PROJECT - MODELING

In this project you learn to use general ODEs and PDEs to model a problem of your choice from Section 5 below. You should determine appropriate data for the ODE/PDE, run simulations, and draw conclusions about the problem from your simulations. You should also identify possible sources of error in your simulations and in your model. The project is carried out in groups of 2-4 students.

1. Examination

Examination consists of two submissions of a 3-part project report (part A-C). The format is the following: a first submission should be a PDF document of maximum 10 pages (parts A, B, C) and after a peer-review by another group, a final report of maximum 10 pages (revised versions of A, B, C), including a title page. You should also submit an archive electronically with all computer code that you have written in your project. You pass the project if you: (i) submit the 2 reports, (ii) write a separate 1 page peer review report on the first report of another group, and (iii) submit and present your maximum 10 page final report in a seminar at the end of the course.

The 3 parts of the reports are:

- A Determine relevant data and use an ODE model to simulate your problem, analyze your results in terms of the underlying problem, and comment on possible sources of errors.
- B Determine relevant data and formulate a PDE model for your problem.
- C Use your PDE model from B to simulate your problem, analyze the results in terms of the underlying problem, and comment on possible sources of errors.

As part of the project you should answer the questions posed in Module 6 (attached to the end of this specification).

2. Extra course DN1242

The extra course DN1242 consists of an additional partial submission for the project in the form of an a posteriori error analysis of the ODE-part of the project, as described in module 4. The submission should be 4 extra pages where the background theory is briefly presented, and then applied to your respective problem. If the error analysis includes the solution of a dual problem, the numerical approximation of that dual problem should be presented along with plots of the dual solution.

3. Goals

Model real world problems using ODE and PDE models.

- Apply a given model to simulate a real world problem.

- Interpret the results from the simulation with respect to the underlying problem.
- Estimate the accuracy of the simulation, and connect to the underlying problem.

4. SOFTWARE INTERFACES

In the project you may use software tools from the modules in the course, which you can modify and complement with new code that you write yourself.

With each project project suggestion, we provide prototype ODE and PDE solvers which you may use if you wish. See the project descriptions for details.

5. PROJECT SUGGESTIONS

Below we present 3 different ODE/PDE models, that can be used to model a range of phenomena. For a full model, coefficients have to be chosen and initial and boundary conditions have to be specified for a complete model.

5.1. **Convection-diffusion-reaction.**

The convection-diffusion-reaction of the concentration of one species u_1, which is consumed by another species of concentration u_2, can be described by the following ODE and PDE models:

ODE:

$$\dot{u}_1 = -\alpha_1 u_1 u_2 \tag{1}$$

$$\dot{u}_2 = \alpha_2 u_1 u_2 - \alpha_3 u_2 \tag{2}$$

Here α_i are reaction coefficients.

Ref: Volterra-Lotka

Prototype: See module 4.

PDE:

$$\dot{u} + \beta \cdot \nabla u - \epsilon \Delta u = f(u) \tag{3}$$

where u and ϵ may be vector-valued with several components:

$$u = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \quad \epsilon = \begin{pmatrix} \epsilon_1 & 0 \\ 0 & \epsilon_2 \end{pmatrix} \tag{4}$$

Here β is a convection velocity vector and ϵ a diffusion coefficient, and $f(u)$ can be the reaction part from the ODE model and a source/sink term.

Choose one of the following problems to model (or come up with one yourself, but verify with a teacher first that it's reasonable):

- An oil leak in the Mexican gulf, with u_1 concentration of oil, and u_2 concentration of bacteria consuming the oil. Choose here $\epsilon = \bar{\epsilon} + h$, with $\bar{\epsilon}$ the physical diffusion coefficient (very small) and $h(x)$ the max edge length of the triangles to avoid instabilities/artificial oscillations in the solution.
- A stirred chemical reaction in a beaker, with u the concentration of a number of chemicals.
  References:
  Convection-diffusion-reaction computer session
- The FitzHugh-Nagumo model for neural wave propagation, see Scholarpedia and DN2266

Prototype: See module 6.

5.2. **Wave models.** Wave phenomena can be modeled by a mass-spring model in an ODE, or using a PDE wave equation:

ODE:

$$\dot{x}^i = v^i \tag{5}$$

$$\dot{v}^i = \frac{F^i}{m^i} \tag{6}$$

$$F^i = \sum_{j=0}^{N} F^{ij} \tag{7}$$

$$F^{ij} = E(r^{ij} - L^{ij})e^{ij} \tag{8}$$

Here E is the spring stiffness, $L^{ij} = 0$ a rest length, $r^{ij} = |x^i - x^j|$ and $e^{ij} = \frac{x^j - x^i}{r^{ij}}$.

Prototype: See module 4.

PDE:

$$\dot{u}_1 = u_2 \tag{9}$$

$$\dot{u}_2 - c^2 \Delta u_1 - \epsilon \Delta u_2 = 0 \tag{10}$$

Here c is a speed of sound in the material and ϵ is a damping coefficient.

These models may be used in 1D to model the sound of a guitar string, given an initial condition on the shape of the string, or in 2D to model the sound of a drum membrane.

Prototype: See module 6.

5.3. **Solid mechanics.** Elasticity can be modeled by a mass-spring model in an ODE, or using a PDE model:

ODE:

$$\dot{x}^i = v^i \tag{11}$$

$$\dot{v}^i = \frac{F^i}{m^i} \tag{12}$$

$$F^i = \sum_{j=0}^{N} F^{ij} \tag{13}$$

$$F^{ij} = E(r^{ij} - L^{ij})e^{ij} \tag{14}$$

Here E is the spring stiffness, $L^{ij} = 0$ a rest length, $r^{ij} = |x^i - x^j|$ and $e^{12} = \frac{x^2 - x^1}{r^{12}}$.

Prototype: See module 4.

PDE: A linear model for small deformations:

$$\dot{u}_1 = u_2 \tag{15}$$

$$\dot{u}_2 - \nabla \cdot \sigma = 0 \tag{16}$$

$$\sigma = \frac{1}{2}E(\nabla u_1 + \nabla u_1^T) \tag{17}$$

Here E is a stiffness modulus.

The model may be extended to model large deformations by moving the domain (and thus, the mesh) along with the deformation. Contact the teachers for a formulation and prototype of the model.

These models can be used to model colliding elastic bodies, by including collision detection and a contact model.

Prototype: See module 6.