid 40x40 cells (47 min.)



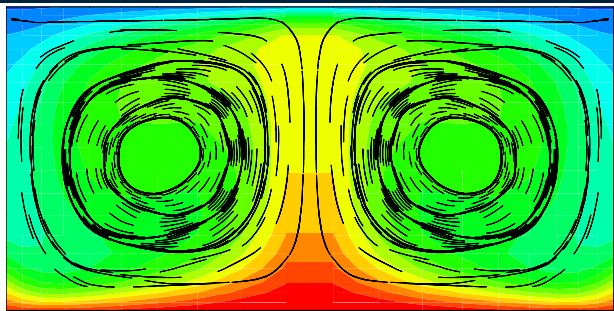
Grid 80x80 (892 min.)



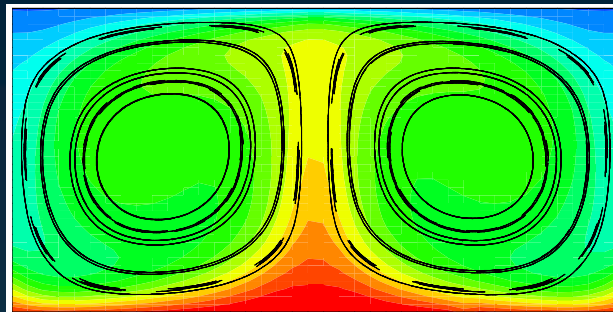
Direct Problem - EHD

→ Natural Convection without solidification ($Ra=1.9 \times 10^5$)

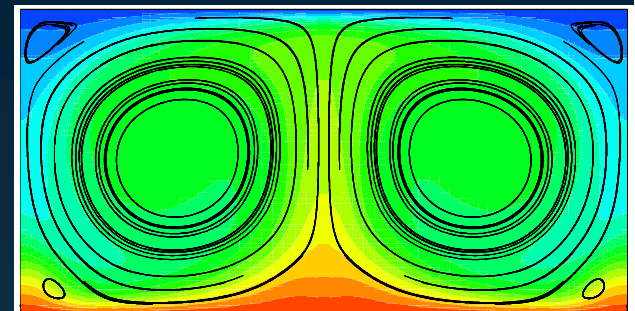
Grid 20x20 cells (8 min.)



Grid 40x40 cells (43 min.)

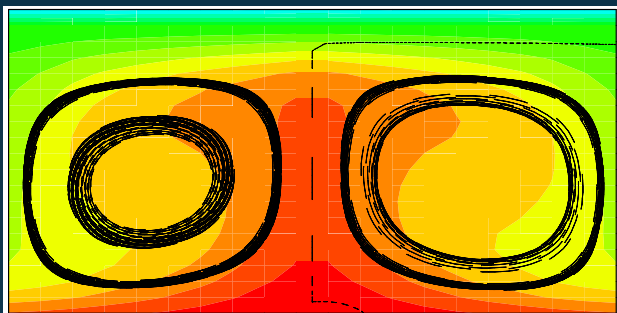


Grid 80x80 (694 min.)

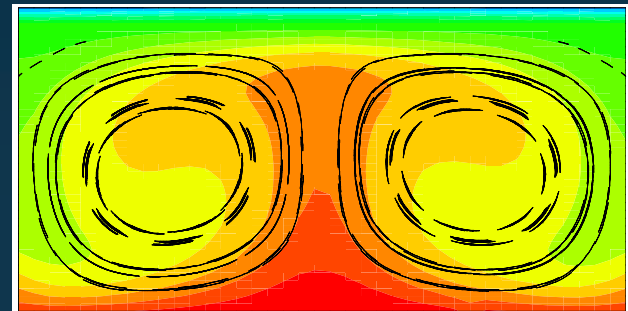


→ Natural Convection with solidification ($Ra=1.9 \times 10^5$)

Grid 20x20 cells (15 min.)



Grid 40x40 cells (116 min.)



Optimization Problem - EHD

→ Motivation

- Control the natural convection effects by the introduction of an externally applied electric field.
- Reduce the internal thermal stresses within the solid material

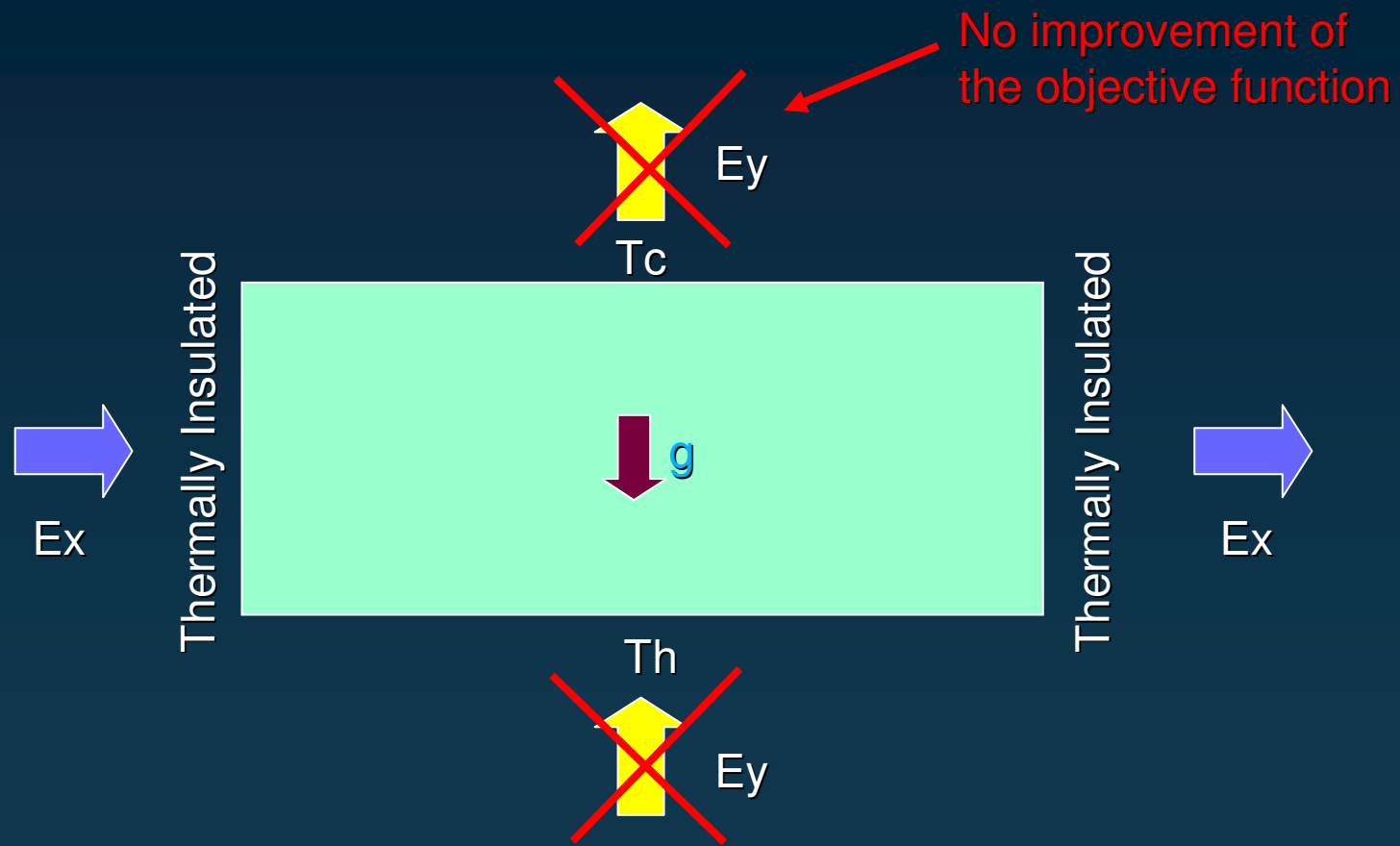
→ Cost function to be minimized

- Reduce the temperature gradients along the x coordinate

$$F = \sqrt{\frac{1}{\#cells} \sum_{i=1}^{\#cells} \left(\frac{\partial T_i}{\partial x_i} \right)^2}$$

Optimization Problem - EHD

- Reduce the natural convection effects by applying an externally electric potential

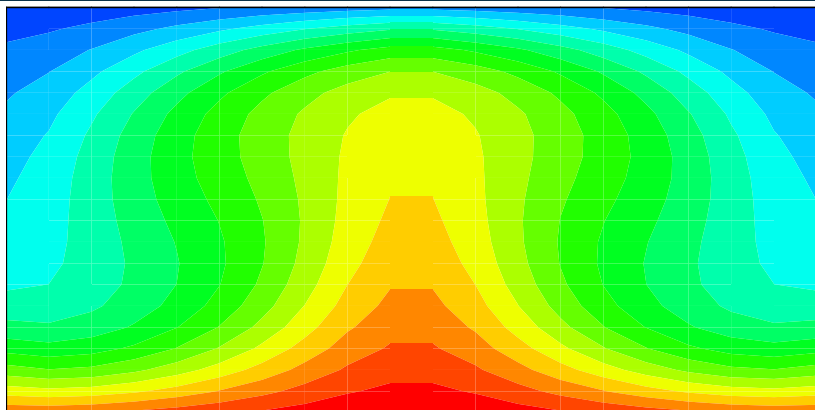
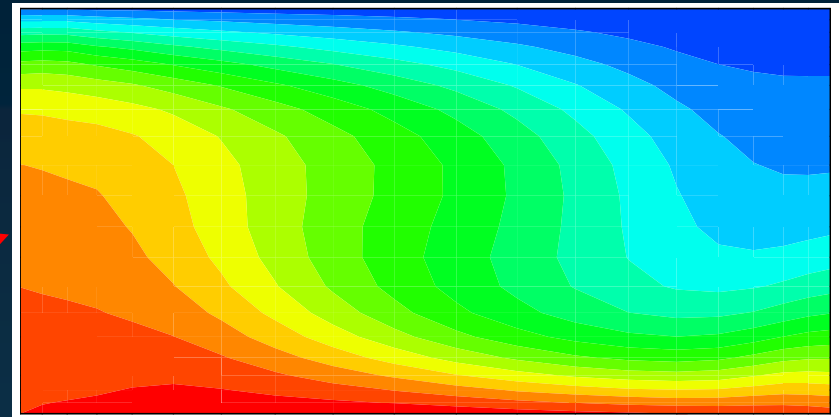


Optimization Problem - EHD

→ Results for the natural convection case without solidification

- 6 parameters per boundary for electric potential discretization
- $Ra=1.9 \times 10^4$

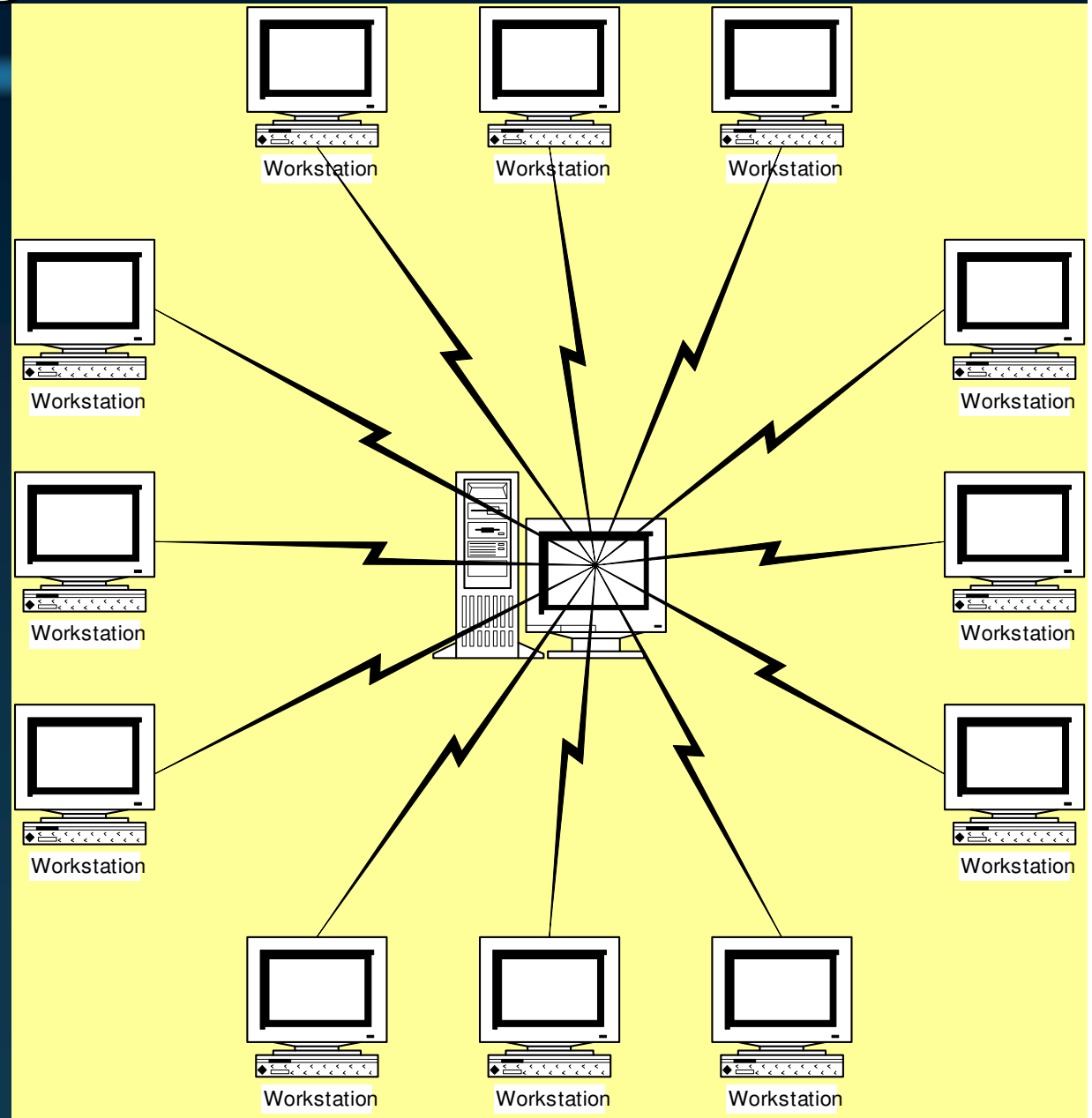
With **optimized** electric potential



Without electric potential

Hybrid Methods

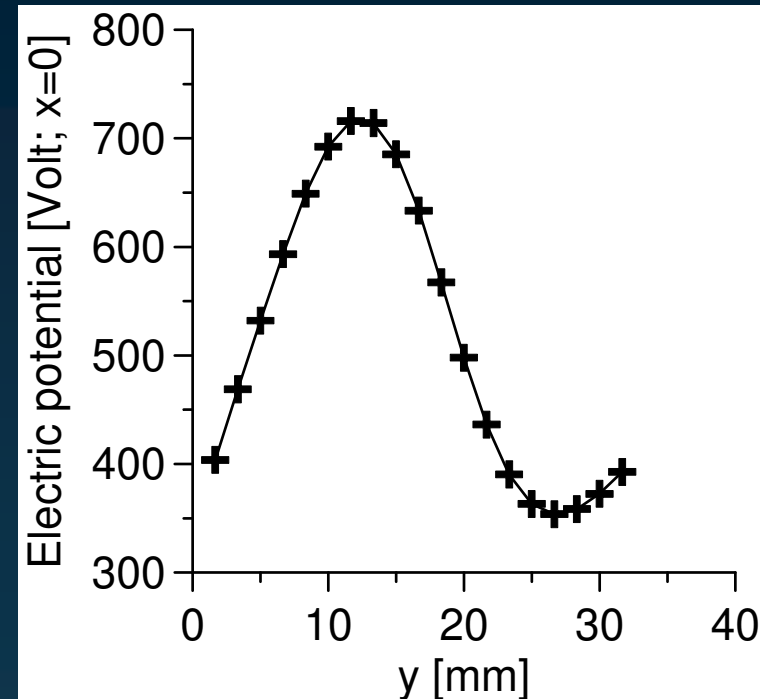
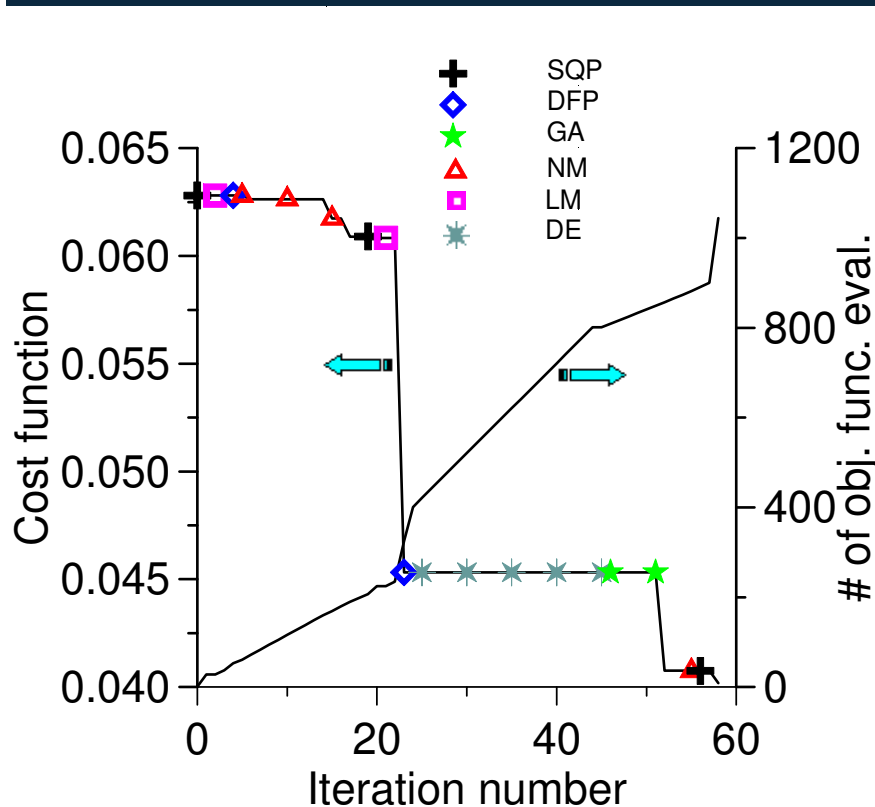
→ Parallel Computing



Optimization Problem - EHD

→ Results for the natural convection case without solidification

- 6 parameters per boundary for electric potential discretization
- $Ra=1.9 \times 10^4$



How long it would take, on a single machine, using:

20x20 grid cells = 7 days

40x40 grid cells = 34 days

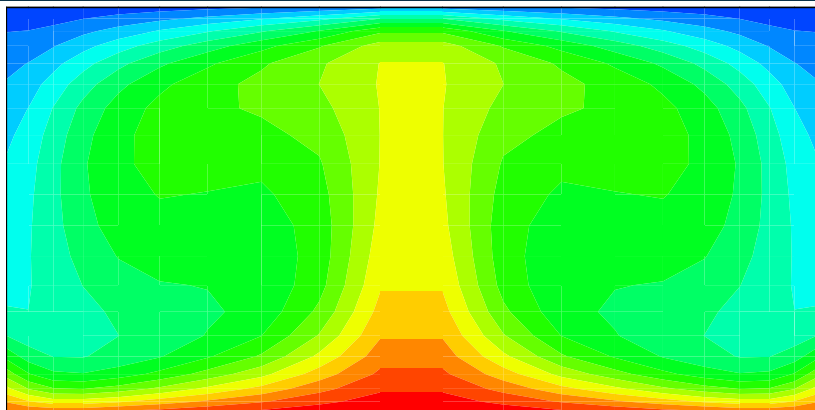
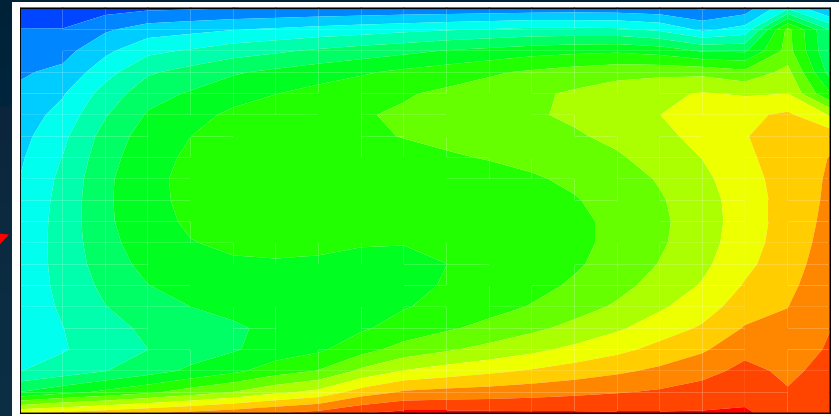
80x80 grid cells = 647 days

Optimization Problem - EHD

→ Results for the natural convection case without solidification

- 6 parameters per boundary for electric potential discretization
- $Ra=1.9 \times 10^5$

With **optimized** electric potential

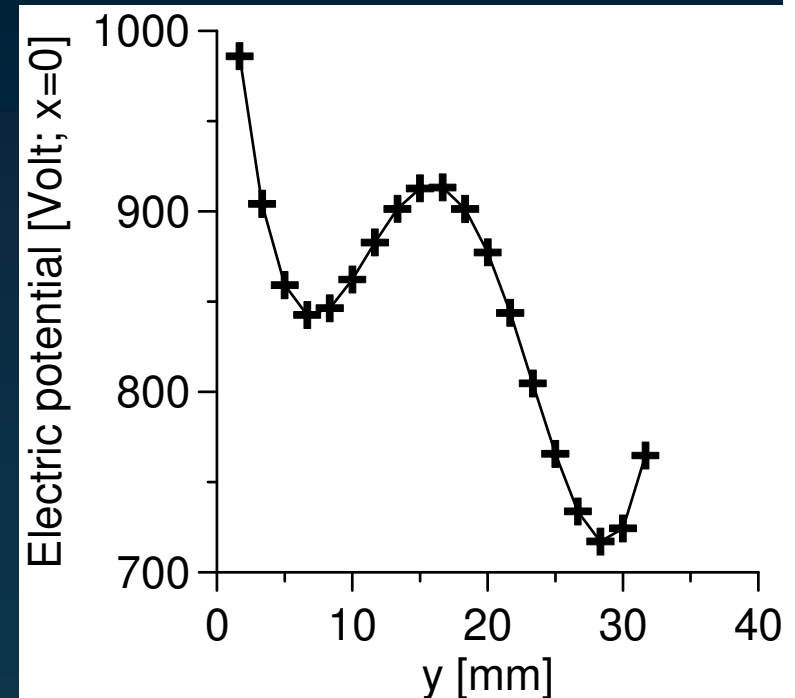
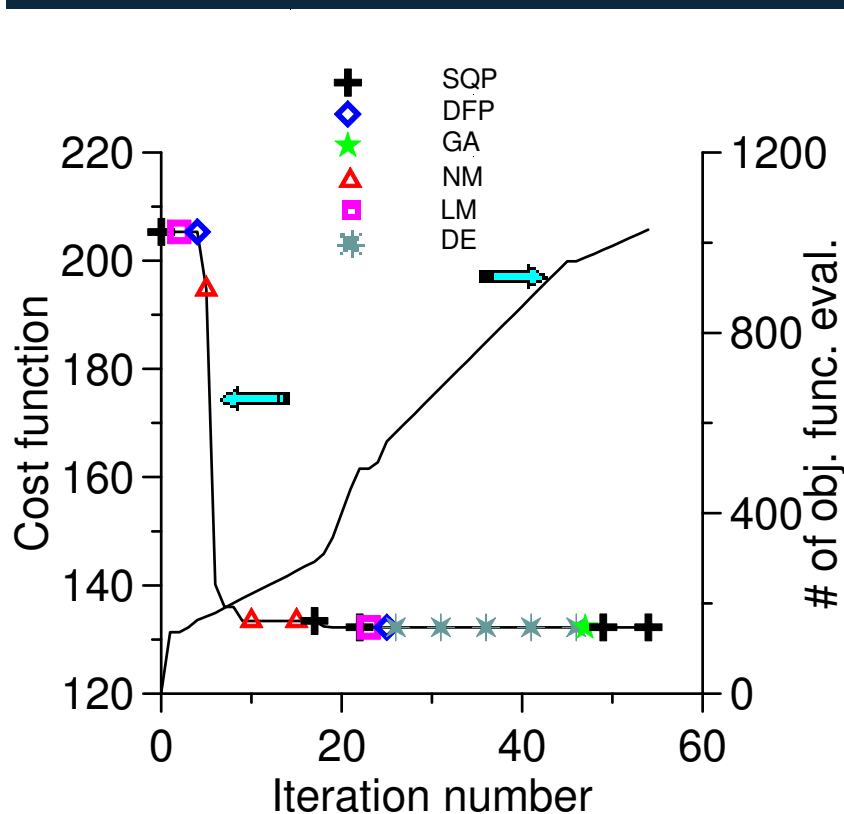


Without electric potential

Optimization Problem - EHD

→ Results for the natural convection case without solidification

- 6 parameters per boundary for electric potential discretization
- $Ra=1.9 \times 10^5$



How long it would take, on a single machine, using:

20x20 grid cells = 6 days

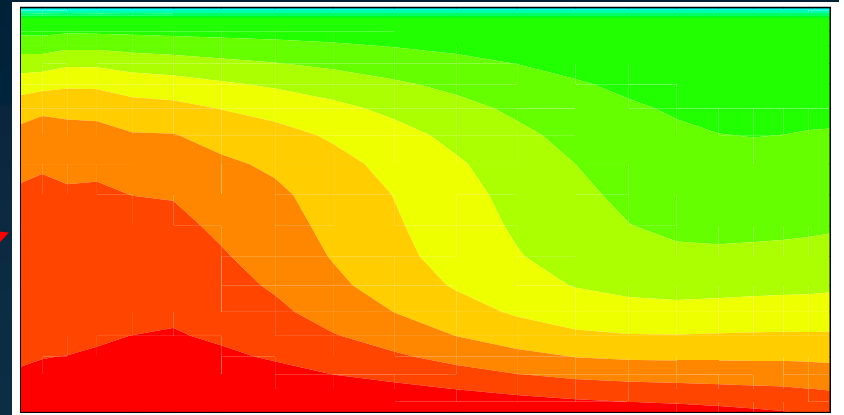
40x40 grid cells = 31 days

80x80 grid cells = 496 days

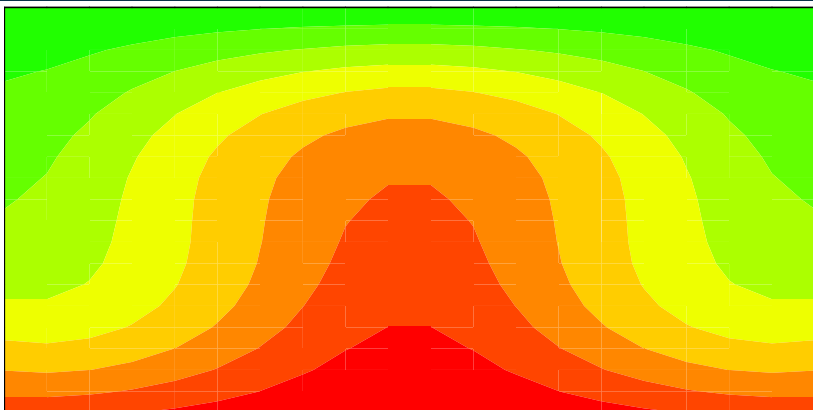
Optimization Problem - EHD

- Results for the natural convection case with solidification
- 6 parameters per boundary for electric potential discretization
 - $Ra=1.9 \times 10^4$

With **optimized** electric potential

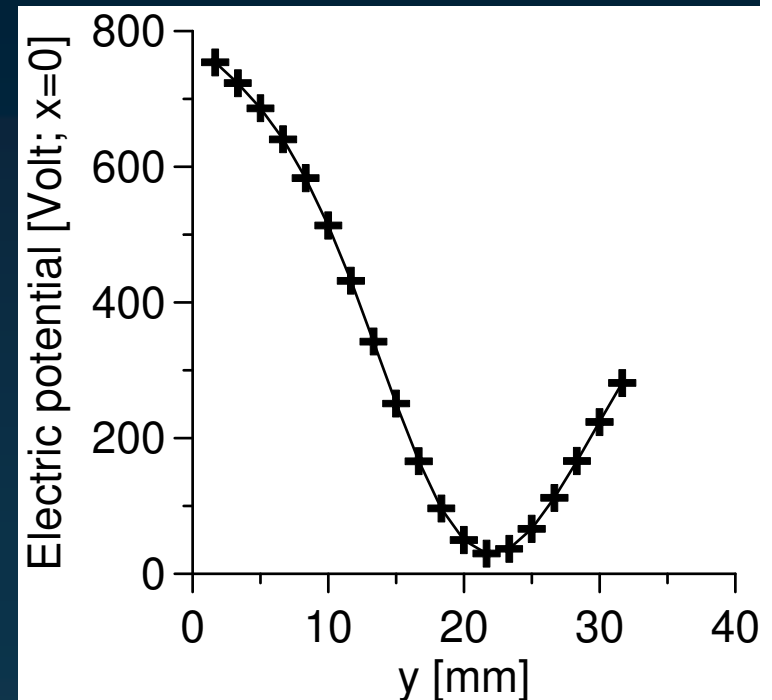
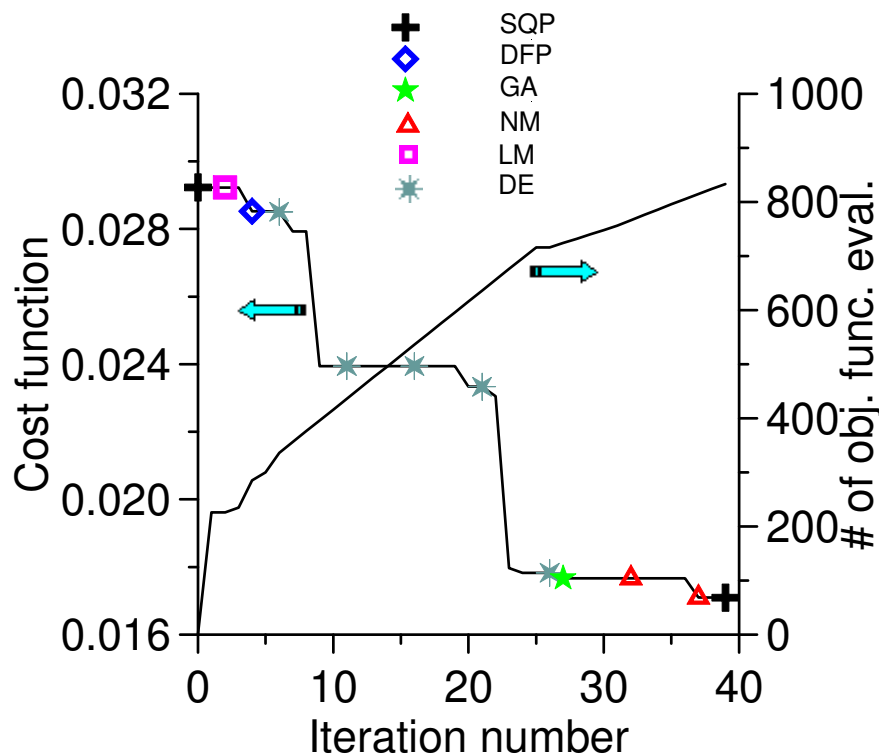


Without electric potential



Optimization Problem - EHD

- Results for the natural convection case with solidification
 - 6 parameters per boundary for electric potential discretization
 - $Ra=1.9 \times 10^4$



How long it would take, on a single machine, using:
 20x20 grid cells = 9 days
 40x40 grid cells = 67 days

Acknowledgments

- CAPES and CNPq, two Brazilian agencies for scientific and technological development.
- IME, Military Institute of Engineering.
- UTA, University of Texas at Arlington.
- FIU, Florida International University.
- UFRJ, Federal University of Rio de Janeiro.

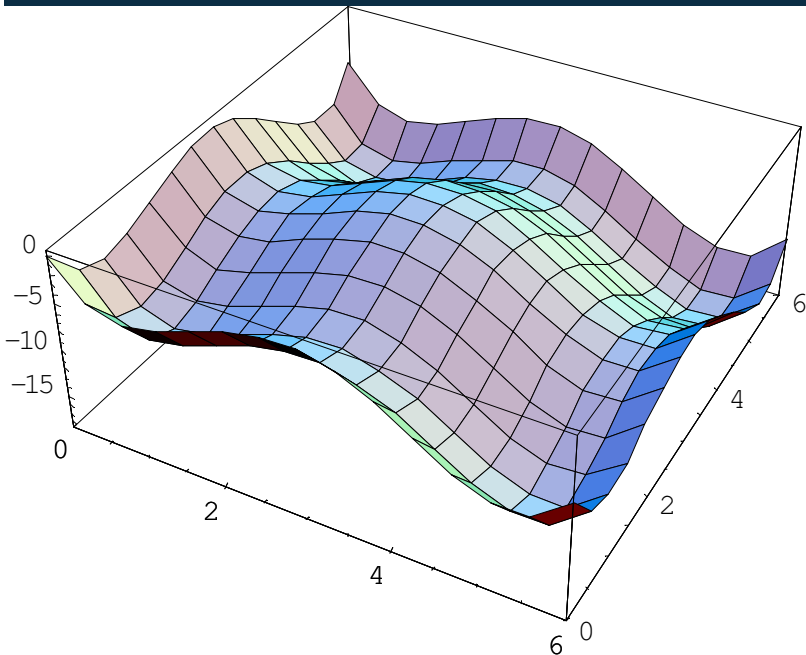
Other people that contributed in this work

- George S. Dulikravich, Florida International University
- Helcio R. B. Orlande, Federal University of Rio de Janeiro
- Brian H. Dennis, University of Texas at Arlington
- Thoman J. Martin, Pratt & Whitney Engine Group

Sample codes

→ Minimization of Rosen's function

- Steepest Descent Method
- Conjugate Gradient Method
- Newton's Method
- Particle Swarm Method



→ RBF

- Multiquadrics in R^N

$$s(x_i) = f(x_i) = \sum_{j=1}^N \alpha_j \phi(|x_i - x_j|)$$

$$\phi(|x - x_j|) = \sqrt{(x - x_j)^2 + c_j^2}$$

Thank you!



Questions?