High order methods for non linear PDE:
Spectral element and reduced basis methods

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From geometry to numerics

Outline

1. Motivation
   - Framework of the approach
   - Parameter dependent problems
   - An example
   - Application to fluid flows

- A lot of problems we have to face in numerical analysis and scientific computing: find u such that

$$\mathcal{F}(u) = 0 \tag{1}$$

can actually be written under a variational form : find $u \in \mathcal{X}$ such that

$$\mathcal{A}(u, v) = < f, v >, \quad \forall v \in \tilde{\mathcal{X}} \tag{2}$$

Where $\mathcal{X}$ and $\tilde{\mathcal{X}}$ are some coherent Banach spaces, $\mathcal{A}$ is an appropriate form, linear in v, and f is a given linear form. For time dependent problem one may specify even : find $u, \forall t, u(t, ;) \in \mathcal{X}$ such that

$$m(\frac{\partial u}{\partial t}, v) + \mathcal{A}(u, v) = < f, v >, \quad \forall v \in \tilde{\mathcal{X}} \tag{2'}$$

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- the Lax Milgram theorem (then $\mathcal{X} = \tilde{\mathcal{X}}$) or
- the Babuška-Brezzi condition.....

that makes explicit conditions under which the problem is well posed : i.e. there exists a unique solution u to problem (1).

For nonlinear problems the conditions are various and more involved.

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The approximation can now proceed. Two families of finite dimensional spaces $\{\mathcal{X}_n\}_n$ and $\{\tilde{\mathcal{X}}_n\}_n$ are provided, that maintain the above mentioned coherence.

and the discrete space reads : find $u_n \in \mathcal{X}_n$ such that

$$\mathcal{A}_n(u_n, v_n) =< f_n, v_n >, \quad \forall v_n \in \tilde{\mathcal{X}}_n \qquad (2_n)$$

or again for time dependent problems : find $u_n, \forall t, u_n(t,;) \in \mathcal{X}_n$ such that

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most often further numerical quadratures are involved leading to slightly modified discrete problems

Framework of the approach.

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- The discrete solutions u_n exist and are unique
- An error bound $\|u - u_N\|_{\mathcal{X}} \leq c \inf_{w_n \in \mathcal{X}_n} \|u - w_N\|_{\mathcal{X}}$ can be derived
- The best fit, $\inf_{w_n \in \mathcal{X}_n} \|u - w_N\|_{\mathcal{X}}$, goes to zero rapidly
- The effective computation of u_n is easy enough
- An a posteriori error providing the size of $\|u - u_N\|_{\mathcal{X}}$ is available
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- Nonlinear approximations/ multiresolution analysis $\mathcal{X}_n$ are based on wavelet approximations
- Reduced basis $\mathcal{X}_n$ are based on previously computed solutions

Framework of the approach.

High order methods

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Spectral methods.
in one dimension

- For any integer N, $I\!P_N$ is the set of all polynomials of degree $\leq N$
- Classical approximation results are known in $\mathcal{C}^0$–norm and reveal infinite order accuracy
- We are interested in Sobolev norms:

$$H^1 = \{v \in L^2, \quad v' \in L^2\}$$

$$H^r = \{v \in L^2, \quad v' \in H^{r-1}\}$$

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in 2 and 3 dimensions

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Spectral methods.

Definition of the problem

- Consider the Navier Stokes problem
- Find $\mathbf{u}$ and p such that

$$\frac{\partial \mathbf{u}}{\partial t} - \nu \Delta \mathbf{u} + \mathbf{u} \nabla \mathbf{u} + \nabla p = \mathbf{f}$$

$$div(\mathbf{u}) = 0$$

- Variational formulation

$$\int_\Omega \frac{\partial \mathbf{u}}{\partial t} \mathbf{v} + \int_\Omega \nabla \mathbf{u} \nabla \mathbf{v} + \int_\Omega \mathbf{u} \nabla \mathbf{u} \mathbf{v} - \int_\Omega p\, div(\mathbf{v}) = \int_\Omega \mathbf{f} \mathbf{v}$$

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$$\int_\Omega \frac{\partial \mathbf{u}}{\partial t} \mathbf{v} + \int_\Omega \nabla \mathbf{u} \nabla \mathbf{v} + \int_\Omega \mathbf{u} \nabla \mathbf{u} \mathbf{v} - \int_\Omega p div(\mathbf{v}) = \int_\Omega \mathbf{f} \mathbf{v}$$

- the spectral approximation : find $\mathbf{u}_N$ and p_N such that

$$\int_\Omega \frac{\partial \mathbf{u}_N}{\partial t} \mathbf{v}_N + \int_\Omega \nabla \mathbf{u}_N \nabla \mathbf{v}_N + \int_\Omega \mathbf{u}_N \nabla \mathbf{u}_N \mathbf{v}_N - \int_\Omega p_N div(\mathbf{v}_N) = \int_\Omega \mathbf{f} \mathbf{v}_N$$

Spectral methods.

Definition of the problem

- Consider the Navier Stokes problem
- Find $\mathbf{u}$ and p such that

$$\frac{\partial \mathbf{u}}{\partial t} - \nu \Delta \mathbf{u} + \mathbf{u}\nabla \mathbf{u} + \nabla p = \mathbf{f}$$

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Spectral methods.

Coherent spaces

- $$\int_\Omega \frac{\partial \mathbf{u}_N}{\partial t}\mathbf{v}_N + \int_\Omega \nabla \mathbf{u}_N \nabla \mathbf{v}_N + \int_\Omega \mathbf{u}_N \nabla \mathbf{u}_N \mathbf{v}_N - \int_\Omega p_N div(\mathbf{v}_N) = \int_\Omega \mathbf{f}\mathbf{v}_N$$
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the degrees of $\mathbf{u}_N$ and p_N cannot be the same.... spurious pressure modes
degree of $\mathbf{u}_N = N$ (idem for $\mathbf{v}_N$) and degree of $p_N = N - 2$ (idem for q_N) leads to a unique solution

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Efficient implementation

- The nonlinear contribution $\int_\Omega \mathbf{u}_N \nabla \mathbf{u}_N \mathbf{v}_N$ is a problem from the computational point of view
- We need to evaluate these contribution efficiently: the idea is to make use of a numerical integration that should not destroy the accuracy : Gauss type formula

$\int_\Omega \mathbf{u}_N \nabla \mathbf{u}_N \mathbf{v}_N$ is evaluated by $\sum_{i,j} \mathbf{u}_N(\xi_{ij}) \nabla \mathbf{u}_N(\xi_{ij}) \mathbf{v}_N(\xi_{ij}) \omega_{ij}$

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Spectral methods.

Extension to curved domains

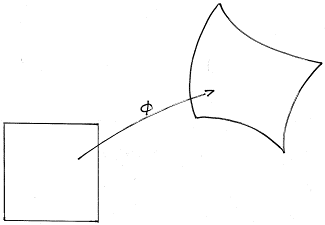

Figure: The domain of interest is obtained as a regular deformation of the square

Spectral methods.
Domain decomposition

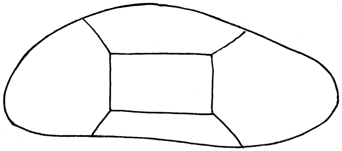

Figure: The domain of interest is decomposed into a union of nonoverlapping deformed squares

This non overlapping domain decomposition $\Omega = \cup \Omega^k$ allows to write simply the integral over Ω as a sum of integrals over each of the subdomains Ω^k.

$$\sum_{k=1}^{K} \sum_{i,j} \frac{\partial \mathbf{u}_N}{\partial t} \mathbf{v}_N(\xi_{ij}^k)\omega_{ij}^k + \sum_{k=1}^{K} \sum_{i,j} \nabla \mathbf{u}_N \mathbf{v}_N(\xi_{ij}^k)\omega_{ij}^k \ldots$$

This way, we do not have to wonder about the matching, only continuity is imposed at the interfaces

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Spectral methods.

Non matching domain decomposition

This variational formulation + numerical integration + non overlapping DD allows also to be able to use different polynomial degree in each subdomain

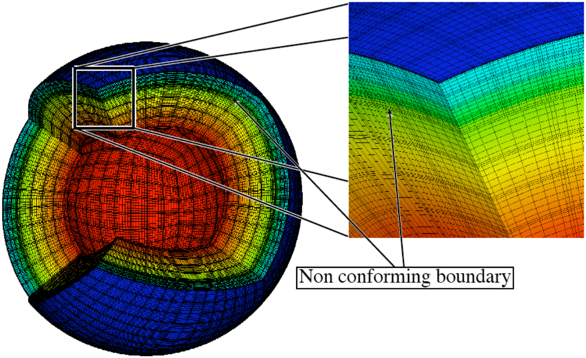

Figure: non matching grids treated by the mortar element method, by Y. Capdeville, E. Chaljub, J.P. Vilotte, J.P. Montagner

If the solution to be approximated is only piecewise regular but globally discontinuous
Spectral approximations lead to furious oscillations.... but a post treatment is possible

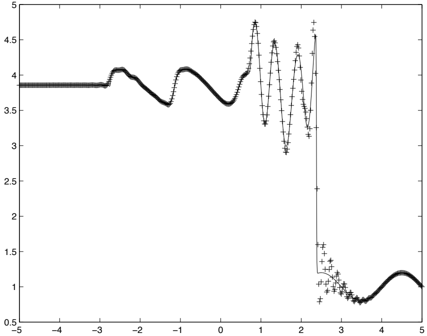

Figure: The solution before post processing, from S.M. Kaber

Spectral methods.

Non regular solutions

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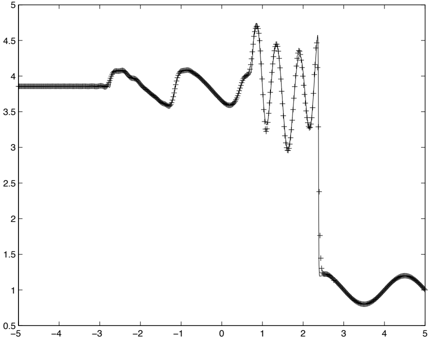
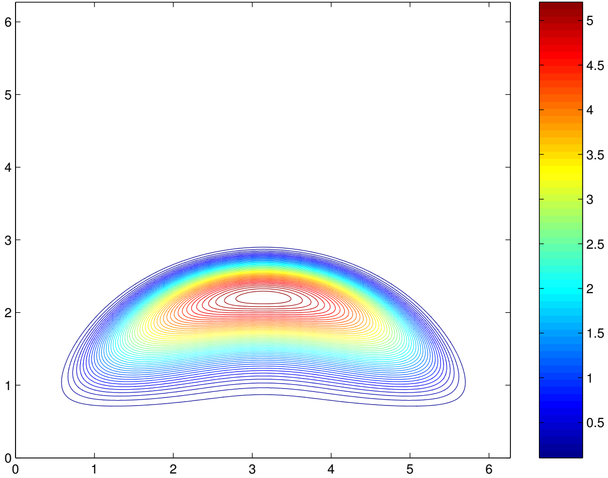


Figure: The solution AFTER the postprocessing, from S.M. Kaber

Spectral methods.

Non regular solutions



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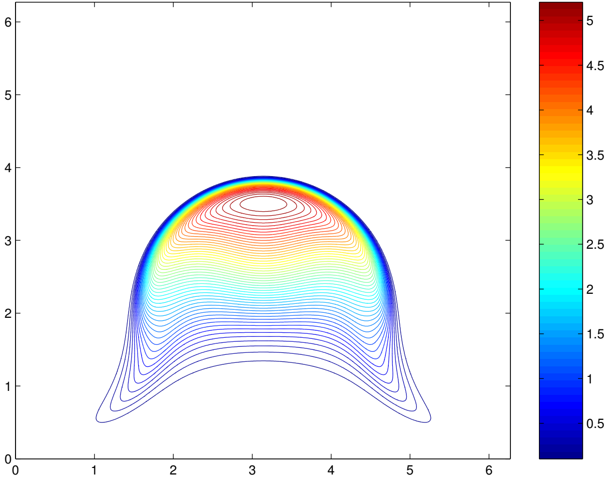

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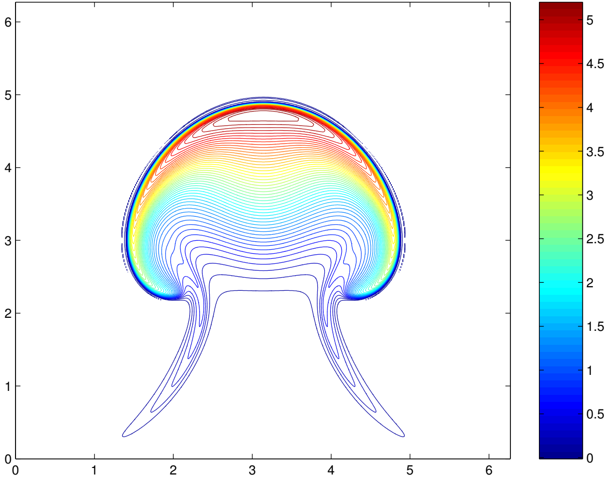

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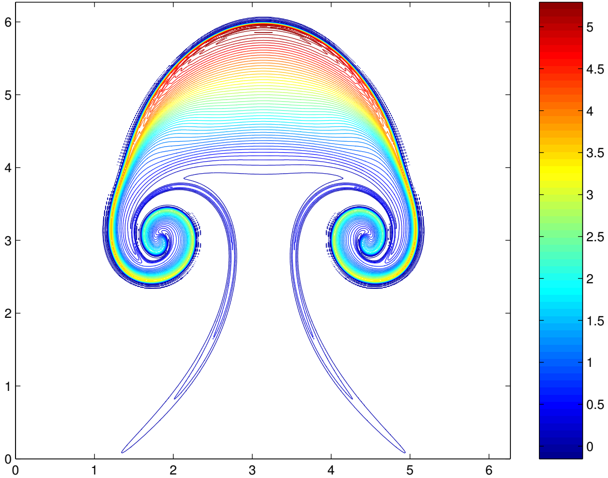

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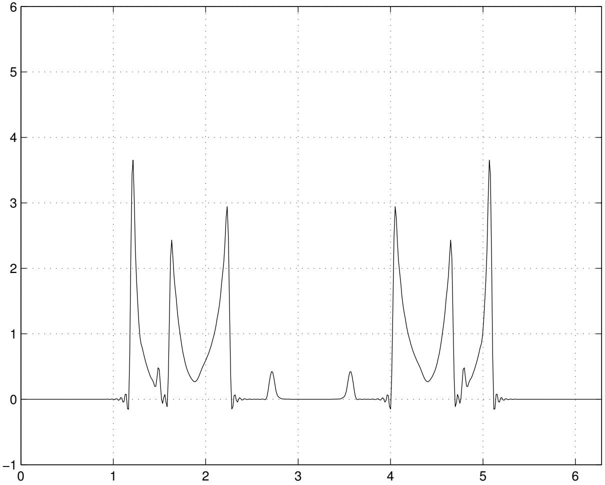

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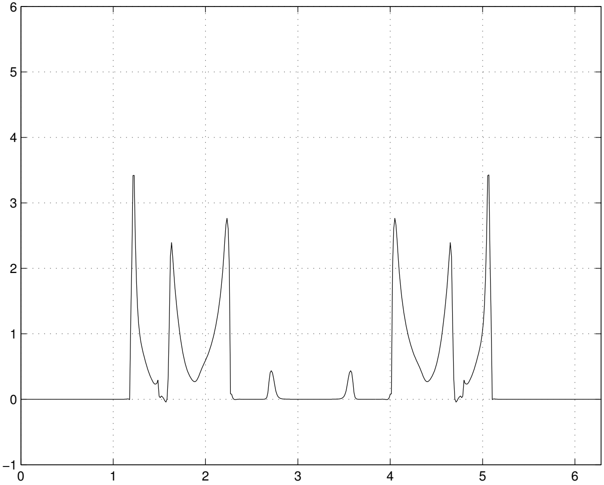

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Here what we want to use is an a priori knowledge of a reduced space X much smaller than $\mathcal{X}$ where the solution to (1) should be sought

We present here two classes of problems where this strategy can be used

- parameter dependent problems
- hierarchical geometry for the domain

in both cases the space X is conceived from the use of a more standard approximation methods you do not have to forget your favorite method... it is more the opposite in a first step

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Outline

1. Motivation
   - Framework of the approach
   - Parameter dependent problems
   - An example
   - Application to fluid flows

Parameter dependent problems.

Basics

Let us consider a class of problems depending on some parameters:

$$\mathcal{F}(u, \mu) = 0 \qquad (1')$$

and the parameter μ belongs to R^d (or some brick in R^d)

- This is the case for instance in a dimensional problem where some parameters have to be optimized for some purpose
- This can equally be the case for an inverse problem in parameter identification.
- The solution $u = u(\mu)$ of (1') is sought in some space $\mathcal{X}$ for any given parameter μ
- The dependancy in μ of the solution $u(\mu)$ is most often regular.

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- Define $X = \text{Span}\{u(\mu),\ \mu \in \mathcal{D}\}$ then looking for the solution in X instead of $\mathcal{X}$ (generally a Sobolev space) is already a valuable indication.....
- In order to apprehend in which sense the good behavior of X should be understood, it is helpfull to introduce the notion of n-width following Kolmogorov

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Parameter dependent problems.

The reduced basis space and approximation

Definition

Let $\mathcal{X}$ be a normed linear space, X be a subset of $\mathcal{X}$ and X_n be a generic n-dimensional subspace of $\mathcal{X}$. The deviation of X from X_n is

$$E(X; X_n) = \sup_{x \in X} \inf_{y \in X_n} \|x - y\|_{\mathcal{X}}.$$

The *Kolmogorov n-width* of A in X is given by

$$\begin{aligned} d_n(X, \mathcal{X}) &= \inf\{E(X; X_n) : X_n \text{ an } n\text{-dimensional subspace of X}\} \\ &= \inf_{X_n} \sup_{x \in X} \inf_{y \in X_n} \|x - y\|_{\mathcal{X}} \ . \end{aligned} \quad (1)$$

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The n-width of X thus measures the extent to which X may be approximated by a n-dimensional subspace of $\mathcal{X}$.

- Of course X is rarely known but $X_n = \text{Span}\{u(\mu_k),\ k = 1, ..., n\}$ where μ_k are properly chosen
- The solution to (1') for other values of μ is then approximated through a Galerkin process.
- The best fit approximation is often exponential in n and a random log repartition of the sample values μ_k is often better than other obvious choices.
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Application to a non affine elliptic problem

We are interested in solving

$$-\Delta u + \mu_1 \frac{e^{\mu_2 u} - 1}{\mu_2} = f$$

the results with the interpolation process are

N	4	8	12	16	20
$\varepsilon^u_{N,M,\max}$	6.53 E-03	1.05 E-03	7.34 E-05	1.30 E-05	5.05 E-06
$\eta^u_{N,M}$	1.94	2.16	2.33	2.36	1.21

Application to a non affine parabolic problem

We are interested in solving

$$\frac{\partial u}{\partial t} - \Delta u + \mu_1 \frac{e^{\mu_2 u} - 1}{\mu_2} = f$$

the reduced basis considers 3 parameters μ_1, μ_2, t... results are similar

N	1	5	10	20	30
$\varepsilon^u_{N,M,\max}$	3.82 E-01	1.36 E-02	1.62 E-03	1.46 E-04	1.88 E-05
$\eta^u_{N,M}$	79	25.9	8.65	8.25	3.82

Rapid evaluation of nonlinear contributions

Similarly as for the spectral method $u(\mu)$ approximated by a sum of $u(\mu_i)$:

e.g. $\exp(u)$

- we use the reduced basis $\exp(u(\mu_i))$, $\rightarrow W_N^{\exp}$
- we select the representative collocation points
- we represent $\exp(u(.,\mu))$ by its interpolation over $W_N^{\exp}$

i.e. let $u(.,\mu)$ be approximated by $\sum_j \alpha_j u(\mu_j)$, then $\exp(u(.,\mu))$ will be approximated by $\sum_j \beta_j \exp(u(\mu_j))$, where the β's are tuned so that

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Some first results in QC

$$u(\mu) = \text{Arg} \inf_{\int u^2 = 1} E(u, \mu)$$

where

$$E(u, \mu) = \frac{1}{2} \int_\Omega |\nabla u|^2 dxdy + \int_\Omega V(., \mu) u^2 dxdy + \int_\Omega \int_\Omega \frac{u^2(x) u^2(y)}{|x - y|} dxdy$$

With the potential

$$V(x, y, \mu) = \frac{\mu_2}{\sqrt{(x + \mu_1/2)^2 + y^2}} + \frac{\mu_2}{\sqrt{(x - \mu_1/2)^2 + y^2)}}$$

Some first results in QC

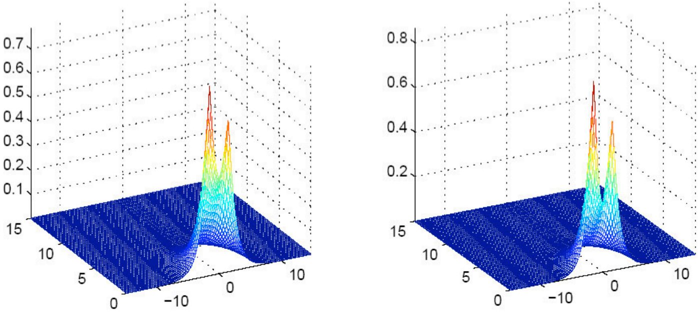

Figure: Different distances between the nuclei.

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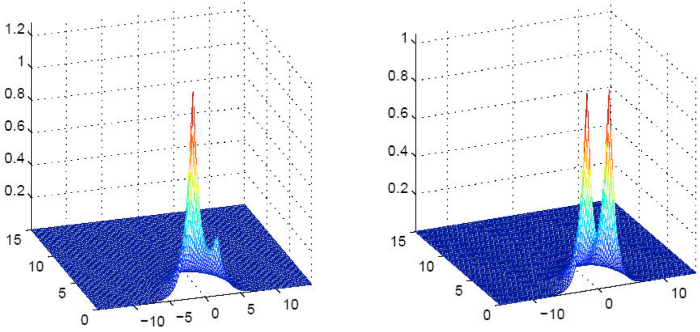

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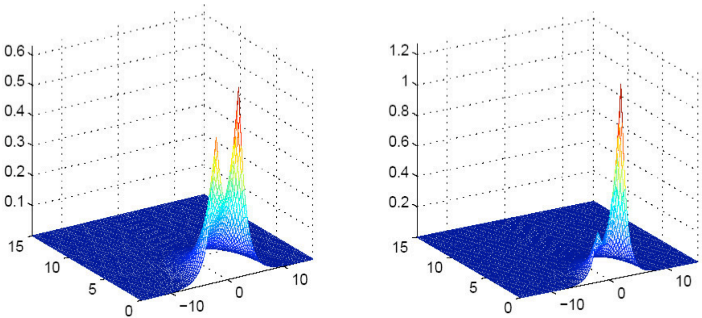

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Reduced Basis Formulation for Kohn Sham Equations

The ground state for the Kohn Sham model
$\hat{\mathbf{u}}_{\rm o}([Z,\mu^*]) \equiv (u_{{\rm o}\,1},\dots,u_{{\rm o}\,n_e})$,

$$\hat{\mathbf{u}}_{\rm o}([Z,\mu]) = \arg\inf_{\hat{\mathbf{w}}_{\rm o}} \Big\{ E_{\rm o}(\hat{\mathbf{w}}_{\rm o} \equiv (w_{{\rm o}\,1},\dots,w_{{\rm o}\,n_e});[Z,\mu]), w_{{\rm o},i} \in Y_{\rm o}, \quad (2)$$

$$\int_{\Omega_o(\mu)} w_{{\rm o}\,i} w_{{\rm o}\,j} = \delta_{ij}, 1 \le i,j \le n_e \Big\},$$

$$\mu^*(Z) = \arg\inf_{\mu} \{ \mathcal{E}_{\rm o}(\hat{\mathbf{u}}_{\rm o}([Z,\mu]);[Z,\mu]); \mu > 0 \}; \quad (3)$$

with $Y_{\rm o} \equiv H^1_{\rm per}(\Omega_{\rm o}(\mu))$

and the electronic energy $E_{\rm o}(\hat{\mathbf{w}}_{\rm o};[Z,\mu])$ is defined as

$$E_{\rm o}(\hat{\mathbf{w}}_{\rm o};[Z,\mu]) = C_w \sum_{i=1}^{n_e} \int_{\Omega_o(\mu)} (\nabla w_{{\rm o}\,i})^2 - \; Z \sum_{i=1}^{n_e} \int_{\Omega_o(\mu)} G_{\rm o}\; {w_{{\rm o}\,i}}^2$$
$$+ \frac{1}{2} C_c \int_{\Omega_o(\mu)} \int_{\Omega_o(\mu)} \left(\sum_{i=1}^{n_e} w^2_{{\rm o}\,i}(y_1) \right) \; G_{\rm o}(y_1 - y_2) \; \left(\sum_{j=1}^{n_e} w^2_{{\rm o}\,j}(y_2) \right) \; dy_1 \; d$$
$$- \; C_x \sum_{i=1}^{n_e} \int_{\Omega_o(\mu)} \left(\sum_{j=1}^{n_e} w^2_{{\rm o}\,j} \right)^{4/3} w^2_{{\rm o}\,i},$$

the periodic Green's function $G_{\rm o}(\cdot\,;\mu)\colon\; \Omega_{\rm o}(\mu) \rightarrow R$ satisfies $-\Delta G_{\rm o} = \left\{ \delta(y) - \frac{1}{|\Omega_{\rm o}(\mu)|} \right\}, \int_{\Omega_o(\mu)} G_{\rm o} = 0$, $|\Omega_{\rm o}(\mu)| = \mu$ is a nucleus geometric parameter.

Reduced Basis Formulation for Kohn Sham Equations

N^u	$\varepsilon^u_{N,M}$	$\varepsilon^{\mathcal{E}}_{N,M}$	$\varepsilon^{\phi}_{N,M}$	$\varepsilon^{\text{ortho}}_{N,M}$
5	7.9044 E−2	4.6557 E−04	1.4647 E+0	5.1756 E−14
6	4.5693 E−2	3.5279 E−05	1.2839 E−1	3.6342 E−3
7	2.1383 E−4	1.3947 E−09	1.0334 E−3	2.1783 E−5
8	9.8819 E−5	8.8168 E−10	3.7635 E−4	1.0686 E−5
9	9.7602 E−6	3.0509 E−10	3.8463 E−5	8.9840 E−7

Table: Variations of the reduced-basis errors $\varepsilon^u_{N,M}$, $\varepsilon^{\mathcal{E}}_{N,M}$, $\varepsilon^{\phi}_{N,M}$ and $\varepsilon^{\text{ortho}}_{N,M}$ with N^u. Here, $n_e = 5$ and $1.5 \leq \mu \leq 5.5$.

Reduced Basis Formulation for Kohn Sham Equations

~~here it is not only~~ but

$$\forall n \le n_e, \quad u_n(\mu) \simeq \sum_{i=1}^{N} \alpha_i u_n(\mu_i)$$

with α_i independant of n

so that the complexity scales with N and not with $n_e \times N$

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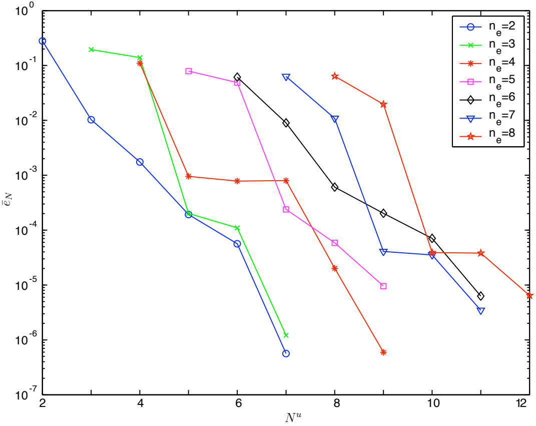

Figure: Convergence of reduced basis error in the vectorial case for $2 \leq n_e \leq 8$.

Reduced element method

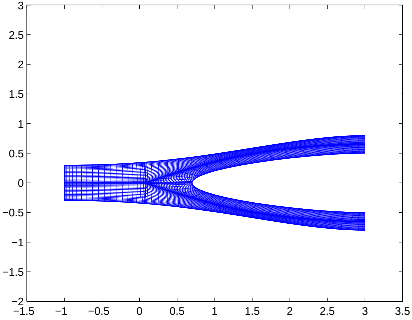

Figure: A first geometry.

Reduced element method

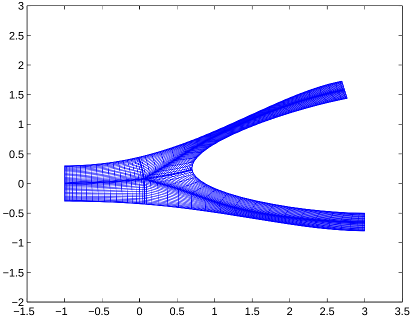

Figure: A second geometry.

Reduced element method

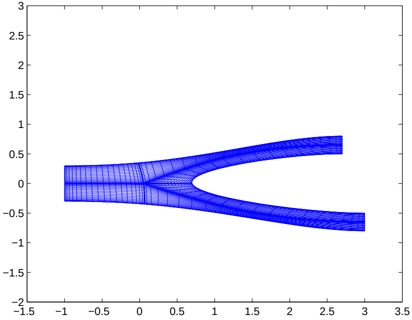

Figure: A third geometry.

Reduced element method

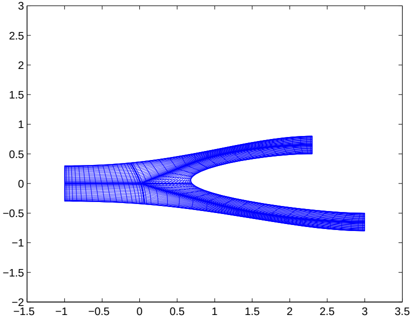

Figure: A fourth geometry.

Reduced element method

As a precomputation, the problem of interest is solved over various deformations of each reference building block and stored, after mapping, on the reference building block.

This gives basis functions $\hat{\zeta}_1, \hat{\zeta}_2, ..., \hat{\zeta}_N$, supposed to be linearly independent

These basics solutions are mapped over each Ω_k^{bb} through φ_k.

The solution corresponding to an unknown, deformed geometry is then represented as a linear combination of these mapped solutions

$$Y_N = \{v_N \in L^2(\Omega) | \quad v_{N|\Omega_k^{bb}} \circ \varphi_k \in \text{span}\{\hat{\zeta}_1, \hat{\zeta}_2, ..., \hat{\zeta}_N\}\} .$$

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Reduced element method

We now define X_N to this purpose by *gluing* the functions of Y_N across the interfaces $\gamma_{k,\ell}^{bb}$ between two stages

$\longrightarrow$ Lagrange multipliers

$$X_N = \{v \in Y_N^1, \quad \forall k,\ell, \quad \forall \psi \in W_{k,\ell}, \int_{\Gamma_{k,\ell}^e} (v^+ - v^-)\psi \, ds \ = \ 0\},$$

where $W_{k,\ell}$ is some well chosen space over $\Gamma_{k,\ell}^e \rightarrow$ nonconforming approximation.

The discrete problem then reads : Find u_N in X_N such that

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Outline

1. Motivation
   - Framework of the approach
   - Parameter dependent problems
   - An example
   - Application to fluid flows

Fluid flows

For flow problems the tranformations between the reference domain and the subdomains are more involved: The PIOLA Transform that allow the work with divergence free discrete spaces

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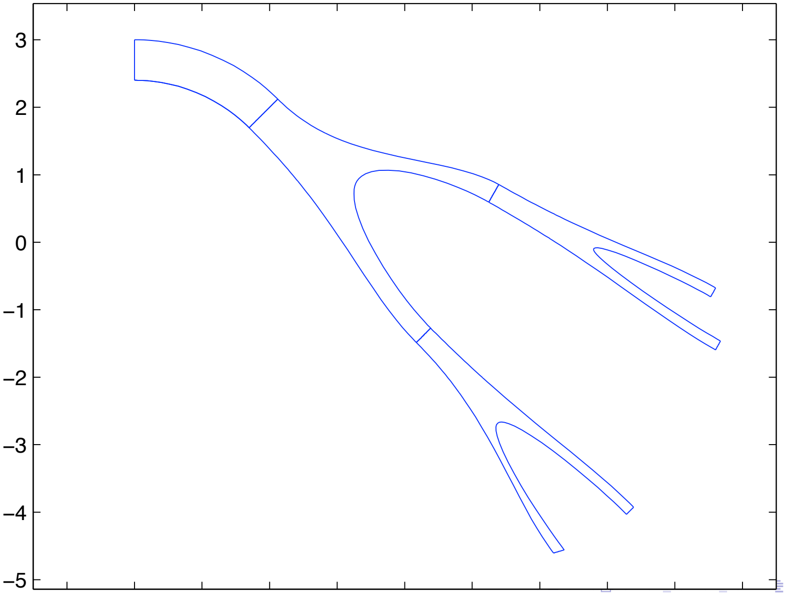

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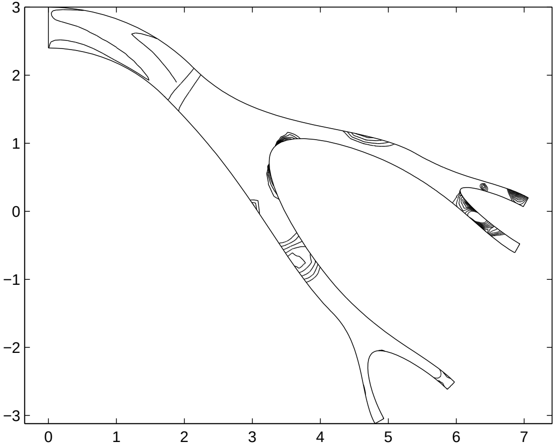


Figure: Error distribution for a new configuration $N_P = 15$, $N_B = 15$ error plot for the pressure max $=3.10^{-2}$, for the velocity error $\simeq 3.10^{-3}$.

Fluid flows

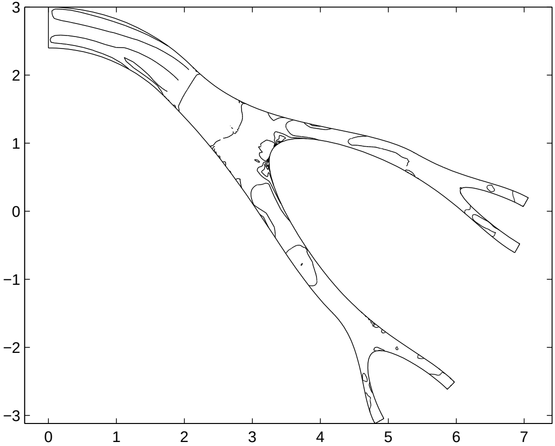


Figure: Error distribution for a new configuration $N_P = 15$, $N_B = 30$ error plot for the pressure max=6.10^{-3}, for the velocity error $\simeq 4.10^{-4}$, size problem

Fluid flows

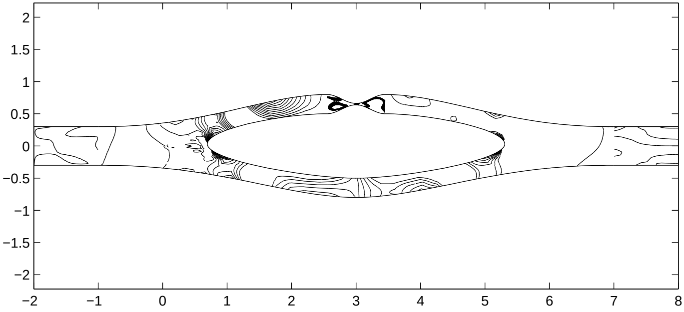
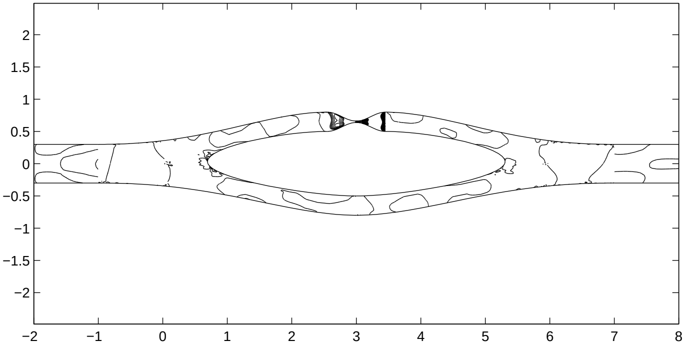


Figure: A stenosis problem with $N_P = 15$, $N_B = 15$.

Fluid flows



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Fluid flows

N	N_1	N_2	$\lvert u_N - u \rvert_{H^1}$	$\lvert\lvert p_N - p \rvert\rvert_{L^2}$
45	9	9	$9.3 \cdot 10^{-3}$	$3.3 \cdot 10$
55	11	11	$3.1 \cdot 10^{-3}$	$5.3 \cdot 10^{-1}$
65	13	13	$2.3 \cdot 10^{-3}$	$9.0 \cdot 10^{-2}$
75	15	15	$1.4 \cdot 10^{-3}$	$5.3 \cdot 10^{-2}$
105	15	30	$5.4 \cdot 10^{-4}$	$3.0 \cdot 10^{-2}$

Table: Steady Stokes solution on a multi-block bypass with three pipe blocks and two bifurcation blocks. Here, $N = 3N_1 + 2N_2$.

Important remarks....

- Note that contrarily to what happens in the parameter dependant problem
- The full problem over the global geometry is never constructed in the reduced element method
- This is a major achievement

- Note also that, more generally, the reduced basis functions have to be suitably prepared

- Finally, do not forget that off-line pre-computations have to be done, involving your favorit approximation method, and that the approach is rapid for online computations.

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