Continuum Modeling: Numerical schemes for linear & nonlinear reaction/diffusion systems, Phase fields Models. Application to Batteries and image processing
Part 2: Numerical Schemes

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Plan

1. Goal

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Fundamentals (theoretical)

- Accuracy
- Stability
- Recover important properties at the discrete level

Fundamentals (practice)

- Efficient algorithms for the effective numerical solution
- Easy to implement

General approach

We deal with evolution PDES : the unknown solution depends both on the time and on the space variables. To approach the solution we

- Spatial discretization, then obtain a finite dimensional differential system
- TIme numerical integration, then produce a sequence of vector which consist in approximation of the solution different discrete times.

Variational framework (simple form)

Let V being a proper linear space V (Hilbert, infinite dimensional). A way to give a sense to the notion of solution of the problem is to consider the **variational problem associated to the PDE**. Consider the Homogeneous Dirichlet Problem, multiply by a test function v and integrate over the domain :

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Now (**Key point**) use integration by part (Green formula)

$$\int_\Omega -\Delta u\mathbf{v}dx = \int_\Omega \nabla u \nabla \mathbf{v}dx - \int_{\partial\Omega} \frac{\partial u}{\partial n}\mathbf{v}d\sigma \tag{2}$$

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Now, if $\mathbf{v} = 0$ on $\partial\Omega$, then

$$\alpha \int_\Omega u\mathbf{v}dx + \int_\Omega \nabla u \nabla \mathbf{v}dx = \int_\Omega f\mathbf{v}dx \quad \forall \mathbf{v} \in V \tag{3}$$

u is said to be the weak solution of the PDE.

Variational framework from minimization

The variational form of the equation is related to a minimization. Consider

$$J(u) = \frac{1}{2}\alpha \int_\Omega u^2 dx + \frac{1}{2}\int_\Omega \|\nabla u\|^2 dx - \int_\Omega fudx \tag{4}$$

We look to the minima of J, say to functions u such

$$J(u) \leq J(u+\lambda w), \forall w \in V, \forall \lambda \in \mathbb{R} \tag{5}$$

They are characterized by the relation $\nabla J(u) = 0$. Developing the expressions we find

$$\begin{aligned} J(u+\lambda w) &= \frac{1}{2}\alpha \int_\Omega (u+\lambda w)^2 dx + \frac{1}{2}\int_\Omega \|\nabla(u+\lambda w)\|^2 dx - \int_\Omega f(u+\lambda w)dx \\ &= J(u) + \lambda\left(\int_\Omega \nabla u \nabla w dx - \int_\Omega fvdx\right) \\ &+\lambda^2 \frac{1}{2}\left(\alpha\int_\Omega w^2 dx + \int_\Omega \|\nabla w\|^2 dx\right) \end{aligned}$$

We can show that

$$J(u) \leq J(u+\lambda w) \iff \left(\alpha\int_\Omega uwdx + \int_\Omega \nabla u \nabla w dx - \int_\Omega fwdx\right) = 0,\ \forall w \in V$$

Solution of the variational problem

The above variational problem can be written as : *Find* $u \in V$ *such that*

$$(\mathcal{V}) = \begin{cases} \underbrace{\alpha \int_\Omega u\mathbf{v}dx + \int_\Omega \nabla u \nabla \mathbf{v} dx}_{\text{bilinear term}} = \underbrace{\int_\Omega f\mathbf{v}dx}_{\text{linear term}} & \forall \mathbf{v} \in V \\ \mathbf{a}(u,\mathbf{v}) = \ell(\mathbf{v}) & \forall \mathbf{v} \in V \end{cases}$$

Mathematical theory

- Under suitable hypothesis (Lax-Milgram Lemma) the problem possesses a unique solution which depends continuously on f
- Under suitable hypothesis, the solution of $(\mathcal{P})$ is solution of $(\mathcal{V})$ and conversely the solution of $(\mathcal{V})$ is solution of $(\mathcal{P})$
- The solution u is regular, say smooth enough to justify finite dimensional approximation, see hereafter.

The finite Element Method (FEM)

All the following will be provided automatically by FreemFem++

- The Finite Element Method (FEM) is a numerical method for solving problems of engineering and mathematical physics.
- Useful for problems with complicated geometries, loadings, and material properties where analytical solutions can not be obtained

- **Key idea 1** : consider $V_h \subset V$ a finite dimensional subspace of V and definite the approach variational problem

$$(\mathcal{V}_h) = \begin{cases} \alpha \int_\Omega u_h \mathbf{v}_h dx + \int_\Omega \nabla u_h \nabla \mathbf{v}_h dx & = \int_\Omega f \mathbf{v}_h dx \quad \forall \mathbf{v}_h \in V_h \\ \mathbf{a}(u_h, \mathbf{v}_h) & = \ell(\mathbf{v}_h) \quad \forall \mathbf{v}_h \in V_h \end{cases}$$

- **Key idea 2** : since V_h is finite dimensional, for every basis ϕ_i of V_h we can write $u_h = \sum_{j=1}^{N} \xi_j \phi_j$ and show that

$$\mathbf{a}(u_h, \mathbf{v}_h) = \ell(\mathbf{v}_h) \ \forall \mathbf{v}_h \in V_h \iff \mathbf{a}(\sum_{j=1}^{N} \xi_j \phi_j, \phi_i) = \ell(\phi_i), \forall i = 1, \cdots, N.$$

Hence $(\mathcal{V}_h)$ is nothing but a linear system $A\xi = F$ where

$$(*) \quad A_{i,j} = \mathbf{a}(\phi_j, \phi_i), \ F_i = \ell(\phi_i).$$

- **Key idea 3** : define V_h such that $\|u - u_h\|$ is "small"
- **Key idea 4** : find a "nice basis" of V_h such that $(*)$ is easy to solve

The finite element method fulfills these lats two points

Building V_h : the Mesh

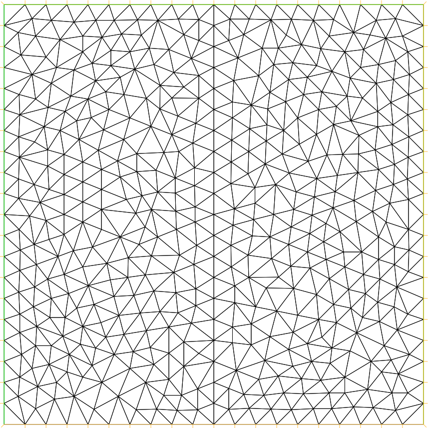

Figure – Mesh when Ω is a rectangle

Building V_h : the Mesh

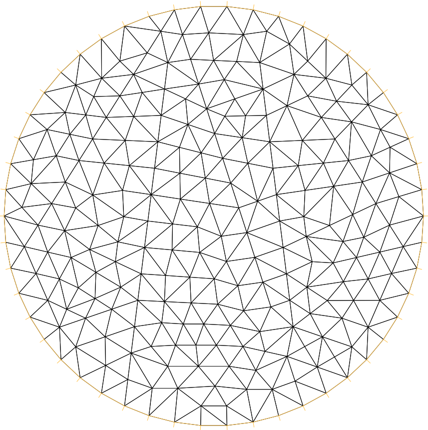

Figure – Mesh when Ω is the unit Disk

Building V_h : the Mesh

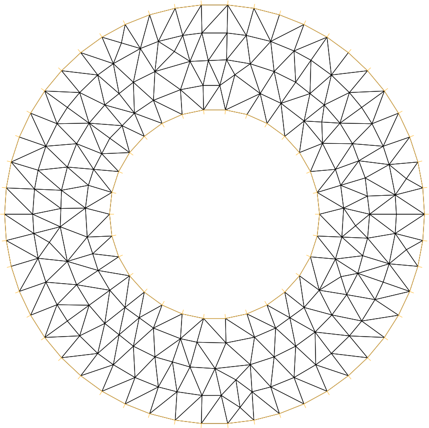

Figure – Mesh when Ω is a Disk with Hole

The simplest way of defining V_h is the following :

$$V_h = \{\mathbf{v}_h : (\mathbf{v}_h)|_T \in \Pi_1, \text{ for any } T \in T_h \text{ (+homogeneous BC in some cases)}\}, \text{ where}$$

- T_h is a regular mesh of Ω
- Π_1 is the space of polynomials whose degree is lower or equal to one

In that way

- The functions of V_h are piecewise polynomial
- The matrix of the system is sparse (the support of the basis functions are essentially disjoints)

Notations

- The matrix $A_{i,j} = \int_\Omega \nabla\phi_j \nabla\phi_i dx$ is called the **STIFFNESS** matrix
- The matrix

$$M_{i,j} = \int_\Omega \phi_j \phi_i dx$$

is called the **MASS** matrix

The Π_1 finite elements approximation produces a linear system whose the solution is a vector containing the approximation of the values of the solution u of the PDE at the nodes of the mesh. When these coefficients are known, we rebuild the (piecewise linear) solution u_h as

$$u_h = \sum_{j=1}^{N} \xi_j \phi_j$$

Notice that it is a (continuous) function defined on Ω. We go back now to the two fundamental examples

- The Dirichlet problem : $-\Delta u = f$ in $\Omega, u = 0$ on $\partial\Omega$
- The Neumann problem : $\alpha u - \Delta u = F$ in $\Omega, \dfrac{\partial u}{\partial n} = 0$ on $\partial\Omega$

The Dirichlet Problem

Here the approximated variational problem is

$$\int_\Omega \nabla u_h \nabla \mathbf{v}_h dx \quad = \int_\Omega f \mathbf{v}_h dx \quad \forall \mathbf{v}_h \in V_h^0$$

where

$$V_h^0 = \{\mathbf{v}_h : (\mathbf{v}_h)|_T \in \Pi_1, \text{ for any } T \in T_h, v_h|_{\partial\Omega} = 0\},$$

The matrix of the problem is the stiffness matrix A_h and is defined by $(A_h)_{i,j} = \displaystyle\int_\Omega \nabla\phi_j \nabla\phi_i dx$. We denote by $\mathbf{u}_h = (\xi_1, \cdots, \xi_{ND})$ the coefficients of u_h in the ϕ_j basis. Then the variational problem is equivalent to

$$A_h \mathbf{u}_h = \mathbf{f}_h$$

with $\mathbf{f}_h = \left(\int_\Omega f\phi_1 dx, \cdots, \int_\Omega f\phi_{ND} dx\right)$

The NeumannProblem

Here the approximated variational problem is

$$\alpha \int_\Omega u_h \mathbf{v}_h dx + \int_\Omega \nabla u_h \nabla \mathbf{v}_h dx \quad = \int_\Omega f \mathbf{v}_h dx \quad \forall \mathbf{v}_h \in V_h$$

where

$$V_h = \{\mathbf{v}_h : (\mathbf{v}_h)|_T \in \Pi_1, \text{ for any } T \in T_h\},$$

The matrix of the problem is a linear combination from the mass matrix M_h and the stiffness matrix A_h ; The variational problem is equivalent to

$$(\alpha M_h + A_h)\mathbf{u}_h = \mathbf{f}_h$$

Numerical methods for solving linear systems

There is a wide variety of algorithms for solving the linear systems, we will use some build-in solvers in `Freefem++`, however, let us cite some of the most used methods

- Iterative, possibly preconditioned methods : GMRES, Conjugate Gradient, Bi-CGSTAB
- Direct methods : LU,Choleski
- Preconditioners : ILU, Choleski, sparse inverses

We first build the variational problem associated to the Heat Equation : starting from

$$\begin{array}{ll} \frac{\partial u}{\partial t} - \Delta u = f & x \in \Omega,\ t \in]0, T) \\ u = 0 & x \in \partial\Omega, t\ t \in (0, T) \\ u(x,0) = u_0(x) & x \in \Omega \end{array}$$

we obtain

$$\begin{array}{ll} \int_\Omega \frac{\partial u}{\partial t}\mathbf{v} dx + \int_\Omega \nabla u \nabla \mathbf{v} dx = \int_\Omega f \mathbf{v} dx & t \in]0, T) \\ u(x,0) = u_0(x) & x \in \Omega \end{array}$$

or

$$\begin{array}{ll} \frac{d}{dt}\int_\Omega u\mathbf{v} dx + \int_\Omega \nabla u \nabla \mathbf{v} dx = \int_\Omega f \mathbf{v} dx & t \in]0, T) \\ u(x,0) = u_0(x) & x \in \Omega \end{array}$$

We can now define the approximated variational differential equation

$$\begin{array}{ll} \frac{d}{dt}\int_\Omega u_h\mathbf{v}_h dx + \int_\Omega \nabla u_h \nabla \mathbf{v}_h dx = \int_\Omega f \mathbf{v}_h dx & t \in]0, T) \\ u_h(0) = Proj_{V_h}(u_0) & \end{array}$$

Space discretization leads to a differential system

$M_h \frac{d\mathbf{u}_h}{dt} + A_h \mathbf{u}_h = \mathbf{f}_h$ (here $\underline{\mathbf{u}}_h$ depends also on t)

Basic Euler Schemes

- Forward Euler's

$$M_h \frac{\mathbf{u}_h^{(k+1)} - \mathbf{u}_h^{(k)}}{\Delta t} + A_h \mathbf{u}_h^{(k)} = \mathbf{f}_h^{(k)}$$

- Backward Euler's

$$M_h \frac{\mathbf{u}_h^{(k+1)} - \mathbf{u}_h^{(k)}}{\Delta t} + A_h \mathbf{u}_h^{(k+1)} = \mathbf{f}_h^{(k+1)}$$

- θ-scheme

$$M_h \frac{\mathbf{u}_h^{(k+1)} - \mathbf{u}_h^{(k)}}{\Delta t} + (1-\theta) A_h \mathbf{u}_h^{(k)} + \theta A_h \mathbf{u}_h^{(k+1)} = (1-\theta)\mathbf{f}_h^{(k)} + \theta \mathbf{f}_h^{(k+1)}$$

Stability of Iterative methods

Fundamental result

The sequence of vectors defined by induction by

$$Z^{(k+1)} = AZ^{(k)}$$

converge to 0 for all initial value $Z^{(0)}$ if and only if $\rho(A) < 1$; here $\rho(A)$ is the **spectral radius** of A, say the modulus of largest eigenvalue of A in modulus.

Let us apply this to Forward Euler's scheme and take $\mathbf{f}_h^{(k)} = 0$ for simplicity we have $M_h\mathbf{u}_h^{(k+1)} = (M_h + \Delta t A_h)\mathbf{u}_h^{(k)}$, say

$$\mathbf{u}_h^{(k+1)} = M_h^{-1}(M_h - \Delta t A_h)\mathbf{u}_h^{(k)} = K\mathbf{u}_h^{(k)}$$

So the scheme is stable iff $\rho(Id - \delta t M_h^{-1} A_h) < 1$

Properties : Stability

Assume that the spectrum of $M_h^{-1}A_h$ is real and contained in $\mathbb{R}_*^+$ then

- Forward Euler's scheme is stable iff $0 < \Delta t < \dfrac{2}{\rho(M_h^{-1}A_h)}$
- Backward Euler's is unconditionally stable ($\forall \Delta t > 0$)
- θ-scheme is stable under the following conditions
    - if $\theta \in [\frac{1}{2}, 1]$ the it is unconditionally stable
    - if $\theta \in [0, \frac{1}{2}[$ it is stable under time step restriction

$$0 < \Delta t < \frac{2}{\rho(M_h^{-1}A_h)(1-2\theta)}$$

Properties : Accuracy

- Euler's schemes and θ-scheme (for $\theta \neq \frac{1}{2}$) are first order accurate in times, say

$$\max_{t\in[0,T]} \|u_h(x,t) - u(x,t)\| \leq C(h + \Delta t)$$

- if $\theta = \frac{1}{2}$, then θ-scheme is second order accurate

For simplicity we consider only semi-implicit and fully implicit Euler's schemes. The first idea is to treat explicitlly the nonlinear term at each time step and to apply the backward Euler's scheme to the linear part.

Semi implicit Euler's scheme

$\mathbf{u}_h^{(0)}$ given
For $k = 0, \cdots$ loop

Find $\mathbf{u}_h^{(k+1)}$ solution of: $M_h \dfrac{\mathbf{u}_h^{(k+1)} - \mathbf{u}_h^{(k)}}{\Delta t} + A_h \mathbf{u}_h^{(k+1)} = -\underline{F}_h(\mathbf{u}_h^{(k)})$

End For

Nice it is easy to implement
But suffers form a hard time step restriction : $0 < \Delta t < C.\epsilon^2$

We now treat implicitly both the linear and the nonlinear part

Fully implicit Euler's scheme

$\mathbf{u}_h^{(0)}$ `given`
`For` $k = 0, \cdots$ `loop`

`Find` $\mathbf{u}_h^{(k+1)}$ `solution of:` $M_h \dfrac{\mathbf{u}_h^{(k+1)} - \mathbf{u}_h^{(k+1)}}{\Delta t} + A_h \mathbf{u}_h^{(k+1)} = -\underline{F}_h(\mathbf{u}_h^{(k+1)})$

`End For`

The big difference here is that $\mathbf{u}_h^{(k+1)}$ is defined implicitly, as the solution of a nonlinear system of equations. We then need to use **at each time step** a numerical method devoted to the numeric solution of such problems. Let us cite two of ones :

- Fixed points methods (to which we focus)
- Newton Method and its variations

Fixed Point

Let $\Phi : \mathbb{R}^n \to \mathbb{R}^n$ a continuous function. X is said to be a fixed point of F if

$$\Phi(X^*) = X^*$$

Fixed Point method : (Emile) Picard's iterates

Assume that X^* exists and is unique. To compute this fixed point, we generate the sequence

$$X^{(k+1)} = \Phi(X^{(k)}),\ k = 0, \cdots$$

If the sequence converges, it is necessary to X^*.

To implement the fully implicit Euler's scheme, we need to plug the fixed point iterations inside the loop in time taking

$$\Phi(X) = (M_h + \Delta t A_h)^{-1}(M_h \mathbf{u}_h^{(k)} - \Delta t F(X))$$

Inside and outside loops

Fully implicit Euler's scheme

$\mathbf{u}_h^{(0)}$ given
OUTSIDE LOOP
For $k = 0, \cdots$ loop
INSIDE LOOP
Set $w_h^{(0,k)} = \mathbf{u}_h^{(k)}$
For $m = 0, \cdots$ loop

Find $\mathbf{w}_h^{(m+1,k)}$ solution of: $M_h \dfrac{\mathbf{w}_h^{(m+1,k)} - \mathbf{u}_h^{(k)}}{\Delta t} + A_h \mathbf{w}_h^{(m+1,k)} = -\underline{F}_h(\mathbf{w}_h^{(m,k)})$

End For
Set $\mathbf{u}_h^{(k+1)} = \mathbf{w}_h^{(m+1,k)}$ (the last computed w)
End For

Here we take into account the gradient flow structure to build schemes that are energy decreasing. A first inconditionally stable scheme is [Elliott,ElliottStuart]

$$\frac{\mathbf{u}_h^{(k+1)} - \mathbf{u}_h^{(k)}}{\Delta t} + A_h \mathbf{u}_h^{(k+1)} + \frac{1}{\epsilon^2} \mathbf{DF}_h(\mathbf{u}_h^{(k)}, \mathbf{u}_h^{(k+1)}) = 0, \tag{6}$$

$$\text{where } \mathbf{DF}_h(u, v) = \begin{cases} \dfrac{\mathbf{F}_h(u) - \mathbf{F}_h(v)}{u - v} & \text{if } u \neq v, \\ f(u) & \text{if } u = v. \end{cases}$$

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proof

We take the scalar product with $\frac{\mathbf{u}_h^{(k+1)} - \mathbf{u}_h^{(k)}}{\Delta t}$, and use the identity $< DF(u,v),(u-v) >=< F(u),\mathbf{1} > - < F(v),\mathbf{1} >$. We get

$$\|\frac{\mathbf{u}_h^{(k+1)} - \mathbf{u}_h^{(k)}}{\Delta t}\|^2 + \frac{1}{2\Delta t} < A_h(\mathbf{u}_h^{(k+1)} - \mathbf{u}_h^{(k)}), \mathbf{u}_h^{(k+1)} - \mathbf{u}_h^{(k)} >$$

$$+ \frac{E(\mathbf{u}_h^{(k+1)}) - E(\mathbf{u}_h^{(k)})}{\Delta t} = 0$$

Then $E(\mathbf{u}_h^{(k+1)}) < E(\mathbf{u}_h^{(k)})$ with $E(\mathbf{u}_h) = \frac{1}{2} < A_h \mathbf{u}_h, \mathbf{u}_h > + \frac{1}{\epsilon^2} \int_\Omega F_h(\mathbf{u}_h)dx$

We start from the coupled system

$$\frac{\partial u}{\partial t} - \Delta\mu = 0, \tag{7}$$

$$\mu = -\Delta u + \frac{1}{\epsilon^2} f(u), \tag{8}$$

$$\frac{\partial u}{\partial n} = 0, \frac{\partial \mu}{\partial n} = 0, \tag{9}$$

$$u(0,x) = u_0(x) \tag{10}$$

we obtain the variational form We start from the coupled system

$$\int_\Omega \frac{\partial u}{\partial t}\mathbf{v}dx + \int_\Omega \nabla\mu\nabla\mathbf{v}dx = 0, \forall\mathbf{v} \in V \tag{11}$$

$$\int_\Omega \mu\mathbf{w}dx = \int_\Omega \nabla u\nabla\mathbf{w}dx + \frac{1}{\epsilon^2}\int_\Omega f(u)\mathbf{w}dx, \tag{12}$$

$$u(0,x) = u_0(x) \tag{13}$$

Semi implicit Euler's scheme

$\mathbf{u}_h^{(0)}$ `given`

`For` $k = 0, \cdots$ `loop` `Find` $[\mathbf{u}_h^{(k+1)}, \mu_h^{(k+1)}]$ `solution of:`

$$\begin{cases} M_h \dfrac{\mathbf{u}_h^{(k+1)} - \mathbf{u}_h^{(k)}}{\Delta t} + A_h \mu_h^{(k+1)} = 0 \\ M_h \mu_h^{(k+1)} = A_h \mathbf{u}_h^{(k+1)} + \dfrac{1}{\epsilon^2} \mathbf{f}_h(\mathbf{u}_h^{(k)}) \end{cases}$$

`End For`

Nice it is easy to implement

But suffers form a hard time step restriction : $0 < \Delta t < C.\epsilon^4$

Fully implicit Euler's scheme

$\mathbf{u}_h^{(0)}$ `given`

`For` $k = 0, \cdots$ `loop` `Find` $[\mathbf{u}_h^{(k+1)}, \mu_h^{(k+1)}]$ `solution of:`

$$M_h \frac{\mathbf{u}_h^{(k+1)} - \mathbf{u}_h^{(k)}}{\Delta t} + A_h \mu_h^{(k+1)} = 0$$

$$M_h \mu_h^{(k+1)} = A_h \mathbf{u}_h^{(k+1)} + \frac{1}{\epsilon^2} \mathbf{f}_h(\mathbf{u}_h^{(k+1)})$$

`End For`

Need to solve a fixed point at each step

Energy decreasing scheme

$\mathbf{u}_h^{(0)}$ `given`

`For` $k = 0, \cdots$ `loop` `Find` $[\mathbf{u}_h^{(k+1)}, \mu_h^{(k+1)}]$ `solution of:`

$$M_h \frac{\mathbf{u}_h^{(k+1)} - \mathbf{u}_h^{(k)}}{\Delta t} + A_h \mu_h^{(k+1)} = 0$$

$$M_h \mu_h^{(k+1)} = A_h \mathbf{u}_h^{(k+1)} + \mathbf{DF}_h(\mathbf{u}^{(k)}, \mathbf{u}_h^{(k+1)})$$

`End For`