An introduction to scientific computing using free software FreeFem++

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Outline of this Lesson

1. **Scientific Computing and FreeFem++**
   - Purpose of the Course
   - Why using FreeFem++
   - Examples of complex problems computed with FreeFem++

Scientific Computing = branch of Applied Maths

Physics	Numerical meth.	Implementation	Results
obs/equations	PDE/num analysis.	algorithm/code	physical detail

Stages in Scientific Computing

- models –> mathematical theory of PDEs,
- numerical analysis –> mathematically sound methods,
- **algorithms –> program (software)**.

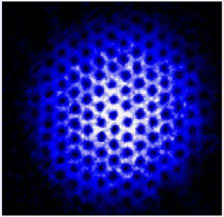
Utility of a free easy-to-use software

- check mathematical theories,
- perform numerical experiments,
- initiate collaborations with physics and industry.

Stages in Scientific Computing: an example

Physics

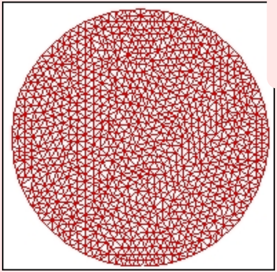
- Bose-Einstein condensate
- experiment



JILA, Colorado

Num method.

- Gross-Pitaevskii (Schrödinger) eq.
- finite elements



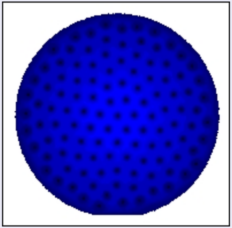
Implementation

- num method
- algorithm
- software: FreeFem++ www.freefem.org

Results

agreement

- qualitative
- quantitative



Why using FreeFem++

FreeFem++ (www.freefem.org)

Free Generic PDE solver using finite elements (2D and 3D)

- syntax close to the mathematical formulation,
- powerful mesh generator,
- mesh interpolation and adaptivity,
- easy to implement weak formulations,
- use combined P1, P2 and P4 elements,
- complex matrices available, etc.

You are welcome to participate in the:

FreeFem++ Days, Paris, December, every year.

FreeFem++ syntax: close to mathematical formulation

- create a mesh and a finite element space

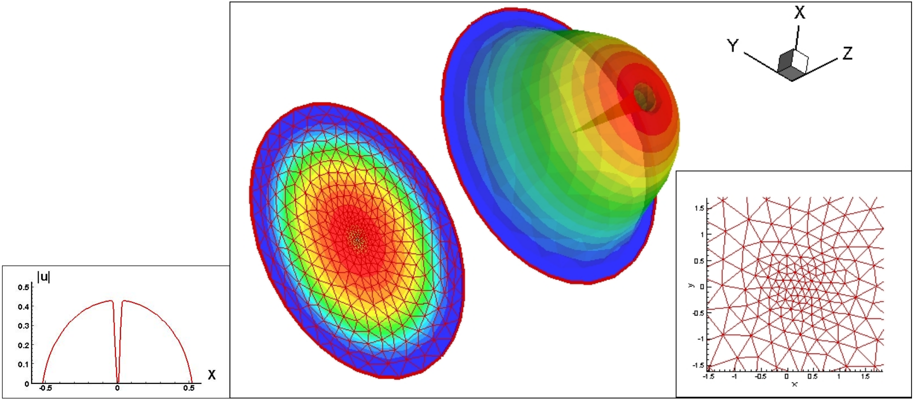
```
border circle(t=0,2*pi)
{label=1;x=Rmax*cos(t);y=Rmax*sin(t);};
mesh Th=buildmesh(circle(nbseg));
fespace Vh(Th,P1);   fespace Vh4(Th,P4);
```

- solve $-\Delta u = f$ in Ω and $u = 0$ on $\partial\Omega$

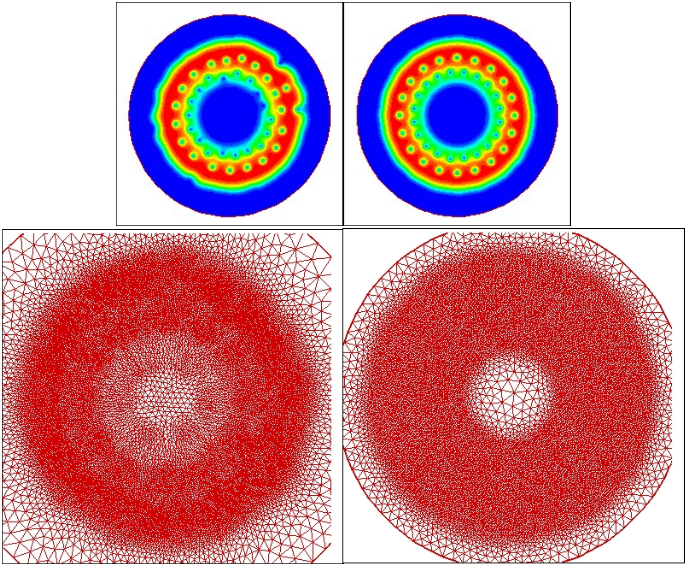
```
Vh u,v ;
problem Lap(u,v) =
int2d(Th)(u*v + dx(u)*dx(v)+dy(u)*dy(v))
- int2d(Th)(f*v)
+ on(1,u=0);

Lap; plot(u);
```

Mesh adaptivity



Mesh isotropy

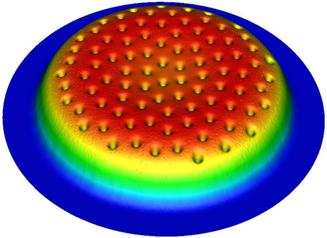


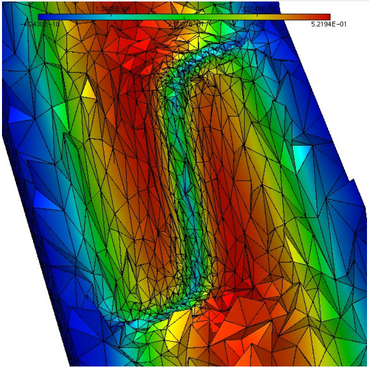
Computation of Bose-Einstein condensates

Developers: G. Vergez (PhD student), I. Danaila, F. Hecht.
submitted to CCP (to freely distribute scripts)!

- stationary Gross-Pitaevskii (Schrödinger) equation

3D anisotropic mesh adaptation, flexibility for boundary conditions,

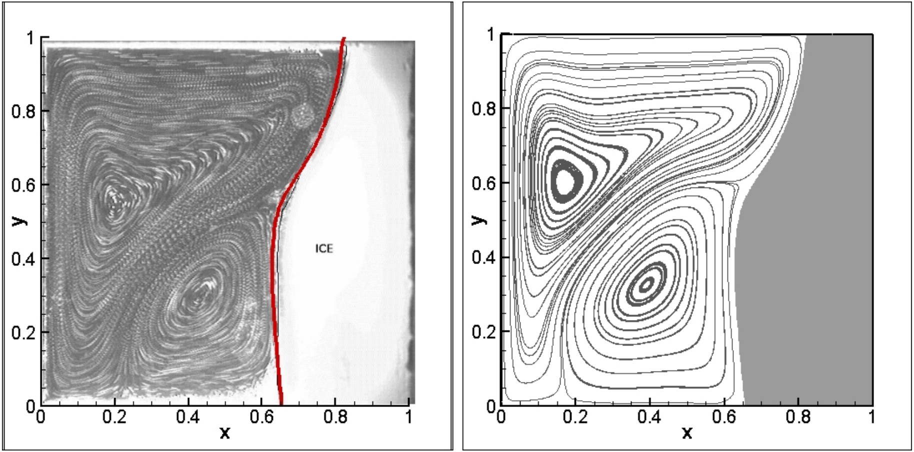




Computation of fluids with phase change

- Navier-Stokes-Boussinesq equations + phase change,
- I. Danaila, R. Moglan, F. Hecht, S. le Masson, JCP, 2014.

ice formation



Kowalewski & Rebow, Int. J. of Comput. Fluid Dynamics, 1999.

How to install FreeFem++

FreeFem++: www.freefem.org

- pre-compiled versions for Windows and MacOS,
- compilation needed for Linux,
- to write programs/scripts: use your preferred Editor (Emacs).

Explore www.freefem.org

- instructions for compilation,
- full documentation, slides from FreeFem++ days, etc
- lots of examples (.edp scripts).

FreeFem++-cs: http://www.ann.jussieu.fr/∼lehyaric/ffcs/

- pre-compiled versions for Windows, MacOS and Ubuntu,
- IDE integrated development environment,
- different graphical interface.