

Master Vietnam-France in HCMC

High Performance computing

TP 1 : You can't Always Hear the Shape of a Drum. Multigrid algorithm



FIGURE 1 – Cocotte (left) and arrow (right)

<http://www.ams.org/samplings/feature-column/fcarc-199706>

This question has a mathematical counterpart that we are going to investigate. It is based on the problem defined in a domain $D \subset \mathbb{R}^2$,

$$\begin{cases} \partial_{tt}u - \Delta u = 0 & \text{in } D \times (0, +\infty) \\ u = 0 & \text{on } \partial D \times (0, +\infty) \\ u = u_0 & \text{on } D \times (0) \\ \partial_t u = u_1 & \text{on } D \times (0) \end{cases} \quad (1)$$

We suppose the initial conditions to be smooth enough ($u_0 \in H_0^1(D) \cap H^2(D)$, $u_1 \in H^1(D)$) so that the theory ensures a unique solution in $C([0, \infty[; H_0^1(D) \cap H^2(D)) \cap C^1([0, \infty[; H_0^1(D)) \cap C^2([0, \infty[; L^2(D))$. We suppose the initial conditions to be smooth enough ($u_0 \in H_0^1(D) \cap H^2(D)$, $u_1 \in H^1(D)$) so that the theory ensures a unique solution in $C([0; 1[; H_0^1(D) \cap H^2(D)) \cap C^1([0; 1[; H_0^1(D)) \cap C^2([0; 1[; L^2(D))$.

1 Radial solutions

We suppose that the membrane is exactly the disc of center O and radius 1.

1. 1. Prove that if the initial data are radial, the solution is radial as well.
1. 2. Using the formula for the laplacian in polar coordinates, find the equation (*) that $v(r, t) = u(x, t)$ satisfies on $(0, 1) \times (0, +\infty)$.

2 Solution of the radial equation by finite differences

1. Write an explicit finite differences scheme to solve (*) with initial data $u_0 = 0$ and $u_1(x; y) = -((\sinh \sqrt{x^2 + y^2})^2 - 1)^2$. Test the stability and the precision of the scheme.
2. Write an implicit finite difference scheme for the same problem. Same questions. Compare with the explicit scheme

3 Solution of the 2 – D problem by finite elements

1. Write the variational formulation and discretize in space-time with a θ -scheme and P_1 finite elements. Use the matlab script delivered. Analyze the stability and the precision with respect to θ , h and dt .
2. Mass lumping. Is there a stage where the system becomes so large that the solution comes too slowly? In that case one uses either “mass-lumping”, or preconditioning. Write a script and compare the two options.

4 Multigrid solution

Each step of the resolution needs the resolution of a big linear system. The tools in the script given to you uses the “backslash” \ of matlab.

3. Apply multigrid at each time step.

5 You can't hear the form of the drum

Consider to the two domains on the first page.

4. Design the geometric mesh (each domain is a gathering of 7 unit triangles) Apply the previous study to compute the solution of the wave equation with oscillatory initial data.

6 Further documents

- *One cannot hear the shape of a drum*, Authors : Carolyn Gordon, David L. Webb and Scott Wolpert, Journal : Bull. Amer. Math. Soc. 27 (1992), 134-138. <http://www.ams.org/journals/bull/1992-27-01/S0273-0979-1992-00289-6/S0273-0979-1992-00289-6.pdf>
- More on this problem https://www.maa.org/sites/default/files/pdf/upload_library/22/Ford/MarkKac.pdf
<https://www.math.ucdavis.edu/~saito/courses/LapEig/lecpdf/lecture15.pdf>

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High Performance computing

TP 2 : You can't Always Hear the Shape of a Drum. Substructuring

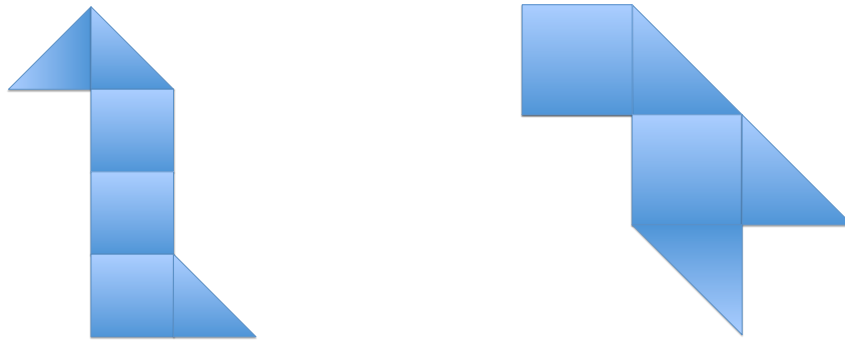


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This question has a mathematical counterpart that we are going to investigate. It is based on the problem defined in a domain $D \subset \mathbb{R}^2$,

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We suppose the initial conditions to be smooth enough ($u_0 \in H_0^1(D) \cap H^2(D)$, $u_1 \in H^1(D)$) so that the theory ensures a unique solution in $C([0, \infty[; H_0^1(D) \cap H^2(D)) \cap C^1([0, \infty[; H_0^1(D)) \cap C^2([0, \infty[; L^2(D))$.

1 Radial solutions

We suppose that the membrane is exactly the disc D_1 of center O and radius 1.

1. 1. Prove that if the initial data are radial, the solution is radial as well.
1. 2. Using the formula for the laplacian in polar coordinates, find the equation (*) that $v(r, t) = u(x, t)$ satisfies on $(0, 1) \times (0, +\infty)$.

2 Radial oscillatory solution of the radial equation by finite differences

2. 1. By separation of variables $v(r, t) = \phi(x)\psi(t)$, show that the solution oscillates in time, and that ϕ is solution of an eigenvalue problem denoted by (**).

2. 2. Write a finite differences scheme to solve (**) and deduce an approximate value of the five first frequencies. Compute and draw the eigenmodes.

3 Oscillatory Solutions of the $2 - D$ problem by finite elements

3. 1. By separation of variables in (1), $u(x; t) = \Phi(x)\Psi(t)$, show that the solution oscillates in time, and that Φ is solution of an eigenvalue problem denoted by (**).

3. 2. Write the variational formulation and obtain a matrix eigenvalue problem when using P_1 finite elements.

3. 3. Use the matlab script delivered to solve the eigenvalue problem in case of the disk D_1 .

3. 4. Compute the first five modes, and compare with the radial modes.

4 You can't hear the difference

Consider to the two domains on the previous page.

4. 1. Design the geometric mesh (each domain is a gathering of 7 unit triangles)

4. 2. Compute the first 10 modes for these domains and compare the results.

4. 3. Apply a substructuring process to compute the eigenmodes. Write the eigenmode problem, and solve it by finite elements.

5 Further documents

— A `matlab` library for finite elements graciously provided by Martin Gander (Genève University) and Felix Kwok (Hong-Kong Baptiste University).

— *One cannot hear the shape of a drum*, Authors : Carolyn Gordon, David L. Webb and Scott Wolpert, Journal : Bull. Amer. Math. Soc. 27 (1992), 134-138. <http://www.ams.org/journals/bull/1992-27-01/S0273-0979-1992-00289-6/S0273-0979-1992-00289-6.pdf>

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High Performance computing

TP 3 : Why is it difficult to resolve the waves. Preconditioning



FIGURE 1 – Waves in a pool

Diving in a pool creates surface waves which can be modeled by the wave equation

$$\begin{cases} \partial_{tt}u - \Delta u = 0 & \text{in } D \times (0, +\infty) \\ u = 0 & \text{on } \partial D \times (0, +\infty) \\ u = u_0 & \text{on } D \times (0) \\ \partial_t u = u_1 & \text{on } D \times (0) \end{cases} \quad (1)$$

We suppose the initial conditions to be smooth enough ($u_0 \in H_0^1(D) \cap H^2(D)$, $u_1 \in H^1(D)$) so that the theory ensures a unique solution in $C([0, \infty[; H_0^1(D) \cap H^2(D)) \cap C^1([0, \infty[; H_0^1(D)) \cap C^2([0, \infty[; L^2(D))$. We suppose the initial conditions to be smooth enough ($u_0 \in H_0^1(D) \cap H^2(D)$, $u_1 \in H^1(D)$) so that the theory ensures a unique solution in $C([0; 1[; H_0^1(D) \cap H^2(D)) \cap C^1([0; 1[; H_0^1(D)) \cap C^2([0; 1[; L^2(D))$.

1 Separation of variables

We suppose that the domain is exactly the square of length 1. The pool is at rest at initial time, $u_1 = 0$. We search a solution in the form $u(x, t) = v(x)\psi(t)$.

1. 1. Show that u and ϕ are solutions of two problems, and give explicitly the equations, the initial equations and the boundary data.

1. 2. Prove that v is solution of the **Helmholtz** equation in D , *i.e.* $\Delta v + \omega^2 v = 0$ in D with Dirichlet data on the boundary. Deduce the behavior of ψ .

1. 3. ω^2 is therefore an eigenvalue of $-\Delta$ in D . By separation of variables again, compute the eigenvalues and eigenfunctions.

2 Solution of the Helmholtz equation

We suppose that a disturbance is injected in the pool, with a frequency k which is NOT an eigenvalue of $-\Delta$ in D . We therefore have to solve

$$\begin{cases} \Delta u + k^2 u = f & \text{in } D \\ u = 0 & \text{on } \partial D \end{cases} \quad (2)$$

2. 1. Write the variational formulation in $H^1(D)$. Does the Lax-Milgram lemma applies? Why? Prove that the bilinear form satisfy a Garding inequality, which ensures well-posedness for this problem (see ref 4).

3 Numerical solution of the Helmholtz equation

3. 1. Discretize in space with P_1 finite elements the Dirichlet problem. The matrix is symmetric but not definite positive!

3. 2. In the FEM script, replace the `matlab` backslash `\` by a Jacobi, Gauss-Seidel algorithm, or Krylov algorithm (choose the last one carefully, the matrix is not definite). Run the algorithm with a source close to a Dirac on the north-east corner. Study the performance of the algorithm with respect to the mesh size (and hence the size of the matrix) and the frequency k . What happens when j is close to an eigenvalue?

3. 3. Propose a preconditioner seen in the lecture for the problem, and study again the performance. Compare with the Laplace equation.

3. 4. Apply a multigrid solver with relaxed Jacobi smoother to the problem. What happens?

4 Further documents

- *When all else fails, integrate by parts, an overview of new and old variational formulations for linear elliptic PDEs*. E.A. Spence. <http://people.bath.ac.uk/eas25/ibps.pdf>
- *Why it is Difficult to Solve Helmholtz Problems with Classical Iterative Methods*, Oliver G. Ernst and Martin J. Gander. <https://www.unige.ch/~gander/Preprints/HelmholtzReview.pdf>

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High Performance computing

TP 4 : The best way to solve to compute acoustics : domain decomposition

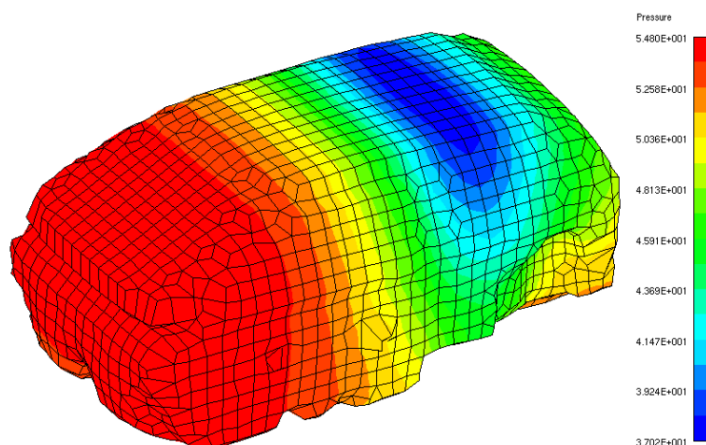


FIGURE 1 – Acoustic computation in a twingo

As seen in TP3, the computation of acoustics in a structure relies on the resolution of the Helmholtz equation

$$\Delta u + k^2 u = f \text{ in } D \quad (1)$$

1 Dimension 1

Consider the interval $D = (-1, 1)$.

1. 1. Show that the problem , with boundary condition $u = 0$ at $x = \pm 1$. as a unique solution $u \in \mathcal{C}^2(D)$ for $f \in \mathcal{C}(D)$, unless k takes the value $\pi/2 + n\pi$, for $n \in \mathbb{Z}$.

1. 2. Show that the problem , with boundary condition $u' = iku$ at $x = -1$ and $u' = -iku$ at $x = 1$. as a unique solution $u \in \mathcal{C}^2(D)$ for $f \in \mathcal{C}(D)$, for any $k \in \mathbb{R}$. (Attention, f is a real function, but the solution u takes complex values) .

1. 3. Build a \mathbb{P}_1 finite element approximation of the two problems, computing $u_n \in V_N = \mathbb{P}_1(x_0, \dots, x_{n+1})$. Theoretical results say that if $hk^2 \leq C$, the finite approximation is quasi-optimal, that is

$$\|u - u_n\|_1 \leq C' \min_{v \in V_n} \|u - v\|_1$$

Estimate the right hand side (to be found in so many textbooks) and check numerically the result, using $f = 1$ on $(-0.5, 0.5)$, 0 elsewhere.

2 Domain decomposition in one dimension

An approximation of the solution is given by dividing the interval into two subdomains $D_1 = (-1, L)$ and $(D_2 = (0, 1)$ with $L > 0$. A sequence of problems is introduced, u_j^n is the solution at step n in D_j ,

$$\begin{array}{l|l} -d_{xx}u_1^n + k^2u_1^n = f \text{ in } D_1 & -d_{xx}u_2^n + k^2u_2^n = f \text{ in } D_2 \\ u_1^n(-1) = 0 \quad u_1^n(L) = u_2^{n-1}(L) & u_2^n(0) = u_1^{n-1}(0) \quad u_2^n(1) = 0 \end{array}$$

With data at step $n = 0$, $u_2^0(L) \equiv g_1$ and $u_1^0(0) \equiv g_2$.

2. 1. Show that the error $u_j^n - u$ is solution of the same algorithm with data $f \equiv 0$, $u_2^0(L) \equiv g_1 - u(L)$ and $u_1^0(L) \equiv g_2 - u(0)$. Show that $u_1^n = a_n \sin k(x + 1)$ and $u_2^n = b_n \sin k(1 - x)$ and find the recursion relation between the a_n and the b_n .

2. 2. Analyze the convergence factor and show that for any k it is convergent except for an numerable set of values of L . What happens when k is large? Draw the curve of convergence of the a_n for various relevant values of k .

2. 3. Compute the sequence by finite elements, and compare the curve of convergence of $\|u - u_j^n\|_{L_2(D_j)}$ to the curve of the a_n for various relevant values of k , h and h .

3 Improvement for domain decomposition in one dimension

We replace the transmission conditions above by

$$(d_x + ik)u_1^n(L) = (d_x + ik)u_2^{n-1}(L), \quad (d_x - ik)u_2^n(0) = (d_x - ik)u_1^{n-1}(0).$$

With data at step $n = 0$, $u_2^0(L) \equiv g_1$ and $u_1^0(0) \equiv g_2$.

3. 1. Show that the error $u_j^n - u$ is solution of the same algorithm with data $f \equiv 0$, $u_2^0(L) \equiv g_1 - u(L)$ and $u_1^0(L) \equiv g_2 - u(0)$. Show that $u_1^n = a_n \sin k(x + 1)$ and $u_2^n = b_n \sin k(1 - x)$ and find the recursion relation between the a_n and the b_n .

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3. 3. Compute the sequence by finite elements, and compare the curve of convergence of $\|u - u_j^n\|_{L_2(D_j)}$ to the curve of the a_n for various relevant values of k , h and h .

4 Further documents

- *When all else fails, integrate by parts, an overview of new and old variational formulations for linear elliptic PDEs.* E.A. Spence. <http://people.bath.ac.uk/eas25/ibps.pdf>
- *Une méthode de décomposition de domaine pour le problème de Helmholtz*, Bruno Després, In french.
- *Why it is Difficult to Solve Helmholtz Problems with Classical Iterative Methods*, Oliver G. Ernst and Martin J. Gander. <https://www.unige.ch/~gander/Preprints/HelmholtzReview.pdf>

Master Vietnam-France in HCMC

High Performance computing

TP 5 : Effective coefficient of a composite material. Preconditioning

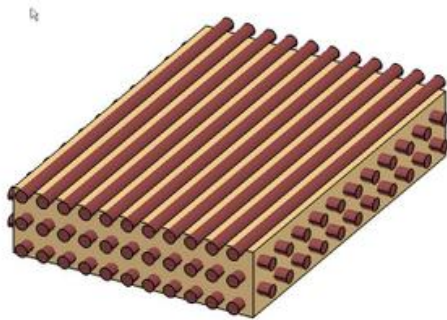


FIGURE 1 – Composite material

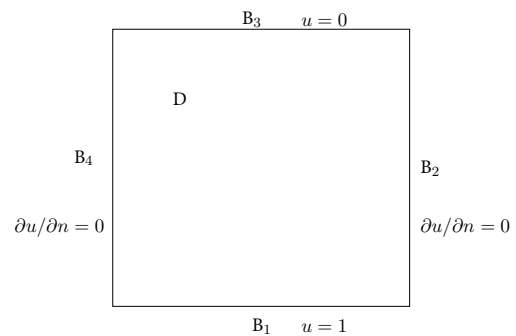


FIGURE 2 – Computational domain

Composite material are everywhere nowadays, in the building, aircrapfts, chairs, etc.. It is important to understand their mechanical and thermal properties.

Start with a heat conducting material, non homogeneous, occupying the space delimité by a square. $a(x)$ denotes the conductivity at point \mathbf{x} , and the heat flux is given by the Ficke law, $J = -a(\mathbf{x})\nabla u$, where u is the temperature. We are interested in computing the apparent conductivity of the material, defined as follows :

The boundaries Γ_1 and Γ_3 are heated to 0 and 1 respectively, and the heat flux across the lateral boundaries Γ_2 and Γ_4 are supposed to be zero. The system is

$$\begin{aligned} -\nabla(a(x)\nabla u) &= 0 \quad \text{in } D \\ \partial_n u &= 0 \quad \text{on } B_2 \cup B_4 \\ u &= 1 \quad \text{on } B_1 \\ u &= 0 \quad \text{on } B_3 \end{aligned} \tag{1}$$

We are searching for a solution $u \in H^1(D)$. The apparent conductivity is the ratio between the mean flux and the temperature gradient, that is

$$a_{app} = - \int_{B_3} a \partial_y u(x, y) dx$$

We will suppose that the square is $(0, 3) \times (0, 3)$, that the conductivity depends on x only and

$$a(x) = 1 \text{ on } (0, 1), \quad a(x) = \epsilon \text{ on } (1, 2), \quad a(x) = 1 \text{ on } (2, 3)$$

The aim of this work is to compute the apparent conductivity.

1 Closed form computations

1. 1. By separation of variables, if $u(x, y) = v(x)w(y)$, give the equations for v and w , together with their boundary conditions. Each of these functions is a solution of an eigenvalue problem for a second order operator in one dimension.

1. 2. Show that the equation in x amounts to solving with $k \in \mathbb{R}$,

$$(a(x)v')' + k^2av = 0 \text{ in } (0, 3), \quad \text{with } v'(0) = v'(3) = 0.$$

show that for $j = 0, \dots, 2$, v_j in $D_j = (j, j + 1)$ is solution of $u'' + k^2u = 0$, and that the transmission conditions are enforced

$$\begin{aligned} v_1(1) &= v_2(1), & v_2(2) &= v_3(2), \\ v_1'(1) &= \epsilon v_2'(1), & \epsilon v_2'(2) &= v_3'(2). \end{aligned}$$

From this compute explicitly the v_j for fixed k up to a constant, and then use the boundary conditions to obtain an equation giving k . Determine k and then w .

1. 3. Therefore we can expand u as $u = \sum_k v^k(x)w^k(y)$. Deduce from that the apparent conductivity of the material with respect to ϵ when keeping N nodes in the sum above.

2 Numerical computations

2. 1. Write a variational formulation and show well-posedness through Lax-Milgram theorem.

2. 2. Use the `matlab` codes available, modify the `newmesh` to deal with the different coefficients. Modify the finite element code to take the Neumann condition into account.

2. 3. Write a routine computing the apparent conductivity.

2. 4. Fix $\epsilon = 0.1$. Compute the apparent conductivity for refined values of the step size, and compare with the solution obtained by keeping N modes in the expansion above.

2. 5. Choose $\epsilon = 10^{-4}$. Compute the apparent conductivity for refined values of the step size, draw the solution, and see what the mesh size must be to be accurate. What is the computational time in this case?

2. 6. The FEM solver furnished are based on the use of the backslash `\` of `matlab`. Change it to a Krylov solver. Answer to the previous question.

2. 7. Add a Incomplete Cholewski preconditioner and compare the computational cost.

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High Performance computing

TP 6 : Effective coefficient of a composite material and domain decomposition

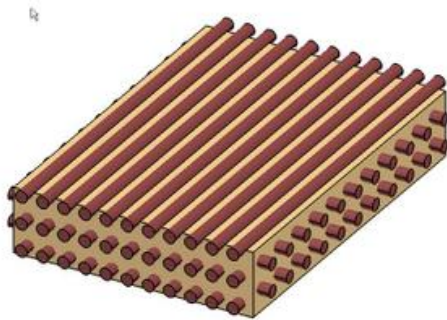


FIGURE 1 – Composite material

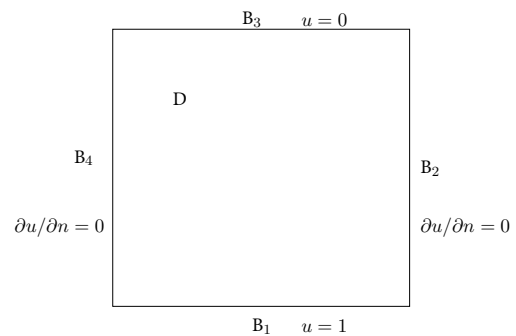


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$$\begin{aligned}
 -\nabla(a(x)\nabla u) &= 0 && \text{in } D \\
 \partial_n u &= 0 && \text{on } B_2 \cup B_4 \\
 u &= 1 && \text{on } B_1 \\
 u &= 0 && \text{on } B_3
 \end{aligned} \tag{1}$$

We are searching for a solution $u \in H^1(D)$. The apparent conductivity is the ratio between the mean flux and the temperature gradient, that is

$$a_{app} = - \int_{B_3} a \partial_y u(x, y) dx$$

We will suppose that the square is $(0, 3) \times (0, 3)$, that the conductivity depends on x only and

$$a(x) = 1 \text{ on } (0, 1), \quad a(x) = \epsilon \text{ on } (1, 2), \quad a(x) = 1 \text{ on } (2, 3)$$

The aim of this work is to compute the apparent conductivity.

1 Global computations

1. -2. Write a variational formulation and show well-posedness through Lax-Milgram theorem.

1. -1. Use the `matlab` codes available, modify the `newmesh` to deal with the different coefficients. Modify the finite element code to take the Neumann condition into account.

1. 0. Write a routine computing the apparent conductivity.

1. 1. Fix $\epsilon = 0.1$. Compute the apparent conductivity for refined values of the step size, and compare with the solution obtained by keeping N modes in the expansion above.

1. 2. Choose $\epsilon = 10^{-4}$. Compute the apparent conductivity for refined values of the step size, draw the solution, and see what the mesh size must be to be accurate. What is the computational time in this case?

2 Domain decomposition in the y direction

An approximation of the solution is given by dividing the domain into two subdomains $D_1 = (0, 3) \times (0, 2)$ and $D_2 = (0, 3) \times (2 + L, 3)$ with $L > 0$. A sequence of problems is introduced, u_j^n is the solution at step n in D_j ,

$$\begin{array}{l|l} -\nabla(a(x)\nabla u_1^n) = 0 \text{ in } D_1 & -\nabla(a(x)\nabla u_2^{n+1}) = 0 \text{ in } D_2 \\ \partial_x u_1^n(0, y) = 0 \quad u_1^n(x, 2 + L) = u_2^{n-1}(x, 2 + L) & u_2^{n+1}(x, 2) = u_1^n(x, 2) \quad \partial_x u_2^{n+1}(3, y) = 0 \end{array}$$

With data at step $n = 0$, $u_2^0(x, L) \equiv g_1$ and $u_1^0(x, 0) \equiv g_2$.

2. 1. Write a solver computing the sequence by finite elements.

2. 2. Take for initialization of the algorithm $g_1 = \sin k\pi x$ and $g_2 = 0$, and show the iterates for various values of k and ϵ . Draw the curve of convergence of $\|u - u_j^n\|_{L_2(D_j)}$ for each k and various relevant values of h and ϵ .

3 Improvement for domain decomposition in one dimension

3. 1. Compute numerically the eigenmodes of the one-dimensional operator in x , that is (λ, v) solution of

$$(a(x)v')' + \lambda av = 0 \text{ in } (0, 3), \quad \text{with } v'(0) = v'(3) = 0.$$

3. 2. What happens in the previous algorithm if the initial guess is the first mode?

3. 3. (optional) Replace the transmission conditions above by

$$(d_y + p)u_1^n(x, L) = (d_y + p)u_2^{n-1}(L), \quad (d_y - p)u_2^{n+1}(0) = (d_y - p)u_1^n(0).$$

Master Vietnam-France in HCMC

High Performance computing

TP 7 : Understanding and computing corner singularities for a vibrating plate

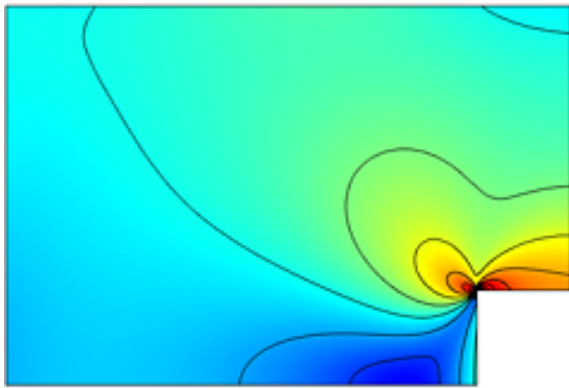


FIGURE 1 – Diffraction by a corner

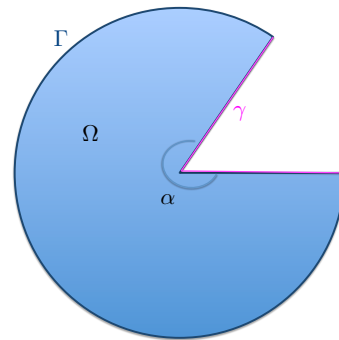


FIGURE 2 – Computational object

This subject aims at exploring the finite element method for elliptic problems, when the geometry is singular and not convex. In that case, the solution is not in $H^2(D)$, and therefore optimal error estimates are not available, for regular finite element methods.

Consider a metallic uniform plane plate, represented by the disk of center O and radius 1, cropped with an angle $\alpha > \pi$, see Figure . The object is fixed on the internal boundary γ , and free to vibrate on the remaining boundary Γ . The vertical vibrations are described by the wave equation

$$\begin{aligned} \partial_t^2 u - \Delta u &= f & \text{in } \Omega \times \mathbb{R}_+ \\ u &= 0 & \text{on } \gamma \times \mathbb{R}_+ \\ \partial_n u &= 0 & \text{on } \Gamma \times \mathbb{R}_+ \end{aligned} \quad (1)$$

and initial conditions u and $\partial_t u$ at initial time.

1 The steady problem

We first consider the steady problem , that is solving

$$\begin{aligned} -\Delta u &= f & \text{in } \Omega \\ u &= 0 & \text{on } \gamma \\ \partial_n u &= 0 & \text{on } \Gamma \end{aligned} \quad (2)$$

1. 1. Let ϕ decreasing and \mathcal{C}^2 on $(0, 1)$, such that $\phi(1) = 0$, $\phi'(0) = \phi(1) = \phi'(1) = 0$ (give an example). Define in polar coordinates

$$u_0(r, \theta) = \phi(r) r^{\frac{\pi}{\alpha}} \sin\left(\frac{\pi}{\alpha}\theta\right)$$

Show that $u_0 \in H^1(\Omega)$, $u_0 = 0$ on γ and $\partial_n u = 0$ on Γ (remember that $\partial_n u = \nabla u \cdot n$, and use the form of gradient and laplacian in polar coordinates

$$\nabla u = \partial_r u e_r + \frac{1}{r} \partial_\theta u e_\theta, \quad \Delta u = \frac{1}{r} \partial_r (r \partial_r u) + \frac{1}{r^2} \partial_\theta^2 u$$

Compute Δu_0 and verify that it belongs to $L^2(\Omega)$. Therefore it is solution of (2).

1. 2. Write the variational formulation of (2) in the space $H_\gamma^1 = \{v \in H^1(\Omega), v = 0 \text{ on } \gamma\}$.

1. 3. Compute the solution with \mathbb{P}_1 finite elements, using the script PDE provided, using $f = \Delta u_0$ as a source. Choose the function ϕ you want.

1. 4. Analysis : What is the numerical convergence order of the approximation : if p is the order, that means that $\|u - u_h\|_{L^2} \sim C(u)h^p$. If you draw the error for three values of h on the same plot in loglog scale, you should recover a straight line, whose slope is p . It can be calculated by

$$p \sim \log_2 \frac{\|u - u_h\|}{\|u - u_{h/2}\|}$$

How the numerical order does it depend on $\alpha \in (0, 2\pi)$. ?

1. 5. For a regular domain, a theoretical result says that $p = 2$. It relies on the following result : if $\Delta u \in L^2(\Omega)$, then $u \in H^2(\Omega) \cap H_0^1(\Omega)$. Does u_0 belong to $H^2(\Omega)$?

2 Singularity coefficient

From now on $\alpha \in]\pi, 2\pi[$. We give below some theory in functional analysis. Let L be the operator

$$\begin{aligned} L : L^2(\Omega) &\rightarrow H_\gamma^1, \\ f &\mapsto u \text{ solution of (2)} \end{aligned}$$

Now define $V = \text{Range}(L)$, then we have

$$H^2(\Omega) \cap V = \{v \in H^2(\Omega) \cap H_\gamma^1(\Omega), \partial_n v = 0 \text{ on } \Gamma\}$$

2. 1. What do you think the convergence rate should be if $u \in H^2(\Omega) \cap V$? Check this numerically.

2. 2. Note $H = L^{-1}(H^2(\Omega) \cap V)$, and D its orthogonal in $L^2(\Omega)$

$$H = \{f \in L^2(\Omega), \exists v \in H^2(\Omega) \cap V, -\Delta v = f\}, \quad D = \{f \in L^2(\Omega), \forall v \in H^2(\Omega) \cap V, \int_\Omega f \Delta v = 0\}.$$

Define the function p in polar coordinates by

$$p(r, \theta) = c_\alpha (r^{\frac{\pi}{\alpha}} + r^{-\frac{\pi}{\alpha}}) \sin \frac{\pi}{\alpha} \theta, \quad c_\alpha = \sqrt{\frac{2}{\alpha} \frac{1 - (\pi/\alpha)^2}{2 - (\pi/\alpha)^2}}$$

Show that $p \in D$ and $\|p\|_{L^2} = 1$. We admit that D is of dimension 1 and H is closed in $L^2(\Omega)$. For $f \in L^2(\Omega)$, we note $c(f)$ and call singular coefficient the quantity $c(f) = (p, f)_{L^2(\Omega)}$.

2. 3. For any $f \in L^2(\Omega)$, define $\tilde{f} = f - c(f)p$. Show that $\tilde{f} \in H$.

2. 4. Write a `matlab` script to compute an approximation of $c(f)$. Verify that the order of approximation is at least 1 (test on $f = p$).

3 Approximation of the singular part

3. 1. Show that $-\Delta u_0 \notin H$. Deduce that for any f in $L^2(\Omega)$, there exists a real number $\beta(f)$ such that $L(f) - \beta(f)u_0 \in H^2(\Omega) \cap V$.

3. 2. (Optional) Note $\beta_0 = \beta(p)$. Then $\beta_0 = 1/(\pi c_\alpha)$.

3. 3. Show that that for any f in $L^2(\Omega)$, $f + c(f)\beta_0\Delta u_0 \in H$. What do you think of the finite element approximation of $L(f + c(f)\beta_0\Delta u_0 \in H)$? ‘

3. 4. Propose and realize an approximation \hat{u}_h of $L(f)$ which is of order two, that is

$$\|u - \hat{u}_h\|_{L^2(\Omega)} \leq Ch^2 \|f\|_{L^2(\Omega)}$$

Verify numerically the order of convergence for $f \equiv 1$.

4 Eigenvalue problem

We admit that there exist a complete set of eigenfunctions of L , that is a sequence $(\phi_n) \subset H^1(\Omega)$ orthonormal in $L^2(\Omega)$, and a sequence $(\lambda_n) \subset \mathbb{R}_+$ with

$$L\phi_n = \lambda_n \phi_n, \quad -\Delta\phi_n = \lambda_n \phi_n, \quad \phi_n = 0 \text{ on } \gamma, \quad \partial_n \phi_n = 0 \text{ on } \Gamma.$$

We want to compute the fundamental mode of the structure, that is the largest eigenvalue of L $1/\lambda_1$, together with the fundamental mode ϕ_1 . We will use the method of power or Von Mises iteration which computes the largest eigenvalue of an operator when it is simple. The initialization is with $v_0 \in L^2(\Omega)$. Then solve

$$\tilde{v}_{k+1} = L(v_k) \text{ or equivalently } -\Delta\tilde{v}_{k+1} = v_k, \quad \tilde{v}_{k+1} = 0 \text{ on } \gamma, \quad \partial_n \tilde{v}_{k+1} = 0 \text{ on } \Gamma.$$

and normalize by $\mu_{k+1} = \|\tilde{v}_{k+1}\|$, $v_{k+1} = \tilde{v}_{k+1}/\mu_{k+1}$. It can be shown that if the eigenvalue λ_1 is simple (which is the case) and v_0 has a non-void component on ϕ_1 , then the sequence v_k converges to $\pm\phi_1$ and the sequence μ_k converges to λ_1 .

4. 4. Write a solver for the method of power iteration, for the problem above with regular solution, that is $\alpha \in (0, \pi)$.

4. 5. Extend the solver to the problem above with singular solution, that is $\alpha \in (\pi, 2\pi)$.

Master Vietnam-France in HCMC

High Performance computing

TP 8 : Computing corner singularities by substructuration

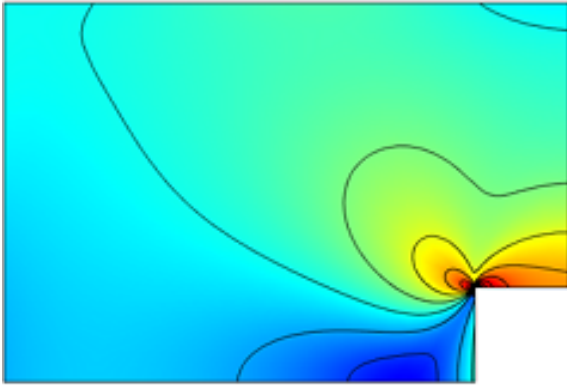


FIGURE 1 – Diffraction by a corner

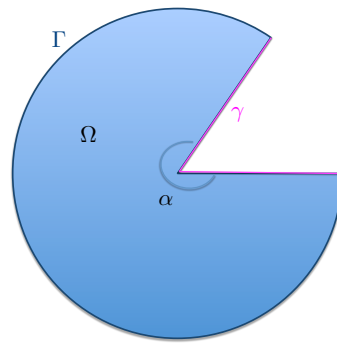


FIGURE 2 – Computational object

This subject aims at exploring the finite element method for elliptic problems, when the geometry is singular and not convex. In that case, the solution is not in $H^2(D)$, and therefore optimal error estimates are not available, for regular finite element methods.

Consider a metallic uniform plane plate, represented by the disk of center O and radius 1, cropped with an angle $\alpha > \pi$, see Figure . The object is fixed on the internal boundary γ , and free to vibrate on the remaining boundary Γ . The vertical vibrations are described by the wave equation

$$\begin{aligned} \partial_t^2 u - \Delta u &= f & \text{in } \Omega \times \mathbb{R}_+ \\ u &= 0 & \text{on } \gamma \times \mathbb{R}_+ \\ \partial_n u &= 0 & \text{on } \Gamma \times \mathbb{R}_+ \end{aligned} \quad (1)$$

and initial conditions u and $\partial_t u$ at initial time.

1 The steady problem

We first consider the steady problem , that is solving

$$\begin{aligned} -\Delta u &= f & \text{in } \Omega \\ u &= 0 & \text{on } \gamma \\ \partial_n u &= 0 & \text{on } \Gamma \end{aligned} \quad (2)$$

1. 1. Let ϕ decreasing and \mathcal{C}^2 on $(0, 1)$, such that $\phi(0) = 1$, $\phi'(0) = \phi(1) = \phi'(1) = 0$ (give an example). Define in polar coordinates

$$u_0(r, \theta) = \phi(r) r^{\frac{\pi}{\alpha}} \sin\left(\frac{\pi}{\alpha}\theta\right)$$

Show that $u_0 \in H^1(\Omega)$, $u_0 = 0$ on γ and $\partial_n u = 0$ on Γ (remember that $\partial_n u = \nabla u \cdot n$, and use the form of gradient and laplacian in polar coordinates

$$\nabla u = \partial_r u e_r + \frac{1}{r} \partial_\theta u e_\theta, \quad \Delta u = \frac{1}{r} \partial_r (r \partial_r u) + \frac{1}{r^2} \partial_\theta^2 u$$

Compute Δu_0 and verify that it belongs to $L^2(\Omega)$. Therefore it is solution of (2).

1. 2. Write the variational formulation of (2) in the space $H_\gamma^1 = \{v \in H^1(\Omega), v = 0 \text{ on } \gamma\}$.

1. 3. Compute the solution with \mathbb{P}_1 finite elements, using the script PDE provided, using $f = \Delta u_0$ as a source. Choose the function ϕ you want.

1. 4. Analysis : What is the numerical convergence order of the approximation : if p is the order, that means that $\|u - u_h\|_{L^2} \sim C(u)h^p$. If you draw the error for three values of h on the same plot in loglog scale, you should recover a straight line, whose slope is p . It can be calculated by

$$p \sim \log_2 \frac{\|u - u_h\|}{\|u - u_{h/2}\|}$$

How the numerical order does it depend on $\alpha \in (0, 2\pi)$. ?

1. 5. For a regular domain, a theoretical result says that $p = 2$. It relies on the following result : if $\Delta u \in L^2(\Omega)$, then $u \in H^2(\Omega) \cap H_0^1(\Omega)$. Does u_0 belong to $H^2(\Omega)$?

2 Singularity coefficient

From now on $\alpha \in]\pi, 2\pi[$. We give below some theory in functional analysis. Let L be the operator

$$\begin{aligned} L : L^2(\Omega) &\rightarrow H_\gamma^1, \\ f &\mapsto u \text{ solution of (2)} \end{aligned}$$

Now define $V = \text{Range}(L)$, then we have

$$H^2(\Omega) \cap V = \{v \in H^2(\Omega) \cap H_\gamma^1(\Omega), \partial_n v = 0 \text{ on } \Gamma\}$$

2. 1. What do you think the convergence rate should be if $u \in H^2(\Omega) \cap V$? Check this numerically.

2. 2. Note $H = L^{-1}(H^2(\Omega) \cap V)$, and D its orthogonal in $L^2(\Omega)$

$$H = \{f \in L^2(\Omega), \exists v \in H^2(\Omega) \cap V, -\Delta v = f\}, \quad D = \{f \in L^2(\Omega), \forall v \in H^2(\Omega) \cap V, \int_\Omega f \Delta v = 0\}.$$

Define the function p in polar coordinates by

$$p(r, \theta) = c_\alpha (r^{\frac{\pi}{\alpha}} + r^{-\frac{\pi}{\alpha}}) \sin \frac{\pi}{\alpha} \theta, \quad c_\alpha = \sqrt{\frac{2}{\alpha} \frac{1 - (\pi/\alpha)^2}{2 - (\pi/\alpha)^2}}$$

Show that $p \in D$ and $\|p\|_{L^2} = 1$. We admit that D is of dimension 1 and H is closed in $L^2(\Omega)$. For $f \in L^2(\Omega)$, we note $c(f)$ and call singular coefficient the quantity $c(f) = (p, f)_{L^2(\Omega)}$.

2. 3. For any $f \in L^2(\Omega)$, define $\tilde{f} = f - c(f)p$. Show that $\tilde{f} \in H$.

2. 4. Write a `matlab` script to compute an approximation of $c(f)$. Verify that the order of approximation is at least 1 (test on $f = p$).

3 Approximation of the singular part

3. 1. Show that $-\Delta u_0 \notin H$. Deduce that for any f in $L^2(\Omega)$, there exists a real number $\beta(f)$ such that $L(f) - \beta(f)u_0 \in H^2(\Omega) \cap V$.

3. 2. (Optional) Note $\beta_0 = \beta(p)$. Then $\beta_0 = 1/(\pi c_\alpha)$.

3. 3. Show that that for any f in $L^2(\Omega)$, $f + c(f)\beta_0\Delta u_0 \in H$. What do you think of the finite element approximation of $L(f + c(f)\beta_0\Delta u_0 \in H)$? ‘

3. 4. Propose and realize an approximation \hat{u}_h of $L(f)$ which is of order two, that is

$$\|u - \hat{u}_h\|_{L^2(\Omega)} \leq Ch^2 \|f\|_{L^2(\Omega)}$$

Verify numerically the order of convergence for $f \equiv 1$.

4 Substructuring

The domain Ω is divided into two parts, in any of these two configurations

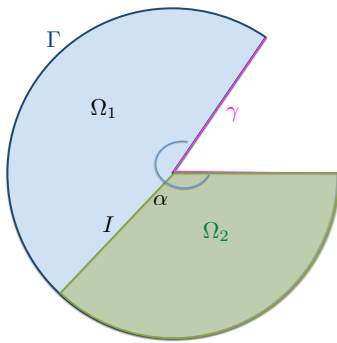


FIGURE 3 – Subdivision 1

Start with the regular case.

4. 1. Split the domain Ω into two domains Ω_j with angle $\alpha/2$ (Figure 4). Design one mesh in each subdomain, with the same interface mesh on I . The substructured problem can be designed as follows : take g on I , solve the problem 2 in each subdomain with data g on I , call $\mathcal{L}_j(f, g)$ the solution in Ω_j . Then the problem to be solved is

$$\mathcal{A}_1(f_1, g) + \mathcal{A}_2(f_2, g) = 0, \quad f_j = f|_{\Omega_j}.$$

This is a linear problem, solved by iteration, like Richardson or Krylov method.

4. 2. Design the iteration process, using Gauss-Seidel algorithm.
4. 3. Plot the iterates, and the convergence history.
4. 4. Do the same for the non regular case.
4. 5. Do the same for Decomposition 1 in Figure 4.

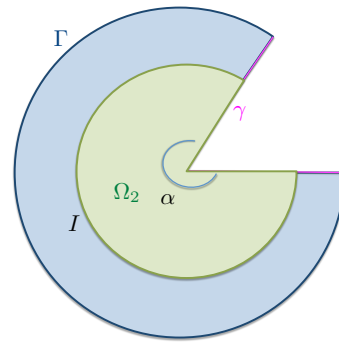


FIGURE 4 – Subdivision 2

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High Performance computing

TP 9 Air conditioning and domain decomposition

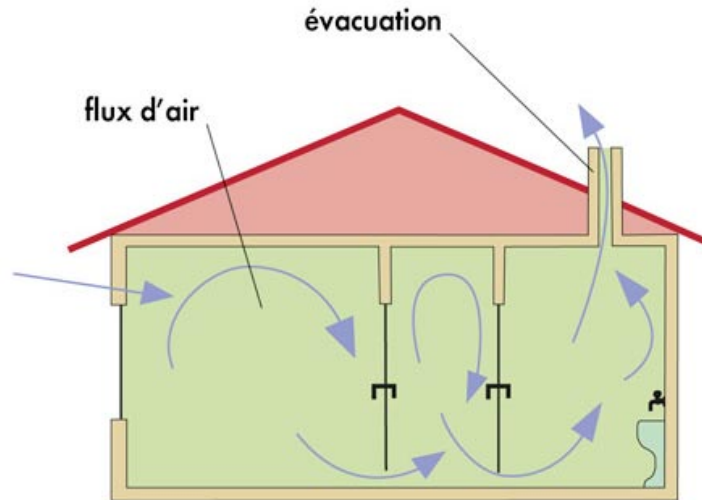


FIGURE 1 – Ventilation in a house

1 Modelisation

1. 1. Draw a scheme of your room with walls, windows, doors and main furnitures.

The temperature in the room occupying a geometrical domain Ω , is subject to variations due to source of heating (or cooling) and boundary conditions on the walls, windows and doors. The Fourier's law asserts that the equation modelizing the temperature in the room is subject to the **heat equation**

$$c(x)\rho(x)\partial_t u - \nabla(K\nabla u) = Q \quad (1)$$

where $c(x)$ is the specific heat, $\rho(x)$ is the density, and $K(x)$ the thermal conductivity of the material at point x . $Q(x, t)$ is used to represent any external sources or sinks (i.e. heat energy taken out of the system) of heat energy. If $Q(x, t) > 0$ then heat energy is being added to the system at that location and time and if $Q(x, t) < 0$ then heat energy is being removed from the system at that location and time.

The initial data u_0 tells us what the initial temperature distribution in the room is.

The **boundary data** tell us what happens on the walls and doors and windows. There are of four different sorts.

Prescribed temperature or Dirichlet boundary condition .

$$u = g$$

Prescribed heat flux or Neumann boundary conditions . Using Fourier's law it can be written

$$-K\partial_n u := -K\nabla u \cdot n = g$$

where n is the exterior unit normal to the boundary. If the boundary is insulated, *i.e.* there is no heat flow out of them then the boundary conditions reduces to $\partial_n u = 0$.

Newton's law of cooling or Robin boundary conditions . These are usually used when the material is in a moving fluid and note we can consider air to be a fluid for this purpose. In a room they can stand for wind coming from a window.

$$-K\partial_n u := H(u - g),$$

where H is a positive quantity that is experimentally determined, and g gives the temperature of the surrounding fluid at boundary.

Periodic boundary conditions They arise from particular geometries like a disk or an infinite channel

we can also mix and match these boundary conditions so to speak.

1. 2. Write a two dimensional model for the temperature in your room, and give precisely the boundary conditions on the wall, doors and windows. The source Q might be a heater (or a cooler!).

2 Insight on the heat equation in one dimension

Suppose the room is compressed into a nail Ω of length L , with constant density, specific heat, and thermal conductivity. Suppose the nail with initial temperature $u_0(x)$, $x \in (0, L)$ is placed between two ice cubes. We assume that the nail is thin enough so that we can consider it to be one dimensional. The ice cubes are naturally at temperature zero, and they touch the nail at both extremities. This defines the boundary conditions of the problem, and therefore we treat the heat equation

$$\partial_t u - \partial_{xx} u = 0 \text{ in } \Omega \times (0, T),$$

with given initial value u_0 .

2. 1. Show that the solution takes the form of a series

$$u(x, t) = \sum_k \phi_k(x) \psi_k(t),$$

and give the explicit form for the basis functions $\phi_k(x)$ and $\psi_k(t)$. For each $j = 1, 5, 10$, $u_0 = \sin(j\pi x/L)$, draw on the same plot the value of u at different times.

2. 2. Suppose now that Neumann conditions are imposed at each end of the nail. What physical meaning does it have? Can you also get the solution explicitly. Draw some snapshots of the solution.

3 The steady state in two dimensions

Suppose again that the room has constant density, specific heat, and thermal conductivity. It seems from the 1-D analysis that a steady state can be reached. Suppose the heat furnished by the heater is $f(x)$ independent of time. At the moment the temperature u is stabilized in the room, it does not depend on time anymore, and is solution of the **Poisson equation**

$$-\Delta u = f$$

If there is no external force, we have the **Laplace equation** $-\Delta u = 0$.

3. 1. Write the the matlab script `NewMesh` into `Myroommesh` to insert the geometry, the material properties, and the boundaries of your room.

3. 2. When the heater is off, and the windows and doors are at $20^\circ C$, draw the temperature repartition.

3. 3. Compute now a very warm day with 30 degrees outside, and the door are $20^\circ C$.

3. 4. Turn the cooler on a temperature of $20^\circ C$.

4 The heat equation in two dimensions

In the same geometry, we now want to solve the heat equation with a θ schéma. Let K be the stiffness matrix and M the mass matrix in the finite element approximation of $-\Delta$ with the boundary conditions designed in Section 3. The *semi-discrete* approximation of the problem (1) (with the simplification in the previous section) is $u_h(t) = \sum \xi_i(t)\phi_i$, where the ϕ are the basis functions in the finite element methods

$$\partial_t - \Delta u = f; M\partial_t \xi + K\xi = G_h$$

where G_h represents all sources contained in the volume and on the boundaries. This is now an ordinary differential equation we solve by the θ scheme. Let a time discretisation of the interval $(0, T)$ with step dt . The approximation of u_h at time t_n is denoted by u_h^n , and the scheme is :

$$M \frac{\xi^{n+1} - \xi^n}{dt} = \theta(G_h^{n+1} - K\xi^{n+1}) + (1 - \theta)(G_h^n - K\xi^n) \quad (2)$$

When $\theta = 0$, it is called forward Euler, when $\theta = 1$, it is called backward Euler, and for $\theta = 1/2$, it is called Crank-Nicolson.

4. 1. Write a `matlab` program called `Heat` taking as entries θ , the data and the spacial geometry, and computing the sequence of values in time. The initial value is a gaussian centered at the center of the room, there is no source, the boundary data are zero everywhere, but on the window where the temperature it is equal to 0.5 for $t \geq 0.1$.

4. 2. It is well establish that for $\theta = 0$ the scheme is stable for θ sufficiently small and of order 1 in time, and inconditionnally stable and of order 1 for $\theta = 1/2$. Illustrate this result by numerical computation (find the relevant theory in reference 6).

5 Substructuring

Suppose the problem is first discretized in time by the implicit Euler scheme

$$\frac{u^{n+1} - u^n}{dt} - \Delta u^{n+1} = G^{n+1}.$$

Split the domain Ω into two rectangular subdomains Ω_j . Design one mesh in each subdomain, with the same interface mesh on I . The substructured problem can be designed as follows : take $g(t)$ on I , solve the problem ?? in each subdomain with data g on I , call $\mathcal{L}_j(f, g)$ the solution in Ω_j . Then the problem to be solved is

$$\mathcal{A}_1(f_1, g) + \mathcal{A}_2(f_2, g) = 0, \quad f_j = f|_{\Omega_j}.$$

This is a linear problem, solved by iteration, like Richardson or Krylov method.

4. 3. Design the iteration process, using Gauss-Seidel algorithm.

4. 4. Plot the iterates, and the convergence history.

6 Further documents

- <http://tutorial.math.lamar.edu/Classes/DE/TheHeatEquation.aspx>
- Quarteroni Valli, *Numerical approximation of partial differential equations*.