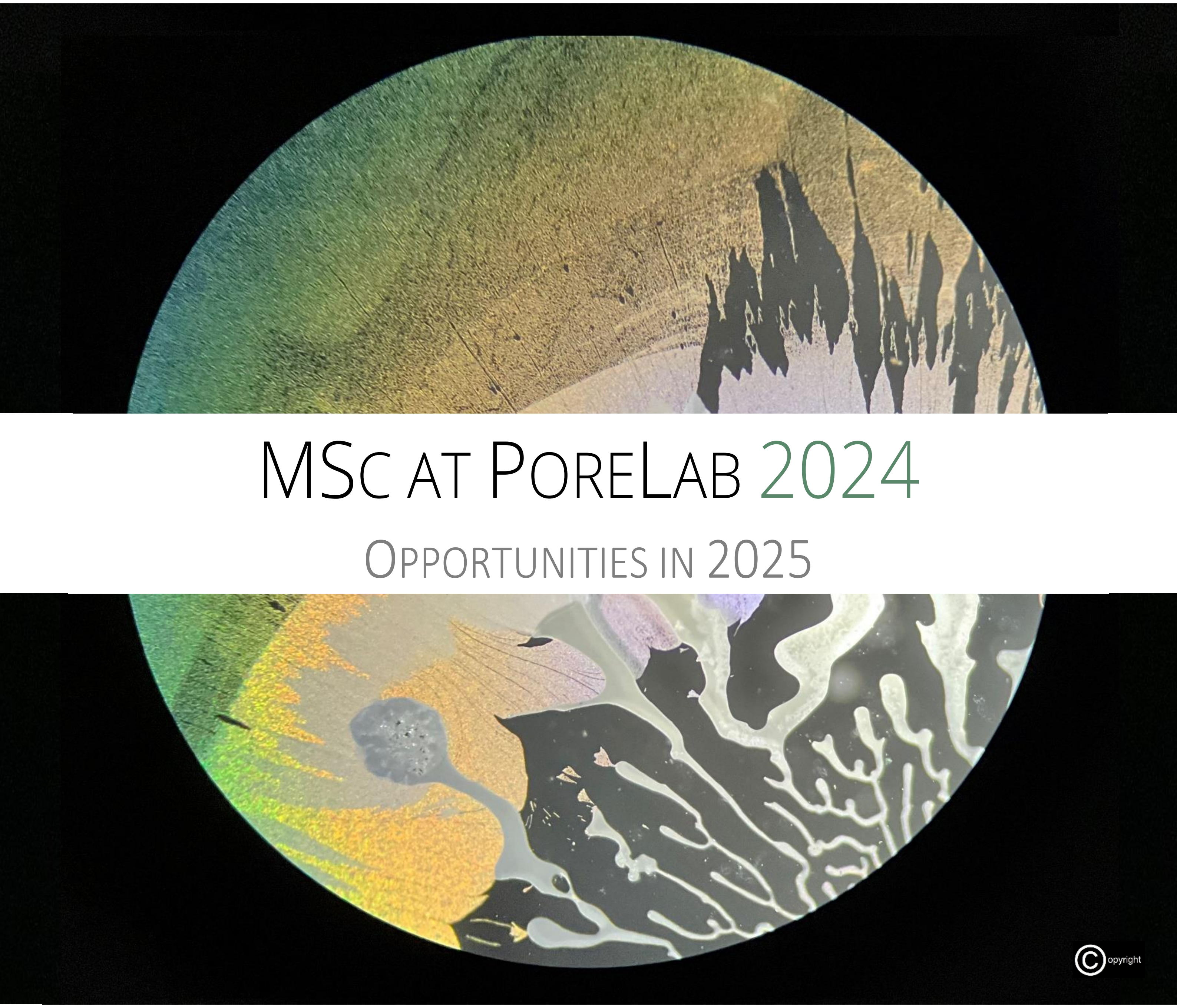
PoreLab
NTNU-UiO Porous Media Laboratory

Norwegian
Centre of
Excellence
The Research Council of Norway

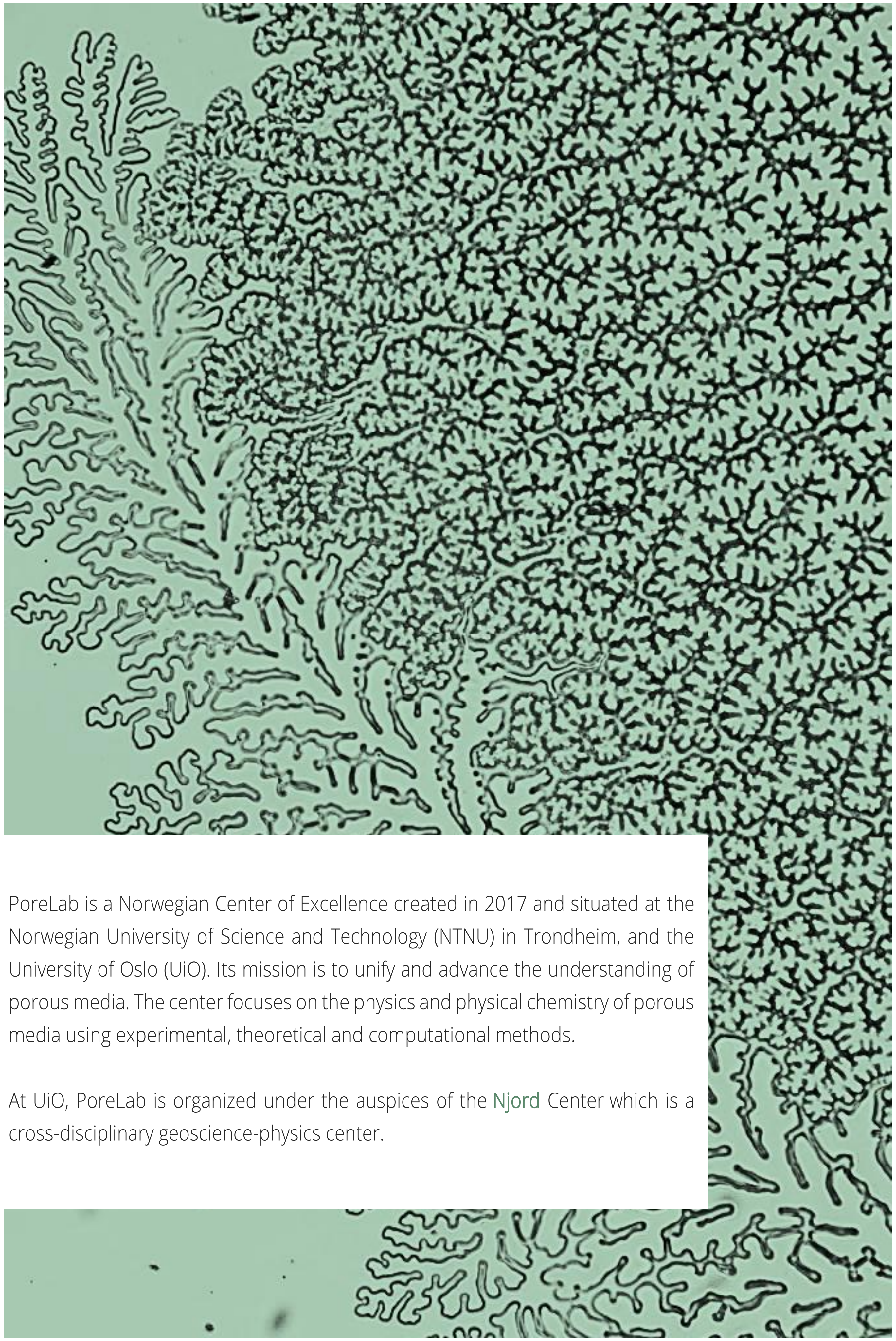


MSc at PoreLab 2024

Opportunities in 2025

NTNU
Norwegian University of
Science and Technology

UiO : University of Oslo



PoreLab is a Norwegian Center of Excellence created in 2017 and situated at the Norwegian University of Science and Technology (NTNU) in Trondheim, and the University of Oslo (UiO). Its mission is to unify and advance the understanding of porous media. The center focuses on the physics and physical chemistry of porous media using experimental, theoretical and computational methods.

At UiO, PoreLab is organized under the auspices of the Njord Center which is a cross-disciplinary geoscience-physics center.

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Dark-field microscopy image showing the drying pattern of a confined colloidal suspension. The colour of the continuous regions is due to scattering white light from a monolayer of colloids. The grey fingers evolve due to an instability of the drying front that stops the further deposition of the colloidal monolayer

Overview – 2024 MSc students

	Title Master thesis	Supervisors
Anders Daltveit Melve	A Real-Space Renormalisation Group Analysis of the Local Load Sharing Fibre Bundle Model	Alex Hansen, Santanu Sinha
Amalie Eveline Hermundstad	Shannon Entropy in Two-Phase Flow in Porous Media	Alex Hansen, Santanu Sinha
Gabriel Paaske	Creating the First Trigel of DNA-Coated Colloids	Erika Eiser
Markus Månum Moen	Polychromatic X-ray Computed Tomography and Dual Energy Computed Tomography	Basab Chattopadhyay and Dag Werner Breiby,
Tuva Coldevin Stavø	Simulating Transport of Therapeutic Agents in Tissue Exposed to Ultrasound and Microbubbles	Natalya Kizilova, Catharina de Lange Davies, Magnus Aa. Gjennestad and Signe Kjelstrup
Henrik Friis and Håkon Nese	NeCT: Neural Computed Tomography for Sparse-View CT and 4D-CT	Dag Werner Breiby, Ole Jakob Mengshoel and Anders Kristoffersen
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Johannes Salomonsen Løken	Predicting the Transport Properties of the Lennard-Jones Spline Fluid using Revised Enskog Theory and Extended Corresponding States Methods	Øivind Wilhelmsen, Morten Hammer, Vegard G. Jervell
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Sigurd Sønvisen Vargdal	Predicting and Generating Transport Properties of Porous Media using Machine Learning	Eirik Flekkøy, Gaute Linga, Henrik A. Sveinsson, Paula K. P. Reis
Håkon Sjøvik Olsen	Fluid Flow Patterns in an Expending Cavity	Eirik G. Flekkøy, Gaute Linga, Fabian Barras
Leroy Leonidas Tzumakaris	Application of the Pressure Dependence of Ideal Gas Xenon to Hydrogen and CO_2 Storage Challenges using the micro-CT scan	Antje van der Net
Nima Hossein Zadeh	Numerical Simulation on CO_2 Dissolution in Aquifers	Carl Fredrik Berg

Welcome to PoreLab

PoreLab would like to have more Master students!

We therefore invite potential students to make contact with anybody in our crew. Contact juniors to learn about our environment. Contact PIs and seniors for project possibilities!

The projects listed in the end of this booklet are only a fraction of the possibilities. We like to tailor new projects to the particular student's wishes and can start a new topic this way. The team's cores activities are presented in the Annual Report, and on our homepage. They serve also as useful starting points.

The climate crisis is a fact, and PoreLab is putting its weight behind the UN sustainability goals! With all our skills and ingenuity, we want to contribute to production of clean water and a more energy efficient world. Some of the master projects refer to that.

Norway has a high competence on transport of oil through porous media. PoreLab sees it as a mission to bring this basic competence to other fields of application.

We recently completed a project to study transport of nanoparticles with in cancerogeneous biological tissue. This is an example of a such a change in direction.

Looking forward to seeing you in PoreLab!

Signe Kjelstrup
Leader of graduate school

A Scientifically Inspiring and Including Working Environment

Training of Master and PhD students, as well as Postdoctoral researchers, is a core activity at PoreLab. An essential part of NTNU's and UiO's mission as universities, is student and researcher education. PoreLab is a valuable contributor in this respect. A vital asset of the center from an educational point of view is that it offers each student and junior researcher a scientifically stimulating and inclusive workday, much above the level of a regular MSc/PhD/Postdoc program.

"*Because we are interdisciplinary group, we work with people from different departments and universities and fields of research, which makes it an excellent learning environment*", says Astrid Fagertun Gunnarshaug, former PoreLab fellow and PhD candidate at the Department of Chemistry, NTNU. This is indeed our ambition at PoreLab, to create an interdisciplinary and international training ground for our juniors.

The aim of this catalogue is to provide an overview of the projects performed by our Master students in 2024 and inspire new students to join the team. PoreLab is an international community. Master students at PoreLab do not only come from NTNU and UiO, but also from our international partners. The Center offers some funds that allow foreign Master students to spend some time with us, as well as to send our own students abroad. The same offer is available for Master students between NTNU and UiO.

A few years ago, we developed a project in collaboration with the French University Paris-Saclay and the Universidade Federal do Ceara (UFC) in Fortaleza, Brazil about non-Newtonian flow in porous media. Funds are available for Master students to do their thesis research not only at the laboratory of the three institutes: PoreLab NTNU/UiO, Laboratoire FAST at the University of Paris-Saclay and Complex Systems Group at UFC, Brazil, but as well with our collaborators worldwide.

As a PoreLab Master student, you will get an office space at PoreLab premises. Being part of the PoreLab team, you will be offered to attend and contribute to all PoreLab events, such as the PoreLab lecture series organized usually every other Wednesday at 13:00. We host this event simultaneously in Oslo and Trondheim, and it is open to all. The PoreLab lecture series are now almost always given by external lecturers.

PoreLab started again the Journal club during the Spring 2024 semester. The idea is to present a recent paper with a short preparation time, so that the juniors (PhD candidates and postdoctoral researchers) can learn how to read papers quickly, understand its main content, and explain it to others. The juniors are given a paper 1-2 days before the presentation. The Journal Club is usually organized one or two times a month, on Thursdays. It is our goal that each PoreLab member should participate with at least one presentation during the course of the year. Master students are welcome to attend.

PoreLab provides a research environment that is centered for working as a team and that allows everyone's talents to flourish. Therefore, open communication is crucial at PoreLab, and we designed the organization to achieve this goal. Ailo Aasen, former PhD candidate at PoreLab, provides a good summary: "*It is an open and social atmosphere with genuinely nice people. I especially like how there is so much interaction between the senior and junior researchers*". Hossein Golestan, former PhD candidate at PoreLab, says that: *"The working environment is excellent, and the colleagues are so eager to share their knowledge. The best side is its international atmosphere with people from different fields of research (Physics, chemistry, Petroleum and so on) and whenever you have a question there is always someone who can help you finding the answer"*.

At PoreLab UiO, the researchers also join forces with the larger team of the Njord Centre, for interdisciplinary collaboration across the fields of physics and geology, as well as larger social gatherings, conferences and other events. As researcher, Marcel Moura puts it: "*The idea 'Simplify it until you understand it', is really in the nature of physics and it has given us quite a lot. However, it is important to remember that sometimes reality is bigger and more complex than our models. Therefore, being in close proximity to scientists who tackle nature at different scales of complexity – geologists, volcanologists, and rock scientists of all types – is excellent to keep our eyes open and our antennas tuned*."

Though PoreLab has dedicated, eager researchers, being at PoreLab does not only mean hard work. The Pore Buzz at PoreLab NTNU and the Junior club at PoreLab UiO are informal events that aims to strengthen connection within our group and integrate new juniors, Master students and guests. The hottest research topics in the field, as well as pizza, are on the menu of these convivial and relaxing events. For more social interaction, we all meet at 10' every day for our coffee break, as well as at lunch time. On Mondays, fruits and cake are served. In addition, a ping-pong table, a table soccer and an ever-present thousand-pieces puzzle became popular playgrounds for all at PoreLab NTNU.

A glimpse of students' activities at PoreLab
1. Coffee break at 10:00 every morning 2. Srutarshi, Hossein, Giulio and Michael take a break. 3. Internal seminar
4. The PoreLab UiO team at the summer's cabin of Joachim Brodin

NTNU – Department of Physics

Anders Daltveit Melve

Department of Physics, NTNU

A Real-Space Renormalisation Group Analysis of the Local Load Sharing Fibre Bundle Model

Fall 2024 – Spring 2025
Supervisors: Alex Hansen, Santanu Sinha

Background:

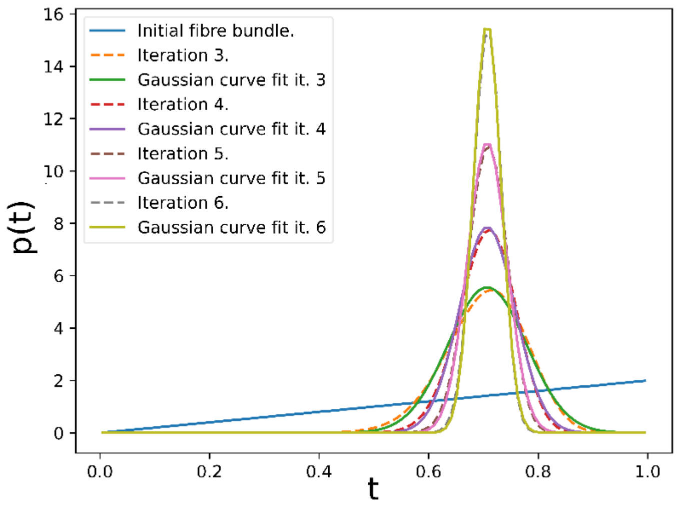
The *fibre bundle model* is a model that aims at providing insights into fracture phenomena in materials. It consists of a set of linear elastic fibres placed between two clamps. Each fibre can hold a certain load before failing, this threshold value being drawn from a given probability distribution. In the *local load sharing* version of this model, the load from a failed fibre is redistributed to its nearest surviving neighbours.

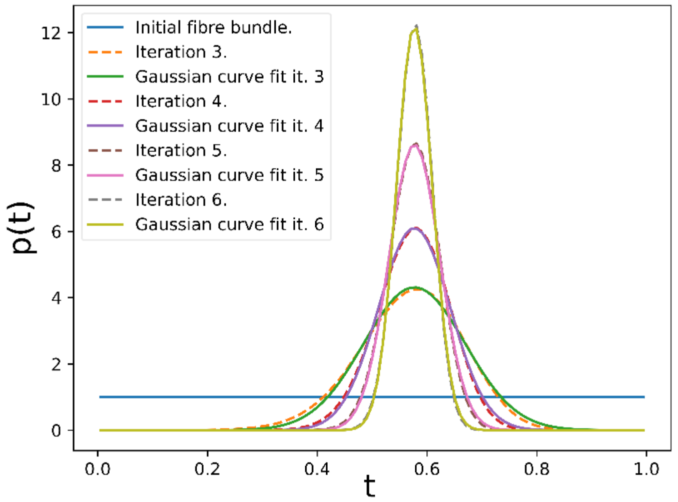
Objectives:

The main goal will be the construction of a renormalisation group for the local load sharing fibre bundle model, focusing on the effect this has on the underlying probability distribution. Being heavily dependent on numerical simulations, this can then be of aid in investigating characteristics of the model, such as critical phenomena and universality.

Results:

Similar techniques have been applied to a simpler version of the fibre bundle model, the *global load sharing* version. For this model, the behaviour of threshold values under transformation was found to depend strongly on whether the starting probability distribution was broad or narrow, the two cases giving rise to different classes of dynamics.





Figures: evolution of two narrow distributions under the renormalisation group transformation on a global load sharing model, curve fitted to Gaussian distributions whose variance is halved with each iteration.

Amalie E. Hermundstad

Department of Physics, NTNU

Shannon Entropy in Two-Phase Flow in Porous Media

Fall 2024 – Spring 2025
Supervisors: Alex Hansen, Santanu Sinha

Background

The complex dynamics of two-phase flow in porous media form a scientific field which serves as a foundation for various phenomena. Two-phase flows in porous media are believed to exhibit self-affine scaling properties, which can be explained more thoroughly by a measure of its entropy.

Objectives

The main objective of my master's thesis is to develop a method for estimating the entropy of configurations with two-phase flows in porous media.

Methodology

By studying several different self-affine structures during the work for my specialization project, a method for estimating the entropy was developed. As self-affine structures exhibit long-range spatial dependencies, a discrete wavelet transform is used to de-correlate the features of the systems into representations by wavelet coefficients in the frequency domain. The entropy is then estimated directly from these coefficients. Figure 1 shows the self-affine trace generated synthetically using a Fast Fourier algorithm, while Figure 2 shows the corresponding distribution of normalized wavelet coefficients. The wavelet coefficients are also used to estimate the Hurst exponent governing the scaling properties of the self-affine traces, as illustrated in Figure 3.

Results

The resulting entropy estimates of the work in my specialization project illustrates the difficulties of estimating a discrete entropy (the Shannon entropy) from a continuous distribution. When extending the entropy estimates to two-phase flows, different definitions of entropy will be investigated.

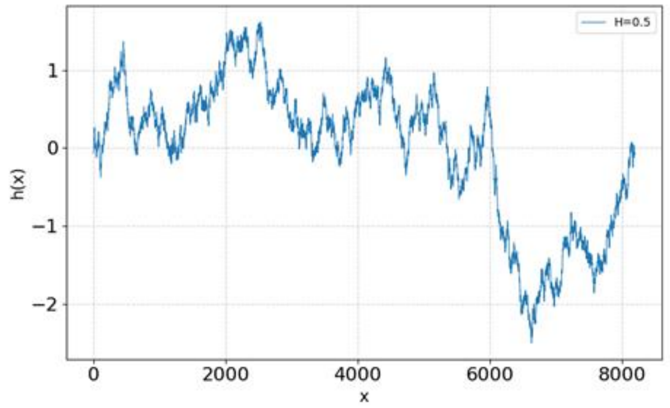


Figure 1: Height as a function of position for a synthetically generated self-affine trace.

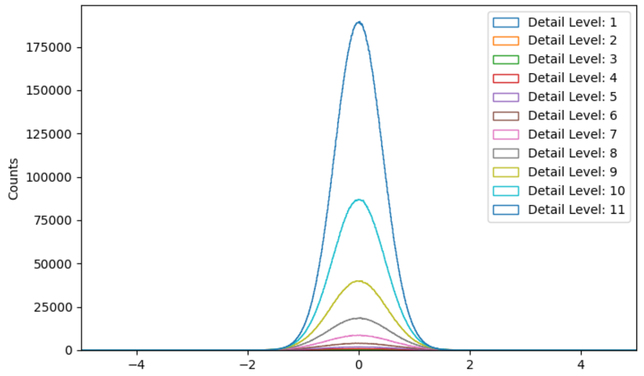


Figure 2: Histogram of normalized wavelet coefficients for a given Hurst exponent.

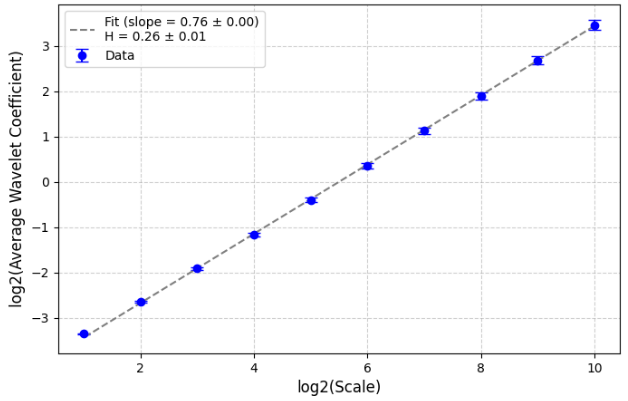


Figure 3: Best-fit regression line used in estimation of Hurst exponents by AWC.

NTNU – Department of Physics

NTNU – Department of Physics

Gabriel Paaske

Department of Physics, NTNU

Creating the First Trigel of DNA-coated Colloids

Fall 2024 – Spring 2025
Supervisors: Erika Eiser

In an upcoming paper, researchers in Brazil and at PoreLab showed that it is theoretically possible to create a large number of spanning clusters in a 3D volume (technically infinite, given infinite size), where each spanning cluster can be non-interacting with the others. In the lab, only gels with two distinct species have been created thus far. This raises the question of whether it is possible to create a gel that consists of three non-interacting species of colloids. For this purpose, DNA-coated colloids is the clear candidate. The selectivity of DNA, as well as its ability to reverse its binding upon heating/cooling means that a gel could be formed with three critical temperatures: below the lowest temperature all three species would bind and form a more rigid gel; between the first and second temperatures only two species would bind, making it less viscous; and between the second and third temperatures, only one species would bind.

In this project, creating such a trigel is attempted. In order to have maximum control over the properties of the gel, first polystyrene nanoparticles were created with the help of the Adolphe Merkle Institute in Switzerland. Then, amphiphilic polymer F127 was functionalized with azide ends and grafted onto the nanoparticles to attach through click chemistry to DBCO-DNA strands. Before DNA addition, the particles and polymer was tested to see that particle size was suitable and monodisperse and that the polymer had correctly been functionalized. Dynamic light scattering and SEM was used for the former and FTIR spectroscopy for the latter. In the coming six months, attaching DNA and creating the trigel will be attempted, as well as characterizing it.

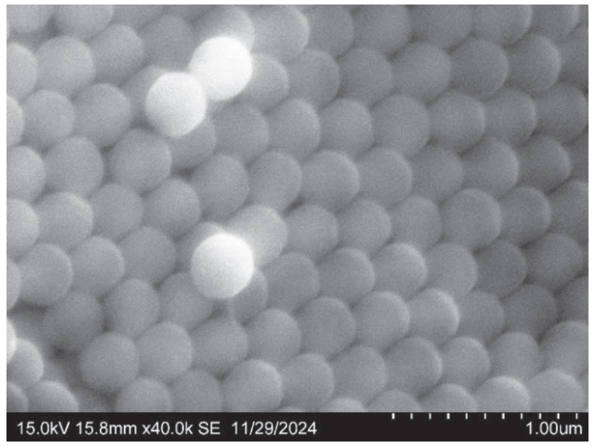


Figure 1: Electron micrograph showing the high degree of monodispersity in the colloids. Most colloids are around 300 nm dry.

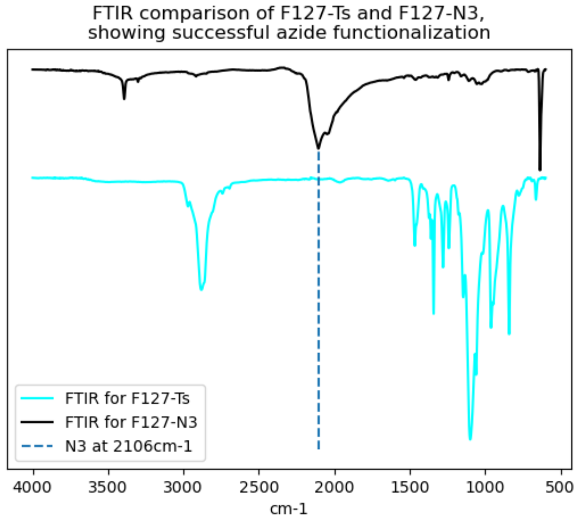


Figure 2: FTIR spectrum showing successful azide functionalization of F127

NTNU – Department of Physics

Markus Månum Moen

Department of Physics, NTNU

Polychromatic X-ray Computed Tomography and Dual Energy Computed Tomography

Spring 2024
Supervisors: Basab Chattopadhyay and Dag Werner Breiby

Background

The motivation behind this study is to better monitor and understand corrosion processes in the caprocks and in the gas pipelines used for carbon capture and storage (CCS). CO_2 under high pressure and temperature is supercritical and highly corrosive. X-ray Computed Tomography (CT) is a non-destructive imaging technique which gives 3D images of the internal structure of samples. The interaction between X-rays and matter is energy dependent and the resulting image will thus depend on the X-ray spectrum used during imaging. This spectrum can be altered by applying filters or changing the acceleration voltage. Dual Energy Computed Tomography (DECT) exploits this energy dependence to extract more information about the sample by comparing images obtained with different energy spectra.

Objectives and methodology

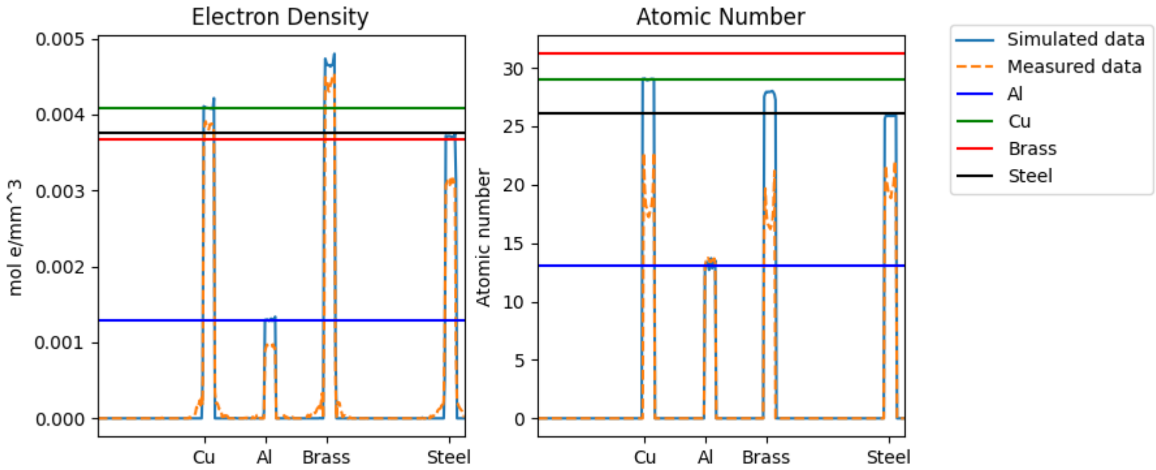
In this work a polychromatic X-ray imaging simulation tool has been developed to find the instrument configurations yielding the highest contrast between different minerals, metals and oxides. In some situations, one requires more information about the sample than what is provided by conventional CT. The DECT method SIRZ [1], giving information about atomic number and electron density, has been implemented and tested on simulated and measured data.

Results

For a solid-liquid interdiffusion sample used as a test case it was shown that the contrast between different regions can be dramatically improved by choosing the optimal configurations. The SIRZ method was found to work well on simulated data. For the measured data, it proved necessary to include the afterglow in the detector to get satisfactory results. Applying the method to a corroded sample gave promising results.

Reference

[1] K. M. Champley *et al.*, "Method to Extract System-Independent Material Properties From Dual-Energy X-Ray CT," in *IEEE Transactions on Nuclear Science*, vol. 66, no. 3, pp. 674-686, March 2019, doi: 10.1109/TNS.2019.2898386.



Picture: *Line plot of reconstruction using SIRZ on simulated and measured data. The horizontal lines illustrate the expected values for the different compounds*

Tuva Coldevin Stavø

Department of Physics, NTNU

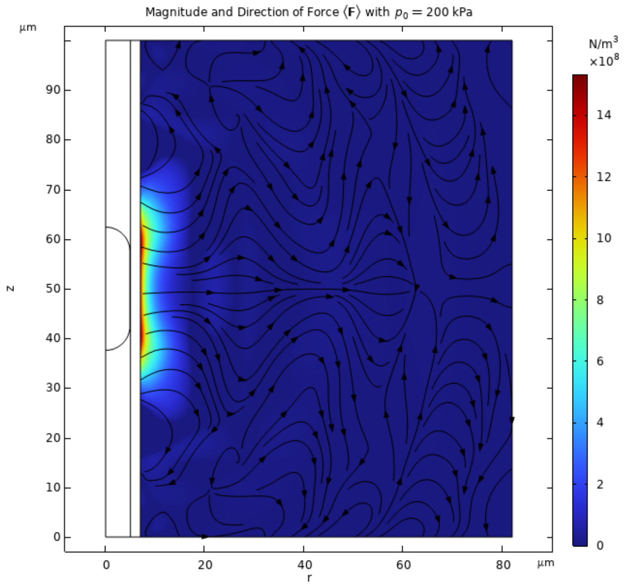
Simulating Transport of Therapeutic Agents in Tissue Exposed to Ultrasound and Microbubbles

Spring 2024
Supervisors: Natalya Kizilova, Catharina de Lange Davies, Magnus Aashammer Gjennestad, Signe Kjelstrup

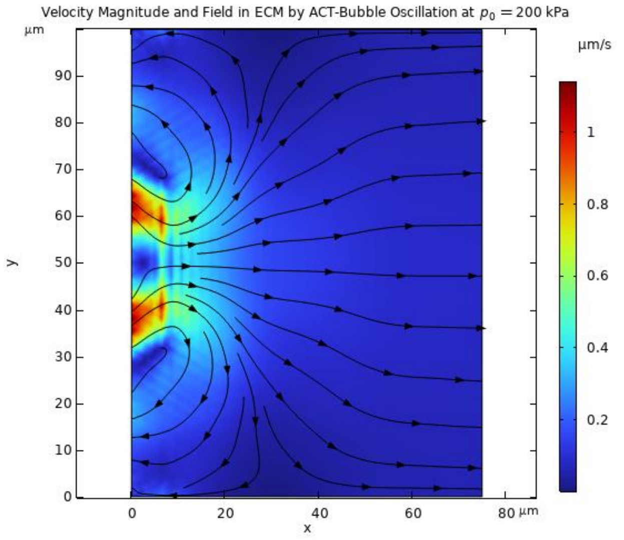
A promising technique to improve cancer treatment and limit its side effects is to encapsulate anti-cancerous drugs into nanoparticles (NPs), facilitating their further delivery to tumor cells. The combination of focused ultrasound (FUS) together with microbubbles (MBs) have been shown to enhance the distribution and uptake of NPs in tumor tissue. However, the exact mechanisms governing the NP transport in extracellular matrix (ECM) remain not fully understood.

Simulations in the software COMSOL Multiphysics were performed to investigate if cavitation of MBs can enhance the NP distribution in ECM. The simulations were divided into two parts. Firstly, generating a displacement field in the surrounding tissue due to cavitation of both a spherical MB and an elongated ACT-bubble, which was further used to calculate an acoustic radiation force (ARF). Secondly, the ARF was used to generate a velocity field in the ECM, macroscopically modeled as a porous medium. This velocity field was further used to study the convective transport of NPs through ECM. The bubbles were able to distribute NPs at depths ranging from 20-60 µm into the ECM, depending on the parameters used in the computational model.

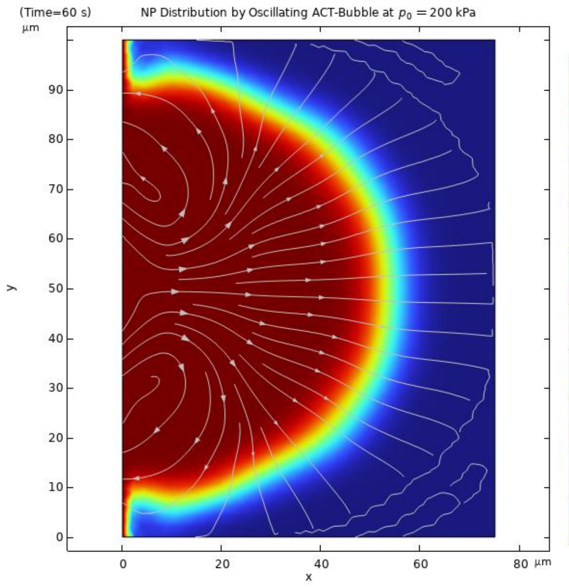
[1] C. Einen et al. 'Nanoparticle Dynamics in Composite Hydrogels Exposed to Low-Frequency Focused Ultrasound'. In: Gels 9 (2023), p. 771.



Picture 1: *ARF in the surrounding tissue generated by sound waves created by a vibrating ACT-bubble.*



Picture 2: Velocity field in ECM created by cavitation of an ACT-bubble.



Picture 3: Distribution of NPs after 60 seconds enhanced by the interstitial fluid flow created by cavitation of an ACT-bubble.

Henrik Friis and Håkon Nese

Department of Physics and Department of Computer Science, NTNU

NeCT: Neural Computed Tomography for Sparse-View CT and 4D-CT

Spring 2024
Supervisors: Dag W. Breiby (IFY), Ole Jakob Mengshoel (IDI) and Anders Kristoffersen (Equinor)

Background

Fast 4D-CT imaging is important for studying dynamic processes like pore-filling events and supercritical CO_2 fingering in porous media. 4D-CT imaging in the home lab is typically slow due to the low photon flux of common CT scanners.

Objectives

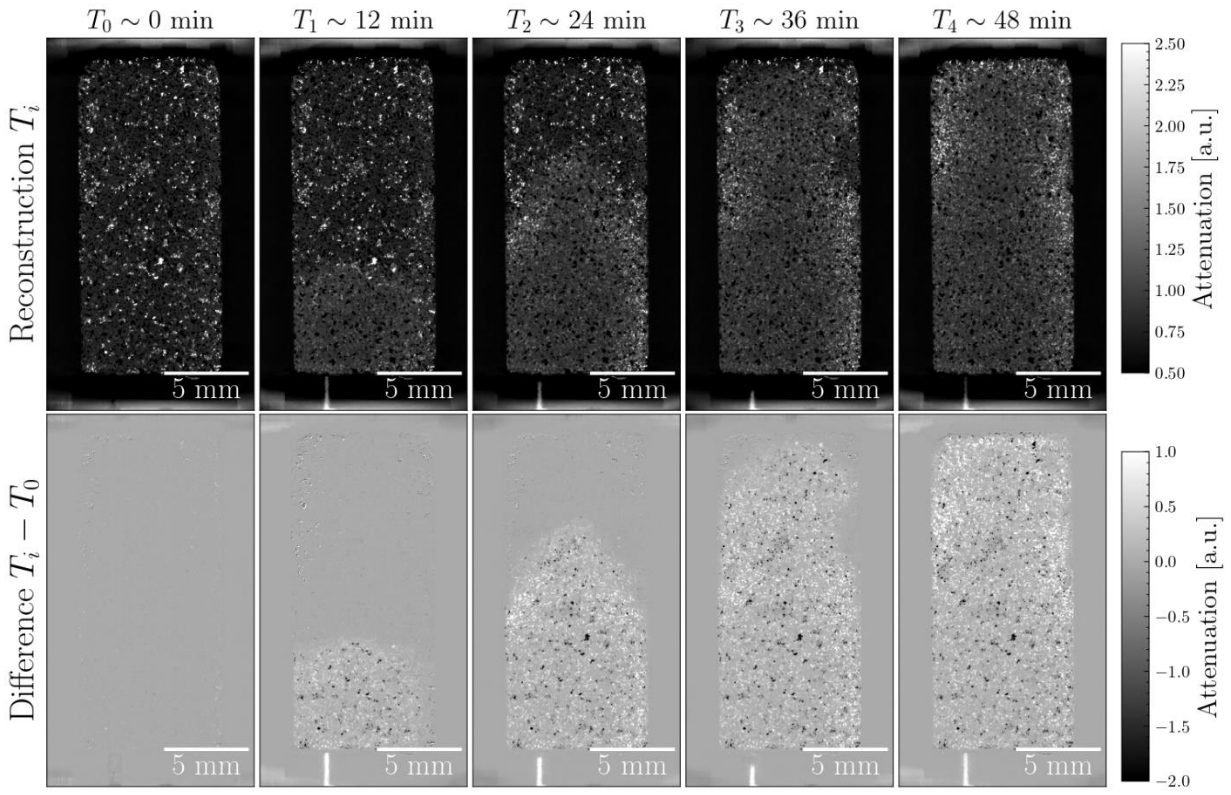
Current methods have a temporal resolution of around one hour, while a sub-minute temporal resolution is necessary for fast dynamic processes.

Methodology

We develop a novel iterative neural network-based optimization algorithm, named Neural Computed Tomography (NeCT), that can reconstruct both the spatial and temporal parts of a CT scan simultaneously.

Results

Our NeCT reconstruction algorithm can reconstruct high-quality CT images and outperforms other analytical, iterative and neural network-based methods. NeCT achieves a temporal resolution down to a single projection, which typically corresponds to a few seconds, thus enabling detailed studies of important mechanisms in porous media



Picture: Selected timesteps from a one-hour long Bentheimer Sandstone reconstruction using NeCT with a temporal resolution on the order of seconds. The brine is injected from the bottom.

Julie Myrmo Lervik

Department of Physics, NTNU

Simulations of Nanoparticle Diffusion in a Course-Grained Collagen Network and the Effect of Ultrasound

Spring 2024
Supervisors: Anders Lervik, Sebastian E. N. Price

Background

Targeted drug delivery remains a challenge in cancer treatment due to inefficiencies and side effects associated with conventional therapies. Nanoparticles combined with focused ultrasound have shown promising results in overcoming biological barriers to improve drug delivery. However, the mechanisms underlying this enhancement are not yet fully understood.

Objectives

To study the mechanisms behind nanoparticle transport in the *extracellular matrix*, this thesis aimed to develop a molecular dynamics model of a collagen network (the largest steric obstacle in the extracellular matrix) to investigate nanoparticle diffusion under the influence of ultrasound. The study sought to understand how nanoparticle-collagen interactions and ultrasound parameters affect diffusion processes in tissue.

Methodology

A coarse-grained collagen network model was created in a Lennard-Jones solvent environment using molecular dynamics simulations performed by LAMMPS software. Solvent particles enabled the study of solvent effects, which according to our literature search, no other previously published model has included. An oscillatory force was applied to the solvent to simulate ultrasound.

Results

The model successfully demonstrated the formation of a coarse-grained collagen network, with pore-size ratios similar to collagen in living organisms. Increasing the nanoparticle-collagen interaction resulted in *subdiffusive behaviour*, while higher ultrasound intensities enhanced diffusion. These findings suggest the model to align with prior studies and simulation models, opening for further investigations on nanoparticle-collagen interactions and ultrasound intensities, together with fluid dynamic effects. Despite the potential of the model, a significant drawback is the extensive runtime, with simulations often taking over 30 days to complete.

Keywords:

* *Extracellular matrix:* is a network of proteins and sugars that surrounds and supports cells, acting as a structural framework for tissues.
* *Subdiffusive behaviour:* occurs when particles move more slowly than expected in normal diffusion

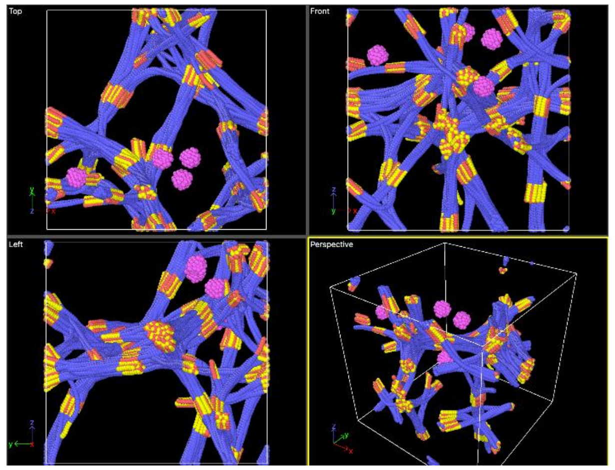


Figure 1: A visual representation of the collagen model, with nanoparticles (pink)

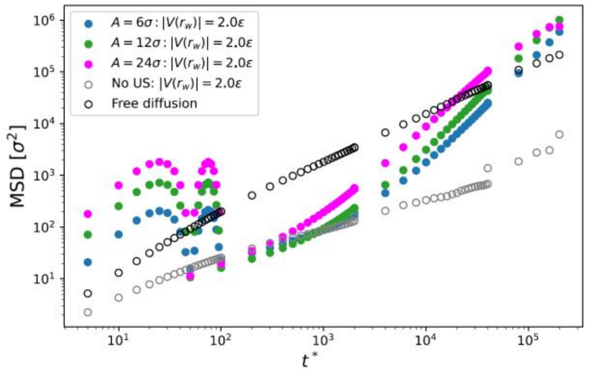


Figure 2: Mean squared displacement (MSD) of four nanoparticles over reduced time, with positive attraction set between nanoparticles and collagen. The colours indicate varying ultrasound amplitudes

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Mats Kjenes

Department of Chemistry, NTNU

Implementation and Evaluation of the TRAPP Model for Calculation of Viscosity of Gas Mixtures

Fall 2024 – Spring 2025
Supervisors: Morten Hammer, Even Solbraa

Objectives

In this project, the SuperTRAPP method will be implemented and evaluated based on fluids containing pure H_2, pure CO_2 and a mixture of both. The primary objective of this project will be to implement the SuperTRAPP model and assess its accuracy in predicting the viscosity of pure CO_2, pure H_2 and a mixture of both. This will be done by comparing the values with experimental measurements.

The TRAPP method

Up until now, the TRAPP model has been implemented, which is the model that SuperTRAPP is based on. The TRAPP model has been implemented in accordance with the corresponding states principle, where the residual viscosity of a pure fluid is related to the residual viscosity of the reference fluid. In this implementation, the reference fluid is propane, and the dilute viscosity is determined based on Chapman-Enskog theory for pure fluids, and Reichenberg's method for mixtures.

The predicted viscosities given by the TRAPP model for the different fluids are given in the three figures. The mean absolute percentage deviation (MAPD) for CO_2 and H_2 were 2.21 % and 5.53 %, respectively. The MAPD for the CO_2/H_2 mixture were 1.06 %. A possible explanation for the deviation between the pure fluids and the mixture is that the pure fluids contain data points under extreme conditions, which results in a high deviation. If limited to 50 bar, the deviation for the pure fluids drops significantly

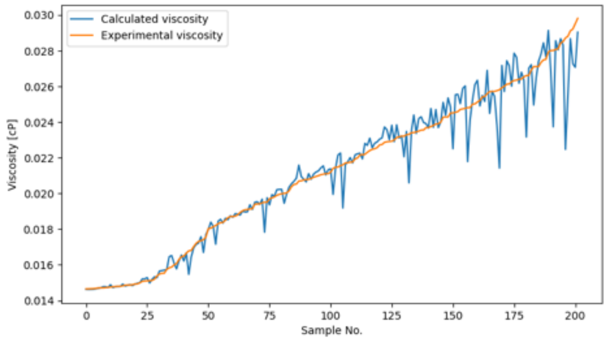


Figure 1: Predicted viscosity for CO_2

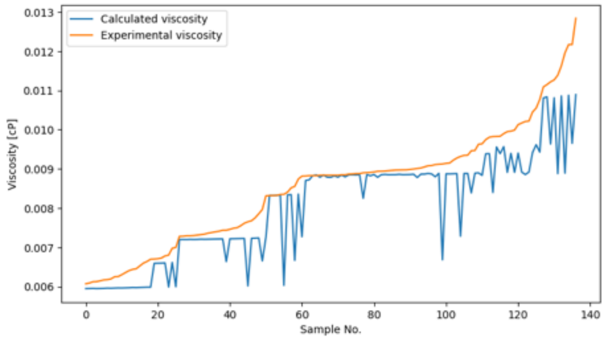


Figure 2: Predicted viscosity for H_2

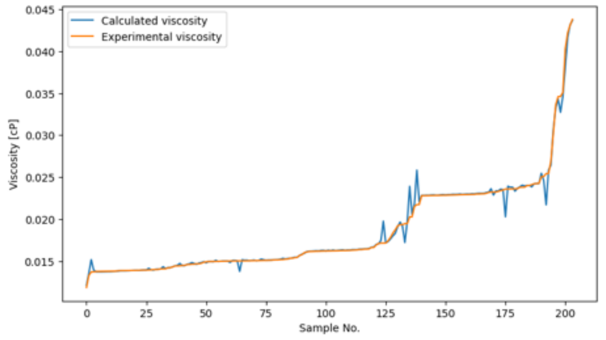


Figure 3: Predicted viscosity for CO_2/H_2

NTNU – Department of Chemistry

Johannes Salomonsen Løken

Department of Chemistry, NTNU

Predicting the Transport Properties of the Lennard-Jones Spline Fluid using Revised Enskog Theory and Extended Corresponding States methods

Fall 2024
Supervisors: Øivind Wilhelmsen, Morten Hammer, Vegard G. Jervell

Background

The Lennard Jones spline (LJ/s) potential is a Lennard Jones potential truncated in a unique way, which makes the interaction potential and the force continuous [1]. As such, it avoids the need for further specification and the risk of ambiguity in how the potential is used in a simulation. The potential is frequently used at PoreLab, and it's also one of the primary examples that will be used in the ERC project, Interlab, where one of the goals is to understand the temperature jump across the vapor-liquid interface.

Objective and methodology:

Revised Enskog Theory (RET) has been used with great success to accurately represent the transport properties of Mie potentials (a generalized version of the full Lennard-Jones potential) from low to moderate densities [2]. This thesis aims to develop a RET for the LJ/s potential, which will be verified by comparing to molecular dynamics (MD) results of the transport properties. The transport properties will also be calculated using extended corresponding states (ECS) methods [3], which involve mapping and scaling the transport properties of a reference fluid onto the LJ/s fluid.

Results:

Figure 1 shows a comparison of the predictions of RET for the shear viscosity η, self-diffusion D, and thermal conductivity λ. The three properties are shown as a function of temperature T, and density ρ. The plot demonstrates that RET can predict the transport properties of the LJ/s potential for low to moderate densities.

References:

[1] Hafskjold, Bjørn, et al. Thermodynamic properties of the 3D Lennard-Jones/spline model. *Molecular Physics* 117.23-24 (2019): 3754-3769.

[2] Jervell, Vegard G., and Øivind Wilhelmsen. Revised Enskog theory for Mie fluids: Prediction of diffusion coefficients, thermal diffusion coefficients, viscosities, and thermal conductivities. *The Journal of Chemical Physics* 158.22 (2023).

[3] Kleint, S.A., et al. An improved extended corresponding states method for estimation of viscosity of pure refrigerants and mixtures. *Int J. Refrig*. 20.3 (1997).

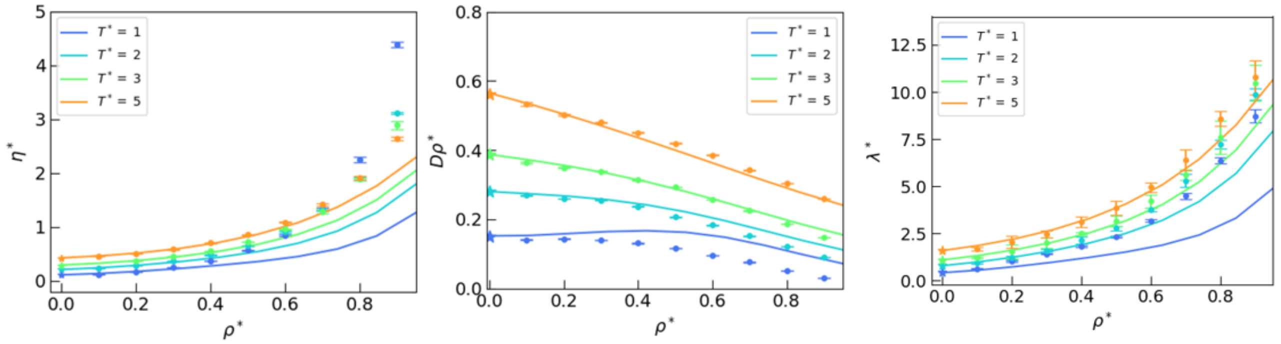


*Figure 1: RET predictions of the shear viscosity, self-diffusion, and thermal conductivity (lines), compared to MD results (points). All properties are in LJ units (indicated by *).*

NTNU – Department of Geosciences

Maria Lorense Rogde

Department of Geosciences, NTNU

Utilizing Electrical Networks to Model Subsurface Transport Systems using Machine Learning Principles

Fall 2024 – Spring 2025
Supervisor: Carl Fredrik Berg

This project focuses on utilizing machine learning techniques in digital models of physical electrical networks, for subsurface flow modeling and optimization of control of subsurface fluid transport systems.

Recent research and advancements have shown that self-learning electrical circuits can be designed to autonomously and efficiently adjust their parameters in order to achieve a desired output.

The overall objective is to bridge the gap between traditional machine learning methods and physical laws, offering practical applications in fields like reservoir management, groundwater modeling, and geoenergy systems. We aim for providing a more accurate, physics-based alternative for modeling subsurface flow optimization.

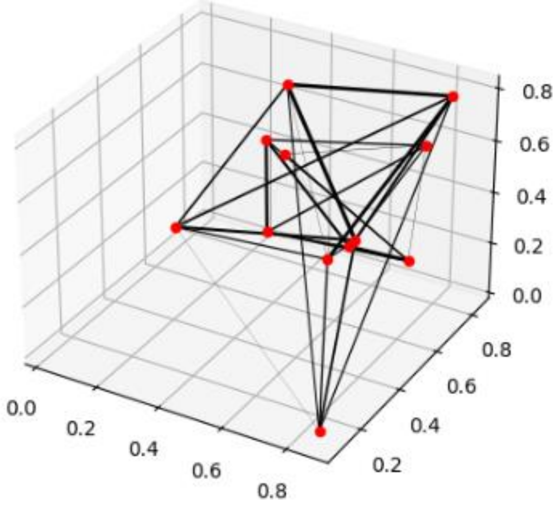


Figure 1: Digital model of electrical network. The link thickness represents the conductance values. We aim to optimizing these values in relation to the actual physical network.

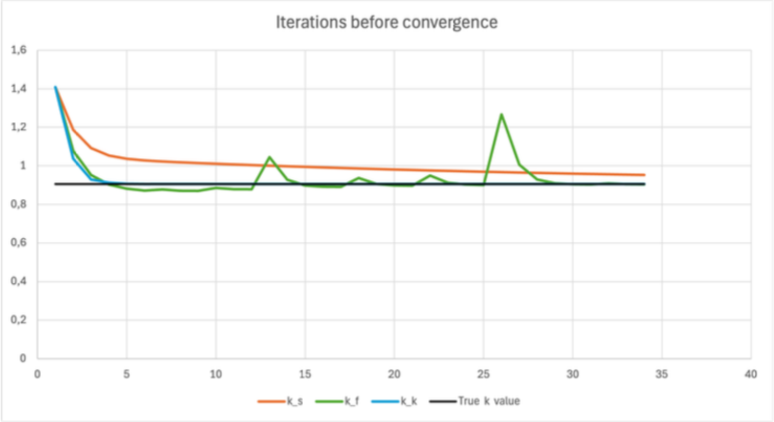


Figure 2: Using the root of the sum of squares, three different approaches for gradient descent-based convergence methods for convergence were compared.

University of Oslo – Department of Physics

Sigurd Sønvisen Vargdal

Department of Physics, University of Oslo

Predicting and Generating Transport Properties of Porous Media using Machine Learning

Fall 2024 – Spring 2026
Supervisors: Eirik G. Flekkøy, Gaute Linga, Henrik A. Sveinsson, Paula K. P. Reis

With the recent surge in development of machine learning methods it has been shown that a neural network may be capable of predicting transport properties such as permeability using the highly successful Convolution Neural Network (CNN).

In recent years the Transformer has been a highly successful architecture for processing data with contextual dependence. By utilizing this property, we aim to compare the permeability prediction from the CNN with the Transformer. Another transport property we want to predict is the mixing rate.

If predictions reach good results, we will extend the mode into a generative adversarial network for generating a porous media with a given transport property.

In addition, we would like to explore the use of the transformer in the U-net architecture diffusion model to generate the flow field based on the geometry of the model.

If time allows it, we want to explore how the use of Physics-Informed Neural Network can help the study of porous media.

Håkon Sjøvik Olsen

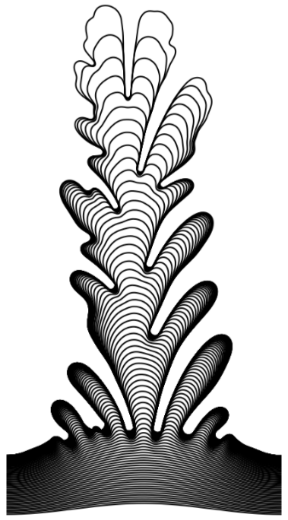
Department of Physics, University of Oslo

Fluid Flow Patterns in an Expanding Cavity

Fall 2024 – Spring 2026
Supervisors: Eirik G. Flekkøy, Gaute Linga, Fabian Barras

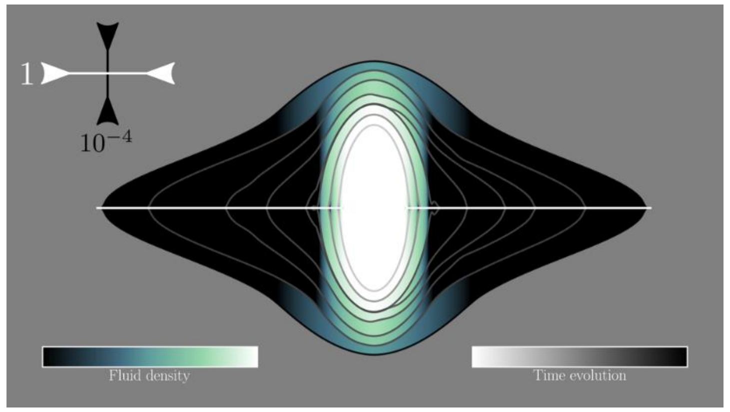
The interaction between fluid flow and solid deformation in dynamically changing geometries, such as expanding fractures, is critical for advancing green energy technologies like geothermal energy extraction and CO_2 sequestration. These processes often require careful management of subsurface conditions to enhance permeability while minimizing the risk of induced seismicity or runaway fractures. Furthermore, natural geohazards like earthquakes and landslides can involve rapid solid deformation that interacts with fluid flow, potentially vaporizing fluids and amplifying instability. A deeper understanding of these interactions at the scale of individual fractures is essential for improving safety and efficiency in energy applications and geohazard mitigation.

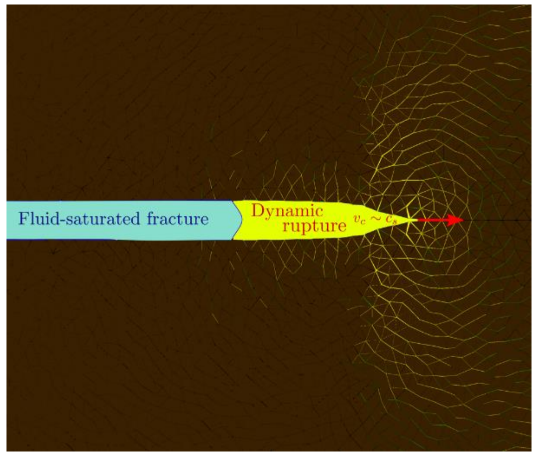
The primary aim of this research is to simulate and study the physics of fluid flow in an expanding cavity, focusing on the feedback mechanisms between fluid dynamics and deforming solid boundaries. This will be done by implementing a numerical model using the finite element method (FEM). The starting point for the model is a two-phase flow setup in the form of a classical Hele-Shaw cell. When the less viscous fluid is injected and displaces the more viscous, we get viscous fingering due to the Saffmann-Taylor instability. Subsequently the confining solid will be adjusted by steps so that the system resembles more of a fracture (i.e. an expanding cavity). As the solid boundaries rapidly expand, and the solid responds elastically to the fluid forces, this will again affect the fluid dynamics and result in a feedback loop. The simulations will be validated against theoretical predictions, as well as experiments conducted at PoreLab UiO.



← *Figure 1: Visualization of viscous fingering due to the Saffmann-Taylor instability, caused by the unstable interface between the two fluids in the Hele-Shaw cell. The front is plotted at equally spaced points in time.*

↓ *Figure 2: Simulation of flow in a rapidly expanding crack cavity. The crack growth is much faster than the lateral spread of the liquid. Thus, the black area corresponds to the formation of a large bubble with negligible fluid density. While this 2D geometry assumes a flat front between the liquid and bubble, we expect Saffmann – Taylor instabilities in the third dimension.*





← *Figure 3: A dynamic fracture running through a saturated poroelastic medium. The solid fracture speed v_c is close to the shear wave velocity c_s, and is too rapid for the pore fluid, causing the formation of a fluid depleted region (yellow) between the fracture tip and liquid front.*

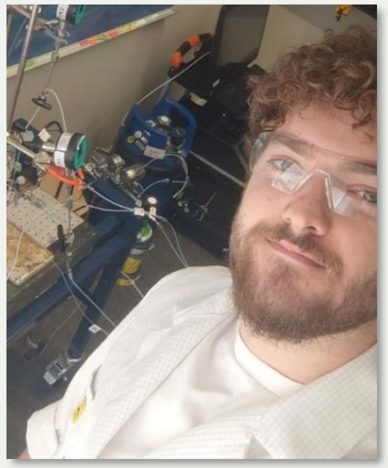
University of Oslo – Department of Physics

Leroy L. Tzumakaris

Technical University of Crete and Department of Geosciences, NTNU

Application of the Pressure Dependence of Ideal Gas Xenon to Hydrogen and CO_2 storage Challenges using the micro-CT scan

4-month Erasmus internship, summer 2024
Supervisor: Antje van der Net at NTNU



Obtaining locally in a porous media, gas pressure data is challenging. Unique micro-CT scan experiments in our lab by Mark Willemsz [1] have shown that the ideal gas Xenon gives in the images at pore scale in a sandstone a pressure dependent signal (color), representing X-ray absorption (attenuation). This research shall be continued to exploit to what extend this physical effect of Xenon pressure dependent X-ray absorption can be applied to understanding multiphase gas flow in porous media. It might create the unique opportunity to visualize with CT scanning local pressure variations in various kind of fluid-gas flow experiments in porous media, beside the known application of Xenon as tracer [2,3]. Applications to explore are for example foam flooding for control of the gas mobility for hydrogen or CO_2 storage [4], capillary pressure curve determination of caprock and use of Xenon as tracer in gas trapping studies.

The Xenon pressure dependent micro-CT scan signal has been studied as single phase in sandstone [1]. The next step is to study whether the presence of a second phase in the pores, brine, will affect the correlations found between Xenon pressure and X-ray attenuation. By introducing brine, also the interaction of Xenon with brine is to be studied. Theoretically Xenon has a solubility in brine, which likely is not neglectable and therefore can affect the contrasts.

I joined the laboratory activities and completed a 4-month internship developing a multiphase core flooding set-up, where the brine can be introduced as a second phase, beside gas, in the porous media. Experiments with different geometries and phases can now be performed (see Figure), to study pressure dependence but also the Xenon diffusion in brine and how the Xenon gas signal is possible dependent on the pore geometry. Preliminary tests were performed proving the set-up functions. This allows further studies to be pursued, currently as master project in the spring semester of 2025. Once the concept is proven, the method can be applied to detect local pressure variations in various kind of multiphase experiments to ultimate describe and predict multiphase flow in porous better.

RECOMMENDED READING

[1] Willemsz M., June 24, 2022, A micro computed tomography-study on the use of Xenon as a pressure indicator in porous media. Internship report NTNU, TU Eindhoven, supervisor A. van der Net, Norwegian University of Technology.

[2] Taber, H. Jana G. Zimmerman, Howard Yonas, William Hart, Robin A. Hurley, 1999, Applications of Xenon CT in Clinical Practice: Detection of Hidden Lesions Katherine J. Neuropsychiatry Clin. Neurosci. 11:4, 423-425.

[3] Akin, S. and A. R. Kovscek,2003, Computed tomography in petroleum engineering research. From: MEES, F., SWENNEN, R., VAN GEET, M. & JACOBS, P. (eds). Applications of X-ray Computed Tomography in the Geosciences. Geological Society, London, Special Publications, 215, 23-38.

[4] van der Net, A., P. Zitha, 2005, A New Method for the Determination of Foam Capillary Pressures in Porous Media *SPE* 96988.

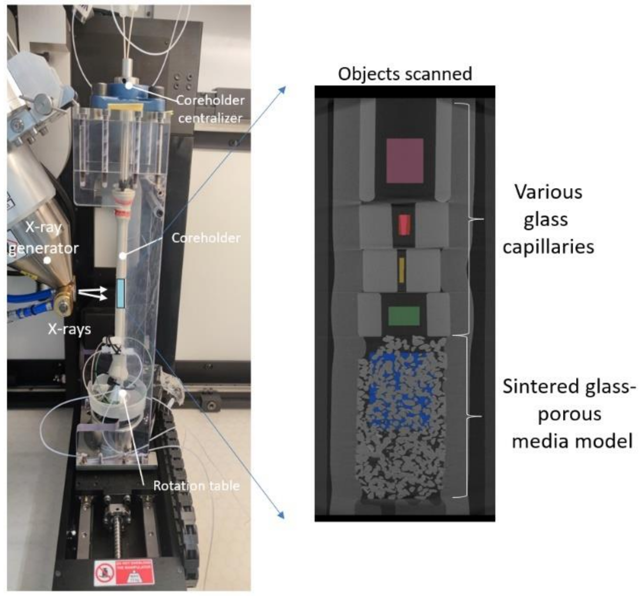


Figure: *The core holder placed in the micro-CT scan(left), where X rays can be sent through the object of interest. Several of these so-called projections are reconstructed into a 3D image. Right an example is given of the resulting 3D image, where the different grey scales represent different levels of X-ray absorption of gas filling the objects. The brighter the grey scale, the more Xray absorption, being dependent on the atomic number and density of the material. The colored regions are the analysed regions where the gas signal (X-ray absorption) is analysed.*

Nima HosseinZadeh

Polytechnic University of Turin, Italy
and Department of Geosciences, NTNU

Numerical Simulation on CO_2 Dissolution in Aquifers

6-month guest student, Fall 2024
Supervisor: Carl Fredrik Berg at NTNU

Background

Geological CO_2 storage is a growing solution to environmental challenges like global warming. Injecting CO_2 into aquifers triggers processes that lead to its permanent storage. CO_2 dissolves over time, beginning with gas diffusion, which increases the density of the top-layer brine, making it heavier than the bottom layer. Gravity and buoyancy effects then cause the heavier brine to sink and lighter brine to rise, enhancing the secure, long-term storage of CO_2 underground.

Objective and Methodology

The project aims to study CO_2 dissolution regimes in formation water using numerical simulations and compare the results with prior laboratory experiments. A reservoir model is developed with porous media and fluid properties matching the laboratory setup.

The model is a 3D symmetric cylindrical reservoir matching the laboratory tank dimensions (60 cm diameter and 60 cm height).

Figure 1 shows snapshots of the model at different simulation times.

Results

Running the simulation for one year and plotting dissolved gas (Rs) over time with a Python script reveals diffusion, convection, and convection impedance. The onset of convection can be roughly estimated by fitting two lines to the diffusion and its deviation, and a similar method estimates when convection impedes. These results align with laboratory experiments and match existing equations for estimating convection onset in the literature. Figure 2 illustrates the onset of convection, while Figure 3 depicts the different dissolution regimes.

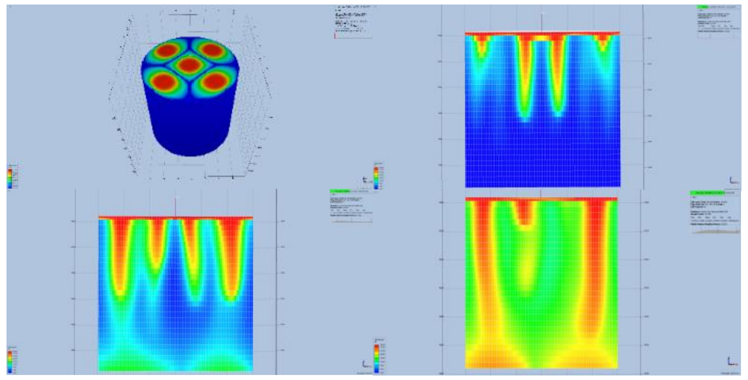


Figure 1*- Diffusion and convection over time*

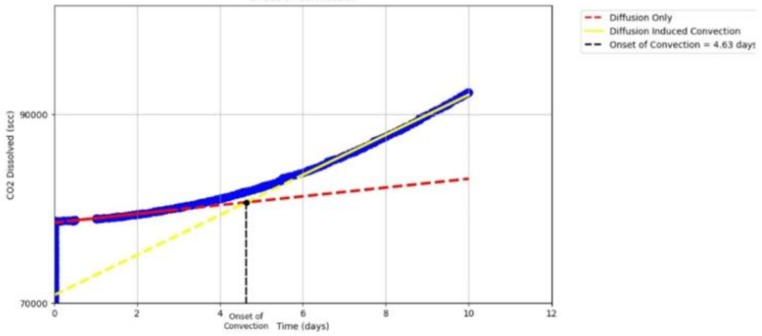


Figure 2*- Onset of Convection*

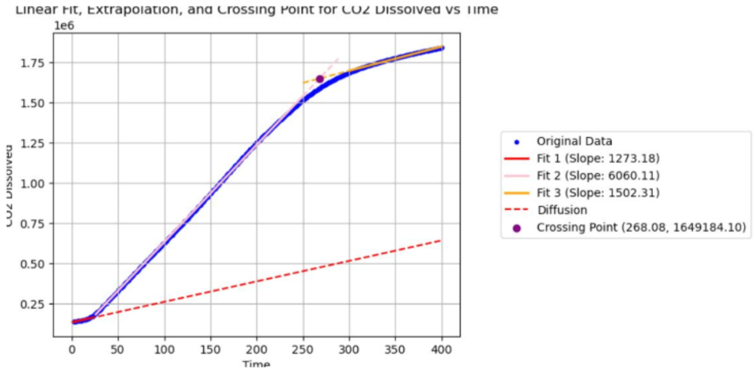


Figure 3*- Different regimes during dissolution*

INSPIRATION FOR MASTER PROJECTS

You find in the following pages a few suggestions for master projects to be performed at PoreLab. These are only a fraction of the possibilities. We like to tailor new projects to the particular student's wishes and can start a new topic this way. We invite therefore potential students to make contact with anybody in our crew at PoreLab.

Proposed Master Project at PoreLab NTNU (department of Physics)

Coarsening in snow

Contact: Quirine Eibhilin Krol (quirine.e.krol@ntnu.no)

Research Question

Ice crystals grow in size throughout the winter season after they have fallen to the ground and begin to sinter, forming the material we refer to as snow. This coarsening process is highly dependent on environmental conditions and remains poorly understood. Grain size, or specific surface area, is one of the most important characteristics for both remote sensing and the physical properties that determine mass and energy transport in snow. The primary thermodynamic driver for crystal shape change is the temperature gradient, which causes vapor in the pore space to deposit on the colder side of the crystal while sublimating on the warmer side. Since vapor fluxes are not directly detectable at the scale of snow grains, we can only observe the resulting changes in crystal morphology through μ-computed tomography. It is therefore essential to understand the origin of grain-growth that leads to coarsening, such that these models can be compared to experimental datasets.

Tasks

This project aims to investigate the role of density, size, and kinetic theory in crystal growth and coarsening rates by simulating growth using an existing pore-network model in one dimension and comparing the results with experimental data. The second objective is to extend this model to two (or three) dimensions and contextualize the results within broader coarsening models such as Gibbs-Thomson and Allen-Cahn theories.

Learning Goals

Throughout this project, you will become familiar with classical coarsening theories relevant to soft-condensed matter, which apply to both natural and industrial phenomena. You will gain practical experience by simulating snow crystal growth using Python and comparing the results to existing μ-computed tomography data. Additionally, you will develop skills in coding, documentation, and software maintenance. The ultimate goal of this master's project is to publish the results in a scientific paper.

The project will be supervised by Dr. Q. Krol. For more information contact: quirine.e.krol@ntnu.no

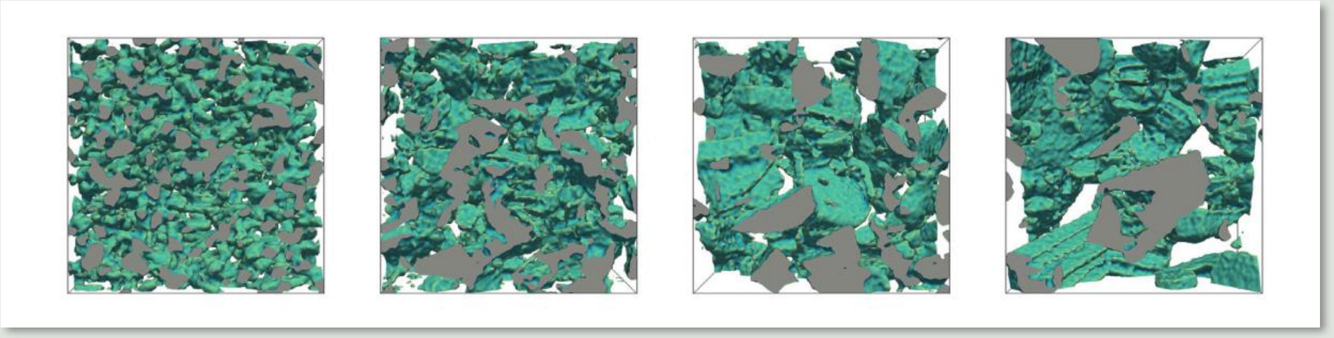


Figure: Visual representation of temperature gradient metamorphism at 4 time steps (Δt = 192 hours and the cube length is 3.51 mm)

Proposed Master Project at PoreLab NTNU (department of Physics)

Effect of gravity on steady-state two-phase flow in porous media

Contact: Santanu Sinha (santanu.sinha@ntnu.no)

Simultaneous flow of two immiscible fluids inside a porous medium shows a wide variety of non-trivial properties. For example, a low-viscosity fluid displacing a high viscosity fluid inside a porous medium at high flow rate creates viscous fingers, the growth of which recently found to depend non-linearly on the local pressure gradient in a certain regime [1]. When a steady state sets in, the total volumetric flow rate in two-phase flow also shows non-linear relationship between the total flow rate and pressure drop in a regime where capillary forces compete with viscous forces. The reason behind these non-linearities is the complex geometrical structure and the wetting properties of the pore space, which create a distribution of capillary barriers at the interfaces between the two fluids.

The importance of two-phase flow lies behind its various applications in industry and geophysics. However, in many applications the porous medium is not horizontal and therefore, in addition to the viscous and capillary forces, the gravitational forces play a significant role when the two fluids have different densities [2].

The goal of this project is to study the effect of gravity on the steady-state two-phase flow by using a dynamic pore-network model [3] where variable gravity can be implemented by adding a tilt to the network. The main tasks will be to find out the relation between the flow rate and the pressure drop, the saturation distribution, and the distribution of clusters in steady-state.

Recommended background:

Adequate skills and interest in programming in C and Python are essential for this project. Furthermore, fundamental understanding of fluid mechanics and statistical physics are recommended.

References:

[1] S. Sinha, Y, Méheust, H. Fyhn, S. Roy and A. Hansen, Phys. Fluids **36**, 033309 (2024).

[2] Y. Méheust, G. Løvoll, K. J. Måløy and J. Schmittbuhl, Phys. Rev. E **66**, 051603 (2002).

[3] S. Sinha, M. A. Gjennestad, M. Vassvik, and A. Hansen, Front. Phys. **8**, 548497 (2021).

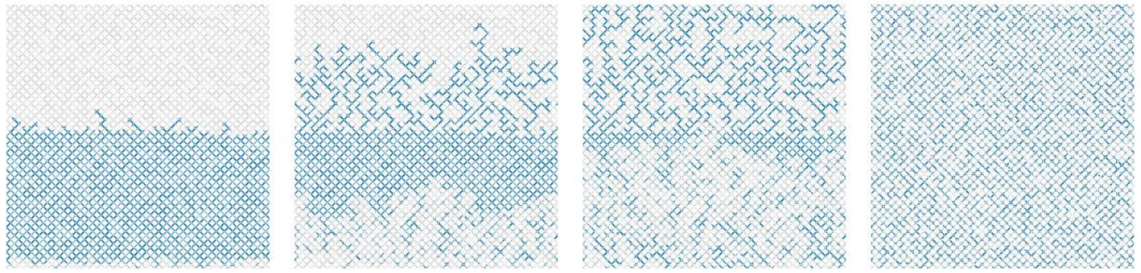
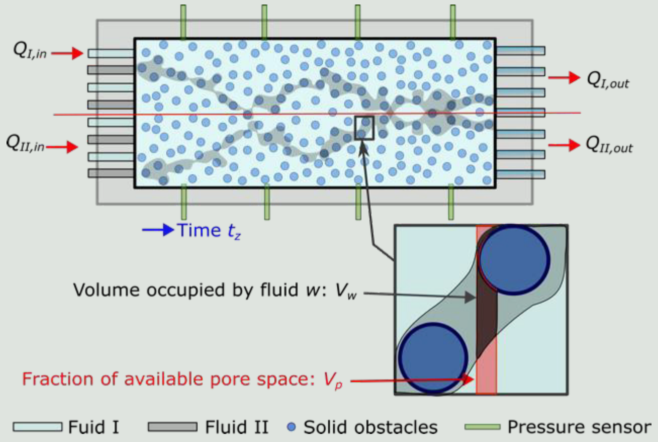


Figure: Dynamic pore-network simulation of two-phase flow in a 2-dimensional network of 64×64 *links where the wetting and non-wetting fluids are indicated by blue and gray colors. The images from left to right indicate the time evolution of the model where the right most image indicates a steady state.*

Proposed Master Project at PoreLab NTNU (department of Physics)

Information entropy in 2-phase flow

Contact: Erika Eiser (erika.eiser@ntnu.no)



Motivation

Clausius introduced the concept of Entropy as a cornerstone of thermodynamics. Boltzmann and Gibbs provided the statistical-mechanical interpretation of Clausius' entropy. Starting with the works of Shannon, Jaynes and Edwards, entropy-like quantities have been proposed characterizing non-thermal systems [1]. But investigating an equivalent of a Second Law of Thermodynamics has been hampered by the fact that many non-thermal systems have no natural time evolution. An exception is 2-phase flow through a porous plug, where we can interpret the distance along the flow direction as the equivalent of time (see Figure above).

Your Project

Using optical imaging, the student will experimentally explore the analogies and differences between fluctuations in this system in steady state, and equilibrium fluctuations in thermodynamic systems. In particular, the build a flow cell, mimicking a porous system with well-defined porosity, coupled to an imaging platform that will allow us to measure the velocities of probe-particles using Particle Flow Velocimetry (PIV). This will allow us to probe the phenomenology of spontaneous fluxes and fluctuations, to deduce the dependence of the flow "entropy" on the control parameters (primarily: flow rate and fluid composition).

Requirements

A background in statistical physics and thermodynamics is essential. Further, a keen interest in building up experiments and delving into image analysis are required.

Other Aspects

The project will be supervised by Professor Eiser, an expert in the rheology and microrheology. Latter derives the viscoelastic properties of probe colloids from their thermal fluctuations. If interested the student can do both simulations and/or experiments.

Reference

[1] CE Shannon. A mathematical theory of communication. The Bell system technical journal, 27(3):379 (1948); ET Jaynes. Information theory and statistical mechanics. Physical Review, 106(4):620 (1957); SF Edwards and RBS Oakeshott. Theory of powders. Physica A, 157(3):1080 (1989)

Proposed Master Project at PoreLab NTNU (department of Physics)

Permafrost – heat transport in porous media

Contact: Erika Eiser (erika.eiser@ntnu.no)

© AWI | Georg Schwamborn | ce wedges (Yedoma) on the Bol'shoy Lyakhovsky, the most southern Island of the New Siberian Archipelago [1]

Motivation

Permafrost is a combination of soil, rocks, and sand, held together by ice. Most of it is below freezing throughout the year. However, the top layer, called the active layer, undergoes a thawing-freezing transition during Earth's winter-summer cycle [2]. The soil in this layer is a densely packed, nanoporous network composed of silica-rich grains and clays, with a large size distribution of pores that are filled or partially filled with water. When below freezing, water in pores typically smaller than 10nm will remain liquid while the water in larger pores will freeze, which is known as Gibbs-Thomson effect. Recent theory by Flekkøy and Hansen (unpublished) finds ***super-diffusive propagation*** of a melting front in a frozen, nanoporous networks [3].

Your Project

To test the theory of super-diffusive propagation in a porous medium experimentally the student will build a nano-porous network in terms of a Hele-Shaw cell, which is a thin cell with flat walls. This will be densely packed with micron-sized silica beads and varying degrees of humidity. Using fluorescent microscopy and heating provided by a focused laser we will study how heat is propagating in such a controlled environment. The experiments will be conducted in a cold room, kept at -10ºC.

Requirements

The applicant should have a very good understanding of thermodynamics and be keen on setting up the cell, including the optics and sample preparation.

Other aspects

The experimental study will be supervised by the Professor Eiser, an experimental physicist at PoreLab (www.porelab.no).

References

[1] https://www.sonnenseite.com/en/science/thawing-permafrost-is-shaping-the-globalclimate/

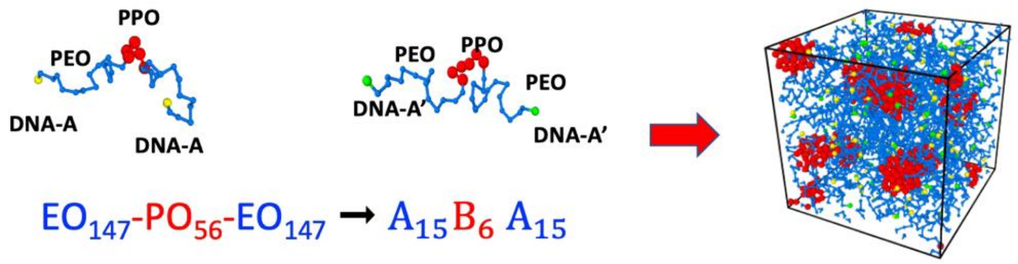
[2] J. Obu, "How Much of the Earth's Surface is Underlain by Permafrost?" J. Geophysical Research: Earth Surface, 126, e2021JF006123 (2021)

[3] E. G. Flekkøy, A. Hansen, B. Baldelli, "Hyperballistic Superdiffusion and Explosive Solutions to the Non-Linear Diffusion Equation" Frontiers in Physics 9, 640560 (2021)

Proposed Master Project at PoreLab NTNU (department of Physics)

Active hydrogels - Simulations

Contacts: Erika Eiser (erika.eiser@ntnu.no) and Raffaella Cabriolu (raffaela.cabriolu@ntnu.no)



Motivation

Hydrogels are solid materials predominantly made of water and a small fraction of self-assembled polymers. In everyday live we encounter hydrogels in form of foods, cosmetics and care products. But they are also essential in applications such as PCR tests, we had to go through in the past 3 years and DNA testing, pharmaceutics and diagnostic tools. Here we are interested in the study of hydrogels made of symmetric, non-ionic triblock copolymers, which are known as Pluronics®. At low temperatures their aqueous solutions are liquid. However, upon heating water becomes a less good solvent for the middle block and the chains start to aggregate to form micelles as shown in the simulation snapshot above[1]. At sufficiently high concentrations the micelles form a soft, gel-like crystal. By adding smart overhands, for instance short, single-stranded DNA, such systems can be made 'active', meaning they will react to an external stimulus.

Your Project

In this project the students will familiarize themselves with a Molecular Dynamics model of these triblock copolymers, previously mapped onto the real system [1], in LAMMPS [2]. As first task the students will perform some tests like, checking the self-assembling behaviour and reproduce a few points in the systems phase diagram [3].

The challenge will be to model the appropriate interactions between the free chain ends in terms of sticky patches with appropriate interaction potentials that will lead to the systems gelation in prescribed parameter settings. If time permits the structure and assembling dynamics will be explored.

Requirements

Background in Soft Matter physics would be advantageous. We would like an applicant who is interested in numerical model.

Other aspects

The project will be supervised by Professor Eiser, an expert in the rheology of self-assembling DNA systems. Associate Professor Cabriolu is an expert in simulation studies of soft matter systems. If interested the student can do both simulations and experiments.

References

[1] Jiaming Yu - PhD thesis: https://www.repository.cam.ac.uk/handle/1810/345675 (2023)

[2] LAMMPS Molecular Dynamics Simulator: https://www.lammps.org/#gsc.tab=0

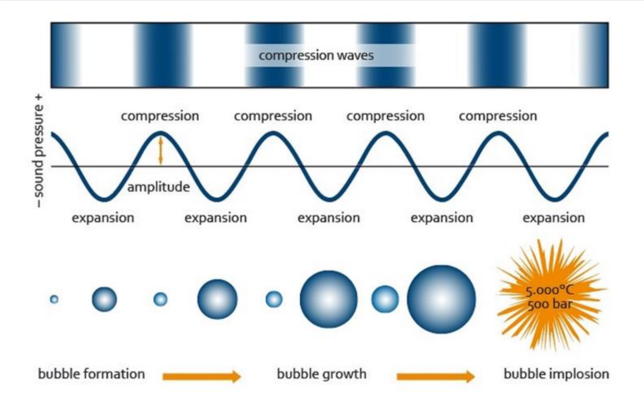
[3] R. Liu, A. Caciagli, J. Yu, X. Tang, R. Ghosh, E. Eiser 'Dynamic Light Scattering based microrheology of End-functionalised triblock copolymer solutions' *Polymers* 15, 481 (2023

Proposed Master Project at PoreLab NTNU (department of Physics)

Bubbles's nucleation and sonochemistry

Contact: Raffaella Cabriolu (raffaela.cabriolu@ntnu.no)

This project can be adjusted to 15, 30, 45 and 60 ECTS.



Compression and rarefaction cycles created by ultrasonic longitudinal pressure waves in a liquid give origin to a variety of effects mediated by the vapor bubbles that nucleate, grow, and interact during the expansion stage of the wave oscillation, and, eventually collapse when the pressure turns from negative to positive. The implosive collapse gives raise to extreme temperatures and pressures that found enormous applications in many fields. For example: ultrasounds are used in water treatments to eliminate pollutants; sonochemistry synthesis of nanoparticles promises more efficient and greener protocols to produce catalysts and to fabricate microelectronics components; furthermore, the ultraviolet light emitted during those processes inactivates microorganisms. Other applications concern food science, medicine, drug delivery and, more in general, bio- and nano-technology. Ideally, the understanding of the nucleation, growth, and implosion of bubbles under ultrasound waves, is essential to achieve the best performance for the desired application.

Your Project

The student will use the GROMACS software to model the formation, growth, and collapse of bubbles in a solution of different types of alcohols (Methanol (MeOH), Ethanol (EtOH), Isopropanol (IPA), 1-butanol (BuOH), and ethylene glycol (EG)) in water. Those solutions are used by experimental collaborators in NTNU that will provide their data against which we can validate our modeling results. The student can decide to approach the problem by performing a pure modeling study or to combine his thesis with some experimental activity.

Requirements

A background in computational physics is a great advantage. This project suits a student interested in modeling, simulation, and programming, and is able to work independently. Experience with C and/or Python is essential. If an experimental activity is also desired, it can be arranged with the experimental group which participates in the project.

Other aspects

This project is in collaboration with Prof. Jaakko Akola from the Department of Physics at NTNU, who will provide quantum approaches expertise, and, with Prof. F. Seland, Prof. S. Sunde, and the Ph.D. H. E. Hansen from the Department of Materials Science and Engineering at NTNU, that will provide the experimental support to the project.

References

[1] Scheme from the website: https://ultrawaves.de/en/ultrasonic/.

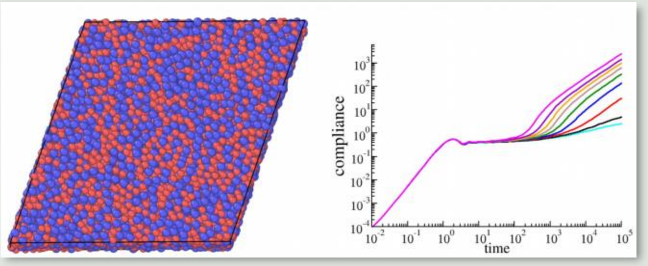
[2] R. Cabriolu, B. Pollet and P. Ballone, *Journal of Physical Chemistry B.*, 127,**7**, 1628-1644, (2023).

[3] Hansen, H. E.; Seland, F.; Sunde, S.; Burheim, O. S.; Pollet, B., *Ultrasonics sonochemistry.* **85**, 105991**,** (2022).

Proposed Master Project at PoreLab NTNU (department of Physics)

Understanding non-Newtonian materials

Contact: Raffaella Cabriolu (raffaela.cabriolu@ntnu.no)



Motivation

Non-Newtonian fluids are ubiquitous in everyday life, but the understanding of the fundamental physical process underlying their properties still remains a big challenge [1]. Why are we able to walk (yes, you can!) on a pool filled by a mixture of cornstarch and water or why toothpaste behave as a liquid when squeezed or sheared? Depending on the applied external force, yield stress materials behave solid- or liquid-like, undergoing peculiar transformations in their dynamics with increasing external load.

Your Project

In this project you will study the stress-strain curves for a Yukawa binary colloidal system representing a typical yield-stress material [2, 3]. In particular, the effect of different friction coefficients and damping parameters on the stress-strain curves will be investigated using Molecular Dynamics simulation. The results will help rationalize complex, irreversible phenomena such as aging and creep in disordered system [3, 4].

Requirements

Background in Soft matter physics would be an advantage. We would like a person interested in modeling, simulation and programming able to work independently. Experience with C or Fortran and/or Python are essentials.

Other aspects

Your study will be supervised by associate professor Cabriolu, who has experience in simulating yield-stress materials. Your computational work will also be supported by Prof. Suman Dutta, whose expertise includes colloidal physics and simulations [4].

Contact:

Raffaela Cabriolu (raffaela.cabriolu@ntnu.no)

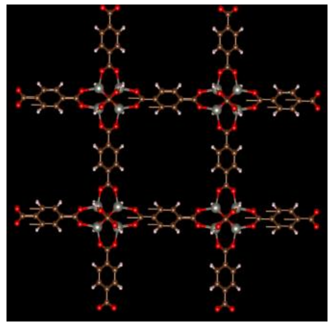
References

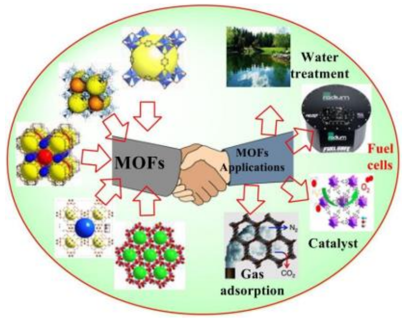
[1] D. Bonn and M. M. Denn , *Science*, **324** , 1401 —1402 (2009).
[2] A. Nicolas, E. E. Ferrero, K. Martens, and J-Louis Barrat, Rev. Mod. Phys., 90, 045006 (2018).
[3] R. Cabriolu, J. Horbach, P. Chaudhuri and K. Martens, Soft Matter, **15**, 415-423, (2019).
[4] S. Dutta, K. Martens and P. Chaudhuri, arXiv:2303.04718 (2023).

Proposed Master Project at PoreLab NTNU (department of Physics)

Classical force fields and machine learnt potentials in material modelling

Contact: Raffaella Cabriolu (raffaela.cabriolu@ntnu.no)





This project can be adjusted to 15, 30, 45, and 60 ECTS.

Motivation

Metal Organic Frameworks (MOFs) constitute a sub-class of nanoporous materials characterized by the combination of organic linkers and metal-ion nodes or vertices. The synthetic and structural versatility of MOFs allows, in principle, to tune their properties through the choice of the linker and/or the metal without changing the underlying topology. This advantage has attracted in the last 10 years large interests for their potential applications in sensing, gas storage and adsorption, chemical separation, and catalysis [1]. Despite the enormous potential in the application and fundamental science, MOF properties are not yet fully understood. Being able to efficiently model those materials, is indeed extremely beneficial to tune and optimize the performances of Metal Organic Frameworks (MOFs) according to our needs.

Your Project

The project will benchmark MACE-MP-0 [1] force field (newly developed Machine Learning potential field) against classical force fields, UFF4MOF, and experimental data to predict the structural and dynamical properties of nanoporous materials. In the first stage, i.e. Specialization project, the students will learn the basics of the Molecular Dynamics technique to predict known structural properties, such as Radial Distribution Function (RDF)m mechanical properties, eg. bulk modulus, and thermodynamical properties, e.g. heat Capacity of mesoporous materials, e.g. MOF-5 [2]. Those properties will be obtained by combining statistical physics and molecular dynamics simulations.

Requirements

Background in condensed matter physics would be an advantage. We would like a person interested in modeling, simulation, and programming able to work independently. Programming experience with Python is essential.

Other aspects

Your study will be supervised by Associate Professor Raffaela Cabriolu, who has experience in Molecular Dynamics simulations. Additionally, your computational work will also be supervised by Dr. Alin Marin Elena, whose interests include developing new Machine Learning interatomic potentials.

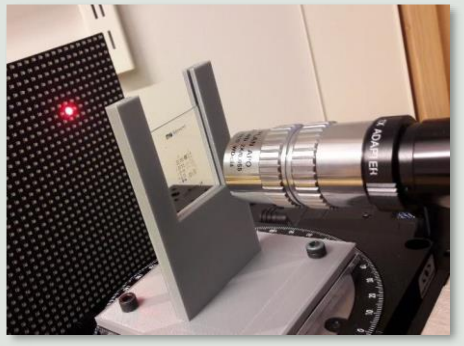
References

[1] https://arxiv.org/abs/2401.00096
[2] https://www.science.org/doi/10.1126/science.1083440

Proposed Master Project at PoreLab NTNU (department of Physics)

Fourier-ptychographic microscopy – a computer does half the imaging job!

Contact: Dag W. Breiby (dag.breiby@ntnu.no)



The FP microscope at NTNU

Fourier ptychography [Zheng 2013] is a microscopy technique based on a standard microscope where the traditional sample illumination has been replaced by a 2D array of partially **coherent** LED lamps, see picture. From each single LED, used one at a time, the light enters the sample with a unique incidence direction. By making one exposure for each LED sequentially, one gets a set of images that can be used to reconstruct both the amplitude and the **quantitative phase** of the imaged object, with a **resolution** well beyond the Rayleigh resolution limit imposed by the hardware. In other words, one single high-resolution wide field-of-view huge (~gigapixel) image can be obtained after the numerical manipulations.

During the last decade, devoted and hard-working master and Ph.D. students in our group have been able to develop a working Fourier ptychographic microscope, see image above. Now, we are keen to further improve the setup and to collect interesting data!

In this project you will:

- Review & understand the physics of Fourier ptychography.
- Choose from a long list of challenges, including:
    - Speed-up and/or miniaturize the image acquisition and reconstruction process (smarter algorithms, better hardware, machine learning, GPU programming)
    - Extension to quantitative polarization-sensitive microscopy for strain mapping
    - Deep 3D imaging of dynamic structures in surfactants: *foams, bubbles and droplets.* (This project requires efforts within instrumentation.)
    - Quantitative imaging of *flaws and fractures in car windscreens* in collaboration with SFI CASA (and European car industry)
    - Use *Machine Learning* methods for image reconstruction.

These projects require good programming skills and an interest in optics.

Co-supervision: The project will be carried out in close collaboration with Prof. M. Nadeem Akram at the University of South-Eastern Norway, located between Horten and Tønsberg.

References:

Zheng et al, Nature Photonics, 2013:
http://www.nature.com/nphoton/journal/v7/n9/full/nphoton.2013.187.html

Proposed Master Project at PoreLab NTNU (department of Physics)

Hyper-spectral X-ray imaging

Contact: Dag W. Breiby (dag.breiby@ntnu.no)

Standard X-ray imaging uses area detectors with pixels recording the number of incoming photons per time and area, i.e., the "intensity". Conventional radiography is poor at distinguishing materials of similar electron densities. In other words, thick & light materials may give the same beam attenuation as thin & dense materials.

Recently, energy-dispersive detectors have been developed, where each pixel is able to record the spectrum of the incoming radiation with good energy resolution. Because different elements give different "fingerprints" in their absorption spectra, these new detectors are radically better at discriminating material phases.

In the X-ray Physics Group, we have acquired an Advacam detector (https://advacam.com/application/non-destructive-testing/), which combines excellent energy resolution with high-speed readout and small pixels for good image resolution. This detector will be used with one of our existing X-ray sources to capture spectral images in 2D. The sample systems will be mainly fluids in porous and soft materials. The project will involve hardware development and experimental challenges. Still, the most demanding part of the project will be to develop computer algorithms to exploit the spectral information for quantitative imaging contrast.

The project requires good computer programming skills. An extension of the project could be corrosion studies of steel in contact with CO_2, in combination with compressed sensing and machine learning.

The project will be co-supervised by other members of the X-ray Physics Group.

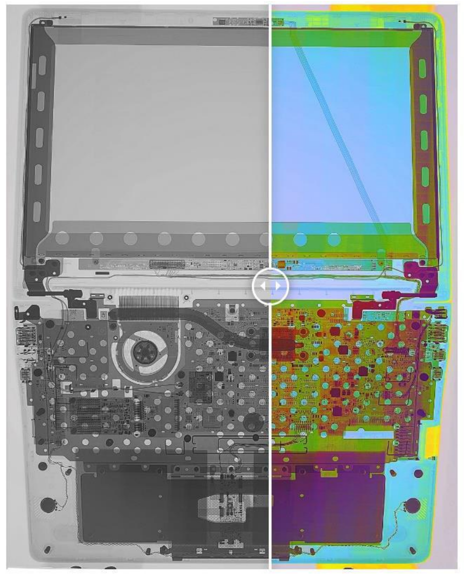


Figure: "Coloured" X-rays reveal additional features in an electronics circuit board. Image by Advacam Inc.

Proposed Master Project at PoreLab NTNU (department of Physics)

Phase contrast microscopy of droplet nucleation

Contacts: Dag W. Breiby (dag.breiby@ntnu.no) and Basab Chattopadhyay (basab.chattopadhyay@ntnu.no)

The scattering of electromagnetic radiation by particles has played an important role in the development of physics, with highlights including Descartes' understanding of the rainbow 400 years ago, Rayleigh scattering by small particles, and Mié's exact solution to the scattering of plane waves by spheres. In this project, we will study light scattering from liquid droplets on transparent functionalized substrates – relating directly to wetting, environmental physics, and CO_2 storage.

Ultimately, the project aims at measuring the condensation properties of CO_2 under conditions of high temperature and pressure – a challenge of high scientific interest and "green" industrial relevance.

Project tasks:

1. Study the relevant models for light scattering, and thermodynamics of liquid wetting and nucleation.
2. Implement an efficient computer program for calculating the near- and far-field (static) light scattering from droplets.
3. Develop a climate chamber (aided by our engineer!) for droplet nucleation. Starting with water, we would like to proceed to CO_2 condensation under high p and T.
4. Work on the inverse problem of resolving the droplet shape based on microscopy data, using numerical optimization techniques, including machine learning.

Co-supervision:
The project will be carried out in collaboration with Dr. Basab Chattopadhyay.

Figure 1 Physics and Nano students with Fourier ptychography microscope

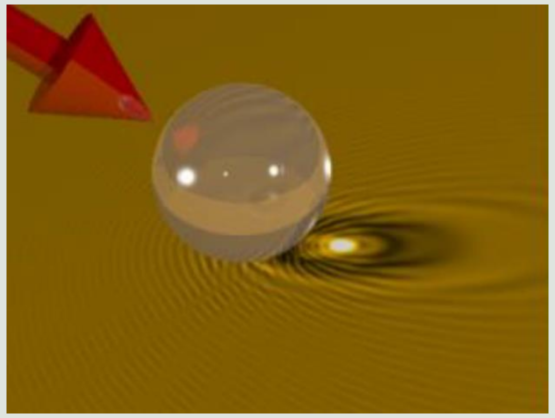


Figure 2. Modelling the light scattering from a translucent spherical object

Proposed Master Project at PoreLab NTNU (department of Physics)

X-ray phase-contrast microscopy & computed imaging

Contacts: Dag W. Breiby (dag.breiby@ntnu.no), Basab Chattopadhyay (basab.chattopadhyay@ntnu.no) and Ragnvald Mathiesen (ragnvald.mathiesen@ntnu.no)

Phase contrast in X-ray images was in fact first described by Einstein. For biological and other soft organic materials, the phase modification imprinted onto the electromagnetic field is stronger than the corresponding amplitude decay caused by beam attenuation, giving much improved image contrast.

A recent trend in optics is to teach microscopes to *think*: computer algorithms can in many situations replace conventional optical hardware (like lenses and filters), enabling 3D imaging, super-resolution, post-focusing, and other desired functionalities. Through phase retrieval algorithms based on ***machine learning***, quantitative images can be obtained. ***Quantitative*** imaging means that rather than measuring only "grey values", the images provide numbers describing for example the local material density.

We have recently purchased a partially coherent laboratory X-ray source ("***NanoTube***" from Excillum AB in Sweden) that we will use for phase-contrast microscopy.

Project tasks:

- Implement a digital twin based on Fourier optics and/or Monte Carlo ray tracing to mathematically describe phase-contrast X-ray microscopy with the *NanoTube* source.
- Demonstrate phase contrast imaging in 2D.
- Extend to 3D tomographic reconstructions. Rat brains and cold-water corals from the Trondheim fjord are particularly adequate samples!

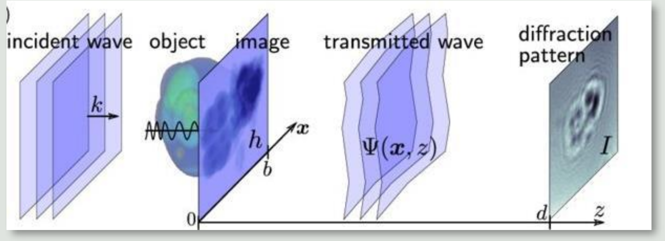


Figure : *Modeling the transmission and scattering of X-rays through an object. [Image Ref.: Maretzke & Hohage, SIAM Journal on Applied Mathematics 77 (2016)]*

Co-supervision: The project will be done in collaboration with Dr. Basab Chattopadhyay and Prof. Ragnvald Mathiesen.

Proposed Master Project at PoreLab NTNU (department of Physics)

4-dimensional computed tomography ("4D-CT") with Equinor

Contact: Dag W. Breiby (dag.breiby@ntnu.no) and Anders Kristoffersen at Equinor

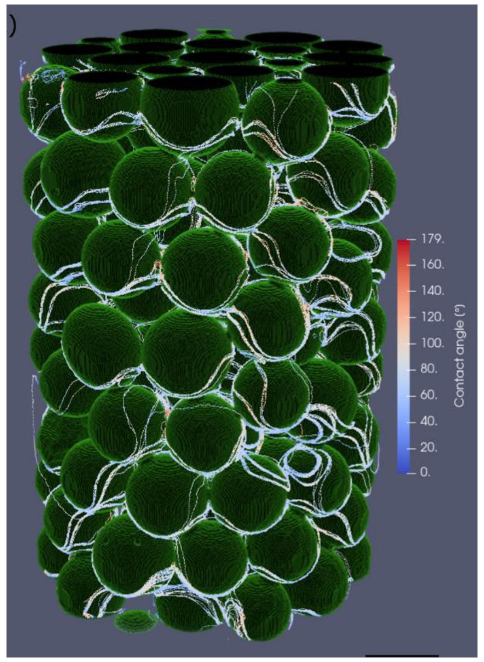


Figure: 4D-CT: Water being extracted from a pack of glass beads. The lines indicate the water level at different times, and the color coding of the lines gives the wetting contact angle [Tekseth, to be published].

We offer an exciting project on experimental porous media physics. Liquids in porous materials are a complicated topic of high relevance to many societal, industrial, medical, and environmental challenges. Examples include CO_2 storage in abandoned oil reservoirs, fresh water supply, and medicine administration across cell walls.

Computed tomography (CT) is a well-known non-destructive technique that gives 3D images of the interior of materials. If the object changes with time, the data will thus be 4-dimensional, hence "4D-CT". There are technical and scientific challenges associated with the 4D-CT measurements, and also with the statistical analysis and modelling of such large data sets (often several terabyte of data). A standard CT measurement of a static sample consists of typically 2000 radiographic projections at different angles and requires at least an hour of measurement time. To achieve a reasonable time resolution for dynamic studies (~minutes), a compromise must thus be found with a reduced number of projections, while still being able to reconstruct the 3D volume. Until recently, "compressed sensing" based on *sparsity* was the favoured technique for such reconstructions; the current trend is to employ Machine Learning.

Phase transitions of liquids in porous media are an applied challenge we would like to pursue. This problem is more complicated than one might immediately think: The freezing point of the liquid might be shifted towards lower temperature owing to the colligative effect of dissolved minerals, while the confinement in the pores tends to increase the freezing point. Additional challenges include i) mineral precipitation, ii) a series of coupled processes between heat and mass transport, and iii) mechanical deformation caused by the stress of the water expanding upon freezing. Many of these phenomena can be followed by CT. There are many challenges in terms of instrumentation, analysis and modelling.

The candidate should ideally have a strong background in physics, but also candidates trained in related topics like nanotechnology, chemistry & thermodynamics, big data, computer programming, mathematics, machine learning and artificial intelligence (AI) are welcome.

The project is partially motivated by better understanding phase transitions associated with CO_2 storage in abandoned oil reservoirs, so-called CCS, which is a prioritized area politically and industrially in Norway. The project is thus closely connected with major activities in Norwegian industry. This challenging problem also connects strongly to other climate processes like thawing of the tundra and subsequent release of methane gas – a potent greenhouse gas.

For exceptional candidates, projects of at least 30 ECTS might be carried out in collaboration with Equinor, being one of Norway's leading energy companies and a highly attractive workplace for graduates.

CT is a technique that is steadily gaining ground in new scientific fields, and the advanced analysis methods that will be used in this project are of high and generic interest. At the same time, the project is of course academically oriented and will be an excellent career step also for further university studies.

In this project you will:

- Review & understand the physics of CT
- Study liquids (wetting, capillarity, thermodynamics, ...)
    - Plan, perform and analyse "climate controlled" X-ray computed tomography experiments to obtain ***quantitative*** 3D **movies** of liquid-related phenomena in porous materials. Suggested studies include: Refinement/building of experimental sample environment
    - Analysis: Improving the image capturing and analysis (smarter algorithms, quantitative image analysis)
    - 3D imaging and simulations of dynamics, for example *multi-phase flow.*
    - *Machine learning approaches to data analysis and modelling.*

The project can be tailored to combine theory, numerical simulations, and experiments.
Co-supervision: Dr. Anders Kristoffersen (Equinor ASA)

Four Proposed Master Projects at PoreLab NTNU (department of Physics)

Ultrasound-mediated drug delivery to tumours and brain

Contacts: Catharina Davies (catharina.davies@ntnu.no) and Sofie Snipstad (sofie.snipstad@ntnu.no)

Web page https://www.ntnu.edu/physics/biophysmedtech/drugdel

Background: Ultrasound mediated delivery of drugs and nanoparticles in tumour tissue

Chemotherapy given alone or combined with radiotherapy or surgery is a common cancer therapy. A prerequisite for successful chemotherapy is that the drugs reach all cancer cells, and toxicity towards healthy tissue is limited. However, upon systemic injection of drugs, it is typically found that less than 1 % accumulates in tumors. Toxic effects on healthy tissue restrict the doses that can be applied and severely limit clinical outcome. A promising strategy for enhancing the accumulation of drugs to tumors, is to encapsulate drugs into nanoparticle carriers (NPs) and take advantage of the enhanced permeability and retention effect (EPR), permitting NPs to cross the leaky tumour capillary walls, but not capillaries in normal tissue. Although the NPs might extravasate across the capillary wall rather easily, the NPs do not to travel far away from the blood vessels and only a small population of cancer cells located close to the blood vessels will be exposed to the cytotoxic drugs as shown in *Figure 1*. The delivery of free drugs or drugs encapsulated into drugs and NPs depend on the vasculature, the transport across the capillary wall, through the extracellular matrix (ECM), and if the final target is intracellularly, the NPs/drugs have to cross the cell membrane (*Figure* 2). In order to improve the distribution of NPs/drugs, the delivery should be combined with a treatment facilitating the delivery.

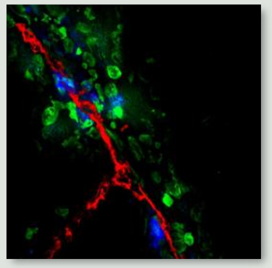


Figure 1: Nanoparticles (blue) do not travel far from the blood vessels (red). The encapsulated drug is taken up by cells (green) close to blood vessels

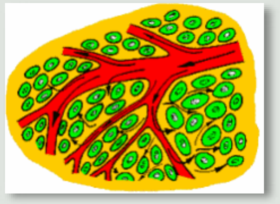


Figure 2: The delivery of nanoparticles/drugs depends on
1) The blood vessel network
2) Transport across the capillary wall
3) Penetration through the ECM
4) Cellular uptake

Delivery of drugs and NPs to brain tissue is even more challenging due to the blood-brain barrier (BBB). The BBB is a complex regulatory and dynamic system that prevents harmful substances from reaching brain tissue. Tight junctions between endothelial cells lining the microvessels form a physical barrier. Thus, to be able to treat diseases in the central nervous system, the BBB has to be opened safely and subsequently the NPs/drugs need to penetrate through the brain interstitium.

Ultrasound (US) focused toward the tumour or brain has been reported to improve drug delivery by different mechanical mechanisms such as acoustic radiation force or acoustic streaming and cavitation. Ultrasound in combination with gas filled microbubbles causes cavitation. Cavitation is the oscillation microbubbles in the acoustic field. Such oscillations can be stable and generate mechanical shear stress on the capillary wall thereby increasing the vascular permeability or the microbubbles can collapse in a violent process generating jet streams and shock waves that increase the vascular permeability, improve the transport through the ECM and increase the cellular uptake of NP. We are using different types of microbubbles such as commercially available microbubbles used for contrast enhanced imaging, SonoVue and Sonazoid, and microbubbles developed for drug delivery such as ACT bubbles explained below. The overall aim of our project is to study to what extent US and microbubbles can improve the delivery of distribution of NPs/drugs in tumour tissue and across the BBB, and to understand the underlying mechanism.

In collaboration with the company EXACT Therapeutics AS (https://www.exact-tx.com), we are studying the concept of Acoustic Cluster therapy (ACT) which is a novel drug delivery platform based on intravenously injection of clusters of microbubbles and microdroplets. After the injections, focused ultrasound is applied to the tumor or brain whereby the microbubbles transfer energy to the microdroplets, which undergo a liquid-to-gas phase shift. Growing in size, these large bubbles transiently block blood flow in a fraction of the capillaries. A second exposure of ultrasound causes these large bubbles to oscillate. The ACT bubbles have a diameter of typically 15-30 μm, whereas regular microbubbles also used at contrast agents for US imaging, have a diameter of 3-6 μm. Thus, the oscillating ACT bubbles generate biomechanical effects on a much larger part of the capillary wall than regular microbubbles. The induce biomechanical effects on the vessel wall enhancing the transport of drugs or NPs across the capillary wall. We have successfully shown that this concept can be used to treat tumors growing in mice. Now we are working on understanding the mechanisms. We are asking the questions: Does ACT change the ECM? Does ACT induce any immune response?

Our results in mice show that the tumor uptake of drugs and NPs and the therapeutic response of both ACT and US and microbubbles in general, vary between tumor types and between tumors of the same type. We have very promising results in prostate cancer, but limited success in pancreatic cancer. Thus, we also need to understand what causes these differences, both within tumor types and between tumor types. When using US and MB combined with chemotherapy in patients, it is important that the treatment is offered to the patients that can benefit from it.

1.Does ACT induce an immune response?

Contacts: Catharina de Lange Davies (catharina.davies@ntnu.no); Håkon Wesche (hakon.f.wesche@ntnu.no)

The cancer patient's immune response against tumour growth might have an impact on the overall survival and effect of cancer therapy. The infiltration of macrophages/neutrophils or cytotoxic T cells into the tumour is in general considered beneficial, eliminating cancer cells through respectively phagocytosis and apoptosis. The aim of this project is to study whether ACT causes infiltration of immune cells (macrophages, neutrophils, cytotoxic T-cells) into tumour tissue. The number of immune cells in tumours is measured by flow cytometry and their distribution in tumour tissue imaged by confocal laser scanning microscopy.

2. Does ACT improve cancer treatment using immune check point inhibitors?

Contacts: Catharina de Lange Davies (catharina.davies@ntnu.no); Håkon Wesche (hakon.f.wesche@ntnu.no)

Immune check point proteins on the surface of cytotoxic T cells (PD-1) recognize and bind to immune check point proteins on tumor cells (PDL-1). This binding prevents the cytotoxic T cells from killing cancer cells. Immune check point inhibitors can block the binding between PD-1 and PDL-1, allowing cytotoxic T cells to kill cancer cells. This is a new promising immunotherapy. However, only some patients respond to the treatment. The immune check point inhibitors are injected into the blood and need to cross the capillary wall and enter into tumour tissue. The aim of this project is to study whether ACT can improve the tumor uptake and microdistribution of immune check point inhibitors in tumours. The distribution of fluorescently labelled immune check point inhibitors will be imaged by confocal laser scanning microscopy.

3. Opening of the blood brain barrier by ultrasound and microbubbles

Contacts: Sofie Snipstad (sofie.snipstad@ntnu.no); Catharina de Lange Davies (catharina.davies@ntnu.no)

We have shown that ACT bubbles can open the BBB safely. Next, we want to use other microbubbles. Monodisperse microbubbles are especially promising as they are expected to give more reproducible and efficient cavitation response compared to polydisperse microbubbles. The efficiency of opening BBB using targeted microbubbles which bind to the vessel wall might also be studied. Opening of the BBB will be verified by MRI. Distribution of drugs or NPs into brain tissue will be imaged by confocal laser scanning microscopy of frozen sections of brain tissue.

4. Distribution of drugs in tumor tissue exposed to ultrasound and microbubbles

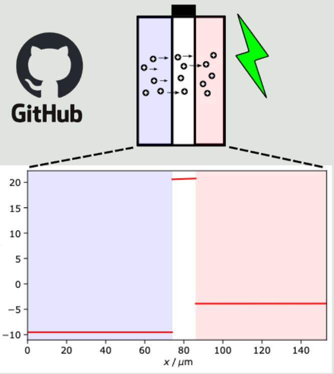
Contacts: Catharina de Lange Davies (catharina.davies@ntnu.no); Veronica Nordlund (veronica.nordlund@ntnu.no)

We have studied the effect of ultrasound and microbubbles on tumor uptake of a small molecular drug, doxorubicin, in two tumor types, colon and pancreatic cancer, which have different vascularization and stiffness. The background for studying the effect of ultrasound and microbubbles on uptake and distribution of small drugs is that at St.Olavs Hospital, we have two clinical studies treating cancer patients with standard chemotherapy in combination with focused ultrasound and microbubbles. We need to understand how ultrasound and microbubbles improve the distribution of small drugs in tumor tissue. Currently a master student is imaging tumor sections using confocal laser scanning microscopy, to determine the microdistribution of doxorubicin in control and treated tumors and estimate how far from a blood vessels doxorubicin is located. These analyses need to be continued. The new student will also image the blood vessels to study whether ultrasound and microbubbles have any effect on number of functional blood vessels and whether number of functional blood vessels correlate with the uptake of doxorubicin.

Proposed Master Project at PoreLab NTNU (Department of Chemistry and Department of Materials Science and Engineering)

Modelling hot spots in battery cells for improved performance and lifetime

Contacts: Signe Kjelstrup (signe.kjelstrup@ntnu.no) and Øystein Gullbrekken (oystein.gullbrekken@nnu.no)



Motivation:
Extreme fast charging of batteries is highly relevant for many current and new applications, such as electric vehicles, electric trucks and electric aircraft. To accelerate the adoption of batteries for existing and new applications, the US Department of Energy has set a target for next-generation batteries of less than 15 minutes charging time to reach 80 % state of charge. We need a better understanding of the internal transport processes of batteries in order to reach this target. However, during real-life battery operations (not inside a laboratory), our knowledge of the internal processes and internal state of the battery is limited. The precise modelling of battery cells is crucial in order to gain a better understanding of the internal processes and to be able to push the performance of the batteries during charging. Fast charging heats the battery and can generate local hot spots inside the cells which are detrimental for the lifetime of the batteries and can be a safety hazard.

Your project:
We have in a previous Master project developed a Python program for the nonisothermal modelling of a battery cell based on nonequilibrium thermodynamics. The battery cell model has a graphite anode and lithium iron phosphate cathode, and a standard mixed carbonate electrolyte with a lithium salt. In the current project, the student will study local heat effects and potential hot spots inside the cells as a function of the current using the existing Python code. Particularly, the student will examine how the properties (e.g. resistances) of the interfaces inside the cells influence the performance. The student will also get the opportunity to expand the program with new functionality, and to study new types of batteries and materials, for example Na-ion batteries, in the existing model framework, if they are interested in doing that.

Recommended background:
Background in thermodynamics is advantageous. An interest in modelling and programming.

Literature:

1. F. Schloms, Ø. Gullbrekken, S. Kjelstrup, Lithium-ion battery modelling for nonisothermal conditions, arXiv. https://doi.org/10.48550/arXiv.2411.14506
2. L. Spitthoff, A.F. Gunnarshaug, D. Bedeaux, O. Burheim, Peltier effects in lithium-ion battery modeling, J. Chem. Phys. 154, 114705 (2021). https://doi.org/10.1063/5.0038168

Proposed Master Project at PoreLab NTNU (department of Mechanical and Industrial Engineering)

Computer simulations of mechanical properties of graphene and other 2d materials

Contact: Astrid de Wijn (astrid.dewijn@ntnu.no)

In this project, we will investigate the mechanisms of solid lubrication using Molecular-Dynamics simulations. In lubrication with a solid powder, small, nm thin flakes of the solid slide easily past each other. While we have some understanding of the behaviour of single sliding flakes, we are only beginning to explore the effects of having multiple flakes that can act collectively, or how multiple layers interact with each other [1]

This project will focus on possible effects of tearing of layers, as well as the interactions between layers. Another possible line of inquiry is the interactions between flakes. You will employ the existing openly available molecular dynamics code LAMMPS in combination with python scripting to create the models and to analyze the results.

[1] *Understanding the friction of atomically thin layered materials*, David Andersson and Astrid S. de Wijn, Nature Communications **11**, 420 (2020).

Recommended background
A basic programming course and an interest in modelling or programming. Tribology, basic statistical mechanics, or classical mechanics.

Supervisor
Astrid S. de Wijn, astrid.dewijn@ntnu.no
Research group: http://syonax.net/science/research.html.
This project is part of the Gemini Centre for the COmputational multi-Scale materials societY (COSY) https://www.ntnu.edu/cosy/cosy

Resources
The project will make use of high-performance computing resources that are already available through NTNU IT's HPC facilities and Sigma2.

Work load
This project is intended for a combined specialization project thesis and master thesis, i.e. 45 or 60 ECTS in total.

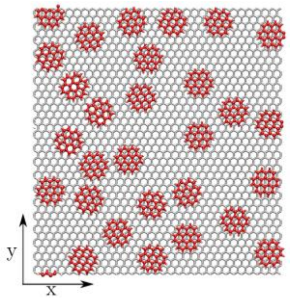


Figure : A top view of a simulation of a single layer of graphene flakes acting as a solid lubrican

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Proposed Master Project at PoreLab NTNU (department of Mechanical and Industrial Engineering)

Modelling spreading phenomena in social networks

Contact: Astrid de Wijn (astrid.dewijn@ntnu.no)

Large networks of interacting components are more common than you might think. Examples are human social interaction, communication networks, power grids, and ecological networks of species. When the components fail (people get sick, communication hubs break down, species go extict), this weakens the network and the other components. Once a few components have failed a cascade of failures can start, spreading rapidly through the network. The spread of a disease through social interaction, such as is happening right now, is an obvious example. Some large power blackouts affect hundreds of thousands of people and can last hours or even days. The purpose of this project is to study how the size of these failures is related to the interaction between the components. We have designed a simple general model for these types of systems, and it will be your task to simulate this model and study the results.

This project will involve a lot of programming to simulate the model, and statistical analysis of the simulations of the model. It may be necessary to study very large networks, which means that your code will need to be efficient. If necessary, you will run simulations on high-performance computing facilities.

Required background
A basic programming course and an interest in modelling or programming.

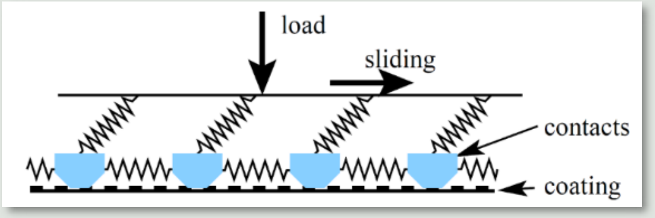
Supervisor
Astrid S. de Wijn, astrid.dewijn@ntnu.no
Research group: http://syonax.net/science/research.html.
This project is part of the Gemini Centre for the COmputational multi-Scale materials societY (COSY) https://www.ntnu.edu/cosy/cosy

Work load
This project is intended for a combined specialization project thesis and master thesis, i.e. 45 or 60 ECTS in total.

Proposed Master Project at PoreLab NTNU (department of Mechanical and Industrial Engineering)

Superlubricity in the real world: modellingmulticontact low-friction sliding

Contacts: Astrid de Wijn (astrid.dewijn@ntnu.no), Bjørn Haugen (bjorn.haugen@ntnu.no)



This project is concerned with structural superlubricity. This is a dramatic effect by which friction is reduced enormously due to structural incompatibility between two surfaces at the atomic level. Macroscopic surfaces in contact in the real-world, however, do not have one large flat contact, but consist of many small contacts.

The goal of the project is to investigate how superlubricity behaves in situations where there are multiple contacts. As part of this project, we will modify an existing model for multi-contact friction to take into account superlubric contacts. You will write and perform simulations of this model, and investigate its behaviour. If necessary, you will run simulations on high-performance computing facilities.

Recommended background
This project will entail a lot of programming, and it helps if you have good understanding of mechanics.

Supervisors
Astrid S. de Wijn, astrid.dewijn@ntnu.no
Bjørn Haugen, bjorn.haugen@ntnu.no

Research environment: http://syonax.net/science/research.html.
This project is part of the Gemini Centre for the COmputational multi-Scale materials societY (COSY) https://www.ntnu.edu/cosy/cosy

Work load
This project is intended for a combined specialization project thesis and master thesis, i.e. 45 or 60 ECTS in total.

Proposed Master Project at PoreLab NTNU (department of Mechanical and Industrial Engineering)

Machine learning aging in nanoscale friction

Contacts: Astrid de Wijn (astrid.dewijn@ntnu.no) and Ondrej Hovorka from the University of Southampton

In this project, you will learn machine learning and other data mining techniques to analyse simulated atomic force microscope (AFM) experiments. Aging in frictional contacts, including in AFM experiments, usually leads to increased friction when the contact is left stationary for some time. You will generate simulated force measurement data, by writing and run simple simulations of various basic models. You will analyse this data and build machine learning models and study how these can recover properties of the model, especially the presence of hidden dynamical degrees of freedom that can lead to aging.

Recommended background
A basic programming course and an interest in modelling or programming. A course dealing with data analysis.

Supervisors
Astrid S. de Wijn, astrid.dewijn@ntnu.no
Ondrej Hovorka, University of Southampton

Research group: http://syonax.net/science/research.html
This project is part of the Gemini Centre for the COmputational multi-Scale materials societY (COSY) https://www.ntnu.edu/cosy/cosy

Work load
This project is intended for a combined specialization project thesis and master thesis, i.e. 45 or 60 ECTS in total.

Proposed Master Project at PoreLab NTNU (department of Mechanical and Industrial Engineering)

Computer simulations of degradation of polymer surfaces into nanoplastics

Contact: Astrid de Wijn (astrid.dewijn@ntnu.no)

In this project, we will investigate the mechanisms by which polymeric materials can degrade under mechanical stress, UV radiation, or a combination of both. In the first stage, we will focus on simulating a small piece of a polymer surface, creating a realistic material with realistic structure. We will randomly break and reform bonds to mimic the effect of UV radiation, and investigate how this impacts the structure. In the second stage, we will subject the simulated material to mechanical stresses.

You will employ the existing openly available molecular dynamics code LAMMPS in combination with python scripting to create the models and to analyze the results.

Recommended background
A basic programming course and an interest in modelling or programming. Basic statistical mechanics or classical mechanics.

Supervisor
Astrid S. de Wijn, astrid.dewijn@ntnu.no

Research group: http://syonax.net/science/research.html
This project is part of the Gemini Centre for the COmputational multi-Scale materials societY (COSY) https://www.ntnu.edu/cosy/cosy

Resources
The project will make use of high-performance computing resources that are already available through NTNU IT's HPC facilities and Sigma2.

Work load
This project is intended for a combined specialization project thesis and master thesis, i.e. 45 or 60 ECTS in total.

Proposed Master Project at PoreLab NTNU (department of Geosciences)

Characterization of capillary trapping of CO₂ in micromodels and micro-CT scanner

Contact: Antje van der Net (antje.van.der.net@ntnu.no)

For flow optimization in porous media both for storage and production, an understanding of phase trapping in the porous media is crucial. This can be relevant for reduction of trapping of oil but for also stimulation of gas trapping in CO_2 flooding as one of the storage mechanisms.

For two phase flooding the concept of the capillary desaturation (CDC) curve correlates how the residual gas, water or oil depends on the capillary number (ratio of viscous and capillary forces), mainly for water wet systems. This concept is in simulation tools used to adapt the end point saturations of the relative permeability curves, dependent on how either viscous or capillary force are changing. The CDC curves are measured in the lab, determining residual oil saturation as a function of flow rate. The question is when this concept of CDC curves is applicable. How to use this concept if the wettability changes? Can variations in CDC curve tell anything about the wettability distribution within the core?

The study shall explore the use and dependencies of CDC curves measured, e.g. dependencies on wettability. Micromodels and core flooding will be used to further explore the effect of wettability on the CDC curve.

Proposed Master Project at PoreLab NTNU (department of Geosciences)

Pore scale imaging of CO₂ storage mechanisms using Xenon in a micro-CT scanner

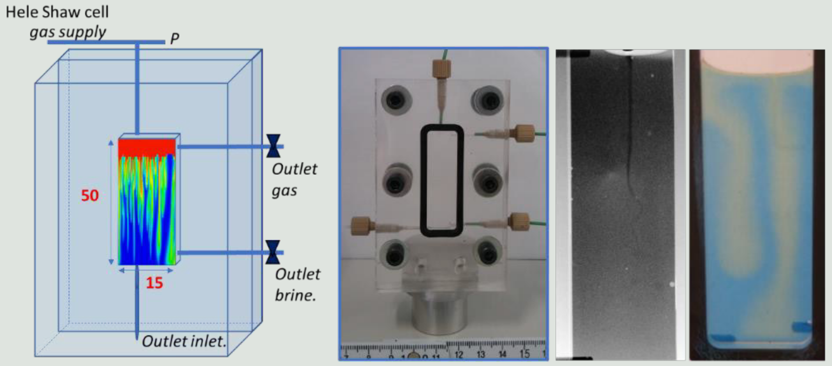
Contacts: Antje van der Net (antje.van.der.net@ntnu.no) and Carl Fredrik Berg (carl.f.berg@ntnu.no)

Multiple storage mechanisms act during CO_2 storage in the subsurface where capillary trapping and solubility trapping are two of them. When injected CO_2 forms a gas cap, the dissolution of gas from the gas cap is significantly enhanced by a natural convective motion, driven by the density difference between the formation brine and CO_2 enriched brine. These convective flows are crucial to distribute the CO_2 saturated brine, reduce the CO_2 gas phase and thereby enhancing the long-term storage potential of the reservoir. These convective flows are however not well understood nor described well in porous media.

The objective of this project is to visualize convective flow in 2D and 3D porous media and characterize capillary trapping by in-situ gas pressure measurements. As dissolved CO_2 is not visible in a mCT scan, we opt to use Xenon, as analogue gas. This shall ultimately lead to an Improved description of CO_2 storage capacity based on CO_2 solubility and transport. Depending on the availability different research objectives can be targeted:

O1. Pore scale visualization of convective flow in 1, 2 and 3 D models (see ***Figure 1*** *under for an example)*
O2. Pore scale monitoring of capillary trapping and Ostwald ripening
O3. Local gas pressure measurements during capillary trapping and Ostwald ripening (see ***Figure 2*** *under)*

The experimental results of O1 and O2 can be used as input for verification of the pore and core scale models. This can be part of the project, or the work can be performed in a team, co-supervised by Carl Fredrik Berg. Collaboration with the University of Oslo is possible concerning the effect of scale of the different 2D models



2M CsCl, 3wt%NaCl solution drop falling in water (CT scan)

CO_2 gas cap on top; Bromocrezol green used as pH indicator

Figure 1; *a 2D model to study convective flow, adapted to be used in the microCt scan*

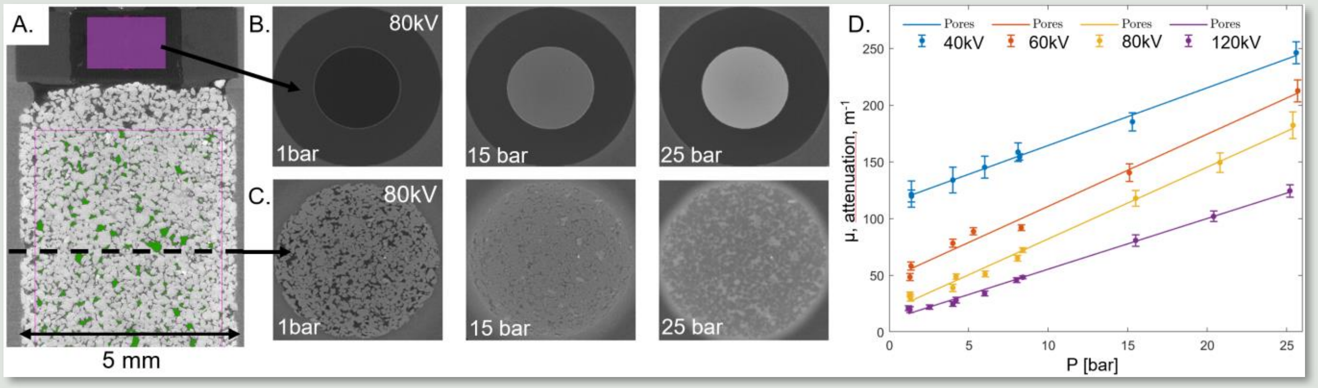


Figure 2; *The pressure dependence of Xenon visualized by mCT scanning of a void space in a plastic ring and a cylindrical Bentheimer sandstone core, both seen in A. The resulting cross sections of the void space and the Bentheimer core at set pressure levels of 1, 15 and 25 bar are presented in B. and C. respectively. In D. the linear correlations between static Xenon pore pressure and attenuation inside the pores are presented dependent on X-ray energy levels. The yellow curved for 80 kV is derived from images C. The ultimate objective is to use these curves to derive pressure from microCT scan images of Xenon gas flow in porous media. [Willemsz2022, A micro computed tomography-study on the use of Xenon as a pressure indicator in porous media. Internship report NTNU-TU Eindhoven, supervisor A. van der Net, NTNU]*

Proposed Master Project at PoreLab NTNU (department of Geosciences)

Low permeable rock characterization, cap rock and reservoir rock

Contact: Antje van der Net (antje.van.der.net@ntnu.no)

For CO_2 sequestration a sealing cap rock is critical. The sealing ability can be characterized by the capillary pressure of the cap rock, specifically the capillary entry pressure of the rock. This is however not exactly representing the breakthrough pressure of the cap rock, causing the actual leakage. This information is important for sealing predications. Similarly, breakthrough through different low permeable aquifer rock formations is of importance to describe the vertical CO_2 plum migration through the reservoir and predicting its leakage potential. There is to our knowledge no comparison made between the parameters of breakthrough capillary pressure and entry pressure combined with visualization of breakthrough.

O1: In this study we like to set-up and compare different methods of capillary entry and break through pressure determination combined with visualization of the fluid distribution using the micro-CT scan for the description of the sealing ability of a rock.

In order to model effects of CO_2 plum migration or understanding the pore network available for CO_2 mineralization reactions, characterization of the pore-network is crucial. The resolution of visualization methods like micro-CT scanning is limited, so microporosity is hard to characterize.

O2: In this study the pore network is to be analyzed using X ray contrast enhancing phases during visualization in the micro-CT scan.
Different contrast enhancers shall be tested and compared, scanning for different rock types, to derive a best practice to be applied in reservoir models.

The projects will be performed in collaboration with professors Philip Ringrose and Carl Fredrik Berg and PhD student Mateja Macut

Proposed Master Project at PoreLab NTNU (department of Geosciences)

CO_2 foam injection, improvement of CO_2 injection volumes by use of foams

Contact: Antje van der Net (antje.van.der.net@ntnu.no)

To store as much CO_2 in the subsurface as possible all the pore space shall be filled with CO_2. While injecting CO_2 or any other fluid in a porous media, not all pores are reached and filled. In order to improve the so-called volumetric sweep efficiency of CO_2 in a given volume, the viscosities of the fluids injected shall match or be higher than the viscosities of fluids in place. Generally, the viscosity of CO_2 in a gas- or supercritical state is always lower than the fluids in the pores. A solution is to inject CO_2 as foam. In these master projects we would like to explore how CO_2 as foam has an effect on the CO_2 injection and storage. Different aspects can be explored with the following objectives (O).

CO_2 stored as a gas cap exerts a gas pressure on the cap rock. This shall not lead to leakage through the cap rock. Gas in the form of foam will reduce the pressure exerted on the rock and will so reduce the risk of leakage. *O1: In this project the objective will be to study the effect of the foam presence and foam structure on the breakthrough pressure of the seal rock.*

One CO_2 storage mechanism is dissolution, which occurs after CO_2 stored in the gas cap will diffuse in the aquifer and create a convective flow based on differences in density. It has not been studied how CO_2 stored as a foam (see Figure 3) will affect the storage mechanism of CO_2 dissolution in the aquifer by convective flow.

O2: In this study a start of this will be made in the 2D visualization cell shown in Figure 1 and different flow patterns will be analyzed dependent on the foam structure, and rock properties.

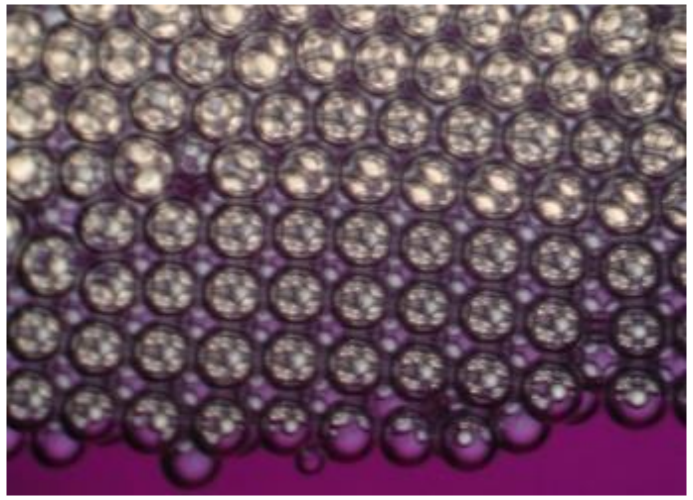


Figure: *Foam with bubbles of similar sizes on top of a liquid*

Proposed Master Project at PoreLab UiO (department of Physics)

CO_2 storage and stability of convection plumes in model aquifers

Contacts : Marcel Moura (marcel.moura@fys.uio.no), Knut Jørgen Måløy (k.j.maloy@fys.uio.no)

When CO_2 is injected into a closed water aquifer, which may be a porous medium closed by a caprock, the CO_2 will rise due to buoyancy to top of the reservoir where it will dissolve partially in water by diffusion and convection and form carbonic acid. The density of carbonic acid is higher than the density of pure water and this will cause the carbonic acid to sink due to buoyancy. This will set up an instable convection pattern which will be stabilized by the viscosity of the fluids, the resistance of the porous medium, and the CO_2 diffusion constant. The main tasks of this project will be to perform systematic experiments in quasi 2D experimental models by changing buoyancy and the permeability of the porous medium. This problem is of central importance to mastering CO_2 Storage in aquifers.

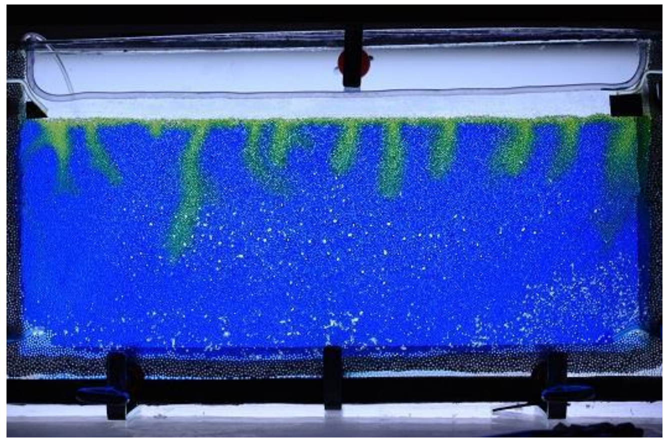


Figure: *A layer of CO_2 above a water-saturated porous medium consisting of glass beads. An indicator acid has been added to the water carbonic acid to turn it blue. Where the CO_2 has been absorbed by the water, carbonic acid forms which turns the color to green. The acid has larger density than water and form sinking plumes*

Proposed Master Project at PoreLab UiO (department of Physics)

3D scanning of porous media flows – mobilization of trapped clusters

Contacts : Marcel Moura (marcel.moura@fys.uio.no), Knut Jørgen Måløy (k.j.maloy@fys.uio.no)

The investigation of porous media flows is a topic of pivotal importance for several aspects of human activity. The extraction of water from natural reservoirs, the remediation of contaminated soils and the recovery of oil from subsea rocks are two examples where the knowledge of porous media physics brings immediate economical and societal impact. Performing experiments in 3D systems in porous media is challenging, as natural rocks and soils are never transparent. At the University of Oslo we have developed an innovative 3D scanning setup that allow us to see inside an artificial porous sample made of glass (https://titan.uio.no/teknologi-fysikk-goy-pa-laben-innovasjon/2020/splitter-ny-3d-skanner-folger-vaesker-fra-hulrom-til-hulrom).

In this project you will have the opportunity to further develop the technique and to apply it to study how different fluids move inside a porous network. In particular, we will employ the setup to study how trapped clusters of a fluid can be washed away from the porous medium by using another fluid moving fast around the first one. This experimental project will give you useful transferable skills related to fluid mechanics, optics, experimental control and programming.

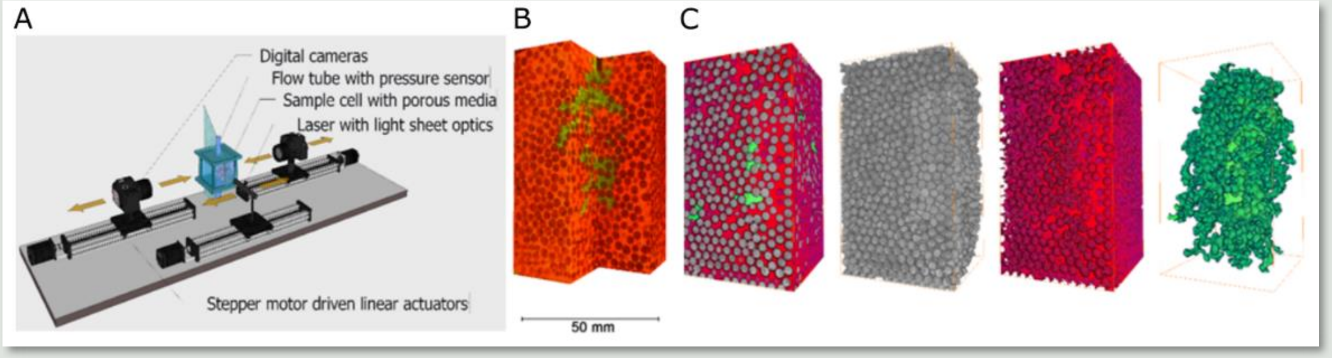


Figure*: A The 3D scanner is based on optical index matching and fluorescence. A random packing of 3 mm glass beads forms the porous medium, index matched with two immiscible fluids. The fluids contain different fluorescent dyes that are excited with a 2D laser sheet that is driven through the sample during a scan. The fluid phases appear on the images with different colors, making them distinguishable through the analysis. B Raw 3D data. The 2D images captured as frames by the cameras are added together to build up the third dimension. C Segmented phases. The porous medium and the two liquid phases are fully separated.*

Proposed Master Project at PoreLab UiO (department of Physics)

Pressure fluctuations in porous media flows

Contacts : Marcel Moura (marcel.moura@fys.uio.no), Knut Jørgen Måløy (k.j.maloy@fys.uio.no)

The investigation of porous media flows is a topic of pivotal importance for several aspects of human activity. The extraction of water from natural reservoirs and the recovery of oil from subsea rocks are two examples where the knowledge of porous media physics brings immediate economical and societal impact. One point that makes experiments in porous media particularly challenging is the fact that natural porous media, such as soils and rocks, are never transparent. By using artificial micromodels, one can overcome this challenge. In this project we will perform experiments in which one fluid will displace another in a quasi-2D porous network. We will take pressure measurements and images of the flow simultaneously and we will try to correlate the outcomes of these two measures. One of the main objectives is to try to use the fluctuations in the pressure signal to obtain indirect information about the properties of the porous network (such as its porosity) and the fluids involved (such as their viscosity contrast). This can provide the means for the development of new measuring techniques based on the pressure signal only, which can be further employed in the investigation of natural porous media

Figure: Detail of the trapped liquid clusters (blue) left behind after air (white) is slowly injected from the left in a quasi-2D porous network previously saturated with the liquid

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Proposed Master Project at PoreLab UiO (department of Physics)

Pollution spreading in porous media

Contacts : Marcel Moura (marcel.moura@fys.uio.no), Knut Jørgen Måløy (k.j.maloy@fys.uio.no)

When a wet portion of the soil gets dry, say after some hours of sunshine following a storm, thin liquid films remain on the surface of the soil grains. These thin films bring an interesting consequence: they can interconnect different parts of the soil, like a whole set of water bridges forming a large network of water streets and avenues. Plant roots can use this network to obtain nutrients from far away, but pollutants can also take a high-speed road to spread quickly in the soil (see figure). In this project, we are interested in understanding the dynamics of the transport of polluted water through a network of thin water films in a porous medium. This is analogous to the scenario in which some polluted water is spilled on the ground and starts to seep through the porous space. We will employ artificial porous samples in our study (either made of glass or 3D printed in a transparent plastic) which allow us to directly track the motion of the pollutant. We have observed that the residual water content in the sample (how wet or dry the soil is) plays a key role in the pollution spreading dynamics. We have found that for intermediate residual water content, the thin liquid films in the sample behave as a network of tiny pumps, which act to spread the pollution very quickly. Once this behavior is properly understood, we believe it will allow us to understand how we can make use of the thin film network for soil remediation measures. The same transport mechanisms that aid the pollution spreading can be tailored to spread a cleaning agent in the soil, to remediate the damage caused by the pollution.

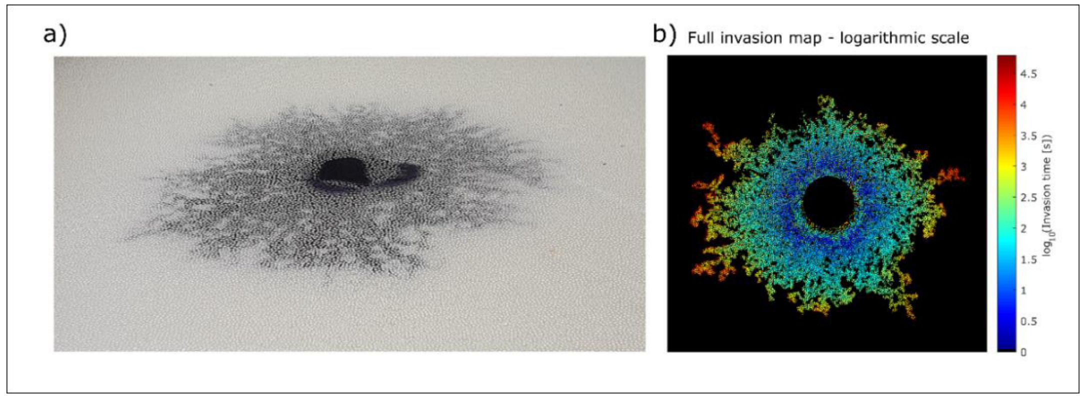

Figure: a) Experiment illustrating how a source of pollution (central dark blob) spreads through a partially wet porous network (here made of glass beads). Water films covering the internal surfaces of the porous medium can act as a fast pathway for the spreading of pollution. b) Spatiotemporal invasion map of a typical experiment. The color code shows the time (in seconds, logarithmic scale) for the pollution to reach a given point in the network.

Proposed Master Project at PoreLab UiO (department of Physics)

Steady state two phase flow experiments in 3D

Contacts : Marcel Moura (marcel.moura@fys.uio.no), Knut Jørgen Måløy (k.j.maloy@fys.uio.no)

Simultaneous flow of two fluid phases in a porous medium will after a transient state often lead to a steady state regime where all measurable quantities have a well defined statistical distribution with well defined averages. Experiments in quasi 2D systems have been performed in the past in our group for horizontal models. The goal of this experiments is to perform steady state experiments in 3D with density matched fluids to prevent buoyancy effects. This project is of central importance for comparison with theoretical model building in PoreLab. In two dimensional systems an unusual scaling relation has been found between the flow rate and the pressure, and we want to investigate the relation between the pressure and the flow rate for a three dimensional system. This project is also of great technological interest for fluid flow in oil and water reservoirs in addition to CO_2 sequestration in porous media.

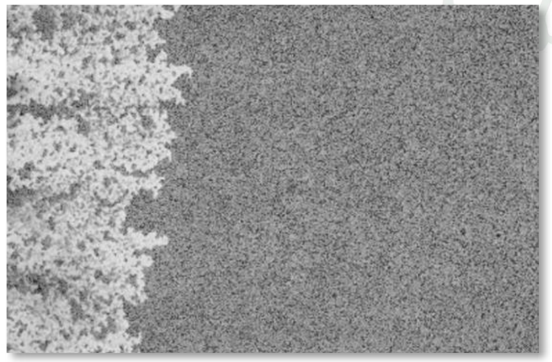

Figure: Steady state flow in a quasi 2D model system. Simultaneous injection of a glycerol/water (black) solution and rapeseed oil (white)

Proposed Master Project at PoreLab UiO (department of Physics)

Steady state two phase flow experiments in 3D

Contacts : Marcel Moura (marcel.moura@fys.uio.no), Knut Jørgen Måløy (k.j.maloy@fys.uio.no)

The investigation of porous media flows is a topic of pivotal importance for several aspects of human activity. The extraction of water from natural reservoirs and the recovery of oil from subsea rocks are two examples where the knowledge of porous media physics brings immediate economical and societal impact. Since the visualization of flows in porous media can be very challenging, numerical simulations have been used to study the morphology and dynamics of flow structures both in fast and slow injection processes. With the development of modern high-resolution and high-speed imaging techniques, we are now in position to address experimentally questions that previously could only be accessed via numerical simulations. In this project we will investigate, both experimentally and analytically, how the invasion dynamics of a pore is affected by speed of the flow.

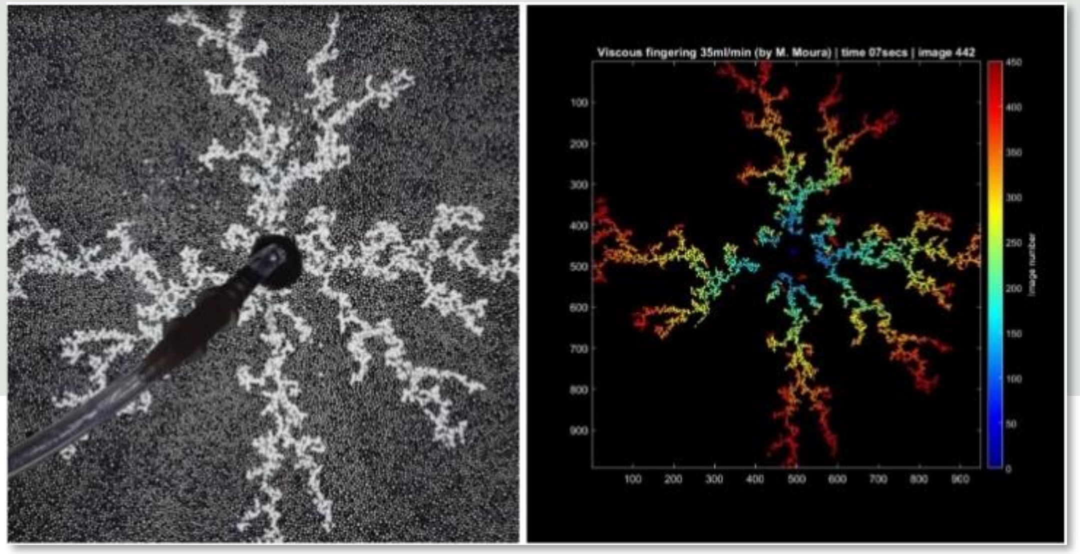

Figure: Viscous fingering pattern (left) observed when air is injected fast in a porous medium previously filled with a viscous liquid (blue). The image analysis (right) shows the time (image number) of injection of each pore

Proposed Master Project at PoreLab UiO (department of Physics)

Steady state two phase flow in a gravitational field

Contacts : Marcel Moura (marcel.moura@fys.uio.no), Knut Jørgen Måløy (k.j.maloy@fys.uio.no)

Simultaneous flow of two fluid phases in a porous medium will after a transient state often lead to a *steady state* regime where all measurable quantities have a well defined statistical distribution with well defined averages. Experiments in quasi 2D systems have been performed in the past in our group for horizontal models. The goal of this project is to investigate the influence of buoyancy effects by changing the gravitational constant in the direction of the flow. This will be done by systematic tilting the models. The goal is to measure the fluid saturation and the distribution of trapped fluid clusters, the pressure drop across the model, and the dynamics linked to snap-off coalescence and migration of clusters. This project is of great interest in comparison with theoretical model building in PoreLab. It is also of great technological interest for fluid flow in oil and water reservoirs in addition to CO_2 sequestration in porous media.

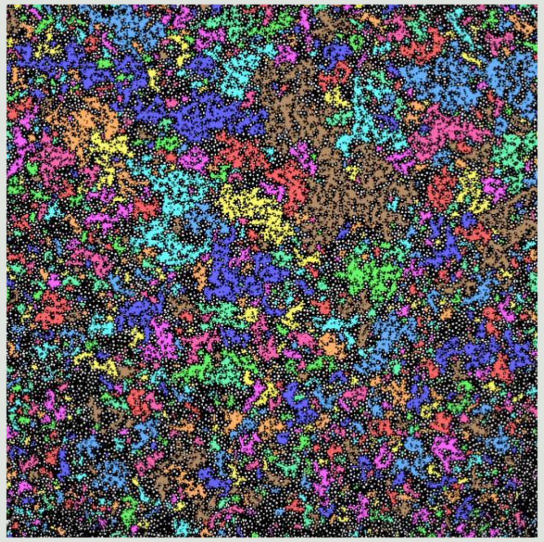

Figure: *Steady state two phase flow experiments in a horizontal quasi 2D porous media. Air and a glycerin water solution are injected simultaneously into the porous medium. The colors indicate different cluster sizes of trapped air*

Proposed Master Project at PoreLab UiO (Njord center, department of Physics)

The role of pore fluid phase transition during earthquake ruptures: insights from an idealized numerical model

Contacts: Fabian Barras (fabian.barras@mn.uio.no), Gaute Linga (gaute.linga@mn.uio.no), Eirik G. Flekkøy (e.g.flekkoy@fys.uio.no)

Motivation

Earthquakes lead to large and fast changes in porosity along the fault and in the surrounding rock. Under water-saturated conditions, this rapid expansion of fluid-filled cavities and fractures could lead to transient phenomena such as vaporisation due to the resulting large pressure drop, impacting the propagating earthquake rupture. However, a proper quantification of the conditions leading to such events and their resulting stresses is needed.

Project description

In this project we propose to investigate the physics of a rapidly expanding fluid-filled cavity. The student will employ and develop a numerical model that fully couples solid and fluid dynamics at the tip of a rapidly growing tensile fracture. We will initially consider a single fluid-filled crack propagating between two semi-infinite solid blocks (see Figure). The compressible fluid dynamics within the expanding cavity will be simulated using a finite element method formulated on a moving mesh. The implementation of the fluid dynamic model will be validated against theoretical predictions. Next, the model will be used to identify the conditions leading to phase transition of the pore fluid and its impact on the surrounding solid, i.e. the formation and eventual collapse of cavitation bubbles. Throughout the project, the candidate will benefit from direct comparison with ongoing experiments at PoreLab UiO investigating cavitation in an analogue setup.

Resources

The candidate will learn how to use High-Performance Computing (HPC) infrastructure and will have access to the computing clusters of the Norwegian HPC infrastructure (Sigma2) as well as the local cluster of PoreLab UiO.

Required background

Basic programming skills (C++, Python) and basic background in fluid mechanics. Some knowledge of solid mechanics and thermodynamics is an advantage.

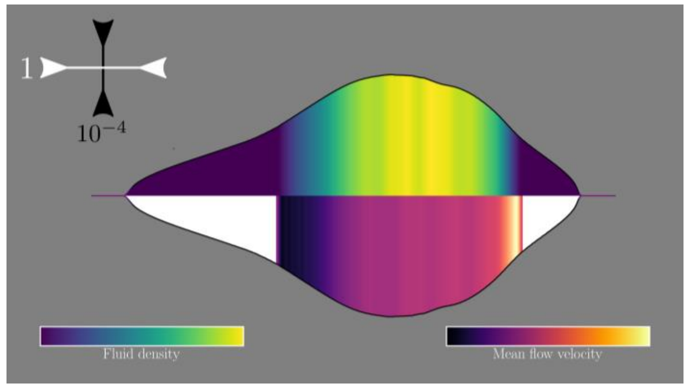

Figure: *Snapshot of dynamic fluid flow simulation (i.e. density and mean fluid velocity) within a rapidly expanding crack cavity. The white area highlights the formation of a fluid-depleted cavity.*

Proposed Master Project at PoreLab UiO (Njord center, department of Physics)

Experimental imaging of chemical transport and mixing in multiphase porous media flows

Contacts : Kevin Pierce (j.k.pierce@mn.uio.no), Marcel Moura (marcel.moura@fys.uio.no), Knut Jørgen Måløy (k.j.maloy@fys.uio.no), Gaute Linga (gaute.linga@mn.uio.no)

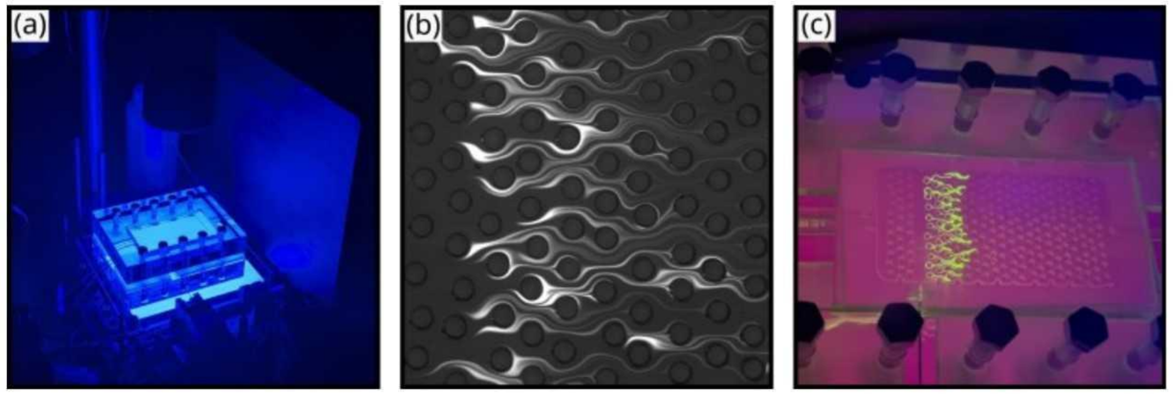

Figure: *(a) Fluorescence imaging experiment, showing blue excitation light; (b) Solute plume in a single phase flow; (c) 3D printed porous model with green fluorescence light from a dye undergoing mixing.*

Motivation:

Solute mixing in porous media is essential to a host of industrial and natural processes, as it dictates the speed of chemical reactions by bringing reactants into contact. The mixing dynamics of steady single-phase flows through porous media are becoming well understood. However, for multiphase flows, e.g. when air and water flow together below Earth's surface, very little is known, despite the prevalence of these flows in the environment.

Project description:

We will employ state-of-the-art fluorescence imaging and stereolithography 3D printing techniques to study the dynamics of mixing in porous media. Our setup resolves the concentrations of initially segregated chemicals in porous media flows through space and time. Image analysis techniques will be developed to analyse the mixing dynamics, and we will assess how different boundary and flow conditions affect the results. Experiments will be compared to numerical simulations performed under similar conditions. This project will provide insights into the fundamental physics underpinning applications from carbon dioxide sequestration to groundwater remediation.

Resources:

The student will learn to use the fluorescence imaging and 3D printing facilities at PoreLab UiO and will have access to dedicated computing resources for image analysis.

Required background:

Interest in fluid dynamics, experimental methods, data analysis. Students with diverse backgrounds are especially encouraged to apply.

Proposed Master Project at PoreLab UiO (Njord center, department of Physics)

Experimental resolution of local flow velocities in multiphase flow through porous media

Contacts : Kevin Pierce (j.k.pierce@mn.uio.no), Marcel Moura (marcel.moura@fys.uio.no), Knut Jørgen Måløy (k.j.maloy@fys.uio.no), Gaute Linga (gaute.linga@mn.uio.no)

Motivation:

Simultaneous flow of gases and liquids is ubiquitous in Earth's porous subsurface, and governs biogeochemical processes ranging from contaminant degradation in groundwater to nutrient cycling in soils. While the velocities of single-phase flows through porous media are relatively well-understood, our understanding of the local flow velocities in multiphase flows remains limited. Partly, this is due to the challenge of measuring flow velocities simultaneously with the moving interfaces between different fluids.

Project description:

The student will innovate new methods to resolve the local flow velocities and interface dynamics in flows through porous media, using the state-of-the-art imaging and 3D printing facilities at the PoreLab UiO laboratories.

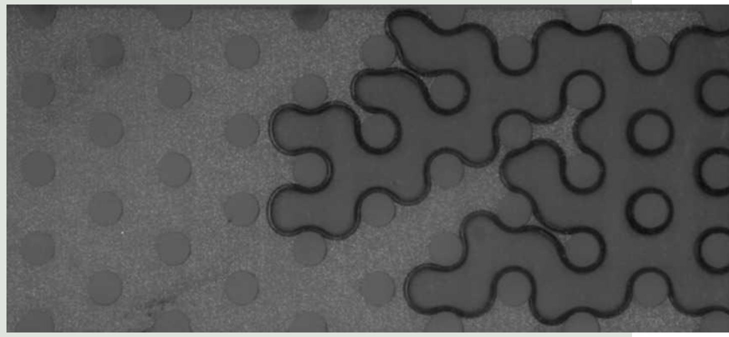

Figure: *Snapshot of microscopic tracer particles in a two-phase flow through a porous model*

Multiphase flows through 3D-printed transparent models will be seeded with microscopic fluorescent tracer particles, and these particles will be tracked in high-speed videos to resolve real-time velocity fields in porous media. Flow characteristics will be quantified for different multiphase flow geometries (i.e., drainage, imbibition) and physical conditions (i.e., interfacial tensions and applied pressure gradients)

Resources:
The student will have access to the laboratory facilities and experimental expertise at PoreLab UiO to construct particle-tracking velocity experiments. Students will benefit from direct comparison with simulations in identical geometries (see also the related computational project). Dedicated computing resources will be made available for image analysis.

Required background:
Interest in fluid dynamics, experimental methods, and data analysis. Students with diverse backgrounds are especially encouraged to apply.

Proposed Master Project at PoreLab UiO (Njord center, department of Physics)

Numerical simulation of mixing in microscale multiphase flow

Contacts: Gaute Linga (gaute.linga@mn.uio.no), August Johansson (SINTEF Digital, august.johansson@sintef.no), Eirik G. Flekkøy (e.g.flekkoy@fys.uio.no)

Motivation:
Solute mixing in porous media is essential to a host of industrial and natural processes, as it dictates the speed of chemical reactions by bringing reactants into contact. The mixing dynamics of steady single-phase flows through porous media are becoming well understood. However, for multiphase flows, e.g. when air and water flows together, very little is known. This partly stems from the fact that it is difficult to numerically resolve flows with strong capillary forces and low solute diffusion.

Project description:
In this project, we will employ a combined Eulerian-Lagrangian representation of two-phase flow with solute transport. We will use a finite-element formulation of a phase-field model to represent the interface between the two immiscible fluids and a (Lagrangian) diffusive strip method to resolve the solute transport. This allows us to characterize fluid stretching at unprecedented accuracy, including measuring the Lyapunov exponent which quantifies chaotic mixing. The MSc project will be tailored to the recruited student, but could include:

- Implementing and comparing different discretization schemes for the 3D fluid flow model. This will allow us to answer under which conditions (fully or partially) implicit schemes, with fewer but larger time steps, are advantageous over more explicit schemes, with more but smaller time steps.
- Investigate how chaotic mixing dynamics are influenced by two-phase flow in 3D periodic porous geometries and microfluidic geometries.
- Numerically and theoretically investigate how the mixing dynamics at finite Peclet number relates to the Lyapunov exponent or other flow properties.

Resources
The student will learn how to use HPC infrastructure and have access to Sigma2 and the PoreLab UiO cluster. The project will benefit from comparison to experiments carried out under similar conditions (see other project).

Required background
Strong interest and basic skills in numerical methods, scientific computing, fluid mechanics. Some knowledge of statistical mechanics is an advantage.

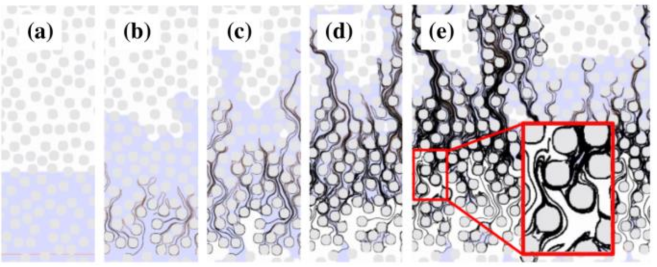

Figure: *Simulations of chaotic mixing in two-phase flow in a 2D porous medium. (a)–(e) show a strip of solute at various instances of time as it is exponentially elongated by a net upward flow*

Proposed Master Project at PoreLab UiO (Njord center, department of Physics)

Modelling pollutant spreading through capillary bridge networks in soils

Contacts: Paula Reis (p.k.p.reis@mn.uio.no), Marcel Moura (marcel.moura@fys.uio.no), Gaute Linga (gaute.linga@mn.uio.no)

Motivation:
When water-saturated granular soils are drained or dried, water in the pore space between grains is replaced by air. This process leaves behind water clusters and bridges which are held in place by capillary forces [1]. These clusters and bridges can together form large-scale connected networks which may act as highways for pollutants or chemical solutes spreading in soils. However, how fast and how far solutes may spread in these networks, under different physical conditions, remains elusive. A better understanding of this process would be of immediate interest e.g. in the context of environmental remediation.

Project description:
In this project, students will develop a numerical pore-network model that incorporates fluid and solute transport in arbitrary capillary bridge networks. We will effectively model flow and solute transport in individual bridges of the network by direct pore-scale simulation in representative geometries. Students will investigate how network structure influences the speed and extent of solute spreading, and characterize and/or theoretically describe the macroscopic behaviour, allowing us to predict critical conditions for pollutant spreading. The candidate will benefit from direct comparison with ongoing experiments at PoreLab UiO (see also the related experimental project).

Resources:
Students will learn how to use national high-performance computing resources (Sigma2) and will have access to Sigma2 as well as the computing clusters of their unit (PoreLab UiO/NTNU).

Required background:
Basic programming skills (Python, MATLAB and/or C++) and basic knowledge of fluid mechanics.

Reference:
[1] P. Reis, M. Moura, G. Linga, P. A. Rikvold, E. G. Flekkøy, K. J. Måløy, A simplified pore-scale model for slow drainage including film-flow effects, Advances in Water Resources 182, 104580 (2023)

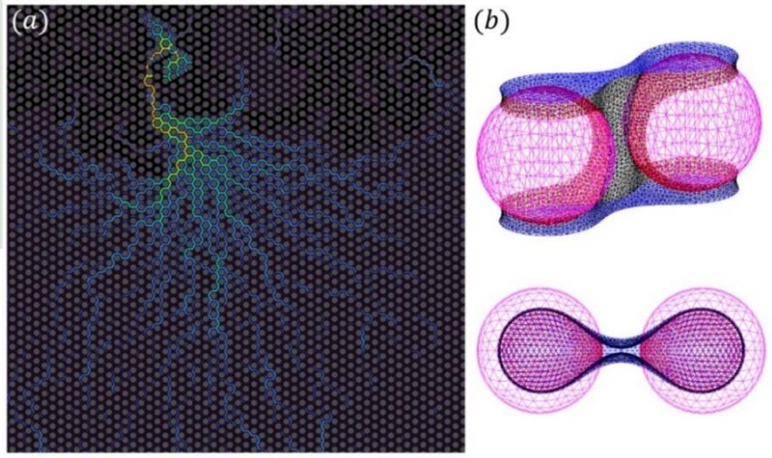

Figure:
(a) Pore-network modeling of a small water cluster draining into a larger cluster via capillary bridge networks. The grains are shown as gray circles, and low (high) local flow rates are indicated by dark blue (yellow)
(b) Example of a single water bridge formed between two spherical grains

EDUCATION

WHY STUDY POROUS MEDIA AND WHAT COURSES TO CHOOSE?

Porous media are all around us. In the ground, water fills the pores of aquifers, and oil is found in porous medium. Pollutants may follow rainwater into the ground which is a porous medium; where do the pollutants end up? When underground water rises during earthquakes, they may push the soil particles apart so that it loses its strength with the results that building topple. Less dramatically, but extremely importantly, the physics and chemistry of nanoporous media is at the core of fuel cells, batteries, and in heterogeneous catalysis. They make up concrete and biological tissue. A better understanding of the flow patterns in these materials will make them much more efficient – an important goal in a world that needs to become greener.

In PoreLab we study phenomena of these and related kinds, aiming to understand, improve and use the porous materials in ways that are more environmentally friendly, and more effective than now. An interdisciplinary PoreLab-environment has been constructed to facilitate contact between different disciplines and speed up this development.

PoreLab offers a range of courses open for all students at our host universities.

The two first courses, PoreLab course 1 and PoreLab course 2 are jointly organized between NTNU and UiO. They were adapted to PoreLab with a special focus on porous media physics.

PoreLab Course 1 – Theory and Simulation of Flows in Complex Media

FYS4465/FYS9465 (Dynamics of Complex Media) at UiO or KJ8210 (Flows in Porous Media) at NTNU

PoreLab course 1 covers hydrodynamics where capillary and viscous forces play a role. It also covers simulation methods, thermodynamics and statistical physics relevant to porous media.

Learning outcome

After completing this course, the student will:

- have knowledge of hydrodynamic and thermodynamic transport processes in porous media.
- have a thorough knowledge of the Navier-Stokes equation and Darcy's law, and also diffusion and dispersion processes.
- be able to program molecular and Brownian dynamics codes as well as the lattice Boltzmann-model and simple network models that are used to simulate flow in complex geometries.
- know the theory behind the simulation models and have an understanding of how small-scale processes affect processes at larger scales. This includes the understanding of percolation theory.

PoreLab course 1 is open for students from both NTNU and UiO. Professor Eirik Flekkøy, PI at PoreLab, is the lecturer for this course.

PoreLab Course 2 – Experimental Techniques in Porous and Complex Systems

FYS4420/FYS9420 (Experimental Techniques in Porous and Complex Systems physics) at UiO

PoreLab course 2 contains four projects that will give students an introduction to important experimental techniques in the field of condensed matter physics. The course will be adapted to the center of excellence PoreLab with a special focus on porous media physics. The teaching is based on four projects at PoreLab in which the students apply techniques on realistic problems.

Learning outcome

After completing the course, the student:

- should know how a PID controller works in an experimental setup with a particular focus on temperature control and has experience with how the temperature in a system can be controlled.
- knows the theory of dynamic light scattering and has experience in using light scattering to study diffusing particles and particles in a convective velocity field. The student has experience in using dynamic light scattering to measure viscosity and the particles diffusion constant and size.
- has experience in setting up a 2D experiment for two-phase flow in porous media and is able to perform image analysis to characterize the structure and the dynamics. The student knows fundamental mechanisms for two-phase flow in porous media and how numerical models can be used to understand the observed pattern formations.
- will have experience in performing a porous media experiment at NTNU PoreLab.
- has acquired skills in collaborating in groups with other students.
- has learned to carry out research projects near the research front and to write a scientific report.

PoreLab course 2 is open for students from both NTNU and UiO. Contact is Professor Knut Jørgen Måløy, PI at PoreLab UiO

Additional courses offered at either NTNU or UiO are relevant for porous media.

Irreversible Thermodynamics

KJ8211/TKJ4200, NTNU

The course extends classical thermodynamics beyond equilibrium and introduces the concept of entropy production. The students will learn what the entropy production is, where it comes from and how it can be used to:

- Formulate consistent transport laws for heat, mass and charge transfer that include coupling. These transport laws will be used to explain thermal diffusion (transport in reservoirs), Peltier and Seebeck effects (energy in space and degradation of batteries), reverse electrodialysis (energy from mixing salt-water and fresh-water), membrane transport, fuel cells and other important examples where renewable energy technologies are in focus.
- Identify, characterize, and minimize lost work and exergy destruction in processes and process equipment. Concepts such as exergy and lost work will be explained, and the students will learn to use them in practice to analyze and improve the energy efficiency of processes and process equipment. Scientifically founded guidelines for energy efficient operation and design will be presented and explained.

The course provides a powerful toolbox, both for students interested in transport phenomena, and for students who want to learn how to improve the energy efficiency; a necessary task to reach many of UN's sustainability goals. The coordinator and lecturer for this course is Professor Øivind Wilhelmsen, PI at PoreLab.

Statistical Physics

TFY4230, NTNU

The course provides an introduction to statistical physics, mainly for systems in thermal equilibrium. The student should understand quantum and classical statistical mechanics for ideal systems and be able to judge when quantum effects are important. The student should understand the connection between microphysics and thermodynamics.

Heat and Mass Transfer in Porous Media

EP8208, NTNU

The course content is as follow:

- Physical and chemical effects of contact between fluid and pore wall
- Heat and mass transport with and without chemical reaction and radiation in the pores
- Analogy between heat and mass transport
- Diffusion and convective heat and mass transport, diffusivity
- Transient and stable mass transport in different phases
- Adsorption and desorption, energy conversion
- Capillary pressure, capillary flow
- Radiation exchange inside pores
- Phenomenological consideration
- Side effects such as shrinkage / swelling, deformation, stress condition
- Practical examples from technical processes
- Mathematical modeling of the transport processes.

The content of the course will be tailored to the students taking the course

Applied Heterogeneous Catalysis

KP8132, NTNU

The course is given every second year, next time in the fall term 2025. The course aims to give an understanding of the relation between modern theories of catalysis and the industrial application for the most important groups of heterogeneous catalysts, metals, metal oxides and zeolites. Assessment of the potential developments and limitations of catalysts will be analyzed through examples from industrial applications or processes under development. This includes the catalyst synthesis, a kinetic description of the different processes involved in a catalytic cycle (adsorption, surface reaction and desorption), mass and heat transfer issues, as well as interpretation of results from experimental and theoretical investigations.

Catalysis, Specialization Course

TKP4515, NTNU

The specialization consists of modules giving a total sum 7,5 credits. Modules are chosen from the following list:

1. Environmental catalysis (3.75 credits).
2. Heterogeneous catalysis (advanced course) - (3.75 credits).
3. Industrial colloid chemistry (3.75 credits).
4. Reactor modelling (3.75 credits).
5. Chemical engineering, special topics (3.75 credits).

Modules from other specializations can be chosen given the approval of the coordinator.

Chemical Engineering Thermodynamics

TKP4107, NTNU

Chemical engineering thermodynamics forms one of the basic pillars for understanding chemical engineering process. In this course, we build on basic principles and learning objectives from subjects such as basic thermodynamics and process engineering. The syllabus is based on updated international standards and it will enable the students to calculate thermodynamics properties of ideal and non-ideal pure component systems as well as mixtures. Furthermore, the students will learn to calculate phase and chemical equilibria. The attained knowledge will help the students to model and simulate existing industrial processes as well as analyzing novel solutions in research and technology development. This competence is needed in order to develop and implement new and possibly more complex technologies, which are necessary in order to achieve future sustainable industry development.

Biophysical Micromethods

FY8906/TFY4265, NTNU

The course gives an introduction into the mode of different types of instrumentation that is important for studies of biological macromolecules, cells and other soft materials. The course provides an understanding of the function of the components that the instrumentation consists of, as well as a theoretical and practical understanding of how to operate the instrument, including calibration procedures and maintenance. Professor Erika Eiser, PI at PoreLab, is the coordinator and lecturer for this course.

Geomechanics and Flow in Porous Media

TPG4112, NTNU

The subject should give basic knowledge about flow in porous media related to reservoir engineering and hydrogeological applications, and basic understanding of geomechanics and its importance in mining operations, tunnel constructions and exploitation of georesources.

The course consists of two parts, one flow part (50%) and one rock mechanics part (50%). The flow part deals with porous media characteristics: Porosity, permeability, flow equations for single- and multi-phase flow, capillary pressure and relative permeability. The flow part also deals with applications in earth sciences, such as seepage through the subsurface, CO_2 sequestration, and the production of georesources such as water and hydrocarbons.

The rock mechanic part deals with tensions and pore pressure in the earth crusts, tectonic tensions, normal and abnormal pore pressures, tension determination, rock mechanic field and laboratory experiments, mechanical properties of rocks, tensions close to wells and subsurface holes. Other topics are: Stability of wells during drilling, sand/particle production, hydraulic fracturing, reservoir compaction and surface setting, the significance of rock mechanics in reservoir control and the use of rock mechanics in relation to rock installations. The course coordinator is Professor Carl Fredrik Berg, PI at PoreLab.

Reservoir Simulation

TPG4160, NTNU

The course aims at giving the students basic knowledge of numerical simulation of fluid flow in porous media. Students will understand partial differential equations for single phase and multiphase flow in porous materials, and numerical solution methods of these using finite difference methods. They will be able to use common modeling tools for numerical prediction of reservoir behavior during production or injection and will be able to do derivation of equations for flow in porous media, and numerical solution of these by using finite difference methods.

This course covers the simulation of flow in porous media during production or storage in subsurface reservoirs, e.g., during CO_2 sequestration, hydrocarbon production, or water production from aquifers. The course derives partial differential equations (PDE's) for one-phase and multi-phase flow in porous materials, and numerical methods for solving these. Topics: Summary of material and fluid properties; derivation of PDE's; numerical solution of PDE's using finite differences; methods for solving linear and non-linear equations; discussion of different types of reservoir simulation models; practical sides of reservoir simulation applications.

Professor Carl Fredrik Berg, PI at PoreLab, is the coordinator and lecturer for this course.

Description and Characterization of Porous Media and Flow by Laboratory Analysis

TPG4116, NTNU

The objective of the course is to learn fundamental principles of flow in porous media, with a specific focus on reservoir engineering including laboratory techniques and understanding the source of lab data as an aid for further studies in reservoir engineering and related subjects. The course content is as follow:

- Basic principles of flow in porous media and corresponding discussion of fundamental properties of the reservoir system to determine fluid distribution, static and dynamic flow properties.
- Determination of fundamental properties of reservoir rock system in the lab.

Topics are;

- Rock properties: Sampling, sample preparation, permeability and porosity, rock types.
- Fluid properties: Density, viscosity, interfacial tension.
- Rock fluid properties: Wettability, capillary pressure, resistivity, relative permeability.
- Additional concepts: Reservoir system, transition zone, Darcy's law, two-phase flow, EOR

Associate Professor Antje van der Net, associated member at PoreLab, is the coordinator for this course.

Numerical Methods in reservoir Simulation

PG8607, NTNU

The course gives an introduction to the various numerical formulations applied in reservoir simulators. The course contains:

- Difference methods,
- Control-volume method.

- Linear equation solvers.
- Stability and numerical dispersion

The subject investigates numerical methods used in reservoir simulation models.

The subject contains:

1. Difference methods.
2. Control-volume methods.
3. Linear equation solvers.
4. Stability and numerical dispersion.
5. Streamline methods.
6. Up-scaling methods.

By completing the course, the candidate will have a deeper understanding of the mathematical building blocks that goes into various reservoir simulators, different numerical representations and solution methods.

Disordered systems and percolation

FYS4460/FYS9460, UiO

The course provides an introduction to methods and problems in modern statistical physics with emphasis on algorithmic and computational methods. The applications addressed and the computational methods introduced are relevant for material science, complex systems, chemistry, solid-state, molecular-, and bio-physics.

The course aims to build understanding for the macroscopic effects of microscopic interactions using numerical simulations of microscopic models coupled with a concurrent development of a relevant theoretical framework.

Statistical Mechanics

FYS4130, UiO

This course will give the student a thorough introduction to thermodynamics and statistical physics, with an emphasis on the fundamental properties of gases, liquids and solids. The course also gives a theoretical foundation for further studies of systems with many particles or degrees of freedom. By completing the course, the student will be able to compute (numerically and analytically) thermodynamic quantities and correlation functions for quantum mechanical and classical models in statistical mechanics using various techniques and approximations. The student will gain experience with models of gases, liquids, electrons in materials, lattice vibrations, and magnetism as well as being able to deduce and mathematically transform thermodynamic identities. The student can also use thermodynamic stability criteria and can characterize phase transitions. The student will have knowledge about terms and concepts related to the renormalization group (RG) and use it to deduce critical exponents. The student will be able to deduce the master equation and use it to construct various Monte Carlo algorithms.

A large delegation from PoreLab, including professors, researchers, postdocs, PhD candidates, and master's students, attended the 15th Annual International Conference on Porous Media organized by InterPore, held from May 22 to 25, 2023, in Edinburgh, Scotland, UK

Porous Media Laboratory
NTNU, UiO

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