FYS-4096 Computational Physics: Exercise 6

Ilkka Kylänpää

Week 7

General:

- You should have access to `ex6_help` on teacher's help file. There you will find various solutions to our previous assignments. These are needed in problem 4.
- **Deadline always before noon on Monday the following week!** That is, for these problems before noon on Monday February 22.

Problem 1: (Pen and paper or equivalent) Derive the weak form for

a) $\nabla^2 u(\mathbf{r}) = f(\mathbf{r})$, where the boundary values include Dirichlet boundary conditions on Γ_D and Neumann boundary conditions on Γ_N.

b) $u'' + 2u' + u = f$ with Dirichlet boundary conditions $u(\pm L) = 0$.

c) $-\frac{1}{2}\frac{\partial^2}{\partial x^2}\phi(x) + V(x)\phi(x) = E\phi(x)$, where $\phi(x)$ is a real valued function in interval $x \in [0, L]$ with Dirichlet boundary conditions $\phi(0) = \phi(L) = 0$.

d) coupled equation set $\nabla^2 u(\mathbf{r}) = f(\mathbf{r}) + v(\mathbf{r})$ and $\nabla^2 v(\mathbf{r}) = g(\mathbf{r}) + u(\mathbf{r})$ with zero Dirichlet boundary conditions.

Problem 2: 1D FEM for Poisson equation

- Solve 1D Poisson equation

$$\frac{d^2\Phi}{dx^2} = -\frac{\rho(x)}{\varepsilon_0} \tag{1}$$

with your own finite element code, when $\rho(x) = \varepsilon_0 \pi^2 \sin(\pi x)$ and boundary conditions are $\Phi(0) = \Phi(1) = 0$.

a) Make a code that utilizes the analytical formulas for the hat function basis (using uniform grid), i.e.,

$$\begin{aligned}
A_{ij} &= \int_0^1 u_j'(x)u_i'(x)dx = \begin{cases} 2/h & \text{for } i = j \\ -1/h & \text{for } i = j \pm 1 \\ 0 & \text{otherwise,} \end{cases} \\
b_i &= \frac{1}{\varepsilon_0}\int_0^1 \rho(x)u_i(x)dx = \frac{\pi}{h}(x_{i-1} + x_{i+1} - 2x_i)\cos(\pi x_i) + \frac{1}{h}\left[2\sin(\pi x_i) - \sin(\pi x_{i-1}) - \sin(\pi x_{i+1})\right]
\end{aligned} \tag{2}$$

  - Test your numerical solution against the analytical solution $\Phi(x) = \sin(\pi x)$ by making a figure and considering some kind of numerical measure for accuracy.

b) Once the code in Problem 2a) is working, make a new function / code where you modify the previous code to also perform the integrations with a numerical integration formula (e.g., trapezoid or Simpson rule).

- The hat functions (for a uniform grid) are given as

$$u_i(x) = \begin{cases} (x - x_{i-1})/h & \text{for } x \in [x_{i-1}, x_i] \\ (x_{i+1} - x)/h & \text{for } x \in [x_i, x_{i+1}] \\ 0 & \text{otherwise,} \end{cases} \tag{3}$$

  where you can choose $h = x_i - x_{i-1}$ due to assuming uniform grid. Modification to non-uniform is trivial. Notice that you also need its first derivative. Notice: once you have coded the hat functions and their derivative it's good to plot them on a grid to validate they are working as expected.

c) In case of finite difference method, you could also solve this as $A\mathbf{x} = \mathbf{b}$. What are your A, $\mathbf{x}$, and $\mathbf{b}$ like in this case (finite difference forms)? Answer these questions by making a function that solves this problem with finite difference, and compare to the analytical solution.

- Notice that in all cases you can use numpy's `linalg.solve(A,b)` for obtaining the solution $\mathbf{x}$ in $A\mathbf{x} = \mathbf{b}$.

Problem 3: Getting familiar with FEniCS software

a) Install FEniCS software on your computer.

b) Solve the Poisson equation with FEniCS following the instructions given at this link.

c) Solve the heat equation with FEniCS following the instructions given at this link.

Problem 4: Evaluation of performance

a) In the teacher's help file repo you will find a folder `ex6_help`.
   - There you will find solutions to the problems made by you and your fellow course participants.
   - Look into the different solutions for the problems. You might find useful coding and/or Python related details.
   - Did you find something of interest in the solutions made by others?

b) Answer the following inquiries:
   - Mention two to four new / useful things you have enjoyed learning thus far in the course.
   - Do you think the subjects so far will benefit you in your future endeavors? Why?
   - How well have you so far done personally? What has been challenging in the course so far? Have you been able to schedule a suitable amount of time for the course?

- Write the answers into a text file problem4.txt and remember to add the file into your repo.

Returning your exercise

1. Make a new folder "exercise6" to your existing Computational Physics repo.
2. In folder "exercise6" write a comma separated list of problems you have solved, e.g., 1,2a,2b,4, into a file called solvedProblems.txt.
3. Make sure all your source files are under version control and push them to GitLab. **Also the derivations related to Problem 1!**
4. Push your commits (and possible tags) to GitLab before noon on Monday February 22:
   ```
   git push --all && git push --tags
   ```