BIOSKINS: Metamodels for a system of fibres

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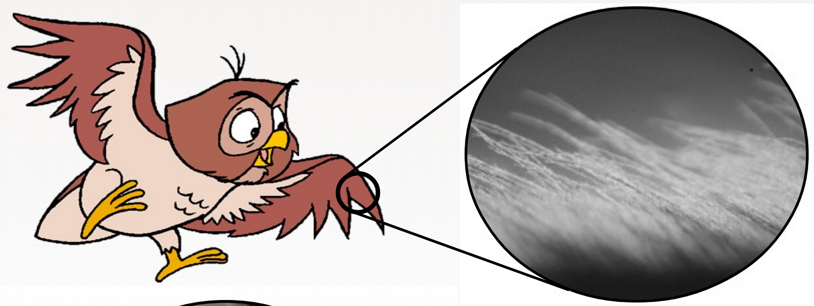
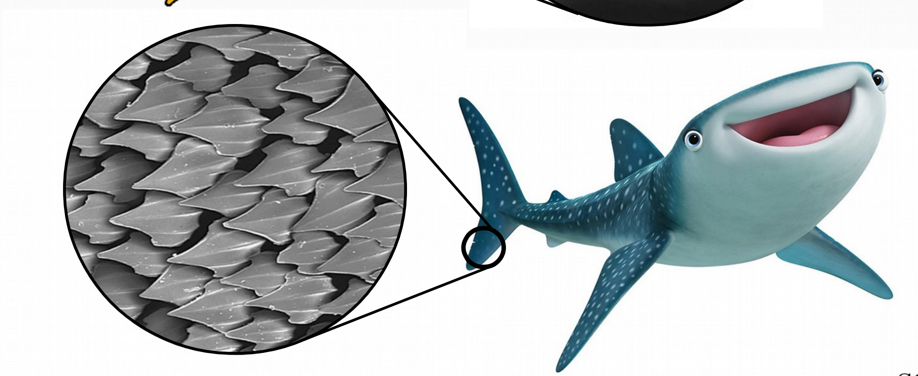
PRESENTATION PLAN

- Introduction
- VANS theory
- CFD: procedure and results
- DACE
- Metamodelling
- Kriging results
- Conclusions

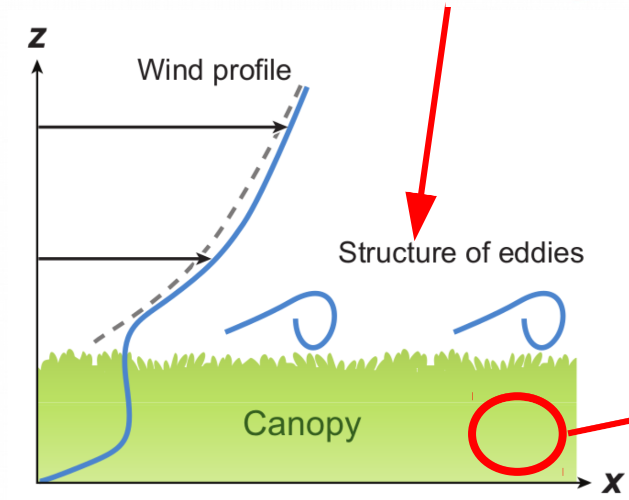
Introduction

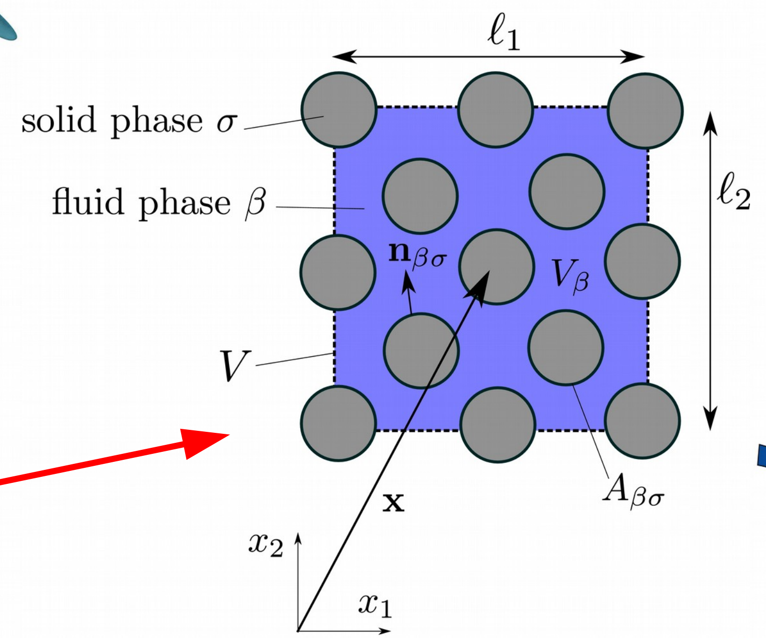




The goal is to find a cheap way to model poroelastic surfaces

The are many problems involved:
- Multiple scales
- Interface coupling
- Fluid structure interaction
- Anisotropy

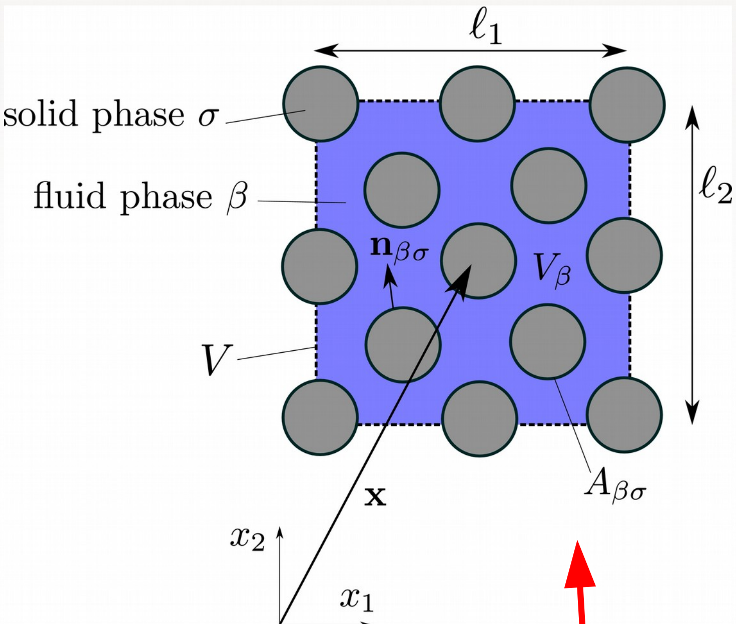


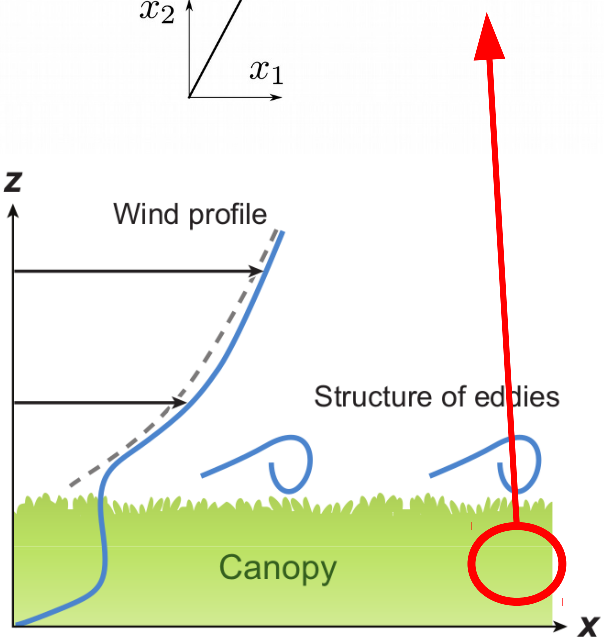


[Luminari, Airiau and Bottaro, "Drag-model sensitivity of Kelvin-Helmholtz waves in canopy flows", Physics of fluids, 2016]

VANS THEORY: 1

REV: Representative Elementary Volume





3D incompressible flow

$$\frac{\partial v}{\partial t} + v \cdot \nabla v = -\frac{1}{\rho}\nabla p + \nu \nabla^2 v$$

$$\nabla \cdot v = 0$$

1) Intrinsic average operator:

$$\langle \psi_\beta \rangle^\beta = \frac{1}{V_\beta} \int_{V_\beta} \psi(x)\, dV_\beta$$

2) Porosity:

$$\varepsilon = \frac{V_\beta}{V}$$

3) Field decomposition:

$$\psi = \langle \psi \rangle^\beta + \tilde{\psi}$$

VANS THEORY: 2

Applying 1) 2) and 3) to the NS system we obtain the VANS:

$$\frac{\partial \langle \mathbf{v}_\beta \rangle^\beta}{\partial t} + \langle \mathbf{v}_\beta \rangle^\beta \cdot \nabla \langle \mathbf{v}_\beta \rangle^\beta = -\frac{1}{\rho_\beta} \nabla \langle p_\beta \rangle^\beta + \nu_\beta \nabla^2 \langle \mathbf{v}_\beta \rangle^\beta + \frac{1}{V_\beta} \int_{A_{\beta\sigma}} (-\frac{\tilde{p_\beta}}{\rho_\beta} \mathbf{I} + \nu_\beta \nabla \tilde{\mathbf{v}_\beta}) \cdot \mathbf{n}_{\beta\sigma} \, dA$$

$$\nabla \cdot \langle \mathbf{v}_\beta \rangle^\beta = 0$$

The fluctuations are still in the equation

4) A closure model is required

micro

$$\mathbf{D} = \frac{1}{V_\beta} \int_{A_{\beta\sigma}} (-\frac{\tilde{p_\beta}}{\rho_\beta} \mathbf{I} + \nu_\beta \nabla \tilde{\mathbf{v}_\beta}) \cdot \mathbf{n}_{\beta\sigma} \, dA$$

MACRO

$$-\nu_\beta \varepsilon \mathbf{K}^{-1} (\mathbf{I} + \mathbf{F} \| \langle \mathbf{v}_\beta \rangle^\beta \|) \langle \mathbf{v}_\beta \rangle^\beta$$

Permeability tensor

Forchheimer tensor

CLOSURE PROBLEMS

$$\begin{cases} 0 = -\nabla \mathbf{d} + \nabla^2 \mathbf{D} + \mathbf{I} \\ \nabla \cdot \mathbf{D} = 0 \\ \mathbf{D} = 0 \qquad at \qquad A_{\beta\sigma} \\ \mathbf{d}(\mathbf{x} + \ell_i) = \mathbf{d}(\mathbf{x}), \qquad \mathbf{D}(\mathbf{x} + \ell_i) = \mathbf{D}(\mathbf{x}) \qquad i = 1, 2, 3 \end{cases}$$

STOKES REGIME

$$\varepsilon \, \langle \mathbf{D} \rangle^i = \mathbf{K}$$

Thanks to the unity matrix the equations are decoupled with triplets
(3x3 equations instead of 9 coupled)

The 3x3 systems have the structure of a Stokes, and Linearized Navier-Stokes problems (we can use the same numerical solvers)

In this case we need also the DNS microscopic field.

The two tensors depend on 4 different flow parameters

$$\begin{cases} \frac{1}{\nu_\beta} \mathbf{v}_\beta \cdot \nabla \mathbf{M} = -\nabla \mathbf{m} + \nabla^2 \mathbf{M} + \mathbf{I} \\ \nabla \cdot \mathbf{M} = 0 \\ \mathbf{M} = 0 \qquad at \qquad A_{\beta\sigma} \\ \mathbf{m}(\mathbf{x} + \ell_i) = \mathbf{m}(\mathbf{x}), \qquad \mathbf{M}(\mathbf{x} + \ell_i) = \mathbf{M}(\mathbf{x}) \qquad i = 1, 2, 3 \end{cases}$$

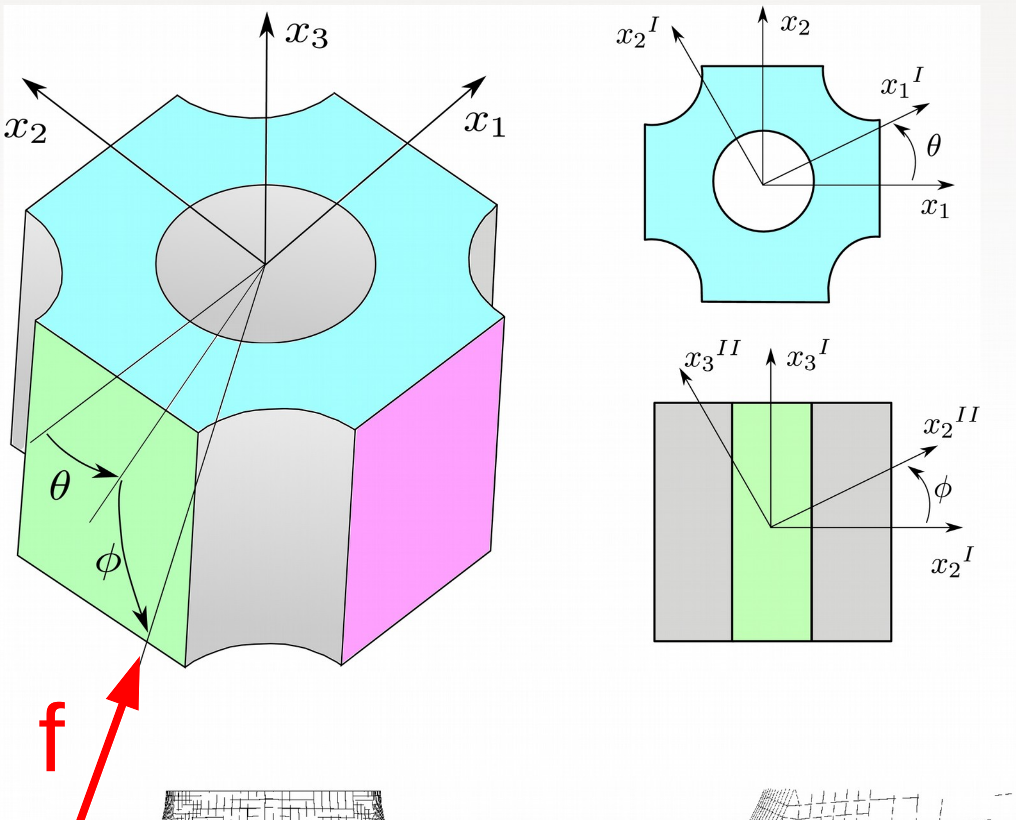
INERTIA REGIME

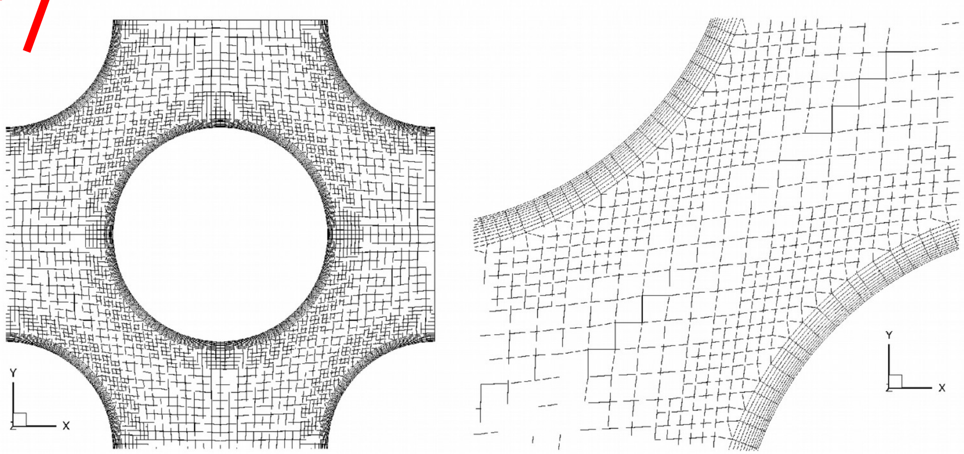
$$\varepsilon \, \langle \mathbf{M} \rangle^i = \mathbf{H}$$

$$\mathbf{H}^{-1} = \mathbf{K}^{-1} (\mathbf{F} + \mathbf{I}) \qquad \Rightarrow \qquad \mathbf{F} = \mathbf{K}\mathbf{H}^{-1} - \mathbf{I}$$

[Whitaker, 1996,Transport in Porous Media]

CFD PROCEDURE





Rigid cylindric filaments in staggered arrangements.

Imposing Re(through f), θ , ϕ, ε

Solve DNS with cyclic b.c.:

$$\frac{\partial \mathbf{v}_\beta}{\partial t} + \nabla \cdot (\mathbf{v}_\beta \mathbf{v}_\beta) = -\frac{1}{\rho}\nabla p_\beta + \nu_\beta \nabla^2 \mathbf{v}_\beta + \mathbf{f}$$

$$\nabla \cdot (\mathbf{v}_\beta) = 0$$

Solve closure problem (form previous slides).

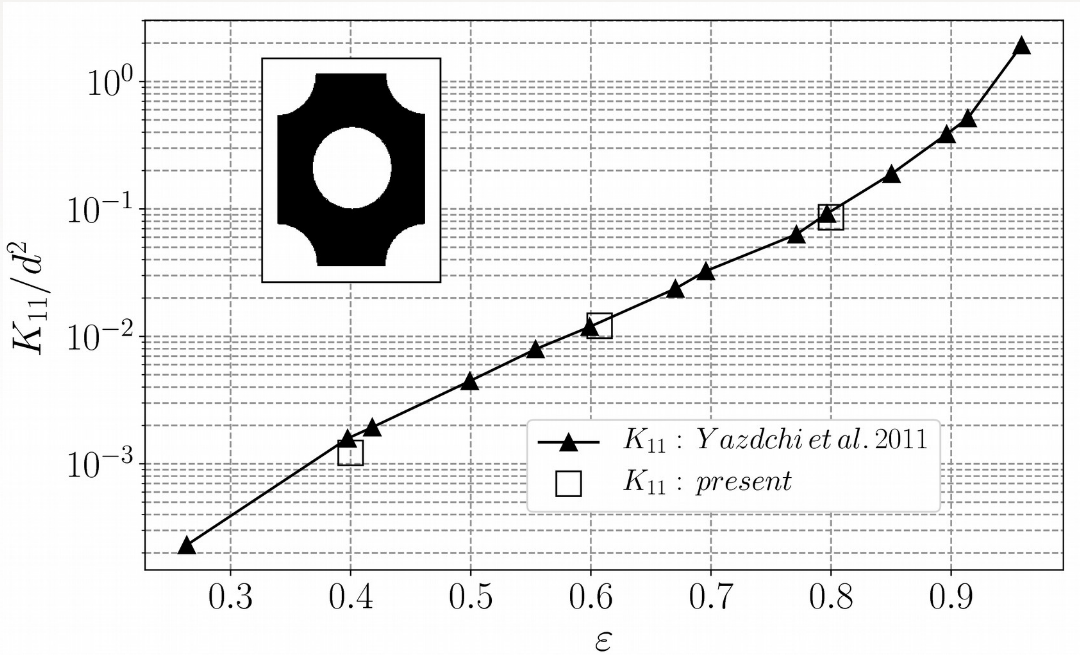
Perform the averaging to obtain the 9 components of **H**.

OpenFOAM

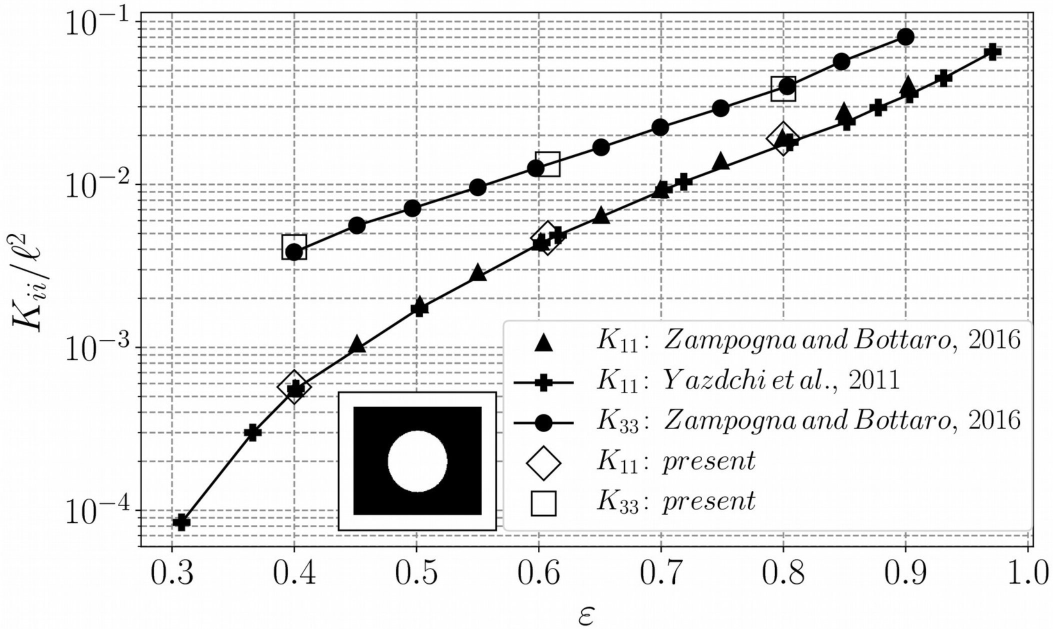
The Open Source CFD Toolbox

VALIDATION

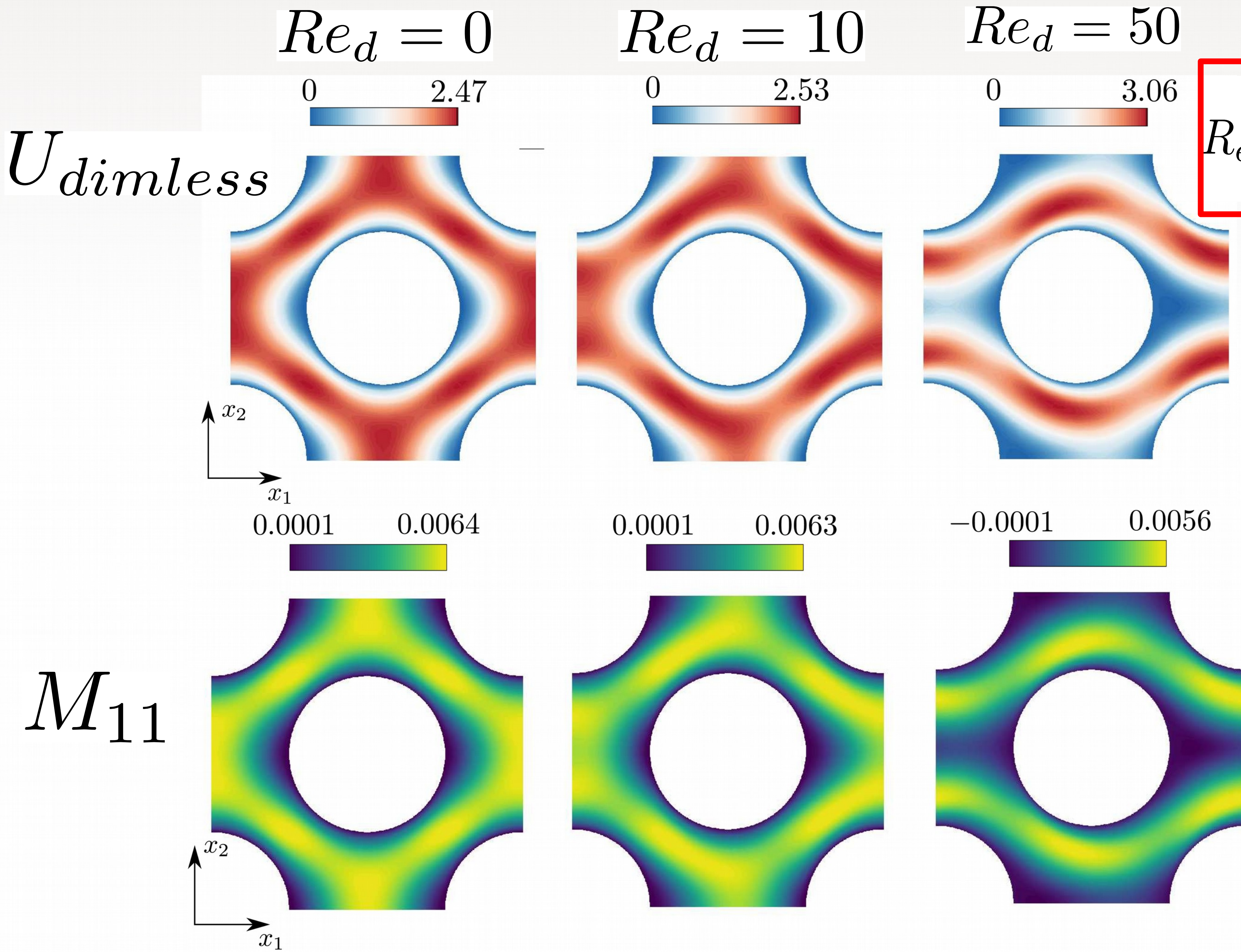
Staggered cylinder arrangement



Centered cylinder arrangement

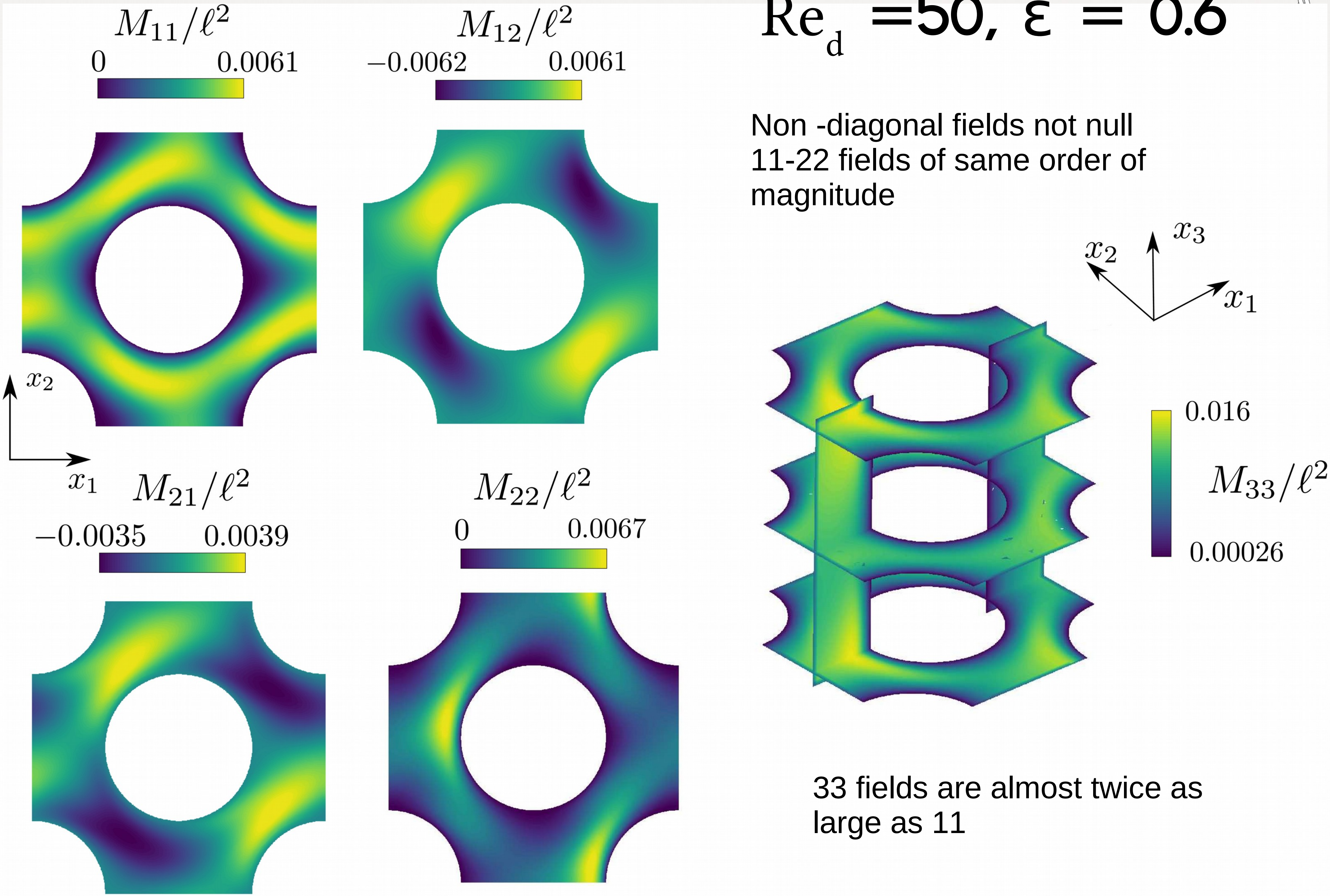


DNS: ε = 0.6



$$R_e = \frac{d < U >^i}{\nu_\beta}$$

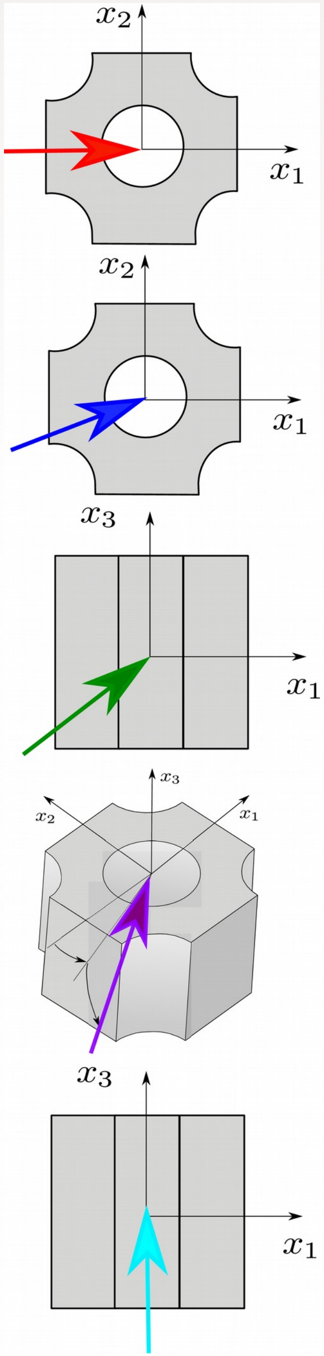
M FIELDS: $\theta = 22.5^\circ$, $\varphi = 45^\circ$, $Re_d = 50$, $\varepsilon = 0.6$



Non -diagonal fields not null
11-22 fields of same order of magnitude

33 fields are almost twice as large as 11

PARAMETERS EXPLORATION



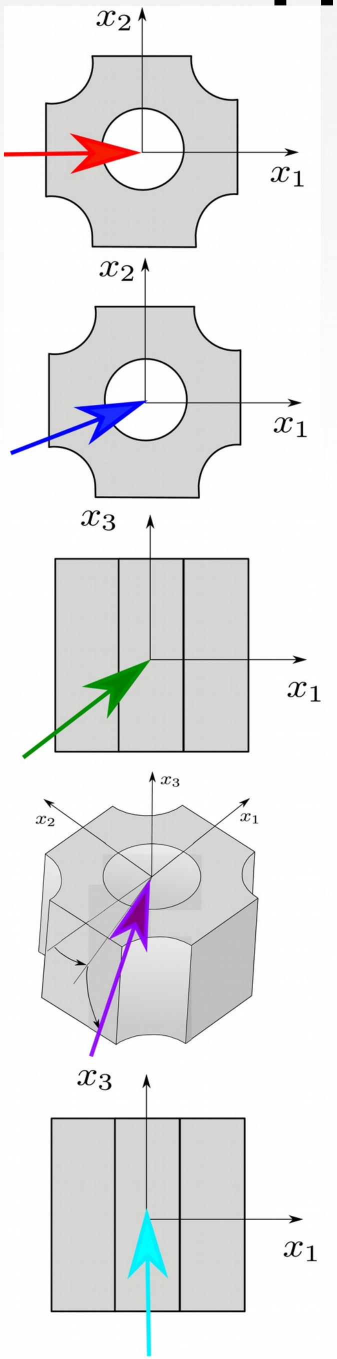
index	θ	ϕ	field properties
1	$0°$	$0°$	2D symmetric
2	$22.5°$	$0°$	2D non-symmetric
3	$0°$	$45°$	3D symmetric
4	$22.5°$	$45°$	3D non-symmetric
5	–	$90°$	3D symmetric

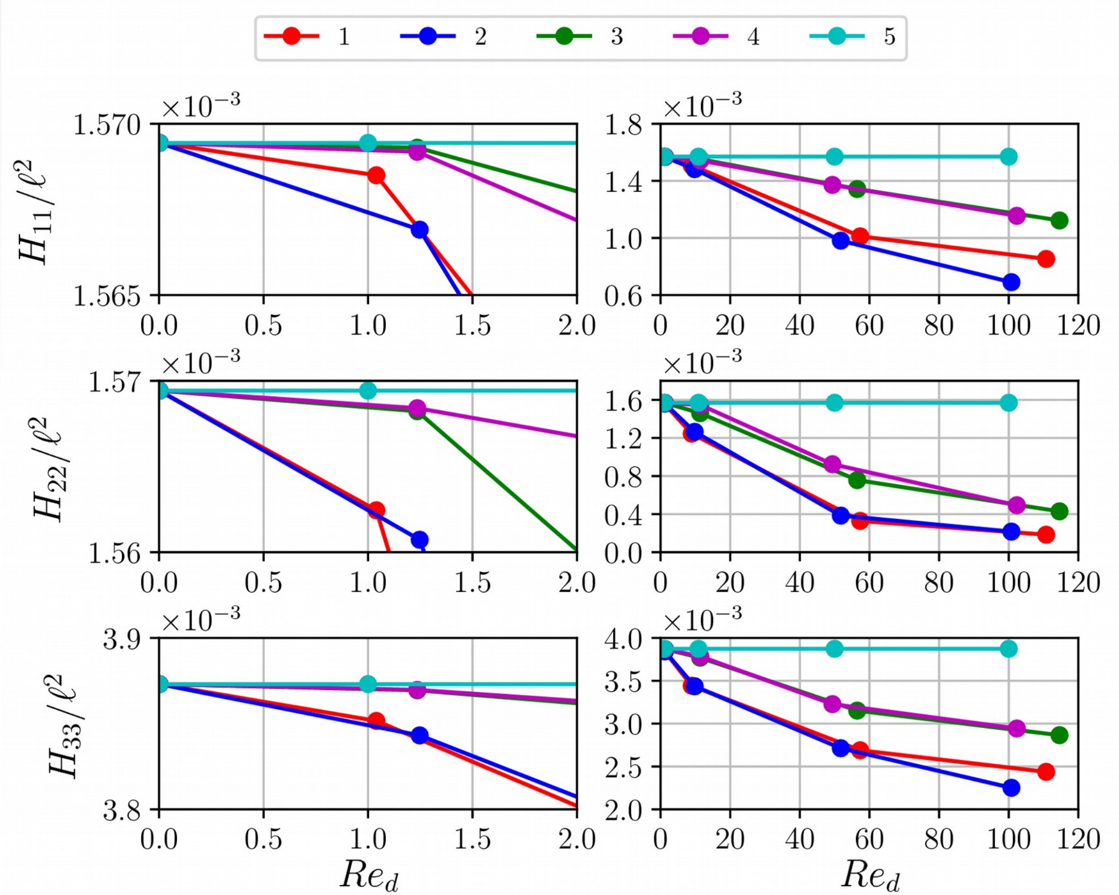
For each of the 5 directions the computation of H is carried out.

The variability of 3 values of porosity 0.4, 0.6, 0.8 are explored

Reynolds number is also changed

H COMPONENTS FOR ε = 0.6

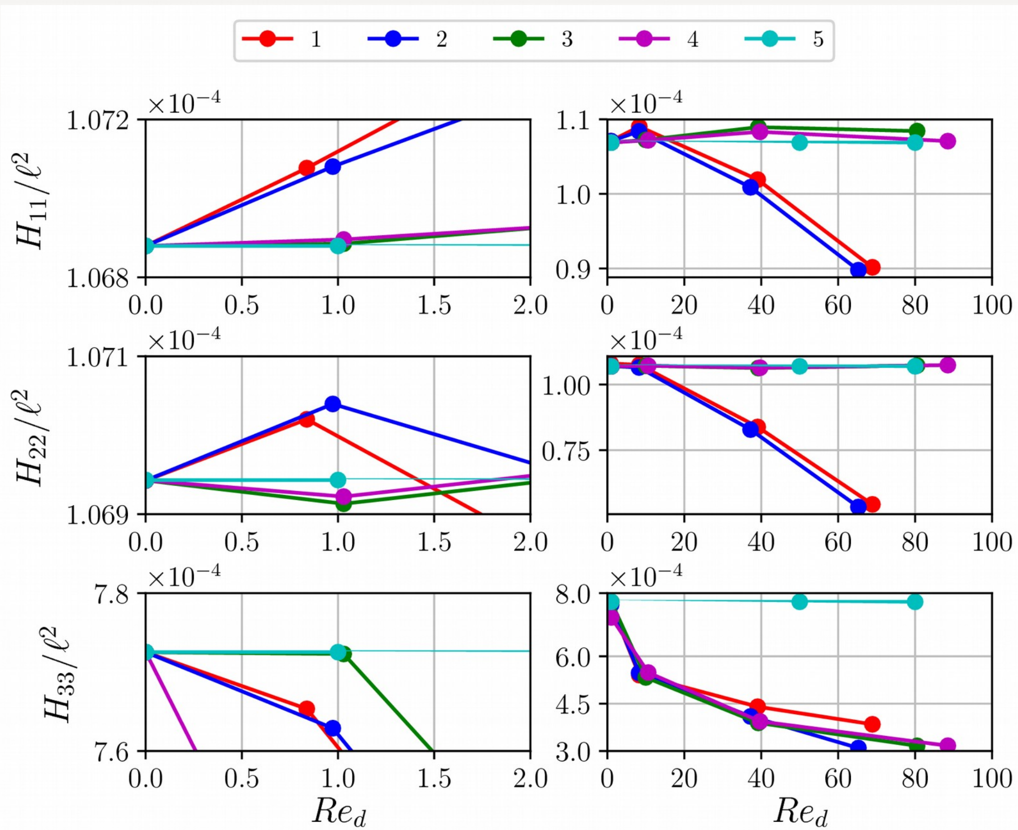




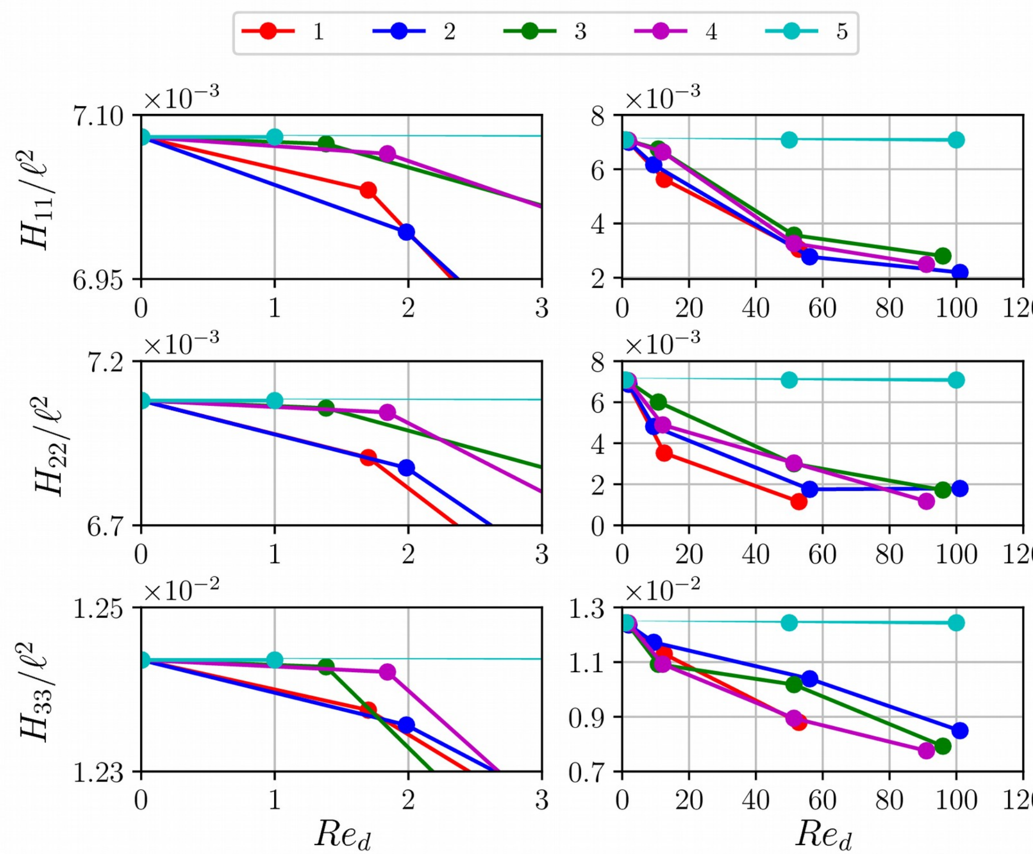
At small Reynolds number the variability is very small

At “high” Reynolds number is possible to distinguish between directions expecially with the angle Φ

H COMPONENTS FOR ε = 0.4, 0.8

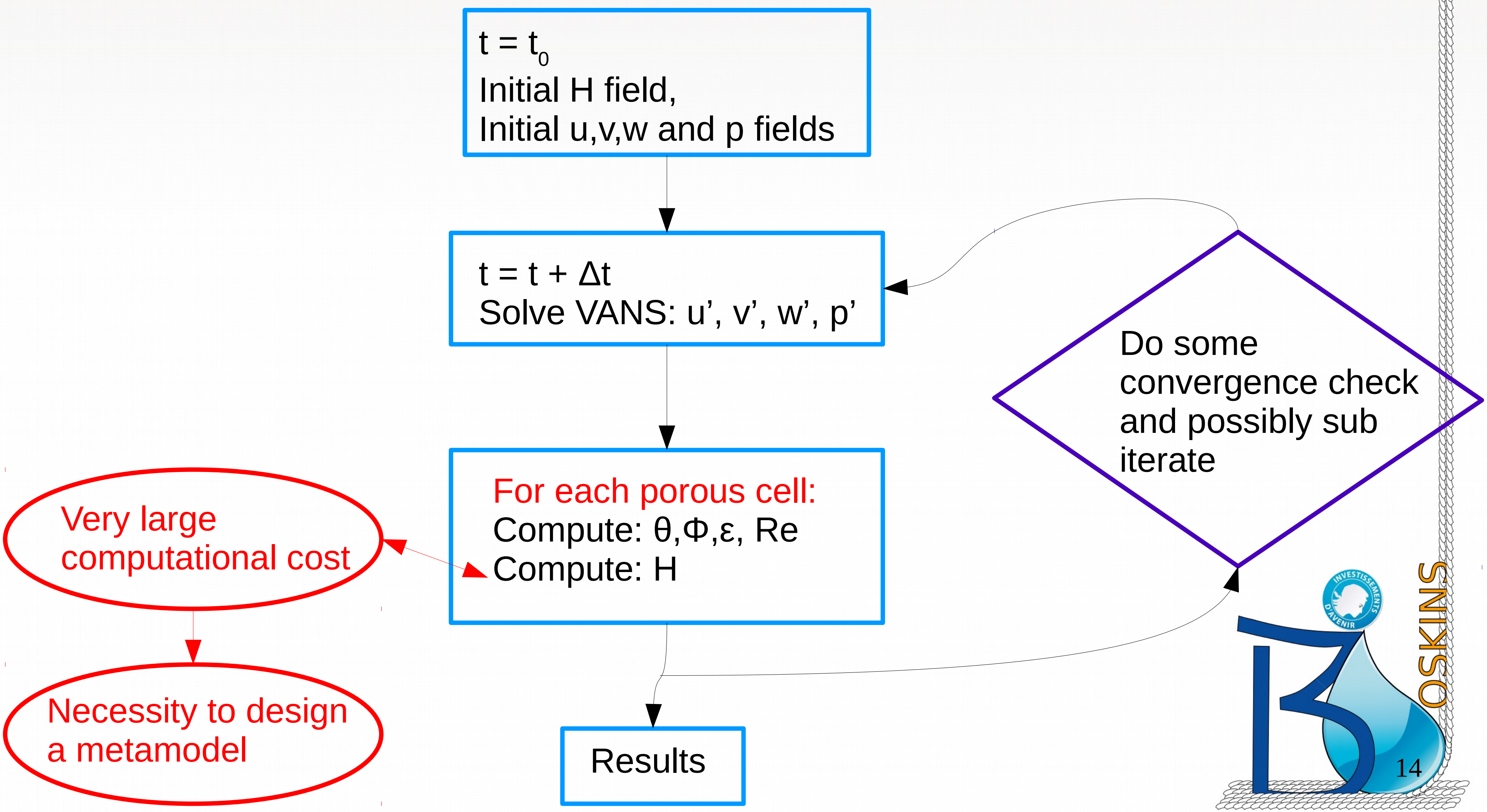


At low porosity (ε = 0.4, on the left) the variability is smaller than before and as before the angle Φ seems to play a bigger role



At low porosity (ε = 0.8, on the right) the curves almost collapse onto one another except for the case with the velocity aligned with the fibre's axis

MACROSCOPIC SIMULATION ALGORITHM:



DACE: Design and Analysis of Computer Experiments

“an experiment is a series of tests in which the input variables are changed according to a given rule in order to identify the reasons for the changes in the output response”[1]

The choice of the “rule” depends on:

- Number of variables (parameters)
- Number of feasible “experimental” runs: N
- Nature of variables (discrete vs continuous)
- Outputs of the experiment

[1] Optimization Methods, Marco Cavazzuti, Springer 2012

DACE ANALYSIS

Random Monte Carlo

- Building response surfaces
- N is a user choice

A jungle of models can be used:

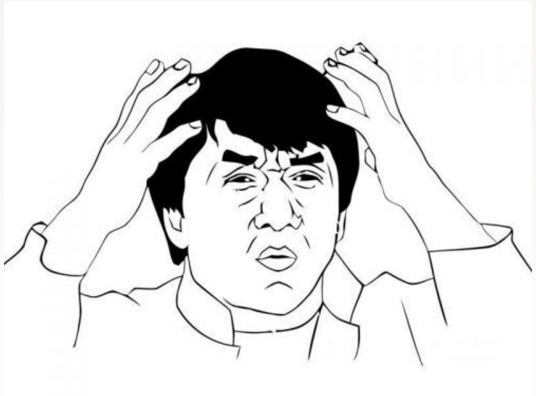
- Tagushi tables
- Full factorial design
- Latin hypercube
- Chebichev polynomials
- ...

parameter	values				
θ	$0°$	$22.5°$	$45°$		
ϕ	$0°$	$22.5°$	$45°$	$67.5°$	$90°$
Re_d	0	10	50	100	
ε	0.4	0.6	0.8		

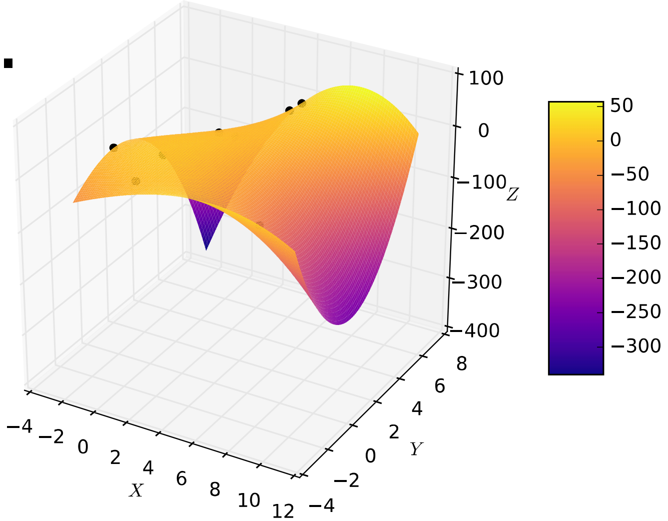
Total numbers of experiments : 118

WHAT IS A METAMODEL?

- "A metamodel is a model of a model..." from wikipedia

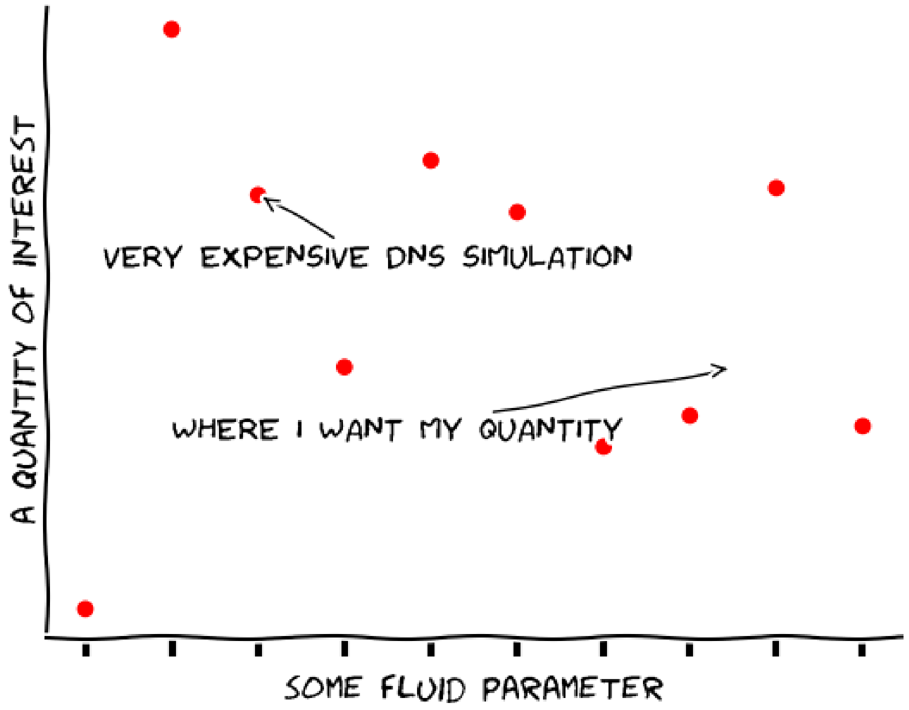


- It is a simpler/cheaper way (simpler than the parent model) to generate new output values of an experiment.



WHEN DO WE NEED IT ?

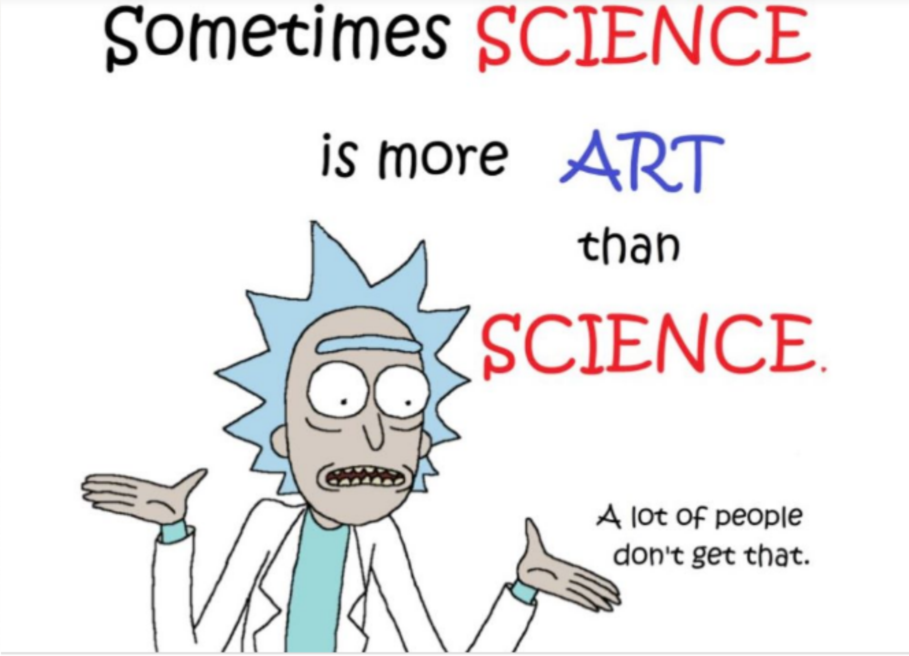
- Whenever your parent model is too “heavy”
- If you do not know the parent model (machine learning)



- Example: Optimization, Uncertainty Quantification, Flow Control

WHICH MODEL IS "THE BEST" ?

- Number of data points
- Distributions of data points
- Availability as library / easyness of implementation
- Domain of applications
- Minimize errors
- Number of variables
- Noise presence, interpolation vs approximation



There is a really jungle of possibilities:

- Least Square regression
- P-th polynomial
- Polynomial chaos
- Radial basis functions
- Deep learning

Kriging Metamodel

- The predictor is a sum of a trend function and a Gaussian process error model

$$y(\mathbf{x}) \approx \hat{f}(\mathbf{x}) = t(\mathbf{x}) + e(\mathbf{x})$$

$t(\mathbf{x})$ → Quadratic Least Square

$e(\mathbf{x})$ → Gaussian process

$$\mathrm{Cov}(y(\mathbf{x_i}), y(\mathbf{x_j})) = \sigma^2 r(\mathbf{x_i}, \mathbf{x_j})$$

$$(\mathbf{x_i}, y(\mathbf{x_i}))$$

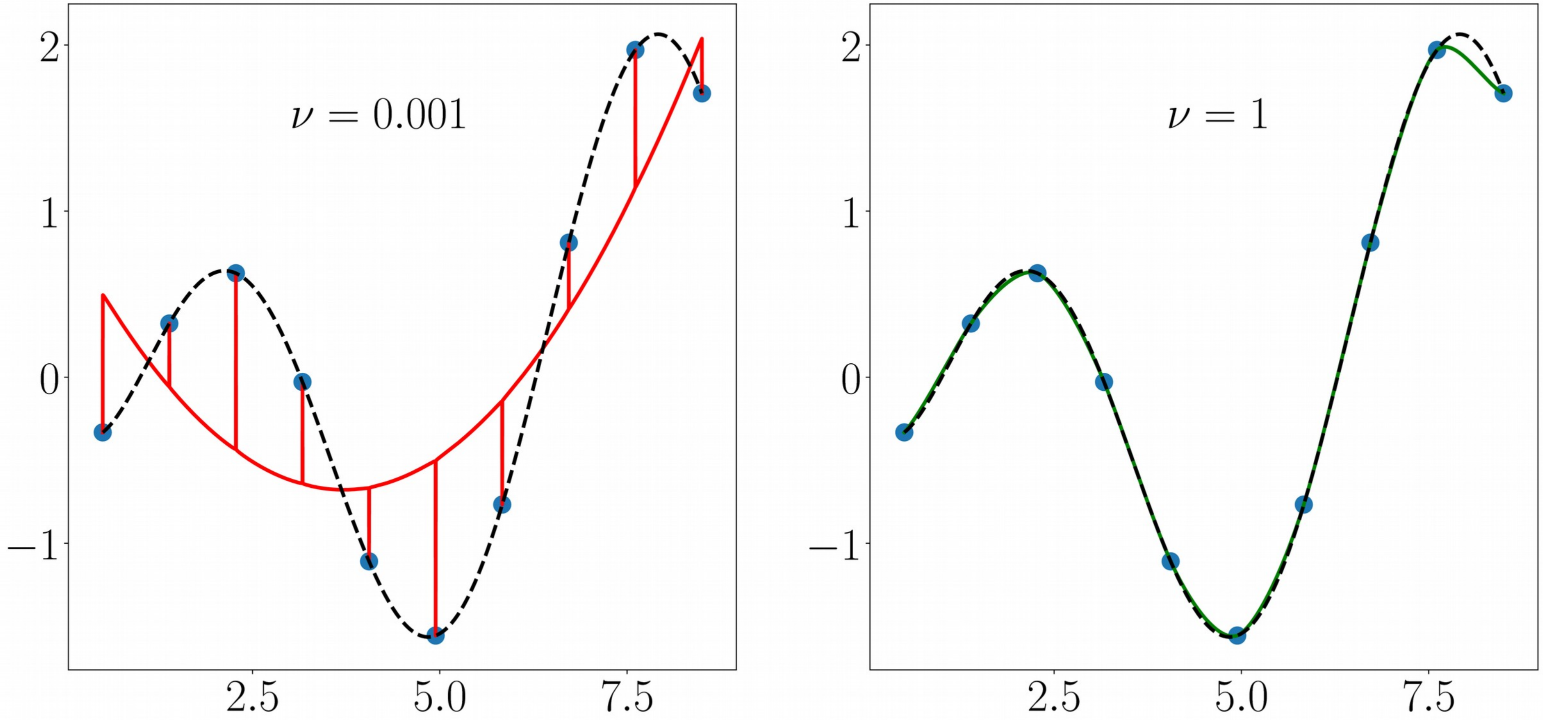
$\mathbf{x_i}$ → $(\theta, \phi, Re_d, \varepsilon)$

$y(\mathbf{x_i})$ → (H_{11}, H_{22}, H_{33})

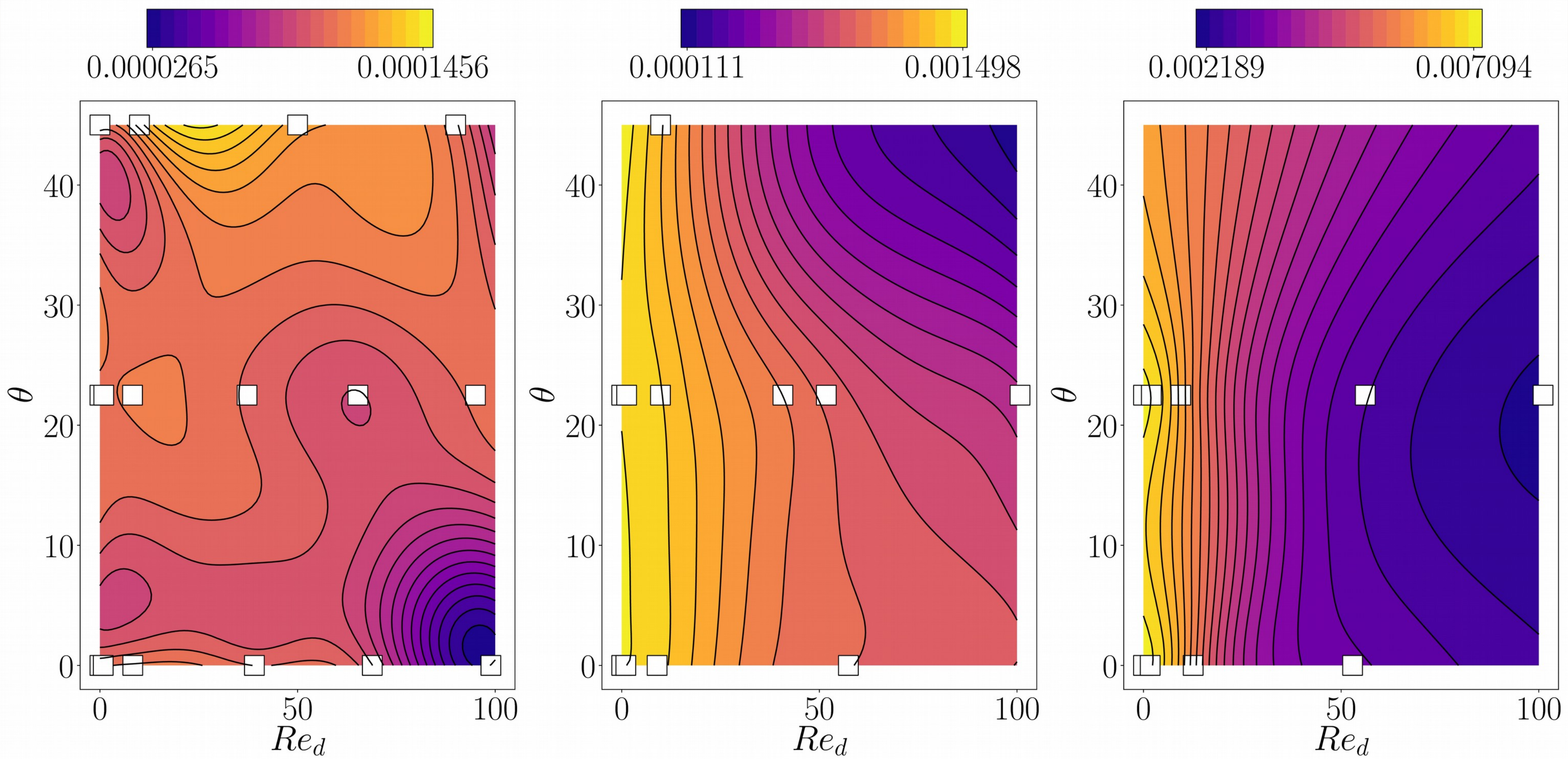
Covariance Model

Matérn covariance model:

$$r(\mathbf{x_i}, \mathbf{x_j}) = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\sqrt{2}\nu|\mathbf{x_i} - \mathbf{x_j}|}{|\lambda|} \right)^{\nu} K_{\nu} \left(\frac{\sqrt{2}\nu|\mathbf{x_i} - \mathbf{x_j}|}{|\lambda|} \right)$$



RESULTS: H_{11} WITH $\varphi = 0°$ AND $\varepsilon = 0.4, 0.6, 0.8$



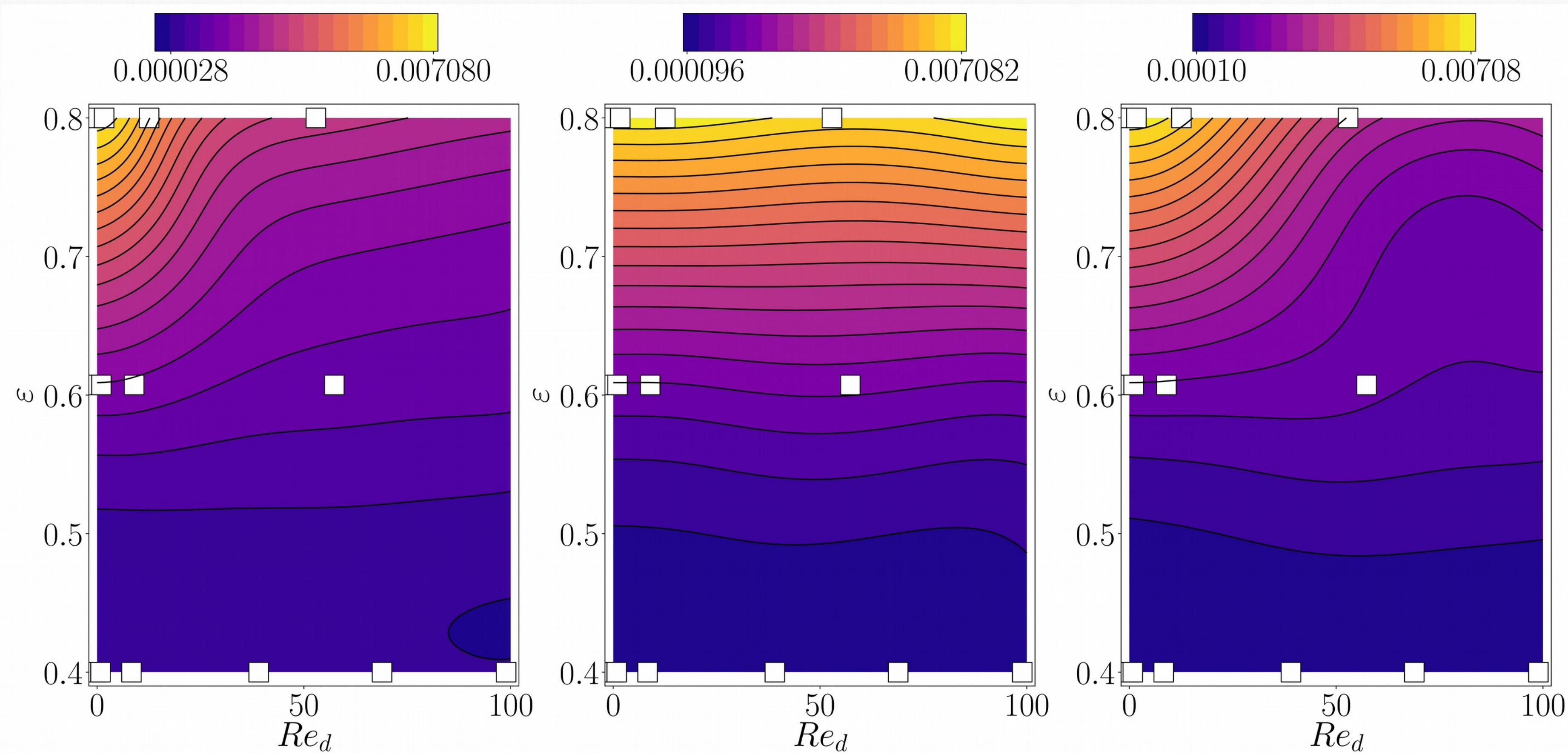
Variation of the apparent permeability with the angle θ is weak

RESULTS: H_{11}

$\phi = \theta = 0^\circ$

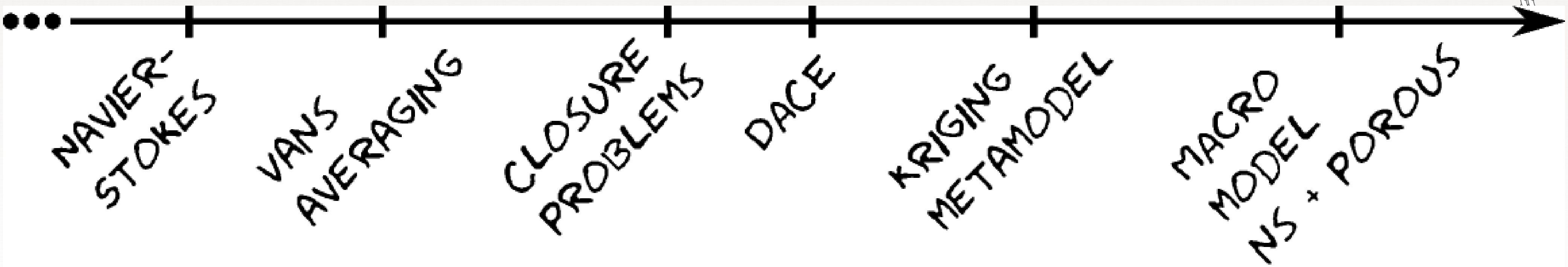
$\phi = 90^\circ$
$\theta = 0^\circ$

$\phi = 45^\circ$
$\theta = 22.5^\circ$



The apparent permeability can change by one order of magnitude in the range of the analysed porosity

Conclusion and future work:



- The work presented has been submitted to “Computer and Fluids”
- We have shown that the tensor H can vary with the fluid flow
- Kriging metamodelling can be a good choice to update H at each time iteration in a NS+porous solver

Next steps:

- Integrate the Kriging metamodel inside the OpenFOAM solver

DACE JUNGLE

Full Factorial:

- Computing the main and the interaction effects
- Building response surfaces
- N is fixed

Taguchi:

- Addressing the influence of noise variables
- N is fixed

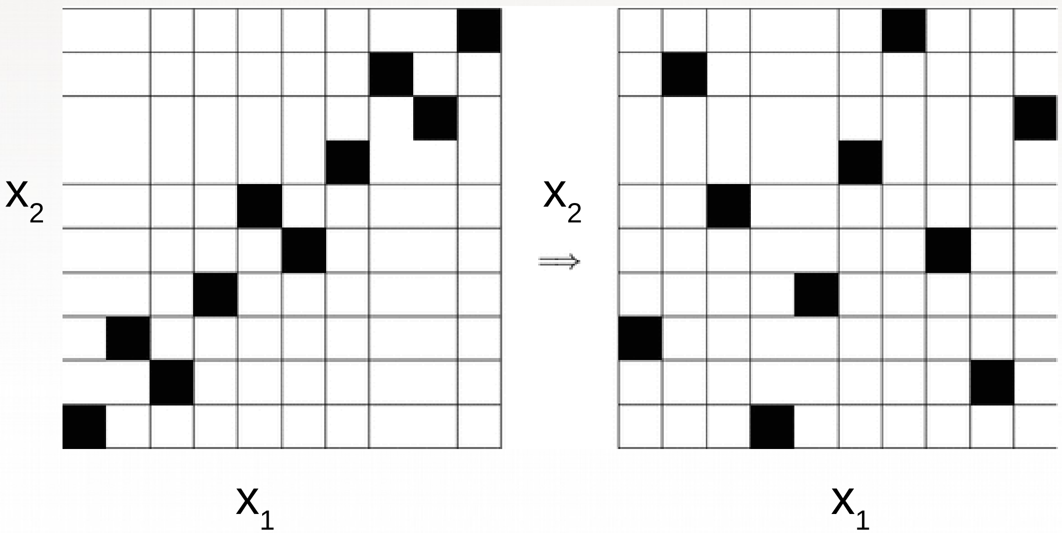
Latin hypercube:

- Building response surfaces
- N is a user choice

Random Monte Carlo

- Building response surfaces
- N is a user choice

DACE VARIABILITY



- LH should be carefully designed but it is often the best choice when we cannot afford large N
- With higher N the results tend to be similar

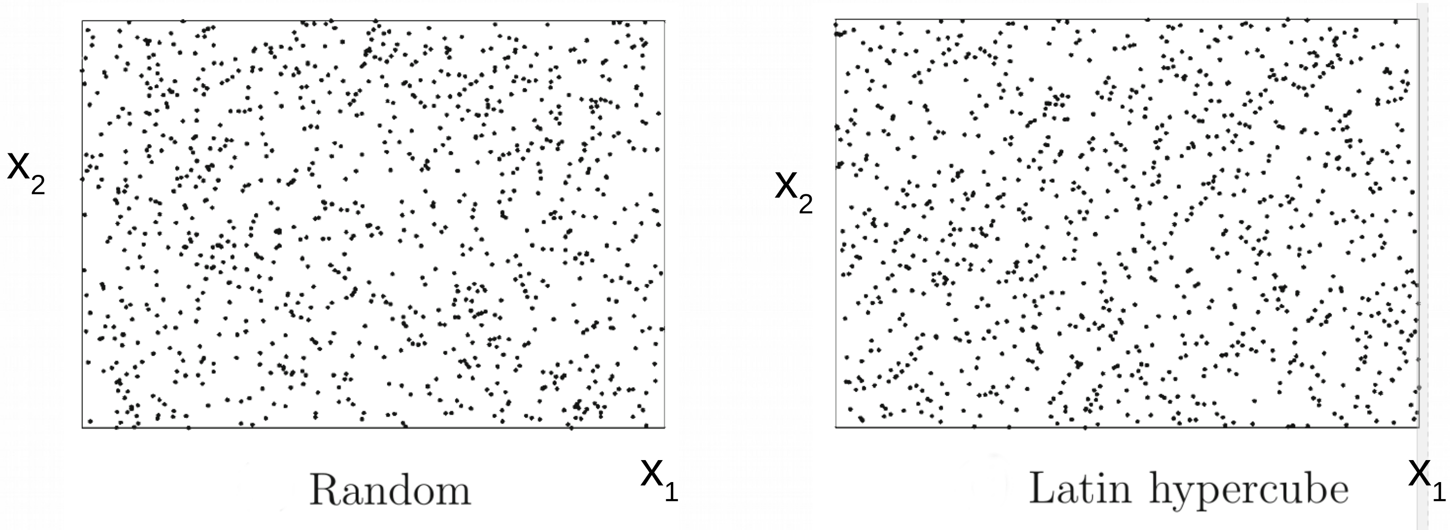


Image from “Optimization Methods”, Marco Cavazzuti, Springer 2012

DATA ANALYSIS

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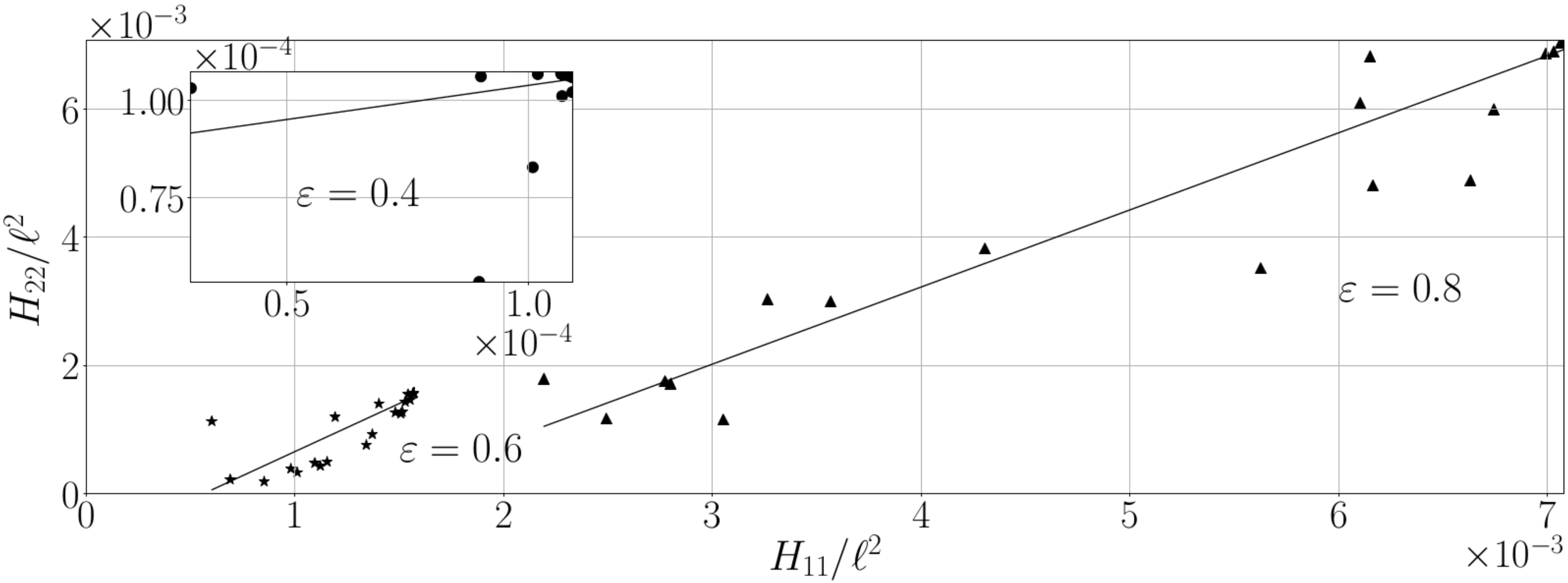
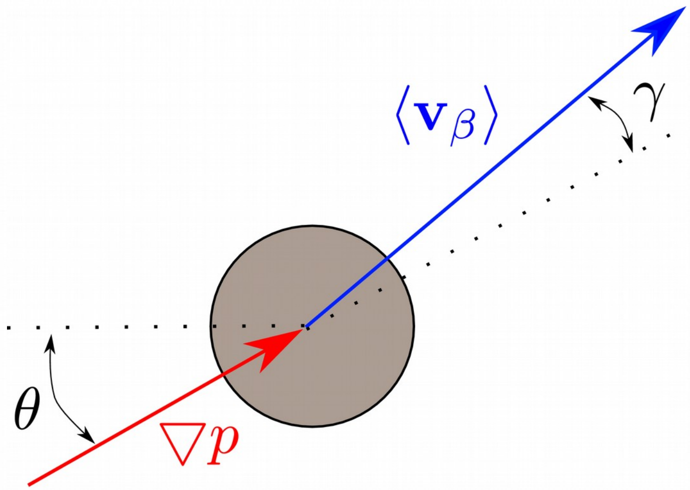
Total numbers of experiments : 118



Correlations appear among the elements of the permeability tensor

Forcing and velocity angles correlation

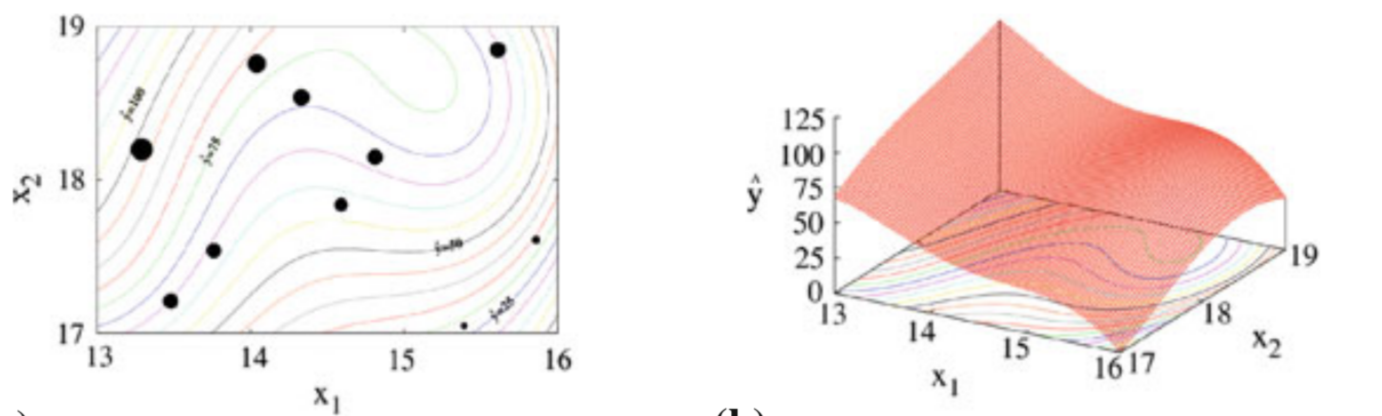
$$(u_\beta, v_\beta, w_\beta) \sim \left(H_{11}\frac{\partial p}{\partial x_1}, H_{22}\frac{\partial p}{\partial x_2}, H_{33}\frac{\partial p}{\partial x_3} \right)$$



$$\tan\,\gamma = \frac{\left(1 - \frac{H_{11}}{H_{22}}\right)\tan\,\theta}{\frac{H_{11}}{H_{22}} + \tan^2\,\theta}$$

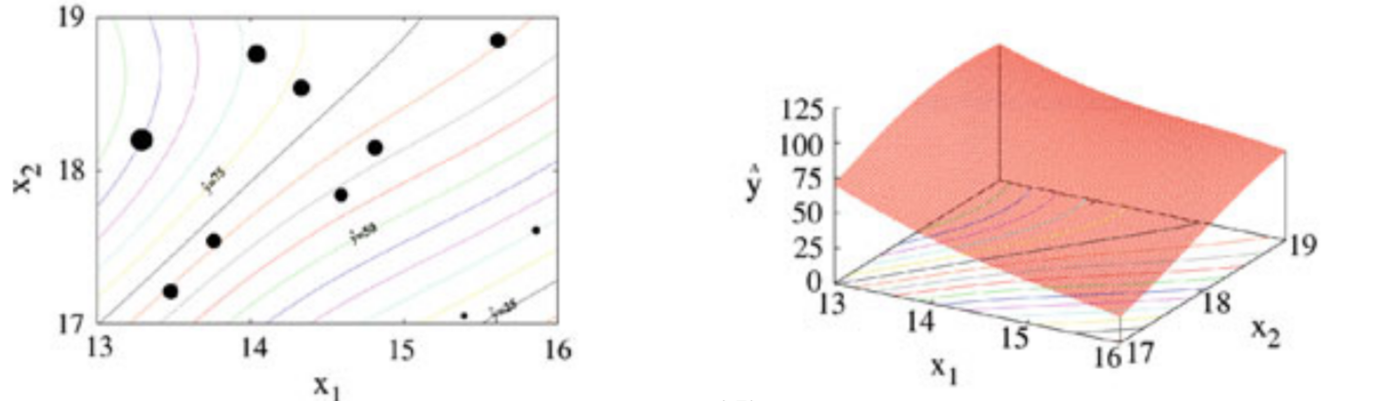
Deviation angles are connected to
the permeability tensor

Kriging variability examples



(a) Gaussian model, $C_0 = 0$, $C_1 = 1478$, $R = 2.68$, $\frac{C_0}{C_1} = 0$, $R_{pr} = 4.66$, contour view

(b) Gaussian model, $C_0 = 0$, $C_1 = 1478$, $R = 2.68$, $\frac{C_0}{C_1} = 0$, $R_{pr} = 4.66$, 3d view



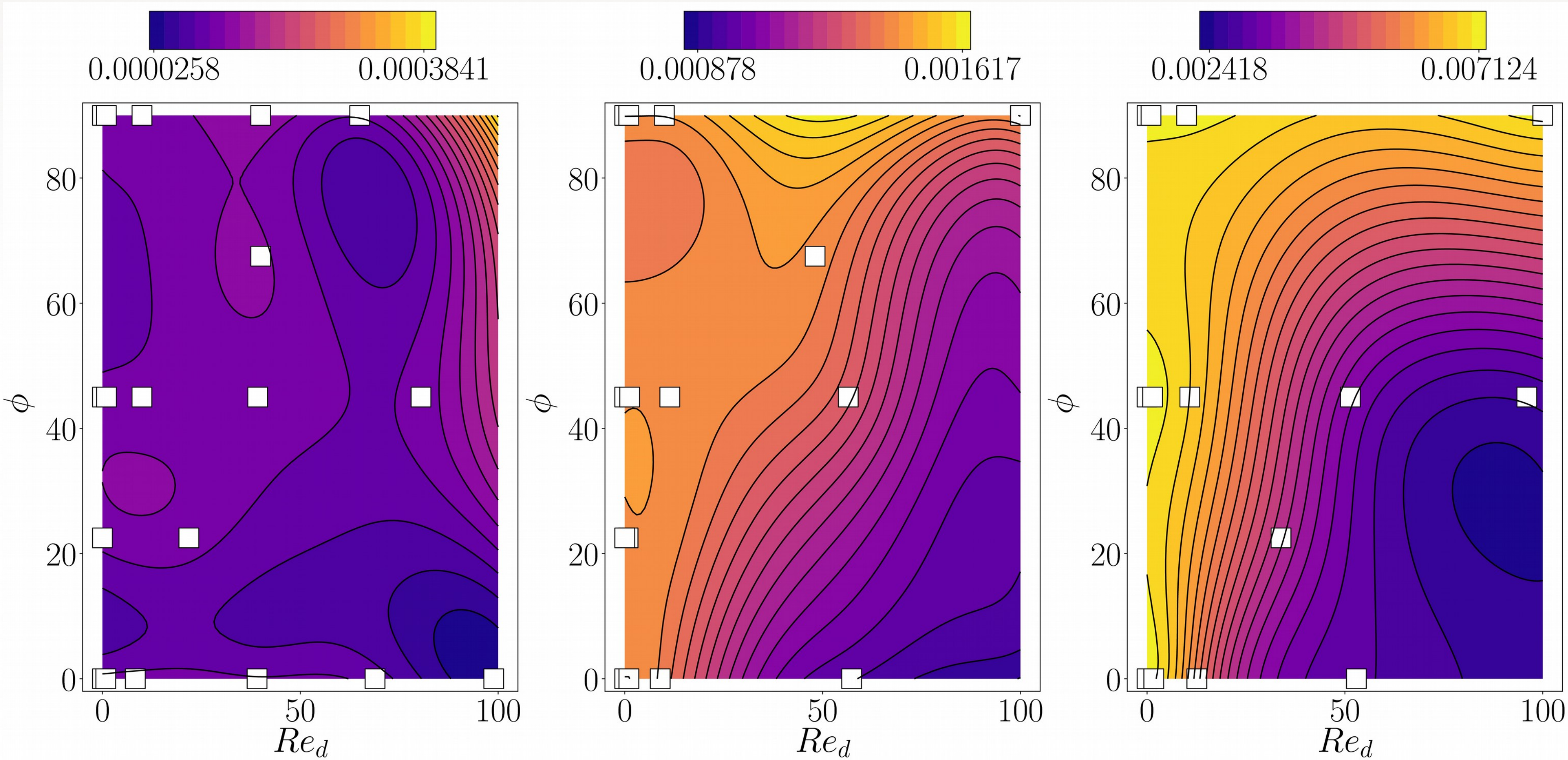
(c) Gaussian model, $C_0 = 7.39$, $C_1 = 1478$, $R = 2.68$, $\frac{C_0}{C_1} = 0$, $R_{pr} = 4.66$, contour view

(d) Gaussian model, $C_0 = 7.39$, $C_1 = 1478$, $R = 2.68$, $\frac{C_0}{C_1} = 0$, $R_{pr} = 4.66$, 3d view

There are a lot of parameters to play with and they can change a lot your model

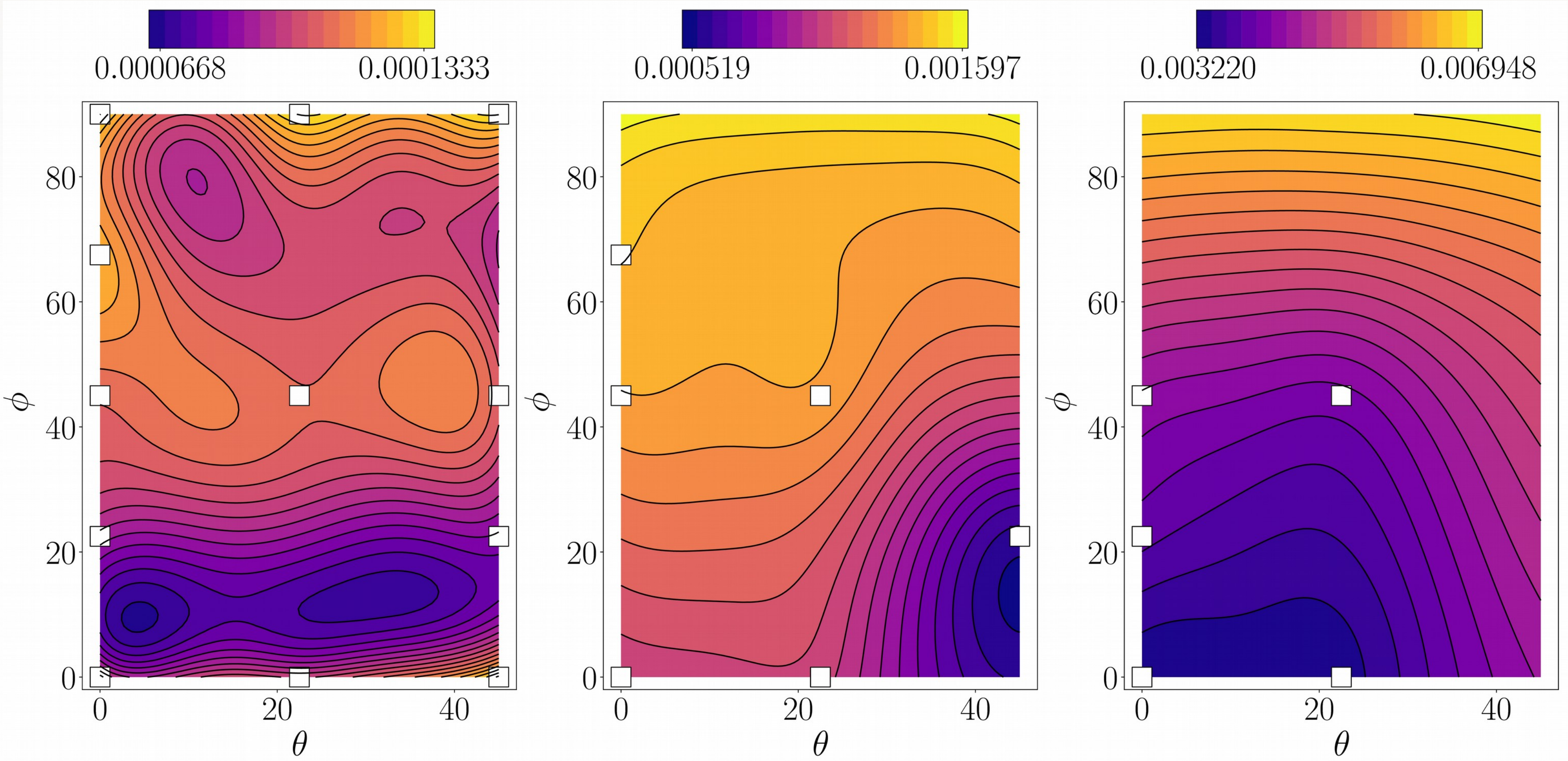
Image from “Optimization Methods”, Marco Cavazzuti, Springer 2012

RESULTS: H_{11} WITH $\theta = 0°$ AND $\varepsilon = 0.4, 0.6, 0.8$



Variations with respect to φ are more pronounced than those found with respect to θ and are due to a real three-dimensionalization of the flow

RESULTS: H_{11} WITH RE = 40 AND ε = 0.4, 0.6, 0.8



H_{11} has a much stronger dependence on φ than on θ, suggesting that the real test of permeability models must include three-dimensional effects