The Sensitivity Equation Method: Characterisation and Optimisation of Flow Systems

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Theme of talk

Computational issues

- Complexity of PDEs modeling the system
- Cost of solving PDEs
- Many parameters ; not all are important
- Accuracy of numerics for optimisation
- Must assess uncertainty due to input data

Tools

- Adaptive FEM for accuracy & efficiency
- SEM : key parameters, optimisation, uncertainty

Outline

- CFD & sensitivities : Context
- Sensitivities : definition and uses
- Flow equations
- FEM & mesh adaptation
- SEM
- Application : Characterisation
- Application : Optimization
- Conclusions

Real Problems

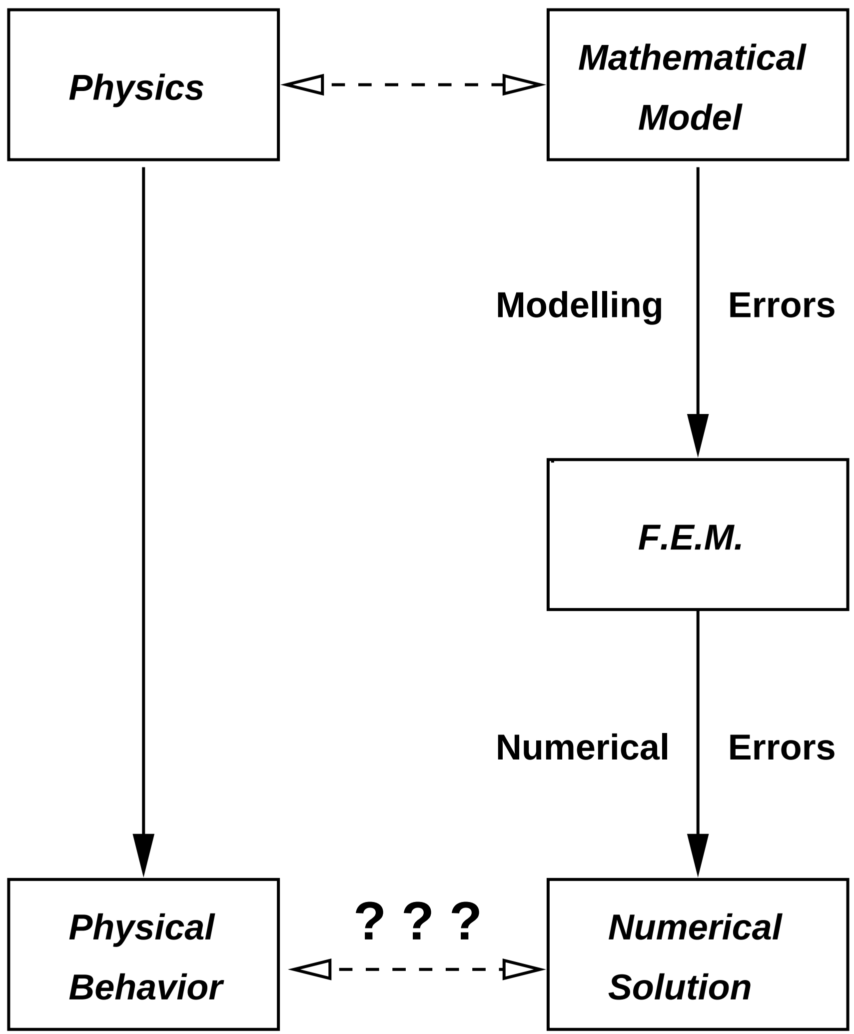
- High Reynolds, Péclet, Rayleigh numbers
- Extreme/Thin geometries
- Extreme/Thin features

1. Unknown kind
2. Unknown location
3. Unknown extent

- Input data uncertainty

- How to design under such conditions ?

Simulation Context



Issues :

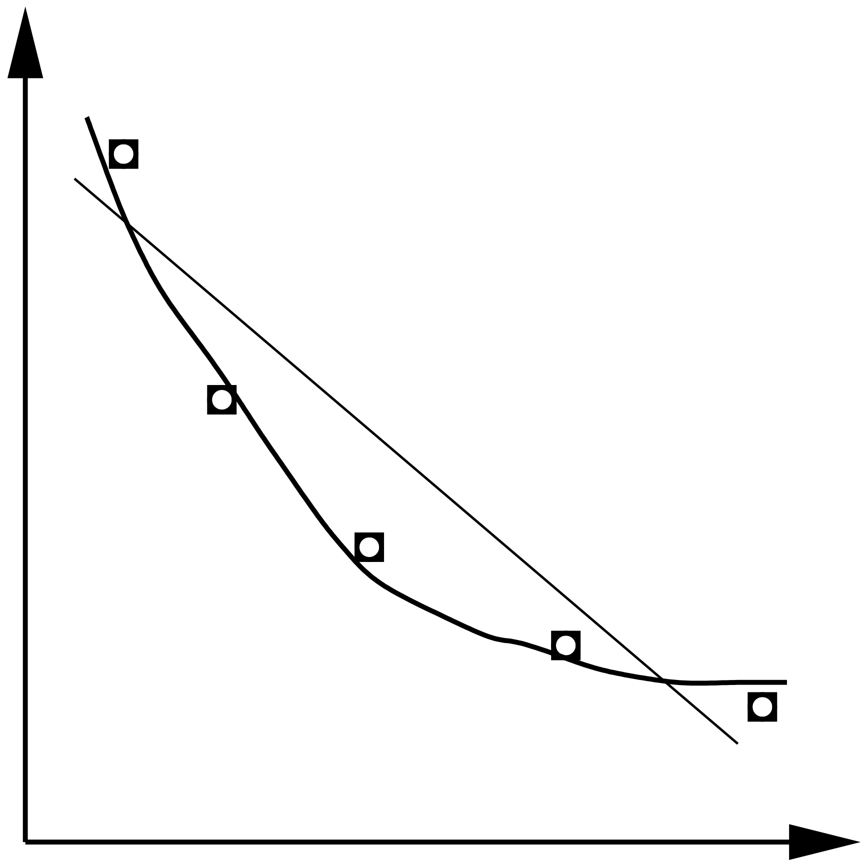
1. Numerical accuracy
2. Modelling errors
3. Input uncertainty
4. Experimental uncertainty

Tools

1, 2 = Mesh adaptation

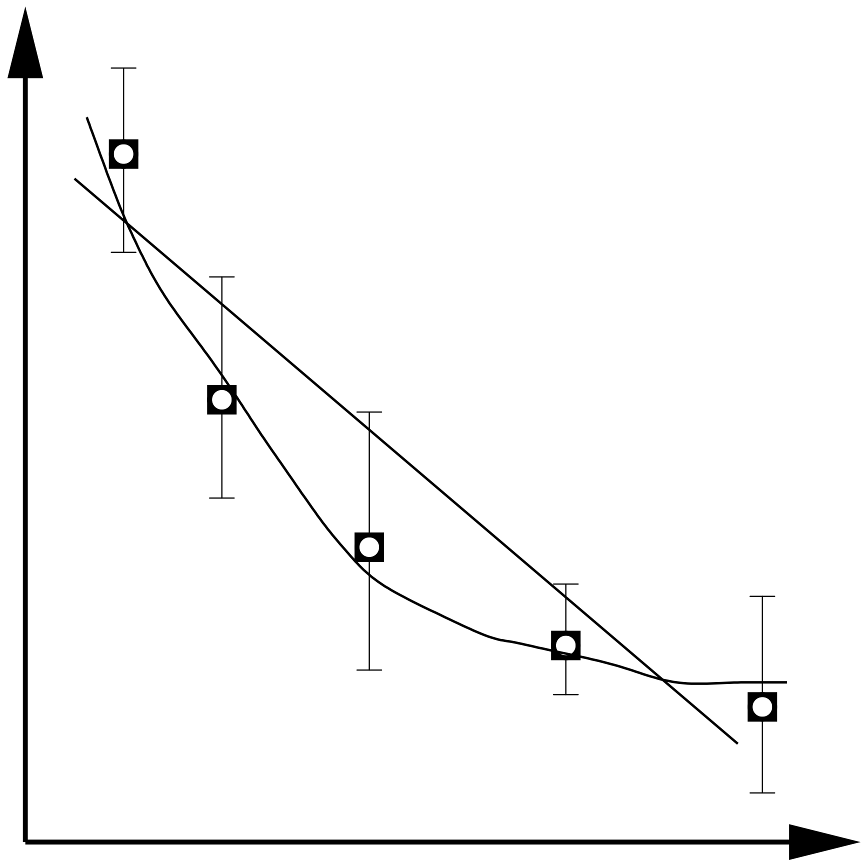
3, 4 = Sensitivities

Modeling & Simulation (1)



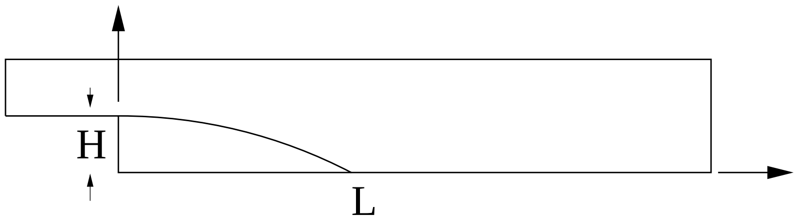
- **Situation :**
  - Linear model
  - Nonlinear model
  - Data points
- **Which is best ?**

Modeling & Simulation (2)

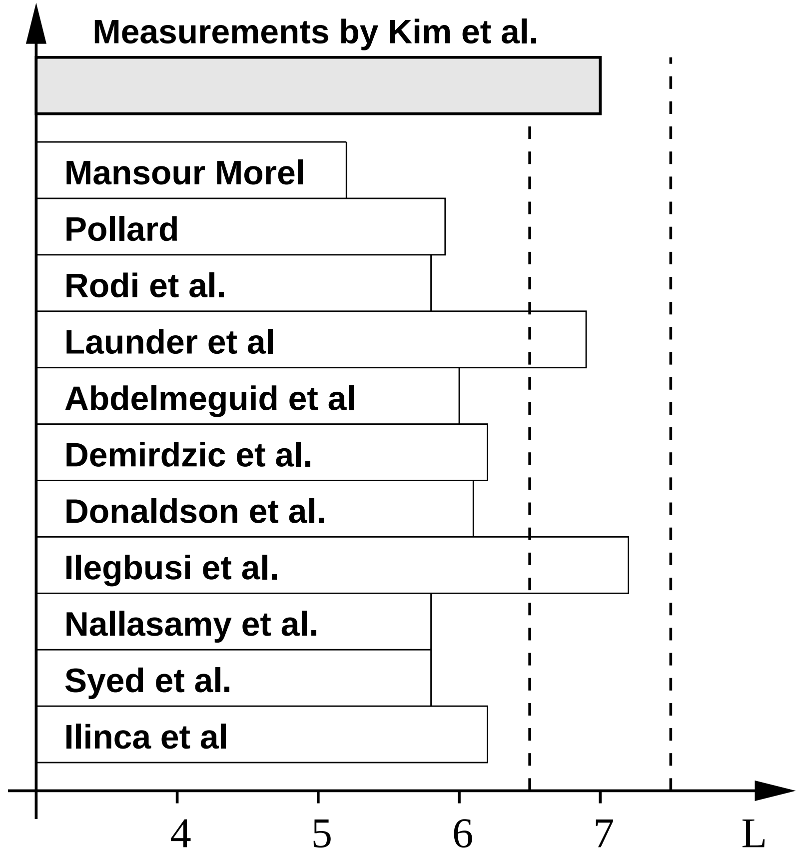


- **Situation :**
  - Linear model
  - Nonlinear model
  - Data points
  - Data uncertainty
- **Which is best ?**

Turbulent flow over step



- Same turbulence model
- Same code
- Except Donalson & Ilinca
- Different meshes



Navier-Stokes : laminar flow

- Free convection
- Variable properties = functions of T

$$\nabla \cdot \boldsymbol{u} = 0$$

$$\rho c_p \boldsymbol{u} \cdot \nabla T = \nabla \cdot (\kappa \nabla T) + q$$

$$\rho \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\nabla p + \nabla \cdot \left[\mu \left(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T \right) \right] - \rho \boldsymbol{g} \beta (T - T_0) + \boldsymbol{f}$$

Boundary conditions

$$\boldsymbol{u}(\boldsymbol{x_b}; a) = \hat{\mathbf{u}}(\boldsymbol{x}_b; a) \qquad \text{on } \Gamma_u$$

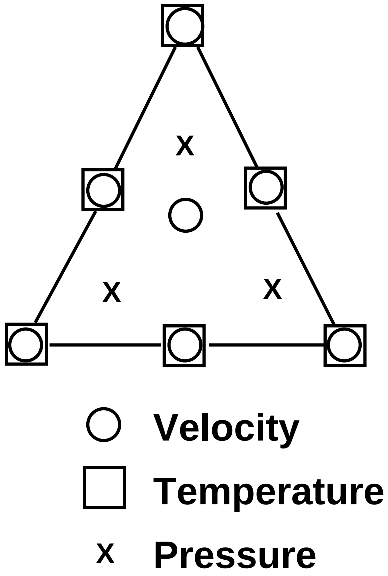
$$\boldsymbol{t}(\boldsymbol{x_b}; a) = \boldsymbol{\sigma} \cdot \hat{\boldsymbol{n}} = \boldsymbol{F}^N(\boldsymbol{x}_b; a) \qquad \text{on } \Gamma_t$$

$$\boldsymbol{\sigma} = \left[-p\boldsymbol{I} + \mu \left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T - \frac{2}{3} \boldsymbol{I} \nabla \cdot \boldsymbol{u} \right) \right]$$

$$T(\boldsymbol{x_b}; a) = \hat{T}(\boldsymbol{x}_b; a) \qquad \text{on } \Gamma_T$$

$$\lambda \nabla T(\boldsymbol{x}_b; a) \cdot \hat{\boldsymbol{n}} = \hat{q}_w(\boldsymbol{x}_b; a) \qquad \text{on } \Gamma_q$$

FEM Solver



- Galerkin FEM + Stabilization
- Primitive variables = (U,V,p) & (T,k,ϵ)
- Augmented Lagrangian
- Newton's Method

Verification and Validation

Verification :

Are we solving the equations **Properly** ?

Validation :

Are we solving the **Proper** equations for the problem at hand ?

Verification

Verification involves :

- mathematics,
- numerical analysis,

For example :

- ? Is scheme/code implementation really $O(\delta x^2)$?
- ? $O(\delta x^2)$? on the case at hand ?

Validation

Validation means having

- the proper physics,
- the proper science,
- an appropriate engineering model.

Requirements :

- detailed experiments,
- high quality measurements.

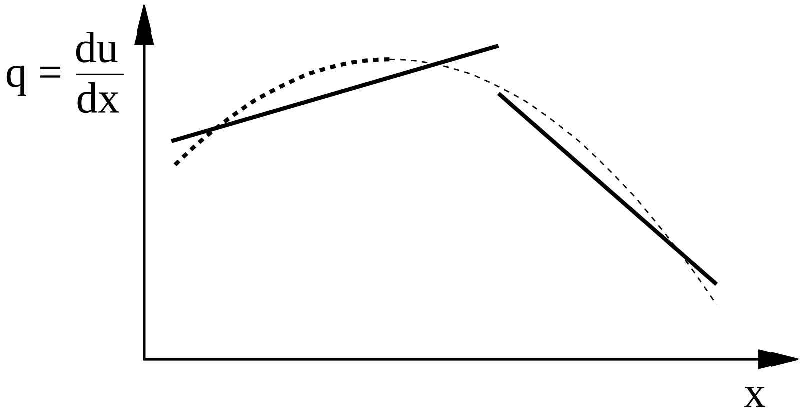
Adaptivity

- M_i : i^{th} adaptive mesh
- P_i : degree of interpolant

0. Initial Discretisation : (M_0, P_0)
1. FEM Solver : U_i
2. Error Estimation : $E_i(M_i, P_i, U_i)$
3. if ($E_i < \epsilon$) $\longrightarrow$ STOP
4. Adaptation $(M_{i+1}, P_{i+1}) = A(M_j, P_j, U_j)$

   Goto 1

Projection Error Estimator



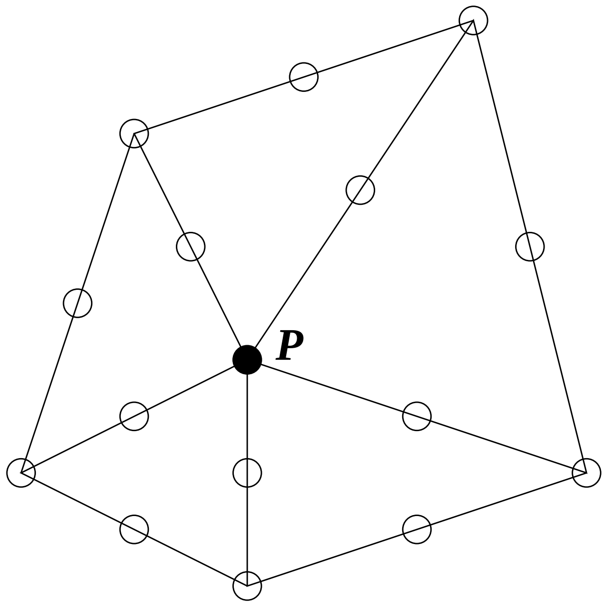
Error in derivative

$$e^2 = \int (q_{ex} - q_h)^2 dx$$

$$e^2 \simeq E^2 = \int (q^* - q_h)^2 dx$$

q^* an approximation of q_{ex}

Projection Error Estimator



$$Min \int_{\Omega_S} (q^* - q_h)^2 \, d\Omega$$

$$q^* = [1, x, y, x^2, xy, y^2][a1, \ldots, a6] = P\vec{a}$$

$$\left[\int_{\Omega_S} P^T P \, d\Omega\right] \{a\} = \left[\int_{\Omega_S} P^T q_h \, d\Omega\right]$$

Projection : Navier-Stokes

$$e_U^2 = \int (\tau^* - \tau_h) : (\tau^* - \tau_h)$$

$$e_P^2 = \int (p^* - p_h)^2$$

$$e_T^2 = \int (\nabla T^* - \nabla T_h) \cdot (\nabla T^* - \nabla T_h)$$

$$\tau = \mu \left[\nabla U + (\nabla U)^T \right]$$

New Mesh

- Target accuracy = $\bar{\eta}\%$
- Target error : $\bar{e} = \bar{\eta}\frac{\|U\|}{\sqrt{N_e}}$
- Equidistribution :
  - $e_i = cte \qquad , \qquad i = 1, .., N_e$
- Asymptotic convergence rate :
  - $e_i = Ch_i^k$
  - $\bar{e} = C\delta_i^k$
- New element size :

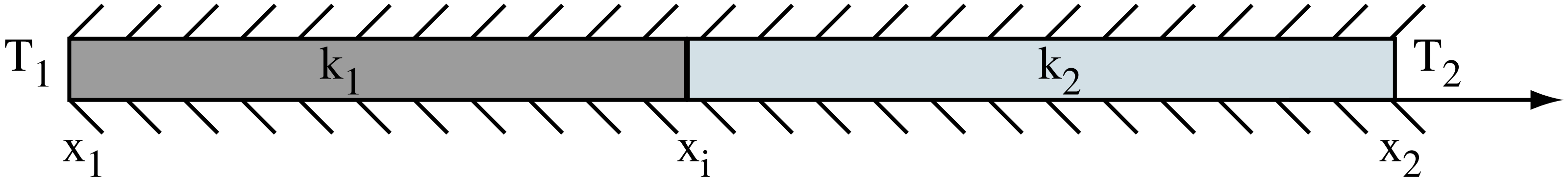
$$\delta_i = \left\{\bar{\eta}\frac{\|U\|}{\sqrt{N_e}\|e_i\|}\right\}^{\frac{1}{k}} h_i$$

Multiple fields

$$
\begin{aligned}
e_U &\longrightarrow \delta_U \\
e_P &\longrightarrow \delta_P \\
e_T &\longrightarrow \delta_T \\
e_k &\longrightarrow \delta_k \\
e_\epsilon &\longrightarrow \delta_\epsilon
\end{aligned}
$$

$$\delta = min\{\delta_i\}$$

Sensitivities



$$T = T(x; T_1, T_2, \kappa_1, \kappa_2, x_1, x_i, x_2)$$

Sensitivity with respect to a

$$s_T = \frac{\partial T}{\partial a}$$

$$a \in \{T_1, T_2, \kappa_1, \kappa_2, x_1, x_i, x_2\}$$

Sensitivities : uses

Gradient based optimization : $\min \; J(\boldsymbol{u}(\alpha), p(\alpha); \alpha)$

$$\frac{dJ}{d\alpha} = \frac{\partial J}{\partial \boldsymbol{u}} \underbrace{\frac{\partial \boldsymbol{u}}{\partial \alpha}}_{\boldsymbol{s}_u} + \frac{\partial J}{\partial p} \underbrace{\frac{\partial p}{\partial \alpha}}_{s_p} + \frac{\partial J}{\partial \alpha}$$

Fast nearby solution via Taylor series

$$C_p(x; \alpha_0 + \delta\alpha) = C_p(x; \alpha_0) + \left. \underbrace{\frac{\partial C_p}{\partial \alpha}} \right|_{\alpha_0} \delta\alpha$$

Uncertainty Analysis

Cascade input data uncertainty into CFD outputs

1st Order statistics : $$\sigma^2_{C_f} \approx \sum_{i=1}^{n} (\underbrace{\frac{\partial C_f}{\partial a_i}}_{s_F^{a_i}} \sigma_{a_i})^2$$

Worst case scenario : $$\delta C_f \approx \sum_{i=1}^{n} |\underbrace{\frac{\partial C_f}{\partial a_i}}_{s_F^{a_i}}||\delta a_i|$$

1st Order Sensitivity PDE

Continuity :

$$\boxed{\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0}$$

SEM : differentiate then discretize

$$\frac{\partial}{\partial a}\left[\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right] = 0 \qquad \longrightarrow \qquad \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial a}\right) + \frac{\partial}{\partial y}\left(\frac{\partial v}{\partial a}\right) = 0$$

$$\boxed{\frac{\partial s_u}{\partial x} + \frac{\partial s_v}{\partial y} = 0}$$

1st Order Energy Sensitivity

$$\frac{\partial}{\partial a}\left[\rho c_p \boldsymbol{u}\cdot\nabla T = \nabla\cdot(\kappa\nabla T) + q_s\right]$$

general approach : all possible dependencies

$$T = T(x, y; a)$$

$$c_p = c_p(T(a); a)$$

$$\Downarrow$$

$$\left(\rho' c_p + \rho c_p'\right)\boldsymbol{u}\cdot\nabla T + \rho c_p\left(\boldsymbol{s}_u\cdot\nabla T + \boldsymbol{u}\cdot\nabla s_T\right)$$

$$= \nabla\cdot(\kappa'\nabla T + \kappa\nabla s_T) + q_s'$$

1st Order Momentum Sensitivity

$$\frac{\partial}{\partial a}\left[\ \rho \boldsymbol{u}\cdot\nabla\boldsymbol{u} = -\nabla p + \nabla\cdot\left[\mu\left(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T\right)\right] - \rho\boldsymbol{g}\beta(T - T_0) + \boldsymbol{f}\ \right]$$

$$\Downarrow$$

$$\begin{aligned}\rho'\boldsymbol{u}\cdot\nabla\boldsymbol{u} + \rho\boldsymbol{s}_u\cdot\nabla\boldsymbol{u} + \rho\boldsymbol{u}\cdot\nabla\boldsymbol{s}_u = -\nabla s_p \\ +\nabla\cdot\left[\mu'\left(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T\right) + \mu\left(\nabla\boldsymbol{s}_u + (\nabla\boldsymbol{s}_u)^T\right)\right] \\ -\left(\rho'\boldsymbol{g}\beta + \rho\boldsymbol{g}'\beta + \rho\boldsymbol{g}\beta'\right)(T - T_0) - \rho\boldsymbol{g}\beta\left(s_T - T_0'\right) + \boldsymbol{f}'\end{aligned}$$

Newton linearization : 1 linear system of PDE / parameter

Variable fluid properties

$$\mu = \mu(\boldsymbol{u}(a), T(a); a)$$

$$\mu' = \frac{\partial \mu}{\partial a} + \frac{\partial \mu}{\partial u} s_u + \frac{\partial \mu}{\partial v} s_v + \frac{\partial \mu}{\partial T} s_T$$

$\rightarrow$ chain rule : all dependencies

Boundary conditions : Dirichlet

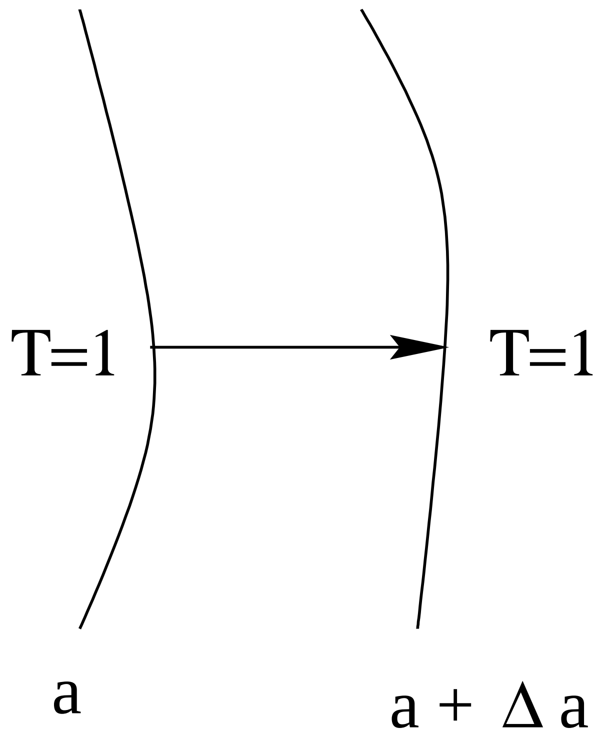
value parameter : $T = T_0$

$$s_T = \frac{\partial T_0}{\partial a}$$

shape parameter

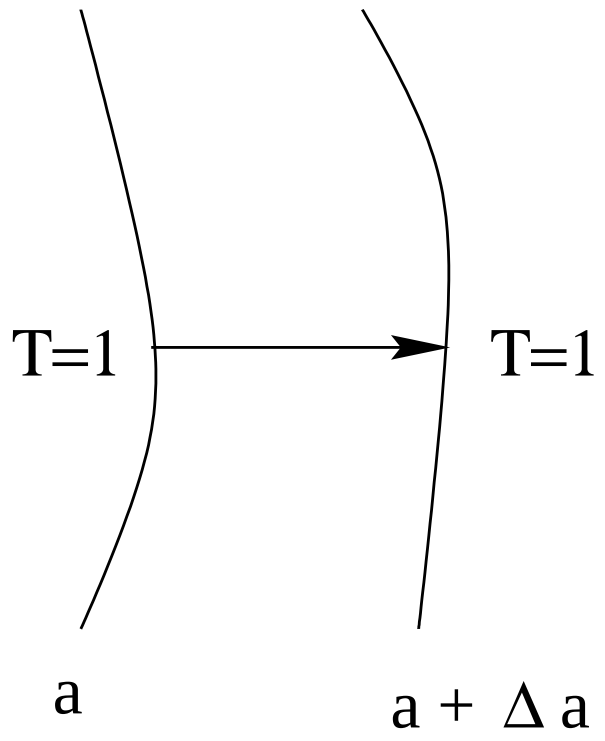
$$T(x_b(a), y_b(a); a) = T_0(x_b(a), y_b(a); a)$$

$$\frac{DT}{Da} = \frac{DT_0}{Da}$$



Boundary conditions : Dirichlet

$$
\begin{aligned}
\frac{DT}{Da} &= \frac{DT_0}{Da} \\
s_T &= -\frac{\partial T}{\partial x}\frac{\partial x_b}{\partial a} - \frac{\partial T}{\partial y}\frac{\partial y_b}{\partial a} + \frac{DT_0}{Da}
\end{aligned}
$$



- Provide $\frac{DT_0}{Da}$, $\frac{\partial x_b}{\partial a}$, and $\frac{\partial y_b}{\partial a}$
- Compute $\frac{\partial T}{\partial x}$ and $\frac{\partial T}{\partial y}$ from the flow solution

Boundary conditions : Neumann

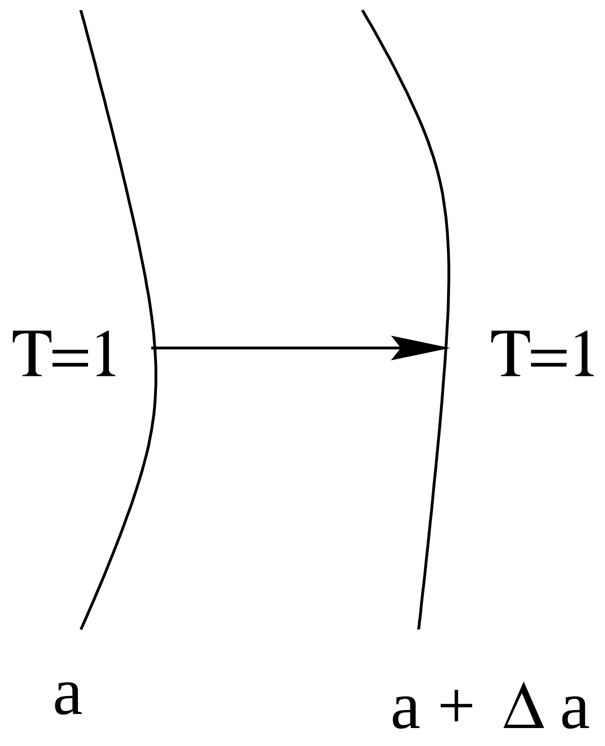
value parameter : $\kappa \nabla T \cdot \hat{\boldsymbol{n}} = q_0$

$$(\kappa' \nabla T + \kappa \nabla s_T) \cdot \hat{\boldsymbol{n}} = q_0'$$

shape parameter

$$\kappa \nabla T \cdot \hat{\boldsymbol{n}} = q_0(x_b(a), y_b(a); a)$$

$$\frac{D}{Da}(\kappa \nabla T) \cdot \hat{\boldsymbol{n}} + \kappa \nabla T \cdot \frac{D\hat{\boldsymbol{n}}}{Da} = \frac{Dq_0}{Da}$$



Boundary conditions : Neumann

<u>shape parameter</u>

$$\frac{D}{Da}\left(\kappa\nabla T\right)\cdot\hat{\boldsymbol{n}}+\kappa\nabla T\cdot\frac{D\hat{\boldsymbol{n}}}{Da}=\frac{Dq_0}{Da}$$

$$\left(\kappa'\nabla T+\kappa\nabla s_T\right)\cdot\hat{\boldsymbol{n}}=\frac{Dq_0}{Da}-\kappa\nabla T\cdot\frac{D\hat{\boldsymbol{n}}}{Da}$$

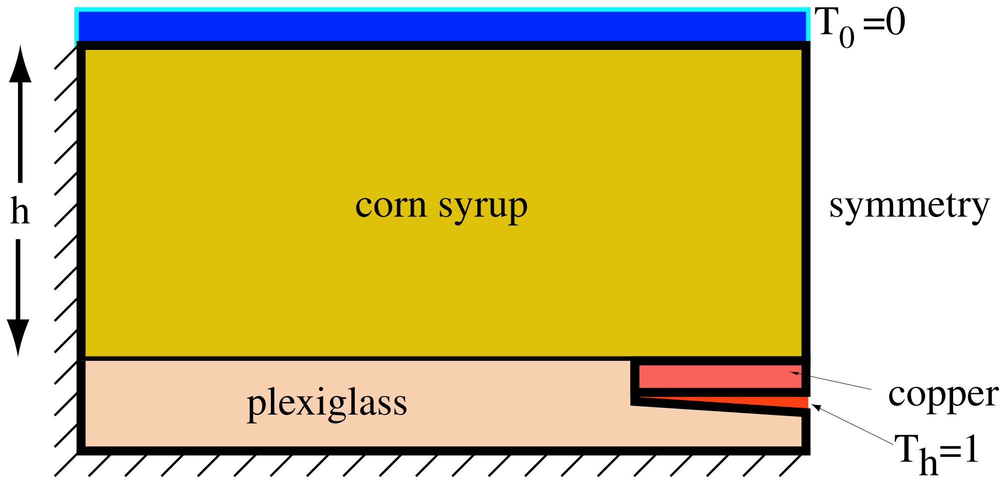
$$-\left[\frac{\partial}{\partial x}\left(\kappa\nabla T\right)\frac{\partial x_b}{\partial a}+\frac{\partial}{\partial y}\left(\kappa\nabla T\right)\frac{\partial y_b}{\partial a}\right]\cdot\hat{\boldsymbol{n}}$$

- Provide $\frac{Dq_0}{Da}$ and $\frac{D\hat{\boldsymbol{n}}}{Da}$
- Compute $\frac{\partial^2 T}{\partial x^2}, \frac{\partial^2 T}{\partial x \partial y}, \frac{\partial^2 T}{\partial x^2}$

Implementation

- General formulation
- FEM
- Numerical Jacobian
- Adaptivity : flow + sensitivities
- Projected flow gradients :
  - BC (shape parameters)
  - PDEs : $\rho c_p \boldsymbol{s}_u \cdot \nabla T$, $\nabla \cdot (\kappa' \nabla T)$

Free Convection in Corn Syrup



$$\mu = a_0 e^{a_1 e^{-T/a_2}}$$

$$\kappa = b_0 + b_1 T$$

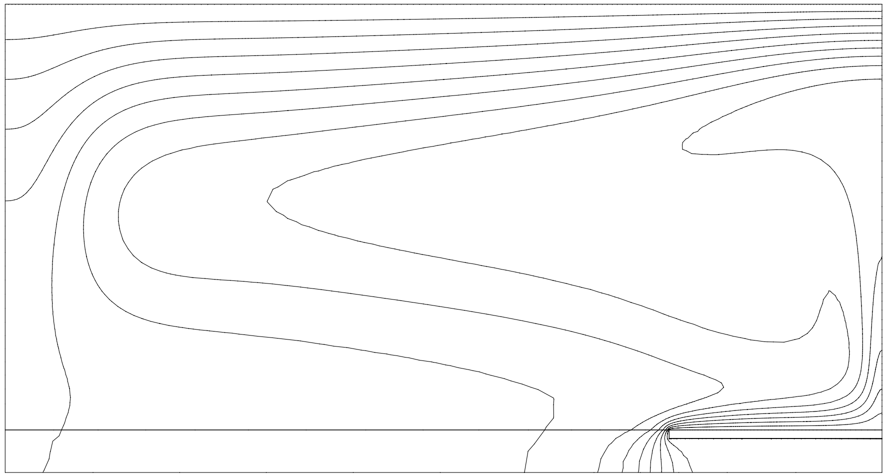
$$c_p = c_0 + c_1 T + c_2 T^2$$

A laboratory model for magma circulation in the earth's mantle

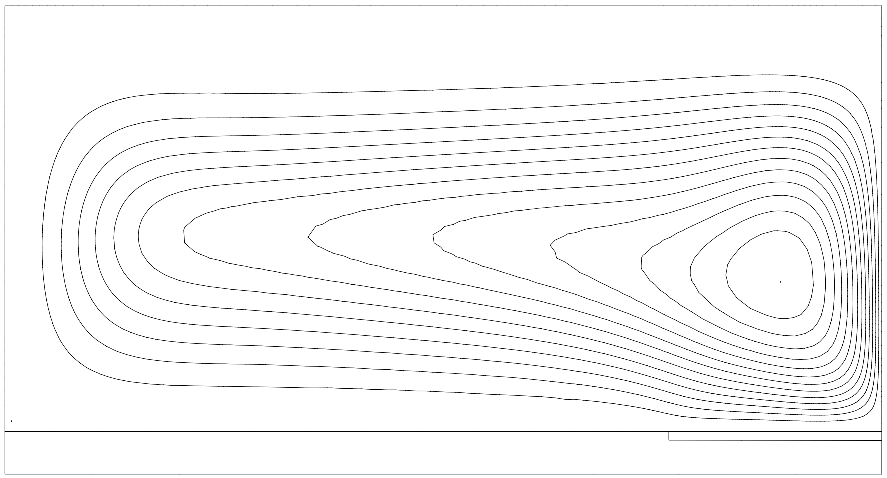
4 parameters :

h, T_h, a_0, and b_0

Free Convection in Corn Syrup

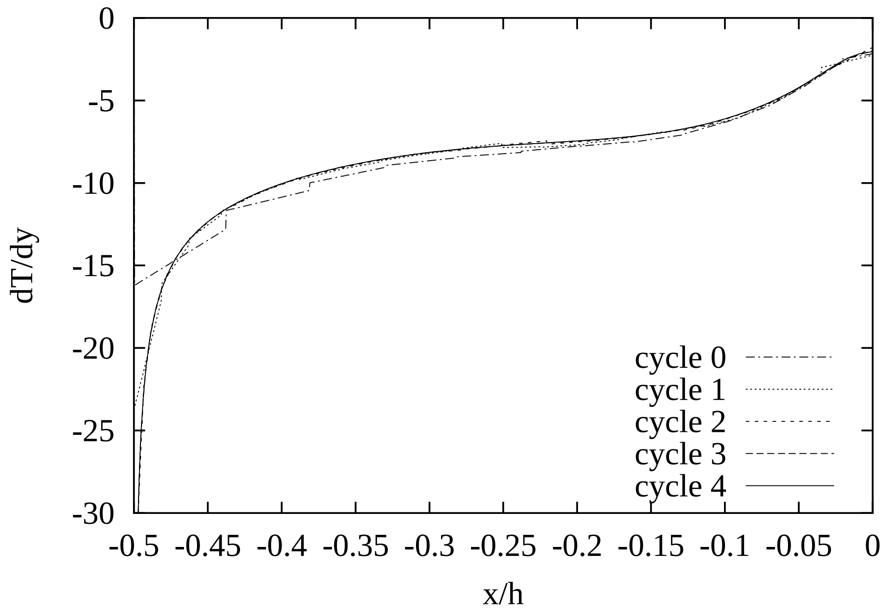


Temperature

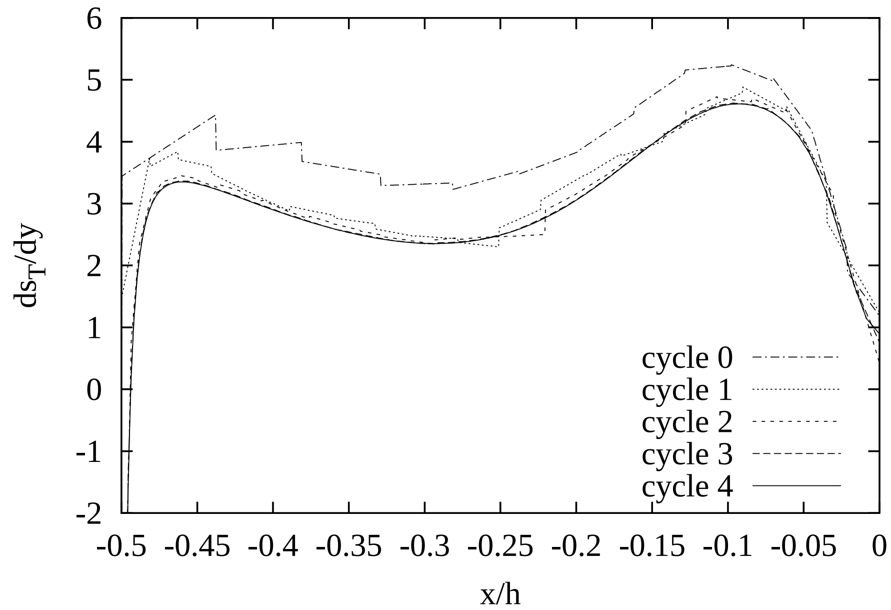


Streamlines

Grid convergence



$$\frac{\partial T}{\partial y}$$



$$\frac{\partial s_T}{\partial y}(b_0)$$

Must adapt mesh to flow & sensitivities

Scaled sensitivities

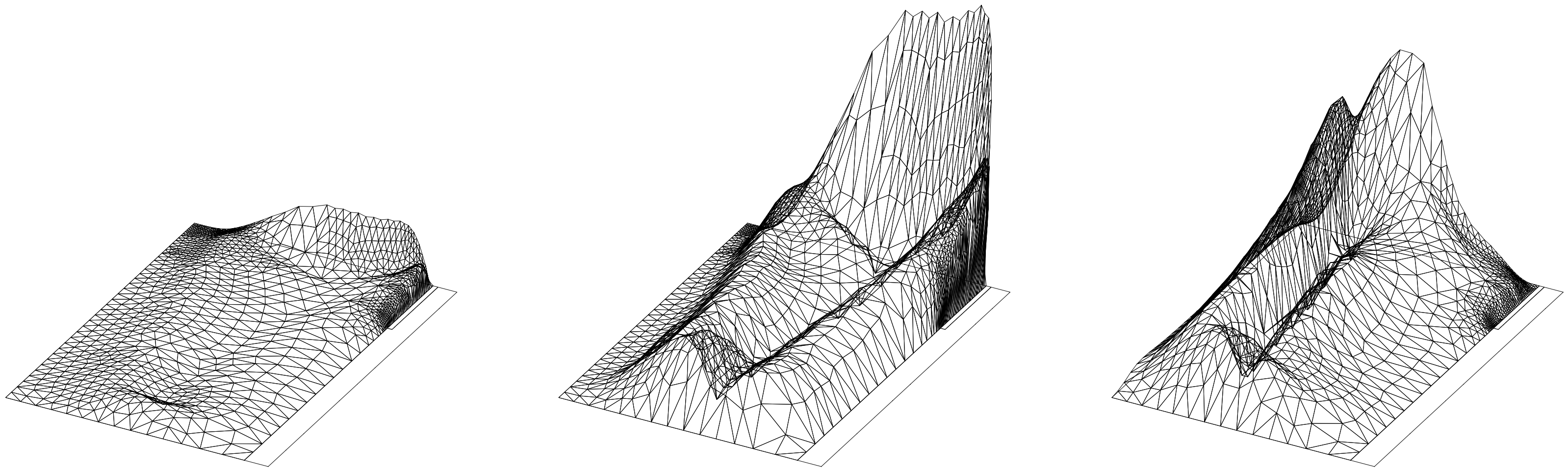
$$T(x; a_i + \Delta a_i) - T(x; a_i) = \frac{\partial T}{\partial a_i} \Delta a_i$$

$$\Delta T = \sum_i \underbrace{\left(\frac{\partial T}{\partial a_i} a_{i_0} \right)}_{\text{scaled sensitivity } \tilde{s}_{T_i}} \times \underbrace{\left(\frac{\Delta a_i}{a_{i_0}} \right)}_{\text{\% change in } a_i}$$

All $\dfrac{\partial T}{\partial a_i} a_{i_0}$ in $^\circ C \rightarrow$ Comparison more meaningful

Scaled Sensitivities : $\|\boldsymbol{s}_u\|$

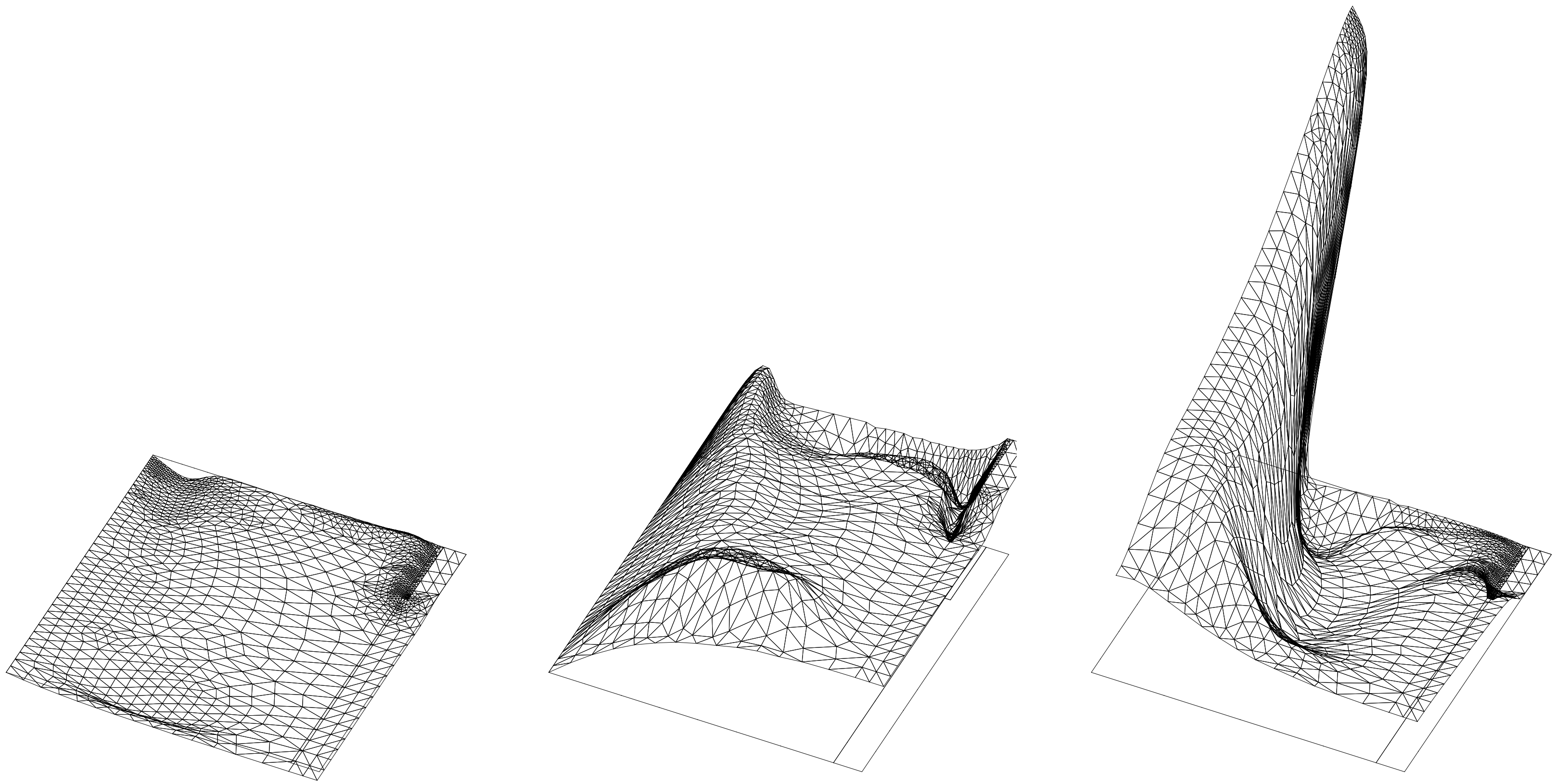
3 Scaled sensitivities of velocity



a_0 T_h h

Scaled Sensitivities : s_T

3 Scaled sensitivities of temperature



b_0 $\qquad$ T_h $\qquad$ h

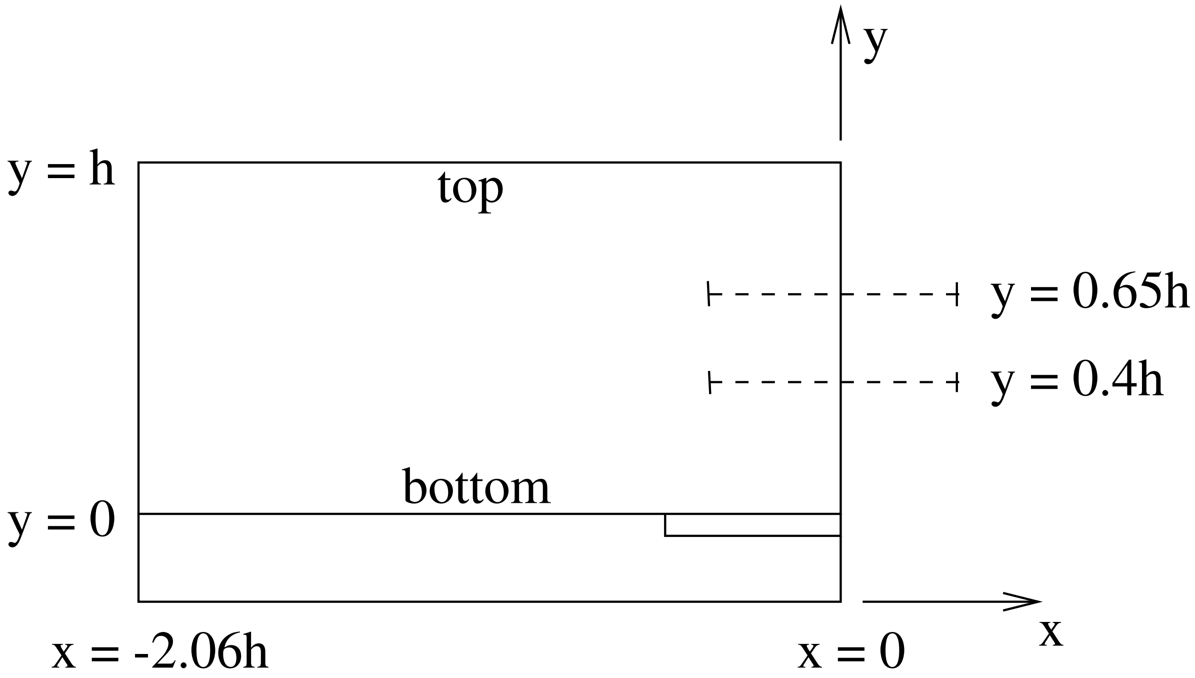
Uncertainty cascade

$$T(\boldsymbol{x};\boldsymbol{a}+\Delta\boldsymbol{a}) = T(\boldsymbol{x};\boldsymbol{a}) + \sum_{i=1}^{n} \frac{\partial T}{\partial a_i}(\boldsymbol{x};\boldsymbol{a})\Delta a_i$$

$$\Delta T = \sum_{i=1}^{n} \frac{\partial T}{\partial a_i}(\boldsymbol{x};\boldsymbol{a})\Delta a_i$$

$$|\Delta T| \leq \sum_{i=1}^{n} \left|\frac{\partial T}{\partial a_i}(\boldsymbol{x};\boldsymbol{a})\right| |\Delta a_i|$$

Cut planes



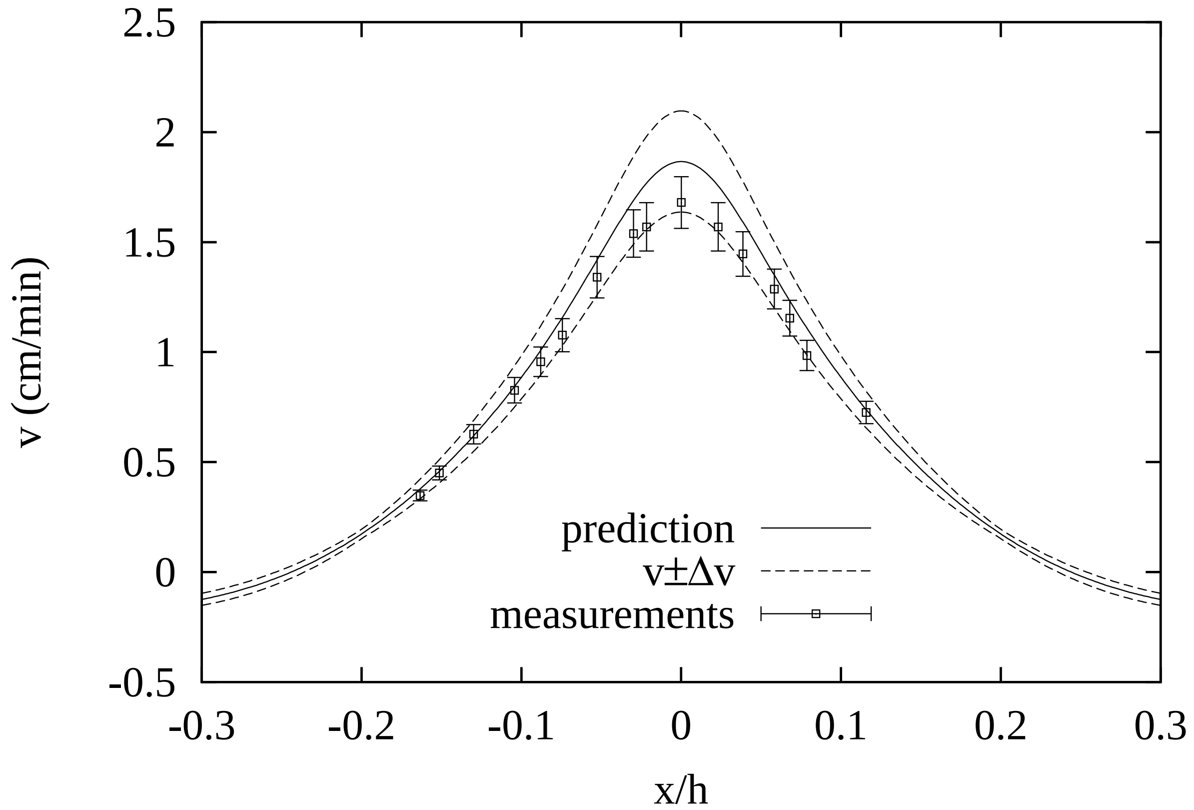
Vertical velocity at $y = 0.4h$

$$\Delta a_0 = 0.065 a_0$$

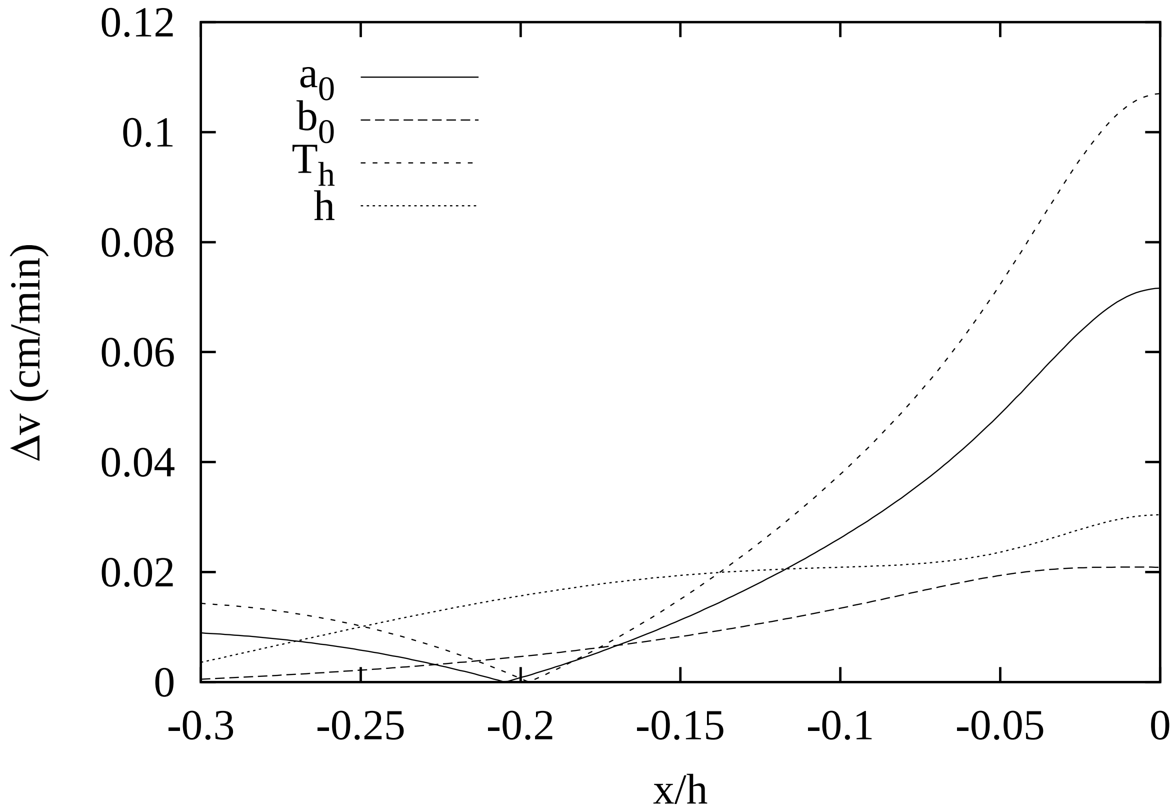
$$\Delta b_0 = 0.03 b_0$$

$$\Delta T_h = 0.02(T_h - T_0)$$

$$\Delta h = 0.02h$$

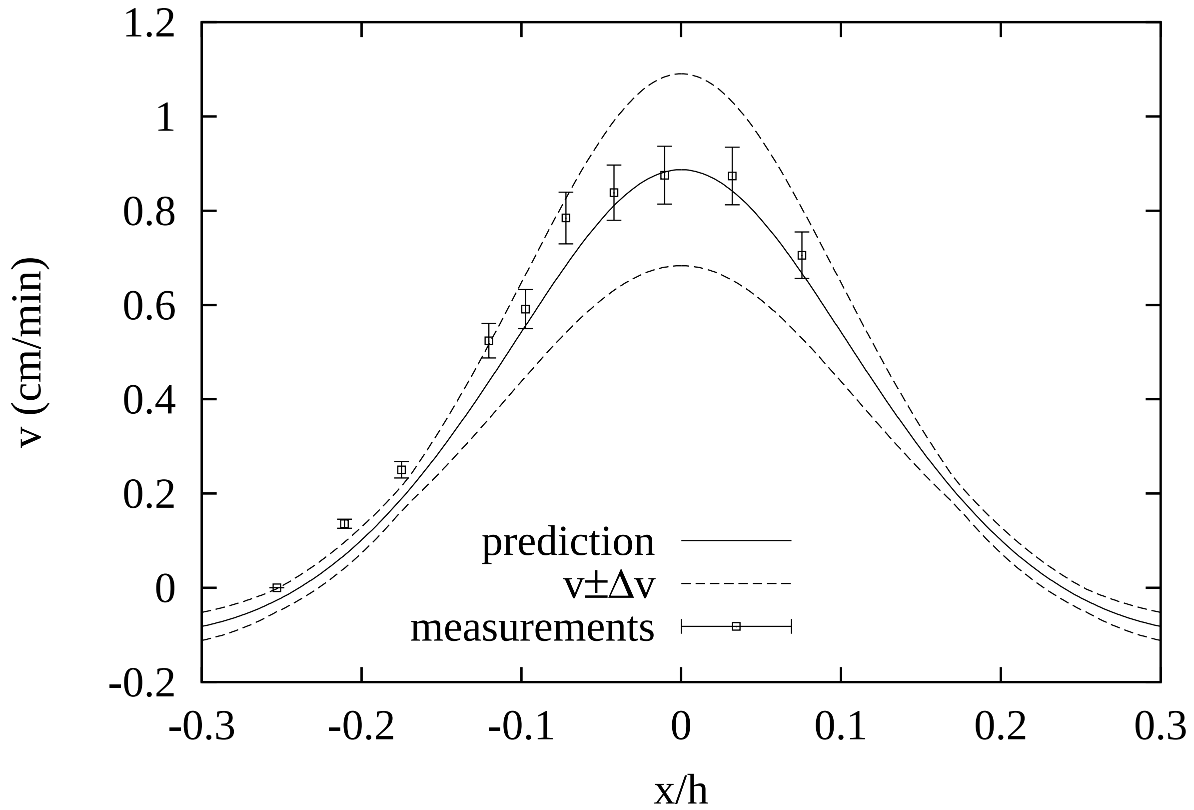


Contributions to Δv at $y = 0.4h$



Vertical velocity at $y = 0.65h$

$$\Delta a_0 = 0.065 a_0$$
$$\Delta b_0 = 0.03 b_0$$
$$\Delta T_h = 0.02(T_h - T_0)$$
$$\Delta h = 0.02h$$



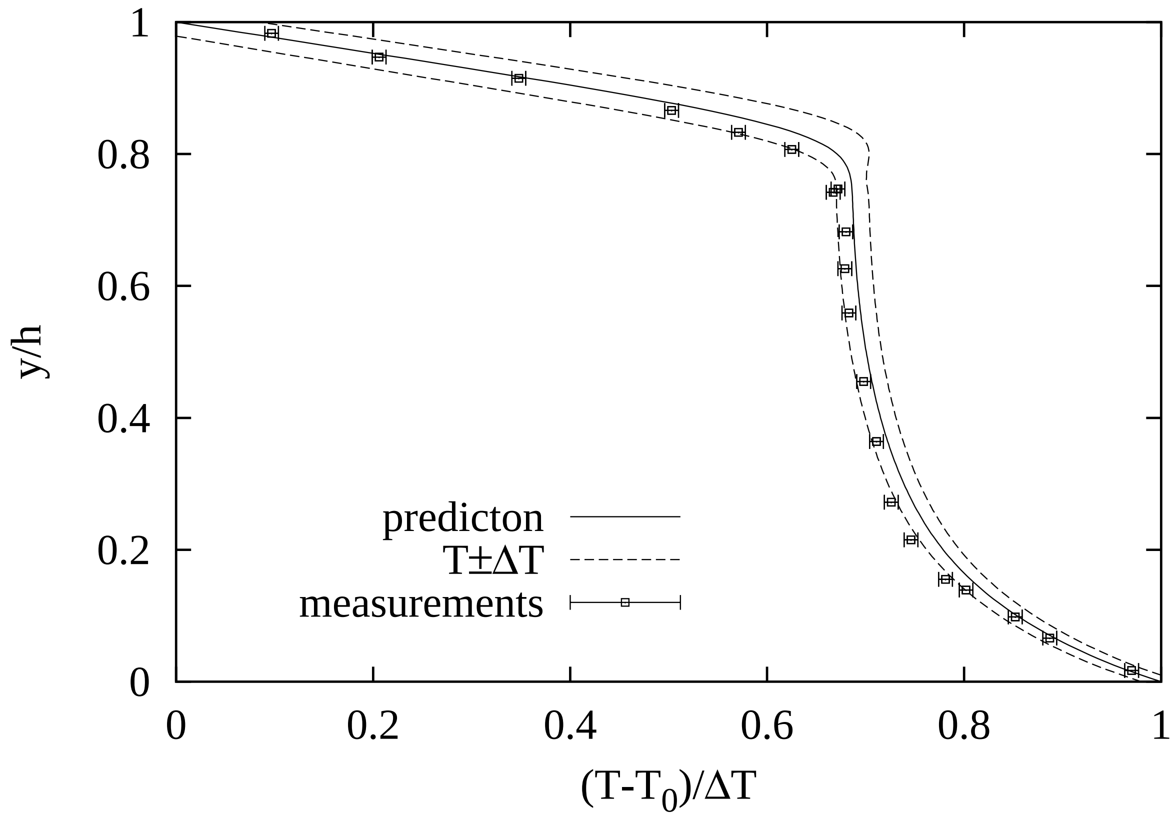
Temperature at $x = 0$

$$\Delta a_0 = 0.065 a_0$$

$$\Delta b_0 = 0.03 b_0$$

$$\Delta T_h = 0.02(T_h - T_0)$$

$$\Delta h = 0.02 h$$



Fast Nearby Solution

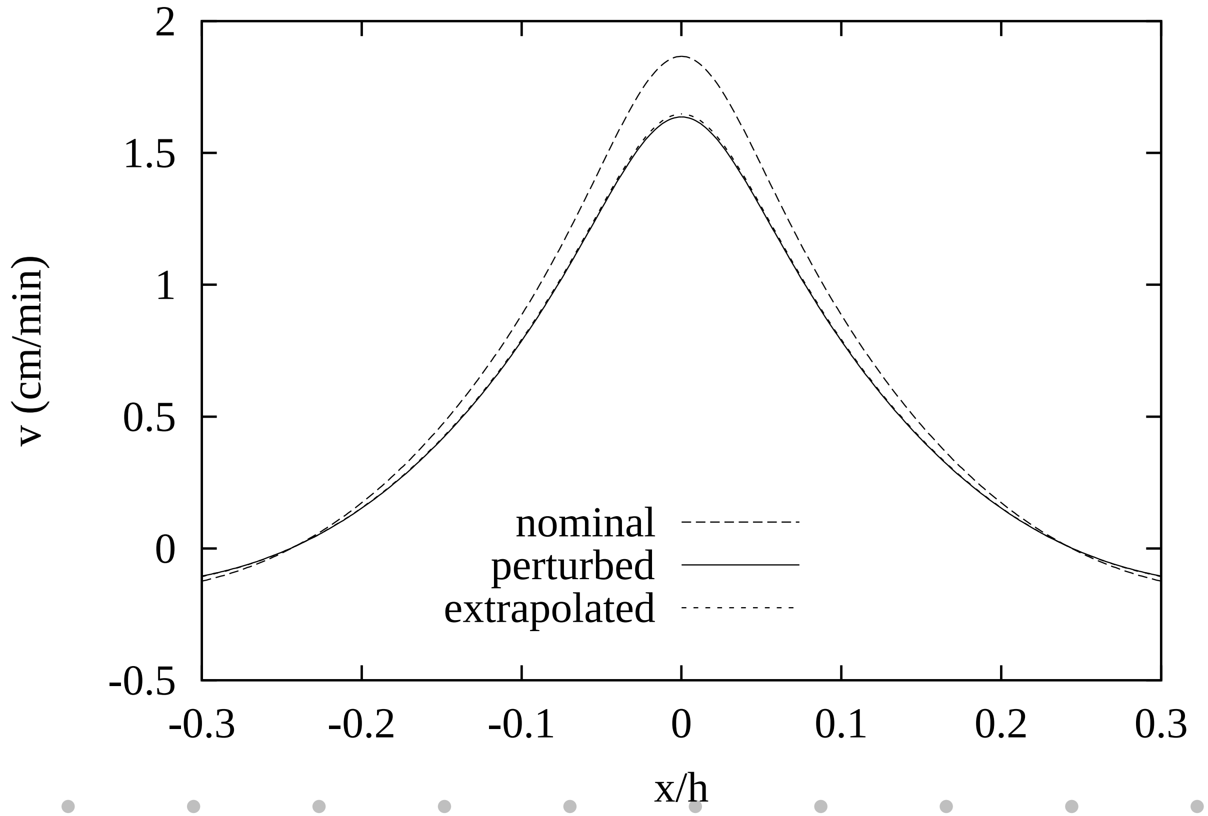
$$v(x; \boldsymbol{a} + \Delta \boldsymbol{a}) = v(x; \boldsymbol{a}) + \sum_{i=1}^{4} \frac{\partial v}{\partial a_i} \Delta a_i$$

$$\Delta a_0 = 0.065 a_0$$

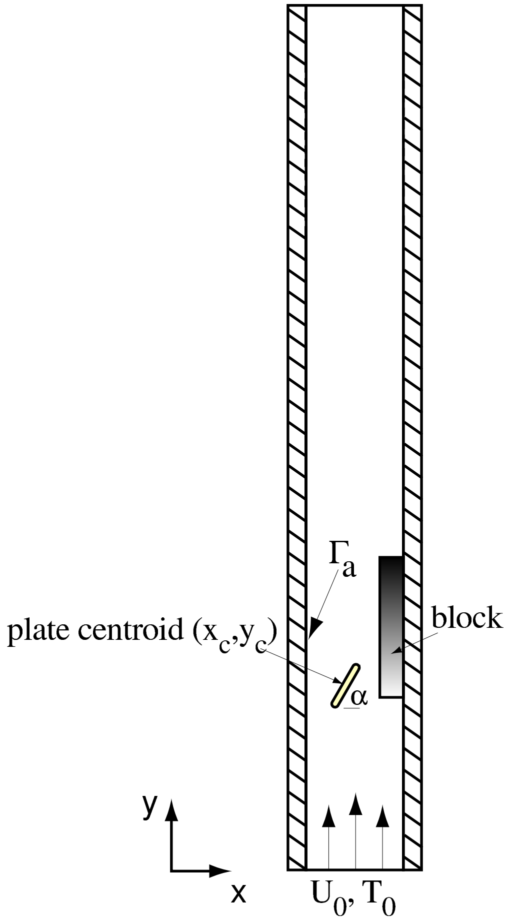
$$\Delta b_0 = 0.03 b_0$$

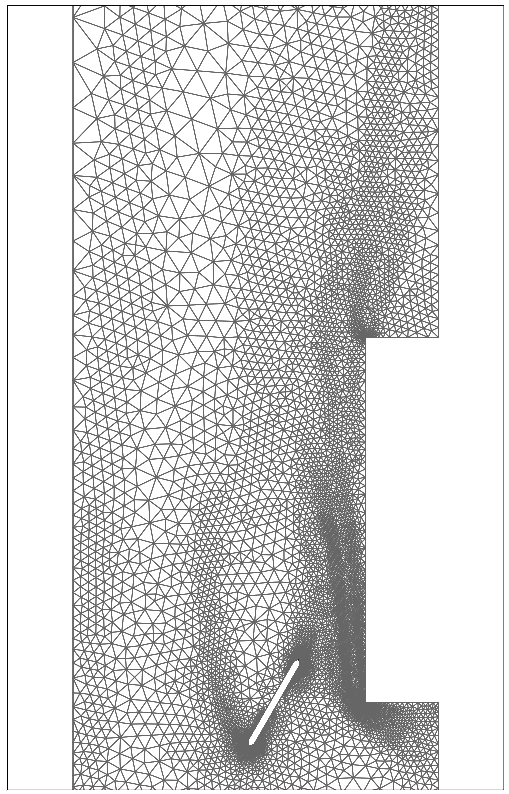
$$\Delta T_h = 0.02(T_h - T_0)$$

$$\Delta h = 0.02 h$$



A simple cooling system





A simple cooling system

Design parameter :

- plate angle α
- centroid coordinates (x_c, y_c)

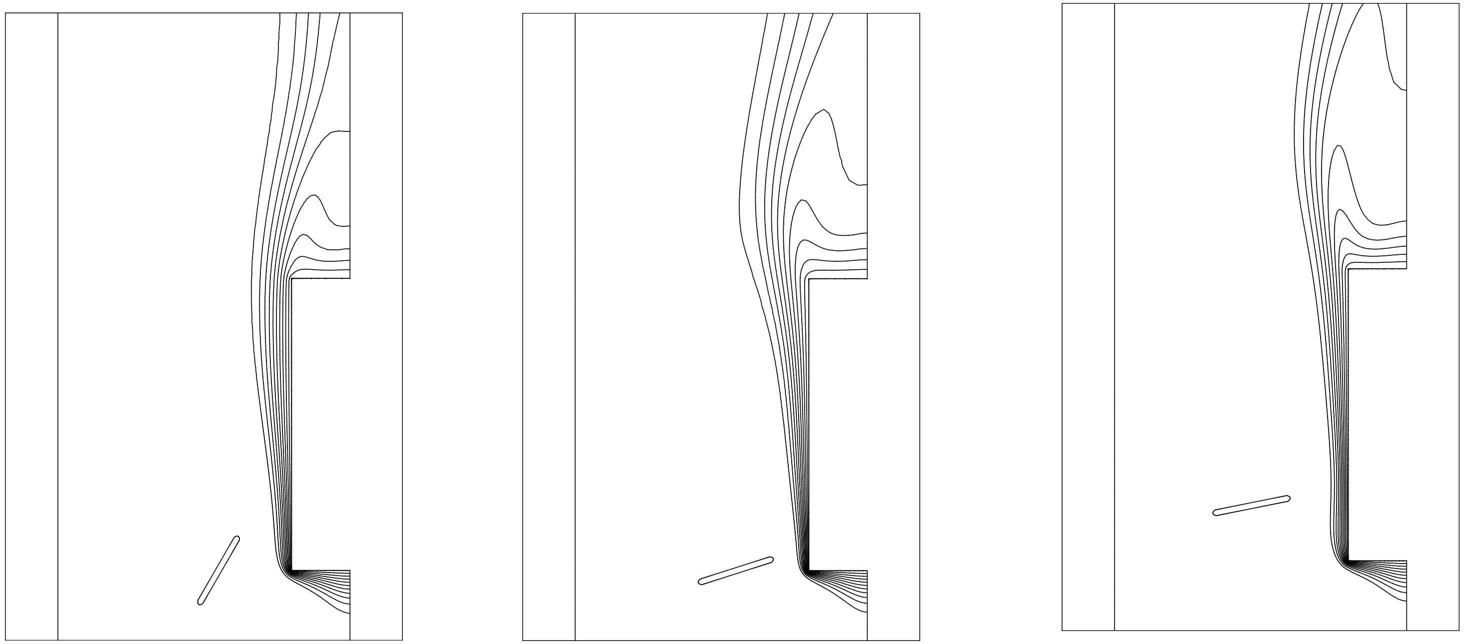
Objective function :

$$\mathcal{J}_1(\alpha, x_c, y_c) = \int_{\Gamma_b} \kappa \nabla T(\mathbf{x}; \alpha, x_c, y_c) \cdot \hat{\mathbf{n}} d\Gamma$$

Gradient of the objective function :

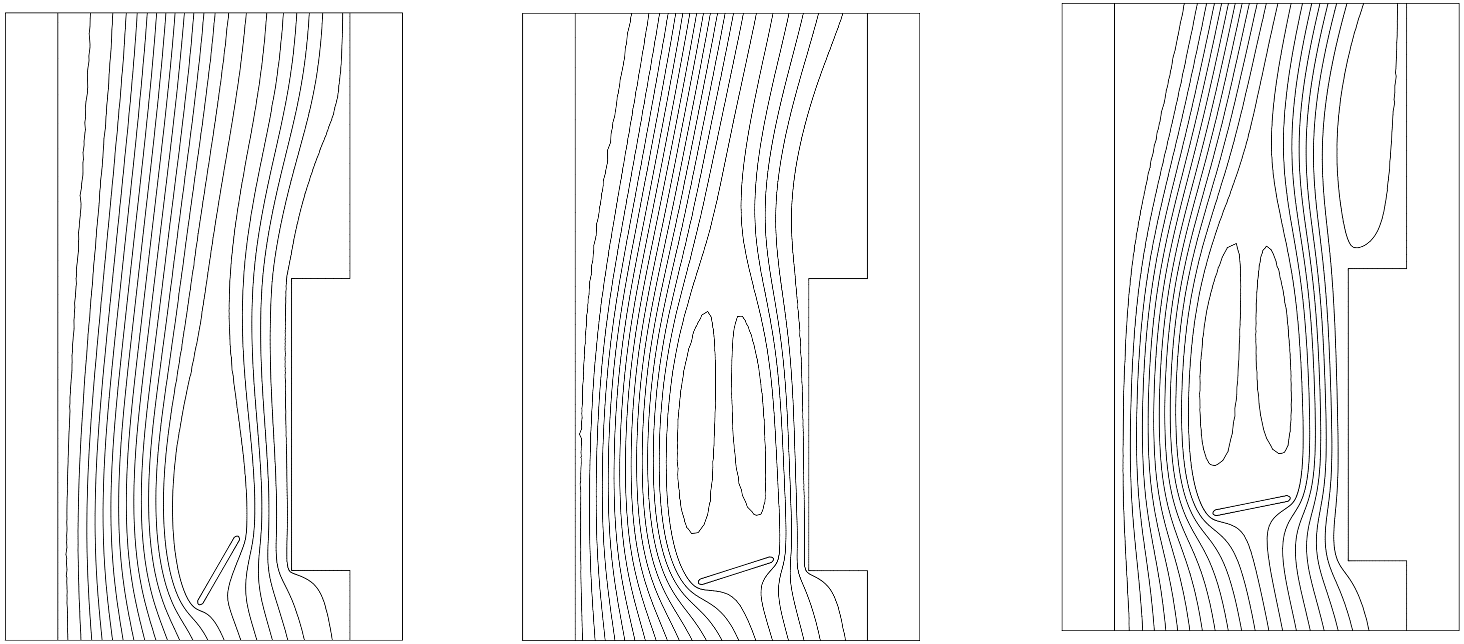
$$\frac{\partial}{\partial a} \mathcal{J}_1(\alpha, x_c, y_c) = \int_{\Gamma_b} \kappa \nabla s_T(\mathbf{x}; \alpha, x_c, y_c) \cdot \hat{\mathbf{n}} d\Gamma$$

Temperature fields



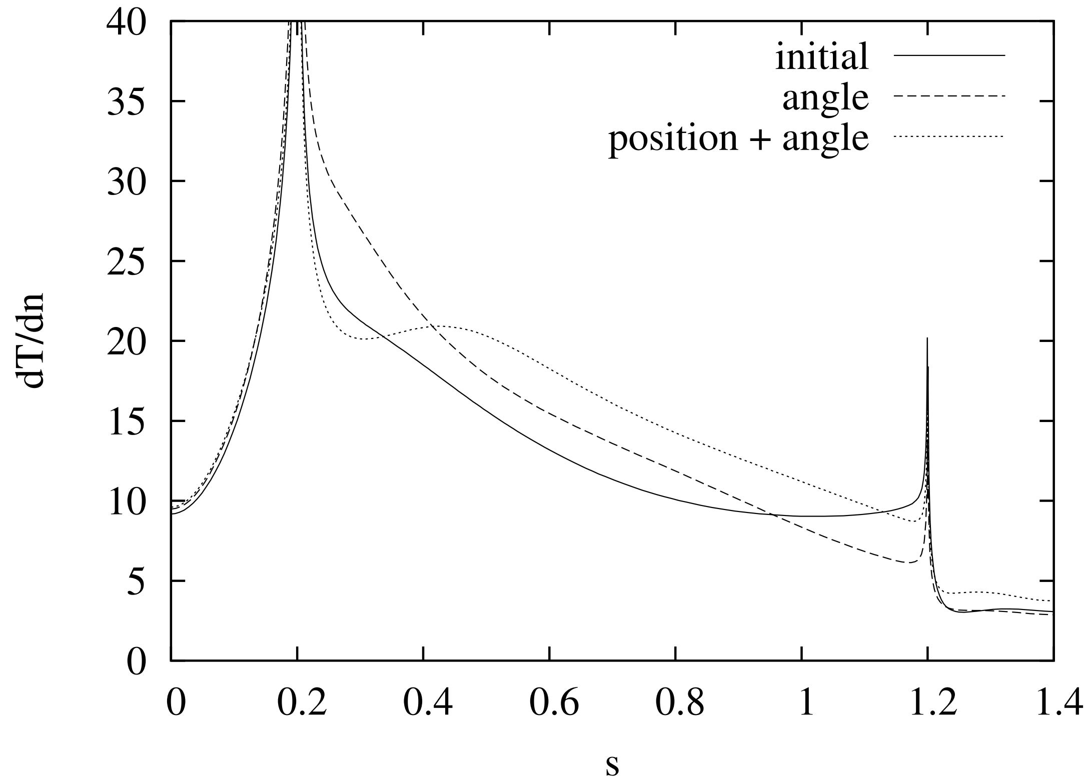
initial α (α, x_c, y_c)

Streamlines



initial α (α, x_c, y_c)

Heat Flux on thee block



Improvements : $\alpha = 10\% \quad (\alpha, x_c, y_c) = 15\%$

Optimisation path : α, x_c, y_c

It.	α	x_c	y_c	$\mathcal{J}$	$\frac{\partial}{\partial \alpha}\mathcal{J}$	$\frac{\partial}{\partial x_c}\mathcal{J}$	$\frac{\partial}{\partial y_c}\mathcal{J}$
0	17.7	0.550	1.000	0.07609	-0.00128	-0.04439	0.03101
1	17.5	0.433	1.082	0.07805	-0.00867	0.02027	0.01717
2	16.3	0.447	1.145	0.07890	-0.00843	0.01645	0.00658
3	14.8	0.454	1.158	0.07906	-0.00849	0.01140	0.02033
4	13.0	0.460	1.186	0.07931	-0.00770	0.01399	0.00168
5	11.4	0.467	1.190	**0.07946**	-0.00741	0.00846	0.01744
6	9.7	0.473	1.198	0.07945	-0.00590	0.00932	-0.00122

Maximum for non-zero gradient

Conclusion

- **Mesh adaptation provides**
  - cost effective solutions
  - accuracy for flow and sensitivities
- **General SEM formulation for complex flows**
  - identify important parameters
  - quantify flow uncertainty due to inputs
  - useful in optimal design
  - nearby flow evaluation : ***what if questions***