(naía-

Offer #2025-08975

Post-Doctoral Research Visit F/M Numerical and metabolic simulation of microbial communities for CO? storage underground

Contract type : Fixed-term contract

Level of qualifications required : PhD or equivalent

Fonction: Post-Doctoral Research Visit

Level of experience : Up to 3 years

About the research centre or Inria department

The Inria center at the University of Bordeaux is one of the nine Inria centers in France and has about twenty research teams.. The Inria centre is a major and recognized player in the field of digital sciences. It is at the heart of a rich R&D and innovation ecosystem: highly innovative SMEs, large industrial groups, competitiveness clusters, research and higher education players, laboratories of excellence, technological research institute...

IFP Énergies nouvelles (IFPEN) is a major public-sector player in research, innovation and training in the fields of energy, transport and the environment. Organized into several centers, the main one of which is located in Rueil-Malmaison, IFPEN relies on research excellence to meet the major challenges of the energy transition. It operates within a rich ecosystem of industrial partners, startups, academic establishments, competitiveness clusters and public institutions, and plays a key role in developing sustainable solutions for industry and society.

Translated with DeepL.com (free version)

Context

Within the framework of a partnership between Inria and IFP Énergies nouvelles (IFPEN) we develop numerical and metabolic models to study the influence of microorganisms that are naturally present in deep geological formations used for **carbon capture storage** (CCS). Our objective is to better understand the interactions between microbial communities, the lithic environment, and the CO? injected in deep carbon storage sites. These interactions produce **biological phenomena** that can influence, beneficially or detrimentally, the efficiency and reliability of carbon storage.

These interactions may include, for example, mineral bioalteration, production of metabolic gases (such as methane or hydrogen sulfide), or even biologically-induced carbonate precipitation (biocarbonatation) that contributes to the permanence of the storage by immobilizing CO? in **mineral** form and **limiting the risk of leaks**. Other effects, such as the formation of biofilms, may have contrasted impacts: in reservoirs, they may reduce injectivity, or increase corrosion in wells in the case of sulfate-reducing bacteria; whereas in geological cover formations, biofilms may reduce permeability and consequently reinforce the efficiency of the geological barrier. Understanding and modeling these mechanisms is thus essential for anticipating their long-term impact on the fitness of storage sites and for orienting risk management strategies.

To simulate these complex phenomena, we will **couple two modeling tools** developed at the IFPEN and Inria in a common framework. Inria provides its expertise in **community-scale microbial metabolic modeling** and codes that can simulate metabolic exchanges in complex microbial networks. With this approach we can anticipate the biological functions activated in a given environment, such as the conditions favorable for biofilm formation. IFPEN provides **nonlinear dynamical models of biogéochemical reactions** and codes that can predict their effects on the geological environment and the associated transformations. By integrating these complementary approaches we will construct a robust simulation workflow that can evaluate the influence of microbial processes on the performance of CO? storage sites.

The principal place of work will be the Inria center at the University of Bordeaux, in the offices of the Pleiade project-team https://team.inria.fr/pleiade/.

Travel between Bordeaux, Toulouse, and Reuil-Malmaison may be necessary from time to time, and expenses will be covered.

Assignment

Assignments: Under the direction of David Sherman (Inria) and Arnaud Pujol (IFPEN), the recruited person will work on coupling two existing codes, one a logicial model developed by Inria to predict metabolic interactions within microbial communities, the other a nonlinear dynamical model developed by IFPEN to simulate biological and geochemical processes over time. Starting from collections of taxa identified by sampling or by literature search, and from nutritional constraints derived from the geological characteristics of each site, Inria's model will identify the biochemical functions that can be activated and potential interspecies interactions, in particuliar those that may produce biofilms. These results will be the entry point for IFPEN's numerical simulation of coupled biological-geological behavior, as well as sensitivity analysis. Forthermore, the combined workflow will make it possible to identify minimal microbial consortia, optimized for a given objective (reinforcement of geological barriers by biofilms, biocarbonatation, ...) thanks to the reasoning tools developed by Inria.

For better knowledge of the proposed research subject:

- 1. *Metage2Metabo, microbiota-scale metabolic complementarity for the identification of key species.* Belcour A, Frioux C, Aite M, Bretaudeau A, Hildebrand F, Siegel A. **eLife**, 2020, 9, ?10.7554/eLife.61968?
- Community-scale models of microbiomes: articulating metabolic modelling and metagenome sequencing. Cerk K, Ugalde-Salas P, Ghassemi Nedjad C, Lecomte M, Muller C, Sherman DJ, Hildebrand F, Labarthe S, Frioux C. Microbial Biotechnology, 2024, ?10.1111/1751-7915.14396?
- Inferring and comparing metabolism across heterogeneous sets of annotated genomes using AuCoMe. Belcour A, Got J, Aite M, Delage L, Collén J, Frioux C, Leblanc C, Dittami SM, Blanquart S, Markov GV, Siegel A. Genome Research, 2023, 33, pp.972 – 987. <u>10.1101/gr.277056.122</u>?
- Modeling acclimatization by hybrid systems: Condition changes alter biological system behavior models. Assar A, Montecino MA, Maass A, Sherman DJ. BioSystems, 2014, 121, pp.43-53. ? 10.1016/j.biosystems.2014.05.007?
- Interplay between microorganisms and geochemistry in geological carbon storage. Kirk MF, Altman SJ, Santillan EFU, Bennett PC. Int. J. Greenhouse Gas Control, 2016, 47, pp. 386-395. <u>10.1016/j.ijggc.2016.01.041</u>?
- Underground gas storage as a promising natural methane bioreactor and reservoir? Molíková A, Vít?zová M, Vít?z T, Buriánková I, Huber H, Dengler L, Hanišáková N, Onderka V, Urbanová I. Energy Storage, 2017, 47.?10.1016/j.est.2021.103631?
- 7. *Life on the Rocks*. Gorbushina AA. **Microbiology**, 2007, 9, pp. 1613-31. ? 10.1111/j.1462-2920.2007.01301.x?
- Enigmatic, ultrasmall, uncultivated Archaea. Baker BJ, Comolli LR, Dick GJ, Hauser LJ, Hyatt D, Dill BD, Land ML, Verberkmoes NC, Hettich RL, Banfield JF. Proc Natl Acad Sci U S A. 2010 May 11;107(19):8806-11. ? 10.1073/pnas.0914470107?
- Bacterial Calcium Carbonate Precipitation in Cave Environments: A Function of Calcium Homeostasis. Banks ED, Taylor NM, Gulley J, Lubbers BR, Giarrizzo JG, Bullen HA, Hoehler TM, Barton HA. Geomicrobiology Journal, 27(5), 444–454. ?10.1080/01490450903485136?

Collaboration : The recruited person will be in contact with experts from the IFPEN in phenomenological modeling in geological environments, and with Inria project-teams concerned with modeling biological systems.

Main activities

Main activities:

- **Perform numerical simulations**, analyze the results and identify microbial mechanisms of interest (biofilm formation, biocarbonatation, ...).
- **Develop and couple simulation tools** for modeling the behavior of microbial communities in the context of geological CO? storage
- **Contribute to the scientific promotion of the project**, through writing publications and reports, and participating in conferences

Additional activities:

- **Present** progress of ongoing work to colleagues and partners
- **Discuss** with scientific collaborators
- **Review** the scientific literature

Skills

Technical skills:

- Experience in software development and a willingness to adopt good software engineering practices.
- Experience in mathematical modeling and a willingness to improve models of biological and chemical systems.
- Optionally, knowledge of executing programs on high-performance computing or on Kubernetes platforms.

Languages:

• Ability to speak and write scientific English.

Relational skills:

- Ability to communicate with colleagues from the biological, chemical, and computer sciences
- Willingness to listen to and learn from these colleagues

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 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

The gross monthly salary will be $2788 \in$ (before social security contributions and monthly witholding tax).

General Information

- Theme/Domain : Computational Biology Scientific computing (BAP E)
- Town/city : Talence
- Inria Center : Centre Inria de l'université de Bordeaux
- Starting date : 2025-10-01
- Duration of contract : 2 years
- Deadline to apply : 2025-07-04

Contacts

- Inria Team : <u>PLEIADE</u>
- Recruiter : Sherman David / David.Sherman@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

We seek excellent candidates with a strong background in either numerical modeling or machine reasoning, and their implementation using good programming practice. An interest in interdisciplinarity will be necessary.

Experience applying these methods to biological systems in general, and microbial consortia in particular, would be appreciated.

A key goal of this work is decarbonisation and in general the Inria and IFPEN teams are heavily invested in adaptation to and mitigation of climate change. We actively seek candidates who are motivated by these challenges.

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

If you are interested by this job, please could you apply on website jobs.inria with the following documents :

- cv
- cover letter

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.