Model Reduction - Trouble with Scales?

Wolfgang Dahmen

Institut für Geometrie und Praktische Mathematik
RWTH Aachen

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Outline

1. Scales and Spatial Dimensionality
   - Upscaling and Transport
   - Transpiration Cooling
2. How to Best Sample the Solution Manifold?
   - Model Reduction - Reduced Basis Method
   - Transport Dominated Problems

What is this Talk about?...

...some obstructions...

- range of relevant scales
  (geometric micro structures, turbulence, porous media...)
- high spatial dimensionality
  (parameter dependence, high dimensional phase space...)

... prediction beyond experiment... any mathematical "shortcuts"?

$\rightsquigarrow$ Certified Reduced Bases for transport dominated problems...

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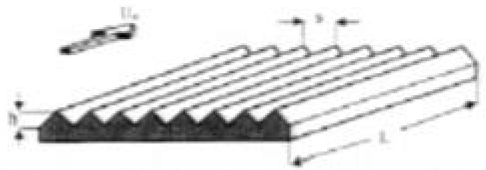
Turbulent Drag Reduction - FOR 1779 - DFG

(Joint work with G. Deolmi, S. Müller)



P.R.Viswanath "Aircraft viscous drag reduction using riblets", *Progress in Aerospace Sciences* **38** (2002) 571-600

Challenges:

- limited experimental accessibility...
- One cannot resolve turbulent flow...
- One cannot discretize flow boundary...
- How to find the best parameters y : frequency, amplitude... ? Feedback control?...

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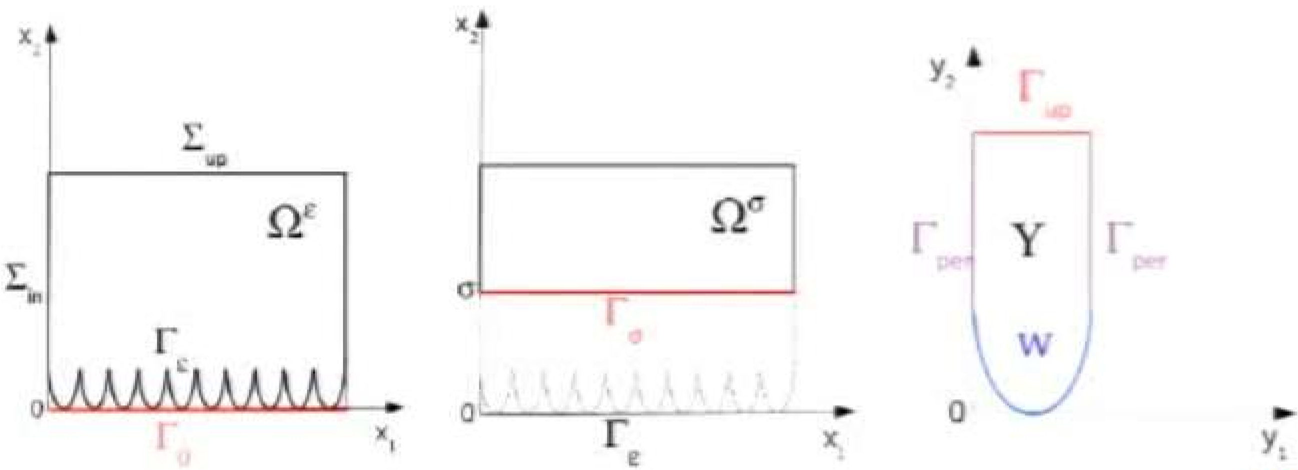
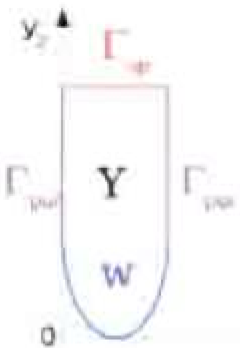
Upscaling... (Dahmen/Deolmi/Müller)

- turbulence modeling $\leftrightarrow$ geometric upscaling
- regularized compressible NS equations on smooth domain Ω^σ
  - find effective boundary conditions depending on $y \in$ {frequency, amplitude, wavelength,... }
  - cell problem $\rightsquigarrow$ parameter dependent convection-diffusion equation



$F(\mathbf{u}^\varepsilon, \rho^\varepsilon, p^\varepsilon) = 0,\qquad F(\mathbf{u}^{eff}, \rho^{eff}, p^{eff}) = 0,\qquad F(\mathbf{u}^0, \rho^0, p^0) = 0$

The Cell Problem



$$\mathbf{y} := \frac{\mathbf{x}}{\epsilon} \quad \eta_\epsilon := \frac{\eta}{\epsilon Re}, \quad k_\epsilon := \frac{k}{\epsilon Re}$$

Beavers-Joseph cond:

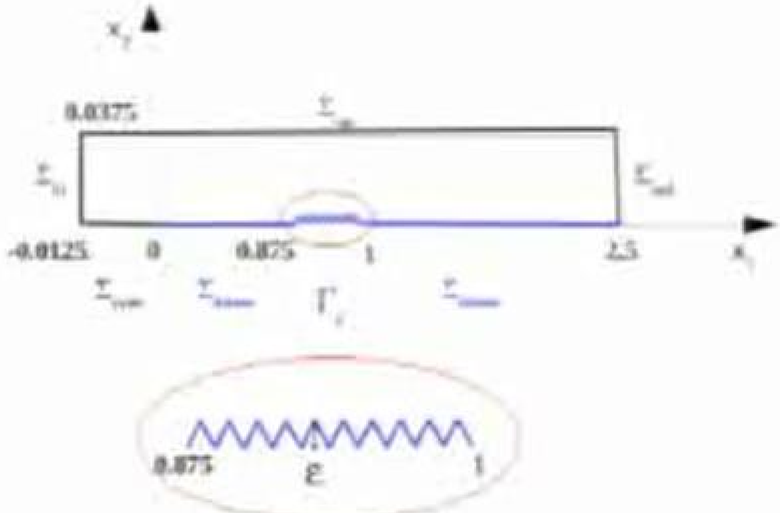
$$\frac{\partial \rho^{eff}}{\partial n} = 0, \ \frac{\partial p^{eff}}{\partial n} = 0, \ \mathbf{u}^{eff} = \frac{\partial u_1^{eff}}{\partial x_2}(\sigma \mathbf{e}_1 + \epsilon\langle\chi\rangle)$$

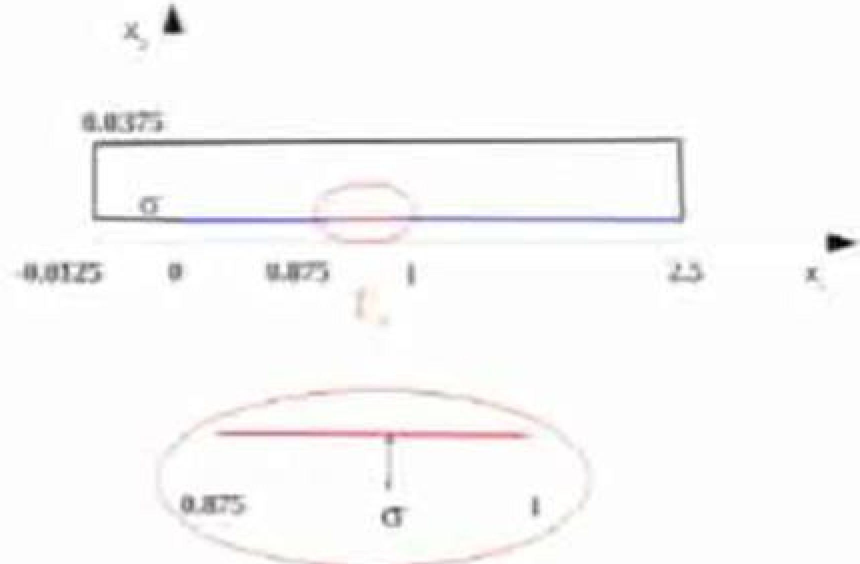
Asymptotic expansions ⇝...

$$\begin{aligned}
(\mathbf{u}^0 \cdot \nabla_y)\phi + \rho^0 \nabla_y \cdot \chi &= 0, \\
\rho^0(\mathbf{u}^0 \cdot \nabla_y)\chi + \nabla_y \pi &= \eta_\epsilon \left(\Delta_y \chi + \tfrac{1}{3}\nabla_y(\nabla_y \cdot \chi)\right), \quad in\ Y \\
(\mathbf{u}^0 \cdot \nabla_y)\pi + \gamma p^0 \nabla_y \cdot \chi &= \frac{\gamma k_\epsilon}{Pr\,\rho^0}\left(\Delta_y \pi - \frac{p^0}{\rho^0}\Delta_y \phi\right)
\end{aligned}$$

... + BC's ...⇝ Parameter dependent convection-diffusion equation

Laminar Flow over Rough Plate: $Re = 5 \cdot 10^5$, $Ma = 0.3$, $\epsilon = 6.25 \cdot 10^{-4}$, $\frac{\epsilon}{\delta} \approx 9\%$ (Dahmen/Deolmi/Müller)





$\epsilon = 6.25 \cdot 10^{-4}$	DNS	Effective
$s = 10\epsilon$	$1.15799 \cdot 10^{-3}$	$1.159905 \cdot 10^{-3}$
$s = 20\epsilon$	$1.189297 \cdot 10^{-3}$	$1.159265 \cdot 10^{-3}$

Dynamic drag coefficient: Flat plate: $c_D = 1.224175 \cdot 10^{-3}$

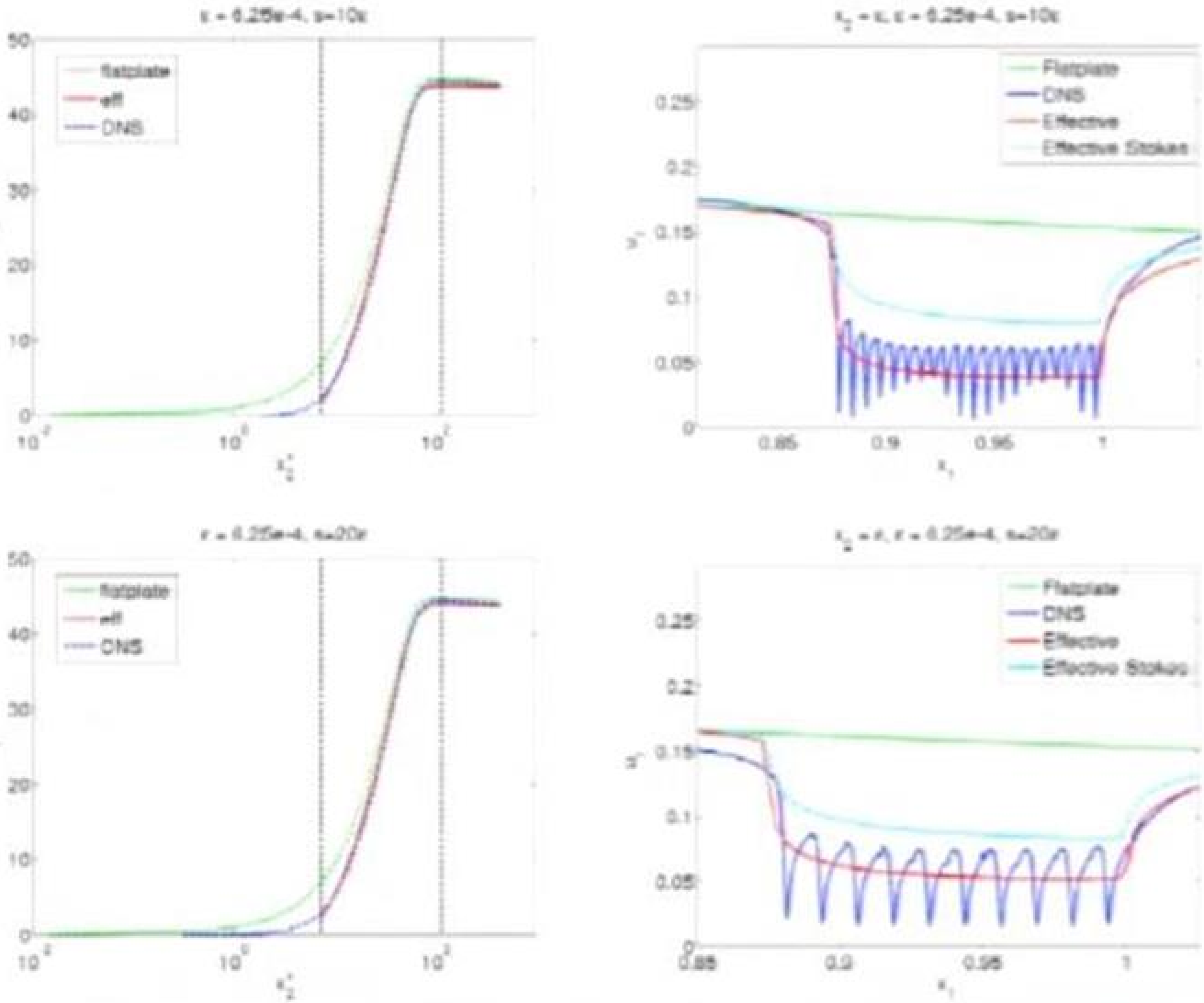
$\epsilon = 6.25 \cdot 10^{-4}$	DNS	Effective
$s = 10\epsilon$	59738	10924
$s = 20\epsilon$	53469	10978

Effective Problem: $\epsilon = 6.25 \cdot 10^{-4}$

wall-normal direction | streamwise profile

$s = 10\epsilon$

$s = 20\epsilon$



Ongoing...

W. Dahmen, G. Deolmi, S. Müller, Effective boundary conditions for compressible flows over rough surfaces, to appear in M^3AS Mathematical Models & Methods in Applied Sciences

So far: proof of principle for small structured area - single cell problem

- incorporate turbulence
- large structured surface: frequent solution of cell problems depending on macro-flow
- feed back loop: reduce macro-flow model... estimate ϵ, λ... from model and data...

Key demand: model reduction for transport dominated problems

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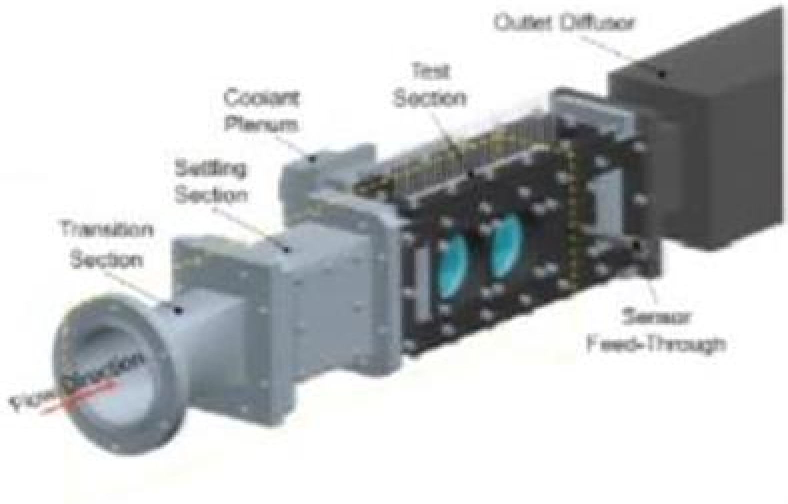
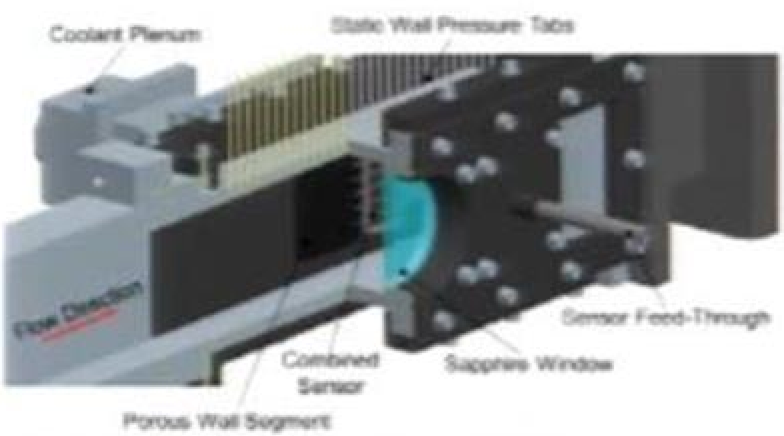
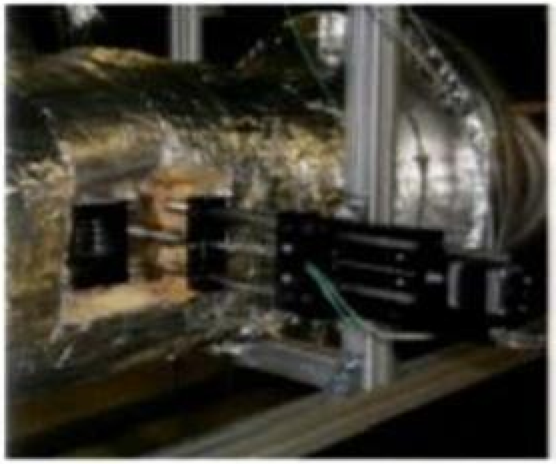
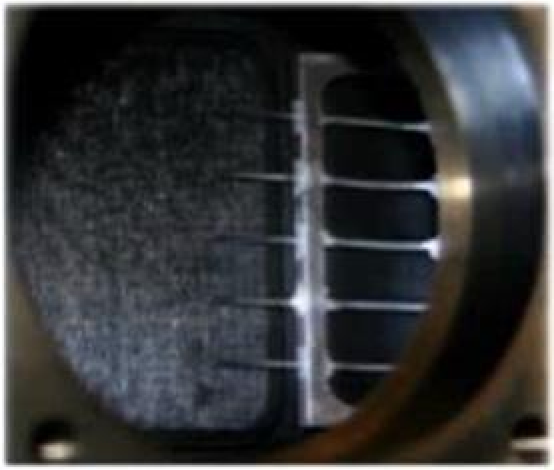
Experimental Setup: DFG-TR40

RWTH Aachen, TU Braunschweig, TU Munich, Un. Stuttgart ... Eckert/Livingood









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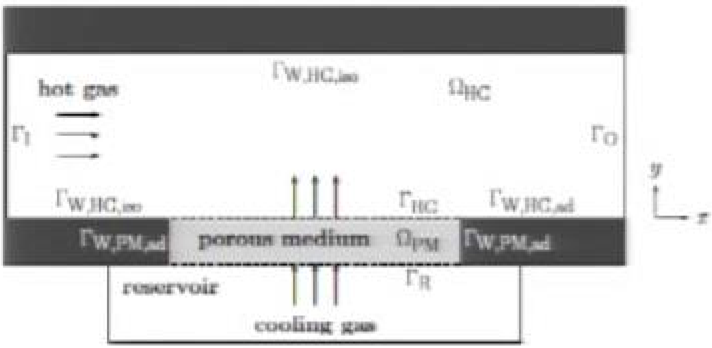
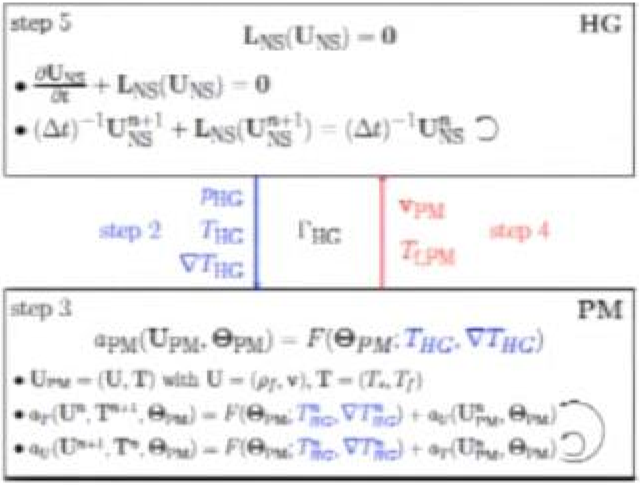
Main Issues

- subsonic turbulent hot gas flow
  (Reynolds averages Navier Stokes equation, Wilcox k, ω-model)
- compressible porous medium
  (Darcy-Forchheimer momentum balance with quadratic drag)
- capture non-equilibrium temperature effects
- no pre-modeled boundary conditions at hot gas interface
  $\rightsquigarrow$ more detailed information of skin-friction and heat flux reduction
- goal: predictability beyond experiment

Computational Model Dahmen/Gotzen/Müller/Rom

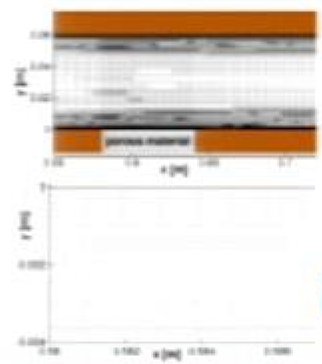




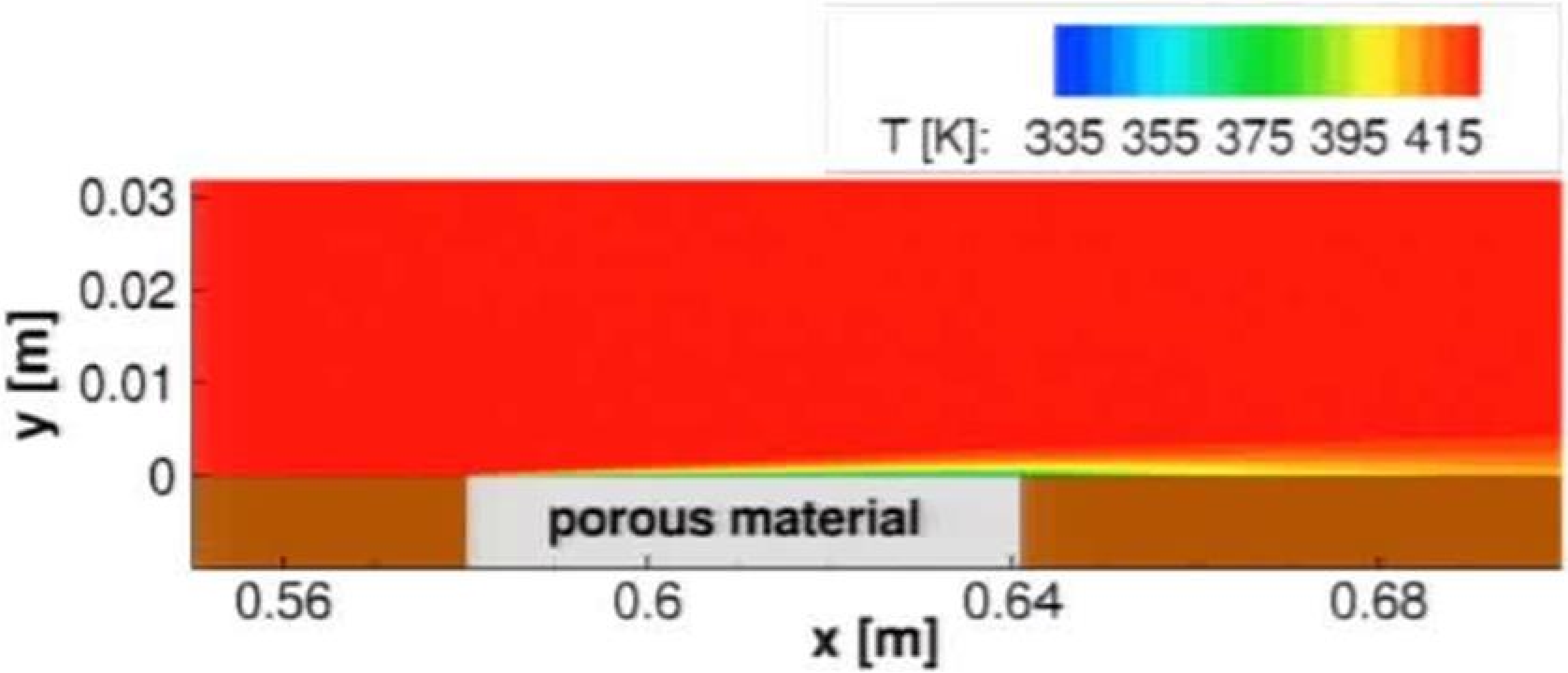
Hot gas: compr. Navier Stokes

porous medium: Darcy-Forchheimer

interface: coupling conditions



Some Numerical Results



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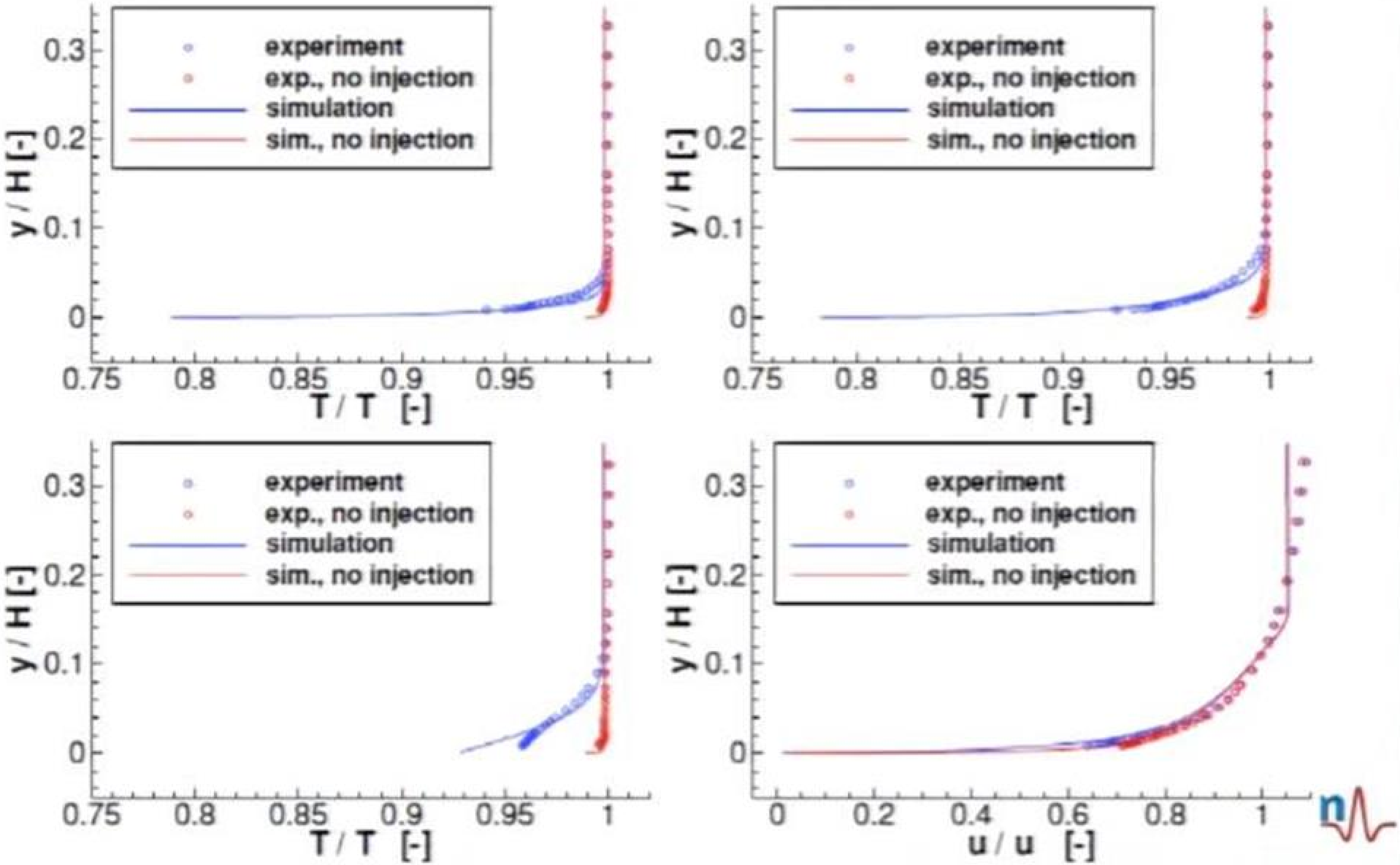

Some Numerical Results

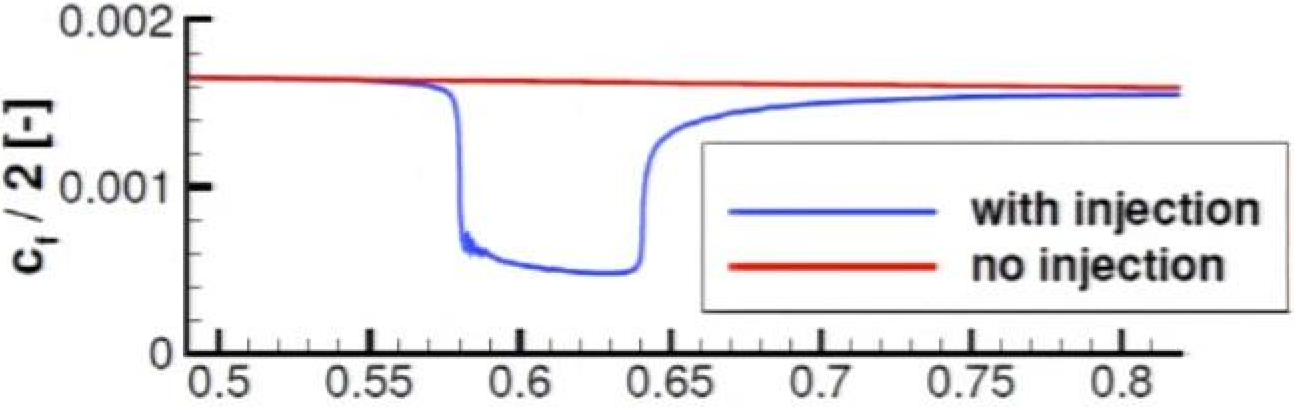

Figure: streamwise variation of skin-friction coefficient

Ongoing...

- parameter (blowing ratio) dependent transport equations in porous medium
- parameter dependent coupling conditions, hot gas flow
- take roughness of porous medium surface into account
- $\rightsquigarrow$ further model reduction for porous medium flow

References:

W. Dahmen, T. Gotzen, S. Müller, M. Rom, Numerical simulation of transpiration cooling through porous material, IGPM Preprint, Juli 2013, RWTH Aachen, to appear in International Journal for Numerical Methods in Fluids.

S. Müller, W. Dahmen, M. Rom, S. Schweikert, M. Selzer, J. von Wolfersdorf, Numerical boundary layer investigations of transpiration-cooled turbulent channel flow, to appear in International Journal of Heat and Mass Transfer

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What are we up to?...

Scenario: parameter dependent family of transport dominated PDEs:

$$F(u, y) = 0, \quad y \in \mathcal{Y}, \quad \rightsquigarrow u(x, y)$$

- High-dimensionality

  sparsity promoting dictionaries

- online parameter optimization: $QI(y) = \ell(u(y)) \to \mathrm{opt}$ is practically infeasible

  frequent query problems, instantaneous solutions

- Data assimilation: state (parameter) estimation based on few measurements

  mitigates undersampling - regularization

... calls for Certified Model Reduction ...

Problem: dominating transport

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Abstract Setting

- Parameter dependent family of PDEs

$$\mathcal{B}_y u = f, \quad y \in \mathcal{Y}, \quad \Leftrightarrow \quad b_y(u, v) = f(v), \quad v \in Y', \quad \Rightarrow \quad u = u(y)$$

- Solution manifold:

$$\mathcal{M} = \{u(y) : y \in \mathcal{Y}\} \subset X$$

- Goal: approximate $\mathcal{M}$ uniformly over $\mathcal{Y}$ by possibly small dimensional reduced space X_n, i.e.,

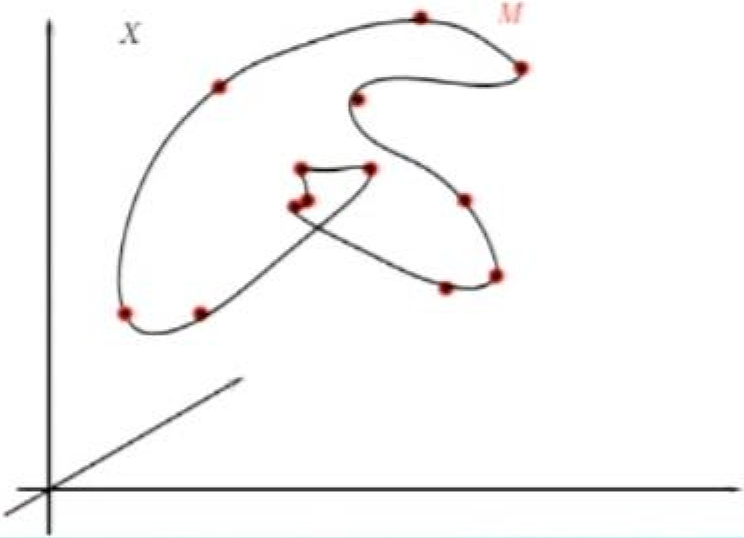
$$\sup_{v \in \mathcal{M}} \inf_{w \in X_n} \|v - w\|_X =: \operatorname{dist}(\mathcal{M}, X_n)_X \overset{!}{\leq} \varepsilon, \quad n = n(\varepsilon) \text{ small !}$$

- Benchmark: Kolmogorov n-widths:

$$d_n(\mathcal{M})_X := \inf_{\dim V_n = n} \operatorname{dist}(\mathcal{M}, V_n)_X$$

Philosophy of the Reduced Basis Method (RBM)

- Offline mode: precompute a "reduced basis" consisting of "suitable" solution samples $\rightsquigarrow$ heavy computational cost in the "truth space"
- Online mode: for each parameter query solve only a small reduced system - with certified accuracy



$$\sum_{j=1}^{n} c_j(y)u(x, y_j) \approx u(x, y)$$

How to get good snapshots?

A Greedy Paradigm... Maday, Patera, Rozza, Prud'homme, Turinici...

- Recall $\mathcal{B}_y : X \to Y'$: $\mathcal{B}_y u(y) = f$, $\mathcal{M} := \{u(y) := \mathcal{B}_y^{-1} f : y \in \mathcal{Y}\}$
- Goal: find $X_n \subset X$ s.t. $\mathrm{dist}\,(\mathcal{M}, X_n)_X \le \varepsilon$ for n small
- Suppose that one has a rapidly computable Surrogate:

$$\inf_{v \in X_n} \|u(y) - v\|_X \le R(y, X_n), \quad y \in \mathcal{Y}, \quad \rightsquigarrow$$

Greedy Algorithm:

- $X_0 := \{0\}$;
- for $n = 1, 2, \ldots,$ given X_{n-1}

$$y_n := \mathrm{argmax}_{y \in \mathcal{P}} R(y, X_{n-1}), \quad X_n := \mathrm{span}\,\{X_{n-1}, \{u(y_n)\}\}$$

Rate-Optimality

THEOREM: [Binev/Cohen/Dahmen/DeVore/Petrova/Wojtaszczyk]

For $\inf_{w \in X_n} \|u(y) - w\|_X = R(y, X_n)$ one has

$$\operatorname{dist}(\mathcal{M}, X_n)_X \leq \frac{2^{n+1}}{\sqrt{3}} d_n(\mathcal{M})_X \quad n \in \mathbb{N}$$

THEOREM: [Binev/Cohen/Dahmen/DeVore/Petrova/Wojtaszczyk]

If surrogate is tight, i.e., $c_S R(y, X_n) \leq \inf_{w \in X_n} \|u(y) - w\|_X \leq R(y, X_n)$

$$d_n(\mathcal{M})_X = \begin{cases} O(n^{-\alpha}), \, n \in \mathbb{N}, \\ O(e^{-cn^{\alpha}}), \, n \in \mathbb{N}, \end{cases} \quad \Rightarrow \quad \operatorname{dist}(\mathcal{M}, X_n)_X = \begin{cases} O(n^{-\alpha}), \; n \in \mathbb{N}, \\ O(e^{-\bar{c}n^{\alpha}}), \; n \in \mathbb{N}, \end{cases}$$

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What are good surrogates?...how to best see the manifold?

- One should have

$$\text{surrogate} \quad \approx \quad \text{best approximation error}$$

- Surrogate should be based on residuals: $f - \mathcal{B}_\mu u_n^*(\mu)$
- One should have for $\mathcal{B}_\mu : X \to Y'$

$$\begin{aligned} \|f - \mathcal{B}_\mu u_n^*(\mu)\|_{Y'} &= \|\mathcal{B}_\mu(u(\mu) - u_n^*(\mu))\|_{Y'} \overset{!}{\sim} \|u(\mu) - u_n^*(\mu)\|_X \\ &\overset{!}{\sim} \|u(\mu) - P_{X_n} u(\mu)\|_X \end{aligned}$$

- Works well for elliptic problems with Galerkin projection: $X = Y = H_0^1(\Omega)$, $Y' = H^{-1}(\Omega)$
- For transport dominated, indefinite, singularly perturbed problems need $X \neq Y$

RBMs for Transport Dominated Problems [Dahmen/Plesken/Welper]

Problem: "elliptic surrogates" don't work

Remedy: instead of $\|f - \mathcal{B}_y \Pi^y_{X_n} u(y)\|_{X'}$ use

- $R(y, X_n) := \|f - B_y \Pi^y_{X_n} u(y)\|_{Y'}$, where Y is chosen properly
- stable variational formulations $b_y(\cdot,\cdot) : X \times Y \to \mathbb{R}$

  [D./Huang/Schwab/Welper, Cohen/D./Welper, Barret/Morton, Cai/Manteuffl...,Demkowicz/Jopalakrishnan...Rozza/Veroy, Patera/Urban (SP problems)...]

- grow pairs of spaces X_n, Y_n, $n = 1, 2, 3, \ldots$ such that corresponding Petrov-Galerkin projections realize near best approximation in X
- construction of the Y_n trough inner stabilizing greedy loop based on equivalent saddle-point formulation

THEOREM: [Dahmen/Plesken/Welper]

The "double greedy" RBM is rate optimal.

An Example

(Pure) Transport Equation: Dahmen/Huang/Schwab/Welper

$\Gamma_-(\mu) := \{x \in \partial\Omega : n(x) \cdot \mu < 0\}, \mu \in S^{d-1}$

$$\mu \cdot \nabla u + cu = f^\circ, \quad \text{in } \Omega = (0,1)^d, \quad u = u_b, \quad \text{on } \Gamma_-(\mu),$$

$$b_\mu(u,v) := \langle u, \underbrace{\mu \cdot \nabla v + cv}_{=\mathcal{B}_\mu{}^* v} \rangle = \langle f^\circ, v\rangle - \int_{\Gamma_-(\mu)} n \cdot \mu u_b v =: \langle f, v\rangle$$

$$\|v\|_{Y_\mu} := \|\mathcal{B}_\mu{}^* v\|_{L_2}, \quad \|u\|_{X_\mu} := \|u\|_{L_2}$$

Transport Equation

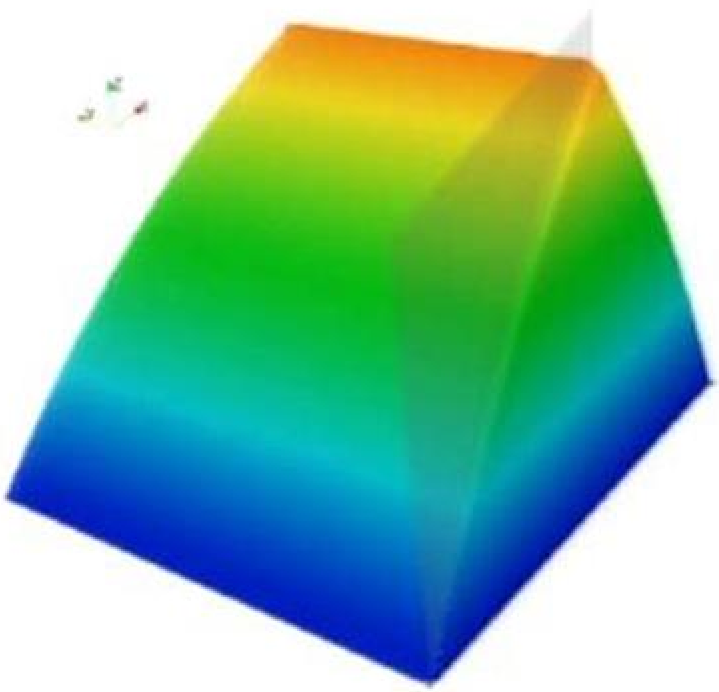

Figure: (1): reduced basis of dimension $n = 24$, $m(n) = 91$, angle $\mu = 0.244579$

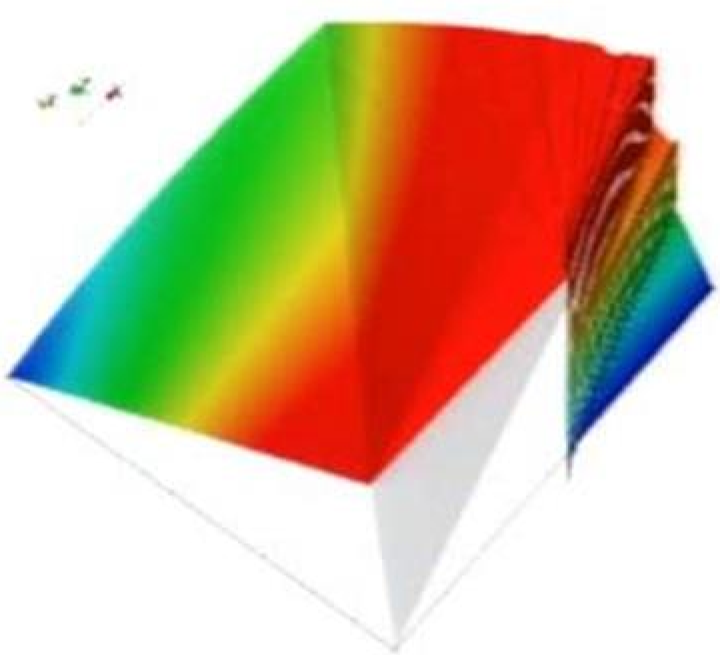

Figure: (2): reduced basis of dimension $n = 24$, $m(n) = 96$, angle $\mu = 0.256311$

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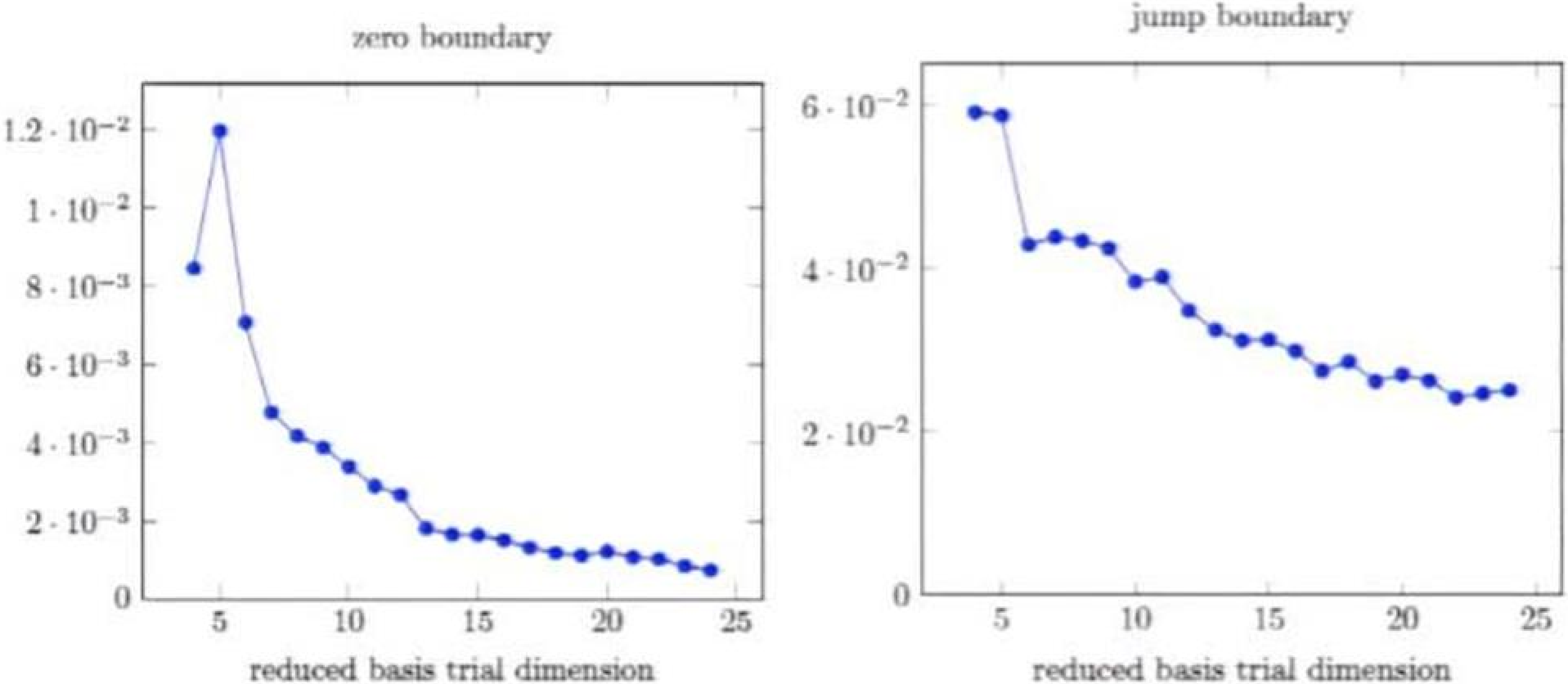
Transport Equation: Convergence



(Pure) Transport Equation (2): truth L_2-error 0.0154

trial	test	δ	surr	rb truth	rb L2	surr/err
4	14	4.97e-01	5.91e-02	1.29e-01	1.30e-01	4.54e-01
8	31	4.29e-01	4.34e-02	7.78e-02	7.95e-02	5.46e-01
12	49	3.71e-01	3.48e-02	7.40e-02	7.53e-02	4.63e-01
16	64	3.74e-01	2.99e-02	6.20e-02	6.41e-02	4.67e-01
20	81	3.73e-01	2.71e-02	5.46e-02	5.62e-02	4.82e-01
24	96	3.91e-01	2.51e-02	4.51e-02	4.79e-02	5.25e-01

Convection-Diffusion Equations

$$-\epsilon\Delta u + \begin{pmatrix}\cos\mu \\ \sin\mu\end{pmatrix}\cdot\nabla u + u = 1, \text{ in } \Omega = (0,1)^2, \quad u = 0, \text{ on } \partial\Omega$$

Choice of the test norm:

$$s_\mu(u,v) := \frac{1}{2}\big(\langle B_\mu u, v\rangle + \langle B_\mu v, u\rangle\big),$$

$$\|v\|_{Y_\mu}^2 := s_\mu(v,v) = \epsilon|v|_{H^1(\Omega)}^2 + \left\|\left(c - \frac{1}{2}\mathrm{div}\, b(\mu)\right)^{1/2} v\right\|_{L_2(\Omega)}^2$$

$+$ boundary penalization at outflow boundary: (see Cohen/Dahmen/Welper, M2AN 2012)

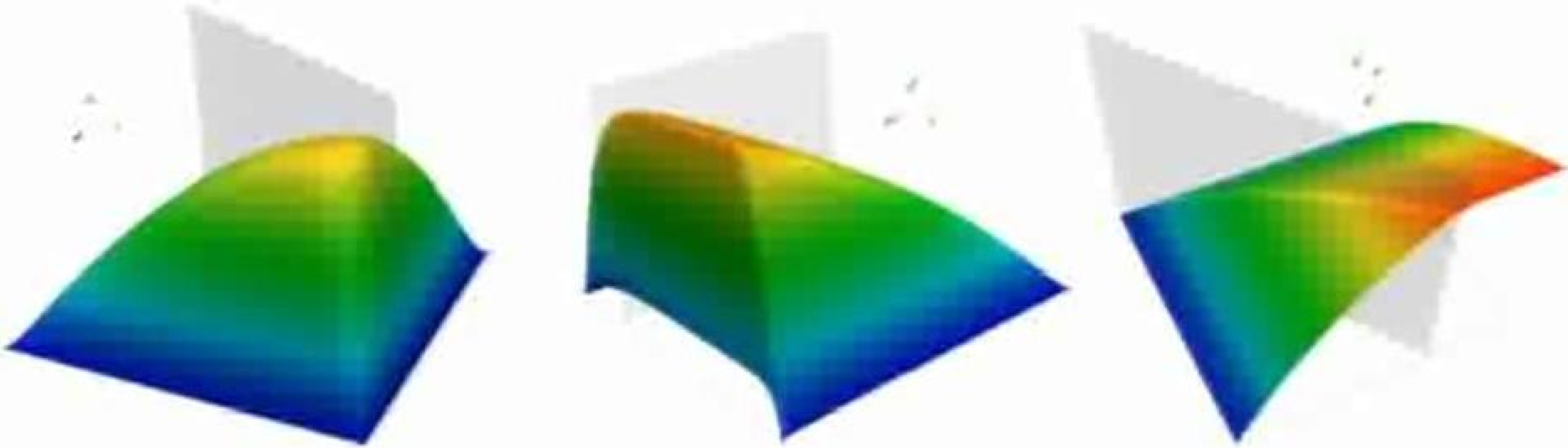
$$\|u\|_{\bar{X}_\mu}^2 := \|\bar{B}_\mu u\|_{\bar{Y}'_\mu}^2 = \|\bar{B}_\mu u\|_{Y'_\mu}^2 + \lambda\|u\|_{H_b(\mu)}^2$$

$H_b(\mu) = H_{00}^{1/2}(\Gamma_+(\mu))$, $\bar{Y}_\mu := Y_\mu \times H_b(\mu)'$

$$u(\mu) = \mathrm{argmin}_{w\in X_-}\{\|\bar{B}_\mu w - f\|_{\bar{Y}'_\mu}^2 + \lambda\|\gamma w\|_{H_b(\mu)}^2\}$$

Convection-Diffusion Equations

Robustness with respect to small diffusion

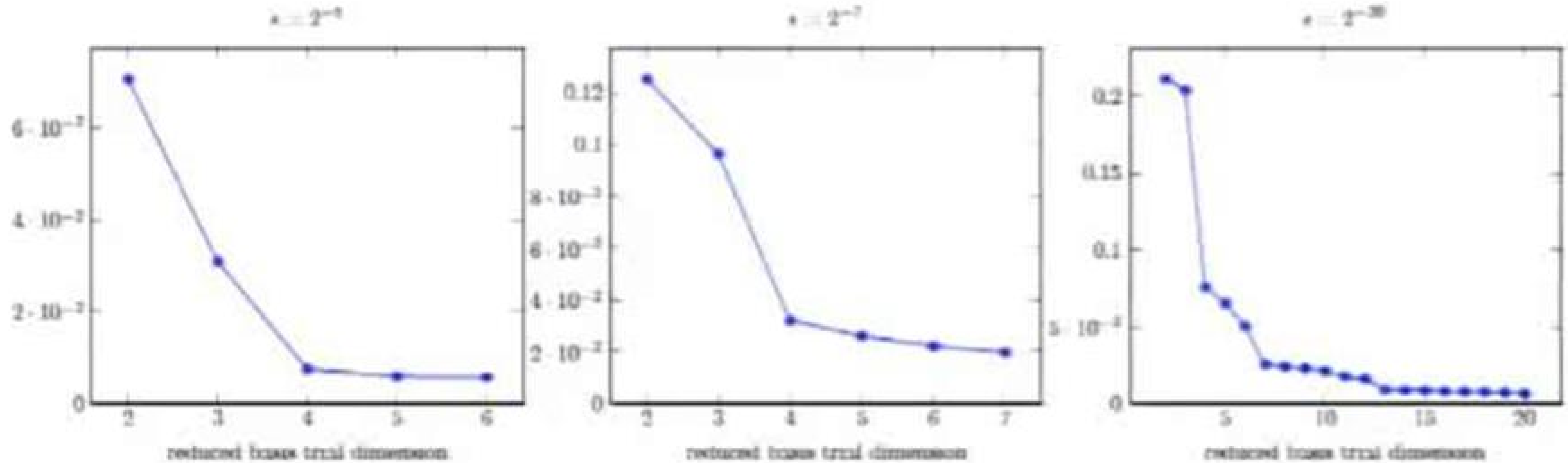


(a) $\epsilon = 2^{-5}$ RB dim $n = 6$, $m(n) = 13$, angle $\mu = 0.885115$,

(b) $\epsilon = 2^{-7}$ RB dim $n = 7$, $m(n) = 20$, angle $\mu = 0.257484$,

(c) $\epsilon = 2^{-26}$ RB dim $n = 20$, $m(n) = 57$, angle $\mu = 0.587137$

Convection-Diffusion Equations



Convection-Diffusion Equations: $\epsilon = 2^{-7}$ a-post. error 0.0197

dim trial	dim test	δ	max surr	surr/a-post
2	5	8.92e-03	1.25e-01	6.37e+00
3	8	1.22e-01	9.65e-02	4.90e+00
4	11	1.13e-02	3.21e-02	1.63e+00
5	14	1.27e-02	2.61e-02	1.32e+00
6	17	5.55e-03	2.21e-02	1.12e+00
7	20	4.82e-03	1.97e-02	1.00e+00

Convection-Diffusion Equations: $\epsilon = 2^{-26}$ a-post. error 0.0011

trial	test	δ	surrogate	a-post	trial	test	δ	surrogate	surr/a-post
2	5	1.35e-03	2.11e-01	2.00e+02	12	33	3.47e-04	1.60e-02	1.52e+01
4	9	1.09e-02	7.58e-02	7.19e+01	14	39	1.10e-04	8.46e-03	8.02e+00
6	15	1.61e-03	5.02e-02	4.76e+01	16	45	9.39e-05	7.87e-03	7.46e+00
8	21	7.99e-04	2.39e-02	2.26e+01	18	51	6.11e-05	7.69e-03	7.29e+00
10	27	3.55e-04	2.10e-02	2.00e+01	20	57	5.28e-05	6.35e-03	6.02e+00

Reference:

W. Dahmen, C. Plesken, G. Welper, Double Greedy Algorithms: Reduced Basis Methods for Transport Dominated Problems, ESAIM: Mathematical Modelling and Numerical Analysis, 48(3) (2014), 623–663. DOI 10.1051/m2an/2013103, http://arxiv.org/abs/1302.5072

Outlook...

- reduced modeling and data assimilation
- inversion: assisting rapid conditioned sampling
- construction of low-rank approximation to kinetic models

$$b(y) \cdot \nabla u(y) + cu(y) = f + \int_{\mathcal{P}} K(y, y')u(y')d\mu' \quad \text{in } \Omega, \;\; u\,|_{\Gamma_-=0}$$

view the function $u(x, y)$ as collection of fibers
$\mathcal{M} = \{u(\cdot, y) =: y \in \mathcal{Y}\}$