Metoda właściwej dekompozycji ortogonalnej, jako narzędzie redukcji stopni swobody, modelowania wielkoskalowego oraz rozwiązywania zadań odwrotnych

Proper Orthogonal Decomposition as a tool of reduced order method, multiscale modelling and solving inverse problems

Ryszard Białecki

Instytut Techniki Cieplnej

Politechnika Śląska

Ziemowit Ostrowski, Adam Klimanek, Wojciech Adamczyk, Marek Rojczyk, Arkadiusz Ryfa ITC
Antoni John, Inst. Mechaniki i Inżynierii Obliczeniowej, Pol. Śl.
Alain Kassab, Eduardo Divo Univ. Central Florida
Helcio Orlande COPPE Rio de Janeiro

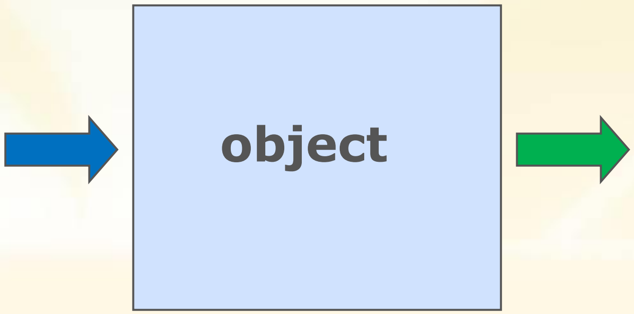
Outline

- Gentle introduction & history
- Theory of Proper Orthogonal Decomposition (POD)
- Trained POD-RBF network
- Applications
  - ✓ Reduced Order Method
  - ✓ Multiscale
  - ✓ Inverse techniques
  - ✓ Bayesian formulation inverse methods
- Conclusions

gentle introduction

Object responses as correlated vectors

excitation sequence $\mathbf{k}_i$



output (snapshot) $\mathbf{u}_i$
sequence of vectors
eg. nodal temperatures
nodal displacements

As all response vectors come from the same physical object, they are correlated. The correlation of multidimensional vectors means that they lay in a hyperplane

gentle introduction

What is POD?

Similarities with Fourier analysis

- POD is a technique of expansion od sets of vectors (snapshots), into a sequence of orthogonal POD modes (basis vectors)

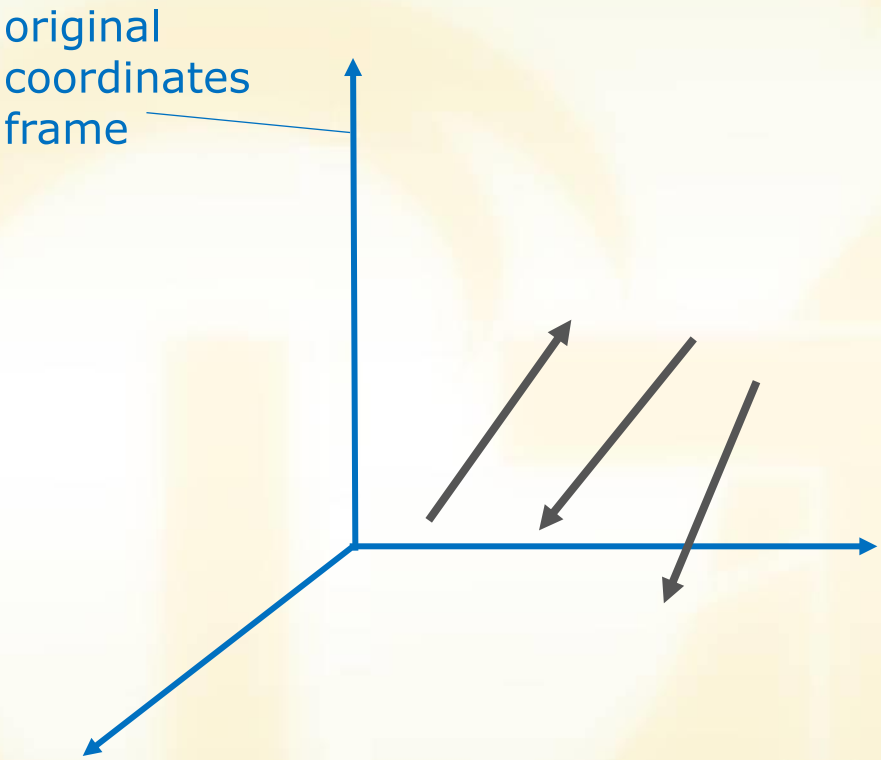
- Modes exhibit optimum approximation property

- Expansion of the set into modes can be truncated after first few dominant modes, practically without affecting the accuracy

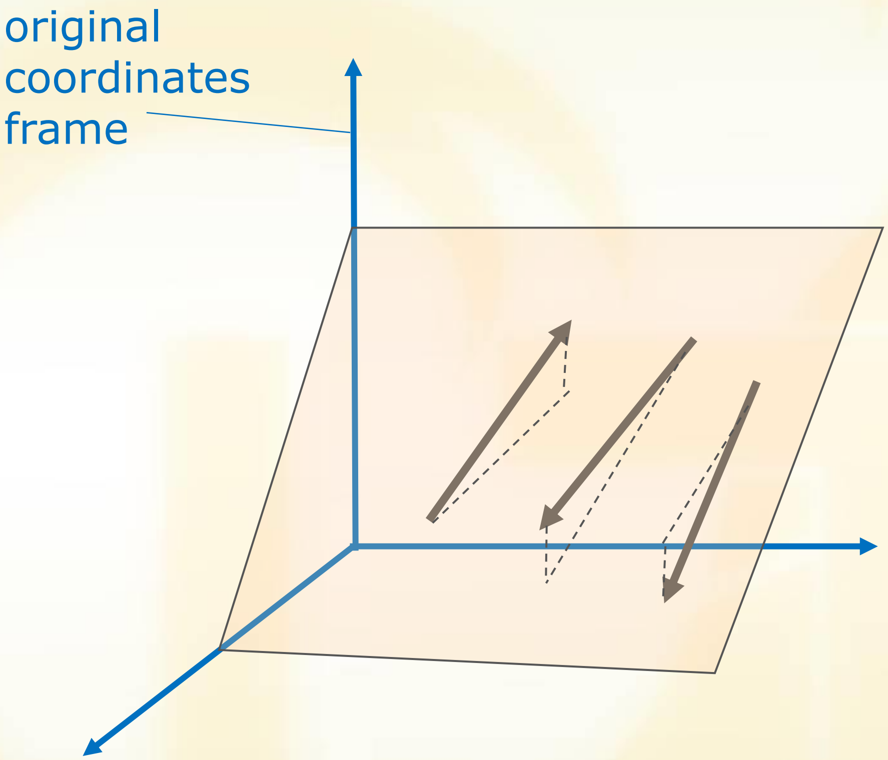
- Leaving out the less important modes results in filtering out the noise

POD modes are constructed using statistical methods to detect the correlations between the vectors in the data set.

principal component analysis PCA

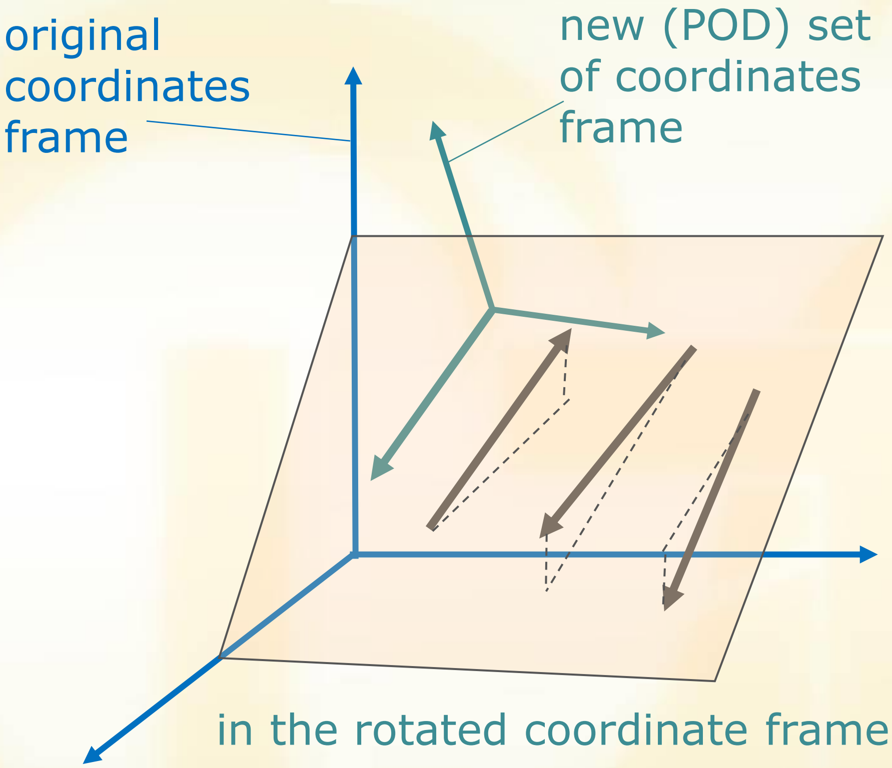


principal component analysis PCA



If vectors are correlated, they form a set of almost in-plane vectors

principal component analysis PCA



in the rotated coordinate frame one coordinate of ALL vectors is negligible.

The dimensionality of the problem is reduced by one. For almost parallel vectors, two coordinates can be neglected, if one axis of the coordinates system is parallel to the vectors.

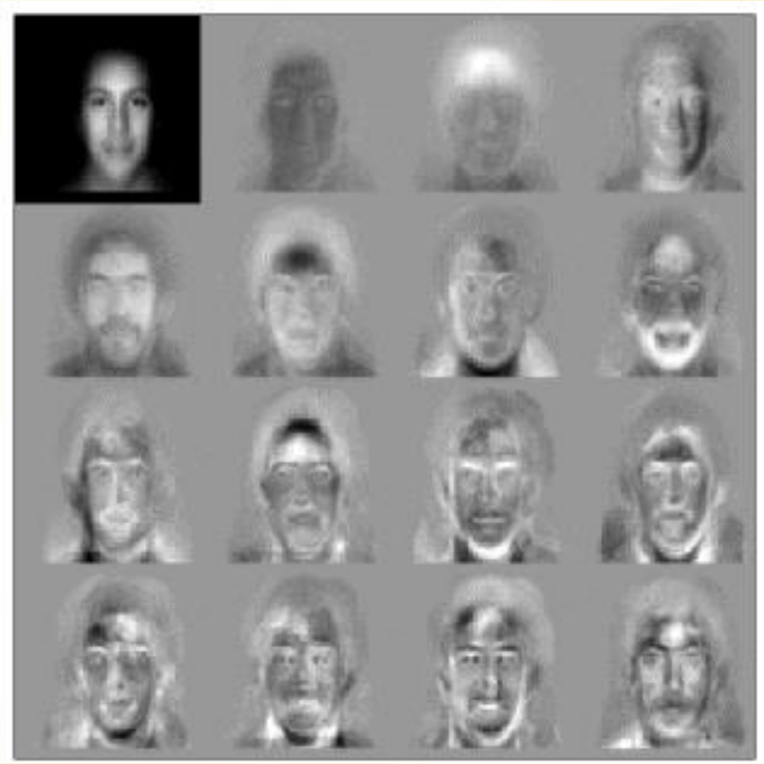
Face recognition

Image identification (whose face is in the picture?)

FERET database: financed by US Department of Defense

Face recognition

each face – 5000 pixels times 256 gray levels
= $1.28\ 10^6$ DOFs



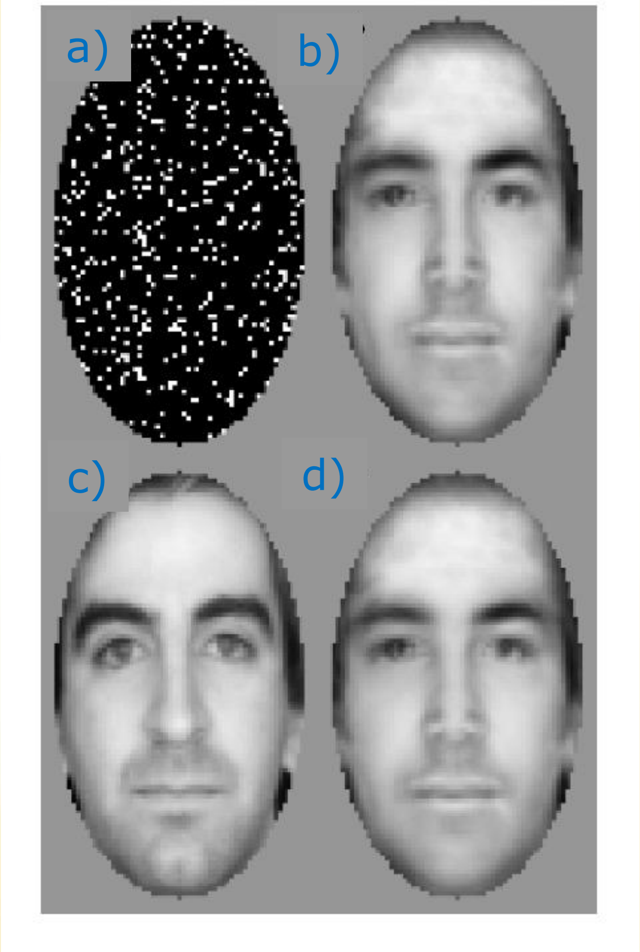
modes
(eigenfaces)

any face can be defined as a linear combination of only 50 DOFs (eigenfaces)

M. **Turk and** A. **Pentland**, "Eigenfaces for Recognition", Journal of Cognitive Neuroscience, vol. 3, no. 1, pp. 71-86, 1991

Face recognition

Available: the face database & some portions of the picture.
WHAT IS THE FULL PICTURE?



a) Known light pixels only.
b) Retrieved face (not included in database) using 50 DOFs and gappy data

c) Source picture (original)
d) Retrieved face (not included in database) using 50 DOFs and entire picture

R. Everson and L. Sirovich, Karhunen–Loeve procedure for gappy data, 1995/J. Opt. Soc. Am. A Vol. 12, No. 8/August 1657

Approximation problem

STANDARD APPROXIMATION	POD APPROXIMATION
1st step: ***guess*** the optimal approximation basis	**1st step:** ***construct*** the optimal approximation basis
2nd step: find the expansion coefficients	**2nd step:** find the expansion coefficients

POD BASE PROPERTIES –
OPTIMALITY w.r.t. APPROXIMATION:

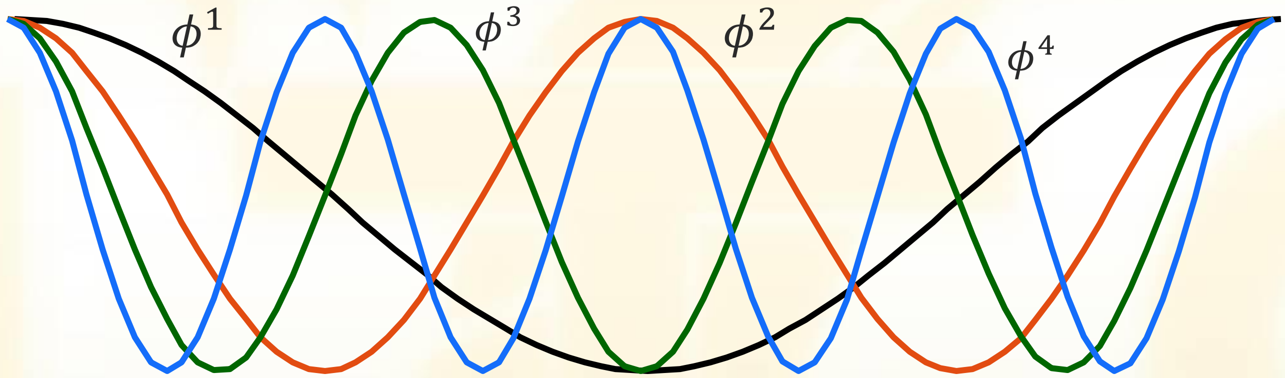
no other basis carries more energy in the same number of modes

Expansion into eigenfunctions

Analytical solution of heat conduction problem

$$T(\mathbf{r},\tau) = \sum_{j=1}^{\infty} A_j(\tau)\,\phi^j(\mathbf{r}) \quad \text{for given BC}$$

A_j amplitude ϕ^j eigenfunction (1,2 or 3D)



truncation of the series removes higher frequencies.

Inverse problems ⇒ advisable to remove higher frequencies

Expansion into eigenfunctions

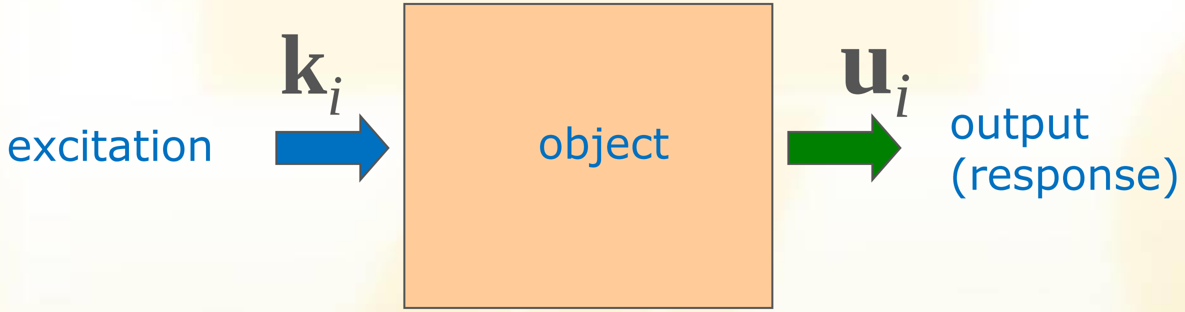
modes as empirical eigenvectors

eigenfunctions of B.V.P have optimal approximation properties.

but

determining eigenfunctions is expensive (most often not possible).

IDEA –find eigenfunctions by studying the response of the system to various excitations



Eigenfunctions can be extracted from the response of the system, even when the B.V.P. is unknown.

Expansion into eigenfunctions

Separation of variables: same type of parametrized boundary conditions, different values of parameter sets $\boldsymbol{k}$, for given set of parameters

$$T(\mathbf{r},\tau) = \sum_{j=1}^{\infty} A_j(\tau)\,\phi^j(\mathbf{r})$$

$\boldsymbol{k}$ – vector of parameters defining the boundary conditions

$\boldsymbol{r}$ – vector coordinate (spatial variable)

τ - time

$$T^1(\mathbf{r},\tau) = \sum_{j=1}^{\infty} A_j^1(\tau)\,\phi^j(\mathbf{r})$$ for 1st set of parameters $\boldsymbol{k}_1$

$$T^2(\mathbf{r},\tau) = \sum_{j=1}^{\infty} A_j^2(\tau)\,\phi^j(\mathbf{r})$$ for 2nd set of parameters $\boldsymbol{k}_2$

$$\vdots$$

$$T^k(\mathbf{r},\tau) = \sum_{j=1}^{\infty} A_j^k(\tau)\,\phi^j(\mathbf{r})$$ for kth set of parameters $\boldsymbol{k}_k$

can be put together as

$$T(\mathbf{r},\tau,\mathbf{k}) = \sum_{j=1}^{\infty} A_j(\tau,\mathbf{k})\,\phi^j(\mathbf{r})$$

Expansion into eigenfunctions

- how to determine the eigenfunctions?
- how to evaluate the amplitudes?

eigenfunctions - analytical methods applicable only to very simple shapes

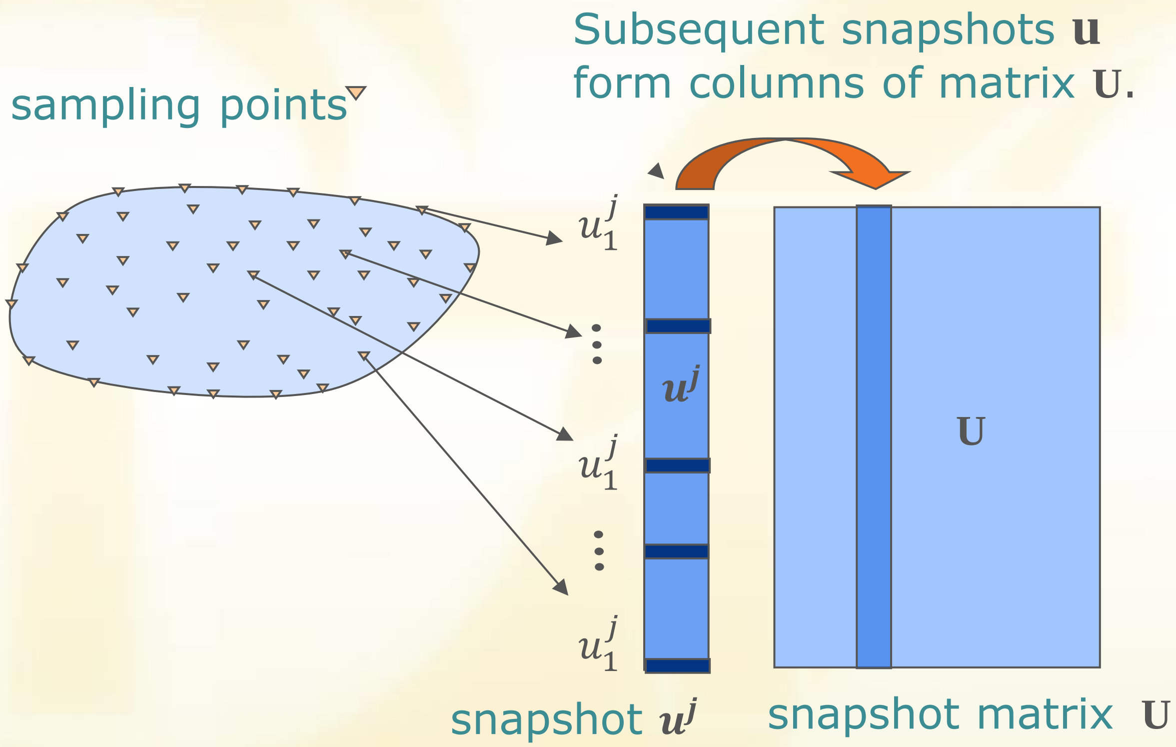
amplitudes - only approximate methods

Proper Orthogonal Decomposition – empirical eigenfunctions

Radial Basis Functions – multidimensional approximation of $A(\tau, \mathbf{k})$

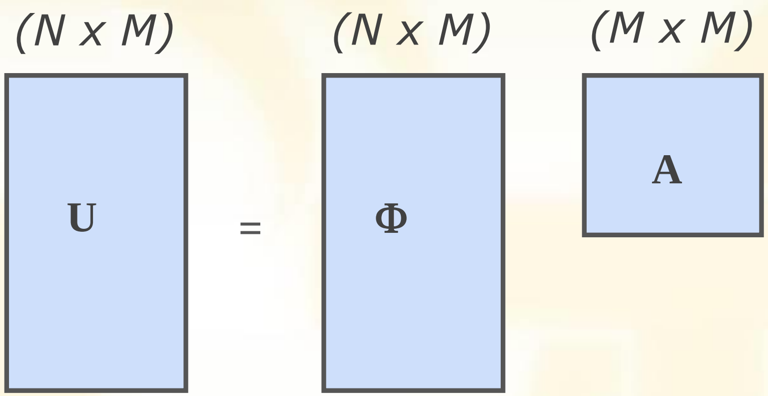
POD idea

SNAPSHOT is a discrete image of the field, corresponding to a chosen excitation (vector of input parameters). May be computed or measured.



POD idea

DECOMPOSITION – snapshot matrix **U** can be expressed as a linear combination of orthogonal basis vectors (modes) ϕ



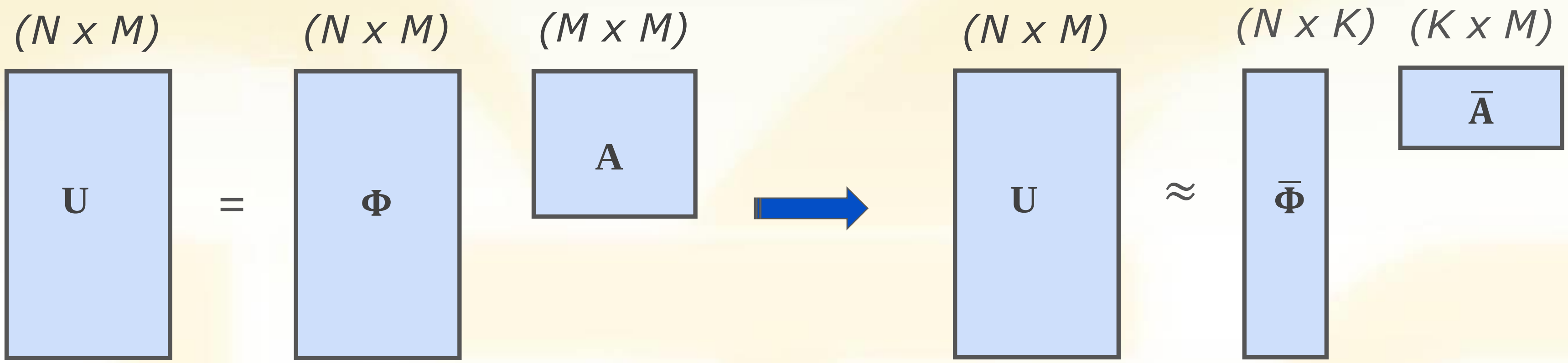
U – snapshot matrix, columns are subsequent snapshots **u**,

Φ – basis vector matrix (coordinates system, modes), columns are subsequent orthogonal basis vectors ϕ^j

A – amplitude matrix (coefficients of the expansion into modes).

POD idea

Truncation – snapshot matrix $\mathbf{U}$ can be approximated by a limited number of POD modes. Insignificant modes might be neglected



$$||\mathbf{U} - \bar{\mathbf{\Phi}} \cdot \bar{\mathbf{A}}|| \rightarrow \min$$

POD basis is optimal w.r.t approximation

POD basis is optimal in a sense that no other basis can contain more energy in the same number of modes

POD idea

How to determine the POD basis

Solve eigenvalue problem for the covariance matrix (other option SVD)

$$(\mathbf{U}\mathbf{U}^{\mathbf{T}})\phi^j = \lambda_j \phi^j$$

eigenvalue of the POD systems is a measure of

- correlation – rapidly decaying eigenvalues indicate strong correlation in the snapshot set
- energy carried by a given POD mode

$$\frac{first\ K\ eigenvalues}{all\ eignevalues} > p$$

p - fraction of the energy that may be neglected. Find the smallest K fulfilling the equation.

DOF reduction
transient heat conduction

time integration of amplitudes

POD as a reduced order method

FEM = weak formulation + Galerkin weighted residuals+locally based trial functions

approximation of temperature

$$T(\mathbf{r}, \tau) = \sum_{i=1}^{N} T_i(\tau) N_i(\mathbf{r})$$

N_i trial (shape) functions
T_j nodal temperature

result of discretization in space

$$\mathbf{K} \cdot \mathbf{T} + \mathbf{M} \cdot \dot{\mathbf{T}} = \mathbf{f}$$

$\mathbf{K}$ stiffness (conductance) matrix

$\mathbf{M}$ mass (capacitance) matrix

$\mathbf{T}$ vector of nodal temperatures

$\dot{\mathbf{T}}$ vector of temporal derivatives of temperatures

POD as a reduced order method

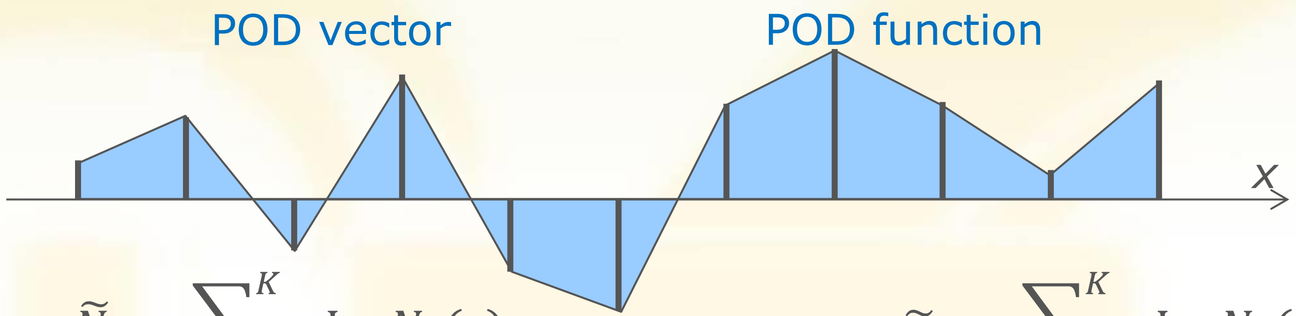
how to construct the POD basis?

Solve the problem using standard time stepping FEM (FDM, FVM) for first few time steps.

Every instantaneous temperature field is treated as a snapshot. POD analysis produces the (truncated) basis.

POD as a reduced order method c

Instead of local shape functions trial and weighting functions are their linear combinations. Coefficients are the entries of the POD basis vectors. Both trial and weighting functions become global.



$$\tilde{N}_k = \sum_{i=1}^{K} \Phi_{ik} N_i\left(\mathbf{r}\right) \qquad \tilde{w}_k = \sum_{i=1}^{K} \Phi_{ik} N_i\left(\mathbf{r}\right)$$

Note: discretization need not be started from scratch. It is enough to transform the existing stiffness matrix and the rhs vector.

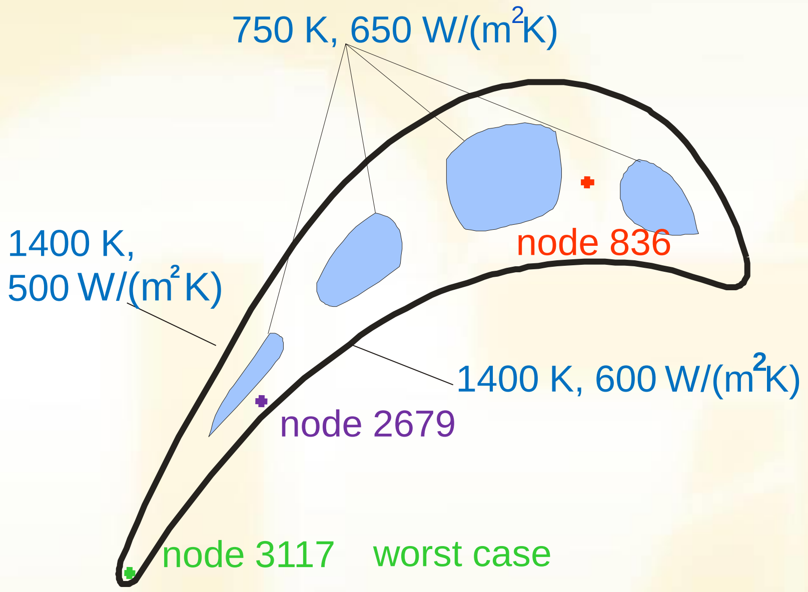
$$T(\mathbf{r},t) = \sum_{k=1}^{K} a_k(t)\tilde{N}_k(\mathbf{r}) \;\Longrightarrow\; \tilde{\mathbf{K}} \cdot \mathbf{a}(t) + \tilde{\mathbf{M}} \cdot \dot{\mathbf{a}}(t) = \tilde{\mathbf{f}}(t)$$

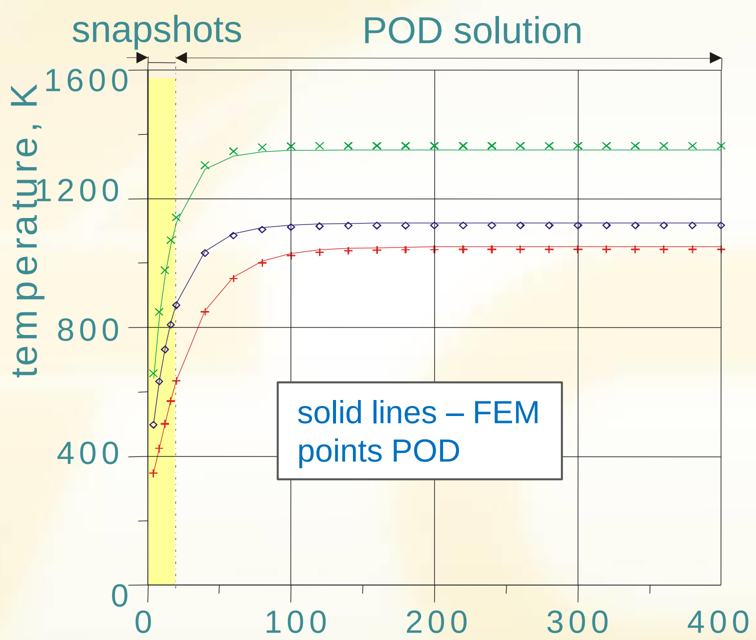
- symmetry of matrices preserved
- dimensionality significantly reduced
- sparsity lost

POD as a reduced order method

Example: heating up a turbine blade

heat conductivity $k=20$ W/mK, specific heat $c\rho=5 \times 10^6$ J/m^3 K. initial condition $T_0 = 300K$.
200 snapshots every 0.1s, central differencing in time





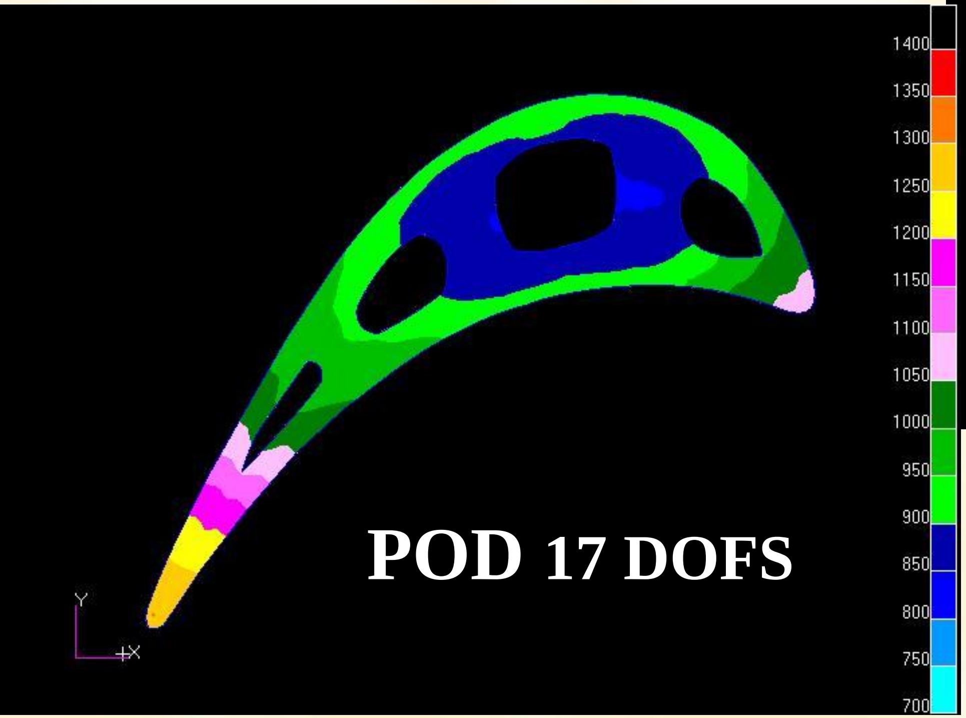
works also with nonlinear material

R.A. Białecki, A.J. Kassab and A. Fic *Proper Orthogonal Decomposition and modal analysis for acceleration of transient FEM thermal analysis*, International Journal for Numerical Methods in Engineering, 62 (2005), pp. 774-797.

A. Fic, R.A. Białecki and A.J. Kassab *Solving transient nonlinear heat conduction problems by Proper Orthogonal Decomposition*, Numerical Heat Transfer, Part B, 48 (2005), pp. 103-124.

POD as a reduced order method

time 40 s



POD as a reduced order method

time 100 s

POD as a reduced order method

time 200 s

multiscale problems

approximation of amplitudes

multiscale problems

separation of variables

$$\mathbf{u}(\mathbf{r},\mathbf{k}) = \sum_{i=1}^{K} \Phi^i(\mathbf{r}) a_i(\mathbf{k}) = \bar{\mathbf{\Phi}} \cdot \mathbf{a}(\mathbf{k})$$

$\mathbf{u}$ – arbitrary discretized field (e.g. temperature)
$\mathbf{k}$ – suitably selected parameters vector (e.g. time, conductivity…)
$\mathbf{r}$ – spatial coordinate
a_i – amplitude (to be found)

known POD basis takes care of the spatial distribution, dependence on other variables accommodated in amplitudes

How to evaluate amplitudes?

- solution of ODEs
- fitting data – approximation of the generated snapshots

$$\mathbf{a}(\mathbf{k}) = \mathbf{B} \cdot \mathbf{g}(\mathbf{k})$$

$\mathbf{B}$ – matrix of unknown, constant coefficients,

$$g_i(\mathbf{k}) = \frac{1}{\sqrt{|\mathbf{k}-\mathbf{k}_i|+r^2}}$$

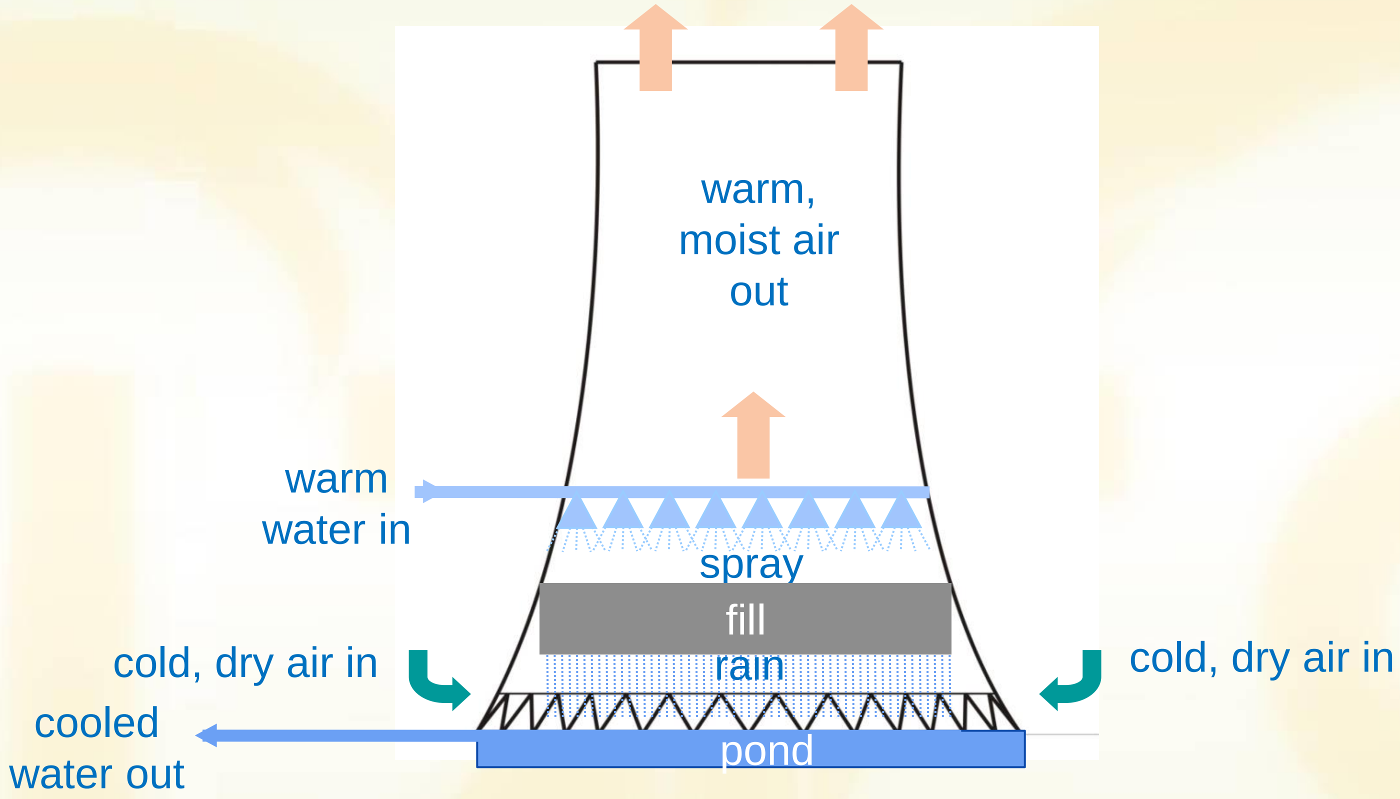
interpolation function – Radial Basis Function (RBF)

$$\mathbf{u}(\mathbf{r},\mathbf{k}) = \bar{\mathbf{\Phi}} \cdot \mathbf{B} \cdot \mathbf{g}(\mathbf{k}) = \mathbf{E} \cdot \mathbf{g}(\mathbf{k})$$

natural draft wet cooling tower

multiscale problems

scheme of a wet cooling tower



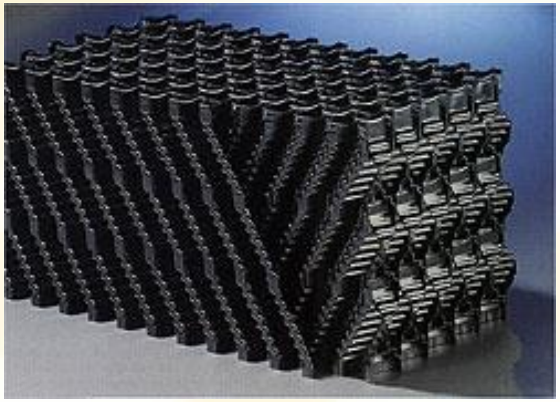
main problem: different geometry scales

outside - kilometers

inside tens of meters

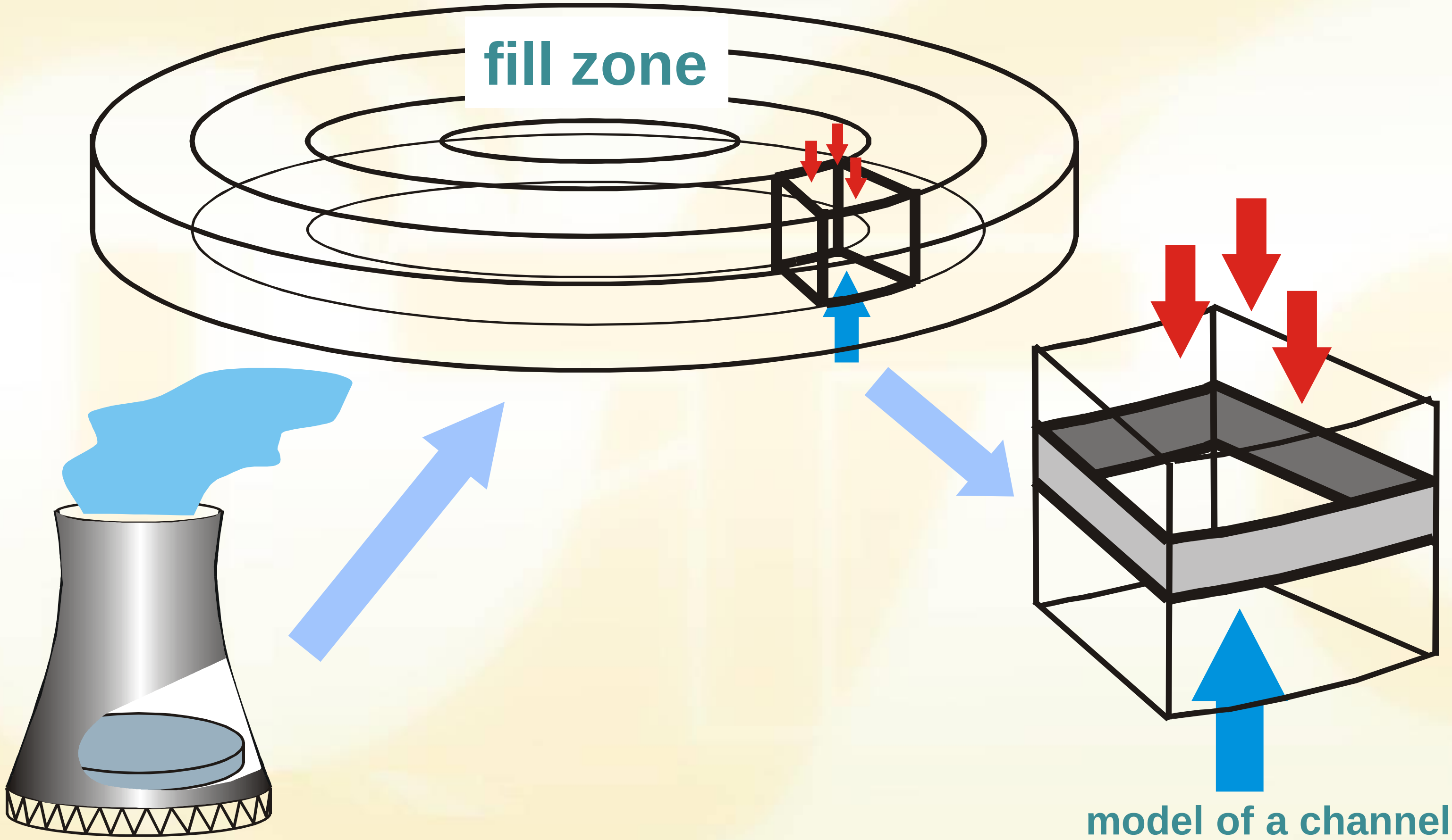
fill - heat and mass exchanger, centimeters

- Large exchange surface: 100-250 m^2/ m^3
- Minimized pressure drop
- High durability
- Material: PP/PVC
- Height in CT: 60-120 cm



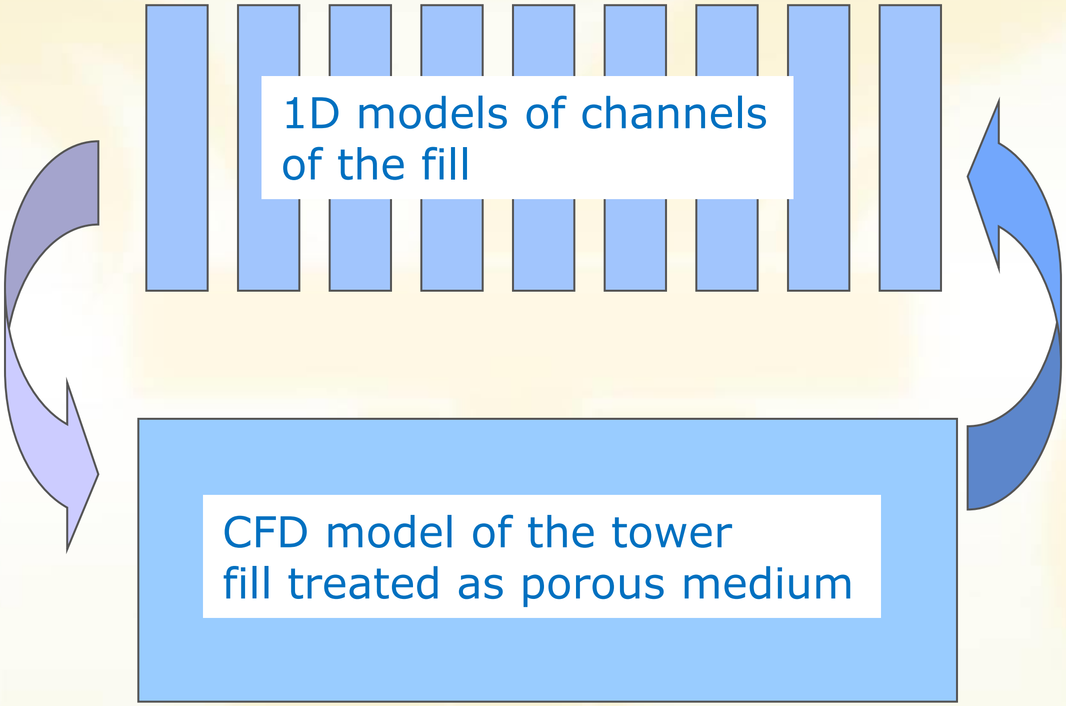
model of the fill zone

vertical channels with no transversal mixing (1D model)



Multiscale approach implemented

distributions
of mass
heat and
momentum
sources
in each
channel



inflow rates
and temperatures
of water
and air, inflow
air humidity

model of the channel - governing equations: 4 ODEs

mass conservation

$$dm_w = m_g dw$$

energy conservation

$$c_w T_w dm_w + m_w c_w dT_w = m_a[c_{pa} dT_a + dw(r + c_{pv} T_a) + w c_{pv} dT_a]$$

mass transfer kinetics

$$dm_w = \beta(w_s - w_a) A dz$$

energy transfer kinetics

$$dQ = (c_w T_w + r)\beta(w_s - w_a) A dz + h(T_s - T_a) A dz$$

flux due to evaporation

flux due to convection

two points problem - implicit self adaptive finite volume technique used in the study

acceleration of the calculations

model of channel invoked frequently, iterative process numerically very intensive.
POD employed to speed up the solution of the model of a single channel

Input data
-inlet mass flow rates of air and water
-inlet temperatures of air and water
-inlet air humidity

input vector $$\mathbf{k} = \{m_w^{in}, m_a, T_w^{in}, T_a^{in}, w^{in}\}$$

Output data
- heat and mass sources at centers of CFD cells within the channel

snapshot vector $$\mathbf{u}^i = \{\mathbf{q}_s^i, \mathbf{m}_s^i\}$$

Low order POD model – functionality of neural network

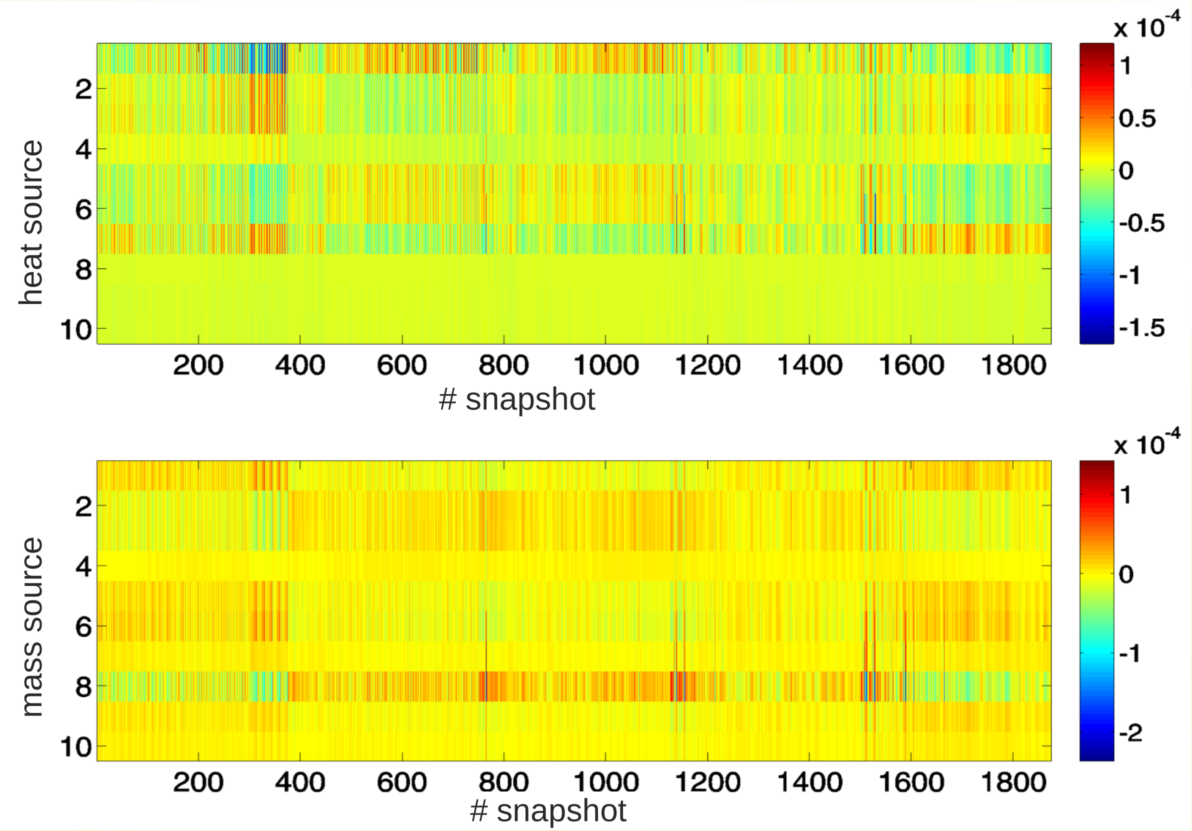
$$\mathbf{u}(\mathbf{k}) = \mathbf{E} \cdot \mathbf{g}(\mathbf{k})$$

acceleration - 100 times, accuracy beter than 1%

multiscale problems

relative error of POD approximation

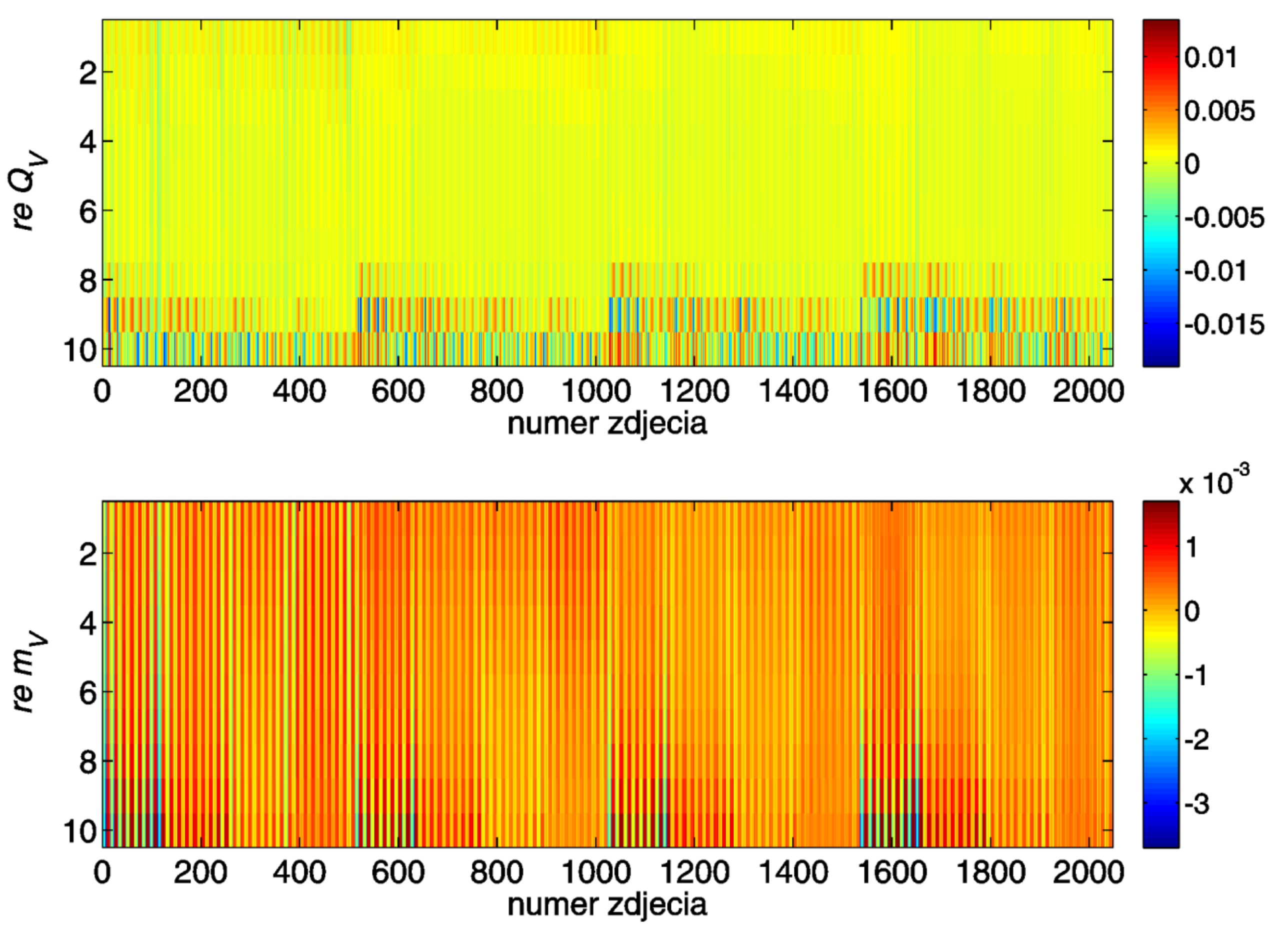
training set



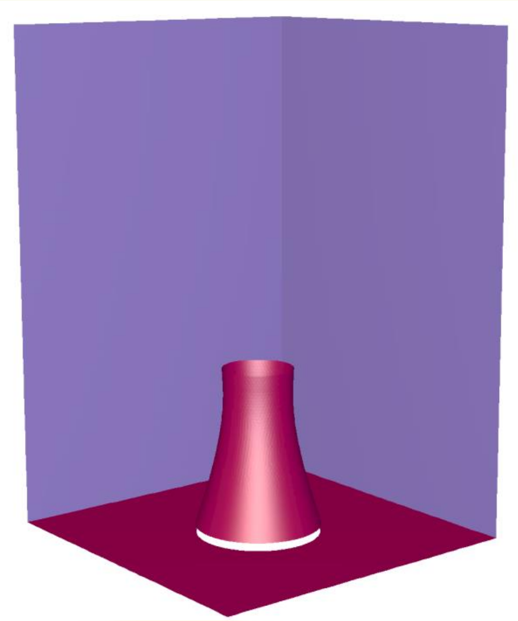
multiscale problems

relative error of POD approximation

testing set

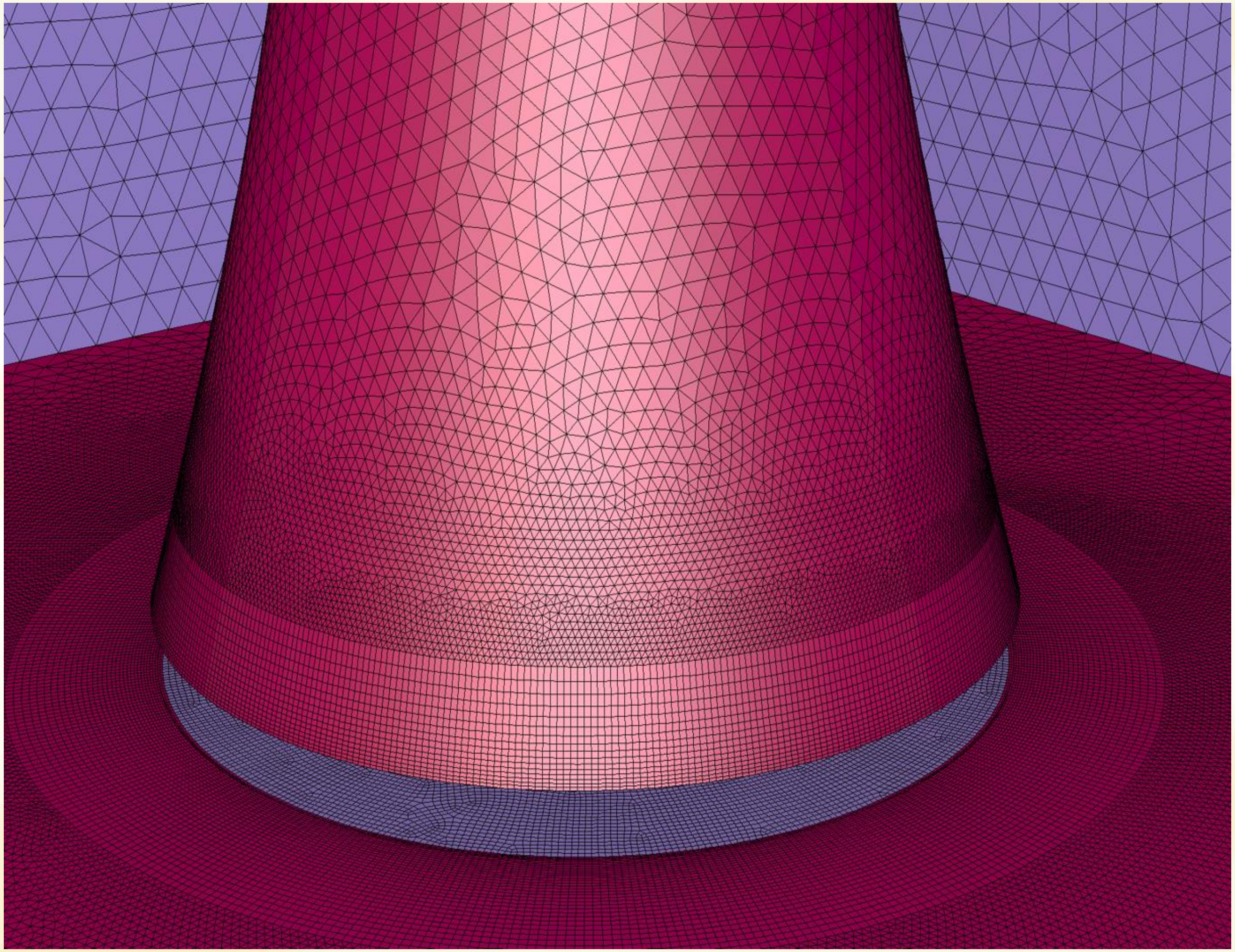


multiscale problems



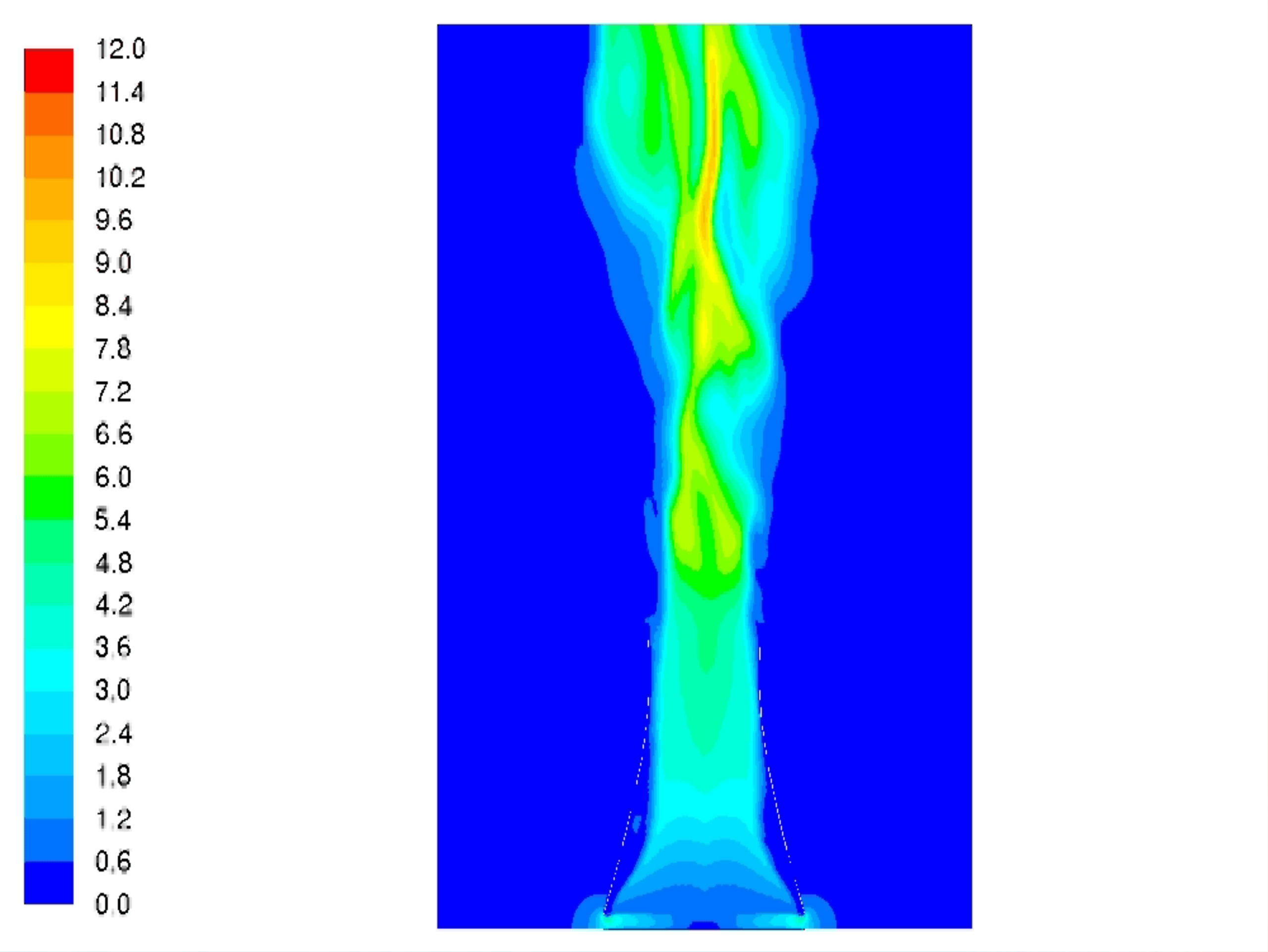
numerical mesh:

4.84 M elements



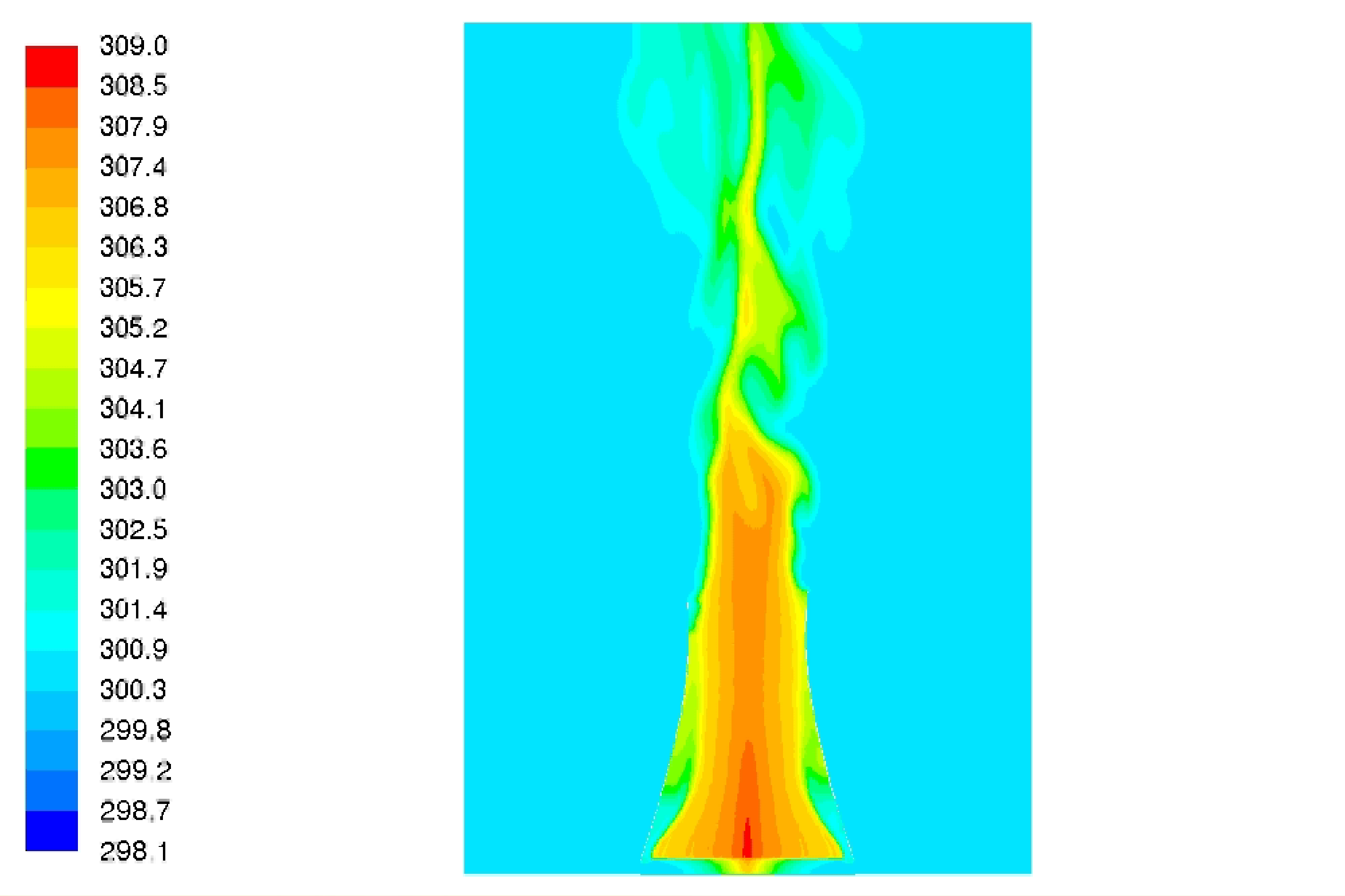
multiscale problems

velocity contours



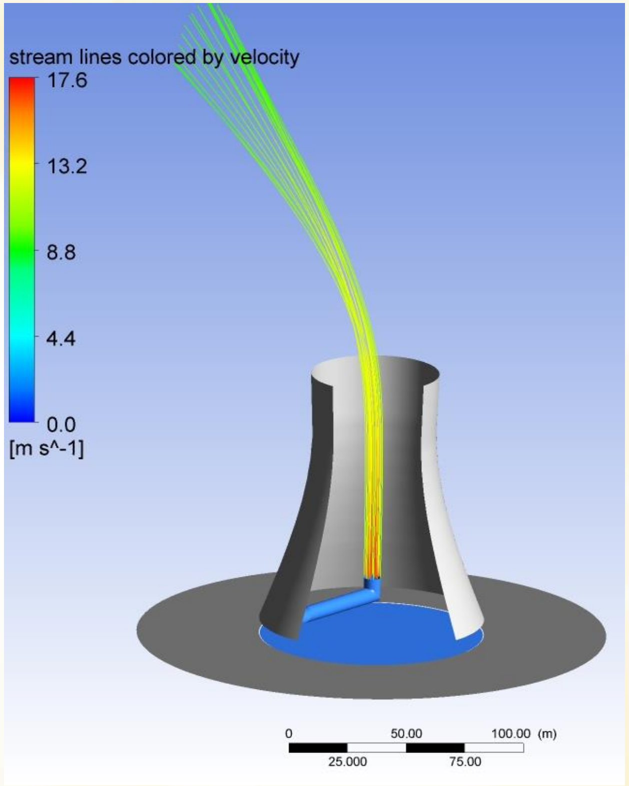
multiscale problems

temperature contours

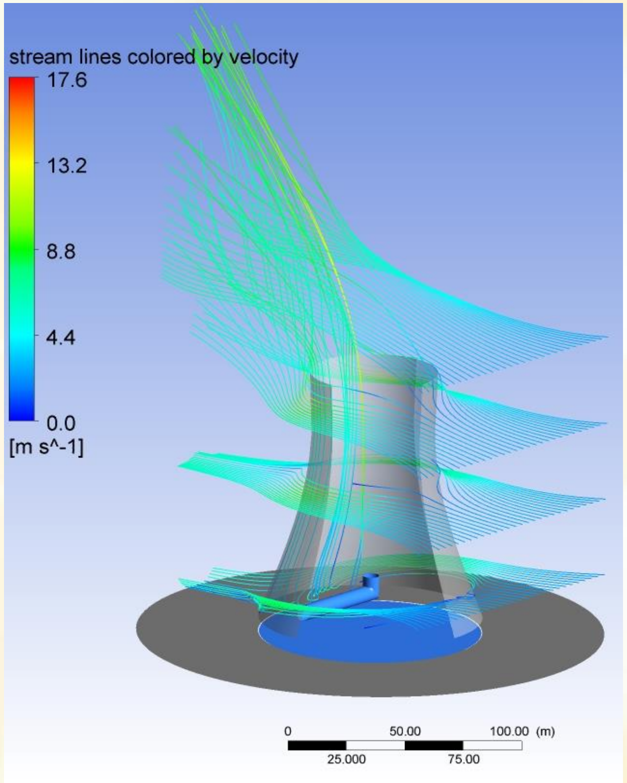


multiscale problems

flue gas discharge through the cooling tower



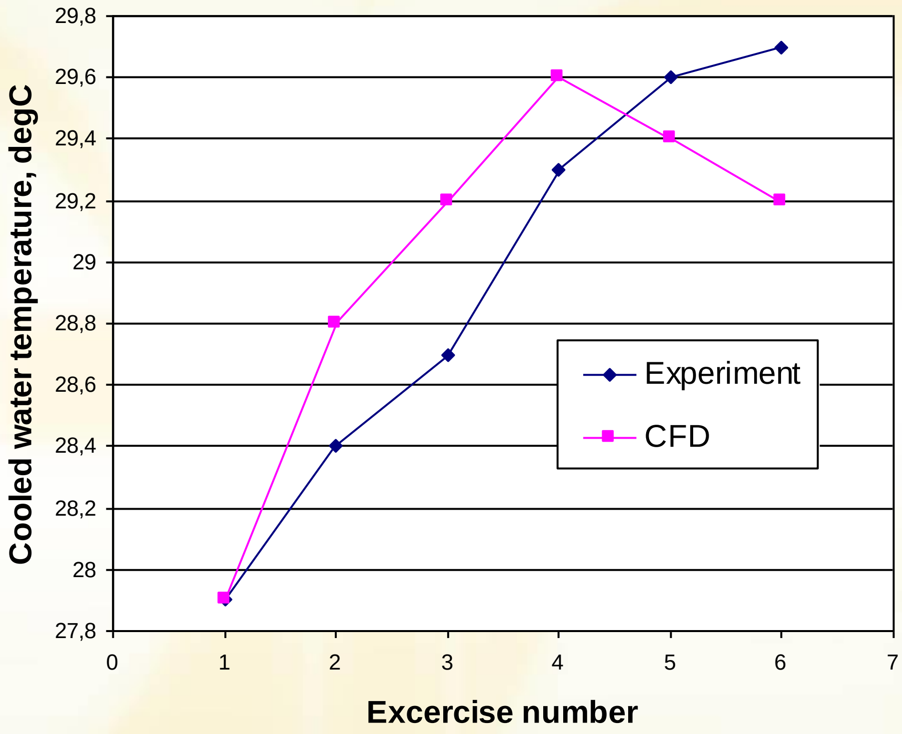
air recirculation in the wake



atmospheric wind profile with u_0 = 1.6 m/s at 2 m

multiscale problems

experimental validation



A. Klimanek, M. Cedzich and R. Białecki *3D CFD modeling of natural draft wet-cooling tower with flue gas injection,* Applied Thermal Engineering, **91** (2015), pp. 824–833, doi:10.1016/j.applthermaleng.2015.08.095

A. Klimanek, R.A. Białecki, Z. Ostrowski, *CFD two scale model of a wet natural draft cooling tower*, Numerical Heat Transfer, Part A: Applications, 57:2, (2010), pp. 119-137

inverse problems

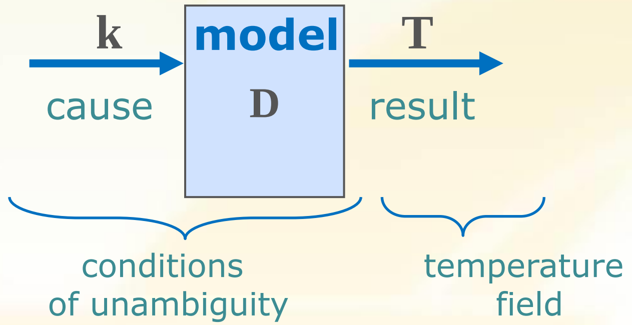
approximation of amplitudes
as in multiscale

inverse problems

direct problem – well defined

all conditions of unambiguity known

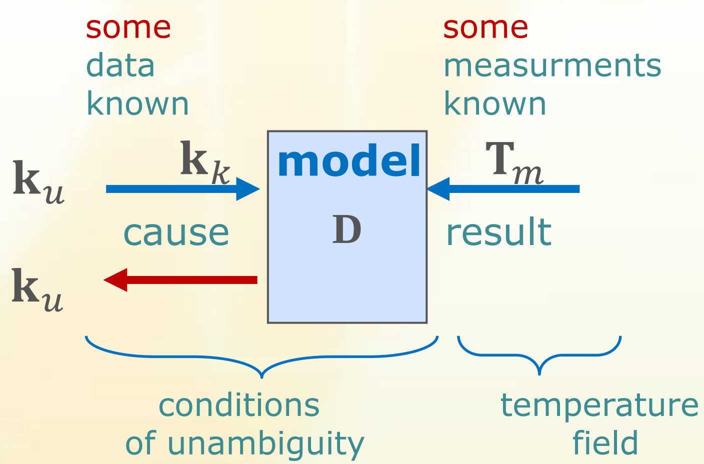
$$D(\mathbf{k}) = \mathbf{T}$$



inverse problem

some conditions of unambiguity unknown, some measured results available

$$D^{-1}(\mathbf{k}_{k,}\mathbf{T}_m) = \mathbf{k}_u$$



ill-posedeness of inverse problems

- solution may not be unique
- results can be unstable w.r.t. small changes in input data

special techniques needed to mitigate ill posedeness

regularization

- reduction of DOF's
- filtering out noise (neglecting higher POD modes)
- modification of the operator (Tikhonov)

ill posed problem → well defined problem

inverse problems

POD/RBF inverse algorithm

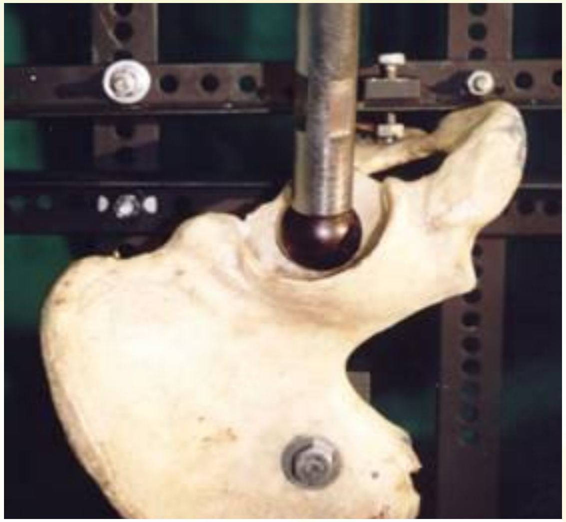
generating the POD base

generating POD basis	training POD-RBF network	solving inverse problem
• produce the snapshot matrix by solving a set of direct problems for a sequence of missing parameters $\mathbf{k}_u$ • generate the POD basis Φ • produce the truncated POD basis $\overline{\Phi}$	• define the radial basis function $g(\mathbf{k}_u)$ • train the POD basis to obtain the interpolation matrix $\mathbf{B}$ • generate the low dimensional model $\mathbf{u}(\mathbf{k}_u) = \mathbf{E} \cdot \mathbf{g}(\mathbf{k}_u)$	• minimize the discrepancy between the measurements $\mathbf{Y}$ and the output of the low dimensional model $\min_{w.r.t.\mathbf{k}_u} \lvert\lvert \mathbf{Y} - \mathbf{T}(\mathbf{k}_u) \rvert\rvert = \min_{w.r.t.\mathbf{k}_u} \lvert\lvert \mathbf{Y} - \mathbf{E} \cdot \mathbf{g}(\mathbf{k}_u) \rvert\rvert$

regularization properties of POD RBF

- **filtering out noise**
- POD basis vectors describe mutual interrelation between physical variables stored at different positions of the snapshot. **Nodal values are not allowed to vary independently**

Example 1
Young moduli of human pelvic bone

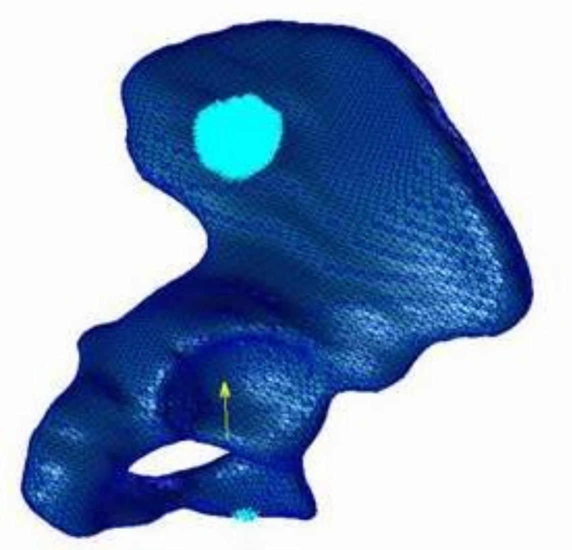


Layered structure of the bone (trabecular and cortical bone tissues) and homogenous (in each region) elastic properties assumed.

Geometry:
coordinate measuring machine & in-house code

Solver of direct problem:
MSC Nastran

Measurements:
Displacements(X,Y,Z) in 3 points
(simulated & experimantal ESPI)



Young moduli of human pelvic bone

POD-RBF model

400 snapshots

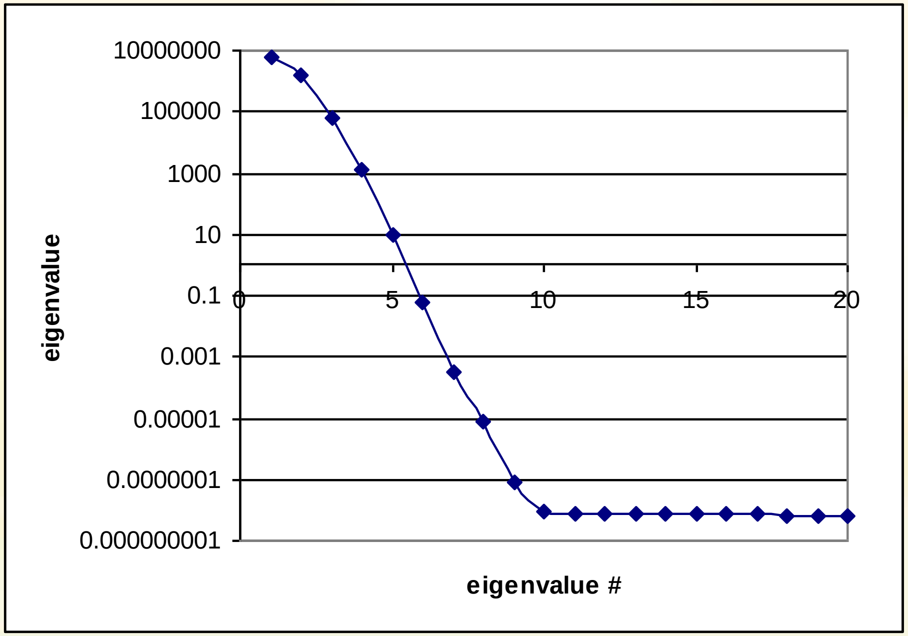
combinations of
various Young Moduli
of cortical and trabecular
bone tissue

Each snapshots stores
displacements (X,Y,Z)
for 28530 nodes
(i.e. 88590 entries)

RBF:
Thin-Plate splines &
Inverse multiquadrics

Eigenvalues:

For only 7 first POD base vectors
neglected energy fraction is 0.993316E-12



inverse problems

Young moduli of human pelvic bone

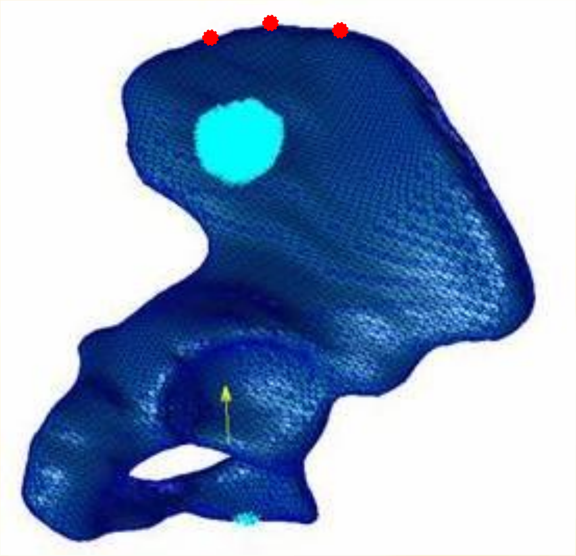
Results

3% simulated
measurements error
(random, uniform distribution)

Inverse multiquadrics RBF
trabecular – rel. error 2.43%
cortical – rel. error -1.09%

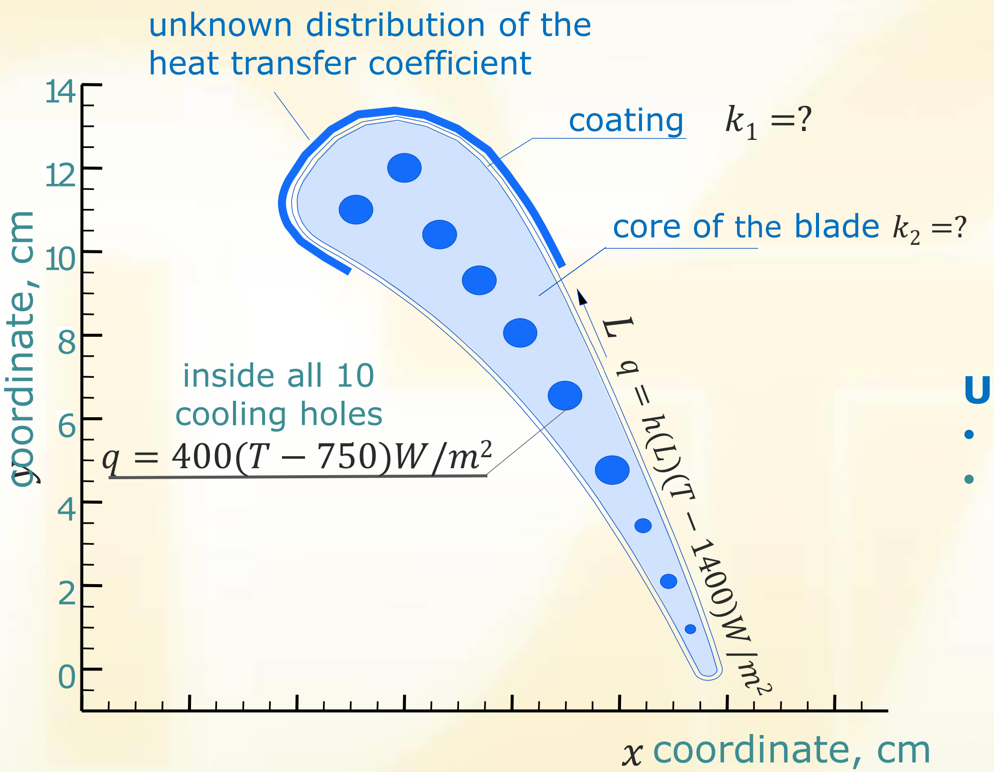
Thin-Plate splines RBF
trabecular – rel. error 2.15%
cortical – rel. error -1.15%

• **m**easurement points



Z. Ostrowski, R. Białecki, A. John, P. Orantek, W. Kuś, *POD-RBF network approximation for identification of material coefficients of human pelvic bone tissues* (Invited Keynote Lecture). In: WCCM8-ECCOMAS 2008 Joint 8th World Congress of Computational Mechanics and 5th European Congress on Computational Methods in Applied Sciences and Engineering, B.A. Schrefler and U. Perego (eds.), Venice, Italy, p.151, ISBN 978-84-96736-55-9, 2008.

Example 2
Identification conductivity and film coefficient



Unknown parameters

- conductivities of core and TBC k_1 & k_2
- distribution of film coefficient $h(L)$
  Lagrange interpolating polynomial
  4 control points

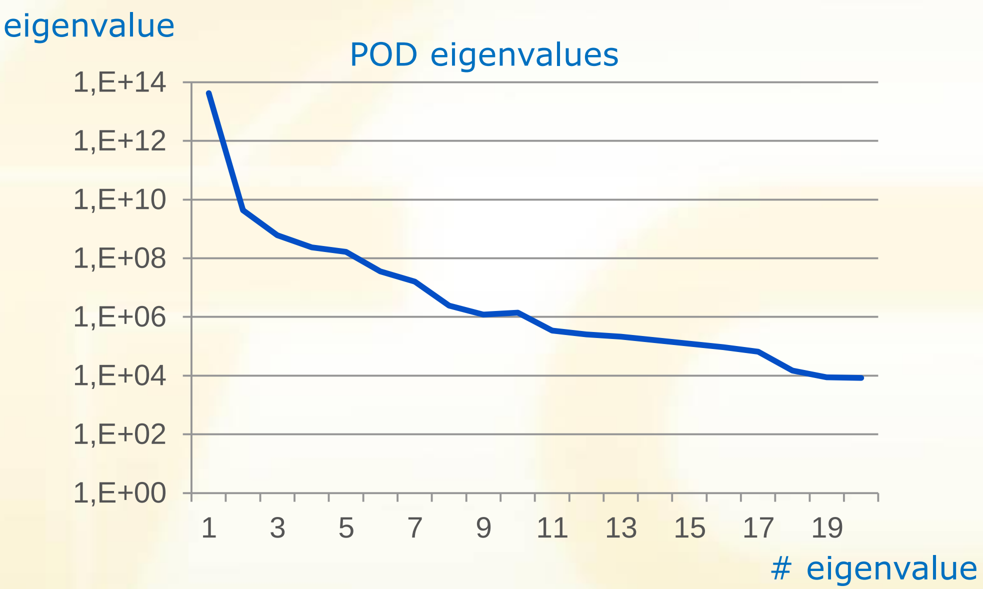
another inverse problem

POD basis model:
729 snapshots

Sampled at:
36479 points (nodes)

Solver:
MSC.Marc (by MSC Software)

Resulting POD base**:**
1.E-9 signal energy neglected
only 20 vectors (POD modes) **used**

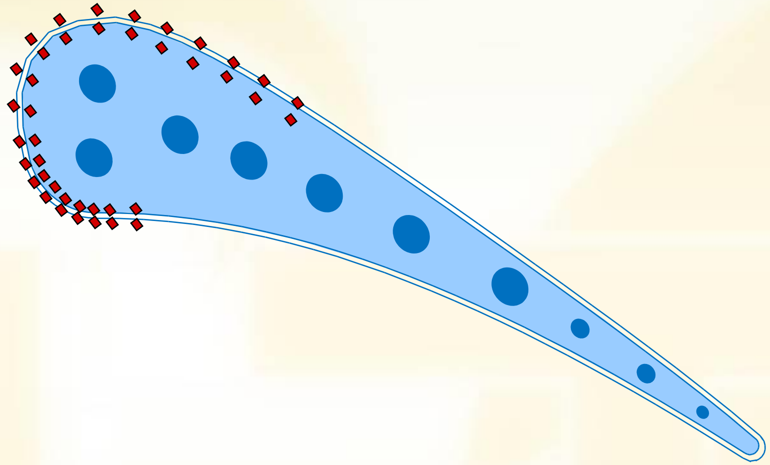


Z. Ostrowski, R.A. Białecki and A.J. Kassab. *Solving inverse heat conduction problems using trained POD-RBF network inverse method*, Inverse Problems in Science and Engineering **16:**1, (2008) pp. 39-54

C.A. Rogers, A.J. Kassab, E.A. Divo, Z. Ostrowski and R.A. Białecki, *An inverse POD-RBF network approach to parameter estimation in mechanics*, Inverse Problems in Science and Engineering 20:5, (2012) pp 1-19

another inverse problem

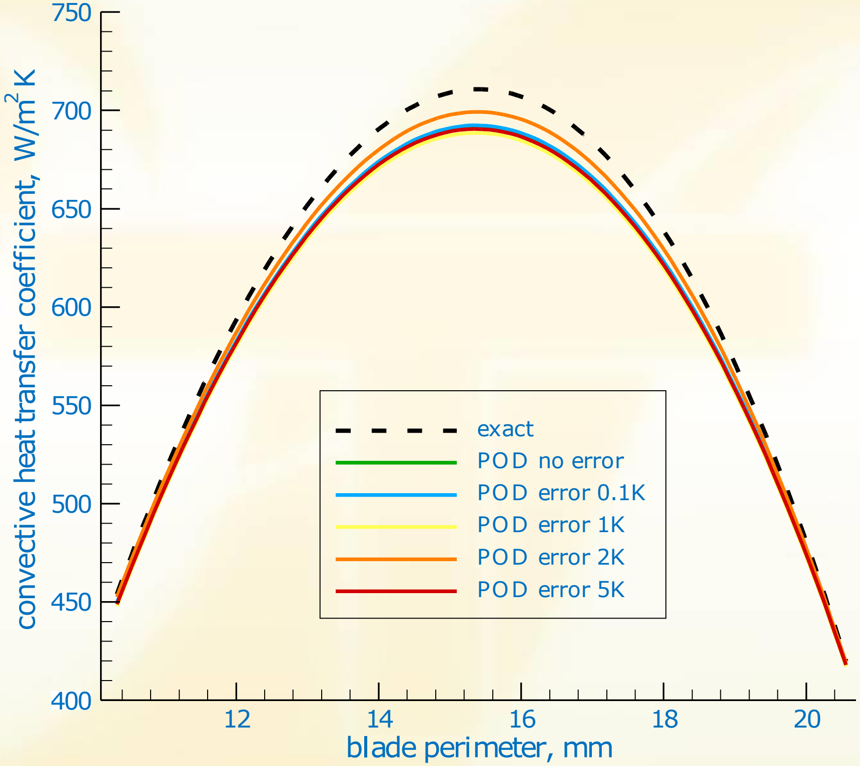
(pseudo) measurements (numerical experiment)



- location of pseudo-sensors, uniform random error distribution, amplitude 0.1, 1.0, 2.0 and 5.0 K

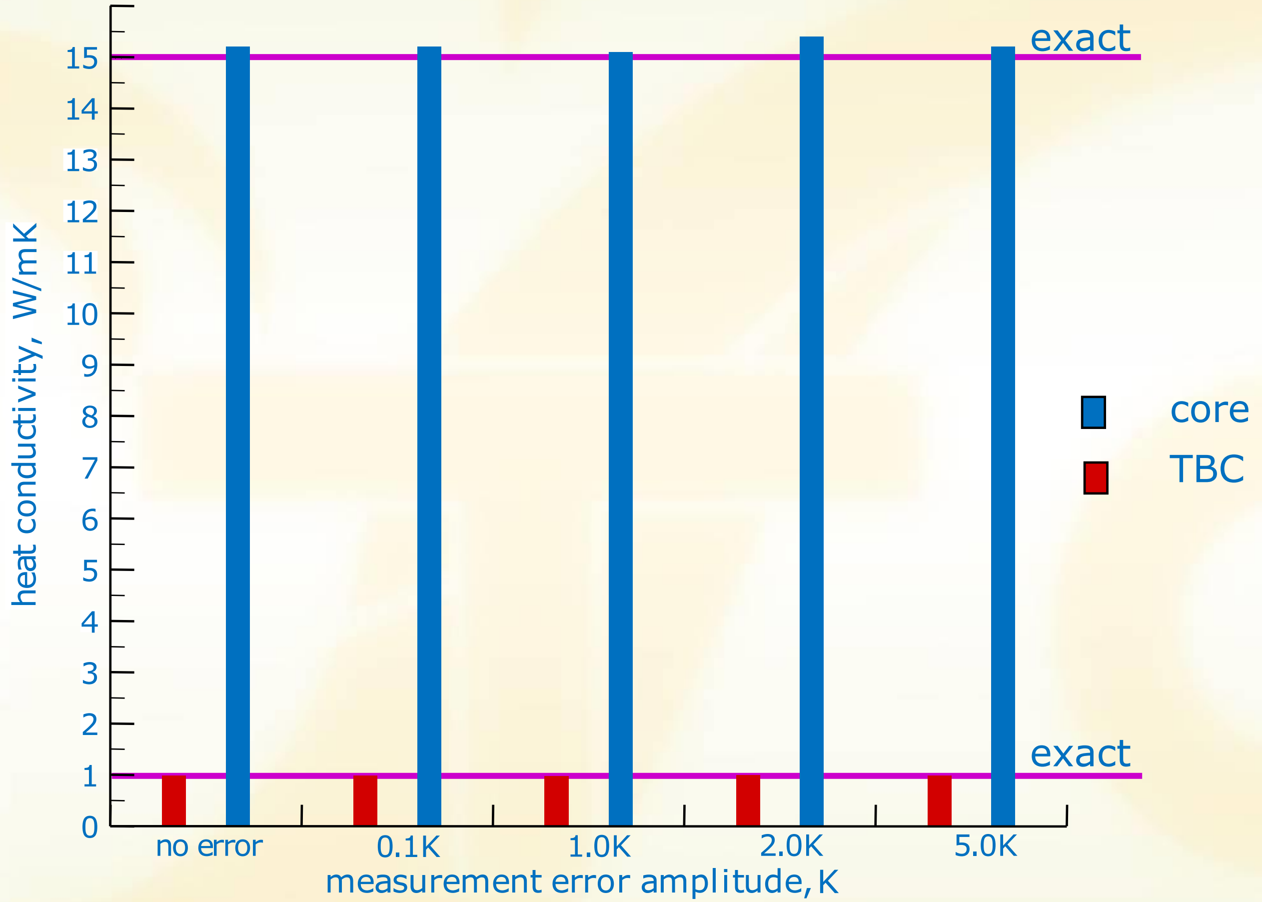
another inverse problem

Retrieved distribution of the film coefficient for different measurement errors



another inverse problem

Retrieved values of heat conductivity for different measurement errors



insensitive to measurement errors

Example 3
Retrieving heat diffusivity – nondestructive method

desired features of techniques of retrieving thermal diffusivity

non-destructive
- cheap
- extracting probes often changes the properties

based on 3D inverse technique
- applicable to bodies of arbitrary shape
- accounting for anisotropy

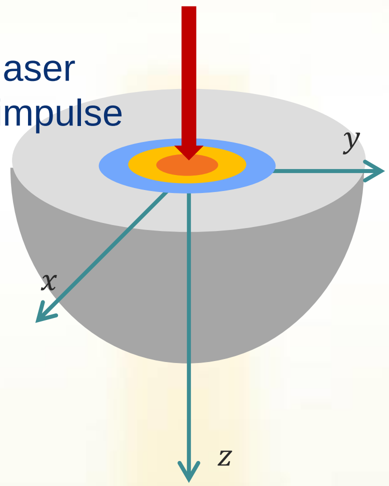
transient
- short time of experiment,
- simple treatment of boundary conditions
- wealth of experimental data

inverse problem, retrieving diffusivity

massive carbon blocks (few tons). International corporation commissioned installation for continuous checking the quality of carbon blocks. Resulting installation embedded in the production line. Operates almost 4 years. **EU and US patent pending.**

IR camera

laser impulse



Principle

Laser short time, small surface area heating. IR camera records the temperature changes. Least squares fit of heat conduction model and measurements.

Model

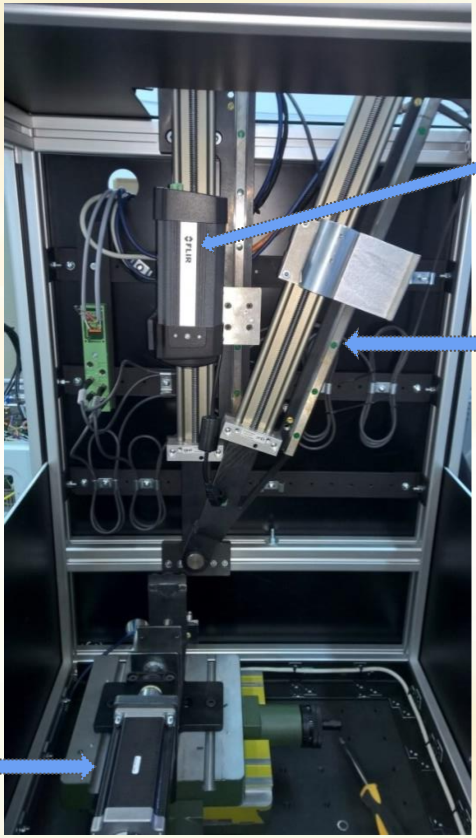
semi-infinite anisotropic body heated by pointwise instantaneous heat impulse. Process lasts about one second, heat losses neglected. Analytic solution: Green's function: temperature ratio (dimensionless). Levenberg Marquardt procedure used to solve the inverse problem, yielding components of the heat diffusivity tensor

$$\Theta(x_i, y_i, z_i = 0, t_1, t_2, D_x, k_y) = \frac{T(x_i, y_i, z = 0, t_1) - T_{init}}{T(x_i, y_i, z = 0, t_2) - T_{init}} = \frac{\sqrt{t_2^3}}{\sqrt{t_1^3}} \exp\left[\frac{1}{4D_x\lambda_y}(\lambda_y x_i^2 + y_i^2)\left(\frac{1}{t_2} - \frac{1}{t_1}\right)\right]$$

inverse problem, retrieving diffusivity

industrial installation

lab installation



inverse problem, retrieving diffusivity

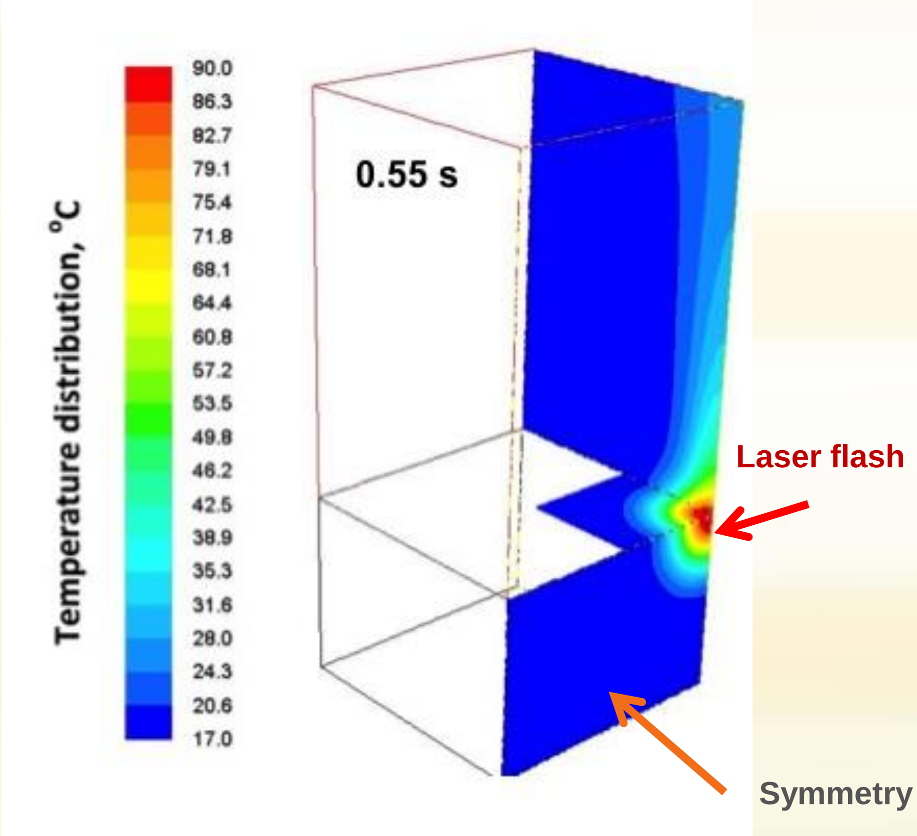
models of heat conduction used in the inverse technique

- analytic, sample of simplified shape, simple BC. Conduction
- numeric, sample of arbitrary shape. Conduction
- numeric sample of arbitrary shape. Conduction in sample CFD in air. Realistic BC
- as previous but with POD-RBG accelerator

Accounting for interaction with convection and radiation

Assumptions:

- arbitrary domain
- short time heat sources acting on a small fraction of the boundary
- **natural convection in the air** in contact with the heated surface accounted for. Businesq model applied
- air treated as a transparent medium
- S2S **radiation model** employed
- equations in the sample and air domains solved simultaneously



inverse problem, retrieving diffusivity

Single direct HT problem solution

Model	Time
Full CFD	12 hours
POD-RBF reduced order	<< 1 sec.

IHTP problem solution

Method	Time
Parker Flash method (destructive)	~20 min
Inverse analysis	
Analytical model	~1 min
Full CFD model	~8 days
Reduced order POD-RBF model	~2 sec.

technique	conductivity
Parker Flash	43.1W/mK
Analytic flash	41.1 W/mK
POD-RBF	43.06 W/mK

Example 4
tumor diagnostics based on response to cooling and heating

Melanoma early diagnostics by primary care physicians. Cooling the suspected area and recording the temperature field. Solving inverse problem for perfusion intensity

joint project of Silesian University of Technology (ITT), Institute of Oncology (Gliwice) and Juvena

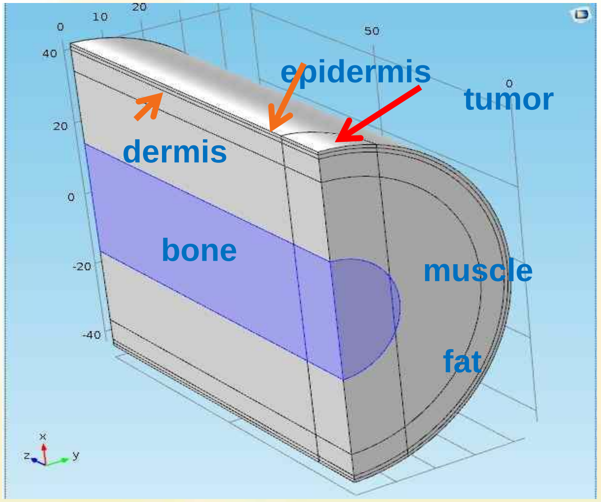
Bayesian inverse problem, tumor diagnostics

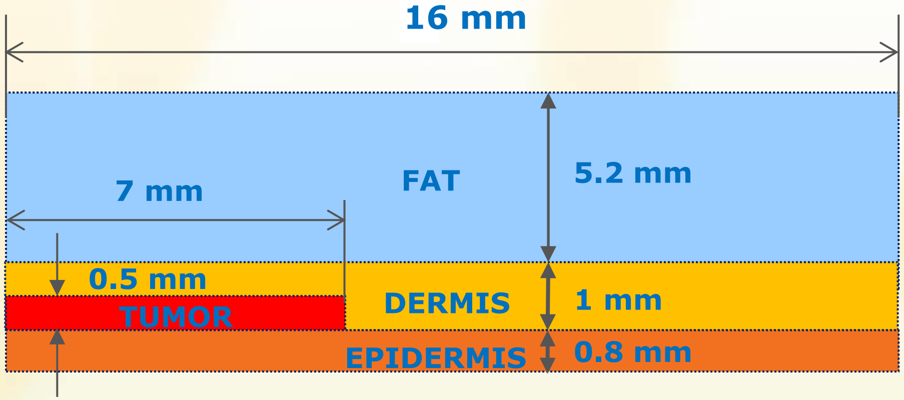
Pennes equation

$$\rho_t c_t \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k_t \frac{\partial T}{\partial x}\right) + \omega_b \rho_b c_b (T_a - T) + \dot{q}_m$$

perfusion metabolism

four parameters characterizing the tissue, $A = \rho_t c_t$, $B = k_t$, $C = \omega_b \rho_b c_b$, $D = \dot{q}_m$





Bayesian formulation

Motto: deterministic inverse problem produce pointwise values of the parameters. Bayesian produce probabilistic distribution thereof

1. parameters $\mathbf{k}$ of the problem are random variables.
2. any information that is available about the unknown parameters (prior).
   Usually the interval within which these parameters are expected is known, so is the probability density function $\pi_{prior}(\mathbf{k})$. These information need not be very precise
3. likelihood function describing the relation between the measurements $\mathbf{Y}$ and results of the direct problem is defined
4. evaluate probability distribution of the unknown parameters once the measurements are known , $\pi(\mathbf{k}|\mathbf{Y})$

Bayesian inverse problem, tumor diagnostics

Bayes equation

$$\pi_{posterior}(\mathbf{k}|\mathbf{Y}) = \frac{\pi_{prior}(\mathbf{k})\,\pi(\mathbf{Y}|\mathbf{k})}{\boldsymbol{\pi}(\mathbf{Y})}$$

$\boldsymbol{\pi}(\mathbf{Y})$ probability density of the measurements (normalizing constant), need not be deterjined

$$posterior \sim prior * likelihood$$

Typical priors

Prior has Gaussian distribution for parameter k_j with mean value μ_j and variance σ_j .

$$\pi(k_j) = \begin{cases} \frac{1}{\sigma_j\sqrt{2\pi}} \exp\left[-\frac{(k_j-\mu_j)^2}{2\sigma_j^2}\right] & if\ a < k_j < b \\ 0 & otherwise \end{cases}$$

$$\pi(k_j) = \begin{cases} \frac{1}{(b-a)} & if\ a < k_j < b \\ 0 & otherwise \end{cases}$$

likelihood function

Let $\mathbf{T}(\mathbf{k})$ denote the simulated values of the measured quantities $\mathbf{Y}$, obtained for a selected set of retrieved parameters $\mathbf{k}$. The measurement errors are assumed to be additive and independent of the parameters $\mathbf{k}$

$$\boldsymbol{\epsilon} = \mathbf{Y} - \mathbf{T}(\mathbf{k})$$

Assuming that the measurement errors $\boldsymbol{\epsilon}$ are Gaussian random variables, with zero means, known covariance matrix $\mathbf{W}$, the likelihood functions becomes

$$\pi(\mathbf{Y}|\mathbf{k}) = (2\pi)^{-D/2}|\mathbf{W}|^{-1/2}\exp\left\{-\frac{1}{2}\boldsymbol{\epsilon}^T\mathbf{W}^{-1}\boldsymbol{\epsilon}\right\}$$
$$= (2\pi)^{-D/2}|\mathbf{W}|^{-1/2}\exp\left\{-\frac{1}{2}[\mathbf{Y} - \mathbf{T}(\mathbf{k})]^T\mathbf{W}^{-1}[\mathbf{Y} - \mathbf{T}(\mathbf{k})]\right\}$$

D number of measurements

Monte Carlo Markov Chain

The posterior $\pi(\mathbf{k}|\mathbf{Y})$ can be evaluated using **Monte Carlo Markov Chain,** so that the that inference on the posterior probability becomes inference on its samples generated eg. by Metropolis Hastings algorithm.

The candidate value $\mathbf{k}^*$ is generated from a user defined distribution (say random walk) for known $\mathbf{k}^{(\mathbf{t})}$ parameter. Then the probability (MH ratio) is evaluated as

$$\alpha\left(\mathbf{k}^*\middle|\mathbf{k}^{(\mathrm{t})}\right) = \min\left[1, \frac{\pi_{posterior}(\mathbf{k}^*|\mathbf{Y})q\left(\mathbf{k}^{(\mathrm{t})}\middle|\mathbf{k}^*\right)}{\pi_{posterior}(\mathbf{k}^{(\mathrm{t})}|\mathbf{Y})q(\mathbf{k}^*|\mathbf{k}^{(\mathrm{t})})}\right]$$

random walk if r is a random number with uniform distribution in (0,1) and w_j is the amplitude, then

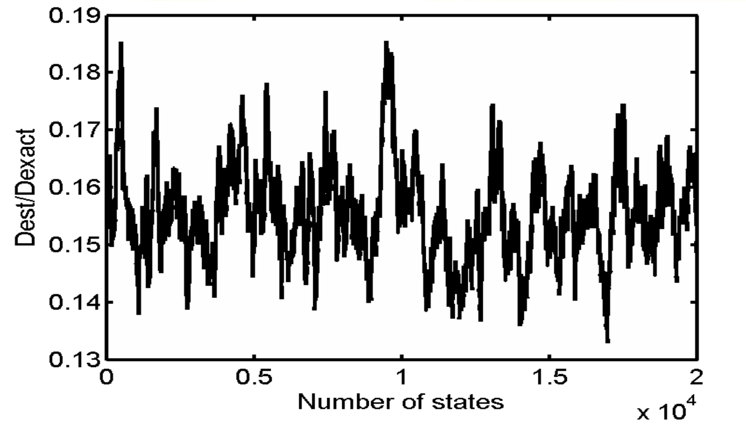
$$k_j^* = k_j^{(t)} + w_j(2r-1)$$

taking advantage of the symmetry of the random walk the Metropolis Hastings ratio simplifies to

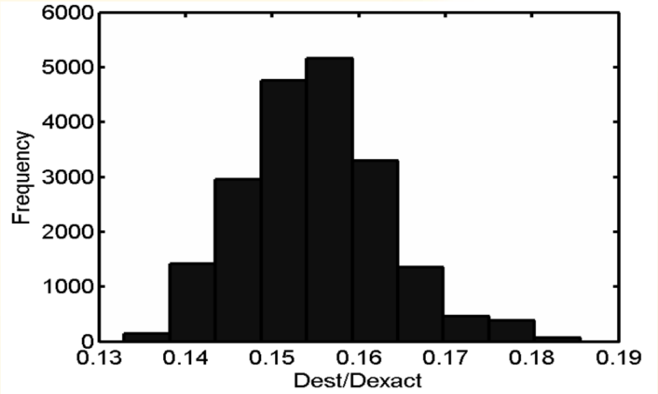
$$\alpha\left(\mathbf{k}^*\middle|\mathbf{k}^{(\mathrm{t})}\right) = \min\left[1, \frac{\pi_{posterior}(\mathbf{k}^*|\mathbf{Y})}{\pi_{posterior}(\mathbf{k}^{(\mathrm{t})}|\mathbf{Y}^*)}\right]$$

a random number U of uniform distribution in $(0,1)$ is generated.
If $U < \alpha, set\ \mathbf{k}^{(\mathbf{t+1})} = \mathbf{k}^{*}$ otherwise, set $\mathbf{k}^{(\mathbf{t+1})} = \mathbf{k}^{(\mathbf{t})}$

The result of the MCMC is a sequence of stochastic vectors. Typical diagram of values of the parameter is shown below. The resulting distribution is obtained by grouping the vectors in bins.



Markov chain, metabolism



distribution for metabolism

Bayesian inverse problem, tumor diagnostics

To use statistical inference, the number of vectors should be large. Each vector corresponds to a solution of one direct problem. **The computational times are prohibitively long.** ROM can be used to speedup the process, here **POD-RBF models come into play.**

The comparison of the exact and ROM models produces a distribution of the error $\boldsymbol{e}(\mathbf{k}) = \mathbf{T}(\mathbf{k}) - \mathbf{T}_{\mathrm{ROM}}(\mathbf{k})$ introduced by the simplified model and its covariance matrix $\mathbf{W}_{ROM}$.

Using the **enhanced error model** i.e. neglecting the dependence of the error on the retrieved parameters produces the modified likelihood defined as

$$\pi(\mathbf{Y}|\mathbf{k}) = (2\pi)^{-D/2}|\widetilde{\mathbf{W}}|^{-1/2}\exp\left\{-\frac{1}{2}[\mathbf{Y} - \mathbf{T}(\mathbf{k}) - \bar{\boldsymbol{e}}]^T\widetilde{\mathbf{W}}^{-1}[\mathbf{Y} - \mathbf{T}(\mathbf{k}) - \bar{\boldsymbol{e}}]\right\}$$

where

$\bar{\mathbf{e}}$ - mean approximation error $\mathbf{e}$

$\widetilde{\mathbf{W}}$ - modified covariance matrix $\widetilde{\mathbf{W}} = \mathbf{W} + \mathbf{W}_{ROM}$

Bayesian inverse problem, tumor diagnostics

FEM vs POD-RBF model

FEM- COMSOL, 1300 elements

POD-RBF 18 modes
Mean approximation error 0.3E-8
MCMC 100 000 iterations – full model two weeks, POD 480s,
online speedup 2500 times

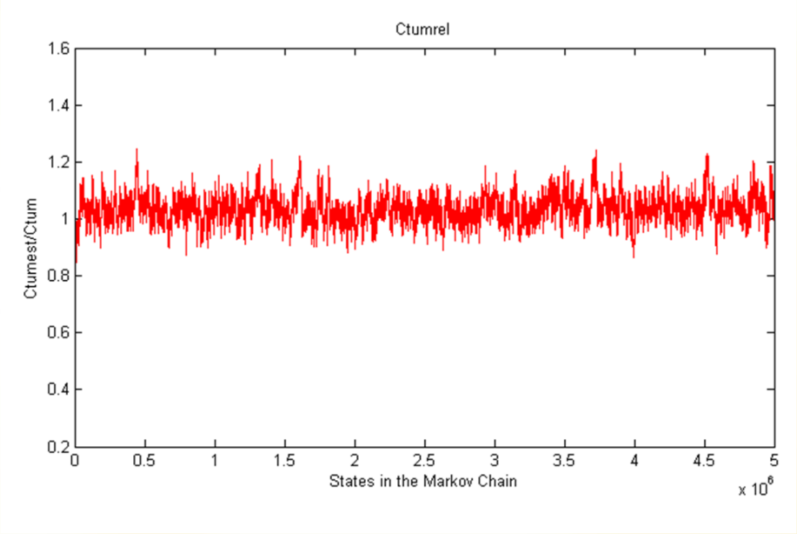
simulated measurements, priors, 10% variation except tumor perfusion, metabolism +- 100%

Parameter	Epidermis	Dermis	Fat	Tumor
$\rho_t, kg/m^3$	1085.0	1085.0	850.0	1085.0 *
$c_t, J/kgK$	3680.0	3680.0	2300.0	3680.0*
$k_t, W/mK$	0.47	0.47	0.16	0.47*
ω_b, s^{-1}	0.0	0.0011	$3.60E-06$	0.00525
$q_m, W/m^3$	0.0	631.0	58.0	6310.0
prior type	Gaussian	Gaussian	Gaussian	Uniform

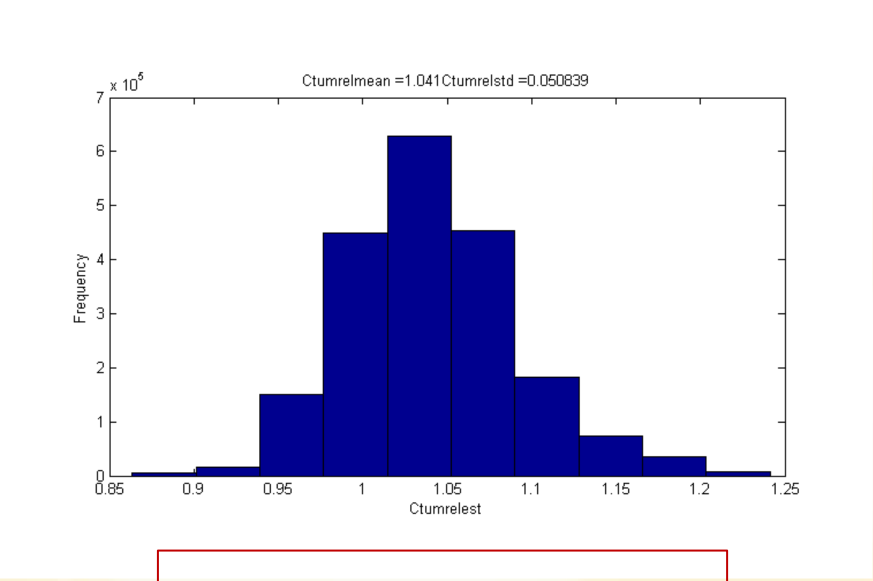
Bayesian inverse problem, tumor diagnostics

retrieved relative tumor perfusion

Markov chain



posterior distribution



mean $C_{mean}/C_{exact} = 1.041$

standard deviation 0.05084

conclusions

POD is a powerful tool of reducing the dimensionality of several classes of numerical models.

Statistical processing leads to an optimal representation of the spatial distribution of the output variable.

The dependence on input parameters can be obtained either by solving a set of differential equations or by resorting to RBFs. In the latter case, the functionality is that of neural network

Application of POD-RBF networks in inverse problems introduces additional regularization by filtering out the noise and additional coupling between DOFs

In the context of the Bayesian formulation of inverse problems, POD-RBF leads to extreme speedup.