Continuum Modeling: Numerical schemes for linear & nonlinear reaction/diffusion systems, Phase fields Modeling

Part 3: Numerical solution with Freefrem++ (a simple introduction)

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- Goal
- Basic structure of the code

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 - The Heat equation
 - Reaction-Diffusion equation

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 - The Heat equation
 - Reaction-Diffusion equation
- Coupled systems

FreeFEM++

is a Free software to solve PDE using the Finite Element Method. It runs on most of available systems: Windows, Linux and MacOS

What FreeFEM++ does

- automatic Mesh Generation
- automatic building of mass and stiffness matrices (taking into account BC)
- Solution of discrete linear systems
- Allows to simulate 2D and 3D problems in many fields such as CFD
- Post-Treatment facilities (Graphics, Text, File generation)

Here a nice basic tutorial

http://homepage.ntu.edu.tw/ twhsheu/twsiamff++/tutorials/2014-Casts/ff-basic-tutorial.pdf



Basic structure of the code Starting with FreeFEM++ Solution of elliptic problem (Poisson) Solution of the variational problem Solution of Evolution equations Coupled systems

- Definition of the geometry then of the mesh
- Definition of the FEM space
- Solution of the variational problem
- Post-treatment (graphics ...)

Download the software at http://freefem/org/f++

Use

- Write the script using a raw editor
- Save it with the file extension .edp
- Run it

What is needed

- Know what a variational formulation is
- (better) Know a little from C++

```
Rectangle
int m=10, n=10;
mesh Th=square(m,n, [x,y]);
plot(Th,wait=1,cmm="The rectangle");
```

```
Disk
int m=30;
border C1(t=0 ,2* pi)x=2*cos (t);y=2*sin (t); label =1;
mesh Th=buildmesh (C1(m));
plot(Th,wait=1,cmm="A disk");
```

```
Torus
int m1=200,m2=100;
border C1(t=0 ,2* pi)x=2*cos (t);y=2*sin (t); label =1;
border C2(t=0 ,2* pi)x=cos (t);y=sin (t); label =1;
mesh Th=buildmesh(C1 (m1)+C2(-m2));
plot(Th,wait=1,cmm="The Torus");
```

Generate Finite Element Space

```
    The most simple
fespace Vh(Th,P1);
    But also other P-elements
fespace Vh(Th,P2);
and
fespace Vh(Th,P3);
```

We look to $u_h \in V_h \subset V$:

$$(\mathcal{V}_h): \int_{\Omega} \nabla u_h \nabla \mathbf{v}_h dx - \int_{\Omega} f \mathbf{v}_h dx = 0 \forall \mathbf{v}_h \in V_h$$

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

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

FreeFem Structure of the problem

```
problem Poisson(u,v)=// Definition of the problem
int2d(Th)(dx(u)*dx(v)+dy(u)*dy(v))// bilinear form
-int2d(Th)(f*v)// linear form
+on(1,2,3,4,u=0); // Dirichlet Conditions
Poisson; // Solve Poisson Equation
```

Exercise 1

A first example, build a FreFem++ code for solving Poisson problem with Homogeneous Dirichlet Boundary conditions

Solution

Not now...

Save: save.edp

```
include "Poisson.edp"; // include previous script
plot(u,ps="result.eps") f=cos(x)*y; // Generate .eps output
save mesh(Th,"Th.msh");// Save the Mesh
of streamfile("potential.txt")
file<<u[];</pre>
```

Read: Read.edp

```
mesh Th=readmesh("Th.msh"); // Read the Mesh
fespace Vh(Th,P1);
Vh u=0;
if stream file("potential.txt"); // Read the potential
plot(u,cmm"The result was correctly saved:)");
```

Exercise 2

A first example, build a FreFem++ code for solving Poisson problem with Mixed Dirichlet-Neumann Boundary conditions

Solution

Not now..

Impossible in Batman school not to consider Robin Boundary conditions!

Impossible in Batman school not to consider **Robin** Boundary conditions! They write as

$$au + \kappa \frac{\partial u}{\partial n} = b$$

and they can be implemented as

border gammar=...

then in the variational problem

int1d(Th,gammar)(a*u*v)-int1d(Th,gammar)(b*v).

Practically, the Numerical solution resumes as a sequence of solutions of approximated variational problems. It suffices then to use a loop structure: first define the problem to be solve at each step.

Exercise 3

Write a FreeFem++ code BackwardEuler for solving the variational problem attached to each step of the Backward Euler Scheme

Solution

Not now..

Consider the reaction-diffusion equation

$$\frac{\partial u}{\partial t} - \Delta u + f(u) = 0$$

A first semi implicit scheme

At first, we apply a semi-implicit scheme :

$$\frac{u^{(k+1)}-u^{(k)}}{\Delta t}-\Delta u^{(k+1)}+f(u^{(k)})=0,$$

to which we associate the variational problem

$$< u^{(k+1)}, v > +\Delta t < \nabla u^{(k+1)}, \nabla v > = < u^{(k)}, v > +\Delta t < f(u^{(k)}), v >$$

The loop structure can be written as

```
for(t=0;t<T;t+=dt){
f=F(u0); BackwardEuler;
u0=u;
}</pre>
```

A fully implicit scheme

At first, we apply a semi-implicit scheme:

$$\frac{u^{(k+1)}-u^{(k)}}{\Delta t}-\Delta u^{(k+1)}+f(u^{(k+1)})=0,$$

This problem is nonlinear and can be solved numerically by using, e.g., a Picard fixed point method, setting also $a(u, v) = \langle u, v \rangle + \Delta t \langle \nabla u, \nabla v \rangle$

Algorithm Fixed point for fully backward Euler's

 $u^{(k,0)} - u^{(k)}$ Set residual=30 Compute

While

 $m < Mmax \& residual > \eta$,

 $a(u^{(k,m+1)}, v) = \langle u^{(k)}, v \rangle + \Delta t \langle f(u^{(k,m)}), v \rangle \forall v \in V$ Solve

residual= $||u^{(k,m+1)} - u^{(k)} - \Delta t \Delta u^{(k,m+1)} + \Delta t f(u^{(k+1,m)})||$ Compute residual

EndFor

 $u^{(k+1)} - u^{(k,m+1)}$ Set

A fully implicit scheme : the whole loop

```
The whole loop structure can be written in FreeFem++ as f=f(u0); for(k=0;k<Kmax;k+=1){ residual=10;p=0; while(p<40 \ residu >0.00000001)){ BackwardEuler; f=F(u); p=p+1; equiv = u; equiv = u;
```

Exercise 4

Write a FreeFem++ code for solving Allen-Cahn equation

The solution of Cahn-Hilliard equation is easier when decoupled in two equations, so the basis of any (semi-)implicit scheme is the solution of a coupled linear system. A nice way to do it, is to generate the block matrix using the command varf. We consider for simplicity first only time integration of the linear part of Cahn-Hilliard equation by a Backward Euler's method.

```
    First define the product of FE spaces
    fespace Vh2(Th, [P1, P1]);
```

- Define the block matrix attached to the coupled variational problem as varf AA([v,w],[phi,psi]) = int2d(Th) (v*phi/dt) int2d(Th)(dx(w)*dx(phi)+dy(w)*dy(phi)) +int2d(Th)(dx(v)*dx(psi)+dy(v)*dy(psi)-w*psi);
- Building the block matrix
 H=AA(Vh2,Vh2, factorize=1, solver=LU);
- initial datum
 [v,w]=[u0,0];
- Solution of the linear system (source is the right hand side

```
v[]=H\land -1*source[];
```

