A fictitious domain-like spectral method for complex geometries

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Introduction

- Motivations
  - Fictitious Domain-like methods allow to avoid the complex task of generating meshes.
  - Fictitious Domain-like methods have the reputation to be low order of accuracy (see V. Girault-R. Glowinski for instance).
  - We had an experience of Fictitious Domain-like method coded in `FreeFEM3D` using FEM.
- Question
  - What about high-order and Fictitious Domain-like methods? Can accuracy be kept?

Outline

1. Description of the method
   - Spectral methods in tensorial domains
   - A fictitious domain-like method in complex geometries
   - *A priori* estimates
2. Numerical simulations
   - Implementation in `FreeFEM3D`
   - Tensorial domains
   - Non-tensorial domains
3. Improving the method efficiency?
4. Conclusions and perspectives

Outline

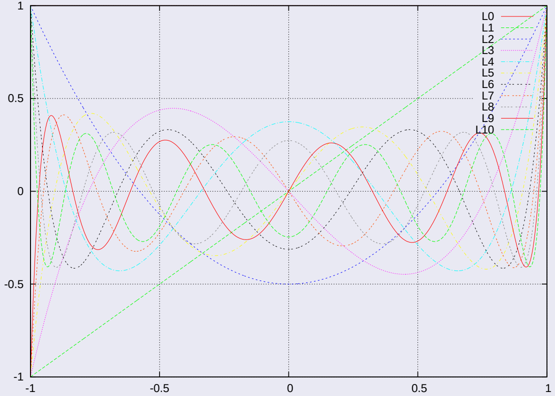
Spectral Methods

- Introduced by Gottlieb-Orszag in the seventies
- The solution is approximated by high-order polynomials
- Approximation space is span by a tensorial basis of **orthogonal** polynomials (Legendre polynomials are $L^2(]-1,1[)$-orthogonal)
- We focus on the **Galerkin** spectral method with numerical quadrature (integration points being **Gauss-Lobatto**'s). *i.e.*:
  Find $u^{\mathbf{N}} \in \mathbb{P}^{\mathbf{N}}$, **s.t.** $\forall v \in \mathbb{P}^{\mathbf{N}},\ a(u^{\mathbf{N}}, v) = \ell(v)$,
  where $\mathbb{P}^{\mathbf{N}} = \mathbb{P}_{N_x} \otimes \mathbb{P}_{N_y} \otimes \mathbb{P}_{N_z}$, so $u^{\mathbf{N}} = \sum_{i,j,k=0}^{N_x,N_y,N_z} u_{ijk} L_i(x) L_j(y) L_k(z)$.
  For the sake of simplicity in the following, we will take $N_x = N_y = N_z = N$, so $\mathbf{N} = (N, N, N)$.
- Comments on the arising linear system:
  - Obtained matrices are not sparse.
  - Assembling the matrix costs $O(N^{3d})$ operations! It is prohibitive.
  - However, the tensorial structure of the discretization allows to compute efficiently the matrix-vector product ($\Longrightarrow$ use of iterative methods)

Legendre Polynomials

Definition (the Legendre Family $(L_n)_{n\geq 0}$)

$(L_n)_{n\geq 0}$ on $]-1,1[$ is the set of polynomials, two by two orthogonal in $L^2(]-1,1[)$, s.t. $\forall n \in \mathbb{N}$, the polynomial L_n is of degree n and satisfies $L_n(1) = 1$.



A priori Estimates 1/3

Theorem (Polynomial approximation errors)

$\forall m \in \mathbb{N}^*$, $\exists c(m, D) \in \mathbb{R}^*$ *s.t.*, $\forall \varphi \in H^m(D)$,

$$||\varphi - \Pi_{\mathbf{N}}^{D}\varphi||_{L^2(D)} \leq cN^{-m}||\varphi||_{H^m(D)},$$

$$||\varphi - \Pi_{\mathbf{N}}^{1,D}\varphi||_{L^2(D)} \leq cN^{-m}||\varphi||_{H^m(D)},$$

and

$$|\varphi - \Pi_{\mathbf{N}}^{1,D}\varphi|_{H^1(D)} \leq cN^{1-m}||\varphi||_{H^m(D)},$$

where $\Pi_{\mathbf{N}}^{D}$ *is the* L^2*-orthogonal-projection operator on* $\mathbb{P}^{\mathbf{N}}$: $\forall \varphi \in L^2(D)$, $\Pi_{\mathbf{N}}^{D}\varphi$ *is*

$$\forall \psi \in \mathbb{P}^{\mathbf{N}}, \quad \int_D \Pi_{\mathbf{N}}^{D}\varphi\,\psi = \int_D \varphi\,\psi$$

and $\Pi_{\mathbf{N}}^{1,D}$ *is the* H^1*-orthogonal-projection operator on* $\mathbb{P}^{\mathbf{N}}$: $\forall \varphi \in H^1(D)$, $\Pi_{\mathbf{N}}^{1,D}\varphi$ *is*

$$\forall \psi \in \mathbb{P}^{\mathbf{N}}, \quad \int_D \Pi_{\mathbf{N}}^{1,D}\varphi\,\psi + \int_D \nabla\Pi_{\mathbf{N}}^{1,D}\varphi \cdot \nabla\psi = \int_D \varphi\,\psi + \int_D \nabla\varphi \cdot \nabla\psi.$$

A priori Estimates 2/3

Natural boundary conditions

Let D be a rectangular domain of $\mathbb{R}^d$.
Let $a(\cdot,\cdot)$ and $l(\cdot)$ be two forms respectively bilinear and linear over $H^1(D)$, a being moreover coercive. Find u in $H^1(D)$ s.t.

$$\forall v \in H^1(D), \qquad a(u,v) = l(v).$$

Let $u^{\mathbf{N}}$ be the solution of the approximate problem:
Find u^N in $\mathbb{P}^{\mathbf{N}}$ s.t.

$$\forall v \in \mathbb{P}^{\mathbf{N}}, \qquad a(u^{\mathbf{N}},v) = l(v).$$

Assuming that $u \in H^m(D)$, there exists a constant c that only depends on D and m such that

- $\|u - u^{\mathbf{N}}\|_{1,D} \leq cN^{m-1}\,\|u\|_{m,D}$,
- $\|u - u^{\mathbf{N}}\|_{0,D} \leq cN^{m}\,\|u\|_{m,D}$.

A priori Estimates 3/3

Dirichlet problem

Let D be a rectangular domain of $\mathbb{R}^d$.
Let $a(\cdot,\cdot)$ and $l(\cdot)$ be two forms respectively bilinear and linear over $H_0^1(D)$, a being moreover coercive. Find u in $H_0^1(D)$ s.t.

$$\forall v \in H_0^1(D), \qquad a(u,v) = l(v).$$

Let $u^{\mathbf{N}}$ be the solution of the approximate problem:
Find u^N in $\mathbb{P}^{\mathbf{N}}$ s.t.

$$\forall v \in \mathbb{P}^{\mathbf{N}}, \qquad a(u^{\mathbf{N}},v) = l(v).$$

Assuming that $u \in H^m(D)$, there exists a constant c that only depends on D and m such that

- $\|u - u^{\mathbf{N}}\|_{1,D} \leq cN^{m-1}\,\|f\|_{m-2,D}$,
- $\|u - u^{\mathbf{N}}\|_{0,D} \leq cN^{m}\,\|f\|_{m-2,D}$,

where $\forall v \in H_0^1(D), \quad l(v) = <f, v>_{H^{-1}(D),H_0^1(D)}$.

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Few examples of spectral methods for complex geometries

- Using domain decomposition: Spectral elements (BERNARDI-MADAY,...).
- Using iso-parametric elements:
  - GORDON-HALL transformations,
  - spectral method applications: MADAY-RØNQUIST,
- These techniques can be mixed (see the book from CANUTO-HUSSAINI-QUARTERONI-ZANG).

A fictitious domain-like spectral method

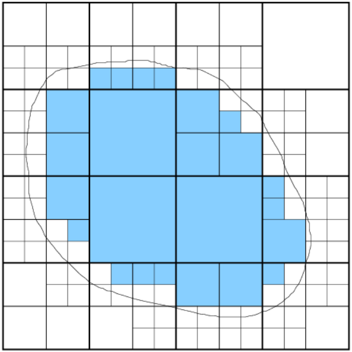
Discrete Space

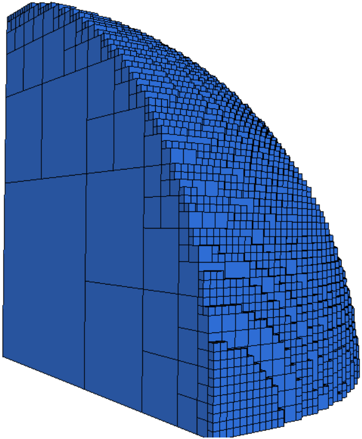
$\mathbb{P}^{\mathbf{N}} = \mathbb{P}_{N_x} \otimes \mathbb{P}_{N_y} \otimes \mathbb{P}_{N_z}$: the set of polynomial of degree $\leq N_{x,y,z}$ in each direction.
Again, we take $N_x = N_y = N_z = N$

The method relies on to main ideas

- Dirichlet boundary conditions are treated by penalty (**Nitsche**'s method): $u = g$ on $\partial\Omega$ is replaced by $\frac{1}{\varepsilon}u + \frac{\partial u}{\partial n} = \frac{1}{\varepsilon}g$ on $\partial\Omega$.
- Geometry is approximated the following way:
  - $\Omega = \cup_{i=0}^{+\infty} D_i$ where D_i are non overlapping rectangular sets.
  - We just use $\Omega_m = \cup_{i=0}^{m} D_i$ build using an octree for instance.
- Beware
  - cost is related to m.
  - loss of orthogonality of the tensorial Legendre basis in Ω_m (condition number is affected **a lot**).

Ω_m Examples





Evaluation of integrals

Volume integrals

Example: solving $\int_\Omega \nabla u \cdot \nabla v = \int_\Omega fv$

$\Longrightarrow$ to evaluate $\int_{D_i} \nabla u \cdot \nabla v = \int_{D_i} fv$, $0 \leq i \leq m$, with the **Gauss-Lobatto-Legendre** formula.

Surface integrals

Method: build a triangular mesh $(T_i)_i$ of $\partial\Omega$ then approximate $\int_{T_i} f$ using a Gauss-like quadrature formula.

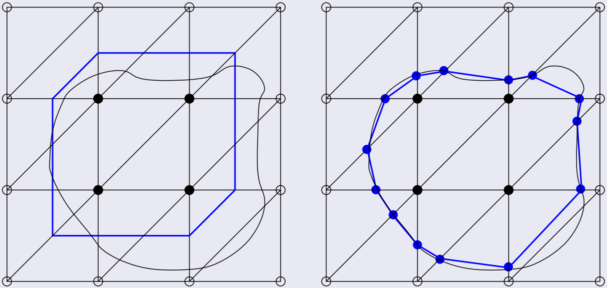
Building surface mesh

An "easy" task...

- Knowing the characteristic function $\mathbf{1}_\Omega$ of the set Ω building a triangular mesh of $\partial\Omega$ is not a big task.
- Moreover it is already coded in `FreeFEM3D`

Technique

- create a tetrahedral structured mesh that contains Ω
- use a slightly improved Marching Tetrahedra algorithm



Summary: an example

Model problem

Find $u \in H_0^1(\Omega)$, **s.t.** $\forall v \in H_0^1(\Omega)$, $\int_\Omega \nabla u \cdot \nabla v = \int_\Omega fv$,
where Ω is a bounded and connected open set of $\mathbb{R}^3$ and $f \in L^2(\Omega)$.

Methodology

- Choose a rectangular domain $D \supset \Omega$ (to build the Legendre basis).
- Penalty: find $u^\epsilon \in H^1(\Omega)$, **s.t.** $\forall v \in H^1(\Omega)$, $\frac{1}{\epsilon}\int_{\partial\Omega} u^\epsilon v + \int_\Omega \nabla u^\epsilon \cdot \nabla v = \int_\Omega fv$.
- Choose N_x, N_y, and $N_z \in \mathbb{N}$ in order to define $\mathbb{P}^{\mathbf{N}} = \mathbb{P}_x^{N_x} \otimes \mathbb{P}_y^{N_y} \otimes \mathbb{P}_z^{N_z}$.
- Build $\Omega_m \approx \Omega$ (e.g. using Octree) and $\Gamma_h \approx \partial\Omega$ (e.g. Marching Tetrahedra).
- Solve $u^{\mathbf{N}} \in \mathbb{P}^{\mathbf{N}}$, **s.t.** $\forall v \in \mathbb{P}^{\mathbf{N}}$, $\frac{1}{\epsilon}\int_{\Gamma_h} u^{\mathbf{N}} v + \int_{\Omega_m} \nabla u^{\mathbf{N}} \cdot \nabla v = \int_{\Omega_m} fv$

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Linear extension

Theorem (Linear extension)

Let $m \in \mathbb{N}^*$. Let Ω be a bounded and connected open set of $\mathbb{R}^d$ with a smooth boundary $\partial\Omega$ of $C^{m-1,1}$ regularity. We fix an open set D such that $D \supset \bar{\Omega}$. There exists a continuous linear extension operator E from $H^m(\Omega)$ to $H_0^m(D)$ such that

$$\left.\begin{array}{l} Ev|_\Omega = v, \text{ and} \\ \|Ev\|_{H^m(D)} \leq c\|v\|_{H^m(\Omega)}, \end{array}\right. \quad \forall v \in H^1(\Omega)$$

where c only depends on the domains Ω, D and on m.

This theorem can be found in **Guilbarg-Trudinger**.

Projection error

Theorem (Projection)

Let Ω bounded and connected open set of $\mathbb{R}^d$, s.t. $\partial\Omega$ is of class $C^{m-1,1}$, and let $u \in H^m(\Omega)$, then there exists a constant $c(\Omega, m) > 0$, s.t.

$$||u - \Pi_{\mathbf{N}}^{\Omega} u||_{L^2(\Omega)} \leq cN^{-m} ||u||_{H^m(\Omega)}, \quad \text{and} \tag{1}$$

$$||u - \Pi_{\mathbf{N}}^{1,\Omega} u||_{H^1(\Omega)} \leq cN^{1-m} ||u||_{H^m(\Omega)}. \tag{2}$$

The proof is based on

- the linear extension theorem, **Guilbarg-Trudinger**,
- the estimates of polynomial approximation in a tensorial domain, **Bernardi-Maday**

Natural boundary conditions

Consider the following variational problem: $\forall v \in H^1(\Omega)$,

$$a(u,v) = \int_\Omega a_0\, uv + \sum_{i,j=1}^{d} \int_\Omega a_{ij} \frac{\partial u}{\partial x_i} \frac{\partial v}{\partial x_j} + \int_{\partial\Omega} b_0\, uv,$$

$$\ell(v) = \int_\Omega fv + \int_{\partial\Omega} gv.$$

Let the approximate problem: find $u^{\mathbf{N}} \in \mathbb{P}^{\mathbf{N}}$ s.t. $\forall v \in \mathbb{P}^{\mathbf{N}}, \quad a(u^{\mathbf{N}}, v) = \ell(v)$.

Theorem

Le Ω be a bounded and connected open set of $\mathbb{R}^d$, such that $\partial\Omega$ is of regularity $C^{m-1,1}$. If $u \in H^m(\Omega)$, there exists a constant $c(\Omega, m, a) \in \mathbb{R}^{+*}$, such that

$$||u - u^{\mathbf{N}}||_{H^1(\Omega)} \leq cN^{1-m}||u||_{H^m(\Omega)}.$$

$$||u - u^{\mathbf{N}}||_{L^2(\Omega)} \leq cN^{-m}||u||_{H^m(\Omega)}.$$

The proof is based on

- le projection theorem (non tensorial case),
- **Céa**'s Lemma
- **Aubin-Nitsche**'s duality argument (for the L^2 error).

Theorem (convergence)

Let H be an Hilbert space endowed with the scalar product $(\cdot,\cdot)$ and $\|\cdot\|$ the associated norm. Let a and b two bilinear, continuous and positive forms such that:

- $\ker a$ *is a finite dimension space,*
- $\exists c > 0$ *such that* $a(v,v) > c\|v\|^2, \forall v \in (\ker a)^{\perp}$, *and*
- $\ker a \cap \ker b = \{0\}$.

Let $\varepsilon > 0$, *and let us define the bilinear form* $a_\varepsilon = a + \frac{1}{\varepsilon} b$.
Let now $f \in H'$ *and let* $H_0 = \ker b$. *We define the following problems*

$$\text{find } u \in H_0 \quad \text{s.t.} \quad \forall v \in H_0, \quad a(u,v) = < f, v >_{H',H}, \tag{3}$$

$$\text{find } u_\varepsilon \in H \quad \text{s.t.} \quad \forall v \in H, \quad a(u_\varepsilon,v) + \frac{1}{\varepsilon} b(u_\varepsilon,v) = < f, v >_{H',H} . \tag{4}$$

Then the two problems are well posed and the sequence $(u_\varepsilon)_\varepsilon$ *converges strongly to* u *in* H *when* ε *goes to 0.*

Many proves can be found see for instance **Aubin, Lions, Maury, etc...**

Consider the following problems
find $u \in H_0^1(\Omega)$ s.t. $\forall v \in H_0^1(\Omega), \quad a(u,v) = \ell(v)$, and
find $u_\varepsilon \in H^1(\Omega)$ such that $\forall v \in H^1(\Omega), a(u_\varepsilon, v) + \frac{1}{\varepsilon}\int_{\partial\Omega} u_\varepsilon v = \ell(v)$.

Theorem (Nitsche,Babuška)

One has the following estimates

$$||u_\varepsilon - u||_{H^1(\Omega)} \leq c\sqrt{\varepsilon}\left|\left|\frac{\partial u}{\partial n}\right|\right|_{L^2(\partial\Omega)}, \quad ||u_\varepsilon - u||_{L^2(\partial\Omega)} \leq \varepsilon\left|\left|\frac{\partial u}{\partial n}\right|\right|_{L^2(\partial\Omega)},$$

et $$||u_\varepsilon - u||_{L^2(\Omega)} \leq c\varepsilon\left|\left|\frac{\partial u}{\partial n}\right|\right|_{L^2(\partial\Omega)}.$$

The proof relies on the

- $u_\varepsilon \longrightarrow u$, in $H^1(\Omega)$ *strong* **(Aubin, Lions, Maury, etc...)**,
- computing $\int_\Omega \nabla(u - u_\varepsilon)\cdot\nabla v + \frac{1}{\varepsilon}\int_{\partial\Omega}(u-u_\varepsilon)v = \int_\Omega fv + \int_{\partial\Omega}\frac{\partial u}{\partial n}v$,
- **Aubin-Nitsche**'s duality argument, for the L^2-error.

A priori error estimate

Let us define the following problems:

$$\text{Find } u \in H_0^1, \qquad \text{s.t.} \qquad \forall v \in H_0^1(\Omega), a(u,v) = l(v), \tag{5}$$

$$\text{Find } u_\varepsilon^{\mathbf{N}} \in \mathbb{P}^{\mathbf{N}}, \qquad \text{s.t.} \qquad \forall v \in \mathbb{P}^{\mathbf{N}}, a(u_\varepsilon^{\mathbf{N}}, v) + \frac{1}{\varepsilon}\int_{\partial\Omega} u_\varepsilon^{\mathbf{N}} v = l(v). \tag{6}$$

Theorem

Let Ω be a bounded connected open set of $\mathbb{R}^d$, whose boundary $\partial\Omega$ has $C^{m-1,1}$ regularity. If $u \in H^m(\Omega)$, there exists $c(\Omega, m) > 0$, such that

$$||u - u_\varepsilon^{\mathbf{N}}||_{H^1(\Omega)} \leq c\left(N^{1-m}||f||_{H^{m-2}(\Omega)} + \sqrt{\varepsilon}\left|\left|\frac{\partial u}{\partial n}\right|\right|_{L^2(\partial\Omega)}\right),$$

$$||u - u_\varepsilon^{\mathbf{N}}||_0 \leq c\left(N^{-m}||f||_{H^{m-2}(\Omega)} + \varepsilon\left|\left|\frac{\partial u}{\partial n}\right|\right|_{L^2(\partial\Omega)}\right).$$

where $\forall v \in H_0^1(D), \quad l(v) =< f, v >_{H^{-1}(D), H_0^1(D)}$.

- $||u - u_\varepsilon^{\mathbf{N}}||_{H^1, L^2} \leq ||u_\varepsilon^{\mathbf{N}} - u_\varepsilon||_{H^1, L^2} + ||u_\varepsilon - u||_{H^1, L^2}$,
- $u \in H^m \implies u_\varepsilon \in H^m$, and $||u_\varepsilon^{\mathbf{N}} - u_\varepsilon||_{H^1, L^2} \leq cN^{\sigma - m}||u_\varepsilon||_{H^m}, \quad \sigma \in \{0, 1\}$,
- $||u_\varepsilon - u||_{H^1, L^2} \leq c_1\varepsilon^{1-\gamma}||u_\varepsilon||_{H^m}, \quad \gamma = 0, \frac{1}{2}$.

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Implementation

FreeFEM3D

- **C++** code of `freefem`'s family
  - 3D Finite element solver (scalar and vectorial problems)
  - driven by a user-friendly language close to the mathematics
  - write weak or strong formulation of the PDE problem
- Geometry
  - unstructured: mesh is provided by the user
  - fictitious domain approach (penalty for Dirichlet): use of CSG for description

Objectives

- integrate spectral method to `FreeFEM3D`:
  - passing from **FEM** to **Spectrale** transparent for the user
  - allow mixing of **FEM** and **Spectral** for a given computation
- Solving in tensorial and non-tensorial domains
- $\mathbb{P}_n - \mathbb{P}_k$

Outline

Solve $-\Delta u = 1$ with $u = 0$ on the boundary.
Boundary condition is approached by: $\frac{1}{\epsilon} u + \nabla u \cdot \mathbf{n} = 0$.

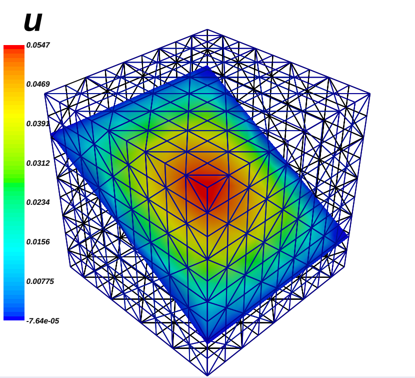
Finite Element Method

```
vector a=(0,0,0); vector b=(1,1,1);
vector n=(10,10,10);
mesh m=tetrahedrize(structured(n,a,b));

femfunction u(m)=0;
solve(u) in m
{
  test(v)
    int[0,1,2,3,4,5](1E3*u*v)
    + int(grad(u)*grad(v))
    = int(v);
}

save(vtk,"u",u,m);
```

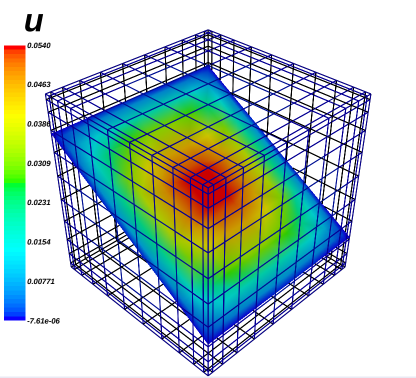
Spectral Method

```
vector a=(0,0,0); vector b=(1,1,1);
vector n=(10,10,10);
mesh m=spectral(n,a,b);

sfunction u(m)=0;
solve(u) in m
{
  test(v)
    int[0,1,2,3,4,5](1E3*u*v)
    + int(grad(u)*grad(v))
    = int(v);
}

save(vtk,"u",u,m);
```

Finite Element Method



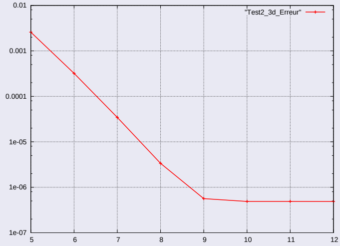
Spectral Method



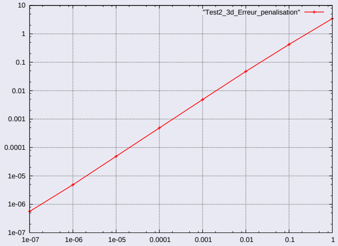
Convergence to the analytical solution of a vectorial problem of the form:

$$-\Delta \mathbf{u} = \mathbf{f}, \text{ dans } \Omega$$
$$\mathbf{u} = \mathbf{g} \text{ sur } \partial\Omega.$$

$N \in \{5, ..., 12\}$ $\varepsilon = 10^{-7}$



$N = 15$ $\varepsilon \in [10^{-7}, 1]$



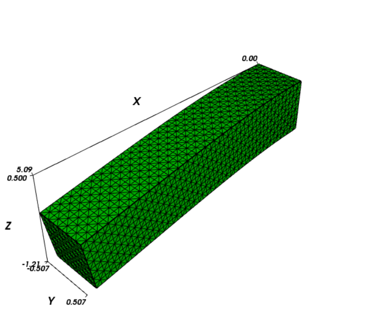
Linear elasticity

Solve the displacement

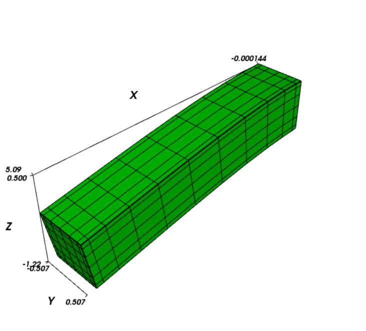
$$\int_\Omega \mu \sum_{ij} \partial_{x_i}\mathbf{u}_j \partial_{x_i}\mathbf{v}_j + \int_\Omega \mu \sum_{ij} \partial_{x_i}\mathbf{u}_j \partial_{x_j}\mathbf{v}_i + \int_\Omega \lambda \sum_{ij} \partial_{x_i}\mathbf{u}_i \partial_{x_j}\mathbf{v}_j = \int_\Omega \mathbf{f}\cdot\mathbf{v},$$

$\Omega =]0,5[\times] -\frac{1}{2},\frac{1}{2}[\times] -\frac{1}{2},\frac{1}{2}[$, $\mu = 500$, $\lambda = 1000$ and $\mathbf{f} = (0,0,-1)$

FEM $50 \times 10 \times 10$



Spectral Method $10 \times 5 \times 5$

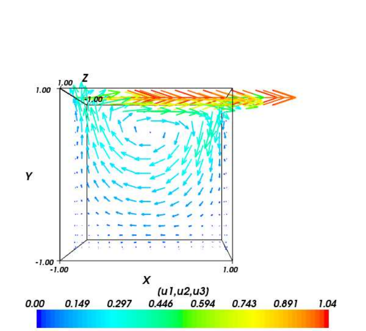


Stokes

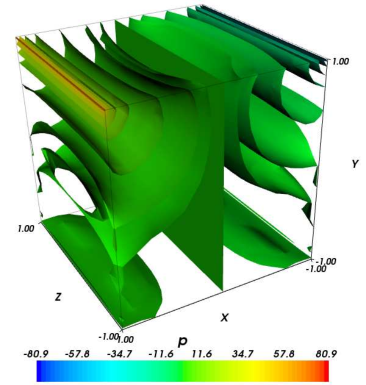
$$-\Delta\, \mathbf{u} + \mathbf{grad}\, p = \mathbf{0}, \quad \text{in } \Omega$$
$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega,$$

Discretization and penalty parameters: $N = 15$, $\varepsilon = 10^{-5}$.

Velocity



Pressure



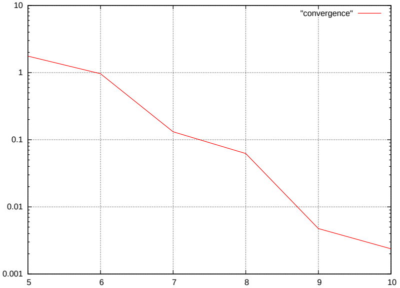
Outline

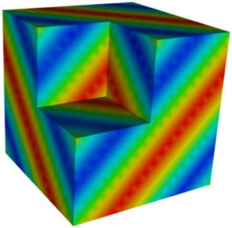
Poisson problem

We consider

$$-\Delta u = 3\pi^2 \sin(\pi(x+y+z)) \quad \text{in} \quad \Omega = \Omega_1 \cup \Omega_2 \cup \Omega_3 \qquad \text{and}$$
$$u = \sin(\pi(x+y+z)) \quad \text{on} \quad \partial\Omega,$$

$\Omega_1 =]-1,0[\times]-1,1[\times]-1,1[$, $\Omega_2 =]0,1[\times]-1,0[\times]-1,1[$,
and $\Omega_3 =]0,1[\times]0,1[\times]-1,0[$.





Preconditioning

- We tried **lots** of strategies to improve the condition number.
- Up to now all failed for various reasons.
- Since the matrix has a **really very bad** condition number a strategy is to change the matrix !
- For instance, use the following iterative procedure:

$$a_D(u^{n+1}, v) = l(v) + a_{D\setminus\Omega}(u^n, v).$$

If it converges, it will converge to the solution of the proposed method. And it converges! See **Bui-Frey-Maury**.

Preconditioning

- We tried **lots** of strategies to improve the condition number.
- Up to now all failed for various reasons.
- Since the matrix has a **really very bad** condition number a strategy is to change the matrix !
- For instance, use the following iterative procedure:

$$a_D(u^{n+1}, v) = l(v) + a_{D\setminus\Omega}(u^n, v).$$

If it converges, it will converge to the solution of the proposed method.
And it converges! See **Bui-Frey-Maury**.

Conclusions and perspective

Conclusions

- 3D-Code **tensorial/ non-tensorial** (Legendre) **integrated** to `FreeFEM3D`
- Implementation goals achieved:
  - Scalar or vectorial problems, $\mathbb{P}_n - \mathbb{P}_k$, elliptic
  - Easy to use, coupling with **FEM** possible,...
- New spectral method in non-tensorial domains
  - Numerical analysis of the method
  - cost and convergence problem
    - Decomposition of $\Omega \implies$ cost
    - loss of orthogonality $\implies$ very bad condition number

Perspectives

- **Numerical analysis:** take into account quadrature error (surface,volume)
- try various techniques to improve convergence (iterative, preconditioning,...)
- reduce cost of the method: aggregation of boxes, reduce the order of the quadrature formulae