Offer #2025-08675

Post-Doctoral Research Visit F/M Fully coupled algorithms for multiphase reactive transport, application to hydrogen storage in porous media

Contract type : Fixed-term contract

Level of qualifications required : PhD or equivalent

Fonction : Post-Doctoral Research Visit

Level of experience : From 3 to 5 years

About the research centre or Inria department

The Inria centre at Université Côte d'Azur includes 42 research teams and 9 support services. The centre's staff (about 500 people) is made up of scientists of di?erent nationalities, engineers, technicians and administrative staff. The teams are mainly located on the university campuses of Sophia Antipolis and Nice as well as Montpellier, in close collaboration with research and higher education laboratories and establishments (Université Côte d'Azur, CNRS, INRAE, INSERM ...), but also with the regiona economic players.

With a presence in the fields of computational neuroscience and biology, data science and modeling, software engineering and certification, as well as collaborative robotics, the Inria Centre at Université Côte d'Azur is a major player in terms of scientific excellence through its results and collaborations at both European and international levels.

Context

The project is part of a collaboration between the Inria Université Côte d'Azur center https://www.inria.fr/fr/centre-inria-universite-cote-azur and Storengy https://www.storengy.fr.

It will be co-supervised by Roland Masson https://math.univ-cotedazur.fr/~massonr (Inria and the J.A. Dieudonné Mathematics Laboratory of Université Côte d'Azur) and Laurent Jeannin (Storengy).

The position will be based at the J.A. Dieudonné Mathematics Laboratory of Université Côte d'Azur https://math.univ-cotedazur.fr on the Valrose campus in Nice.

Assignment

In the context of the energy transition, Storengy is studying and developing underground hydrogen (H2) storage solutions, either in mixtures or pure form, in porous media. On one hand, the production of natural gas from new industrial-scale processes such as methanation and pyro-gasification leads to changes in the composition of the stored gas (which is mainly composed of methane, but H2 can reach a few percent of the molar composition of the stored gas). On the other hand, within the framework of the development of the hydrogen sector in Europe, H2 (pure) produced from renewable electricity through electrolysis can not only contribute to the decarbonization of electricity production and certain industrial processes but also provide flexibility to energy networks when stored. This involves studying the storage of gaseous hydrogen underground. The objective of this study is to examine the behavior of underground H2 storage in an aquifer, whether it is pure or in a mixture. One of the challenges is to account for chemical processes that could alter the composition of the gas in storage. For example, methanation or sulfate-reduction reactions, linked to the presence of certain bacteria, can enrich the gas with methane or hydrogen sulfide.
The aim of this study is to numerically model two-phase water/gas flows in porous media while considering geochemical or biogeochemical reactions in the medium.

We consider chemical systems typically including species in aqueous, gaseous and mineral phases and comprising phase-change reactions assumed to be at equilibrium, homogeneous reactions in the aqueous phase and heterogeneous reactions between the aqueous phase and minerals. Solving these systems, which couple molar conservation laws, chemical equilibrium laws, kinetic laws, and total volume conservation, presents numerous challenges due to the large number of chemical species, the stiffness, and the degeneracies induced by chemical reactions and phase transitions.
The resolution of these systems presents numerous challenges related to the large number of chemical species, the stiffness of the system induced by chemical reactions, and the degeneracies caused by phase transitions. Most formulations are based on splitting algorithms that sequentially solve (i) a two-phase flow sub-model

considering only phase-change reactions to compute the properties of the aqueous and gaseous phases (velocities, volume fractions, pressures) and (ii) a reactive transport sub-model calculating the molar concentrations of species with given phase properties.These algorithms offer advantages in terms of modularity, reusability of existing solvers, and cost. However, they suffer from splitting errors related to the loss of molar or volumetric conservation, which can significantly restrict time steps. Additionally, they assume that the aqueous phase cannot disappear, which typically prevents the consideration of drying phenomena near gas injection wells.

To overcome these limitations, the project will focus on fully coupled algorithms. In particular, we will investigate the extension of natural variable formulations to the reactive framework [1] and address the difficulties associated with the disappearance of the aqueous phase and multiphase chemical equilibria [2].
These algorithms will be implemented in 1D and radial 2D, and their efficiency will be studied on multiphase reactive transport benchmarks from the literature [3,4].
Subsequently, the modeling will integrate mineralogical and petrophysical data from Storengy sites as well as realistic operating conditions, including injection and withdrawal flow rates at wells. The development and operation phases of the storage will then be modeled.

[1] Yaqing Fan, Louis J. Durlofsky, and Hamdi A. Tchelepi. A fully-coupled flow-reactive- transport formulation based on element conservation, with application to co2 storage sim- ulations. Advances in Water Resources, 42:47–61, 2012.

[2] I. Ben Gharbia, C. Cancès, T. Faney, M. Jonval, and Q.H. Tran. Robust resolution of single- phase chemical equilibrium using parametrization and Cartesian representation techniques. working paper or preprint, 2023.

[3] Etienne Ahusborde, Brahim Amaziane, Stephan de Hoop, Mustapha El Ossmani, Eric Flauraud, François P. Hamon, Michel Kern, Adrien Socié, Danyang Su, K. Ulrich Mayer, Michal Toth, and Denis Voskov. A benchmark study on reactive two-phase flow in porous media: Part 2 - results and discussion. Computational Geosciences, 2024.

[4] Stephan de Hoop, Denis Voskov, Etienne Ahusborde, Brahim Amaziane, and Michel Kern. A benchmark study on reactive two-phase flow in porous media: Part 1 - model description. Computational Geosciences, 28(1):175–189, 2024.

Main activities

- Design fully coupled formulations of multiphase reactive transport models
- Implement these numerical methods on a prototype code
- Validate these numerical methods on academic benchmarks
- Extend the model to account for gas storage operational conditions and storengy data sets
- Write reports and articles
- Present the results at workshops and conferences

Skills

Research experience in the design of efficient numerical methods for coupled systems of PDEs

Very good experience in scientific programming for the numerical simulation of PDEs using languages like Fortran, Python

Good experience in writing scientific reports using Latex

Ability to present his work in english and to team working

Benefits package

- Subsidized meals
- Partial reimbursement of public transport costs
- Leave: 7 weeks of annual leave + 10 extra days off due to RTT (statutory reduction in working hours) + possibility of exceptional leave (sick children, moving home, etc.)
- Possibility of teleworking (after 6 months of employment) and flexible organization of working hours
- Professional equipment available (videoconferencing, loan of computer equipment, etc.)
- Social, cultural and sports events and activities
- Access to vocational training
- Social security coverage

Remuneration

Gross Salary: 2788 € per month

General Information

- **Town/city :** Université Côte d'Azur, Campus de Valrose
- **Inria Center :** Centre Inria d'Université Côte d'Azur
- **Starting date :** 2025-09-01
- **Duration of contract :** 1 year, 6 months
- **Deadline to apply :** 2025-06-30

Contacts

- **Inria Team :** AT-SOP AE
- **Recruiter :**
  Masson Roland / Roland.Masson@inria.fr

About Inria

Inria is the French national research institute dedicated to digital science and technology. It employs 2,600 people. Its 200 agile project teams, generally run jointly with academic partners, include more than 3,500 scientists and engineers working to meet the challenges of digital technology, often at the interface with other disciplines. The Institute also employs numerous talents in over forty different professions. 900 research support staff contribute to the preparation and development of scientific and entrepreneurial projects that have a worldwide impact.

The keys to success

PhD in the fields of numerical methods for PDEs and scientific computing.

Experience in porous media flows and reactive transport models will be a plus

Interest in applications in geosciences and chemistry

Good communication skills (oral and written)

Ability to teamwork.

Warning : you must enter your e-mail address in order to save your application to Inria. Applications must be submitted online on the Inria website. Processing of applications sent from other channels is not guaranteed.

Instruction to apply

Defence Security :
This position is likely to be situated in a restricted area (ZRR), as defined in Decree No. 2011-1425 relating to the protection of national scientific and technical potential (PPST).Authorisation to enter an area is granted by the director of the unit, following a favourable Ministerial decision, as defined in the decree of 3 July 2012 relating to the PPST. An unfavourable Ministerial decision in respect of a position situated in a ZRR would result in the cancellation of the appointment.

Recruitment Policy :
As part of its diversity policy, all Inria positions are accessible to people with disabilities.