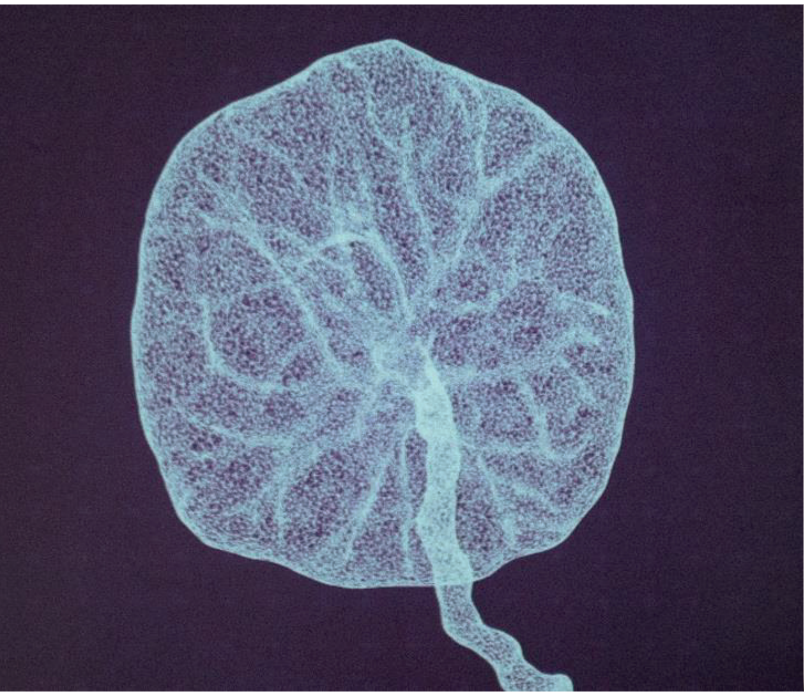
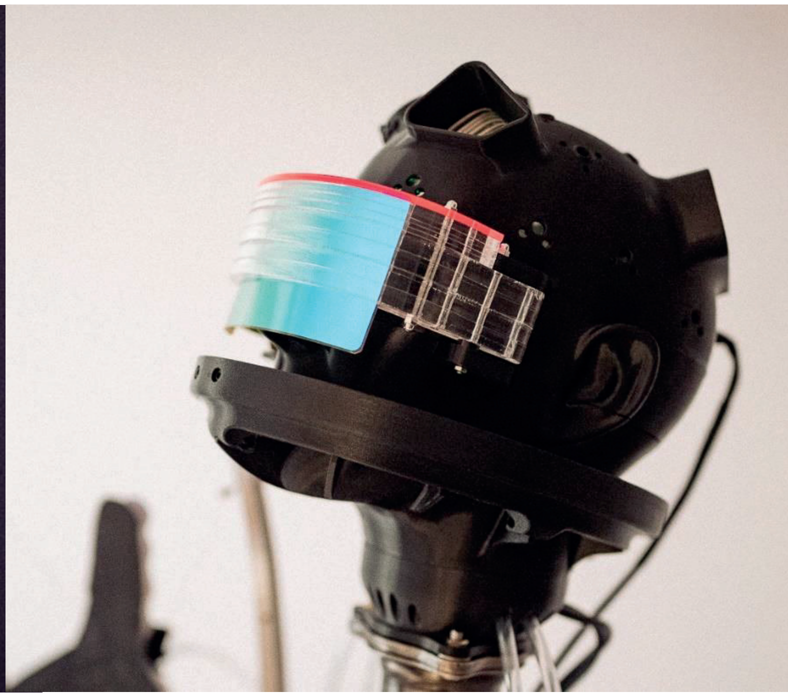
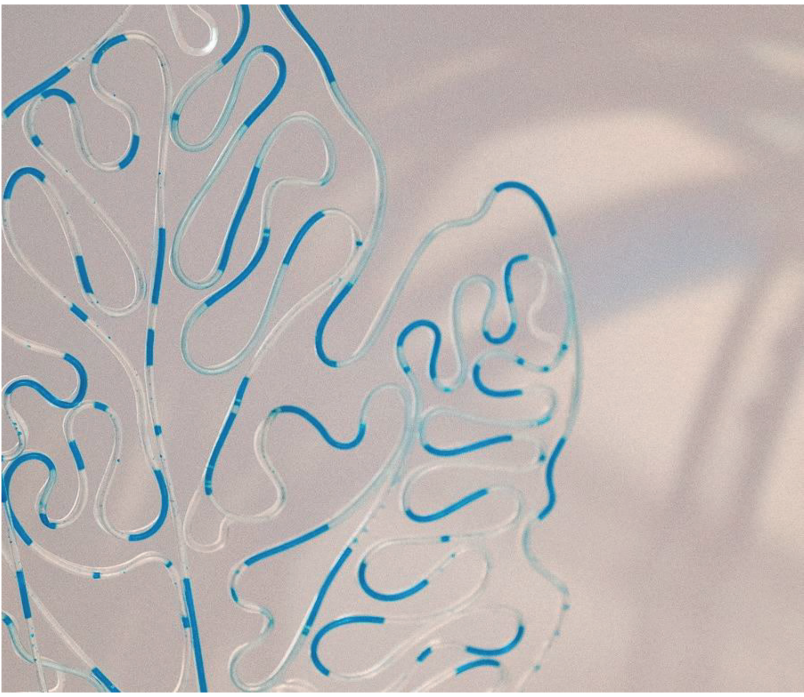
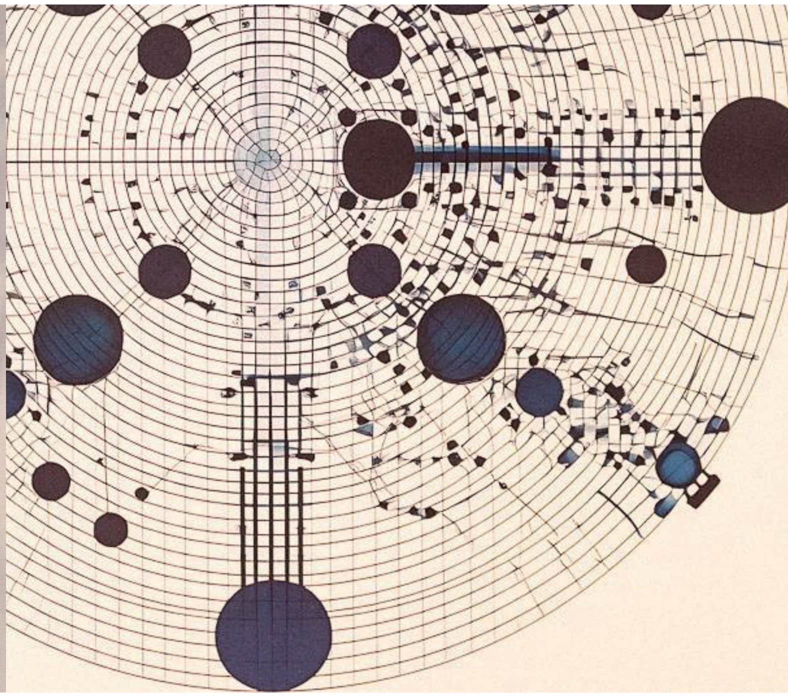
PoreLab
NTNU-UiO Porous Media Laboratory

Norwegian Centre of Excellence
The Research Council of Norway

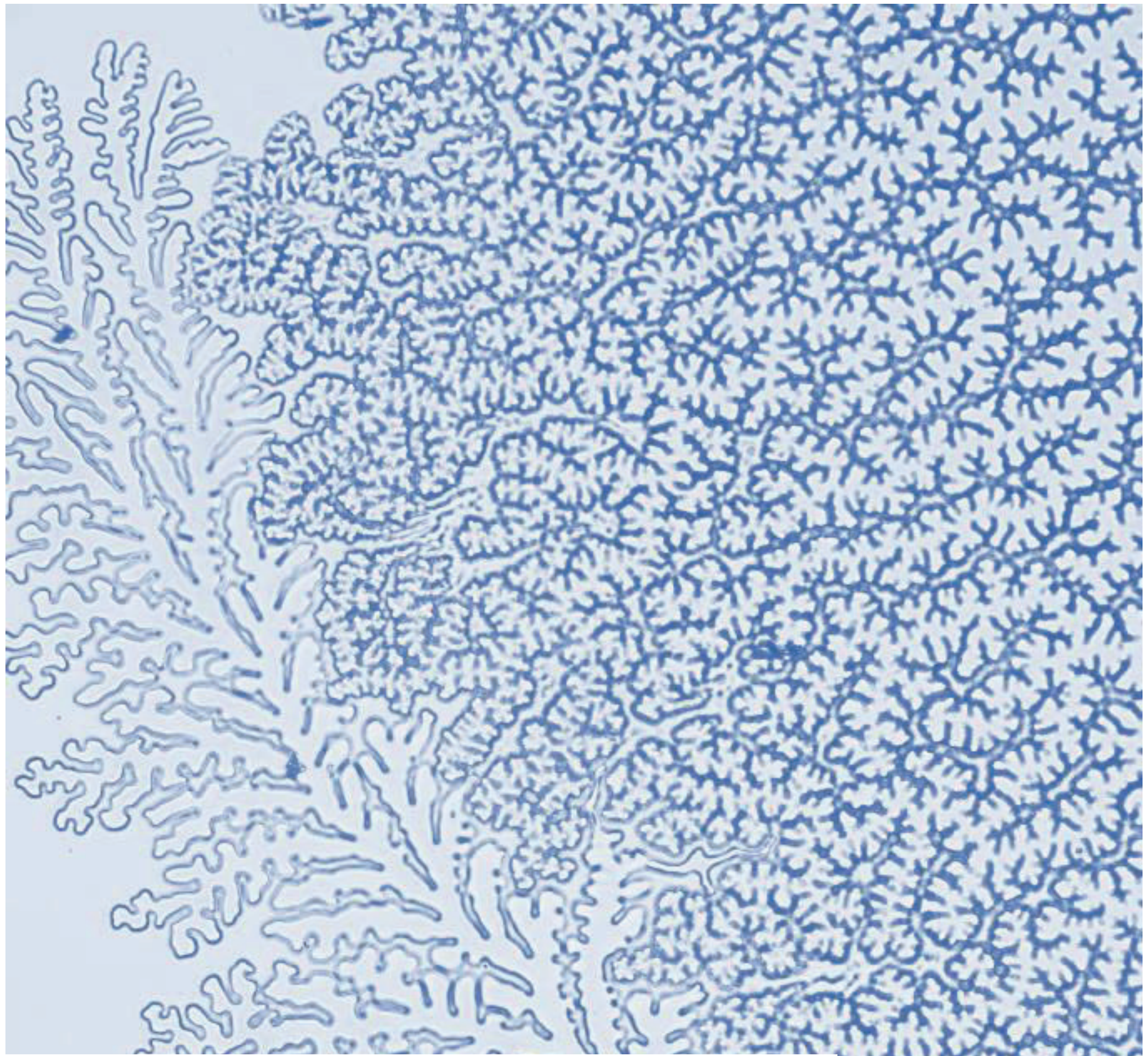
# MSc at PoreLab 2023

## Opportunities in 2024

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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*Cover page:*
*Clockwise from top/left: "Cyborg Placenta" by María Castellanos, "H111 – unfortunate Cookies" by Cosmin Haias, "Fluid processor for ecological computing" by Stahl Stenslie, "Internal flow Studies" by Floriama Cândea*
*Photo credit: Benjamin Bledea for META Spațiu contemporary art gallery*

# Overview – 2023 MSc students

| Name | Title Master thesis | Supervisors |
|---|---|---|
| Kristian Polanco Olsen | The co-molar volume in a miscible binary fluid mixture | Alex Hansen, Bjørn Hafskjold |
| Viktoria Christine Vahlin | Time reversal and parity symmetry breaking in two-phase flow in porous media | Alex Hansen, Carl Fredrik Berg |
| Arne Kristian Kramprud Hjelt | Thermal conductivity of low-dimensional systems | Raffaela Cabriolu |
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| Johannes Salomonsen Løken | Modeling thermo-osmosis in a slit-pore membrane using non-equilibrium thermodynamics and molecular dynamics | Øivind Wilhelmsen, Bjørn Hafskjold and Signe Kjelstrup, |
| Christian Ulrichsen | Electrochemical Noise Monitoring of Corrosion Rates under Insulation | Øivind Wilhelmsen, Signe Kjelstrup, Åsmund Ervik, Ole Meyer, Andreas Erbe |
| Wang Hou | Extending NPV calculation in FieldOpt for $CO_2$ sequestration | Carl Fredrik Berg and Thiago Lima Silva |
| Oluwole Alex Iperepolu | Automated Petrophysical Rock Typing Using Data Analytics And Machine Learning Algorithms | Carl Fredrik Berg, Damiano Varagnolo |

| Name | International Collaboration | Supervisors |
|---|---|---|
| Felix Schloms | Modelling Temperature and Concentration Profiles in Lithium Battery Related Electrochemical Cells | Joachim Groß at the University of Stuttgart, Signe Kjelstrup and Øystein Gullbrekken at NTNU |



# 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 obtained a new 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 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 2023 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.

As an example, we have developed a new 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 at either laboratory of the three institutes: PoreLab NTNU/UiO, Laboratoire FAST at the University of Paris-Saclay and Complex Systems Group at UFC, Brazil.

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. We host this event simultaneously in Oslo and Trondheim, and it is open to all. The PoreLab lecture series are almost always given by external lecturers.

Similarly, all master students are encouraged to submit abstracts and present posters or lectures at national and international conferences in close collaboration with their supervisors. Expenses are covered by PoreLab. As an example, both master students Elias Lundheim and Andreas Hennig travelled to Edinburgh in Scotland, UK, to attend the 15th Annual International Conference on Porous media organized by InterPore from 22 to 25 May 2023. Elias Lundheim presented his poster on "*Stress Concentration in the local load sharing fiber bundle model*", and Andreas Hennig gave an oral presentation on "*Pore-Network Simulations of yield stress fluids in porous media*".

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, 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, a chess board and an ever-present thousand-pieces puzzle became popular playgrounds for all at PoreLab NTNU


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2


3


4

*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*

# Kristian Polanco Olsen

Department of Physics, NTNU

## The co-molar volume in a miscible binary fluid mixture

Fall 2023
Supervisors: Alex Hansen and Bjørn Hafskjold

### Background:

Hansen et al. (2018) introduced a set of equations relating the different seepage and thermodynamic velocities in an immiscible two-phase flow in porous media. The purpose of their work was to present a set of new equations, under the theory of flow in porous media, based on thermodynamic considerations. Later, Roy et al. (2022) published a paper considering a similar relation. In both papers, the name of co-moving velocity was defined for this relation. The results presented by Roy et al. (2022), show a linear behaviour.

### Objective:

The main objective is to study a possible similar linear relation in ordinary thermodynamics, which relates the thermodynamic partial molar volumes and the measurable molar volumes occupied by the different substances in a binary mixture. This relation is called the co-molar volume.

### Methodology:

Contrary to the continuum approach (e.g. use of REV) used in the theory adopted by Hansen et al. (2018), this work focuses on a smaller scale using molecular dynamics (MD) simulations, as well as geometrical analysis by the implementation of Voronoi-tessellations, to study the relationship between the partial molar volumes in three different mixtures.

### References:

[1] Hansen, A., Sinha, S., Bedeaux, D., Kjelstrup, S., Gjennestad, M. A., & Vassvik, M. (2018). Relations between seepage velocities in immiscible, incompressible two-phase flow in porous media. *Transport in Porous Media*, 125.

[2] Roy, S., Pedersen, H., Sinha, S., & Hansen, A. (2022). The co-moving velocity in immiscible two phase flow in porous media. *Transport in Porous Media*, 143.

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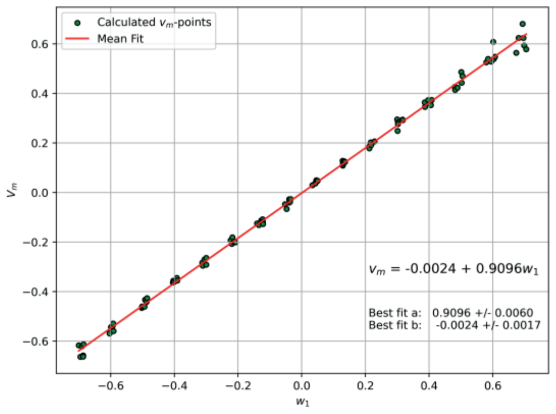
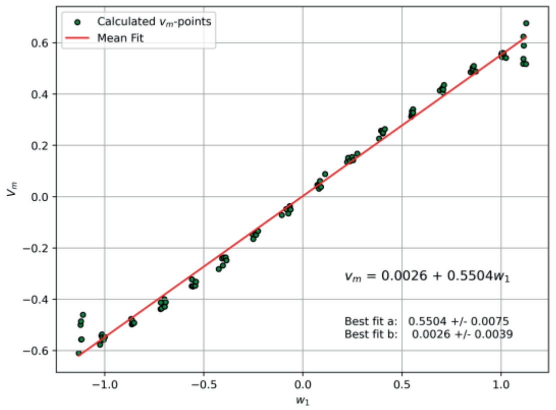
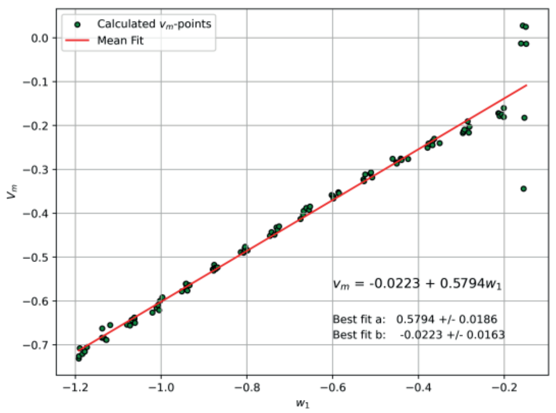



(a) $v_m(w_1) \approx 0.91w_1$ for mixture 1.




(b) $v_m(w_1) \approx 0.55w_1$ for mixture 2.




(c) $v_m(w_1) \approx 0.58w_1 - 0.02$ for mixture 3.

*Figure 1*:The co-molar volume for three different binary mixtures



# Viktoria Christine Vahlin

Department of Physics, NTNU

## Time reversal and parity symmetry breaking in two-phase flow in porous media

Fall 2023/Spring 2024
Supervisors: Alex Hansen and Carl Fredrik Berg

### Background

The complex dynamics of two phase flow in porous media form a scientific field which serves a foundation for various phenomena. This has been governed by an engineering approach as the concepts are developed on phenomenological laws. Numerous approaches has been studied to develop new theory to describe multiphase flow in porous media in a more general and rigorous manner. A part of this work is the research surrounding time reversibility and parity symmetry.

### Objectives

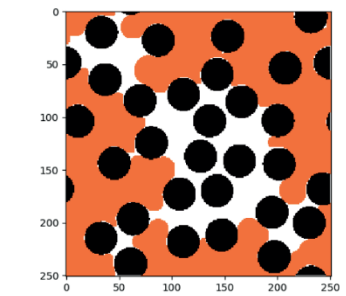
The mail objective is to investigate the time reversibility and parity symmetry of two phase flow through porous media. The effective permeability of flow is studied in the search for different behavior depending on the direction of which the fluids flow.

### Methodology

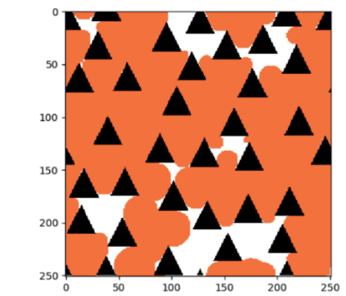
Numerical methods were utilized to simulate fluids of two phases flowing through a constructed porous media. This was done using the open-source tool Lattice Boltzmann methods for Porous Media (LBPM) delivered by the Open Porous Media Project. Ensembles of quasi-two-dimensional porous media were investigated, where the media consisted of a distribution of either solid disks or triangles. This is illustrated in figure 1. Here the black indicates the solid part, the orange is the non-wetting fluid, and the white is the wetting fluid.

### Results

The porous media consisting of solid triangles were used in a comparative analysis of the effect of the triangle orientation. An increased effective permeability for the wetting fluid was found when the triangles were oriented in the same direction as the flow, referred to as case 1. For the non-wetting fluid, an increased effective permeability was found when oriented in the opposite direction as the flow, referred to as case 2. One of the results which substantiates this is illustrated in figure 2. Here the difference in the effective permeability between case 1 and case 2 is plotted. As the majority of the points is below zero for the wetting fluid, and above zero for the non-wetting fluid within its standard deviation, most of the results obey the trend described above. This indicates time reversal and parity symmetry breaking.

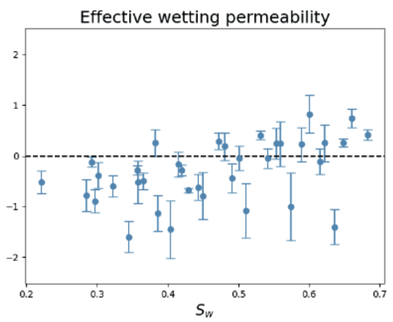


(a) Disk structured porous medium.

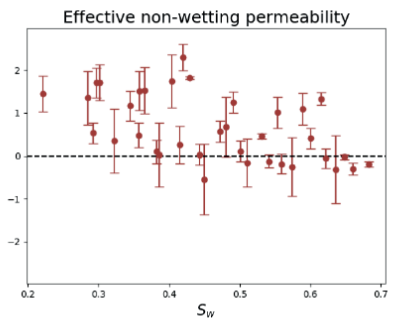


(b) Triangle structured porous medium.

*Figure 1: Illustrations of the constructed porous media used in simulations. The black indicates the solid parts, the orange is the non-wetting fluid, and the white is the wetting fluid.*




(a)




(b)

*Figure 2: The difference between the effective permeability between the fluid flowing through porous media with triangles pointing in the same and in the opposite direction to the flow. The results for the triangles pointing the same direction as the flow, is subtracted from the results of the triangles pointing in the opposite direction to the flow. The dotted line represents the zero reference line.*

# Arne Kristian Kramprud Hjelt

Department of Physics, NTNU

## Thermal conductivity of low-dimensional systems

Spring 2023
Supervisor: Raffaela Cabriolu

The successful synthesis of freestanding graphene has provided the opportunity to experimentally study heat transport in low-dimensional systems. As predicted by theoretical models, reduced-dimensional systems exhibit thermal transport behavior that is markedly different from their 3-dimensional counterparts. Despite the importance of this matter for technological and industrial applications, a deep understanding of this phenomenon has not been clearly established. The exceptionally high thermal conductivity of graphene has been measured to be up to 4000 $Wm^{-1}K^{-1}$ under certain conditions [1]; however, the experimental results vary depending on the length and size of the sample.

In this work, we investigated the low-dimensional thermal conductivity of Graphene NanoRibbons (GNRs) using the Approach to Equilibrium Molecular Dynamics (AEMD) simulation technique. The aim of our study was to explore how the thermal conductivity changes as layers of carbon are stripped off from the GNRs, approaching the ideal case of a one-dimensional (1D) system. Since graphene has two axes of symmetry, both the "zigzag" (Z-GNR) and the "armchair" (A-GNR) orientations have been investigated (Fig. 1).

In general, all the simulations show that the thermal conductivity of GNR depends on the sample orientation (Fig. 2). In particular, as concluded in previous experimental and simulation studies [2,3,4], the Z-GNR shows higher thermal conductivity compared to the A-GNR. Additionally, while the thermal conductivity of A-GNR decreases, the thermal conductivity of Z-GNR increases as the layers of the ribbon decrease to the 1D case (Fig. 2).

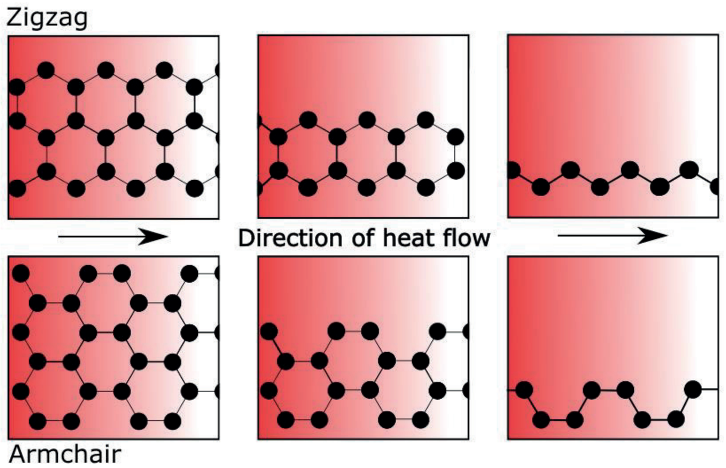



*Figure 1: Here we can see a small section of long GNR's in the zigzag and the armchair orientation. In the left box the GNR's are 3 strips wide, in the middle 2 strips wide, and to clarify what a single strip is, it is shown in the box to the right. The length of the simulated samples was 2μm long.*

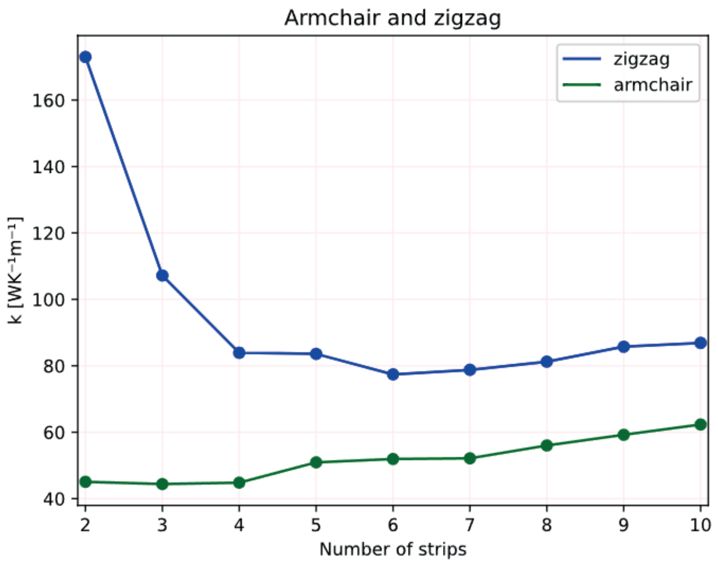



*Figure 2: Calculated values for the thermal conductivity of 2μm long GNR's simulated with the AEMD method. The thermal conductivity along the two different axes of symmetry acts very differently as the GNR's approach the 1D case.*

References:

[1] M. Sang, J. Shin, K. Kim and K. J. Yu, Nanomaterials (Basel), vol. 9(3), p. 374, 2019.
[2] Z. Guo, D. Zhang and X.-G. Gong, Applied physics letters, vol. 95, no. 16, 2009.
[3] K. He, G.-D. Lee, A. W. Robertson, E. Yoon and J. H. Warner, Nature communications, vol. 5, no. 1, p. 3040, 2014.
[4] J. Chen and B. Liu, The European Physical Journal Plus, vol. 136, no. 4, p. 379, 2021.





# Parul Parul

Department of Chemical Engineering, NTNU

## Alternative materials in battery frames

Fall 2023
Supervisors: Erika Eiser and Kristofer Gunnar Paso

### Background

The introduction of electrified vehicles requires a large battery pack with a complex geometry. Each battery pack has an external component, a frame made of aluminum, which ensures that the battery cells and all other battery critical components are shielded from external forces, such as mechanical shock, crash, water intrusions. Furthermore, it must comply with electromagnetic compatibility (EMC), both external and internal, and be light enough so the vehicle has more load carrying capacity.

### Objective

We investigated the possibility of different combinations of materials for the battery frames. We approached companies for possible material combinations and simultaneously ran simple CFD and FEM on the chosen materials. After procuring the most promising material, simplified physical and mechanical tests were performed to compare it with existing materials. Overall, we tried to formulate alternative material for the existing battery frames for a target to achieve lightweight battery housing.

### Results

My work delivered a study of alternative materials for Battery Housing, which is presented in Figure 1.

Other Companies working on material development would also be INEOS Composites US LLC, Johns Manville, Lanxess AG, LyondellBasell and Westlake Epoxy.

Validating the literature and market study together with the following Ashby chart given in Figure 2.

The current material properties are compared with various materials to show the possibilities of alternative material and comparing them against different parameters to attain a holistic image on the selection of material.

| S. No. | Company | Composite Name | Polymer Matrix | Fibre Reinforcement | Processing Technique Used | Notes |
|---|---|---|---|---|---|---|
| 1 | Mitsubishi Chemical Group Corp. | GMT and GMTex | Polyamide or Polypropylene | Glass fiber | Compression molding | 5 min exposure to a 1,000°C flame |
| 2 | SABIC's Petrochemicals | | Polypropylene | Glass fiber | Injection molded thermoplastic | Leads to self-extinguishing |

*Figure 1: Possible alternatives of material and the properties*

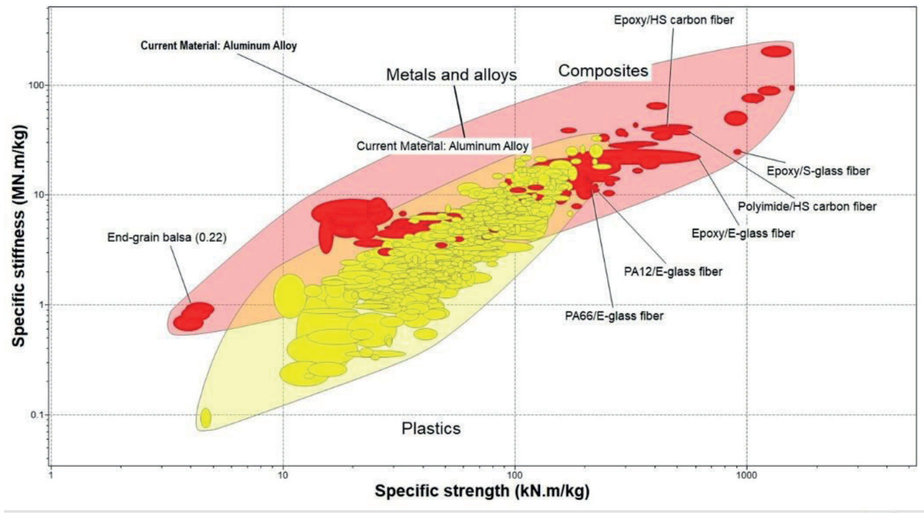



*Figure 2: Ashby Charts typically compare physical and economic properties of different materials. Here we compare the stiffness versus strength properties of different alternative materials (yellow) with those currently used (red).*

NTNU - Department of Chemistry

# Johannes Salomonsen Løken

Department of Chemistry, NTNU

## Modeling thermo-osmosis in a slit-pore membrane using non-equilibrium thermodynamics and molecular dynamics

Fall 2023/Spring 2024

Supervisors: Øivind Wilhelmsen, Bjørn Hafskjold and Signe Kjelstrup

### Background

The thermo-osmotic effect is a phenomenon that potentially can be used to extract mechanical energy from the waste heat of industrial processes. The effect involves the creation of a pressure gradient when a fluid in a porous medium is subjected to a temperature gradient, and thus converts a difference in temperature to a mechanical force.

### Objectives and methodology

Non-equilibrium molecular dynamics simulations have been used to study the effect in a slit-pore membrane system (depicted in figure 1). The simulation results are compared to a non-equilibrium thermodynamics model, which separates the effect into contributions from the membrane surfaces and the middle part of the membrane. The goal is used these model to gain a better understanding of the mechanisms behind the thermo-osmotic effect.

### Results

For a membrane of porosity $\phi = 0.4$ and neutral fluid-membrane interactions, the results show that the surfaces are the main contributor to the effect. The effect of varying the fluid-membrane interactions and other parameters will also be investigated, as this is known to influence the thermo-osmotic effect.

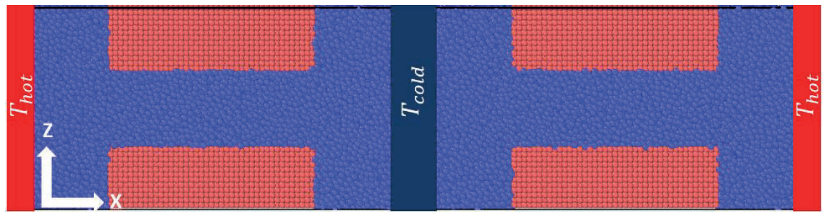



*Figure 1: The NEMD system setup. Blue particles are fluid, and red are the solid particles of the membrane.*

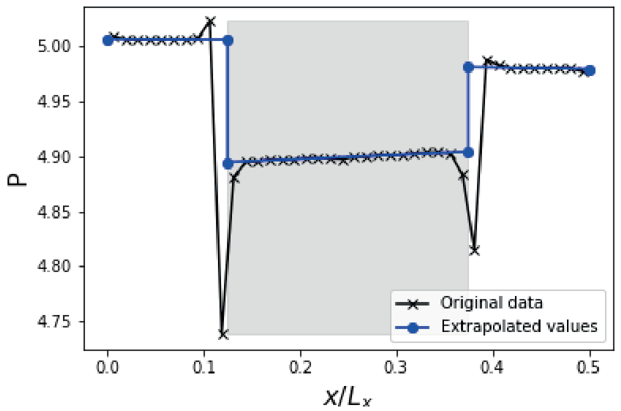



*Figure 2: The pressure profile of the system (grey area corresponds to the slit-pore membrane).*



# Christian Ulrichsen

Department of Chemistry, NTNU
In collaboration with SINTEF Energy AS

## Electrochemical Noise Monitoring of Corrosion Rates under Insulation

Fall 2023/Spring 2024

Supervisors: Ø. Wilhelmsen, S. Kjelstrup, Å. Ervik, O. Meyer, A. Erbe

Corrosion under porous media is relevant for a number of industrial applications, for example in any situation where pipelines are insulated and water can travel through the porous insulation to the surface of the pipe. Monitoring the corrosion on the metal surface is made difficult by the insulation inhibiting direct observation, and the already complex corrosion process is further complicated by the need to also consider transport of corrosion factors such as water, oxygen, and electrolytes through the porous medium to the surface of the metal.

In this work, electrochemical noise monitoring techniques will be combined with theoretical modelling to monitor and estimate corrosion rates under mineral wool insulation. Custom test cells will be designed and 3D-printed for use in the experiments. In addition, a mathematical model will be developed and compared to the experimental results. The experiments and the model will be used to explore correlations between relative humidity, adsorption isotherms of the insulation, and corrosion rate. The work falls under Porelab's Research Theme 8.

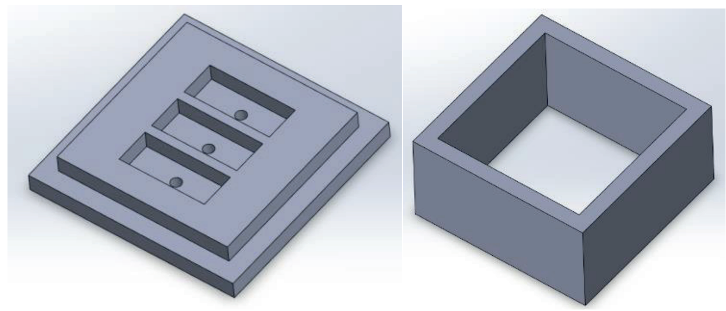


*Figure 1: Modular corrosion cell design. The base portion (left) has metal samples slotted into the indentations, connected to electrical leads passing through the holes in the bottom for electrochemical monitoring. The wall portion (right) is then slotted over the base, and holds both corrosive salt solution and insulation material in place on top of the metal samples during testing.*

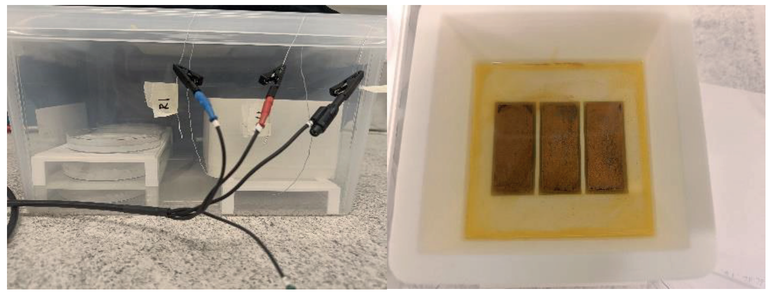


*Figure 2: Experimental setup. On the left is the experimental setup of the corrosion cell in a humidity-controlled box. On the right is an example of steel coupons after corroding for 10 days.*

NTNU - Department of Chemistry

# Wang Hou

Department of Geoscience and Petroleum, NTNU

## Extending NPV calculation in FieldOpt for $CO_2$ sequestration

Fall 2023 – Spring 2024
Supervisor: Carl Fredrik Berg and Thiago Lima Silva

### Background

$CO_2$ sequestration is central for reducing the $CO_2$ concentration in the atmosphere. For $CO_2$ sequestration in aquifers, a series of time-consuming simulation studies is essential to investigate the geological storage capacity under the premise of maximizing the economic value.

### Objective and Methodology

FieldOpt[1] is an open-source software developed by the NTNU petroleum cybernetic group for optimization of reservoir models. This software was initially designed for oil and gas activities. The objective for this master thesis is to extend the software capabilities towards $CO_2$ sequestration.

The flow chart displays the simplified process of how FieldOpt handles optimization problems. The software is modular-based and object-oriented, which facilitates the adaptation and extension of the existing framework to add a new feature, such as $CO_2$ injection optimization. The objective section is the entry point to acquire the software architecture, class, attributes, and methods for NPV calculations. Given the complex syntax of C++, one potential solution would be to replace the internal NPV calculations with an API to an externally run Python interface for NPV calculations. This could possibly simplify implementation of complex constraints and penalty conditions, e.g., a limit on caprock formation pressure.

### Result

New NPV opportunities implemented in FieldOpt for optimization of $CO_2$ sequestration, including a $CO_2$ injection and water production model that act as an example case.

### Reference

[1] Einar J.M. Baumann, Stein I. Dale, Mathias C. Bellout,. 2020. *"FieldOpt: A powerful and effective programming framework tailored for field development optimization"* Computers & Geosciences.

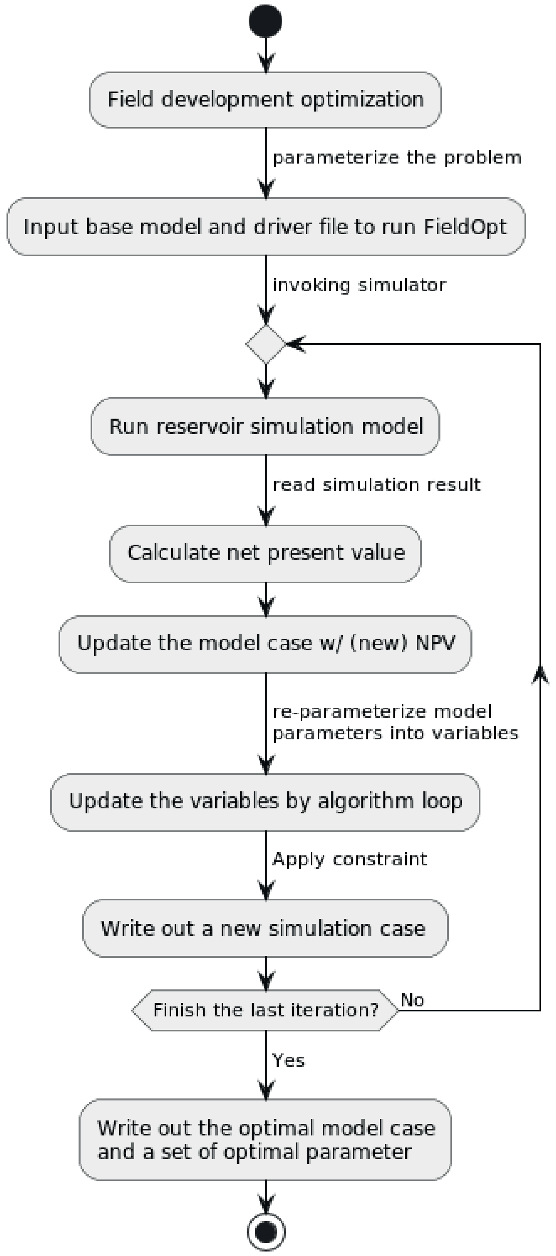



*Figure:* *FieldOpt flow chart*

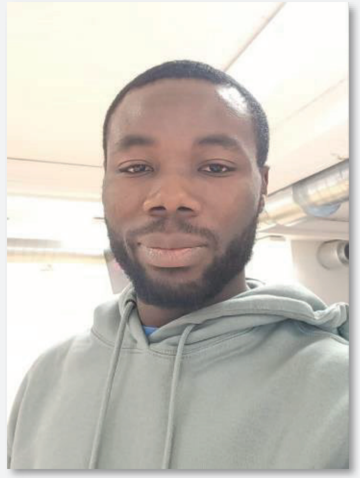


# Oluwole Alex Iperepolu

Department of Geoscience and Petroleum, NTNU

## Automated Petrophysical Rock Typing Using Data Analytics And Machine Learning Algorithms

Fall 2023 – Spring 2024
Supervisor: Carl Fredrik Berg and Damiano Varagnolo



### Background

In reservoir characterization and modeling, rock typing plays a pivotal role. Diverse data sources, such as log data and core measurements, are integrated during rock typing. Archie's [1] insight highlights similar characteristics among rocks of the same type. Employing integrated data, a systematic methodology identifies rocks with similar petrophysical attributes, grouping them into distinct types. Over time, various methods, including theoretical and empirical approaches, have been employed in rock typing. Machine learning has also emerged as a prominent tool for automated and efficient rock type characterization.

### Objectives

The primary goal is to employ data analysis and machine learning to classify rock types based on capillary pressure data. Extracted features, representing curve shape and height, indicative of underlying rock structure and wettability, will be input into a K-means clustering algorithm for classifying capillary pressure curves into distinct petrophysical rock types.

### Methodology

The classification of rock types utilizes an unsupervised machine learning algorithm. Specifically, unsupervised machine learning technique. Principal component analysis (PCA) was applied for dimensionality reduction of extracted features. Subsequently, K-means clustering was employed to categorize the data into distinct rock types.
This clustering approach is implemented on capillary pressure data to group it into various rock types, with a focus on the primary drainage capillary pressure in this instance.

### Results

Principal Component Analysis (PCA) was applied on five extracted features which are porosity, permeability, connate water saturation, pore size distribution and entry pressure. k means was then employed to cluster the reduced dataset. Three rock types were identified. Rock type 0, Rock type 1 and Rock type 2. Rock type 0 has the best rock quality. Rock type 1 has an immediate rock quality, while rock type 2 has a poor rock quality.

### References

[1] Archie, G.E. (1952). 'Classification of Carbonate Reservoir Rocks and Petrophysical Considerations'. In: AAPG Bulletin 36, pp. 278–298

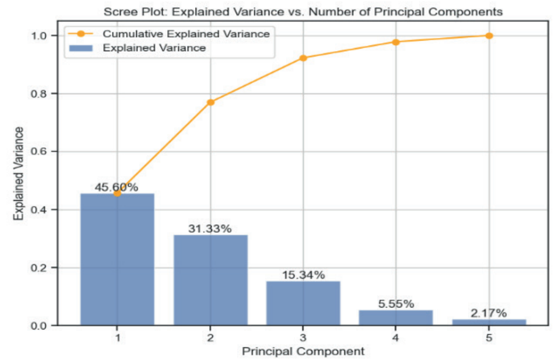



*Figure 1:* *Screen plot showing the principal component analysis order of importance*

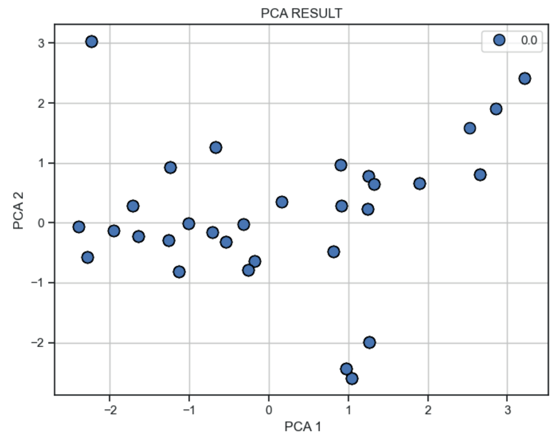



*Figure 2:* *Principal component analysis result*

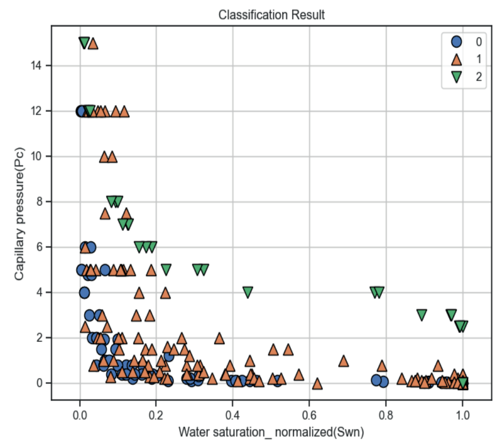



*Figure 3:* *Rock types classification (RT 0, RT 1, & Rock 2)*

International Collaboration

# Felix Schloms

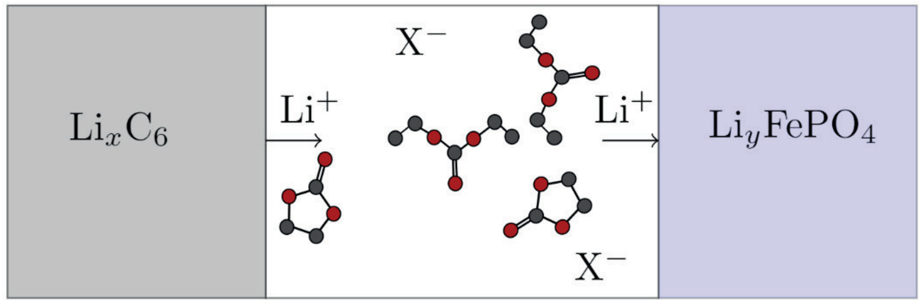

Institute of Technical Thermodynamics and Thermal Process Engineering at the University of Stuttgart and Department of Chemistry at NTNU


## Modelling Temperature and Concentration Profiles in Lithium Battery Related Electrochemical Cells

Internship period: Fall 2023
Supervisors: Joachim Groß, Signe Kjelstrup and Øystein Gullbrekken

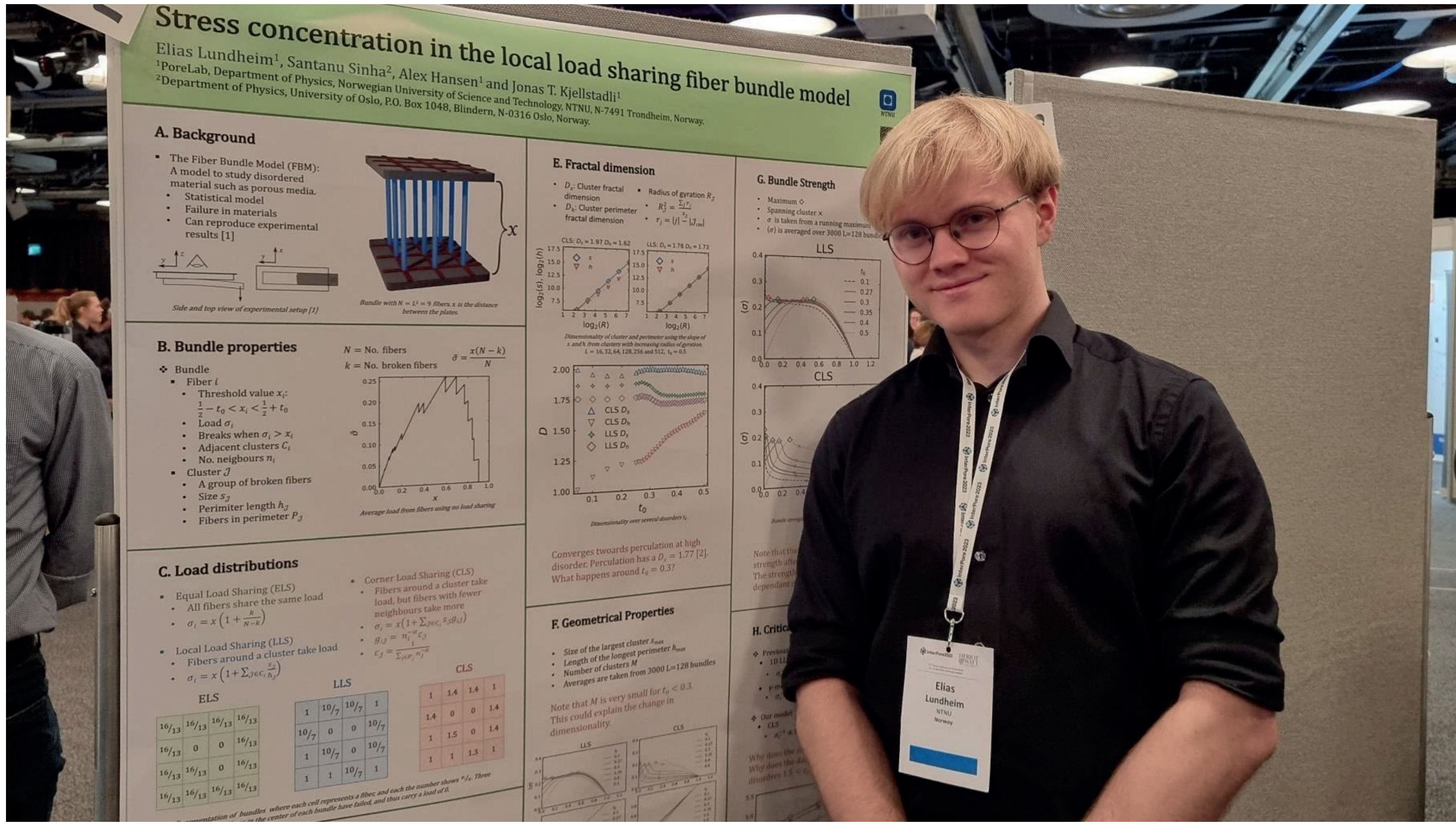
We formulated a lithium-ion battery cell model based on the non-equilibrium thermodynamics, taking all coupling of heat, mass and charge into account. The theory maintains thermodynamic consistency, ensuring strictly positive entropy production. Irreversible and reversible sources of heat are derived within this framework. Subsequently, we validate the veracity of our model by calculating entropy through two distinct methods. Building upon the work of Spitthoff et al. our model incorporates materials and assumptions introduced in their work while extending it to account for Peltier effects and diffusion contributions. The model consists of three bulk phases strictly separated by an interface. We looked at one dimensional transport, formulated the entropy production for each subsystem and derived an expression for the temperature profile by utilizing flux-force relations and balance equations.

The potential gradient observed in the electrolyte bulk phase indicates that concentration polarization has a significant contribution while thermal polarization appears to be negligible. Further we demonstrate that the commonly used assumption of a uniform temperature distribution within a single cell may lead to an underestimation of local temperature peaks. Our findings demonstrate that the primary contributors to these temperature peaks and lows are the local Peltier effects at the surface. Thermal runaway, a critical concern, may initially manifest as a localized phenomenon, triggered at a specific hotspot. Consequently, relying solely on the average temperature of a cell is inadequate for identifying the onset of thermal runaway. Our approach should be considered to provide a more accurate representation of the thermal behavior. The primary objective of the model is not to determine precise values for a single cell but rather to enhance the understanding of the intricate interplay among various effects. This knowledge will facilitate a more informed and effective approach to addressing these factors in subsequent stages. A program code is available at GitHub.




$$j/F = J_{Li^+}$$

*Figure: A schematic illustration of the lithium battery.*
*The electrodes contain intercalated metal.*
*The electrolyte contains a salt LiX and two organic solvents.*
*The potential profile across is computed, when electric current j/F and heat is conducted through.*




*Glimpse from PoreLab attendance to InterPore 2023 in Edinburgh, Scotland, UK*
*Top: Master student Elias Lundheim presented his poster on "Stress Concentration in the local load sharing fiber bundle model"*
*Bottom: Great lineup of PhD candidates and master students at the poster session*

# 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.

Please notice that Dr. Gaute Linga, researcher at PoreLab UiO was appointed Onsager Fellow at NTNU from the fall 2024. Over the next academic year, he will be available as the main supervisor of master students from NTNU who wish to write their thesis in Oslo.

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) and Alex Hansen (Alex.Hansen@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).

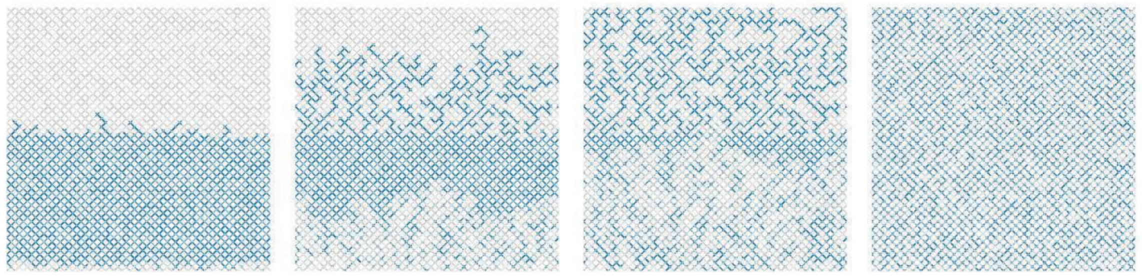



*Figure: Dynamic pore-network simulation of two-phase flow in a 2-dimensional network of* $64 \times 64$ *links where the wetting and non-wetting fluids are indicated by blue and gray colors. The images from left to right indicate the time evolution of the model where the right most image indicates a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

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Proposed Master Project at PoreLab NTNU (department of Physics)

## Measuring the co-moving velocity

Contact: Alex Hansen (Alex.Hansen@ntnu.no) and Santanu Sinha (Santanu.Sinha@ntnu.no)

How do immiscible fluids simultaneously flow in porous media? Answering this question seems straight forward. We know all the fundamental equations of hydrodynamics including those governing the motion of immiscible fluid mixtures. The porous medium acts as boundary conditions for the equations. Take a big computer and voilà.



No, sorry, that is not how it works. The trouble with porous media is that the internal surface area scales in the same way as the volume. The boundary effects never go away, even in the continuum limit, i.e., the limit where the pores are so small compared to the length scales at which we observe the porous medium so that it appears continuous. The boundary conditions then mix with the equations in such a way that a completely new description is necessary.

Since 1936, relative permeability theory has been the leading description of immiscible two-phase flow in porous media at scales much larger than the pore scale. Central to this theory are the two relative permeabilities, one for each fluid, which measures the reduction of mobility each fluid experiences due to the presence of the other fluid. The theory assumes the two relative permeabilities to be functions of the saturation (i.e., relative concentration) alone. When there are saturation gradients present, a third parameter comes into play, the capillary pressure. This is also assumed to depend on the saturation alone.

Such a theory is clearly quite limited in that it makes many strong assumptions. Yet, it is essentially the only one that is used for practical calculations. Can one do better? That is, come up with a theory that is closer to the physics that is going on and at the same does not drown in complexity? Our answer is yes: we have proposed such a theory based on statistical mechanics [1-8].
A central concept in this new theory is the *co-moving velocity*. This velocity has remarkable properties that hints at something deeper which is yet to be uncovered.

The aim of this project is to measure the co-moving velocity directly using a dynamic pore network model [9]. This is laying the groundwork for experimental measurements.

*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] A. Hansen, S. Sinha, D. Bedeaux, S. Kjelstrup, M. Aa. Gjennestad and M. Vassvik, *Relations between seepage velocities in two-phase flow in homogeneous porous media*, Transp. Porous Med. **125**, 565 (2018); doi:10.1007/s11242-018-1139-6.
[2] S. Roy, S. Sinha, and A. Hansen, *Flow-area relations in immiscible two-phase flow in porous media*, Front. Phys. **8**, 4 (2020); doi:10.3389/fphy.2020.00004.
[3] S. Roy, H. Pedersen, S. Sinha, and A. Hansen, *The co-moving velocity in immiscible two-phase flow in porous media*, Transp. in Porous Media, **143**, 69 (2022); doi:10.1007/s11242-022-01783-7.
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[8] J. Feder, E. G. Flekkøy, and A. Hansen, *Physics of Flow in Porous Media*, (Cambridge University Press, 2022).
[9] S. Sinha, M. A. Gjennestad, M. Vassvik, and A. Hansen, *Fluid meniscus algorithms for dynamic pore-network modeling of immiscible two-phase flow in porous media*, Front. Physics, **8**, 548497 (2021); doi:10.3389/fphy.2020.548497.


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Proposed Master Project at PoreLab NTNU (department of Physics)

## Onsager symmetry in immiscible two-phase flow in porous media

Contact: Alex Hansen (Alex.Hansen@ntnu.no)

We have recently proposed a new approach to steady-state immiscible two-phase flow in porous media based on equilibrium statistical mechanics [1]. Here, "steady state" refers to the macroscopic parameters describing the flow fluctuating around well-defined and constant averages. The central idea behind the new approach is to consider the statistics of fluid configurations in cuts orthogonal to the flow direction and the flow direction as a pseudo time axis. Under steady-state flow, the statistics of the fluid configurations in the cuts will be in equilibrium.
We are now attempting to go beyond steady-state flow. If this is to succeed, it is necessary to verify whether Onsager symmetry - i.e., time reversal symmetry - applies to the extensive variables that appear in the theory.
This MSc project consists of using a dynamic pore network model to check whether the symmetry is obeyed or not.


[1] A. Hansen, E. G. Flekkøy, S. Sinha and P. A. Slotte, *A statistical mechanics framework for immiscible and incompressible two-phase flow in porous media*, Adv. Water Res. 171, 104336 (2023); https://doi.org/10.1016/j.advwatres.2022.104336.


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Proposed Master Project at PoreLab NTNU (department of Physics)

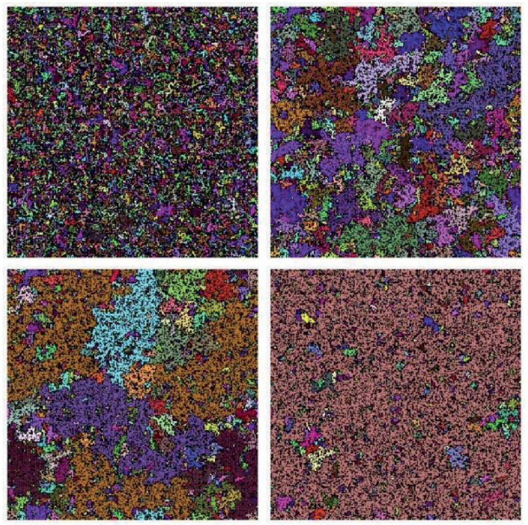
## Role of system disorder and thermal noise in fracture growth

Contact: Santanu Sinha (Santanu.Sinha@ntnu.no), Alex Hansen (Alex.Hansen@ntnu.no)

Material stability is of key importance in industrial applications. Appearance of fractures and their growth in a material depend on the competition between the disorder in the material strength and the local stress concentration. The heterogeneities delocalize the fracture growth and offset the failure point at which a crack becomes unstable. With a bundle of linear elastic fibers, called as a fiber bundle model, it was shown that the transition from a sparse to a localized fracture growth can be of first or second order depending on the type of the disorder distribution [1].

There is another type of fracture process that can cause a material to fail over time even if the applied stress is below the failure point. This is called creep failure which is influenced by external factors such as temperature. Presence of thermal noise can delocalize a localized fracture growth and can make it a percolation-like process [2]. One such growth simulated with a local load sharing fiber bundle model is shown in the figure where the black and colored pixels correspond the intact and broken fibers respectively.

A fiber-bindle model consists of a set of elastic fibers placed in between two clamps under an external force. Each fiber has an elongation threshold beyond which it fails and the load it was carrying is distributed to all (equal load sharing) or nearby (local load sharing) intact fibers. The aim of this MSc project will be to use a fiber bundle model to study the creep failure for different types of threshold distributions and to find out how the two types of disorders, one related to the thermal noise and the other related to the thresholds, control the fracture growth.



*References*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[2] S. Sinha, S. Roy and A. Hansen, Phys. Rev. Res. **2**, 043108 (2020).


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## Proposed Master Project at PoreLab NTNU (department of Physics)
## Shape of Clusters in Immiscible Two-Phase Flow in Porous Media
Contact: Alex Hansen (Alex.Hansen@ntnu.no) and Santanu Sinha (Santanu.Sinha@ntnu.no)

When two immiscible fluids flow simultaneously through a porous medium, they will self-organize into complex pattern that are describable using the language of critical phenomena. This has profound consequences for the properties of the flow.

Underlying this self-organization is a competition between the viscous forces, i.e. the usual hydrodynamic forces and the capillary forces coming from the interfacial tension between the fluids and the wetting properties between the fluids and the pore walls.

The self-organization manifests itself through how the fluids distribute themselves into clusters, which – when they move – are called ganglia. Ganglia dynamics is very rich and still rather poorly understood despite a huge effort to study these experimentally.

It is the aim of this MSc project to use a dynamic network model (i.e. a numerical model) to characterize the shape of trapped clusters and ganglia geometrically. We know, e.g. that there are length scales associated with the two types of forces involved, viscous and capillary. How do these length scales influence the shapes? To answer these questions, we will use the machinery developed in connection with percolation theory – the quintessential example of a non-thermal critical system. We will then go on to correlate the shape of the ganglia with their speed. Is there a typical shape? How does speed correlate with their size?

The findings in this project will open for later experimental studies.

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## Proposed Master Project at PoreLab NTNU (department of Physics)
## Renormalization Group Technique for Local Load Sharing Fiber Bundle Model
Contact: Alex Hansen (Alex.Hansen@ntnu.no)

Ken Wilson won the 1982 Nobel Prize in physics for devising the renormalization group technique. Here is the essence of the idea behind it: We have a system that consists of many interacting parts. We wish to find a description of the macroscopic variables that reflects the underlying behavior of the interacting parts. The renormalization group technique consists of finding a way to replace the original system by another coarse-grained one – one that consists of fewer interacting parts, but which leads to the same behavior of the macroscopic variables. By making the coarse-graining incremental, we keep track of how the relation between the coarse-grained interacting parts and the macroscopic variables changes. We repeat the coarse graining over and over and a pattern of change emerges. This pattern tells us how the macroscopic variables behave.

The fiber bundle model consists of elastic fibers placed between two clamps. Each fiber has a maximum load it can take before it fails. The question is what the force on the clamps versus elongation of the distance between the clamps looks like. In 2018, we constructed a renormalization group procedure for this problem [1], which combining fibers pairwise into "super"-fibers.



There is a version of the fiber bundle model which is much more complex than the one I just described: The local load sharing fiber bundle. When a fiber fails in this model, the force it was carrying is given to the nearest surviving fibers. This makes the model much more complex. The aim of this project is to construct a renormalization group for this problem. This is a hard but not impossible problem.

This work would be in collaboration with Professor Purusattam Ray at the Institute of Mathematical Sciences in Chennai, India


[1] S. Pradhan, A. Hansen and P. Roy, Front. Phys. https://doi.org/10.3389/fphy.2018.00065.


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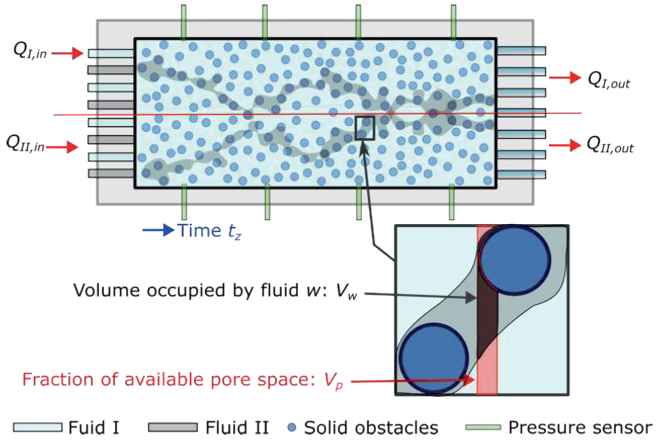
## Proposed Master Project at PoreLab NTNU (department of Physics)
## Information Entropy in 2-phase flow
Contact: Erika Eiser (erika.eiser@ntnu.no) and Alex Hansen (alex.hansen@ntnu.no)




*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 the Professor Eiser, an expert in the rheology and microrheology. Latter derives the viscoelastic properties of probe colloids from their thermal fluctuations. Professor Hansen is a world leader in the theory of 2-phase flow. If interested the student can do both simulations and/or experiments.

*Contact Persons*
Eiser Erika (erika.eiser@ntnu.no) & Alex Hansen (alex.hansen@ntnu.no)

*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)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## Proposed Master Project at PoreLab NTNU (department of Physics)
## Micro-Rheology in Percolating Systems
Contact: Erika Eiser (erika.eiser@ntnu.no) and Alex Hansen (alex.hansen@ntnu.no)

*Motivation*
Percolation theory is a mathematical description describing when a system of sticky spheres or connectors will span a 3-dimensional space such that the system will be able to sustain a shear or normal stress. Generally, it was believed that there can only be one percolating cluster. However, recent work showed that double-percolating solids can be formed when using the high binding-specificity of short DNA-strands attached to colloids [1]. However, little is known about the viscoelasticity of such systems because they often are difficult to prepare on a large scale, and often are fragile.

*Your Project*
In this project the student will use diffusing wave spectroscopy [2] to study the viscoelastic properties of thermally reversible double- and triple-percolating colloidal gels as function of temperature and other physical parameters. This work will also involve learning how to prepare DNA-functionalized colloids, synthesis of those and many other

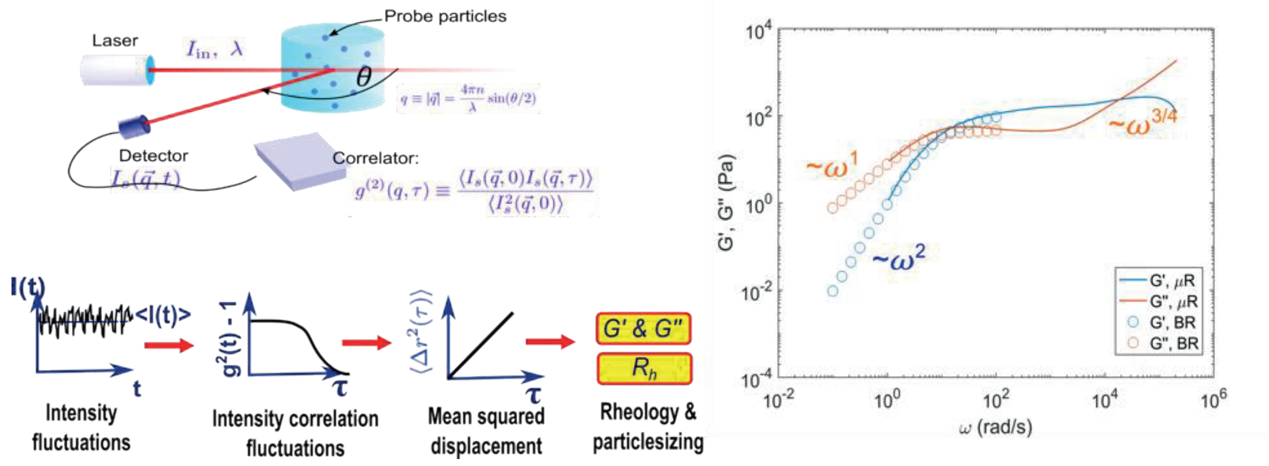
experimental tools. In addition, the student will learn how the rheological properties of complex systems can be derived from the thermal fluctuations of the colloidal particles involved.

*Requirements*
A background in statistical and Soft Matter physics. Further, a keen interest in building up experiments and delving into image analysis are required.

*Other Aspects*
The project will be supervised by the Professor Eiser, an expert in the rheology and microrheology. Latter derives the viscoelastic properties of probe colloids from their thermal fluctuations. Professor Hansen is a world leader in the theory of percolating and porous systems.

*Contact Persons*
Eiser Erika (erika.eiser@ntnu.no) & Alex Hansen (alex.hansen@ntnu.no)

*References*
[1] L. Di Michele et al., *Nature Communications* **4**:2007 (2013); Di Michele et al., *Soft Matter* **10**, 3633 (2014); M. Zupkauskas et al. Chem. Sci., 8, 5559 (2017)
[2] Z. Xing, A.Caciagli, et al. 'Microrheology of DNA-Hydrogels' PNAS 115, 8137 (2018); I.D. Stoev, A. Caciagli, Z. Xing, E. Eiser, SPIE – Proceedings of Optical Trapping and Optical Micromanipulation XV, 107232D (2018)

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## Proposed Master Project at PoreLab NTNU (department of Physics)
## Permafrost – Heat Transport in Porous Media
Contact: Erika Eiser (erika.eiser@ntnu.no) and Alex Hansen (alex.hansen@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 -10°C.

*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, and Alex Hansen a theoretician, PoreLab (www.porelab.no).

*References*
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[2] J. Obu, "How Much of the Earth's Surface is Underlain by Permafrost?" J. Geophysical Research: Earth Surface, 126, e2021JF006123 (2021)
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## Proposed Master Project at PoreLab NTNU (department of Physics)
## Using Soft Matter Physics to Develop Bacterial-DNA
Contact: Erika Eiser (erika.eiser@ntnu.no)

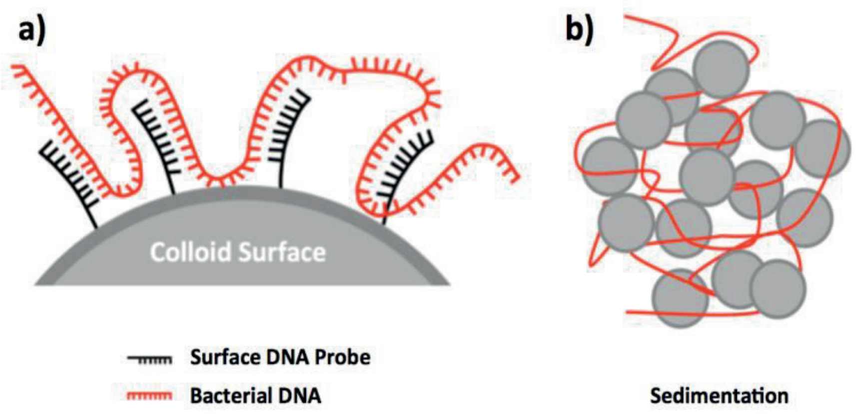


**Figure: (a)** Cartoon of a DNA-coated colloidal particle binding to repeating, short DNA sequences that are complementary to that of a long bacterial genomic DNA. **(b)** Sedimentation resulted from cooperative binding of many DNA-coated particles to a single bacterial DNA.

*Motivation*
Quickly identifying pathogens that cause infections remains challenging, leading to over-prescription of antibiotics, and increase in antibiotic resistance. The main problem is the lack of cheap, fast, and highly selective diagnostic tools. Recently, the Eiser group has introduced a new diagnostic tool based on colloidal probes, densely coated with the short DNA probes tailored to the bacterium to be detected [1]. Our approach uses a new concept of multivalent binding and the high specificity between complementary DNA strands, which were optimized to detect whole bacterial genomes, which have typically over a million base pairs, such as E.coli or tuberculosis caused by the Mycobacterium tuberculosis [2]. However, this approach is not sufficiently sensitive to detect the much shorter viral DNA or RNA.

*Your Project*
In this experimental project we will use a modified multivalency approach, developed in silico. For this the student will learn how to coat colloids with well-defined DNA sequences, how to select them using an "in-house" bioinformatics algorithm [2]. Tests will be done on the filamentous fd-virus solutions. The genome-induced aggregation will be studied using confocal microscopy.

*Requirements*
A strong interest in statistical and Soft Matter physics is required. Further, a keen interest in experimental and computational skills is important.

*Other Aspects*
The project will be supervised by the Professor Eiser, an expert in DNA- coated colloidal systems. Interactions with simulation groups around the world are possible.

*Contact Person*
Eiser Erika (erika.eiser@ntnu.no)

*References*
[1] P. Xu, T. Cao, Q. Fan, X. Wang, F. Ye, E. Eiser 'Whole-Genome Detection using Multivalent DNA-Coated Colloids' PNAS 120 (37), 2305995120; DOI: 10.1073/pnas.2305995120 (2023)
[2] T. Curk, C. A. Brackley, J.D. Farrell, Z. Xing, D. Joshi, S. Direito, U. Bren, S. Angioletti-Uberti, J. Dobnikar, E. Eiser, D. Frenkel, R.J. Allen 'Computational design of probes to detect bacterial genomes by multivalent binding.' PNAS 117, 8719-8726; DOI: 10.1073/pnas.1918274117 (2020)

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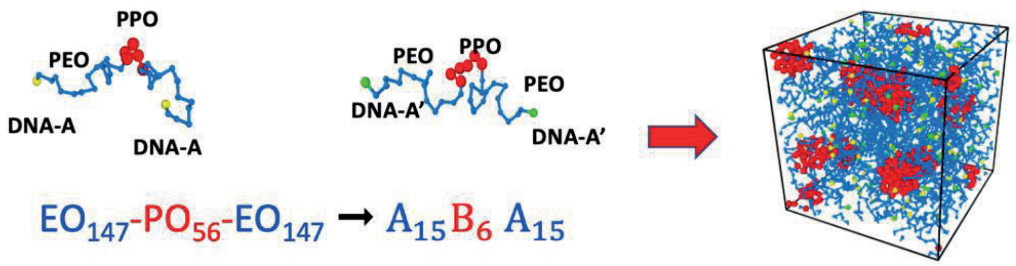
Proposed Master Project at PoreLab NTNU (department of Physics)

## Active Hydrogels - Simulations

Contact: 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)

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Proposed Master Project at PoreLab NTNU (department of Physics)

## Stabilizing Quicksand – Simulations

Contact: Raffaella Cabriolu (raffaela.cabriolu@ntnu.no), Erika Eiser (erika.eiser@ntnu.no) and Astrid de Wijn (astrid.dewijn@ntnu.no)

*Motivation*

The ground in Norway is rich in clay, a natural sheet-like crystalline mineral that is held together via ionic bonds. Thousands of years ago the land was under saline sea water stabilizing this clay-rich ground mainly via a combination of electrostatic and van der Waals forces. Today, when exposed to rain or an earthquake the force balance is disturbed, causing massive landslides or the 'drowning' of buildings like the Tasmanian devil in the figure above [1]. Building roads and constructions in a safe way requires the use of large quantities of cements which is bad for the environment. We want to explore new, sustainable ways to achieve the stability of ground.

*Your Project*

In this project the student will first develop a Molecular Dynamics model of two clay surfaces interacting with each other across an aqueous layer [2, 3], using the software package LAMMPS. The challenge will be finding the appropriate force fields to realistically reflect the interactions between the particles. In a second step we will explore how these interactions can be modified by the presence of various salts or other natural materials such as plant or bacterial based bio-polymers [4].

*Requirements*

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

Other aspects

The main supervisor will be the Associate Professor Cabriolu, expert in molecular simulation studies of condensed, soft matter and yield-stress fluids. The project is in collaboration with Prof. Eiser, who is an experimental expert in the rheology of self-assembling DNA systems and soft matter, and with Prof. De Wijn, who is an expert in theory and modelling analytical of tribology and surface science.

*References*

[1] A. Khaldoun, E. Eiser, G. Wegdam, D. Bonn, 'Liquefaction of quicksand under stress' *Nature* **437**, 635 (2005)

[2] B. Ruzicka et al. 'Observation of empty liquids and equilibrium gels in a colloidal clay' *Nature Materials* 10, 56 (2011)

[3] P. Bacle et al., 'Modeling the transport of water and ionic tracers in a micrometric clay sample' *Applied Clay Science* **123**, 18 (2016)

[4] P. Xu, T. Erdem, E. Eiser, 'A Facile Approach to Prepare Self-Assembled, Nacre-Inspired Clay/Polymer Nano-Composites', *Soft Matter* **16**, 3385 (2020)

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Proposed Master Project at PoreLab NTNU (department of Physics)

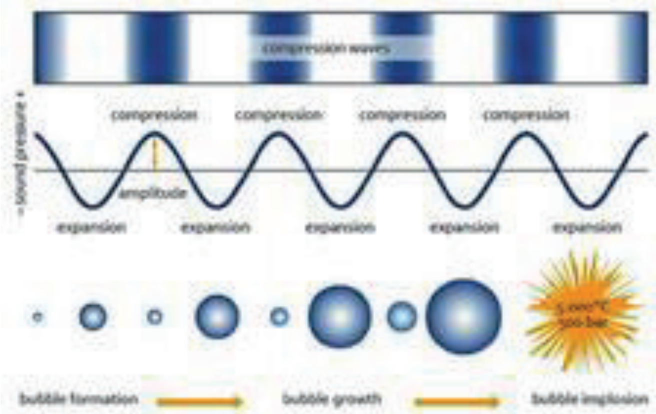
## Bubbles's nucleation and sonochemistry

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

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

*Motivation*

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/.

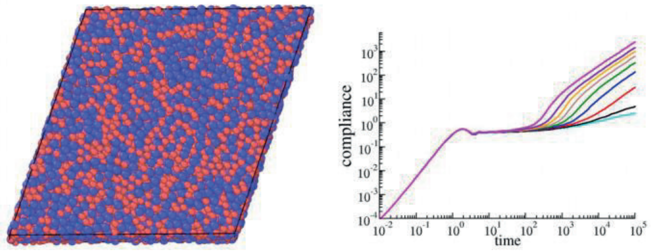
[2] R. Cabriolu, B. Pollet and P. Ballone, *Journal of Physical Chemistry B.*, 127,**7**, 1628-1644, (2023).

[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).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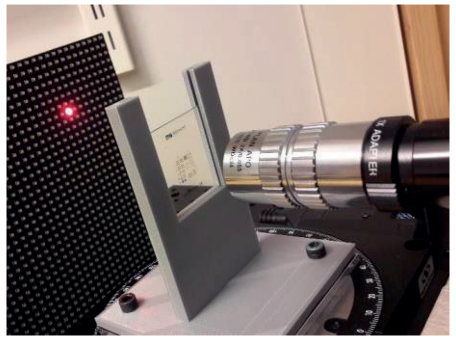
## Proposed Master Project at PoreLab NTNU (department of Physics)

# 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 CO2, in combination with compressed sensing and machine learning.

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

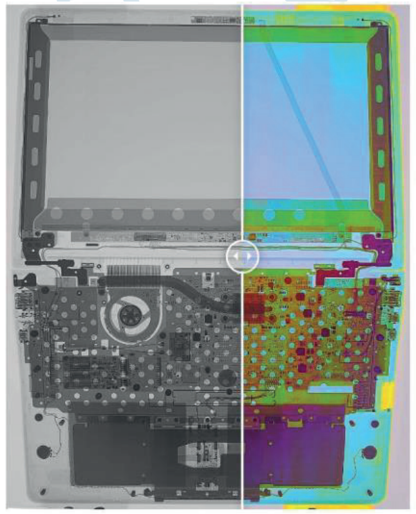


***Figure**:. "Coloured" X-rays reveal additional features in an electronics circuit board. Image by Advacam Inc.*

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## Proposed Master Project at PoreLab NTNU (department of Physics)

# Phase contrast microscopy of droplet nucleation

Contact: 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.*

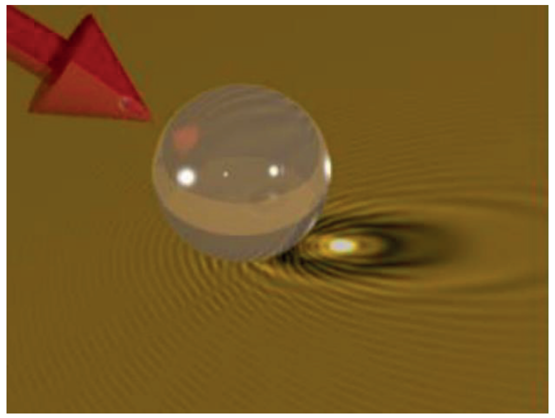

***Figure 2.** Modelling the light scattering from a translucent spherical object*

### Proposed Master Project at PoreLab NTNU (department of Physics)

## X-ray phase-contrast microscopy & computed imaging

Contact: 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!

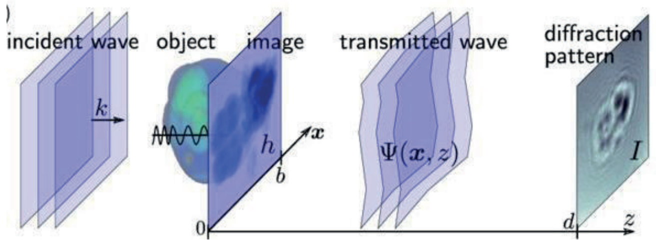


***Figure :*** *Modeling the transmission and scattering of X-rays through an object. [Image Ref.: Maretzke & Hohage, SIAM Journal on Applied Mathematics 77 (2016)]*

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

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### Proposed Master Project at PoreLab NTNU (department of Physics)

## X4-Dimensional Computed Tomography ("4D-CT") with Equinor

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

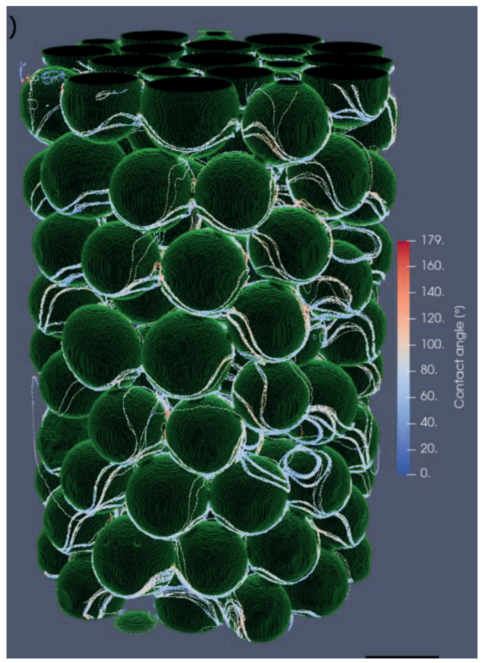


*Figure: 4D-CT: Water being extracted from a pack of glass beads. The lines indicate the water level at different times, and the color coding of the lines gives the wetting contact angle [Tekseth, to be published].*

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 *multiphase 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)

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### Nine Proposed Master Projects at PoreLab NTNU (department of Physics and department of Chemistry)

## Ultrasound-mediated drug delivery to tumours and brain

Contact: 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 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.

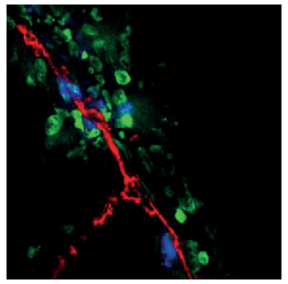

*Figure 1: Nanoparticles (blue) do not travel far from the blood vessels (red). The encapsulated drug is taken up by cells (green) close to blood vessels*

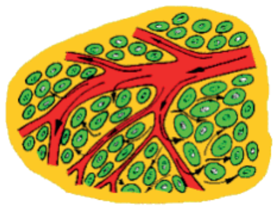

*Figure 2: The delivery of nanoparticles/drugs depends on*
*1) The blood vessel network*
*2) Transport across the capillary wall*
*3) Penetration through the ECM*
*4) Cellular uptake*

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
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?

Contact: 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?

Contact: 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

Contact: 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

Contact: 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.

## 5.The impact of tumor protein composition on uptake of drugs in tumors exposed to ultrasound and microbubbles

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

We have seen that treatment with ultrasound and microbubbles can increase the uptake of cancer drugs in solid tumors, however, the variations are large, and we need to understand more about why certain tumors respond better than others. The protein composition of a tumor may impact the effect of the treatment, and the protein expression can vary greatly between different tumors. We have performed proteomic analyses on untreated tumors and tumors treated with the cancer drug doxorubicin in combination with ultrasound and microbubbles. The student will use the software R to perform statistical analyses on proteomic datasets and examine correlations between protein composition and the uptake of doxorubicin in tumors treated with and without ultrasound and microbubbles.

## 6.Multicellular spheroids as a model for drug delivery studies

Contact: Catharina de Lange Davies (catharina.davies@ntnu.no); Caroline Einen (caroline.einen@ntnu.no)

Multicellular spheroids consist of cells in an extracellular matrix and can be a good model to study transport of drugs and nanoparticles. We have previously established a method to make spheroids of cancer cells and fibroblasts. Currently a master student is studying the infiltration of nanoparticles into spheroids, and the uptake of nanoparticles in cancer cells and fibroblast. Next we want to study the effect of ultrasound and microbubbles on penetration of nanoparticles into spheroids.

## 7.Characterizing activation of ACT bubbles and number of activated ACT bubbles within a tumour

Contact: Catharina de Lange Davies (catharina.davies@ntnu.no); Petros Yeman (petros.t.yemane@ntnu.no)

GE healthcare and EXACT Therapeutics are developing a new formulation of the microbubble Sonazoid, called Ready-to-Use (RtU). Sonazoid is the microbubble which together with microdroplet forms the microclusters in ACT. The RtU formulation will be compared with old formulation in terms of number of activated bubbles and longevity of ACT bubbles in tumours. The goal of this project is to develop a method to process the recorded ultrasound data and estimate the number of activated bubbles and longevity of ACT bubbles within the tumour. The developed method should produce high quality display and quantification of the ACT bubbles. Image processing involves motion correction, background subtraction and counting.

<u>Projects using modelling and simulations</u>

## 8.Molecular simulation of nanoparticle transport under ultrasound streaming through model hydrogels

Contact: Rita S. Días (rita.dias@ntnu.no); Pablo Blanco (pablb@ntnu.no)

One of the key factors in drug delivery therapy is the transport of the drug carriers (typically nanoparticles) through the extracellular matrix. The extracellular matrix is a complex and dense physical hydrogel which can hinder or even prevent nanoparticles from reaching the target of the therapy. Recent experimental studies suggest that the transport of nanoparticles can be enhanced by focused ultrasound irradiation in the target tumor. In this project, we will use coarse-grained models to study the transport of nanoparticles through hydrogels using the Extensible Simulation Package for Research on Soft Matter ESPResSo (https://espressomd.org/wordpress/). We will use Molecular Dynamics to study the effect of the properties of the hydrogel (density, structure, charge), the nanoparticle (size, charge) and the streaming caused by the ultrasound in the transport of the nanoparticle. The project requires basic scripting skills in Python, and the student will also learn to use common tools for software development like Git.

## 9.Simulation of biomolecule adsorption and the effect of nanoparticle coating

Contact: Anders Lervik (anders.lervik@ntnu.no); Signe Kjelstrup (signe.kjelstrup@ntnu.no); Sebastian Everard Nordby Price (sebastian.n.price@ntnu.no)

The blood circulation time of the nanoparticles is substantially reduced by protein adsorption. Coating the nanoparticle with surfactants, for instance, polyethylene glycol can mitigate this issue. The effectiveness of the coating will depend on the type of surfactant used and its characteristics (e.g. length). We will perform atomistic simulations (e.g., molecular dynamics) to investigate and understand the interactions between coated nanoparticles and biomolecules such as proteins and biopolymers on an atomistic scale. We aim to investigate how the interactions change depending on the surfactant's and nanoparticle's characteristics, how this influences the transport, and how we can use this knowledge to suggest more efficient coatings. The project is theoretical, involving computer simulations, programming, and modelling.

This project is in collaboration with the Center of Excellence PoreLab https://porelab.no/

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Proposed Master Project at PoreLab NTNU (department of Chemistry)

## Nature-inspired water and ice-repelling nanostructured surfaces

Contacts: Signe Kjelstrup (signe.kjelstrup@ntnu.no)

Recently, many nanofabricated surfaces with unique physical and chemical properties like super sticky, self-cleaning, hydrophilic, hydrophobic, ice-phobic, anti-fouling properties and with their combinations (multi-purpose smart surfaces) have been elaborated.

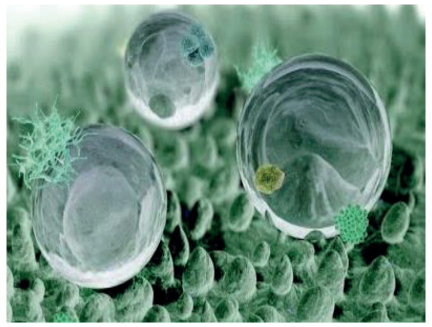
Many important physical and geometric principles of their structure and function can be taken from nature, for instance self-cleaning lotus leaf, super sticky glue from mussels, super-hydrophobic surfaces of insects, air-accumulating surfaces of some leaves and water insects, ice-phobic insect eyes and many others. Modern water and ice-repelling surfaces must sustain different ambient conditions (temperature, pressure, humidity, wind), that needs elaboration of smart nanostructures of different materials.

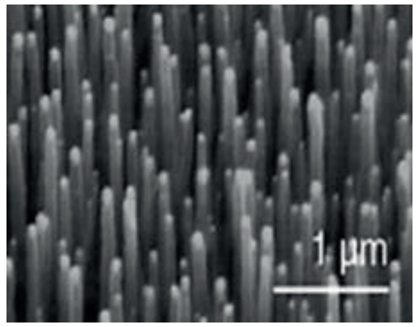
In this project, the student will familiarize with irreversible thermodynamics at the microscale and learn how the surface geometry and physical parameters influence its water- and ice-repelling abilities. The project will be carried out according to the following steps:

1. Classification of the nanostructured natural surfaces discovered in plants and animals and studied in literature.
2. Discussion of the physical and chemical mechanisms of the "smartness".
3. Elaboration of simplifies models of the nanostructured natural surfaces and computations of their surface energy.
4. Comparative analysis of their smart properties and propositions for experimental verification of theoretical results and discussion of possible application.

*Literature*


1. Jeevahan J., M. Chandrasekaran, G. Britto Joseph, R.B. Durairaj,G. Mageshwaran, Superhydrophobic surfaces: a review on fundamentals,applications, and challenges, J. Coat. Technol. Res. 15 (2018) 231–250.
2. Nguyen-Tri P., H.N. Tran, C.O. Plamondon, L. Tuduri, D.-V.N. Vo, S. Nanda,A. Mishra, H.-P. Chao, A.K. Bajpai, Recent progress in the preparation, propertiesand applications of superhydrophobic nano-based coatings and surfaces: areview, Prog. Org. Coat. 132 (2019) 235–256.
3. Yancheshme A.A., G. Momen, R. Jafari Aminabadi, Mechanisms of ice formation and propagation on superhydrophobic surfaces: a review, Adv. Colloid Interface Sci. 279 (2020) 102155.

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

## Superlubricity of Quasicrystals: modelling extremely low friction of exotic materials

Contact: Astrid de Wijn (astrid.dewijn@ntnu.no) and Raffaela Cabriolu (raffaela.cabriolu@ntnu.no)

In this project, you will focus on a particular class of crystalline materials that have an unusual structure: quasicrystals. The discovery of quasicrystals was awarded the Nobel Prize in chemistry in 2011. The project is concerned with how the quasi-crystal structure will affect the friction of these surfaces, through structural superlubricity. This is a dramatic effect by which friction is reduced enormously due to structural incompatibility between two surfaces at the atomic level. You will write a simple numerical simulation to compute interactions of contacts with quasicrystalline surfaces, and whenever possible do analytical calculations to accompany them.

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

*Supervisor*
Astrid S. de Wijn, astrid.dewijn@ntnu.no
Supervisor in physics: Raffaela Cabriolu, raffaela.cabriolu@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.

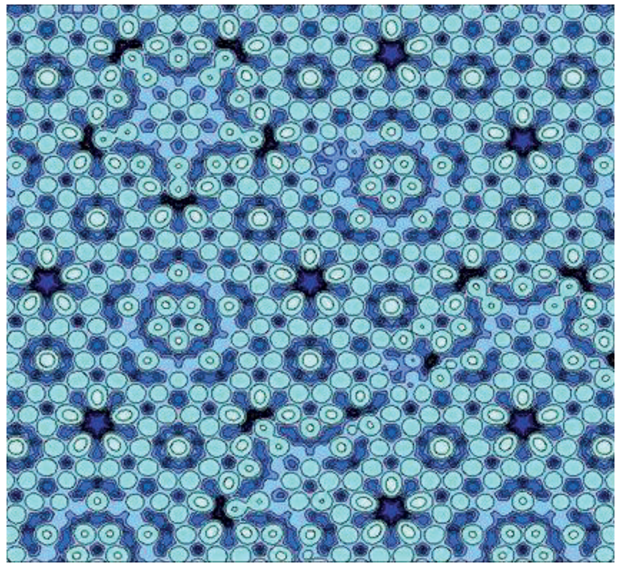

*Figure*: *Example of a quasicrystal surface, atomic model of fivefold icosahedral-Al-Pd-Mn. (Picture from Wikimedia Commons)*



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) and Raffaela Cabriolu (raffaela.cabriolu@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.

*Supervisors*
Astrid S. de Wijn, astrid.dewijn@ntnu.no
Supervisor in physics: Raffaela Cabriolu, raffaela.cabriolu@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.

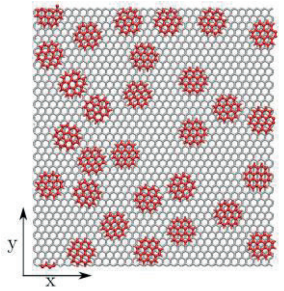


*Figure : A top view of a simulation of a single layer of graphene flakes acting as a solid lubrican*

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

## Superlubricity in the real world: modellingmulticontact low-friction sliding

Contact: Astrid de Wijn (astrid.dewijn@ntnu.no), Bjørn Haugen (bjorn.haugen@ntnu.no) and Rafaella Cabriolu (rafaella.cabriolu@ntnu.no)

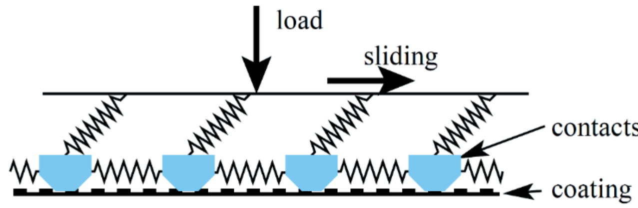
This project is concerned with structural superlubricity. This is a dramatic effect by which friction is reduced enormously due to structural incompatibility between two surfaces at the atomic level. Macroscopic surfaces in contact in the real-world, however, do not have one large flat contact, but consist 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
Supervisor in Physics: Raffaela Cabriolu, Raffaela.cabriolu@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)

## Simulating growth of cancer and the immune system

Contact: Astrid de Wijn (astrid.dewijn@ntnu.no), Rian Friedman (ran.friedman@lnu.se) and Raffaela Cabriolu (raffaela.cabriolu@ntnu.no)

In this project, we will investigate the effect of the patient's own immune system on the growth and death of tumor cells under treatment. Chemotherapy and many other cancer treatments have the ability to kill or severely limit the growth of cancer cells. However, because these medications are typically toxic, they also limit the patient's immune system, which then is not able to fight the cancer itself to the same degree. This is a problem because the patient's own immune system often contributes to fighting the cancer as well, and because it impairs the use of immunotherapy cancer treatments.

This project will focus on modelling the dynamics of populations of cancerous cells in acute myeloid leukemia. We will include the effects of the treatment as well as the immune system on the growth and death of the cells.

You will write a numerical simulation of a model that we will construct in collaboration with Prof. Ran Friedman, from the Department of Chemistry and Biomedical Sciences, Linnæus University in Kalmar, Sweden. You will run the simulations, perform parameter studies, and analyse the results. If necessary, you will run the simulations on high-performance computing facilities.

*Recommended background*
A basic programming course and an interest in modelling or programming. Basic knowledge of thermodynamics or statistical mechanics.

*Supervisors*
Astrid S. de Wijn, astrid.dewijn@ntnu.no
Ran Friedman, ran.friedman@lnu.se
Supervisor in Physics: Raffaela Cabriolu, Raffaela.cabriolu@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

*Resources*
The project may need to make use of high-performance computing resources that are already available through NTNU IT's HPC facilities.

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

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

## Superlubricity in the real world: designing low friction surfaces with patterning

Contact: Astrid de Wijn (astrid.dewijn@ntnu.no), Bjørn Haugen (bjorn.haugen@ntnu.no), Melisa Gianetti (melisa.m.gianetti@ntnu.no), Viet Hung Ho (viet.h.ho@ntnu.no) and Raffaela Cabriolu (raffaela.cabriolu@ntnu.no)

In this project, we will investigate the contact mechanics of patterned surfaces with low-friction coatings. This project is related to 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 this project is to explore different designs for patterning of surfaces that lead to arrays of contacts with specific properties, that will reduce the problematic consequences of surface roughness.

In the computational part of this project, you will perform numerical calculations of nearly perfect arrays of spherical particles and possibly other structures in contact with each other. You will set up calculations for the deformation in the material using Hertz contact mechanics and other approaches. You will write and perform simulations and investigate the behaviour of the system. If necessary, you will run simulations on high-performance computing facilities.

*Figure*: A homemade set of patterned surfaces with low friction due to macroscale structural mismatch between the arrays of ball bearings. This device was built by second year undergraduate students in Dublin.

*Recommended background*
Tribology, basic statistical mechanics, or classical mechanics. Computational: A basic programming course and an interest in modelling or programming.
Experimental: The experimental student should come from an engineering background and have an interest in material science.

*Supervisors*
Astrid S. de Wijn, astrid.dewijn@ntnu.no
Bjørn Haugen, bjorn.haugen@ntnu.no
Melisa Gianetti, melisa.m.gianetti@ntnu.no
Viet Hung Ho, viet.h.ho@ntnu.no
Supervisor in Physics: Raffaela Cabriolu, Raffaela.cabriolu@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

*Resources*
The project may need to make use of high-performance computing resources that are already available through NTNU IT's HPC facilities.

*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

Contact: Astrid de Wijn (astrid.dewijn@ntnu.no) and Raffaela Cabriolu (raffaela.cabriolu@ntnu.no)

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.

*Supervisor*
Astrid S. de Wijn, astrid.dewijn@ntnu.no
Ondrej Hovorka, University of Southampton
supervisor in physics: Raffaela Cabriolu, raffaela.cabriolu@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.

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Proposed Master Project at PoreLab NTNU (department of Geoscience and Petroleum)

## Pore scale imaging of $CO_2$ 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.

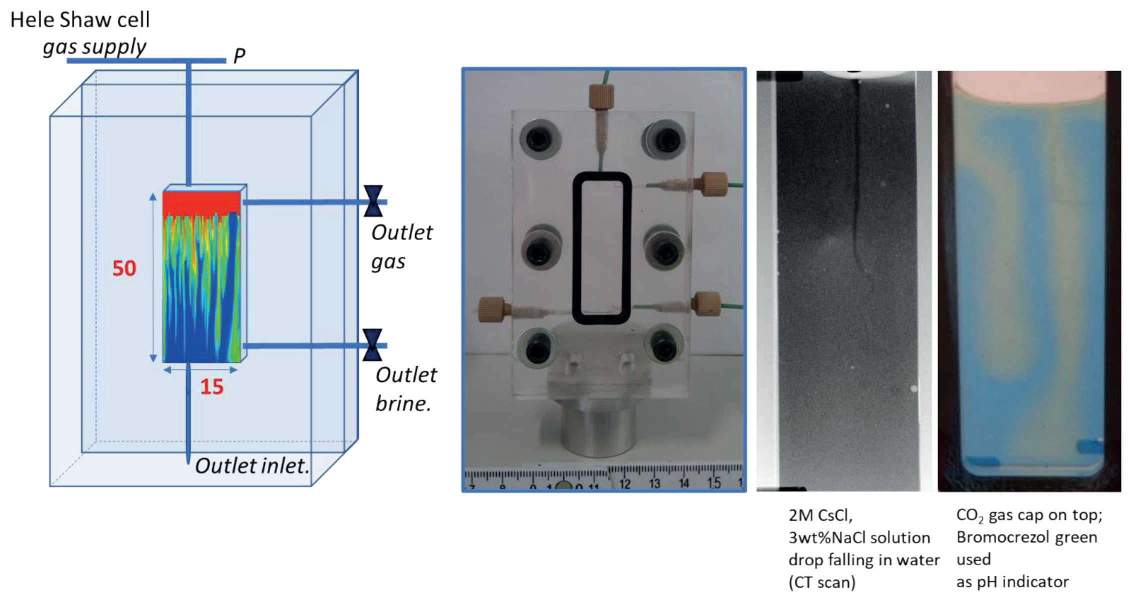


*Figure 1; a 2D model to study convective flow, adapted to be used in the microCt scan*

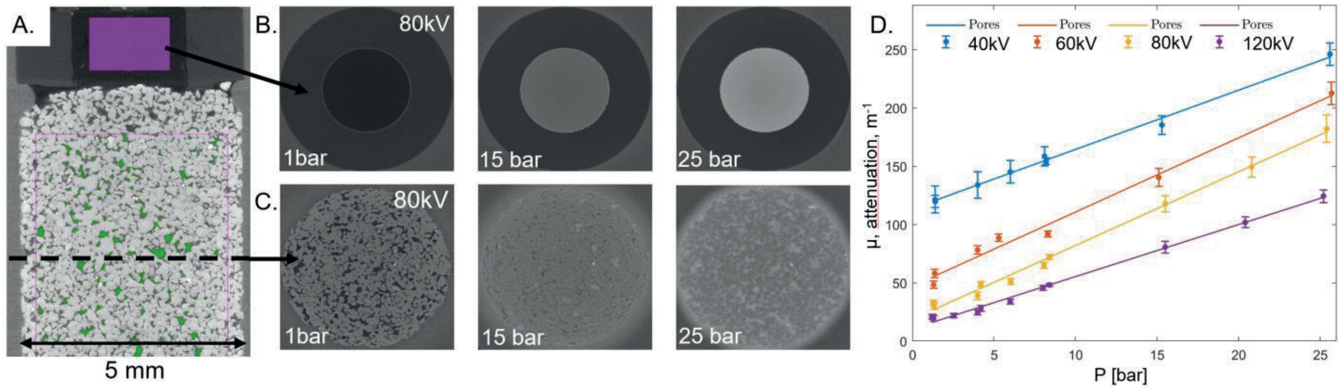


*Figure 2; The pressure dependence of Xenon visualized by mCT scanning of a void space in a plastic ring and a cylindrical Bentheimer sandstone core, both seen in A. The resulting cross sections of the void space and the Bentheimer core at set pressure levels of 1, 15 and 25 bar are presented in B. and 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]*

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## Proposed Master Project at PoreLab NTNU (department of Geoscience and Petroleum)
## Characterization of capillary trapping of $CO_2$ in micromodels and micro-CT scanner
Contacts: 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.

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## Proposed Master Project at PoreLab NTNU (department of Geoscience and Petroleum)
## Pore-scale investigation of low salinity waterflooding in Sandstones
Contact: Antje van der Net (antje.van.der.net@ntnu.no)

For research on understanding multiphase flow description in porous media wettability is one of the important parameters studied. New methods are considered for a better description of wettability changes in multiphase flow, of interest for example for low salinity flooding where wettability change is one of the underlying mechanisms. The measurement of zeta potential is one of these new methods. Zeta potential statically characterizes the transition zone between rock and liquid regarding the surface charge and fluid interaction.

In this project, the objective is to proof whether the zeta-potential measurements of rock-brine system can be used to predict the surface characteristics behavior during low salinity waterflooding and consequently additional oil recovery. Detectable with zeta-potential measurements are double-layer expansion and surface force modification, parameters recognized as important mechanisms of low salinity waterflooding.

The zeta-potential measurements of glass beads/crushed sandstone are used to investigate the sandstone-brine surface properties at different salinities and pH. Afterwards, the optimum chemical condition of the injection brine is examined in two-phase displacement micromodel experiments for a better understanding of pore-scale mechanisms of low salinity waterflooding EOR method.



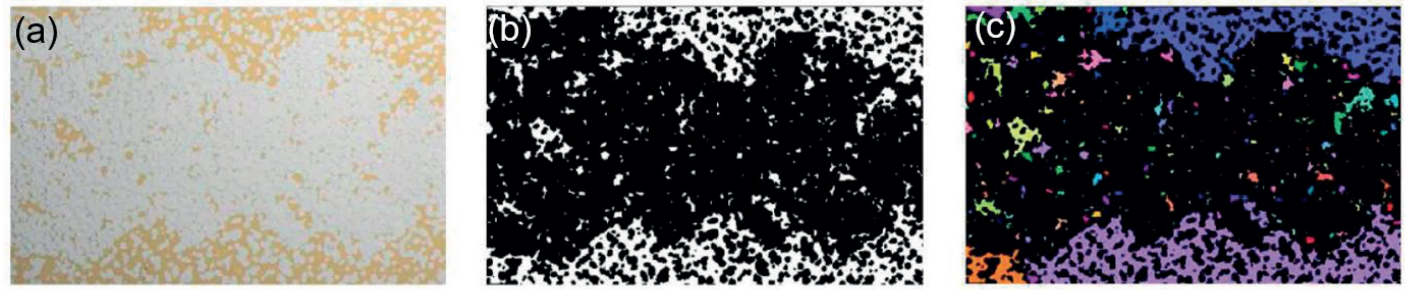


*Figure (a) Pre-processing image of a microchip after water flooding (oil = gold, glass and brine transparent). (b) Segmented, binary image to enable quantitative analysis (oil in white). (c) Oil clusters colored individually for qualitative analysis. [from Aadland et al. Nanomaterials **2020**, 10, p.1296]*

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## Proposed Master Project at PoreLab NTNU (department of Geoscience and Petroleum)
## Oil mobilization with reduced interfacial tension, a study using computational fluid dynamics and micromodels
Contact: Antje van der Net (antje.van.der.net@ntnu.no)

Cleaning processes and mobilization of trapped oil in confined systems can be improved by reducing interfacial tension (IFT). The full understanding of the mechanism behind the phase mobilization in different porous geometries is still unclear and with a better understanding, improvements to the flow processes in porous media can be made, e.g. for trapping $CO_2$ as well as for optimization of oil production.

In this project the importance of IFT, wettability and flow geometry are to be studied in micromodels using biosurfactants combined with computational fluid dynamics modelling for the design of the models and explanation of the effect. As part of the study low interfacial tension solutions are to be found by phase behavior testing with surfactants.

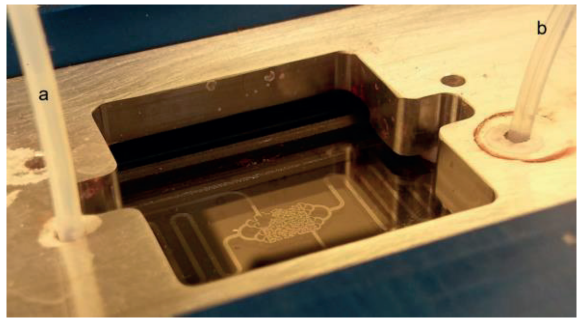


*Figure: Example of a 2D micromodel representing a porous media, connected with an inlet and outlet flow line (a,b)*

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## 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.

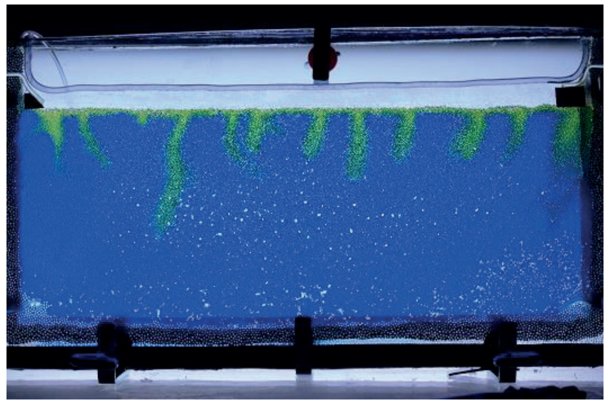

*Figure: A layer of $CO_2$ above a water-saturated porous medium consisting of glass beads. An indicator acid has been added to the water carbonic acid to turn it blue. Where the $CO_2$ has been absorbed by the water, carbonic acid forms which turns the color to green. The acid has larger density than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

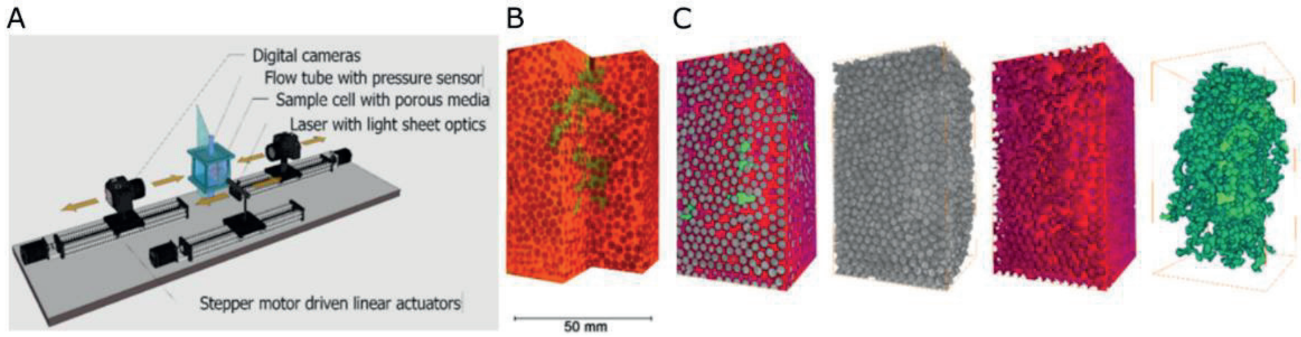


*Figure: A The 3D scanner is based on optical index matching and fluorescence. A random packing of 3 mm glass beads forms the porous medium, index matched with two immiscible fluids. The fluids contain different fluorescent dyes that are excited with a 2D laser sheet that is driven through the sample 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.*

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## 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.

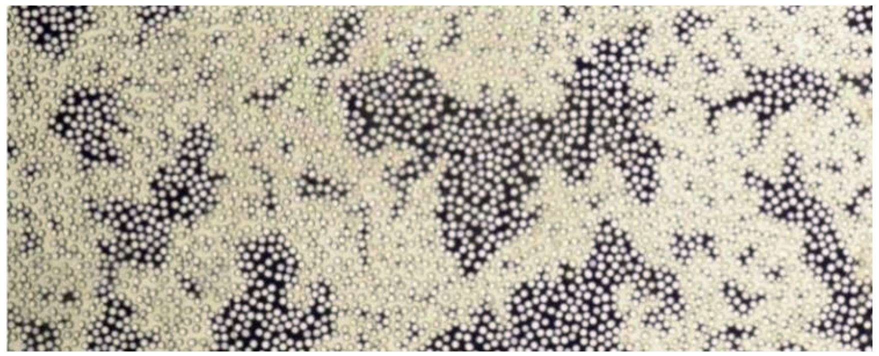

*Figure: Detail of the trapped liquid clusters (blue) left behind after air (white) is slowly injected from the left in a quasi-2D porous network previously saturated with the liquid*



## 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.

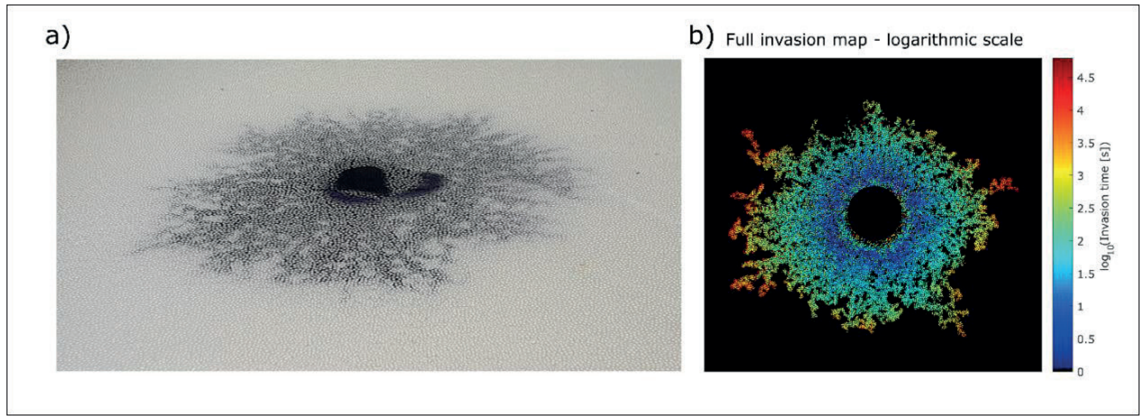


*Figure: a) Experiment illustrating how a source of pollution (central dark blob) spreads through a partially wet porous network (here made of glass beads). Water films covering the internal surfaces of the porous medium can act as a fast pathway for the spreading of pollution. b) Spatiotemporal invasion 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.*

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## 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.

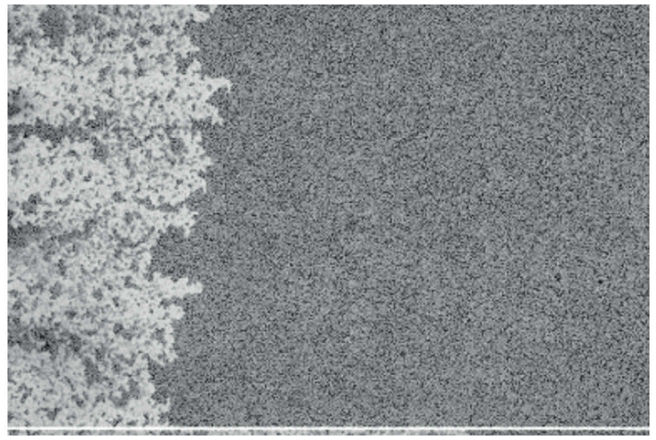

*Figure: Steady state flow in a quasi 2D model system. Simultaneous injection of a glycerol/water (black) solution and rapeseed oil (white)*

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.

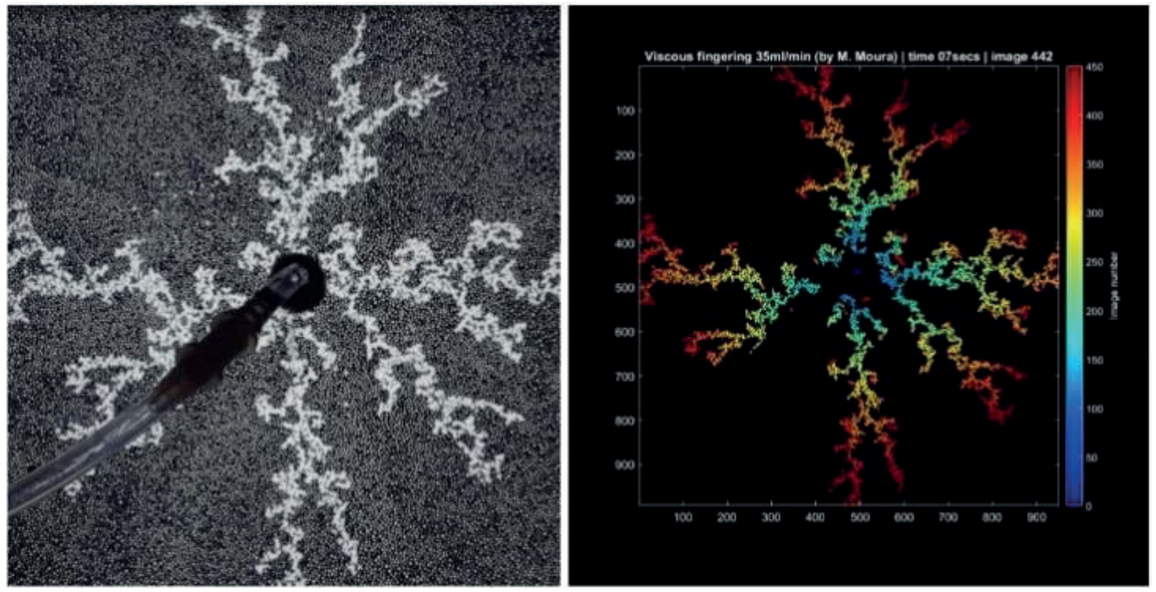

*Figure: Viscous fingering pattern (left) observed when air is injected fast in a porous medium previously filled with a viscous liquid (blue). The image analysis (right) shows the time (image number) of injection of each pore*

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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.

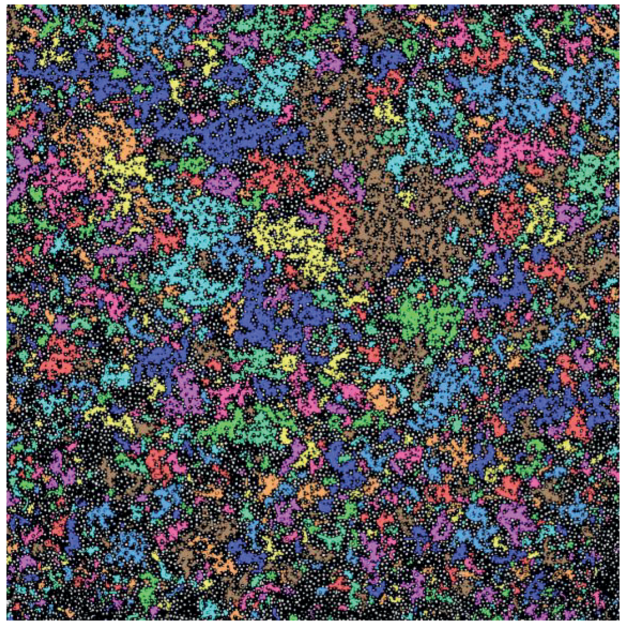

*Figure: Steady state two phase flow experiments in a horizontal quasi 2D porous media. Air and a glycerin water solution are injected simultaneously into the porous medium. The colors indicate different cluster sizes of trapped air*



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.

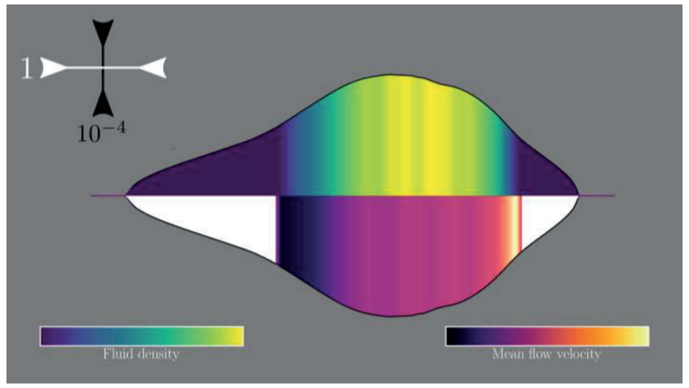


*Figure: Snapshot of dynamic fluid flow simulation (i.e. density and mean fluid velocity) within a rapidly expanding crack cavity. The white area highlights the formation of a fluid-depleted cavity.*

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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)

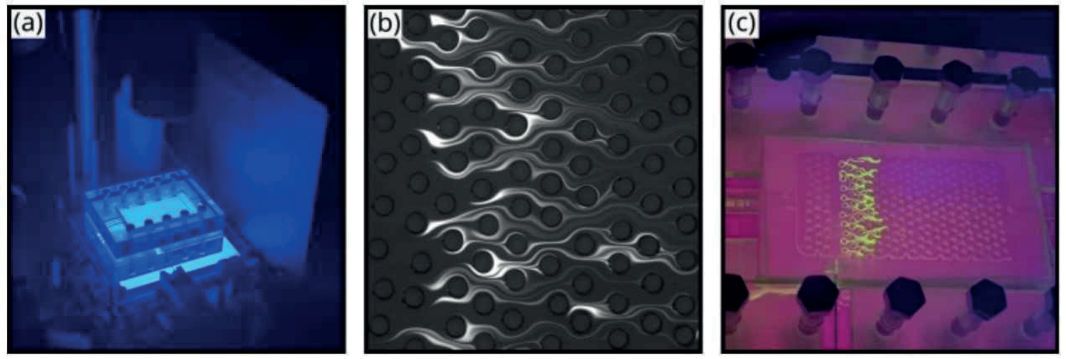


*Figure: (a) Fluorescence imaging experiment, showing blue excitation light; (b) Solute plume in a single phase flow; (c) 3D printed porous model with green fluorescence light from a dye undergoing mixing.*

*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.

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## 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. 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.

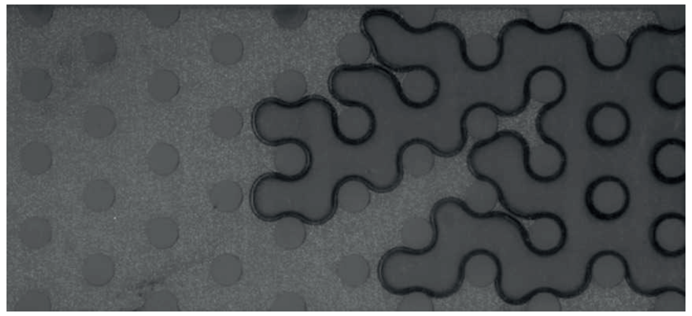

*Figure:* *Snapshot of microscopic tracer particles in a two-phase flow through a porous model.*

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## 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.

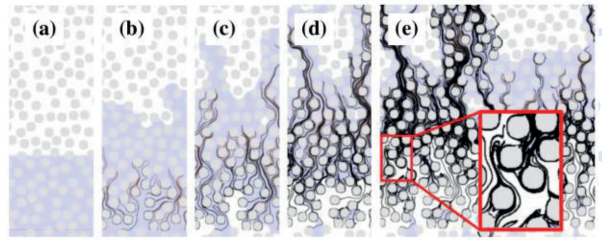


*Figure:* *Simulations of chaotic mixing in two-phase flow in a 2D porous medium. (a)–(e) show a strip of solute at various instances of time as it is exponentially elongated by a net upward flow.*

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## 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)

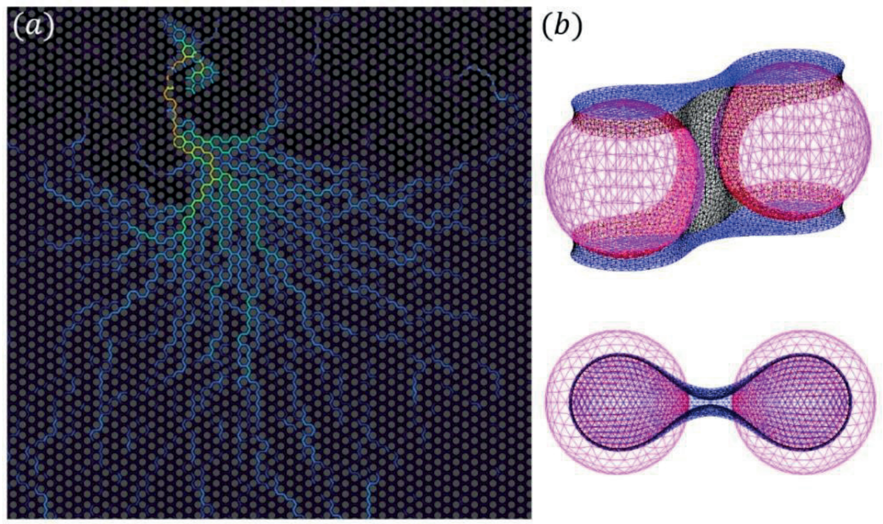


*Figure:*
*(a) Pore-network modeling of a small water cluster draining into a larger cluster via capillary bridge networks. The grains are shown as gray circles, and low (high) local flow rates are indicated by dark blue (yellow)*
*(b) Example of a single water bridge formed between two spherical grains.*

# 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 the 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. You have experience with how the temperature in a system can be controlled.
- knows the theory of dynamic light scattering and have experience in using light scattering to study diffusing particles and particles in a convective velocity field. You have 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 you are able to perform image analysis to characterize the structure and the dynamics. You know 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 the NTNU PoreLab node.
- 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.

### Mass and Heat 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 will be individual adapted to the actual students taking the course.

### Applied Heterogeneous Catalysis

KP8132, NTNU

The course is given every second year. Lessons are not given in the academic year 2022/2023. 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 aims at providing an understanding of the mode of function of the components that the instrumentation consists of as well as a theoretical and practical understanding of how to operate the instrument, including i.e. 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 petroleum resources.

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, relative permeability and applications in earth sciences and petroleum engineering.

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, significance of rock mechanics in reservoir control and 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 petroleum reservoirs. 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 of oil and gas and will be able to do derivation of equations for flow in porous media, and numerical solution of these by using finite difference methods.

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 are as follow: Summary of rock 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 methods; 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 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 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.
- Time integration.
- 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. Time integration.
4. Linear equation solvers.
5. Stability and numerical dispersion.
6. Streamline methods.
7. 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. Professor Carl Fredrik Berg, PI at PoreLab, is the course's coordinator.

### 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. S(he) 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. S(he) will be able to deduce the master equation and use it to construct various Monte Carlo algorithms.

*A large delegation from PoreLab of Professors, researchers, postdocs, PhD candidates and Master Students gathers at the 15th Annual International Conference on Porous media organized by InterPore from 22 to 25 May 2023, in Edinburgh, Scotland, UK.*

# Porous Media Laboratory
# NTNU, UiO


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