

Uncertainty quantification for the Navier–Stokes equations



Tiger SHARK-FV

May 20th, 2019, Ofir, Portugal

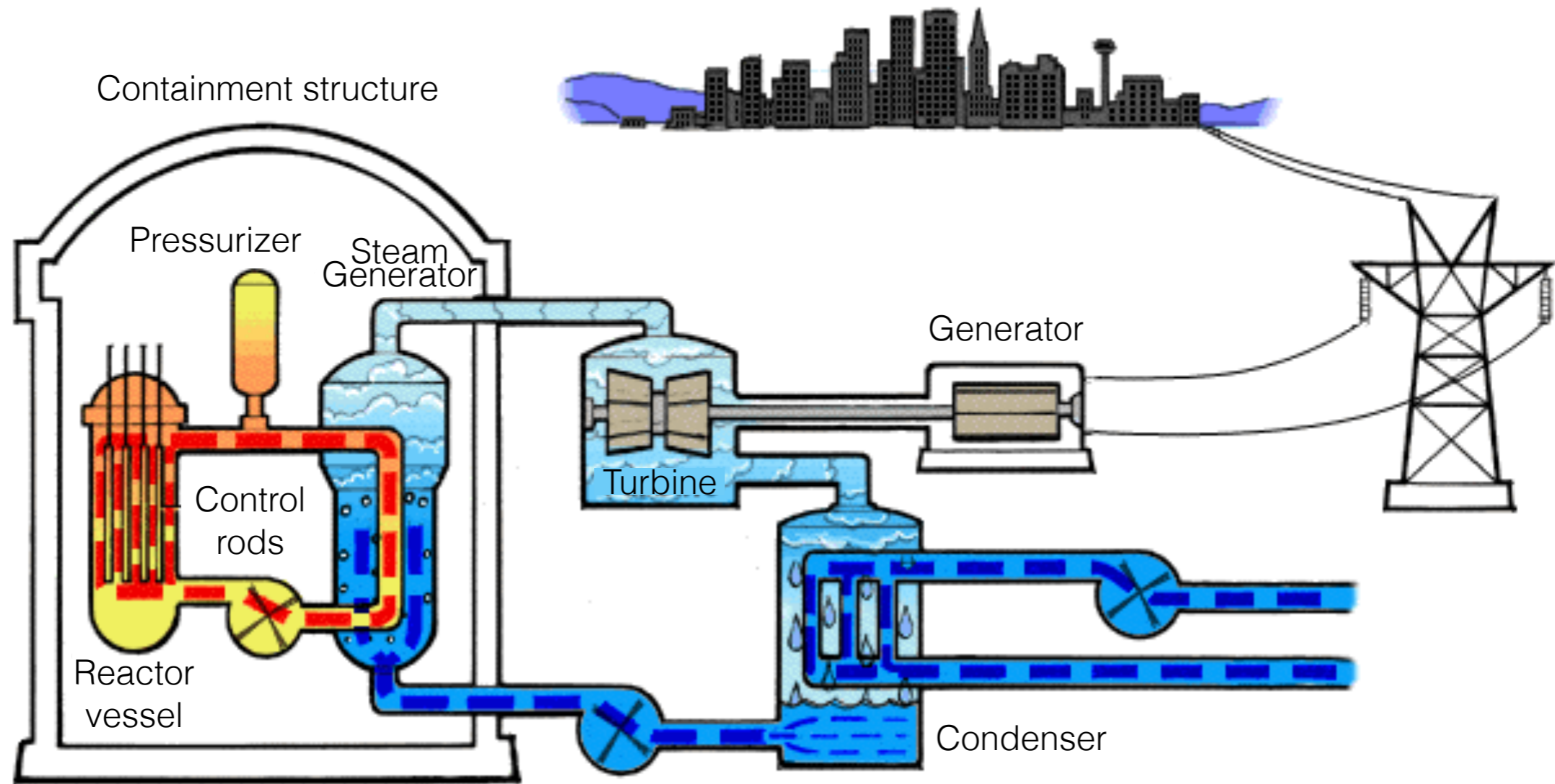
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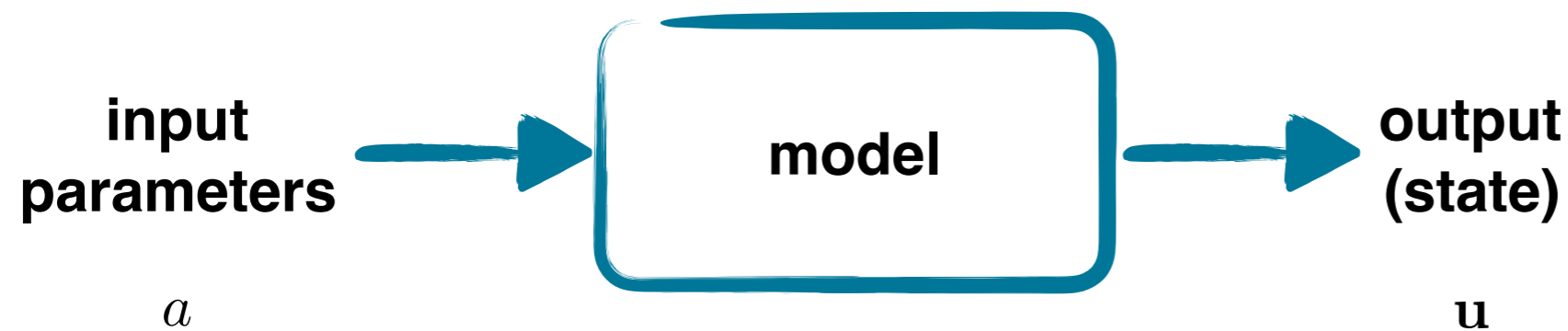


Code TRUST TrioCFD:

- ▶ Developed at CEA
- ▶ Open source
- ▶ Solves 2D and 3D Navier-Stokes
- ▶ **No uncertainty quantification tools**

prediction of the *worst case scenario*
important for security reasons

Sensitivity analysis (SA) : study of how changes in the **inputs** of a model affect the **outputs**



Sensitivity :

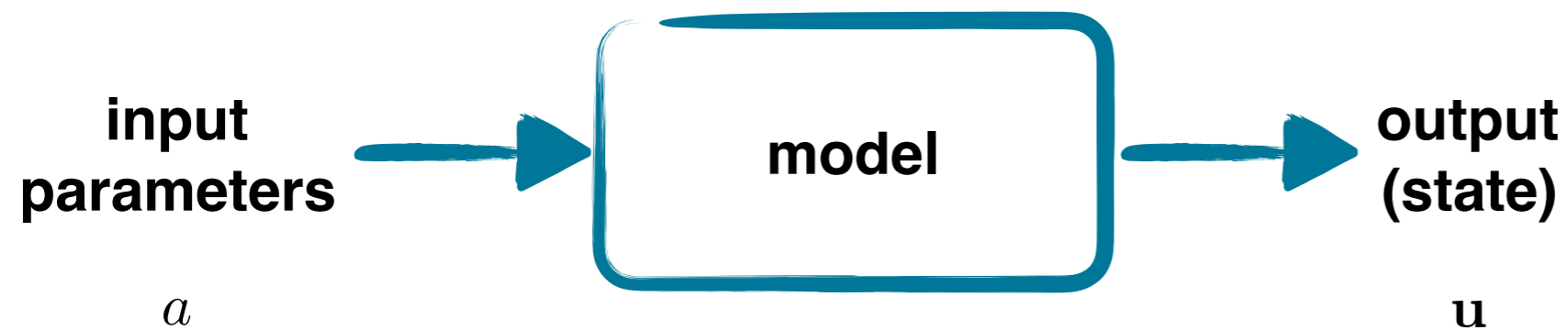
$$\frac{\partial \mathbf{u}}{\partial a} = \mathbf{u}_a$$

Continuous sensitivity equation (CSE) method :

$$\partial_t \mathbf{u} + \mathcal{L}(\mathbf{u}) = \mathbf{f} \quad \Omega, t > 0$$

+ initial and boundary conditions.

Sensitivity analysis (SA) : study of how changes in the **inputs** of a model affect the **outputs**



Sensitivity :

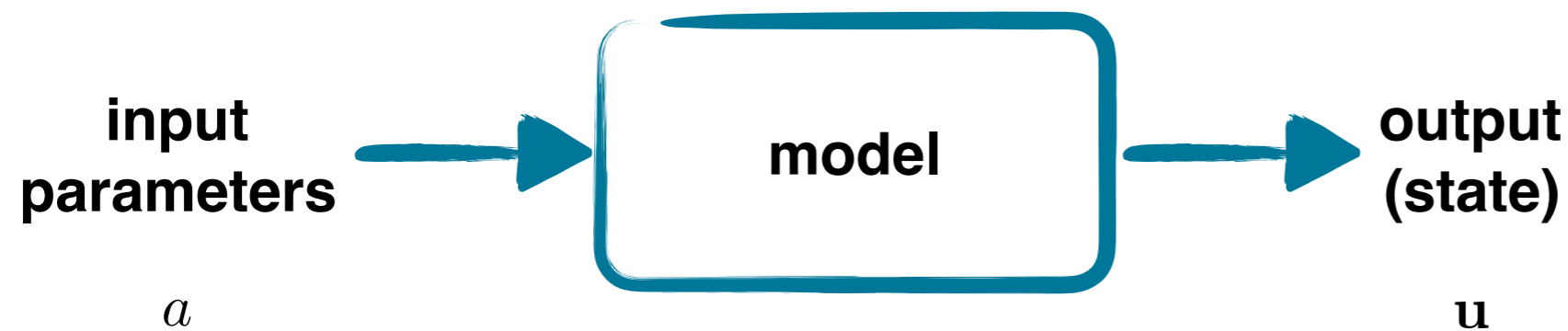
$$\frac{\partial \mathbf{u}}{\partial a} = \mathbf{u}_a$$

Continuous sensitivity equation (CSE) method :

$$\partial_a \partial_t \mathbf{u} + \partial_a \mathcal{L}(\mathbf{u}) = \partial_a \mathbf{f} \quad \Omega, t > 0$$

+ initial and boundary conditions.

Sensitivity analysis (SA) : study of how changes in the **inputs** of a model affect the **outputs**



Sensitivity :

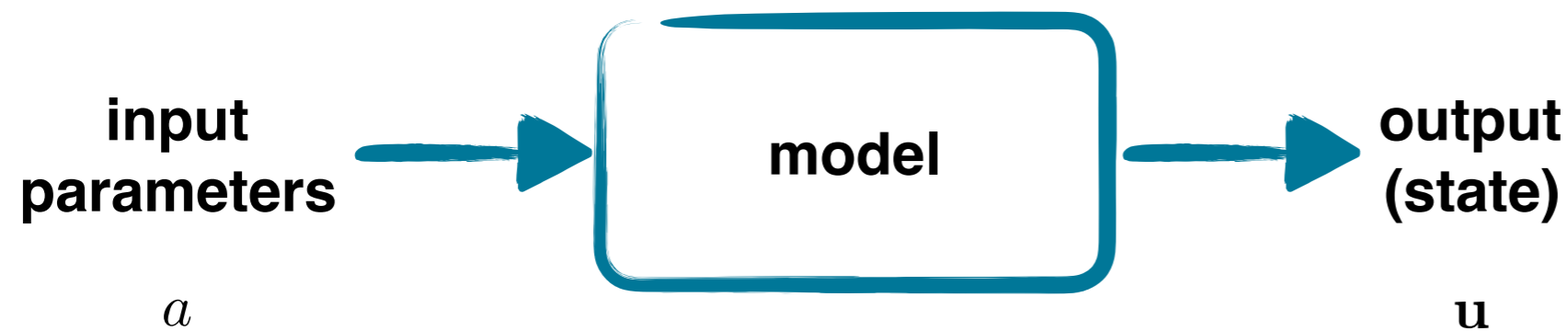
$$\frac{\partial \mathbf{u}}{\partial a} = \mathbf{u}_a$$

Continuous sensitivity equation (CSE) method :

$$\overset{\curvearrowright}{\partial_a} \overset{\curvearrowright}{\partial_t} \mathbf{u} + \overset{\curvearrowright}{\partial_a} \mathcal{L}(\mathbf{u}) = \partial_a \mathbf{f} \quad \Omega, t > 0$$

+ initial and boundary conditions.

Sensitivity analysis (SA) : study of how changes in the **inputs** of a model affect the **outputs**



Sensitivity :

$$\frac{\partial \mathbf{u}}{\partial a} = \mathbf{u}_a$$

Continuous sensitivity equation (CSE) method :

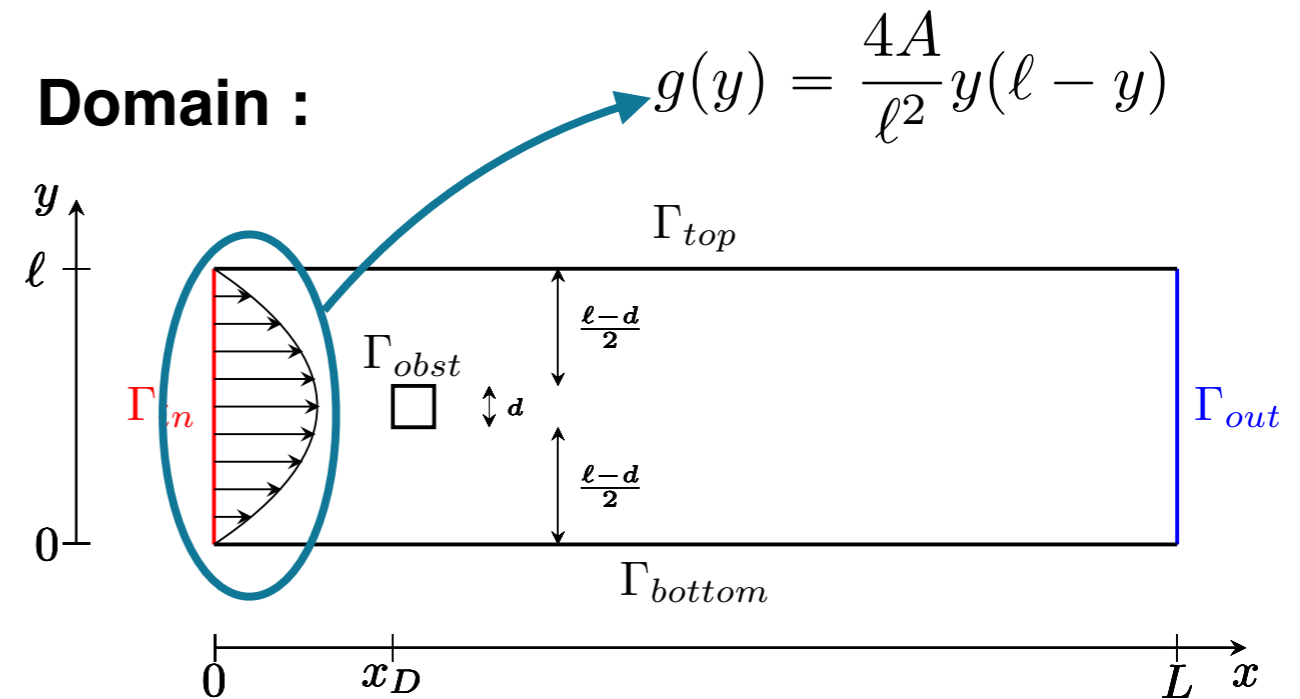
$$\partial_t \mathbf{u}_a + \mathcal{L}(\mathbf{u}, \mathbf{u}_a) = \mathbf{f}_a \quad \Omega, t > 0$$

+ initial and boundary conditions.

The Navier–Stokes equations :

$$\begin{cases} \partial_t \mathbf{u} - \nu \Delta \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla p = \mathbf{f} & \Omega, t > 0, \\ \nabla \cdot \mathbf{u} = 0 & \Omega, t > 0, \\ \mathbf{u}(\mathbf{x}, 0) = 0 & \Omega, t = 0, \\ \mathbf{u} = -g(y) \mathbf{n} & \text{on } \Gamma_{in}, \\ \mathbf{u} = 0 & \text{on } \Gamma_w, \\ (\nu \nabla \mathbf{u} - pI) \mathbf{n} = 0 & \text{on } \Gamma_{out}. \end{cases}$$

Domain :



$$\Gamma_w = \Gamma_{obst} \cup \Gamma_{top} \cup \Gamma_{bottom}$$

The sensitivity equations :

$$\begin{cases} \partial_t \mathbf{u}_a - \nu \Delta \mathbf{u}_a + (\mathbf{u}_a \cdot \nabla) \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u}_a + \nabla p_a = \bar{\mathbf{f}}_a & \Omega, t > 0, \\ \nabla \cdot \mathbf{u}_a = 0 & \Omega, t > 0, \\ \mathbf{u}_a(\mathbf{x}, 0) = 0 & \Omega, t = 0, \\ \mathbf{u}_a = -g_a(y) \mathbf{n} & \text{on } \Gamma_{in}, \\ \mathbf{u}_a = 0 & \text{on } \Gamma_w, \\ (\nu \nabla \mathbf{u}_a - p_a I) \mathbf{n} = 0 & \text{on } \Gamma_{out}. \end{cases}$$

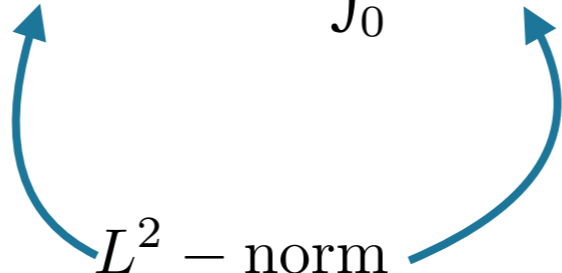
$$\bar{\mathbf{f}}_a = \partial_a \mathbf{f} + \partial_a \nu \Delta \mathbf{u}$$

Remark : these are known as the Oseen equations.

Proposition 1 *Let \mathbf{R}_g be a sufficiently smooth stationary ¹ function such that $\nabla \cdot \mathbf{R}_g = 0$ in Ω and $\mathbf{R}_g = \mathbf{u}$ on $\Gamma_{in} \cup \Gamma_w$. Then, if $\mathbf{u} \cdot \mathbf{n} \geq 0$ on Γ_{out} the following stability estimate holds for some $\gamma > 0$:*

$$\|\mathbf{u}\|^2 \leq \frac{1}{2\nu} \int_0^T \|\tilde{\mathbf{f}}(t)\|_{H^{-1}(\Omega)}^2 dt + \gamma \|\mathbf{R}_g\|_{H^1(\Omega)}^2,$$

where $\tilde{\mathbf{f}} = \mathbf{f} + \nu \Delta \mathbf{R}_g - (\mathbf{R}_g \cdot \nabla) \mathbf{R}_g$, and the norm $\|\cdot\|$ is defined as follows:

$$\|\mathbf{u}\|^2 := \|\mathbf{u}(T)\|^2 + C \int_0^T \|\nabla \mathbf{u}(t)\|^2 dt.$$


L^2 - norm

¹ If the boundary conditions depend on time, \mathbf{R}_g cannot be taken stationary.

Proposition 2 Let \mathbf{R}_{g_a} be a sufficiently smooth stationary function such that $\nabla \cdot \mathbf{R}_{g_a} = 0$ in Ω and $\mathbf{R}_{g_a} = \mathbf{u}_a$ on $\Gamma_{in} \cup \Gamma_w$. Then, if $\mathbf{u} \cdot \mathbf{n} \geq 0$ on Γ_{out} and if

$$\exists \kappa_1 = \kappa_1(\mathbf{u}, \Omega) : - \int_{\Omega} [(\mathbf{u}_a \cdot \nabla) \mathbf{u}] \cdot \mathbf{u}_a \leq \kappa_1 \|\nabla \mathbf{u}_a\|^2$$

the following stability estimate holds for some $\gamma_1 > 0$:

$$\|\mathbf{u}_a\|^2 \leq \frac{1}{2\nu} \int_0^T \|\tilde{\mathbf{f}}_a(t)\|_{H^{-1}(\Omega)}^2 dt + \gamma_1 \|\mathbf{R}_{g_a}\|_{H^1(\Omega)}^2,$$

where $\tilde{\mathbf{f}}_a = \bar{\mathbf{f}}_a + \nu \Delta \mathbf{R}_{g_a} - (\mathbf{R}_{g_a} \cdot \nabla) \mathbf{R}_{g_a}$.

“Morally” it is $\|\nabla \mathbf{u}\|$

$$- \int_{\Omega} [(\mathbf{u}_a \cdot \nabla) \mathbf{u}] \cdot \mathbf{u}_a \leq \|\mathbf{u}_a\|_{L^4}^2 \|\nabla \mathbf{u}\| \leq C \|\nabla \mathbf{u}\| \|\nabla \mathbf{u}_a\|^2$$

$\begin{array}{c} | \\ H^1 \subset L^4 \end{array}$

A number of different time schemes are implemented in the code TRUST TrioCFD:

- ▶ Forward Euler
- ▶ Runge Kutta
 - 2nd, 3rd and 4th order
- ▶ Semi-implicit Euler
 - implicit diffusion
 - explicit convection

The code TRUST TrioCFD is based on a **finite elements volumes** method (FEV).

Ingredients:

\mathcal{T}_h triangulation of the domain Ω

$K_j \in \mathcal{T}_h$ triangles $j = 1, \dots, N_T$

\mathbf{x}_i nodes $i = 1, \dots, N_N$

ω_i control volume

Spaces:

$Q_h = \{q_h : \forall K \in \mathcal{T}_h, q_h|_K \in P_0(K)\},$

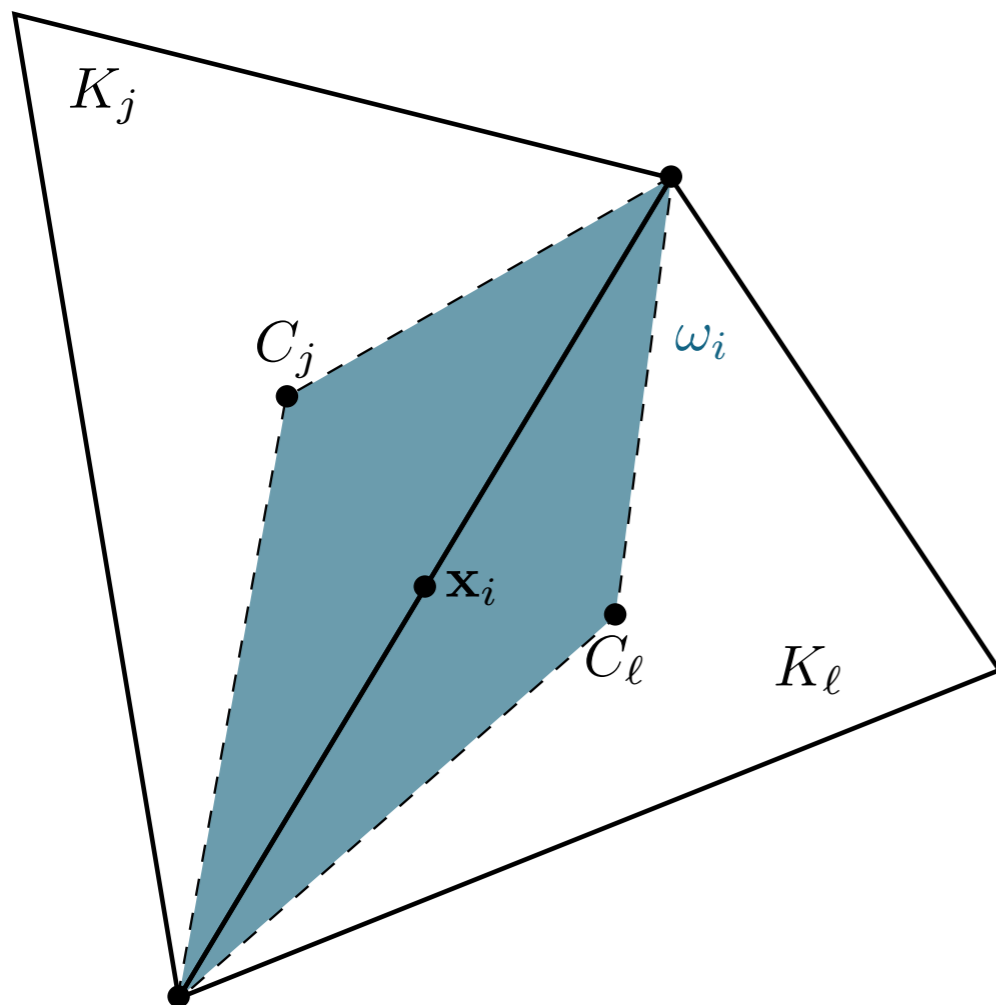
$V_h = \{w_h \text{ continuous in } \mathbf{x}_i : \forall K \in \mathcal{T}_h, w_h|_K \in P_1(K)\},$

$\mathbf{V}_h = \{\mathbf{w}_h = (w_x, w_y)^t : w_x, w_y \in V_h\}.$

Basis functions : $\varphi_i(\mathbf{x}_j) = \delta_{i,j}$ for V_h

χ_K for Q_h

Remark : $V_h \not\subset H^1(\Omega)$



We integrate the mass equation and its sensitivity over the triangles and the momentum equation and its sensitivity over the control volumes :

$$\begin{aligned}
 \int_{\partial K_j \setminus \Gamma_D} \mathbf{u}_h \cdot \mathbf{n} &= - \int_{\partial K_j \cap \Gamma_D} \mathbf{u}_h \cdot \mathbf{n} \quad \forall K_j \in \mathcal{T}_h, \\
 - \int_{\partial \omega_i \setminus \Gamma_N} (\nu \nabla \mathbf{u}_h - p_h I) \mathbf{n} + \int_{\partial \omega_i} (\mathbf{u}_h \otimes \mathbf{u}_h) \mathbf{n} &= \int_{\omega_i} \mathbf{f} \quad \forall \omega_i, \\
 \int_{\partial K_j \setminus \Gamma_D} \mathbf{u}_{a,h} \cdot \mathbf{n} &= - \int_{\partial K_j \cap \Gamma_D} \mathbf{u}_{a,h} \cdot \mathbf{n} \quad \forall K_j \in \mathcal{T}_h, \\
 - \int_{\partial \omega_i \setminus \Gamma_N} (\nu \nabla \mathbf{u}_{a,h} - p_{a,h} I) \mathbf{n} + \int_{\partial \omega_i} (\mathbf{u}_{a,h} \otimes \mathbf{u}_h + \mathbf{u}_h \otimes \mathbf{u}_{a,h}) \mathbf{n} &= \int_{\omega_i} \bar{\mathbf{f}}_a \quad \forall \omega_i.
 \end{aligned}$$

Using the basis functions of the spaces previously introduced one has :

$$\begin{aligned}
 \mathbf{u}_h(\mathbf{x}) &= \sum_{i=1}^{N_N} \mathbf{u}_h(\mathbf{x}_i) \varphi_i(\mathbf{x}), & p_h(\mathbf{x}) &= \sum_{j=1}^{N_T} p_h(K_j) \chi_{K_j}, \\
 \mathbf{u}_{a,h}(\mathbf{x}) &= \sum_{i=1}^{N_N} \mathbf{u}_{a,h}(\mathbf{x}_i) \varphi_i(\mathbf{x}), & p_{a,h}(\mathbf{x}) &= \sum_{j=1}^{N_T} p_{a,h}(K_j) \chi_{K_j}.
 \end{aligned}$$

$$\sum_{i \in \mathcal{I} \cup \mathcal{N}} \mathbf{u}_h(\mathbf{x}_i) \cdot \int_{\partial K_j \setminus \Gamma_D} \varphi_i \mathbf{n} = - \sum_{i \in \mathcal{D}} \mathbf{u}_h(\mathbf{x}_i) \cdot \int_{\partial K_j \cap \Gamma_D} \varphi_i \mathbf{n} \quad \forall K_j \in \mathcal{T}_h,$$

$$- \sum_{j \in \mathcal{I}} \int_{\partial \omega_i} (\nu \mathbf{u}_h(\mathbf{x}_j) \otimes \nabla \varphi_j) \mathbf{n} + \sum_{j=1}^{N_T} p_h(K_j) \int_{\partial \omega_i} \chi_{K_j} \mathbf{n} + \int_{\partial \omega_i} \mathbf{u}_h(\mathbf{u}_h \cdot \mathbf{n}) = \int_{\omega_i} \mathbf{f} \quad \forall \omega_i,$$

$$\sum_{i \in \mathcal{I} \cup \mathcal{N}} \mathbf{u}_{a,h}(\mathbf{x}_i) \cdot \int_{\partial K_j \setminus \Gamma_D} \varphi_i \mathbf{n} = - \sum_{i \in \mathcal{D}} \mathbf{u}_{a,h}(\mathbf{x}_i) \cdot \int_{\partial K_j \cap \Gamma_D} \varphi_i \mathbf{n} \quad \forall K_j \in \mathcal{T}_h,$$

$$- \sum_{j \in \mathcal{I}} \int_{\partial \omega_i} (\nu \mathbf{u}_{a,h}(\mathbf{x}_j) \otimes \nabla \varphi_j) \mathbf{n} + \sum_{j=1}^{N_T} p_{a,h}(K_j) \int_{\partial \omega_i} \chi_{K_j} \mathbf{n} + \int_{\partial \omega_i} \mathbf{u}_{a,h}(\mathbf{u}_h \cdot \mathbf{n}) + \mathbf{u}_h(\mathbf{u}_{a,h} \cdot \mathbf{n}) = \int_{\omega_i} \bar{\mathbf{f}}_a \quad \forall \omega_i,$$

$$\sum_{i \in \mathcal{I} \cup \mathcal{N}} \boxed{\mathbf{U}_i} \boxed{\mathbf{u}_h(\mathbf{x}_i)} \cdot \boxed{B_{j,i}} \int_{\partial K_j \setminus \Gamma_D} \varphi_i \mathbf{n} = \boxed{D_j} - \sum_{i \in \mathcal{D}} \mathbf{u}_h(\mathbf{x}_i) \cdot \int_{\partial K_j \cap \Gamma_D} \varphi_i \mathbf{n} \quad \forall K_j \in \mathcal{T}_h,$$

$$- \sum_{j \in \mathcal{I}} \int_{\partial \omega_i} \boxed{A_{i,j}} (\nu \mathbf{u}_h(\mathbf{x}_j) \otimes \nabla \varphi_j) \mathbf{n} + \sum_{j=1}^{N_T} \boxed{P_j} p_h(K_j) \int_{\partial \omega_i} \boxed{C_{i,j}} \chi_{K_j} \mathbf{n} + \int_{\partial \omega_i} \boxed{[L(\mathbf{U})\mathbf{U}]_i} \mathbf{u}_h(\mathbf{u}_h \cdot \mathbf{n}) = \boxed{F_i} \int_{\omega_i} \mathbf{f} \quad \forall \omega_i,$$

$$\sum_{i \in \mathcal{I} \cup \mathcal{N}} \boxed{\mathbf{U}_{a,i}} \boxed{\mathbf{u}_{a,h}(\mathbf{x}_i)} \cdot \boxed{B_{j,i}} \int_{\partial K_j \setminus \Gamma_D} \varphi_i \mathbf{n} = \boxed{D_{a,j}} - \sum_{i \in \mathcal{D}} \mathbf{u}_{a,h}(\mathbf{x}_i) \cdot \int_{\partial K_j \cap \Gamma_D} \varphi_i \mathbf{n} \quad \forall K_j \in \mathcal{T}_h,$$

$$- \sum_{j \in \mathcal{I}} \int_{\partial \omega_i} \boxed{A_{i,j}} (\nu \mathbf{u}_{a,h}(\mathbf{x}_j) \otimes \nabla \varphi_j) \mathbf{n} + \sum_{j=1}^{N_T} \boxed{P_{a,j}} p_{a,h}(K_j) \int_{\partial \omega_i} \boxed{C_{i,j}} \chi_{K_j} \mathbf{n} + \int_{\partial \omega_i} \boxed{[L(\mathbf{U}_a)\mathbf{U} + L(\mathbf{U})\mathbf{U}_a]_i} \mathbf{u}_{a,h}(\mathbf{u}_h \cdot \mathbf{n}) + \mathbf{u}_h(\mathbf{u}_{a,h} \cdot \mathbf{n}) = \boxed{F_{a,i}} \int_{\omega_i} \bar{\mathbf{f}}_a \quad \forall \omega_i,$$

$$AU + B^t P + L(\mathbf{U})\mathbf{U} = \mathbf{F}$$

$$BU = D$$

$$AU_a + B^t P_a + L(\mathbf{U}_a)\mathbf{U} + L(\mathbf{U})\mathbf{U}_a = \mathbf{F}_a$$

$$BU_a = D_a$$

We consider explicit Euler in time with homogeneous Dirichlet b.c. for simplicity's sake:

$$\begin{cases} M \frac{\mathbf{U}^{n+1} - \mathbf{U}^n}{\Delta t} = -A\mathbf{U}^n - L(\mathbf{U}^n)\mathbf{U}^n - B^t P^{n+1} + F^n \\ B\mathbf{U}^{n+1} = 0 \end{cases}$$

$$M \frac{\mathbf{U}^* - \mathbf{U}^n}{\Delta t} = -A\mathbf{U}^n - L(\mathbf{U}^n)\mathbf{U}^n - B^t P^n + F^n$$

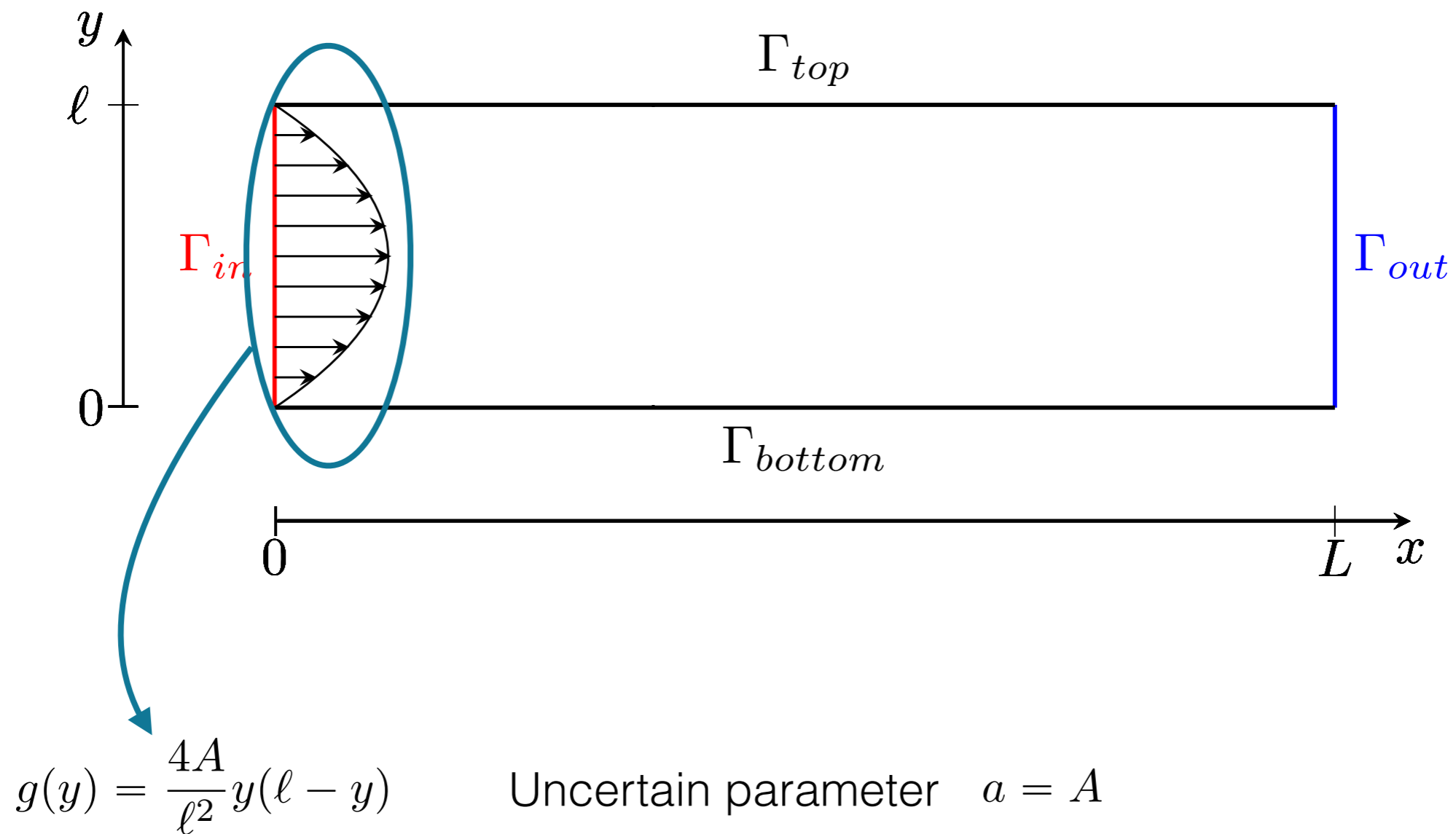
$$(BM^{-1}B^t)\delta P = \frac{1}{\Delta t}B\mathbf{U}^*$$

$$\mathbf{U}^{n+1} = \mathbf{U}^* - \Delta t M^{-1} B^t \delta P$$

$$P^{n+1} = P^n + \delta P$$

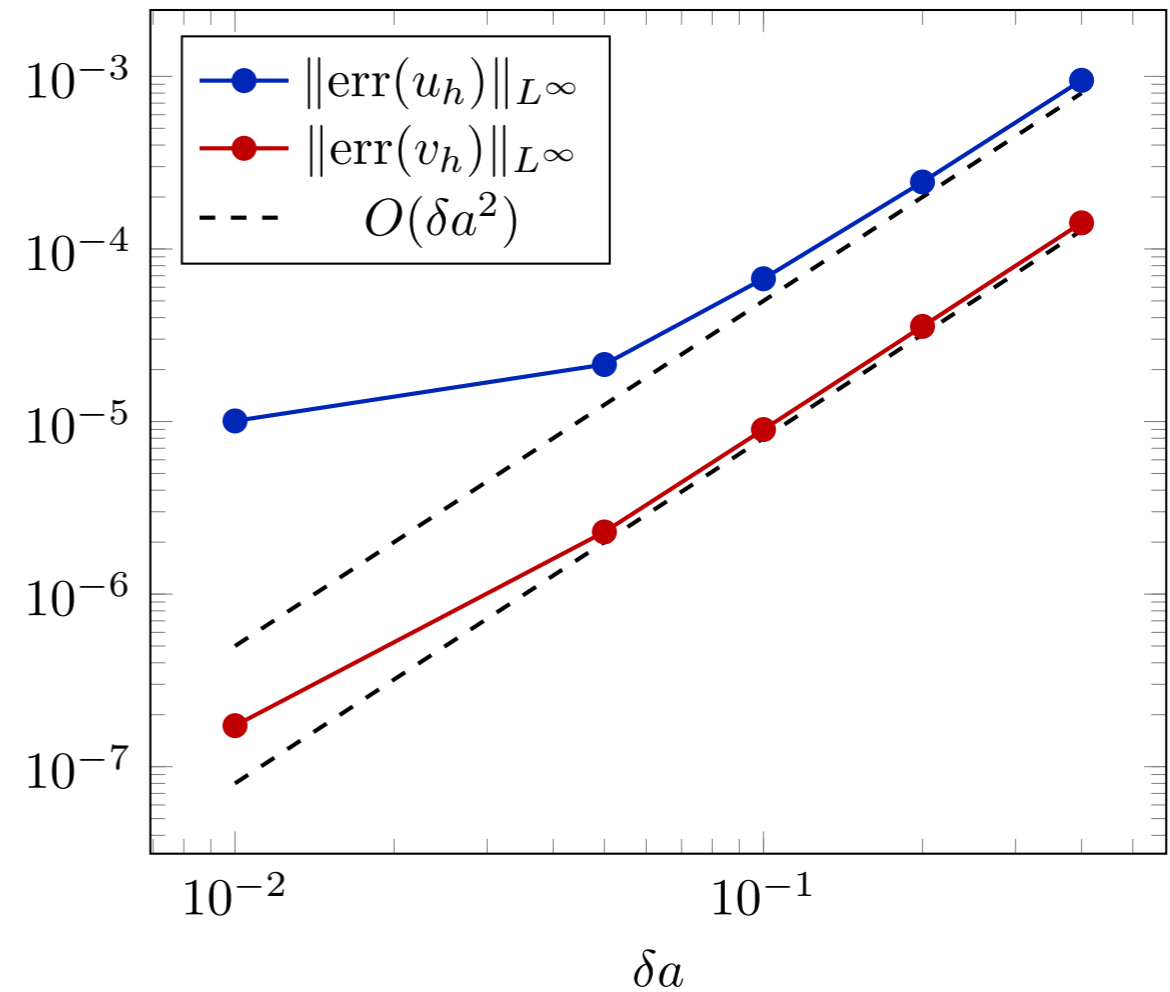
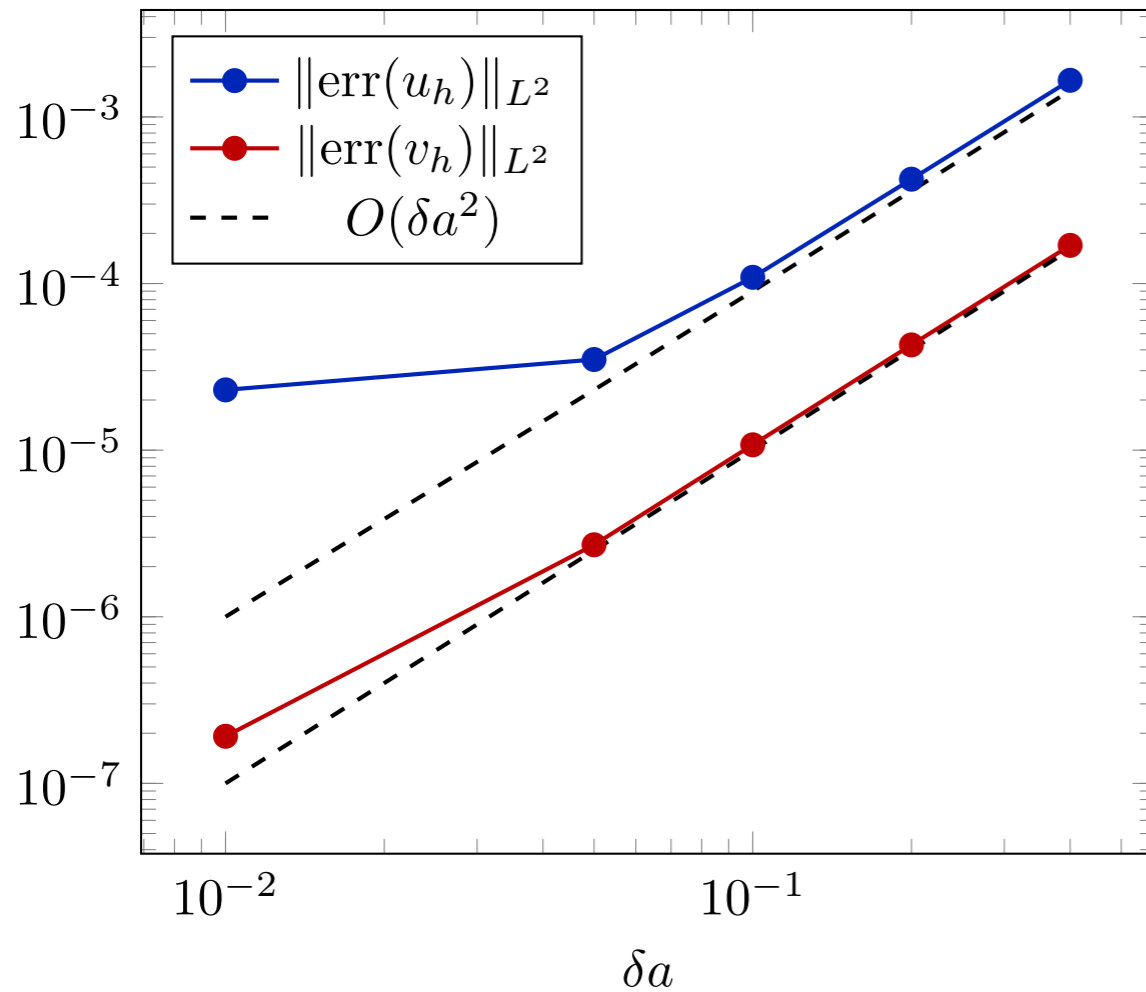
Test case description

Domain :



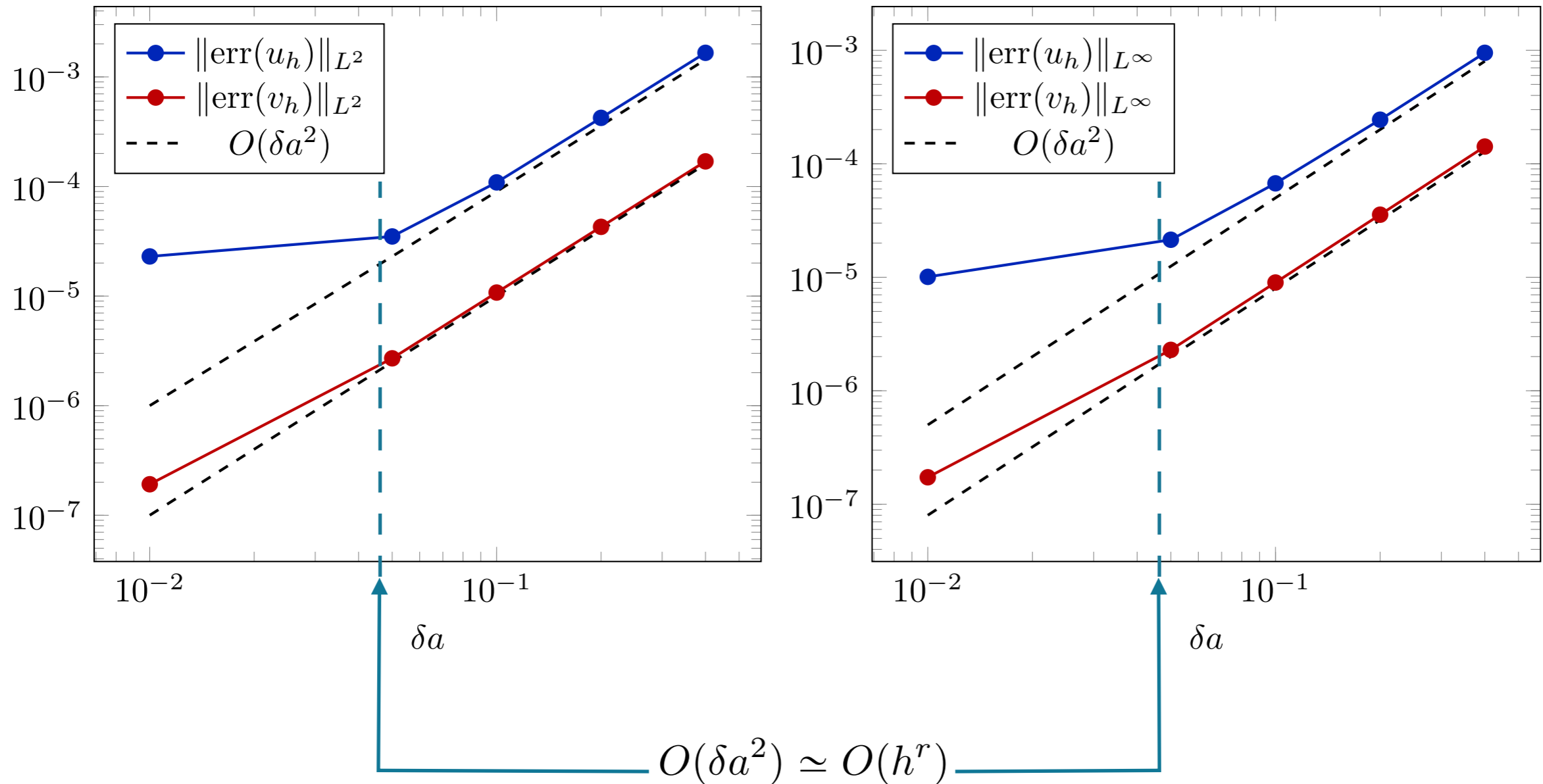
Results

$$\text{err}(\mathbf{u}) = \mathbf{u}(x, T; a + \delta a) - \mathbf{u}(x, T; a) - \delta a \mathbf{u}_a(x, T; a) \simeq O(\delta a^2)$$



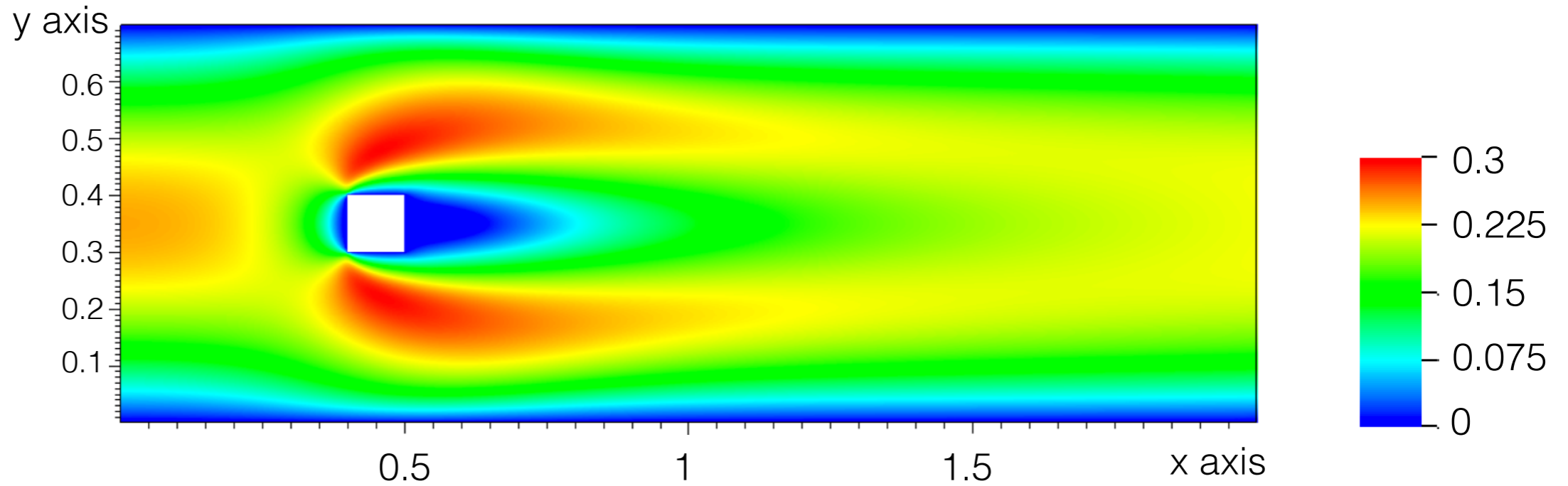
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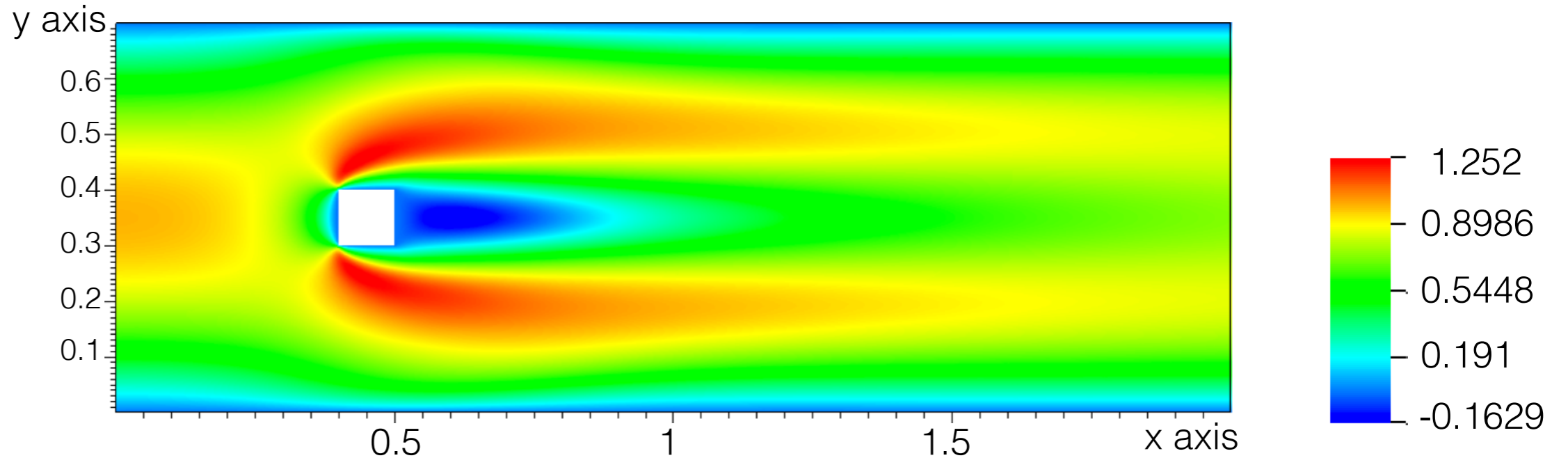


Steady case : x-component of the velocity and its sensitivity

State

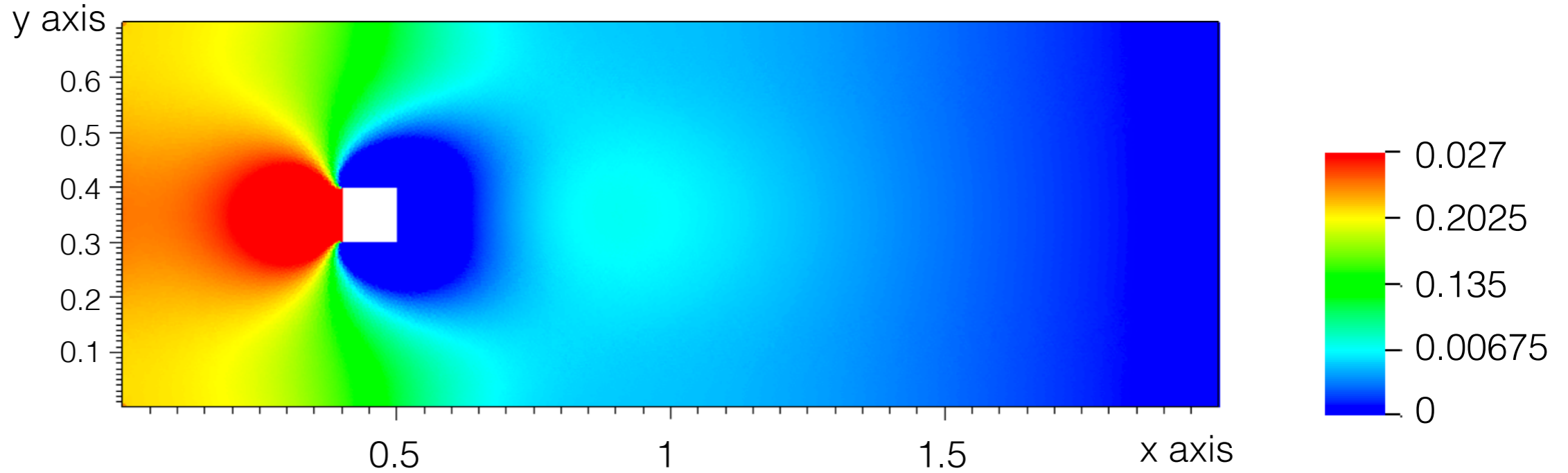


Sensitivity

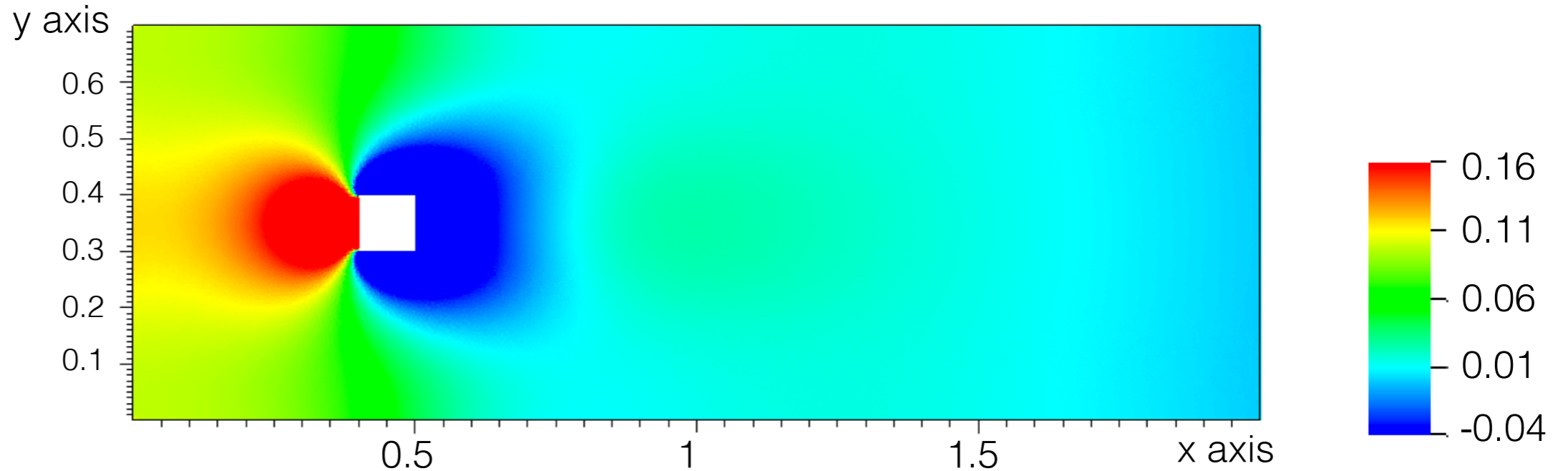


Steady case : pressure and its sensitivity

State

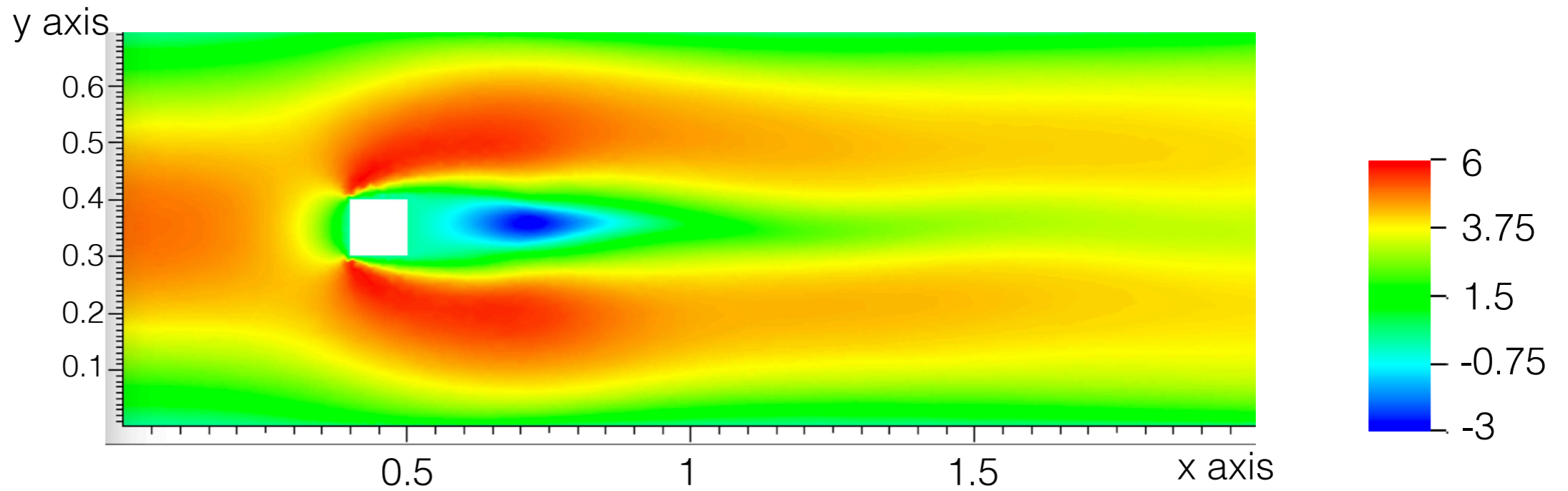


Sensitivity

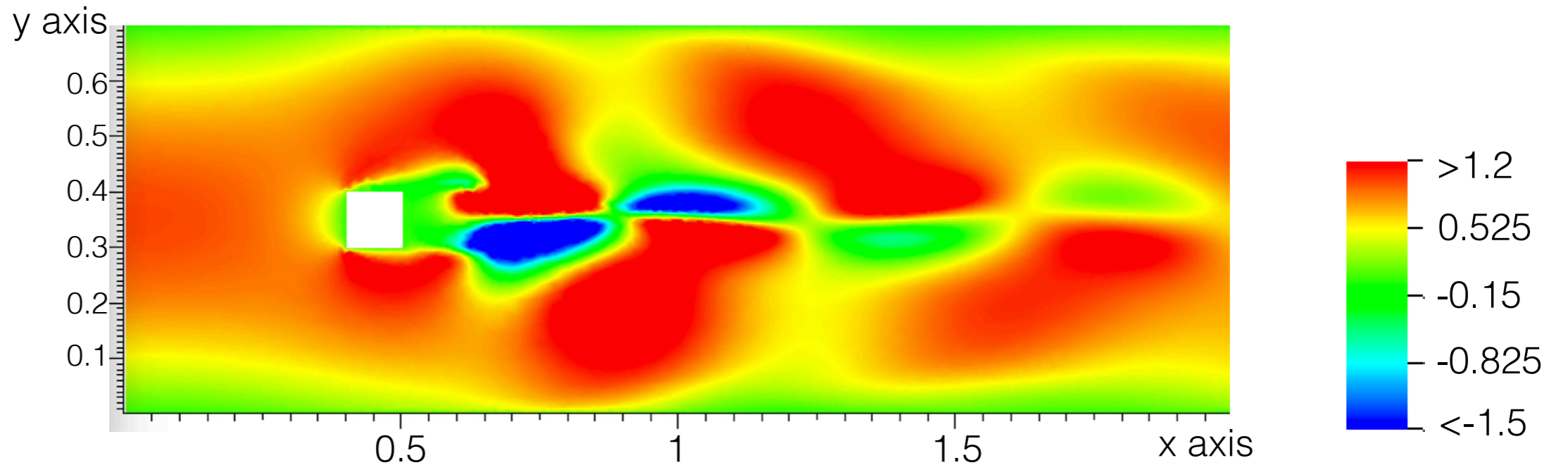


$t = 0.680104$

State



Sensitivity



$t = 0.680104$

y axis
0.6
0.5

State

Proposition 2 Let \mathbf{R}_{g_a} be a sufficiently smooth stationary function such that $\nabla \cdot \mathbf{R}_{g_a} = 0$ in Ω and $\mathbf{R}_{g_a} = \mathbf{u}_a$ on $\Gamma_{in} \cup \Gamma_w$. Then, if $\mathbf{u} \cdot \mathbf{n} \geq 0$ on Γ_{out} and if

$$\exists \kappa_1 = \kappa_1(\mathbf{u}, \Omega) : - \int_{\Omega} [(\mathbf{u}_a \cdot \nabla) \mathbf{u}] \cdot \mathbf{u}_a \leq \kappa_1 \|\nabla \mathbf{u}_a\|^2$$

the following stability estimate holds for some $\gamma_1 > 0$:

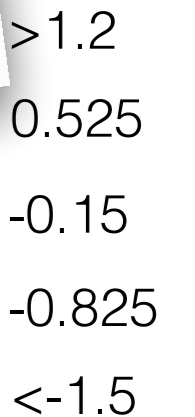
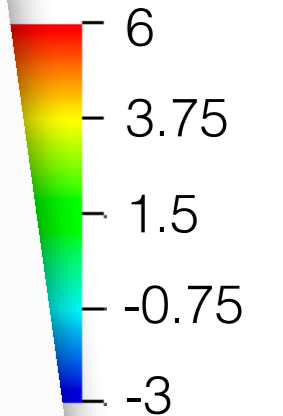
$$\|\mathbf{u}_a\|^2 \leq \frac{1}{2\nu} \int_0^T \|\tilde{\mathbf{f}}_a(t)\|_{H^{-1}(\Omega)}^2 dt + \gamma_1 \|\mathbf{R}_{g_a}\|_{H^1(\Omega)}^2,$$

where $\tilde{\mathbf{f}}_a = \bar{\mathbf{f}}_a + \nu \Delta \mathbf{R}_{g_a} - (\mathbf{R}_{g_a} \cdot \nabla) \mathbf{R}_{g_a}$.

$$- \int_{\Omega} [(\mathbf{u}_a \cdot \nabla) \mathbf{u}] \cdot \mathbf{u}_a \leq \|\mathbf{u}_a\|_{L^4}^2 \|\nabla \mathbf{u}\| \leq C \|\nabla \mathbf{u}\| \|\nabla \mathbf{u}_a\|^2$$

$H^1 \subset L^4$

“Morally” it is $\|\nabla \mathbf{u}\|$



0.5 1 1.5 x axis

Sensitivity

Let \mathbf{a} be a gaussian random vector, with the following average and variance:

$$\mu_{\mathbf{a}} = \begin{bmatrix} \mu_{a_1} \\ \vdots \\ \mu_{a_M} \end{bmatrix}, \quad \sigma_{\mathbf{a}} = \begin{bmatrix} \sigma_{a_1}^2 & \text{COV}(a_1, a_2) & \dots & \text{COV}(a_1, a_M) \\ \text{COV}(a_1, a_2) & \sigma_{a_2}^2 & \dots & \text{COV}(a_2, a_M) \\ \vdots & \vdots & \ddots & \vdots \\ \text{COV}(a_1, a_M) & \dots & \dots & \sigma_{a_M}^2 \end{bmatrix},$$

Aim: determine a **confidence interval** $CI_X = [\mu_X - d(\sigma_X), \mu_X + d(\sigma_X)]$
 $P(X \in CI_X) \geq 1 - \alpha$

Monte Carlo approach: N samples of the state X_k

$$\mu_X = \frac{1}{N} \sum_{k=1}^N X_k \quad \sigma_X^2 = \frac{1}{N-1} \sum_{k=1}^N |\mu_X - X_k|^2$$

Sensitivity approach: let us consider the following first order Taylor expansion

$$X(\mathbf{a}) = X(\mu_{\mathbf{a}}) + \sum_{i=1}^M (a_i - \mu_{a_i}) X_{a_i}(\mu_{\mathbf{a}}) + o(\|\mathbf{a} - \mu_{\mathbf{a}}\|^2)$$

Then, computing, the average one has:

$$\mu_X = E[X(\mathbf{a})] = X(\mu_{\mathbf{a}}) + \sum_{i=1}^M X_{a_i}(\mu_{\mathbf{a}}) E[a_i - \mu_{a_i}] = X(\mu_{\mathbf{a}}),$$

And for the variance:

$$\begin{aligned} \sigma_X^2 &= E[(X(\mathbf{a}) - \mu_X)^2] = E \left[\left(\sum_{i=1}^M X_{a_i}(\mu_{\mathbf{a}}) (a_i - \mu_{a_i}) \right)^2 \right] = \\ &= \sum_{i=1}^M X_{a_i}^2(\mu_{\mathbf{a}}) E[(a_i - \mu_{a_i})^2] + \sum_{\substack{i,j=1 \\ i \neq j}}^M X_{a_i}(\mu_{\mathbf{a}}) X_{a_j}(\mu_{\mathbf{a}}) E[(a_i - \mu_{a_i})(a_j - \mu_{a_j})]. \end{aligned}$$

Therefore, we have the following first order estimates:

$$\mu_X = X(\mu_{\mathbf{a}}), \quad \sigma_X^2 = \sum_{i=1}^M X_{a_i}^2 \sigma_{a_i}^2 + \sum_{\substack{i,j=1 \\ i \neq j}}^M X_{a_i} X_{a_j} \text{cov}(a_i, a_j).$$

Monte Carlo approach:



Provides information on the distribution of the output

Smaller confidence intervals



Computational cost

SA approach :



Reasonable computational cost (depending on the number of parameters)



No insight on the distribution of the output
Valid for small variation of the input

How to compute a confidence interval for an unknown distribution?

Chebyshev's inequality: $P(|X - \mu_X| \geq \lambda) \leq \frac{\sigma_X^2}{\lambda^2} \quad \forall \lambda > 0$

Which implies: $P(X \in (\mu_X - \lambda, \mu_X + \lambda)) \geq 1 - \frac{\sigma_X^2}{\lambda^2}$.

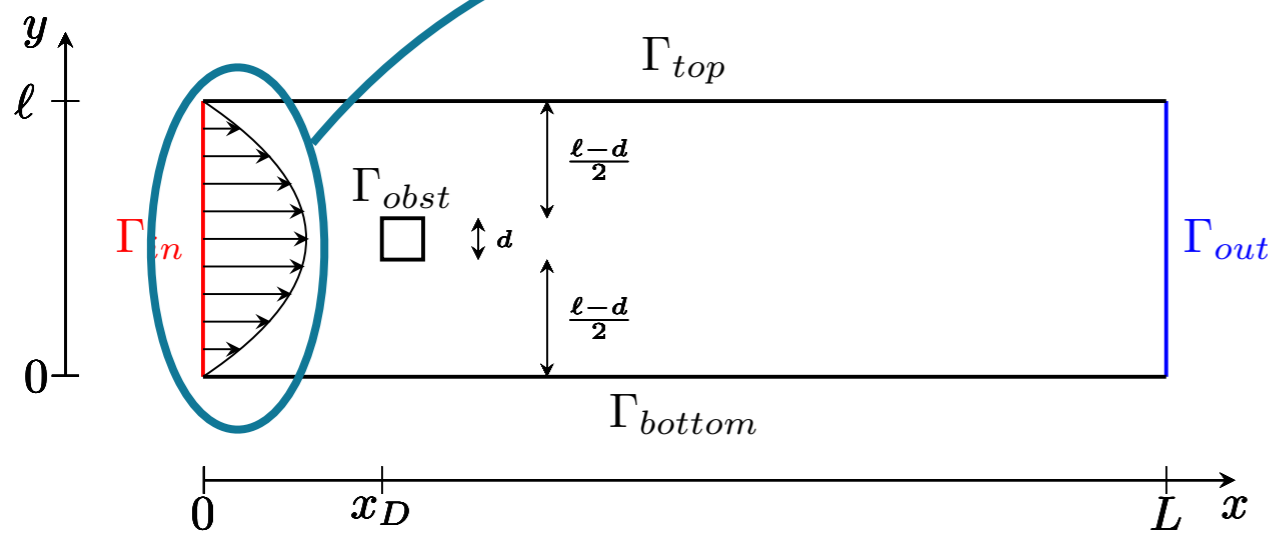
Now, by asking for $1 - \frac{\sigma_X^2}{\lambda^2} = 1 - \alpha$ one obtains $\lambda = \frac{\sigma_X}{\sqrt{\alpha}}$.

Remark: if the variable X was gaussian, to obtain a 95% confidence interval the half amplitude should be $1.96\sigma_X$, whilst with this method we obtain $4.47\sigma_X$.

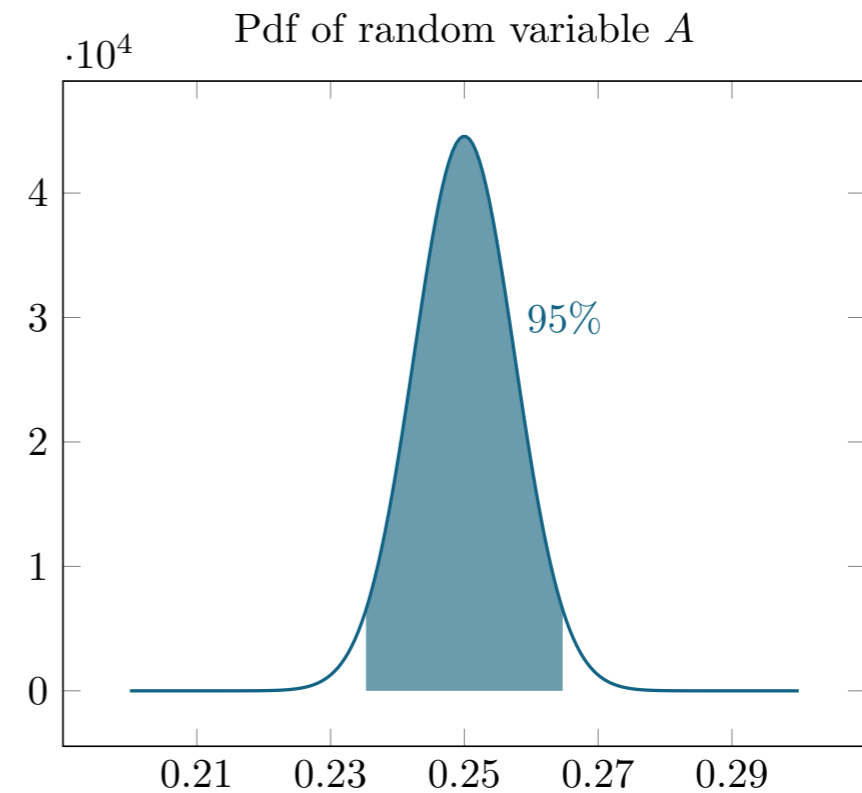
Domain :

uncertain
parameter

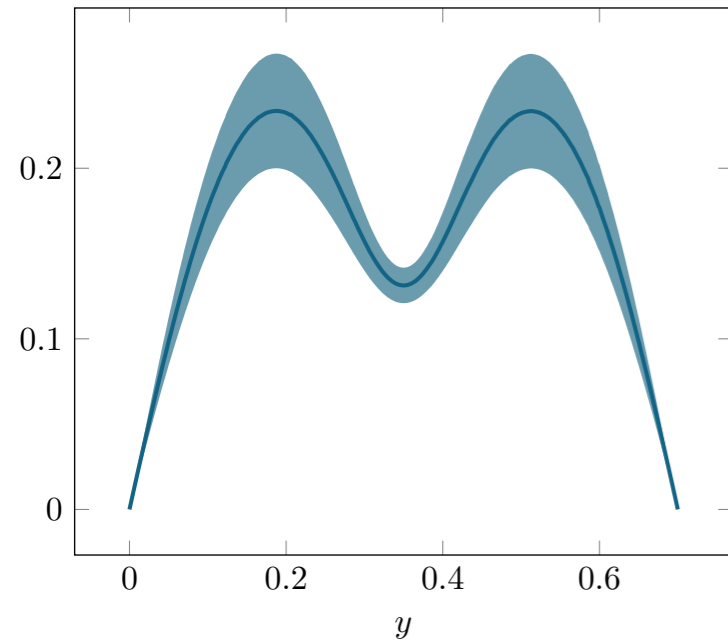
$$g(y) = \frac{4A}{\ell^2} y(\ell - y)$$



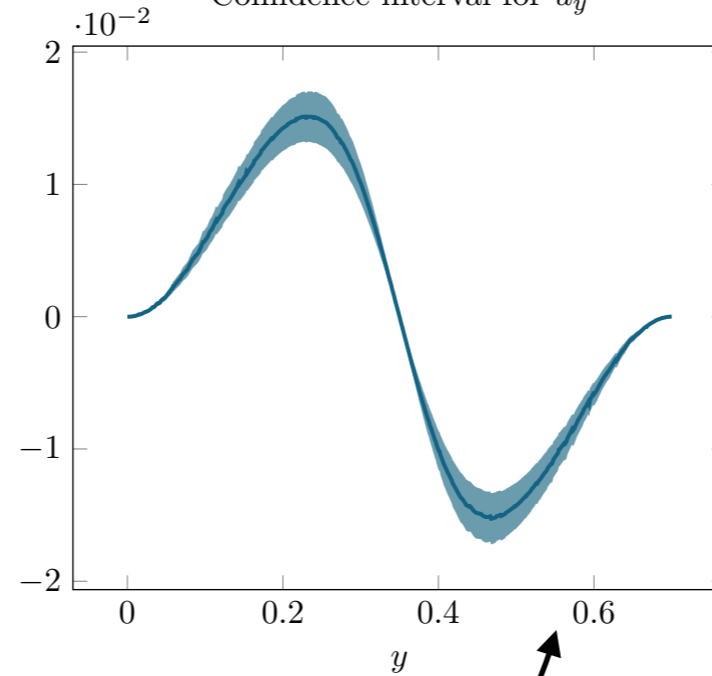
$$\Gamma_w = \Gamma_{obst} \cup \Gamma_{top} \cup \Gamma_{bottom}$$



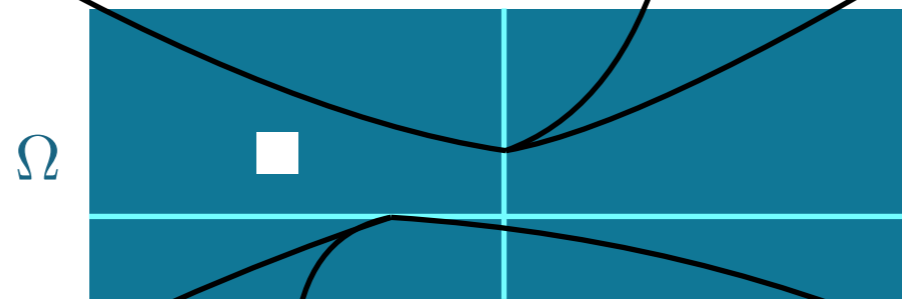
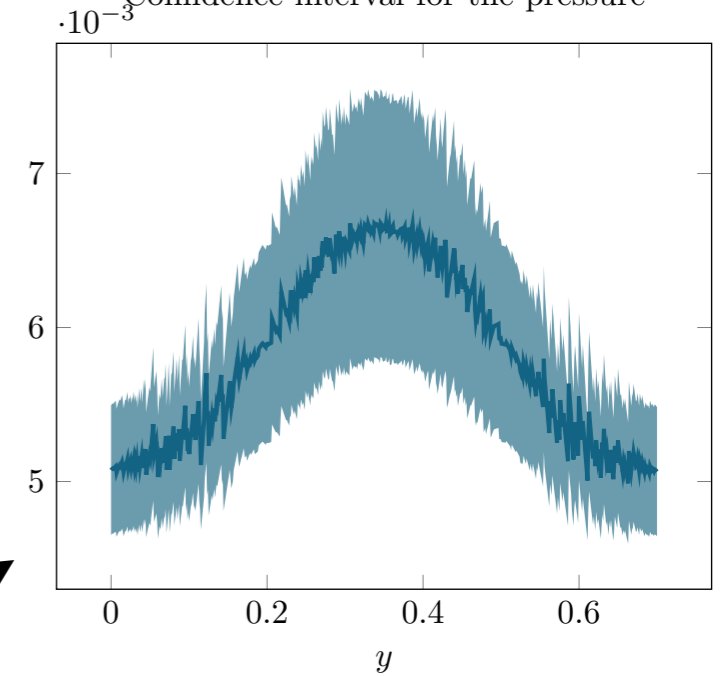
Confidence interval for u_x



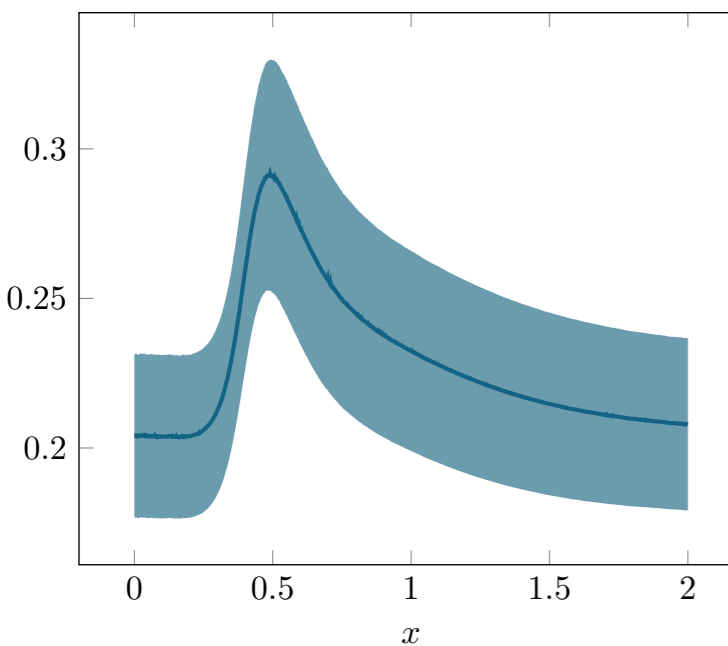
Confidence interval for u_y



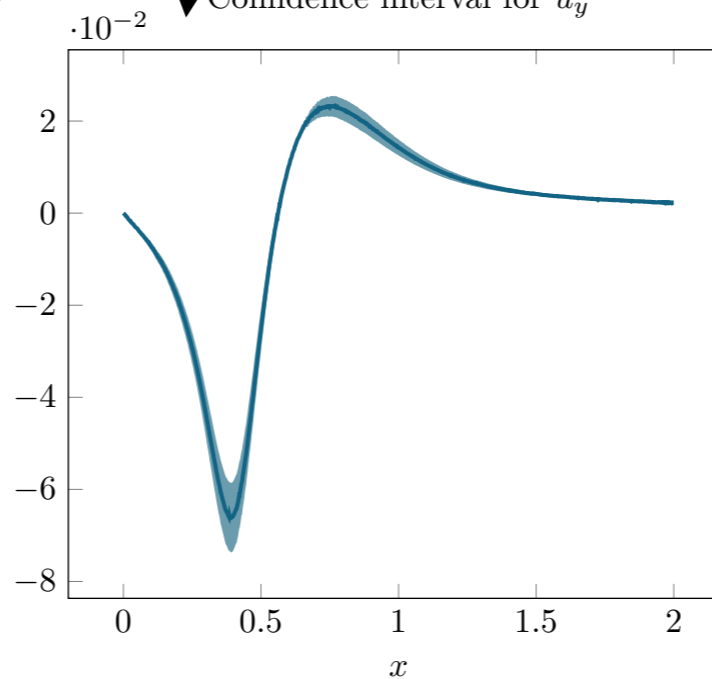
Confidence interval for the pressure



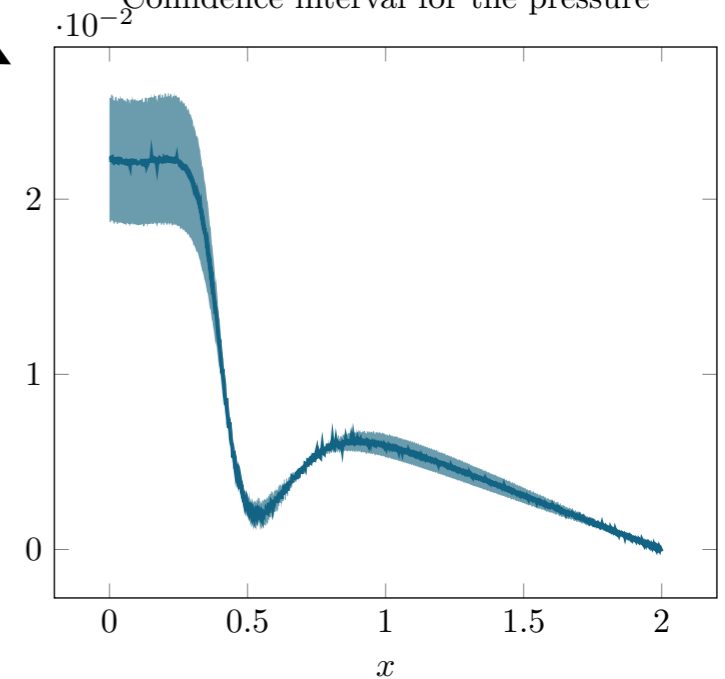
Confidence interval for u_x



Confidence interval for u_y



Confidence interval for the pressure



- ▶ Publish the sensitivity module of the code
- ▶ Higher order schemes in space
- ▶ Extension to 3D
- ▶ Coupling with a temperature equation
- ▶ More realistic simulations
- ▶ Turbulence models

**Thank you
for your attention!**