Doctorant F/H Simulation numérique d’écoulements multi-phasiques couplés à la température en LBM par un potentiel chimique

Contract type: Fixed-term contract

Level of qualifications required: Graduate degree or equivalent

Fonction: PhD Position

About the research centre or Inria department

The Inria Rennes – Bretagne Atlantique Centre is one of Inria’s eight centres and has more than thirty research teams. The Inria Center 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 PMEs, large industrial groups, competitiveness clusters, research and higher education players, laboratories of excellence, technological research institute, etc.

Context

Team Presentation

The project is jointly carried out by the I4S research team at Inria and the LMSF laboratory at CEA.

Inria: Inria is the French institute for research in digital science and technology. This public research center of scientific excellence is at the forefront of digital transformation in France. Research in computer science, mathematics, artificial intelligence (AI), software development, innovation in high-impact technological disciplines, and entrepreneurial risk (DeepTech) constitute the DNA of the institute. Inria is ranked 16th in the global AI Research ranking and is the first European institute for exploratory research in digital science.

I4S: The I4S team (Inferences for Structures) is a joint team between Inria and Gustave Eiffel University, specialized in Structural Health Monitoring (SHM), i.e. attempting to predict, categorize, locate, and quantify defects or damage that may appear in civil, electrical, (bio)-mechanical, energy, or aeronautical structures, etc.. To do this, it is necessary to combine multiple data and expertise, such as numerical physical simulation, data processing, sensor development, embedded electronics integration, statistical uncertainty propagation, etc.

CEA: The French Alternative Energies and Atomic Energy Commission (CEA) is a French research and development organization dedicated to energy, defense, and emerging technologies. Its research covers a wide range of fields, from nuclear and quantum physics to renewable energies, significantly contributing to technological advances and understanding contemporary issues.

LMSF: Within the Department of Modeling of Systems and Structures (DM2S), the Thermohydraulics and Fluid Mechanics Service (STMF) specializes in the design, development, and qualification of simulation software in thermohydraulics and fluid mechanics, adapted to reactors and nuclear installations, as well as processes related to the fuel cycle. It also conducts experimental programs to support the understanding of phenomena and validate the physical models of software, while performing studies and expertise for nuclear and energy applications. The Laboratory of Modeling and Simulation in Fluid mechanics (LMSF) develops numerical methods and calculation codes related to fluids, transfers, and thermodynamics.
General Context

Numerical simulation of multi-phase flows coupled to temperature in LBM by a chemical potential CEA and Inria study multiphase flows in porous media interacting with the porous matrix and temperature field. These flows are inherently more complex to solve due to the nature of the phenomena involved: thermo-mechanical coupling, interface mobility, high density ratio, and so on. However, such flows are of great interest as they are encountered in applications related to energy production, energy management in cities, and for the health diagnosis of porous structures.

On the other hand, the Lattice Boltzmann Method (LBM) [2] is a numerical method that allows the simulation of physical problems modeled by partial differential equations, such as those involved in crystal growth, fractional equations, and fluid flows. The basis of the method is to perform a collision step followed by a displacement step of a distribution function on a regular Cartesian grid. This algorithmic simplicity gives the method good numerical properties, such as good scalability and ease of coupling.

The LBM method has been implemented in a C++ code at CEA: LBM_saclay [4]. It is dedicated to simulating multiphase flows with or without liquid-gas phase change and is executable on different hardware architectures (multi-CPUs and multi-GPUs) [5]. In parallel, Inria has implemented different calculation codes developed in Python and Fortran for liquid-solid or liquid-gas phase change coupled with temperature.

Among the techniques used by LBM to understand multiphase flows, two categories of approaches stand out: phase field approaches and pseudo-potential approaches. Phase field approaches have the advantage of being less sensitive to large density ratios and are theoretically justified from Landau's free energy, allowing easy integration with theoretical and numerical tools in the chemical industry. However, they are more numerically demanding, as they rely on an additional equation (such as the Allen-Cahn equation) and its coupling. This approach is currently used by CEA.

Pseudo-potential approaches have the advantage of being less computationally demanding, as they do not require an additional equation, and offer natural coupling with temperature [3]. Nevertheless, these approaches are more sensitive to large density ratios and are more difficult to justify in terms of free energy (without the addition of an additional term), making them less easily integrated with chemical processes. This approach is used by the I4S team at Inria.

At the interface between these two approaches, another category has emerged in recent years. In parallel, a new category of method for multiphase flows in LBM is beginning to emerge: the use of chemical potential [1, 6]. These approaches derive free energy to obtain the chemical potential that can be related to the phase field and then replaces the pseudo-potential in terms associated with the pressure tensor.

This approach, although interesting as it represents a compromise between the previous approaches, remains subject to many developments. This thesis proposes to focus on multiphase flows in LBM using chemical potentials during thermal couplings. Furthermore, Physically Informed Neural Networks (PINN) integrate physical knowledge into their architecture and provide a powerful framework for modeling complex phenomena in multiphase flows. Thus, once trained with an LBM solver, a PINN will be able to simulate, accurately and very efficiently, direct and inverse problems encountered in the teams of Inria and CEA.

References
Main activities

Thesis Objectives and Directions
— A first part, inherent to the thesis work, will be to acquire a detailed understanding of multiphase flows using the LBM method and chemical potential approaches from the literature. This understanding will also involve getting familiar with the LBM_saclay calculation code and practical experimentation.
— Next, the student will address multiphase problems (solid-liquid-gas) through thermal (or enthalpic) coupling and a possible adaptation of the equation of state.
— This extension will be accompanied by an interaction loop between the proposed model and implementations in LBM_saclay tools.
— Special attention will be given to the thermodynamic consistency and surface tension of the proposed model from both theoretical and numerical perspectives (with error terms).
— Benchmarking will be conducted to study stability criteria, precision, computation time, and scalability of the proposed method.
— The model will then be used for solving direct problems as well as inverse problems through its incorporation into PINNs. Depending on the candidate’s interests, several extensions will be possible, such as refining the chemical potential in terms of fugacity, integrating simple chemical reactions, binary (or ternary) liquid equilibrium, or integrating numerical acceleration methods in AI.

Skills

Technical skills and level required:

Languages:

Relational skills:

Other valued appreciated:

Benefits package

- Subsidized meals
- Partial reimbursement of public transport costs
- Possibility of teleworking (90 days per year) and flexible organization of working hours
- Partial payment of insurance costs

Remuneration

Monthly gross salary amounting to:
- 2082 euros for the first and second years and
- 2190 euros for the third year

General Information

- Theme/Domain: Optimization and control of dynamic systems
- Scientific computing (BAP E)
- Town/city: Rennes
Starting date: 2024-10-01
Duration of contract: 3 years
Deadline to apply: 2024-02-21

Contacts
- Inria Team: I4S
- PhD Supervisor: Noel Romain / romain.noel@irisa.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
There you can provide a “broad outline” of the collaborator you are looking for what you consider to be necessary and sufficient, and which may combine:
- tastes and appetencies,
- area of excellence,
- personality or character traits,
- cross-disciplinary knowledge and expertise...

This section enables the more formal list of skills to be completed and ‘lightened’ (reduced):
- “Essential qualities in order to fulfil this assignment are feeling at ease in an environment of scientific dynamics and wanting to learn and listen.”
- “Passionate about innovation, with expertise in Ruby on Rails development and strong influencing skills. A thesis in the field of **** is a real asset.”

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
Please submit online: your resume, cover letter and letters of recommendation eventually
For more information, please contact romain.noel@irisa.fr

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.