

**Molecular simulation of fluid confinement and crystallisation effects
(NewPores project)**

NewPores research project presentation

NewPores is an international hub dedicated to the mechanics and physics of porous materials, which intends to answer to new Energy and Environment challenges. This is a joint effort of the group on Geomechanics and Porous Materials (G2MP) of the Laboratoire des Fluides Complexes et leurs Réservoirs at E2S UPPA (France), the Centre for Sustainable Engineering of Geological and Infrastructure Materials (SEGIM) at Northwestern University (USA), the University of Vigo (Spain), the Technical University of Madrid (Spain) and University of Liège (Belgium).

Multiscale analysis of porous materials by DFT/Enhanced-poromechanics modelling

Porous materials are composed of a solid skeleton with partially interconnected voids filled by a variety of fluids (liquid, vapour, gas). When pores are large and completely saturated with a single fluid, poromechanics is rather well understood. This is not the case for various situations that depart from this assumption, and most particularly for micro and nanoporous materials. Without being exhaustive, the following examples illustrate such shortcomings:

- in nano-porous materials containing fluid phases, many results show that pressures applied on the pore surfaces by the fluid may be very high. Swelling of the material is observed upon application of an external pressure on saturated nano-porous material, which is qualitatively the opposite of what is predicted by classical poromechanics;
- whenever phase changes are expected, e.g. precipitation of salt in the fluid phase or freezing of water typically, a complex crystal-solid skeleton interaction occurs. This interaction leads authors to the concept of “crystallisation pressure” whose exact form has been rather controversial (e.g. over simplified) in the literature. One reason is that the crystal to solid skeleton interaction should be mediated by the presence of a thin fluid film (a few nanometre thick) located in between them. The accurate kinetics and thermodynamic description of this three constituent system remain to be elucidated.

The common denominator in these two examples is that the continuum description lacks information that is located at the nano-scale. Phenomena occurring at the scale of *a small aggregate of atoms forming pore walls, that of a fluid confined in pores of the nanometre size, that of the liquid-vapour- solid interface, or that of a thin confined film of fluid* govern the macro-scale response. Classical poromechanics needs to be revisited in order to be able to capture these nano-scale effects.

Within the NewPores project, the key challenge is therefore to develop and validate against experiments and molecular simulations, a comprehensive DFT (*Density Functional Theory*) that should be capable to encompass the solid and fluid interacting phases in a porous material when nano-scale phenomena are predominant, including phase changes in the fluid.

2-years postdoc candidate objectives

Within the NewPores project, the 2-year postdoc candidate will be in charge of building a numerical database based on Gromacs molecular simulations allowing the validation on given configurations of the DFT/Enhanced-poromechanics model developed otherwise by two PhD students on adsorption-induced deformation and water crystallisation respectively.

Candidate's profile

The candidate should hold a PhD degree in physics, statistical physics, mechanics, material sciences or a similar field. Previous experience with molecular simulations (MS) is mandatory (with Gromacs or other MS tools). Previous experience with the characterization of multi-physics couplings appearing in porous media

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(phase transition, adsorption-induced strain etc.) is an asset. The candidate should have a strong interest in performing numerical work in a multi-disciplinary team. Proficiency in English is mandatory for both oral and writing communication. Basics in Spanish or French may be helpful but are not mandatory.

Job details

The successful candidate will be hosted in the G2MP research team at LFCR laboratory (UMR5150, UPPA-CNRS-Total SA) but long research residencies will be organised at the University of Vigo (Spain) and the Technical University of Madrid (Spain).

The candidate will be supervised by:

- Pr. Manuel Martínez Piñeiro (University of Vigo)
- Dr. María M. Conde (Technical University of Madrid)
- Dr. Christelle Miqueu (E2S UPPA/LFCR/G2MP)
- Pr. David Grégoire (E2S UPPA/LFCR/G2MP)

The postdoc position may start in Novembre 1st, 2020, will last 2 years and the position includes full social security coverage and a gross salary of approx. 2 984 € per month. This salary encompasses 20h of teaching hours at E2S UPPA per year.

Evaluation procedure

Candidates will be ranked in a first phase based on their submitted application.

In a second phase, an interview will be organized with the selected candidates (via Skype).

Applications should include a cover letter, CV, transcripts of diplomas and lists of courses attended (with grades obtained), recommendation letters, and names and contact details of at least two references.

Calendar

<u>Application deadline:</u>	August 31th, 2020
<u>Application review:</u>	Sept. 1st / Sept. 10th, 2020
<u>Interview (visioconferencing):</u>	Sept. 14th / Sept. 24th, 2020
<u>Final selection:</u>	Sept. 25th, 2020
<u>Job starting date:</u>	Nov. 1st, 2020

Application website

https://docs.google.com/forms/d/e/1FAIpQLSfTx0i-gO_IFTehiVOqz64QQZ12BXS5_qpAmlw4iRBYEmXRCA/viewform

Contact

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