Offre n°2025-08675

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

Le descriptif de l'offre ci-dessous est en Anglais

Type de contrat : CDD

Niveau de diplôme exigé : Thèse ou équivalent

Fonction : Post-Doctorant

Niveau d'expérience souhaité : De 3 à 5 ans

A propos du centre ou de la direction fonctionnelle

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.

Contexte et atouts du poste

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.

Mission confiée

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.

Principales activités

- 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

Compétences

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

Avantages

- 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

Rémunération

Gross Salary: 2788 € per month

Informations générales

- **Ville :** Université Côte d'Azur, Campus de Valrose
- **Centre Inria :** Centre Inria d'Université Côte d'Azur
- **Date de prise de fonction souhaitée :** 2025-09-01
- **Durée de contrat :** 1 an, 6 mois
- **Date limite pour postuler :** 2025-06-30

Contacts

- **Équipe Inria :** AT-SOP AE
- **Recruteur :**
  Masson Roland / Roland.Masson@inria.fr

A propos d'Inria

Inria est l'institut national de recherche dédié aux sciences et technologies du numérique. Il emploie 2600 personnes. Ses 215 équipes-projets agiles, en général communes avec des partenaires académiques, impliquent plus de 3900 scientifiques pour relever les défis du numérique, souvent à l'interface d'autres disciplines. L'institut fait appel à de nombreux talents dans plus d'une quarantaine de métiers différents. 900 personnels d'appui à la recherche et à l'innovation contribuent à faire émerger et grandir des projets scientifiques ou entrepreneuriaux qui impactent le monde. Inria travaille avec de nombreuses entreprises et a accompagné la création de plus de 200 start-up. L'institut s'e?orce ainsi de répondre aux enjeux de la transformation numérique de la science, de la société et de l'économie.

L'essentiel pour réussir

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.

Attention: Les candidatures doivent être déposées en ligne sur le site Inria. Le traitement des candidatures adressées par d'autres canaux n'est pas garanti.

Consignes pour postuler

Sécurité défense :
Ce poste est susceptible d'être affecté dans une zone à régime restrictif (ZRR), telle que définie dans le décret n°2011-1425 relatif à la protection du potentiel scientifique et technique de la nation (PPST). L'autorisation d'accès à une zone est délivrée par le chef d'établissement, après avis ministériel favorable, tel que défini dans l'arrêté du 03 juillet 2012, relatif à la PPST. Un avis ministériel défavorable pour un poste affecté dans une ZRR aurait pour conséquence l'annulation du recrutement.

Politique de recrutement :
Dans le cadre de sa politique diversité, tous les postes Inria sont accessibles aux personnes en situation de handicap.