

# FreeFem++

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# Introduction

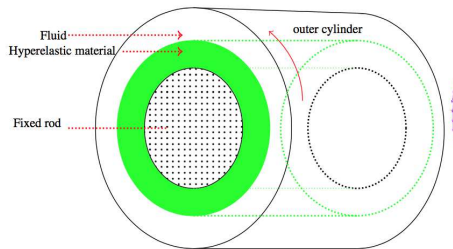
I suggest you choose, according to your level

- ▶ Beginners : Follow the slides
- ▶ Others 1 : Follow today's example
- ▶ Others 2 : Suggest an example and receive help to program it.

Today's example :

$$\rho \partial_t v - \frac{1}{r} \partial_r [\xi^f r \partial_r v + \xi^s r \partial_r d] = 0, \quad \partial_t d = v, \quad r \in (R_0, R_1), \quad v|_{R_0} = 0, \quad v|_{R_1} = 3,$$

with  $\rho = \rho^s \mathbf{1}_{r \leq R} + \rho^f \mathbf{1}_{r > R}$ ,  $\xi^s = 2c_1 \mathbf{1}_{r \leq R}$ ,  $\xi^f = \mu \mathbf{1}_{r > R}$ , and with  $d(r, 0) = 0$ .



## Example

A cylinder contains a fixed rigid cylindrical rod in its center, a cylindrical layer of hyperelastic material around the rod and the rest is filled with a fluid (see figure 3). First the system is at rest and then a constant rotation is given to the outer cylinder. This cause the fluid to rotate with an angular velocity which depends on the distance  $r$  to the main axis; in turn because the friction of the fluid at the interface the hyperelastic material will be dragged into a angular velocity  $\omega$  which is also only a function of  $r$  and time . Due to elasticity  $\omega$  will oscillate with time until numerical dissipation and fluid viscosity damps it.

In a two dimensional cut perpendicular to the main axis, the velocities and displacements are two dimensional as well. Hence the geometry is a ring of inner and outer radii,  $R_0$  and  $R_1$ , with hyperelastic material between  $R_0$  and  $R$  and fluid between  $R$  and  $R_1$ . Because of the incompressibility of the fluid and axial symmetry,  $R$  is constant.

In this test  $R_0 = 3$ ,  $R = 4$ ,  $R_1 = 5$ . The solid is an hyperelastic incompressible material with  $c_1 = 2$  and  $\rho^s = 2$ . The Newtonian fluid has  $\mu = 2$ ,  $\rho^f = 1$ . The velocity of the outer cylinder has magnitude 3. As everything is axisymmetric the computation can be done in polar coordinates  $r, \theta$ , and the fluid-solid system reduces to

$$\rho \partial_t v - \frac{1}{r} \partial_r [\xi^f r \partial_r v + \xi^s r \partial_r d] = 0, \quad \partial_t d = v, \quad r \in (R_0, R_1), \quad v|_{R_0} = 0, \quad v|_{R_1} = 3, \quad (24)$$

with  $\rho = \rho^s \mathbf{1}_{r \leq R} + \rho^f \mathbf{1}_{r > R}$ ,  $\xi^s = 2c_1 \mathbf{1}_{r \leq R}$ ,  $\xi^f = \mu \mathbf{1}_{r > R}$ , and with  $d(r, 0) = 0$ .

# Example

```
load "pipe"
real R0=1,R1=2,R2=3,rhof=1,rhos=2,nu=1,kappa=5,v=3,T=0.8,dt=0.025;
      //    / semi-analytic solution by solving a 1d problem //
mesh Th=square(100,5,[R0+(R2-R0)*x,0.1*y]);
fespace Wh(Th,P1,periodic=[[1,x],[3,x]]);
fespace W0(Th,P0);
Wh d=0,w,wh,wold=0;
W0 nnu=nu*(x>R1)+2*kappa*dt*(x<=R1), Rho=rhof*(x>R1)+rhos*(x<=R1);
problem AA(w,wh) = int2d(Th)(Rho*x*w*wh/dt+x*nnu/2*dx(w)*dx(wh) )
+ int2d(Th)(-Rho*x*wold*wh/dt +x*nnu/2*dx(wold)*dx(wh)
+ 2*kappa*(x<=R1)*(x*dx(d)*dx(wh) ))
+on(2,w=-v)+on(4,w=0); //    this is the one-d axisymmetric problem
pstream pgnuplot("gnuplot" );           //    //// prepare gnuplot ////
int J=40;  real dr = (R2-R0)/(J-1);
for(int i=0;i<T/dt;i++){
    AA; d=d+(w+wold)*dt; wold=w;
    ofstream f("aux.gp");
    for(int j=0;j<J;j++) f << j*dr << "    " << w(R0+j*dr,0.05) << endl;
    pgnuplot << "plot 'aux.gp' u 1:2 w l " << endl;
    sleep(1); flush(pgnuplot);
}
```



# Outline

## Introduction

- The main characteristics

## Basics

## Academic Examples

- Weak form

- Poisson Equation

## Tools

- Remarks on weak form and boundary conditions

## Mesh generation

- Mesh tools

- 3d Poisson equation with mesh adaptation

## Linear PDE

- Linear elasticity equation

- Stokes equation

## Numerics Tools

- Eigenvalue

- Eigenvalue/ Eigenvector

- Optimization : lpopt interface

## Incompressible Navier-Stokes equations

- Boussinesq equation

## Phase change with Natural Convection



# Introduction

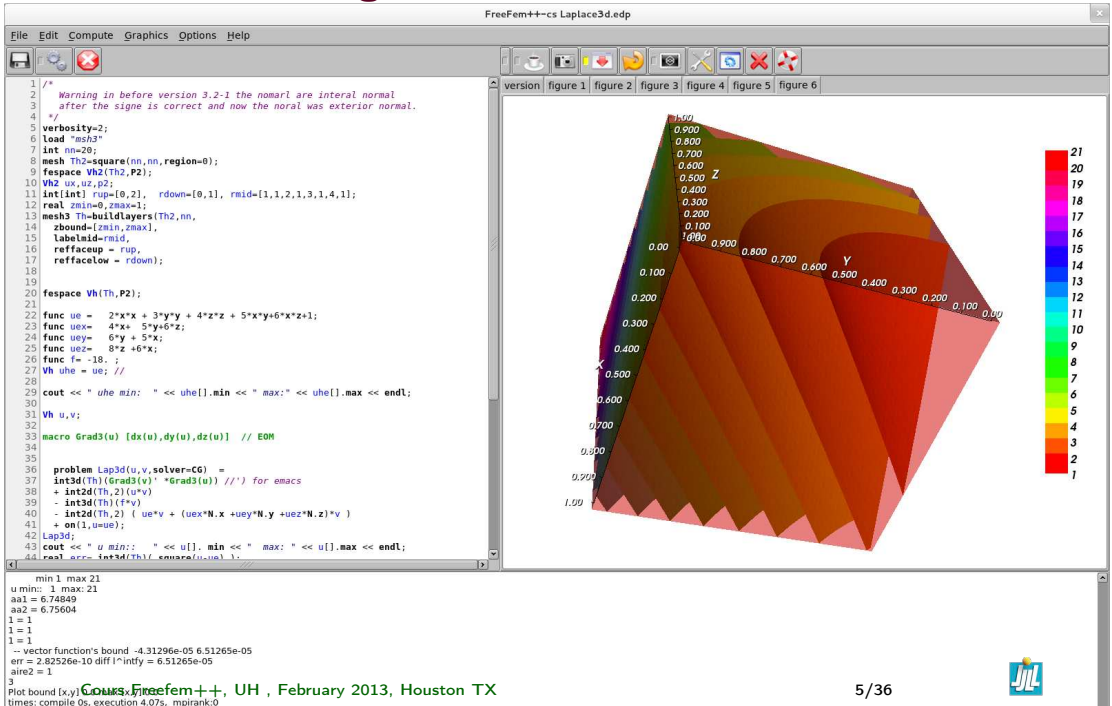
- ▶ Except COMSOL software to solve PDE are application oriented, like NASTRAN, PamCrash, Abaqus, Fluent, OpenFOAM etc.
- ▶ FreeFem++ is a software born in 2000 to solve numerically partial differential equations (PDE) in  $\mathbb{R}^2$  and in  $\mathbb{R}^3$  with finite elements methods.
- ▶ It has its own language, as close to the mathematics as possible : the FreeFem++ script which overwrites C++.
- ▶ All PDEs are specified in variational form.
- ▶ At the root FreeFem++ solves linear steady state problem and convection problems.
- ▶ For time depend, nonlinear and coupled problem the user must specify the algorithm.
- ▶ It can do mesh adaptation , compute error indicator, etc ...

FreeFem++ is a freeware and this run on Mac, Unix and Window architecture, in parallel with MPI.



- ▶ Wide range of finite elements : continuous P1,P2 elements, discontinuous P0, P1, RT0,RT1,BDM1, elements ,Discontinuous-Galerkin, ...
- ▶ Automatic interpolation of data from a mesh to an other one, so a finite element function is view as a function of  $(x, y, z)$  or as an array on the degree of Freedom.
- ▶ Complex or real functions with access to vectors and the matrices.
- ▶ LU, Cholesky, Crout, CG, GMRES, UMFPack, SuperLU, MUMPS, HIPS , SUPERLU\_DIST, PASTIX. ... sparse linear solver ; eigenvalue and eigenvector computation with ARPACK.
- ▶ Optimization Algorithms : GMRES, IPOPT, MEWUOA, CMAES etc.
- ▶ Automatic mesh generator, based on Delaunay-Voronoi. (2d,3d (tetgen) )
- ▶ Mesh adaptation based on automatic metric, possibly anisotropic (only in 2d).
- ▶ Link with other soft : paraview, gmsh , vtk, medit, gnuplot
- ▶ Dynamic linking to add plugin. Full MPI interface
- ▶ Online graphics with OpenGL/GLUT/VTK, C++ like syntax.
- ▶ An integrated development environment FreeFem++-cs

# FreeFem++-CS integrated environment





# Element of syntax 1/2

```
x,y,z , label, N.x, N.y, N.z,           // some reserved variables
int i = 0;                               // an integer
real a=2.5;                               // a reel
bool b=(a<3.);
real[int] array(10);                      // a real array of 10 value
mesh Th;                                  // a 2d mesh
fespace Vh(Th,P2);                        // Def. of 2d finite element space;
      Vh u=x; // a finite element function or array
fespace V3h(Th,[P2,P2,P1]); V3h u;
      u(.5,.6,.7); u[];
Vh3<complex> uc = x+ 1i *y;                // complex valued FE
V3h [u1,u2,p]=[x,y,z];                    // a vectorial finite element
macro div(u,v) (dx(u)+dy(v))              // EOM a macro
varf a([u1,u2,p],[v1,v2,q])=
      int2d(Th)( Grad(u1)'*Grad(v1) +Grad(u2)'*Grad(v2)
      -div(u1,u2)*q -div(v1,v2)*p)
+on(1,2)(u1=g1,u2=g2);
matrix A=a(V3h,V3h,solver=UMFPACK);
real[int] b=a(0,V3h);
u2[] =A^-1*b;                             // or you can put also u1[]= or p[].
```



## Element of syntax 2/2

```
func Heaveside=(x>0); // a formal line function
func real g(int i, real a) { .....; return i+a;}
A = A + A'; A = A'*A; A = [ [ A,0],[0,A'] ];
int[int] I(15),J(15); // two array for renumbering
matrix B;
B = A; B=A(I,J); // B(i,j) = A(I(i),J(j))
B=A(I^-1,J^-1); // B(I(i),J(j))= A(i,j)
B.resize(10,20); // resize the sparse matrix
int[int] I(1),J(1); real[int] C(1);
[I,J,C]=A; // get of the sparse term of the matrix A
A=[I,J,C]; // set a new matrix
matrix D=[diagofA]; // set a diagonal matrix D
real[int] a=2:12; // set a[i]=i+2; i=0 to 10.
a formal array is [ exp1, exp1, ..., expn]
complex a=1,b=2,c=3i;
func va=[ a,b,c]; // is a formal array in [ ]
a =[ 1,2,3i]'*va; cout « a « endl; // hermien product
matrix<complex> A=va*[ 1,2,3i]'; cout « A « endl;
a =[ 1,2,3i]'*va*2.; a =(va+[ 1,2,3i])'*va*2.;
va./va; va*/va; // term to term / and term to term *
```

# Laplace equation, weak form

Let a domain  $\Omega$  with a partition of  $\partial\Omega$  in  $\Gamma_2, \Gamma_e$ .

Find  $u$  a solution in such that :

$$-\Delta u = f \text{ in } \Omega, \quad u = g \text{ on } \Gamma_2, \quad \frac{\partial u}{\partial \vec{n}} = h \text{ on } \Gamma_e \quad (1)$$

Denote  $V_g = \{v \in H^1(\Omega) / v|_{\Gamma_2} = g\}$  .

The Basic variationnal formulation with is : find  $u \in V_g(\Omega)$  , such that

$$\int_{\Omega} \nabla u \cdot \nabla v = \int_{\Omega} f v + \int_{\Gamma} h v, \quad \forall v \in V_0(\Omega) \quad (2)$$

The finite element method is just : replace  $V_g$  with a finite element space, and the `FreeFem++` code :

# Poisson equation in a fish with FreeFem++

The finite element method is just : replace  $V_g$  with a finite element space, and the FreeFem++ code :

```
mesh3 Th("fish-3d.msh");           // read a mesh 3d
fespace Vh(Th,P1);                  // define the P1 EF space

Vh u,v;                             // set test and unknown function in Vh.
macro Grad(u) [dx(u),dy(u),dz(u)]  // EOM Grad def
func f=1;
solve laplace(u,v,solver=CG) =
    int3d(Th) ( Grad(u)'*Grad(v) )
    - int3d(Th) ( f*v)
    + on(2,u=2);                      // int on  $\gamma_2$ 
plot(u,fill=1,wait=1,value=0,wait=1);
```

Run:fish.edp      Run:fish3d.edp



# Build Mesh 2d

a L shape domain  $]0, 1[^2 \setminus [\frac{1}{2}, 1[^2$

```
border a(t=0,1.0){x=t;    y=0;    label=1;};
border b(t=0,0.5){x=1;    y=t;    label=1;};
border c(t=0,0.5){x=1-t;  y=0.5;label=1;};
border d(t=0.5,1){x=0.5;  y=t;    label=1;};
border e(t=0.5,1){x=1-t;  y=1;    label=1;};
border f(t=0.0,1){x=0;    y=1-t;label=1;};
plot(a(6)+b(4)+c(4)+d(4)+e(4)+f(6),wait=1);          //      to see
mesh Th2 = buildmesh (a(6)+b(4)+c(4)+d(4)+e(4)+f(6));
```



# boundary mesh of a Sphere

```
load "tetgen"
mesh Th=square(10,20,[x*pi-pi/2,2*y*pi]);          //  $[-\frac{\pi}{2}, \frac{\pi}{2}] \times [0, 2\pi]$ 
func f1 =cos(x)*cos(y); func f2 =cos(x)*sin(y); func f3 = sin(x);
           // the partial derivative of the parametrization DF
func f1x=sin(x)*cos(y); func f1y=-cos(x)*sin(y);
func f2x=-sin(x)*sin(y); func f2y=cos(x)*cos(y);
func f3x=cos(x); func f3y=0;
                                           //  $M = DF^t DF$ 
func m11=f1x^2+f2x^2+f3x^2; func m21=f1x*f1y+f2x*f2y+f3x*f3y;
func m22=f1y^2+f2y^2+f3y^2;
func perio=[[4,y],[2,y],[1,x],[3,x]];
real hh=0.1/R; real vv= 1/square(hh);
Th=adaptmesh(Th,m11*vv,m21*vv,m22*vv,IsMetric=1,periodic=perio);
int[int] ref=[0,L]; // the label of the Sphere to L ( 0 -> L)
mesh3 ThS= movemesh23(Th,transfo=[f1*R,f2*R,f3*R],orientation=1,
    label=ref);
```

Run:Sphere.edp Run:sphere6.edp

# Mesh tools

- ▶ `change` to change label and region numbering in 2d and 3d.
- ▶ `movemesh` `checkmovemesh` `movemesh23` `movemesh3`
- ▶ `triangulate` (2d) , `tetgconvexhull` (3d) build mesh for a set of point
- ▶ `emptymesh` (2d) built a empty mesh for Lagrange multiplier
- ▶ `freeyams` to optimize surface mesh
- ▶ `mmg3d` to optimize volume mesh with constant surface mesh
- ▶ `mshmet` to compute metric
- ▶ `isoline` to extract isoline (2d)
- ▶ `trunc` to remove peace of mesh and split all element (2d,3d)
- ▶ `splitmesh` to split 2d mesh in no regular way.



# A corner singularity

adaptation with metric

The domain is an L-shaped polygon  $\Omega = ]0, 1[^2 \setminus [\frac{1}{2}, 1]^2$  and the PDE is

Find  $u \in H_0^1(\Omega)$  such that  $-\Delta u = 1$  in  $\Omega$ ,

The solution has a singularity at the reentrant angle and we wish to capture it numerically.



example of Mesh adaptation



## FreeFem++ corner singularity program

```
int[int] lab=[1,1,1,1];
mesh Th = square(6,6,label=lab);
Th=trunc(Th,x<0.5 | y<0.5, label=1);

fespace Vh(Th,P1);          Vh u,v;          real error=0.1;
problem Problem1(u,v,solver=CG,eps=1.0e-6) =
    int2d(Th)( dx(u)*dx(v) + dy(u)*dy(v) )
    - int2d(Th)( v ) + on(1,u=0);
for (int i=0;i< 7;i++)
{ Problem1;                  // solving the pde
  Th=adaptmesh(Th,u,err=error,nbvx=100000);
                               // the adaptation with Hessian of u
  plot(Th,u,wait=1,fill=1);    u=u;
  error = error/ (1000.^(1./7.)); };
```

Run:CornerLap.edp

# Poisson equation with 3d mesh adaptation

```
load "msh3" load "tetgen" load "mshmet" load "medit"
int nn = 6;
int[int] l1111=[1,1,1,1],l01=[0,1],l11=[1,1]; // label numbering
mesh3 Th3=buildlayers(square(nn,nn,region=0,label=l1111),
    nn, zbound=[0,1], labelmid=l11,labelup = l01,labeldown = l01);
Th3=trunc(Th3,(x<0.5)|(y < 0.5)|(z < 0.5) ,label=1); // remove ]0.5,1[3

fespace Vh(Th3,P1); Vh u,v; // FE. space definition
macro Grad(u) [dx(u),dy(u),dz(u)] // EOM
problem Poisson(u,v,solver=CG) =
    int3d(Th3) ( Grad(u)'*Grad(v) ) -int3d(Th3) ( 1*v ) + on(1,u=0);

real errm=1e-2; // level of error
for(int ii=0; ii<5; ii++)
{
    Poisson; Vh h;
    h[]=mshmet(Th3,u,normalization=1,aniso=0,nbregul=1,hmin=1e-3,
        hmax=0.3,err=errm);
    errm*= 0.8; // change the level of error
    Th3=tetgreconstruction(Th3,switch="raAQ"
        ,sizeofvolume=h*h*h/6.);
    medit("U-adap-iso-"+ii,Th3,u,wait=1);
}
```

Run:Laplace-Adapt-3d.edp



# Linear Lamé equation, weak form

Let a domain  $\Omega \subset \mathbb{R}^d$  with a partition of  $\partial\Omega$  in  $\Gamma_d, \Gamma_n$ .

Find the displacement  $\mathbf{u}$  field such that :

$$-\nabla \cdot \sigma(\mathbf{u}) = \mathbf{f} \text{ in } \Omega, \quad \mathbf{u} = \mathbf{0} \text{ on } \Gamma_d, \quad \sigma(\mathbf{u}) \cdot \mathbf{n} = \mathbf{0} \text{ on } \Gamma_n \quad (3)$$

Where  $\varepsilon(\mathbf{u}) = \frac{1}{2}(\nabla \mathbf{u} + {}^t \nabla \mathbf{u})$  and  $\sigma(\mathbf{u}) = \mathbf{A} \varepsilon(\mathbf{u})$  with  $\mathbf{A}$  the linear positif operator on symmetric  $d \times d$  matrix corresponding to the material propriety. Denote

$V_{\mathbf{g}} = \{\mathbf{v} \in H^1(\Omega)^d / \mathbf{v}|_{\Gamma_d} = \mathbf{g}\}$  .

The Basic displacement variational formulation is : find  $\mathbf{u} \in V_0(\Omega)$ , such that :

$$\int_{\Omega} \varepsilon(\mathbf{v}) : \mathbf{A} \varepsilon(\mathbf{u}) = \int_{\Omega} \mathbf{v} \cdot \mathbf{f} + \int_{\Gamma} ((\mathbf{A} \varepsilon(\mathbf{u})) \cdot \mathbf{n}) \cdot \mathbf{v}, \quad \forall \mathbf{v} \in V_0(\Omega) \quad (4)$$

# Linear elasticity equation, in FreeFem++ The finite element method

is just : replace  $V_g$  with a finite element space, and the FreeFem++ code :

```
load "medit"    include "cube.idp"
int[int]  Nxyz=[20,5,5];
real [int,int]  Bxyz=[[0.,5.],[0.,1.],[0.,1.]];
int [int,int]  Lxyz=[[1,2],[2,2],[2,2]];
mesh3 Th=Cube(Nxyz,Bxyz,Lxyz);

                                                                    //      Alu ...
real rhoAlu = 2600, alu11= 1.11e11 , alu12 = 0.61e11;
real alu44= (alu11-alu12)*0.5;
func Aalu = [  [alu11, alu12,alu12,    0.    ,0.    ,0.    ],
               [alu12, alu11,alu12,    0.    ,0.    ,0.    ],
               [alu12, alu12,alu11,    0.    ,0.    ,0.    ],
               [0.    ,  0.    ,  0.    , alu44,0.    ,0.    ],
               [0.    ,  0.    ,  0.    ,  0.    ,alu44,0.    ],
               [0.    ,  0.    ,  0.    ,  0.    ,0.    ,alu44]  ];
real gravity = -9.81;
```



# Linear elasticity equation, in FreeFem++

```
fespace Vh(Th, [P1,P1,P1]);
Vh [u1,u2,u3], [v1,v2,v3];
macro Strain(u1,u2,u3)
  [ dx(u1), dy(u2), dz(u3),
    (dz(u2) +dy(u3)), (dz(u1)+dx(u3)),
    (dy(u1)+dx(u2)) ]
solve Lamé([u1,u2,u3],[v1,v2,v3])=
  int3d(Th) (
    Strain(v1,v2,v3)'*(Aalu*Strain(u1,u2,u3))
- int3d(Th) ( rhoAlu*gravity*v3)
  + on(1,u1=0,u2=0,u3=0) ;

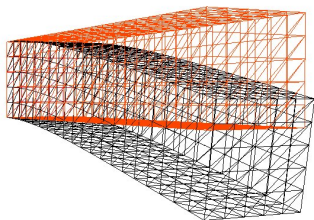
real coef= 0.1/u1[]*linfty;  int[int] ref2=[1,0,2,0];
mesh3 Thm=movemesh3(Th,
  transfo=[x+u1*coef,y+u2*coef,z+u3*coef],
  label=ref2);
plot(Th,Thm, wait=1,cmm="coef amplification = "+coef );
medit ("Th-Thm",Th,Thm);
```

// EOM

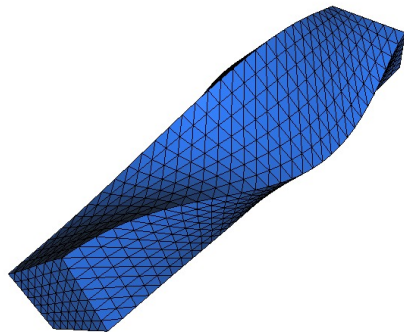


# Lame equation / figure

coef amplification = 3997.95



Run:beam-3d.edp



Run:beam-EV-3d.edp

Run:beam-3d-Adapt.edp

# Stokes equation

The Stokes equation is find a velocity field  $\mathbf{u} = (u_1, \dots, u_d)$  and the pressure  $p$  on domain  $\Omega$  of  $\mathbb{R}^d$ , such that

$$\begin{aligned} -\Delta \mathbf{u} + \nabla p &= 0 && \text{in } \Omega \\ \nabla \cdot \mathbf{u} &= 0 && \text{in } \Omega \\ \mathbf{u} &= \mathbf{u}_\Gamma && \text{on } \Gamma \end{aligned}$$

where  $\mathbf{u}_\Gamma$  is a given velocity on boundary  $\Gamma$ .

The classical variational formulation is : Find  $\mathbf{u} \in H^1(\Omega)^d$  with  $\mathbf{u}|_\Gamma = \mathbf{u}_\Gamma$ , and  $p \in L^2(\Omega)/\mathbb{R}$  such that

$$\forall \mathbf{v} \in H_0^1(\Omega)^d, \forall q \in L^2(\Omega)/\mathbb{R}, \quad \int_{\Omega} \nabla \mathbf{u} : \nabla \mathbf{v} - p \nabla \cdot \mathbf{v} - q \nabla \cdot \mathbf{u} = 0$$

or now find  $p \in L^2(\Omega)$  such than (with  $\varepsilon = 10^{-10}$ )

$$\forall \mathbf{v} \in H_0^1(\Omega)^d, \forall q \in L^2(\Omega), \quad \int_{\Omega} \nabla \mathbf{u} : \nabla \mathbf{v} - p \nabla \cdot \mathbf{v} - q \nabla \cdot \mathbf{u} + \varepsilon p q = 0$$

# Stokes equation in FreeFem++

```
... build mesh .... Th (3d) T2d ( 2d)
fespace VVh(Th, [P2,P2,P2,P1]);           // Taylor Hood FE.
macro Grad(u) [dx(u),dy(u),dz(u)]         // EOM
macro div(u1,u2,u3) (dx(u1)+dy(u2)+dz(u3)) // EOM
VVh [u1,u2,u3,p],[v1,v2,v3,q];
solve vStokes([u1,u2,u3,p],[v1,v2,v3,q]) =
  int3d(Th) (
    Grad(u1)'*Grad(v1)
    + Grad(u2)'*Grad(v2)
    + Grad(u3)'*Grad(v3)
    - div(u1,u2,u3)*q - div(v1,v2,v3)*p
    - 1e-10*q*p )
+ on(1,u1=0,u2=0,u3=0) + on(2,u1=1,u2=0,u3=0);
```

Run:Stokes3d.edp





# Eigenvalue/ Eigenvector example

The problem, Find the first  $\lambda, u_\lambda$  such that :

$$a(u_\lambda, v) = \int_{\Omega} \nabla u_\lambda \nabla v = \lambda \int_{\Omega} u_\lambda v = \lambda b(u_\lambda, v)$$

the boundary condition is make with exact penalization : we put  $1e30 = tgv$  on the diagonal term of the lock degree of freedom. So take Dirichlet boundary condition only with  $a$  variational form and not on  $b$  variational form , because we compute eigenvalue of

$$w = A^{-1}Bv$$

Otherwise we get spurious mode.

Arpack interface :

```
int k=EigenValue (A,B, sym=true, value=ev, vector=eV) ;
```

# Eigenvalue/ Eigenvector example code

```
...
fespace Vh(Th,P1);
macro Grad(u) [dx(u),dy(u),dz(u)] // EOM
varf a(u1,u2)= int3d(Th) ( Grad(u1)'*Grad(u2) + on(1,u1=0) ;
varf b([u1],[u2]) = int3d(Th) ( u1*u2 ); // no BC
matrix A= a(Vh,Vh,solver=UMFPACK),
        B= b(Vh,Vh,solver=CG,eps=1e-20);

int nev=40; // number of computed eigenvalue close to 0
real[int] ev(nev); // to store nev eigenvalue
Vh[int] eV(nev); // to store nev eigenvector
int k=EigenValue(A,B,sym=true,value=ev,vector=eV);
k=min(k,nev);
for (int i=0;i<k;i++)
    plot(eV[i],cmm="ev "+i+" v =" + ev[i],wait=1,value=1);
Execute Lap3dEigenValue.edp Execute LapEigenValue.edp
```



# Ipopt optimizer

The IPOPT optimizer in a FreeFem++ script is done with the `IPOPT` function included in the `ff-Ipopt` dynamic library. IPOPT is designed to solve constrained minimization problem in the form :

$$\begin{aligned} \text{find } x_0 = \operatorname{argmin}_{x \in \mathbb{R}^n} f(x) \\ \text{s.t. } \begin{cases} \forall i \leq n, x_i^{\text{lb}} \leq x_i \leq x_i^{\text{ub}} & \text{(simple bounds)} \\ \forall i \leq m, c_i^{\text{lb}} \leq c_i(x) \leq c_i^{\text{ub}} & \text{(constraints functions)} \end{cases} \end{aligned}$$

Where `ub` and `lb` stand for "upper bound" and "lower bound". If for some  $i, 1 \leq i \leq m$  we have  $c_i^{\text{lb}} = c_i^{\text{ub}}$ , it means that  $c_i$  is an equality constraint, and an inequality one if  $c_i^{\text{lb}} < c_i^{\text{ub}}$ .

```
func real J(real[int] &X) {...} // Fitness Function,
func real[int] gradJ(real[int] &X) {...} // Gradient
func real[int] C(real[int] &X) {...} // Constraints
func matrix jacC(real[int] &X) {...} // Constraints jacobian
matrix jacCBuffer; // just declare, no need to define yet
func matrix jacC(real[int] &X)
{... return jacCBuffer; } // fill jacCBuffer
```



# Stochastic Optimizer

This algorithm works with a normal multivariate distribution in the parameters space and try to adapt its covariance matrix using the information provides by the successive function evaluations. Syntax : `cmaes(J,u[],..)` ( )

From <http://www.lri.fr/~hansen/javadoc/fr/inria/optimization/cmaes/package-summary.html>

```
load "mpi-cmaes"
```

```
real mini = cmaesMPI(J,start,stopMaxFunEval=10000*(al+1),  
                    stopTolX=1.e-4/(10*(al+1)),  
                    initialStdDev=(0.025/(pow(100.,al))));  
SSPToFEF(best1[],best2[],start);
```

Run:cmaes-VarIneq.edp



## incompressible Navier-Stokes equation with characteristics methods

$$\frac{\partial u}{\partial t} + (u \cdot \nabla)u - \nu \Delta u + \nabla p = 0, \quad \nabla \cdot u = 0$$

with the same boundary conditions and with initial conditions  $u = 0$ .

This is implemented by using the interpolation operator for the term  $\frac{\partial u}{\partial t} + (u \cdot \nabla)u$ , giving a discretization in time

$$\begin{aligned} \frac{1}{\tau}(u^{n+1} - u^n \circ X^n) - \nu \Delta u^{n+1} + \nabla p^{n+1} &= 0, \\ \nabla \cdot u^{n+1} &= 0 \end{aligned} \tag{5}$$

The term  $X^n(x) \approx x - \tau u^n(x)$  will be computed by the interpolation operator or convect operator.

Or better we use an order 2 schema, BDF1

$$\frac{\partial u}{\partial t} + (u \cdot \nabla)u \approx \frac{(3u^{n+1} - 4u^n \circ X_1^n + u^{n-1} \circ X_2^n)}{2\tau}$$

with  $u^* = 2u^n - u^{n-1}$ , and  $X_1^n(x) \approx x - \tau u^*(x)$ ,  $X_2^n(x) \approx x - 2\tau u^*(x)$

Run: NSCaraCyl-100-mpi.edp



# Natural Convection

The coupling of natural convection modeled by the Boussinesq approximation and liquid to solid phase change in  $\Omega = ]0, 1[^2$ , No slip condition for the fluid are applied at the boundary and adiabatic condition on upper and lower boundary and given temperature  $\theta_r$  (resp  $\theta_l$ ) at the right and left boundaries.

The model is : find the field : the velocity  $\mathbf{u} = (u_1, u_2)$ , the pressure  $p$  and temperature  $\theta$  :

$$\left\{ \begin{array}{ll} \partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla \cdot \mu \nabla \mathbf{u} + \nabla p &= -C_T(\theta - \theta_0) \mathbf{e}_2 & \text{in } \Omega \\ \nabla \cdot \mathbf{u} &= 0 & \text{in } \Omega \\ \partial_t \theta + (\mathbf{u} \cdot \nabla) \theta + \nabla \cdot k_T \nabla \theta &= 0 & \text{in } \Omega \end{array} \right. \quad (6)$$

Where  $C_T(\theta - \theta_0) \mathbf{e}_2$  correspond to the Archimedes forces due to the affine dependence of density with the temperature and where  $\theta_0$  is temperature of the reference density.

Run: [boussinesq2d.edp](#)

Run: [boussinesq3d.edp](#)

Run: [boussinesq3d-mpi.edp](#)

# Phase change with Natural Convection

The starting point of the

problem is Brainstorming session (part I) of the third FreeFem++ days in december 2011, this is almost the Orange Problem is describe in web page <http://www.ljll.math.upmc.fr/~hecht/ftp/ff++days/2011/Orange-problem.pdf>.

The coupling of natural convection modeled by the Boussinesq approximation and liquid to solid phase change in  $\Omega = ]0, 1[^2$ , No slip condition for the fluid are applied at the boundary and adiabatic condition on upper and lower boundary and given temperature  $\theta_r$  (resp  $\theta_l$ ) at the right and left boundaries.

The model is : find the field : the velocity  $\mathbf{u} = (u_1, u_2)$ , the pressure  $p$  and temperature  $\theta$  :

$$\left\{ \begin{array}{lll} \mathbf{u} & \text{given} & \text{in } \Omega_s \\ \partial_t \mathbf{u} + (\mathbf{u} \nabla) \mathbf{u} + \nabla \cdot \mu \nabla \mathbf{u} + \nabla p & = -c_T \mathbf{e}_2 & \text{in } \Omega_f \\ \nabla \cdot \mathbf{u} & = 0 & \text{in } \Omega_f \\ \partial_t \theta + (\mathbf{u} \nabla) \theta + \nabla \cdot k_T \nabla \theta & = \partial_t S(T) & \text{in } \Omega \end{array} \right. \quad (7)$$

Where  $\Omega_f$  is the fluid domain and the solid domain is  $\Omega_s = \Omega \setminus \Omega_f$ .

# Phase change with Natural Convection

The enthalpy of the change of phase is given by the function  $S$ ;  $\mu$  is the relative viscosity,  $k_T$  the thermal diffusivity.

In  $\Omega_f = \{x \in \Omega; \theta > \theta_f\}$ , with  $\theta_m$  the melting temperature the solid has melt.

We modeled, the solid phase as a fluid with huge viscosity, so :

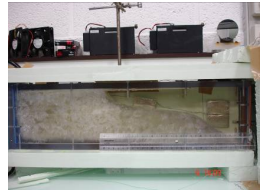
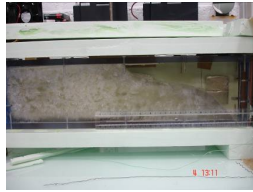
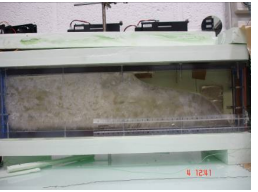
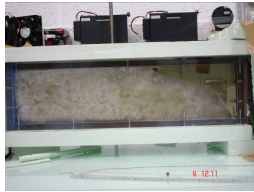
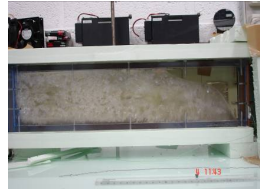
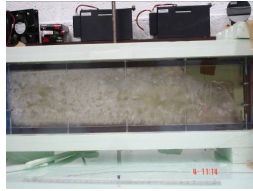
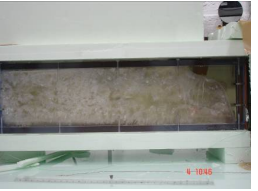
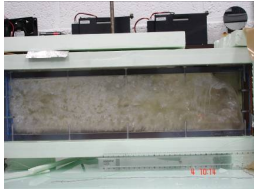
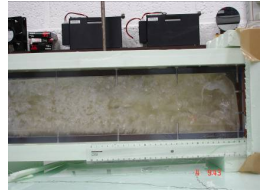
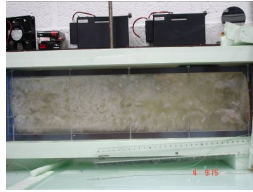
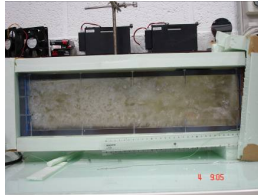
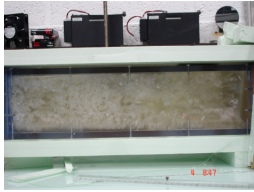
$$\mu = \begin{cases} \theta < \theta_f & \sim 10^6 \\ \theta \geq \theta_m & \sim \frac{1}{\text{Re}} \end{cases},$$

The Stefan enthalpy  $S_c$  with defined by  $S_c(\theta) = H(\theta)/S_{th}$  where  $S_{the}$  is the stefan number, and  $H$  is the Heaviside function with use the following smooth the enthalpy :

$$S(\theta) = \frac{\tanh(50(\theta - \theta_m))}{2S_{te}}.$$



# The Physical Device



# the Algorithm

We apply a fixed point algorithm for the phase change part (the domain  $\Omega_f$  is fixed at each iteration) and a full no-linear Euler implicit scheme with a fixed domain for the rest. We use a Newton method to solve the non-linearity.

- ▶ if we don't make mesh adaptation, the Newton method do not converge
- ▶ if we use explicit method diverge too,
- ▶ if we implicit the dependance in  $\Omega_s$  the method also diverge.

**Implementation** The finite element space to approximate  $u_1, u_2, p, \theta$  is defined by

**fespace** Wh (Th, [P2, P2, P1, P1]) ;

We do mesh adaptation a each time step, with the following code :

```
Ph ph = S(T), pph=S(Tp);  
Th= adaptmesh(Th, T, Tp, ph, pph, [u1, u2], err=errh,  
               hmax=hmax, hmin=hmax/100, ratio = 1.2);
```

This mean, we adapt all variables, the 2 melting phase a time  $n + 1$  and  $n$  and smooth the metric with a ratio of 1.2 to account for the motion of the melting front.



# The Newton loop

the fixed point are implemented as follows

```
real err=1e100,errp ;
for(int kk=0;kk<2;++kk) // 2 step of fixe point on  $\Omega_s$ 
{ nu = nuT; // recompute the viscosity in  $\Omega_s, \Omega_f$ 
  for(int niter=0;niter<20; ++ niter) // newton loop
  { BoussinesqNL;
    err = ulw[].linfty;
    cout << niter << "_err_NL_" << err << endl;
    u1[] -= ulw[];
    if(err < tolNewton) break; } // convergence ..
}
```



# The linearized problem

```
problem BoussinesqNL([u1w,u2w,pw,Tw],[v1,v2,q,TT])
= int2d(Th) (
    [u1w,u2w,Tw]'*[v1,v2,TT]*cdt
  + UgradV(u1,u2,u1w,u2w,Tw)'*[v1,v2,TT]
  + UgradV(u1w,u2w,u1,u2,T)'*[v1,v2,TT]
  + ( Grad(u1w,u2w)'*Grad(v1,v2)) * nu
  + ( Grad(u1,u2)'*Grad(v1,v2)) * dnu* Tw
  + cmT*Tw*v2 + grad(Tw)'*grad(TT)*kT
  - div(u1w,u2w)*q -div(v1,v2)*pw - eps*pw*q
  + dS(T)*Tw*TT*cdt )
- int2d(Th) (
    [u1,u2,T]'*[v1,v2,TT]*cdt
  + UgradV(u1,u2,u1,u2,T)'*[v1,v2,TT]
  + ( Grad(u1,u2)'*Grad(v1,v2)) * nu
  + cmT*T*v2 - eps*p*q + grad(T)'*grad(TT)*kT
  - div(u1,u2)*q -div(v1,v2)*p
  + S(T)*TT*cdt - [u1p,u2p,Tp]'*[v1,v2,TT]*cdt
  - S(Tp)*cdt*TT)
+ on(1,2,3,4, u1w=0,u2w=0)+on(2,Tw=0)+on(4,Tw=0) ;
```

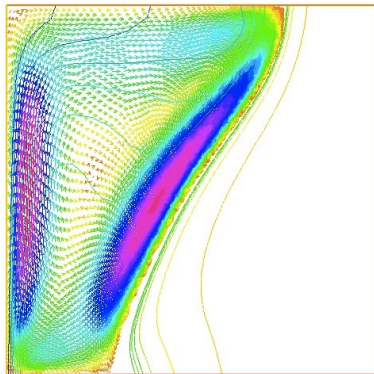
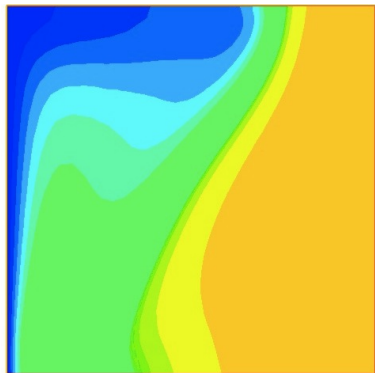
# The parameters of the computation

take case 2 from

Shimin Wang, Amir Faghri, and Theodore L. Bergman. A comprehensive numerical model for melting with natural convection. *International Journal of Heat and Mass Transfer*, January 2010.

$\theta_m = 0$ ,  $Re = 1$ ,  $S_{te} = 0.045$ ,  $Pr = 56.2$ ,  $Ra = 3.27 \cdot 10^5$ ,  $\theta_l = 1$ ,  $\theta_r = -0.1$  so in this case  $cmT = c_T = -Ra/Pr$ ,  $kT = k_T = 1/Pr$ ,  $eps = 10^{-6}$ , time step  $\delta t = 10^{-1}$ ,  $cdt = 1/\delta t$ , at time  $t = 80$  and we get a good agreement with the article.

# Phase change with Natural Convection



So now, a real problem, get the physical parameter of the real experiment.  
Run:Orange-Newton.edp

# Conclusion/Future

Freefem++ v3.20 is

- ▶ very good tool to solve non standard PDE in 2D/3D
- ▶ to try new domain decomposition domain algorithm

The the future we try to do :

- ▶ Build more graphic with VTK, paraview , ... (in progress)
- ▶ Add Finite volume facility for hyperbolic PDE (just begin C.F. FreeVol Projet)
- ▶ 3d anisotrope mesh adaptation
- ▶ automate the parallel tool

Thank for you attention.

