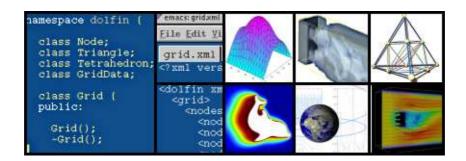
Project Course in Scientific Computing 08

Suggestions for projects



Johan Jansson Computer Science and Communication KTH

General guidelines

This document contains a list of suggested projects. Since these are only suggestions, you are welcome with your own ideas. Regard the list as an inspiration, and perhaps a hint on the expected level of your projects.

Concerning grades, the projects are divided into two parts: basic level and advanced level. Basic level means maximum grade C and advanced level means maximum grade A. It is also required that your report match the level of your project.

Good luck! Johan

 $\mathbf{2}$

1 Chemical reactions

Simulate the following system of chemical reactions, where the substances A and B react to form $C: A + B \rightarrow C$.

Consider a beaker containing a solution of A with given concentration. To this beaker, we add a drop of B every second until finally A has "completely" reacted with B. Try to find a suitable reaction to simulate in a chemistry book. Maybe the reaction you want to simulate is instead given by $2A + 3B \rightarrow 4C$, or perhaps $5A + 2B + C \rightarrow 2C$?

Model this as a system of reaction-diffusion equations, where $u_1(x,t)$ and $u_2(x,t)$ are the two concentrations to be determined.

Implement your 2D/3D solver in FEniCS/DOLFIN.

Advanced

Consider error control and adaptivity.

References

- 1. Applied Mathematics: Body and Soul, by Eriksson, Estep, and Johnson, Springer Verlag 2003.
- 2. Computational Differential Equations, by Eriksson, Estep, Hansbo, and Johnson. Studentlitteratur 1996.
- 3. Some suitable book on chemistry.

2 Heat equation

Implement a solver for the heat equation in 2D/3D and apply the solver to a realistic problem. Compute error estimates (energy norm and/or some quantity of the solution). Compare your results to known data or a model problem with exact solution and study convergence with regard to mesh size h and time step k.

Advanced

Implement space-time adaptivity.

References

- 1. *Applied Mathematics: Body and Soul*, by Eriksson, Estep, and Johnson, Springer Verlag 2003.
- 2. Computational Differential Equations, by Eriksson, Estep, Hansbo, and Johnson. Studentlitteratur 1996.

3 The Navier-Stokes equations

Implement a solver for the Navier-Stokes equations in 2D or 3D.

Advanced

Nothing extra is needed for advanced level.

References

- 1. Applied Mathematics: Body and Soul, by Eriksson, Estep, and Johnson, Springer Verlag 2003.
- 2. Computational Differential Equations by Eriksson, Estep, Hansbo, and Johnson. Studentlitteratur 1996.
- 3. Computational Turbulent Incompressible Flow by Hoffman and Johnson. Springer, 2007 http://www.springer.com/math/cse/book/978-3-540-46531-7.

4 Elasticity

Implement a solver for linear elasticity in 2D/3D and consider adaptivity.

Advanced

Consider large displacements/deformations or a multiphysics application (fluid-structure interaction, elasticity-electromagnetics, etc.)

References

 Beyond the Elements of Finite Elements: General Principles for Solid and Fluid Mechanics Applications by Hansbo. Department of Solid Mechanics, Chalmers University of Technology, 2002

5 The Wave equation

Read the technical report by L.Beilina and implement the hybrid method in 2D.

Advanced

Implement the absorbing boundary condition.

References

- 1. A Hybrid Method for the Wave Equation, by L. Beilina, Technical report, Chalmers Finite Element Center (2001)
- 2. Applied Mathematics: Body and Soul, by Eriksson, Estep, and Johnson, Springer Verlag 2003.
- 3. Computational Differential Equations by Eriksson, Estep, Hansbo and Johnson. Studentlitteratur 1996.

6 Bistable equation

Write a solver in Dolfin for the bistable equation in 2D/3D, which is an easy example of a nonlinear PDE, consider fixed-point iteration and Newton's method.

Advanced

Consider error estimation and adaptivity using duality.

References

1. Body and Soul computer sessions (Reaction-Diffusion): http://www.phi.chalmers.se/bodysoul/sessions/.

7 The compressible Euler equations

Implement a solver for the compressible Euler equations in FEniCS (very advanced) with a simple model problem. Contact me for further details.

Advanced

Nothing extra is needed for advanced level.

References

- 1. *Applied Mathematics: Body and Soul*, by Eriksson, Estep, and Johnson, Springer Verlag 2003.
- 2. Computational Differential Equations by Eriksson, Estep, Hansbo, and Johnson. Studentlitteratur 1996.

8 Maxwell's equations

Implement a solver for Maxwell's equations in FEniCS (fairly advanced). You can choose to use edge elements (Nedelec) or a stabilized method achieve this. Ask the teacher for material on computational electromagnetics if you are interested in such a project.

Advanced

Nothing extra is needed for advanced level.

References

- 1. *Applied Mathematics: Body and Soul*, by Eriksson, Estep, and Johnson, Springer Verlag 2003.
- 2. Computational Electromagnetics by Bondeson, Rylander and Ingelstrm. Springer 2005.