Chalmers / University of Gothenburg
University of Copenhagen
University of Oslo

2017

Nordic Graduate Course on

Computational Mathematical Modeling

Project guidelines and suggestions

Guidelines

Between the first and second course weeks, students should complete a project assignment to be presented during the second course week in Oslo (August 14–18 2017).

- Assignments should be carried out in project teams consisting of two students.
- Project teams should be composed of students from different countries/schools.
- Use online tools for collaboration (Slack, Git, Bitbucket, GitHub, quay.io, Docker Hub, etc) during the summer.
- The first assignment is to choose and plan a project and outline the project plan in a two-page document. The project plan should be submitted by **June 1 2017** to **carlun@chalmers.se** for approval.
- The project should be presented at the second course week, both as a 10 minute oral presentation and in the form of a scientific poster.
- This document contains a list of project ideas for inspiration. Project ideas can be modified or extended, or you may choose to suggest an entirely different project.

Project 1: Virtual City CFD

Project proposal by Anders Logg <logg@chalmers.se>

Task

Simulate the flow of wind through a virtual city.

Background

One of the major forces of our modern society is urbanization. More and more people are moving into cities and it is predicted that by 2050, 70% of the world's population will live in cities. Our cities are getting bigger, higher and more important. In addition, migration is challenging the supply of housing in existing urbanizations and calls for development of new areas and modernization of existing settlements.

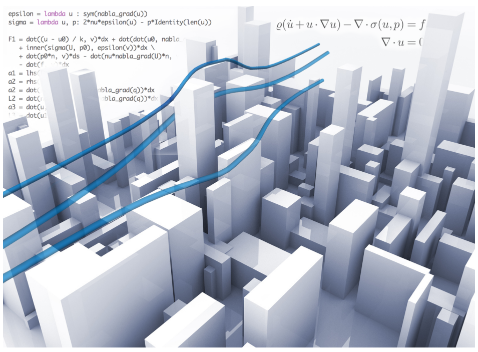
In face of the importance of cities and the rapid growth of new cities, it becomes important to simulate cities in order to study effects of wind, temperature, pedestrian flow, traffic flow etc. In other words, this calls for the development of *virtual cities* that can be simulated, analyzed and optimized before the actual city is built.

Guidelines

- Write a Navier–Stokes solver in FEniCS.
- Generate mesh data for a city (or part of a city) based on 2.5D data using FEniCS mshr (or another mesh generation tool of choice).
- Simulate the flow of wind through the city under realistic assumptions.
- Visualize the results by building a 3D model of the city in the Unity Game Engine. Add textures to create an appealing visualization.

Resources

- `https://unity3d.com/`
- `https://en.wikipedia.org/wiki/3D_city_models`
- `http://www.3dcitydb.net/3dcitydb/3dcitydbhomepage/`



Project 2: Fluid–structure interaction (FSI)

Project proposal by Anders Logg `<logg@chalmers.se>`

Task

Implement a fluid–structure interaction solver.

Background

Fluid–structure interaction (FSI) is an important multiphysics problem involving both fluid flow (described by, e.g., the incompressible Navier–Stokes equations) and the deformation of elastic bodies (described by, e.g., a hyperelastic model). Applications include the deformation of bridges, propellers, aircraft flutter, heart valve mechanics and many more.

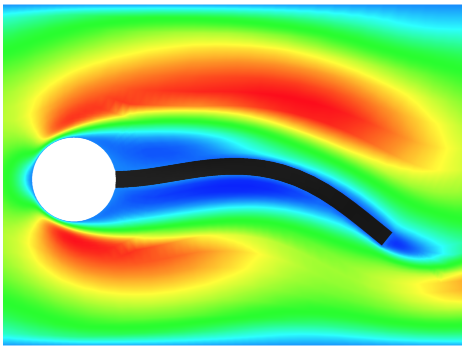
The FSI problem can be solved either using a *monolithic approach*, where one big system is solved for both the fluid and structure degrees of freedom in each time step, or using a *segregated approach*, where one solver is used for the fluid and another for the structure, with iterative updates between the two solvers.

Guidelines

- Write a fluid–structure interaction solver in FEniCS.
- Choose either a monolithic or segregated approach.
- Study the effect of the relative densities of the fluid and the structure. In particular, study the effect of the efficiency the iterative solver and stability of the FSI formulation when the density of the structure becomes relatively small in comparison to the fluid.
- Test your solver on the FLUSTRUK FSI benchmark.

Resources

- `https://folk.uio.no/selim/new_thesis.pdf`
- `https://fenicsproject.org/pub/workshops/fenics13/slides/Balaban.pdf`
- `http://www.featflow.de/en/benchmarks/cfdbenchmarking/fsi_benchmark.html`



Project 3: The elasticity of the brain

Project proposal by Kent-Andre Mardal `<kent-and@simula.no>`

Background

Various forms of dementia are associated with reduced compliance and amplified intracranial pressure pulsations. In this project we will conduct several numerical experiments to gain an understanding of the biomechanics of the brain.

Guidelines

Let us assume that the brain consists of a linear elastic material with Young´s modulus of 5kPa. The brain is bathed in water (cerebrospinal fluid) and the pressure in the water pulsate between 0-5 mm Hg during the cardiac cycle. It is also known that the deformation of the brain during one cardiac cycle is around 1 cc (cm^3). Because the brain is bathed in water, we have to use Neumann conditions everywhere to impose the pressure. We suggest that the method of Lagrange multipliers are used to remove the rigid motions instead of pin-pointing.

a) Write up problem with proper units. Because the mesh is in mm, the canonical choice would be mm, s, g.

b) Implement a simulator that works for both the unit cube and the brain mesh. Scale the unit cube such that its volume is similar to the brain. Use the method of manufactured solutions to generate a test problem and verify the simulator on both the unit cube and brain mesh.

c) Compute the compression cause by a pressure of 5 mmHg. Compare the result of the unit cube and the brain mesh.

c) Compute the compression cause by a pressure of 5 mmHg with Poisson ratio 0.3, 0.4, 0.45, 0.49, and 0.49.

d) Compute the ten lowest eigenvalues and eigenvectors by solving a generalized eigenvalue problem as described in the notes.

Resources

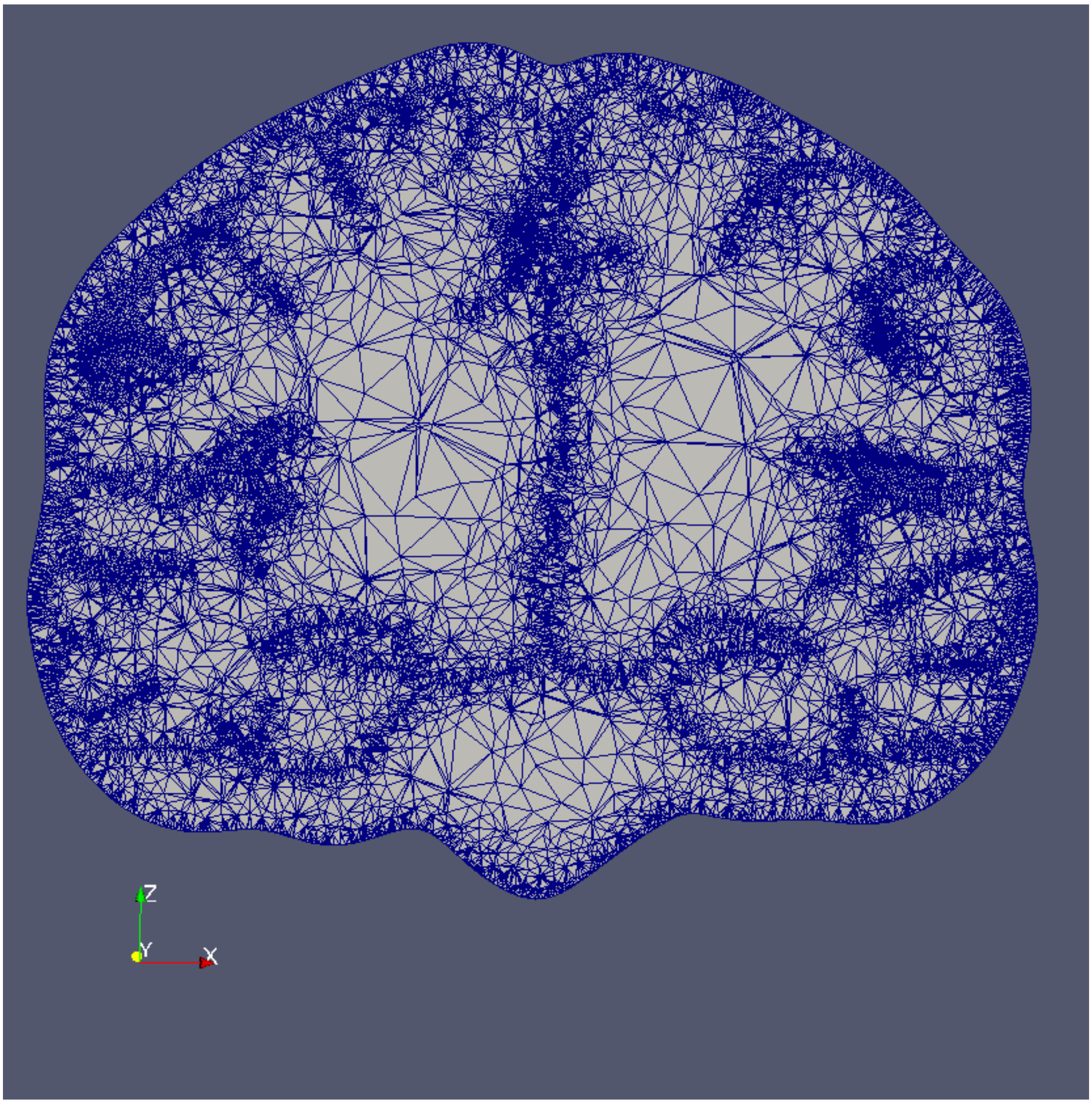
Data: http://http://folk.uio.no/kent-and/cmm/

Readings (of more involved modeling):

K. H. Støverud, M. Alnæs, H. P. Langtangen, V. Haughton, and K.-A. Mardal. Poro-elastic modeling of syringomyelia–a systematic study of the effects of pia mater, central canal, median fissure, white and gray matter on pressure wave propagation and fluid movement within the cervical spinal cord. Computer methods in biomechanics and biomedical engineering, 19(6):686–698, 2016.

P. K. Eide. The correlation between pulsatile intracranial pressure and indices of intracranial pressure- volume reserve capacity: results from ventricular infusion testing. Journal of neurosurgery, 125(6): 1493–1503, 2016.

Vardakis, John C., Brett J. Tully, and Yiannis Ventikos. Multicompartmental poroelasticity as a platform for the integrative modeling of water transport in the brain."Computer models in biomechanics. Springer Netherlands, 2013. 305-316.



Project 4: Electroconvulsive therapy

Project proposal by Kent-Andre Mardal `<kent-and@simula.no>`

Background

Major depression is currently the world's primary cause of disability. Electroconvulsive therapy is a treatment option that leads to improvement in 50-70% and is hence the therapy with best effect. Still, the treatment remains stigmatized. The electroconvulsive therapy induces an epileptic seizure. In this project we will investigate whether the Bidomain equations permit seizure developement under reasonable conditions.

Guidelines

The Bidomain equations are:

$$
\begin{aligned}
u_t &= \nabla \cdot (M_e \nabla(u)) + \nabla \cdot (M_e \nabla(v)) && (1)\\
0 &= \nabla \cdot (M_e \nabla(ue)) + \nabla \cdot (M_{i+e} \nabla(v). && (2)
\end{aligned}
$$

Here, u and v are the unknown extracellular and transmembrane potential, respectively, and M_i and M_e are the intracellular and extracellular conductivities and $M_{i+e} = M_i + M_e$. We may assue that $M_i = 3$ S/m and $M_e = 0.2$ S/m and S is the Simens unit.

a) Write up problem with proper units. Because the mesh is in mm, the canonical choice would be mm, s, and perhaps μS.

b) Implement a simulator that works for both the unit cube and the brain mesh. Scale the unit cube such that its volume is similar to the brain. Use the method of manifactured solution to generate a test problem and verify the simulator on both the unit cube and brain mesh.

c) Use a boundary condition which is $u_{bc} = A\sin(bt)(\exp(-a(x-x_0)^2) + \exp(-a(x-x_1)^2))$, with $a = 0.1, 1.0,$ and 10.0 and $v_{bc} = 0$, with $A = 200mA$. Here x_0 and x_1 are typically points at the left side and the top of the head. Duration of puls is typically 0.5 ms.

d) Compute the ten lowest eigenvalues and eigenvectors by solving a generalized eigenvalue problem as described in the notes.

Resources

Data: http://http://folk.uio.no/kent-and/cmm/

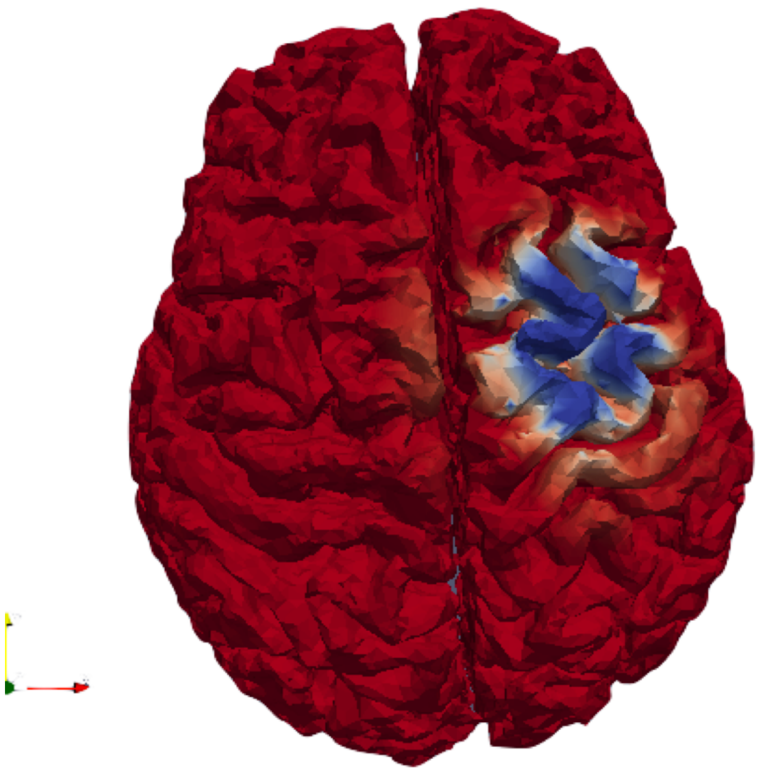
Readings (of more involved modeling):

Sundnes J, Lines GT, Cai X, Nielsen BF, Mardal KA, Tveito A. Computing the electrical activity in the heart. Springer Science & Business Media; 2007 Jun 26.

Lee WH, Lisanby SH, Laine AF, Peterchev AV. Comparison of electric field strength and spatial distribution of electroconvulsive therapy and magnetic seizure therapy in a realistic human head model. European Psychiatry. 2016 Aug 31;36:55-64

Deng ZD, Lisanby SH, Peterchev AV. Controlling stimulation strength and focality in electroconvulsive therapy via current amplitude and electrode size and spacing: comparison with magnetic seizure therapy. The journal of ECT. 2013 Dec;29(4):325.

Lisanby SH. Electroconvulsive therapy for depression. New England Journal of Medicine. 2007 Nov 8;357(19):1939-45.



Project 5: Zebrafish and Cancer

Project proposal by Kent-Andre Mardal `<kent-and@simula.no>`

Background

Zebrafish is a popular laboratory animal that is commonly used for studying various diseases. The control of the DNA of the fish allows scientists to create (among other things) transparent animals which allow detail investigation of the interior. Cancer cells are known to manipulate the vasculature in order to amplify delivery of nutritions, by making the vasculature more torturous, permeable and more numerous near the tumor. Zebrafish infected with human cancer cells is therefore used to gain an understanding of cancer.

Guidelines

In this project we will model the blood flow in the vasculature of a zebrafish to investigate the pressure and shear stress involved in the blood flow of a zebra fish. We assume that the viscosity of blood is $\mu = 3.5$mPa s, the flow is assumed laminar and stationary with an inlet velocity of $v_i = 1$mm/s and pressure drop is expected to be less than 1 mmHg per mm.

a) Write up problem with proper units. Notice that the mesh is in μm. Compute the Reynolds number.

b) Implement a simulator that works for both the unit cube and the zebra fish mesh. Scale the unit cube such that its volume is similar to the zebra fish. Use the method of manifactured solution to generate a test problem and verify the simulator on both the unit cube and zebra fish mesh.

c) Check if the expected convergence rates are satisifed for the manifactured solution with $P_2 - P_1$ elements and with a stabilized $P_1 - P_1$ method.

d) Estimate the mesh size required to obtain an estimate of the shear-stress at the wall within 5% error.

Resources

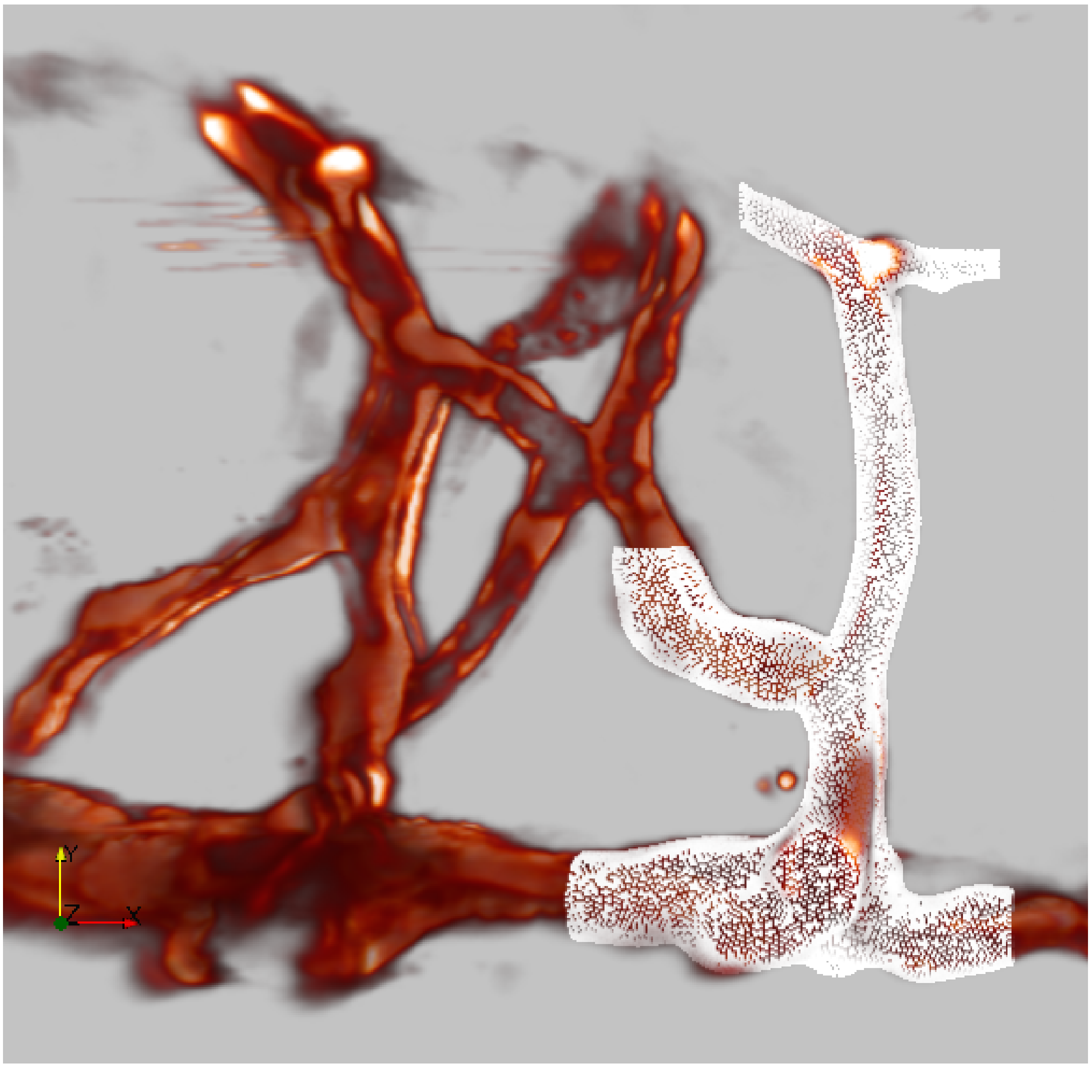
Data: http://http://folk.uio.no/kent-and/cmm/

Readings (of related modeling):

Baxter LT, Jain RK. Transport of fluid and macromolecules in tumors. I. Role of interstitial pressure and convection. Microvascular research. 1989 Jan 31;37(1):77-104.

Evensen L, Johansen PL, Koster G, Zhu K, Herfindal L, Speth M, Fenaroli F, Hildahl J, Bagherifam S, Tulotta C, Prasmickaite L. Zebrafish as a model system for characterization of nanoparticles against cancer. Nanoscale. 2016;8(2):862-77.

Luca Fieramonti, Efrem A Foglia, Stefano Malavasi, Cosimo D'Andrea, Gianluca Valentini, Franco Cotelli, and Andrea Bassi. Quantitative measurement of blood velocity in zebrafish with optical vector field tomography. Journal of biophotonics, 8(1-2):52–59, 2015.



Vasculature of a zebrafish

Project 6: Moving mesh and image registration

Project proposal by Klas Modin <klas.modind@chalmers.se>

Background

Greatly improved medical imaging techniques allow us to capture detailed 3D images of inner organs without surgery. A central problem in mathematical imaging is *registration*. The problem consists in finding warps to match anatomical correspondences between images, thereby allowing voxel-by-voxel comparisons; an illustrative 2D example is given in the figure below. Computational anatomy (CA) is the new paradigm of image registration, rigorously founded in several established fields of mathematics, particularly fluid dynamics and PDE analysis.

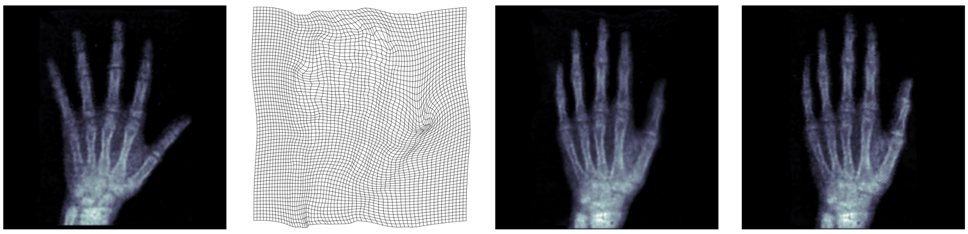
In the CA, the registration problem is formulated as a flow equation (PDE) evolving on a manifold. The image warp can be thought of as a moving mesh. The project at hand consists in using FEniCS to solve the moving mesh PDE in CA. This approach to CA is completely novel, with great promise.

Guidelines

- Study the gradient flow equations of computational anatomy.
- Suggest a FEM setup based on a moving mesh formulation.
- Test the method for 2D and 3D registration.

Resources

- https://en.wikipedia.org/wiki/Computational_anatomy
- http://dx.doi.org/10.1137/151006238



(a) Template (b) Mesh warp (c) Transformed (d) Target

Project 7: Numerical homogenization

Project proposal by Axel Målqvist `<axel@chalmers.se>`

Task

Computing effective material parameters using Homogenization

Background

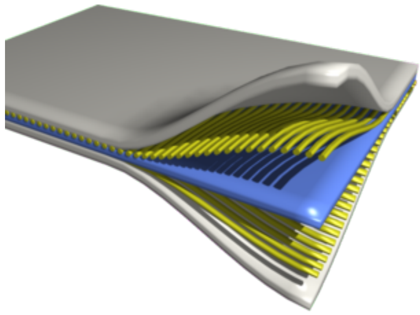
A composite material is made out of two or more constituent materials with different physical properties. By combining materials one can achieve designed materials that e.g. are lighter, stronger, or cheaper than conventional materials. Because of these advantages composites are used in various engineering applications such as cars, airplanes, and buildings. Numerical simulation is crucial in design and evaluation of composites. However, the rapid variation in data (between the constituent materials) poses challenges both for on discretization techniques and linear algebra solvers.

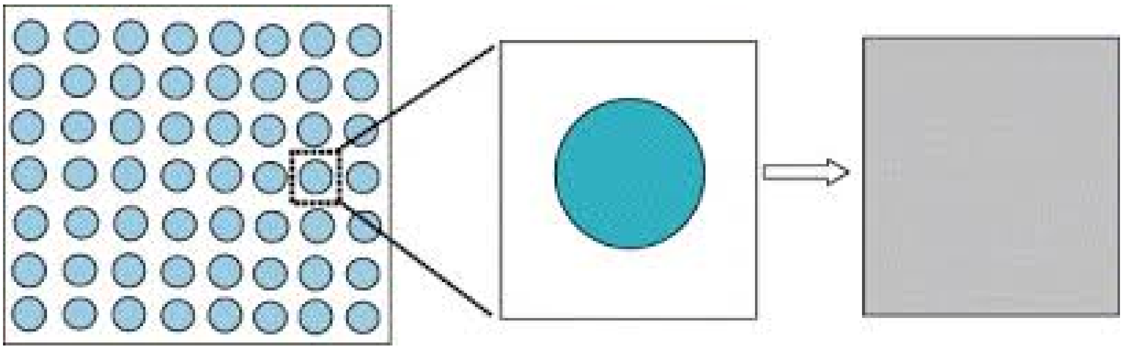
Guidelines

- Show in a one dimensional example that the mesh needs to resolve the data variation in order to converge at optimal rate for the P1 finite element method. Consider the Poisson equation, $-\nabla cdot A \nabla u = f$ in 1D with e.g. $A(x) = (2 + \cos(\frac{2\pi x}{\epsilon}))^{-1}$, $f(x) = 1$, with homogeneous Dirichlet boundary conditions, where ϵ is a small parameter.
- Consider now the Poisson equation in 2D or 3D on a unit square or cube. Use homogenization theory to numerically (using FEniCS) compute an effective diffusion coefficients, for problems with periodic diffusion. Implement periodic boundary conditions and solve the cell problem to compute the effective diffusion coefficient.
- Compare the result to the finite element method and study how the error depends on the period ϵ and the mesh size h. Also investigate the accuracy in the Homogenized solution for more complicated computational domains.
- Investigate how the convergence of iterative solvers depend on frequency and amplitude of the periodic data in the finite element approximation.

Resources

- `https://en.wikipedia.org/wiki/Composite_material`
- `http://www.cmap.polytechnique.fr/~allaire/homog/lect1.pdf`
- `https://en.wikipedia.org/wiki/Asymptotic_homogenization`





Project 8: Simulated interaction between liquids and clothes

Project proposal by Marco Fratarcangeli <*marcof@chalmers.se*>

Task

Simulate the interaction between liquids (e.g., water) and a piece of cloth.

Background

The problem of modeling 3D soft objects (like thick clothes made of different textile materials, virtual flesh, etc.), is of prominent importance in many theoretical and industrial fields including computational design and medical fields. Such kind of objects usually demonstrates complex shape changes under external interactions, which makes them challenging to simulate, in particular when short response times are needed for virtual prototyping.

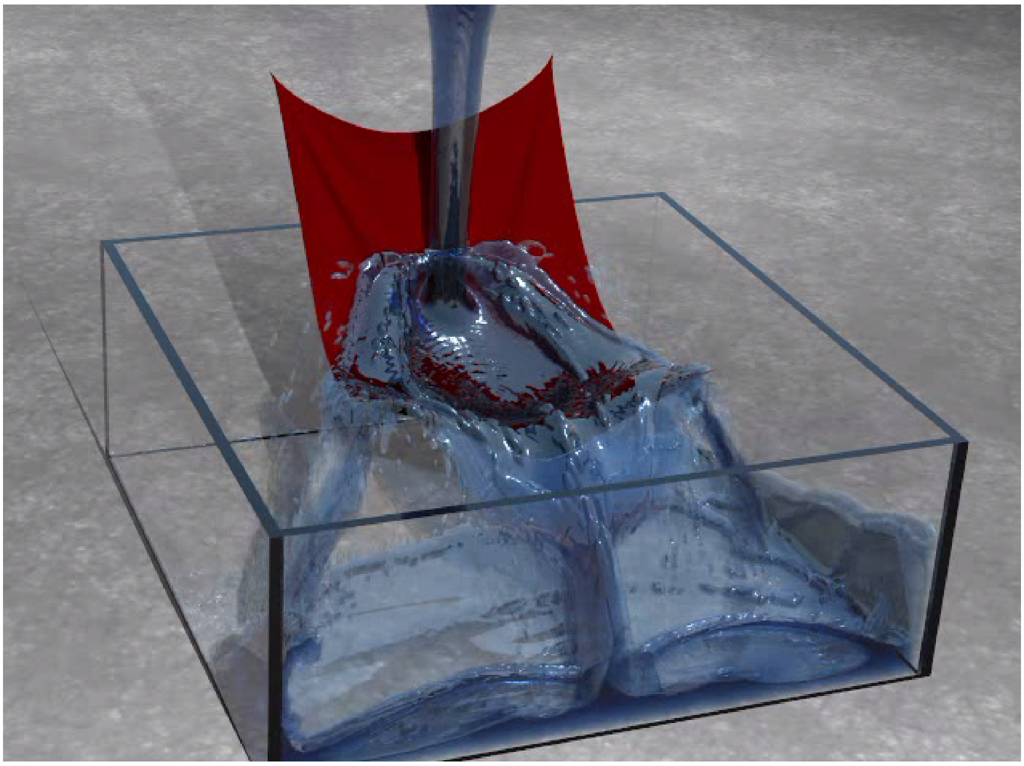
The interaction between soft bodies and liquids is interesting for its high degree of deformation. Being able to replicate the behaviour of a virtual cloth with water, for example, can unlock novel designs in architecture and engineering. The aim of this project is to model and implement the interaction between a tablecloth and water using FEniCS. The computation shall be carried out in the shortest time possible to achieve a minimal level of interactivity. To this end, it is strongly suggested the use of the novel *Projective Dynamics* model [Liu2013, Bouaziz2014] recently introduced by the Computer Graphics community.

Guidelines

- Write the fast mass-spring solver for virtual clothes [?] in FEniCS. Use it for a cloth with a simple rectangular shape.
- Write a Navier–Stokes solver for water (SPH) in FEniCS.
- Model the interaction between water and cloth using collision constraints.
- Visualize the results of the simulation by building a simple OpenGL application or in the Unity Game Engine.

Resources

- `https://unity3d.com/`
- `http://graphics.berkeley.edu/papers/Liu-FSM-2013-11/`
- `https://www.cs.utah.edu/~ladislav/bouaziz14projective/bouaziz14projective.html`



Project 9: Wind flow near a free form shell CFD

Project proposal by Mats Ander <Mats.Ander@chalmers.se>

Task

Simulate the flow of wind near a free form shell.

Background

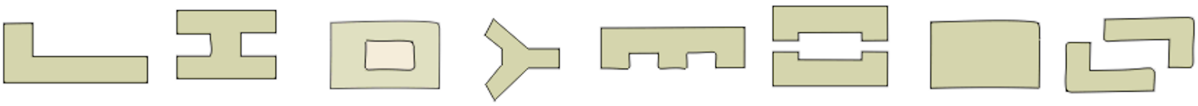
The micro climate near a building is not only dependent on the local weather conditions and the surrounding terrain, but also by the positioning and design of a building or a group of buildings. Compare for example the module constructed long blocks of social housing put in parallel ("miljon-programmet" early seventies), where the space in between the buildings or open court yards almost constantly seems very windy. As more complex architectural shapes such as free form shells are becoming more common, the need for wind flow analysis near these type of buildings is crucial to ensure a comfortable micro climate. Some questions to consider is how openings in the shell surface can effect the flow. Is it possible to design openings to promote a better natural ventilation of the building?

Guidelines

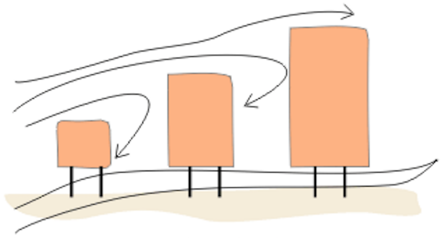
- Write a Navier–Stokes solver in FEniCS.
- Generate mesh data for a free form shell using FEniCS mshr (or another mesh generation tool of choice).
- Simulate the flow of wind near/arround/through the free form shell under realistic assumptions.
- Use the model to generate qualitative results for comparison of different shells designs, orientations and shell surface openings
- Visualize the results by building a 3D model of the shell bulding in the Unity Game Engine. Add textures to create an appealing visualization.

Resources

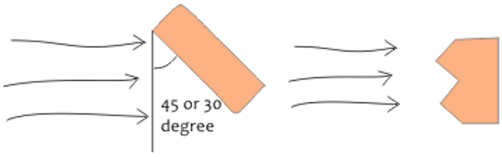
- `https://unity3d.com/`
- `https://en.wikipedia.org/wiki/3D_city_models`
- `http://www.3dcitydb.net/3dcitydb/3dcitydbhomepage/`



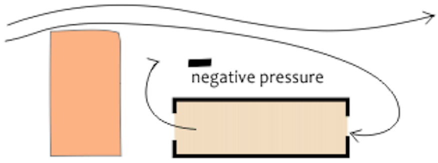
Orient longer facades along the north. This will provide glare free light in summer from north without shading and winter sun penetration from the south.



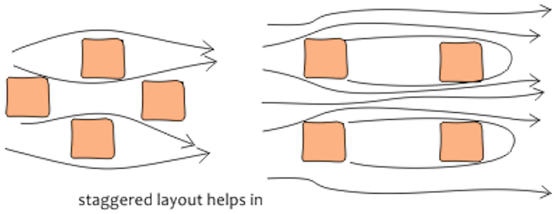
if a site has multiple buildings, they should be arranged in ascending order of their heights and be built on stilts to allow ventilation



Place buildings at a 30 or 45 degree angle to the direction of wind for enhanced ventilation. Form can be staggered in the wind facing direction also to achieve the same result.



Taller forms in the wind direction of prevailing wind can alter the wind movement pattern for low lying buildings behind them



staggered layout helps in accentuating wind movement