Multiscale Modeling of Thermally Induced Damage in Cement-Based Materials

Supervisors:

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Introduction

Cement-based materials and concrete in particular are the most widely used building materials and their global daily consumption is second only to water. Despite extensive research on mechanical properties and durability, the vulnerability to explosive spalling under high temperatures is a critical yet often underestimated aspect. This Ph.D. position aims to address this gap by delving into the small-scale mechanisms governing thermally induced damage in cement-based materials (CBM) using advanced molecular modeling and simulations.

Project Overview

The project will focus on investigating the complex phenomenon of spalling, which involves the detachment of concrete layers exposed to elevated temperatures. This poses a significant risk to structural integrity, as it reduces the working cross-section of the material and exposes reinforcements, potentially leading to structural failure. The research will specifically target the interplay between thermal load, evolving moisture content, and changing permeability at the fundamental level — a dimension often overlooked in traditional structural design.

Research Objectives

The primary objectives of this Ph.D. position include:

1. Developing a molecular-scale approach to enhance insights into the physics of water dynamics and structural/chemical transformations in CBM.

2. Quantifying the dehydration process in cement paste upon heating, with a focus on microstructural changes and water mass loss within the porous structure of Calcium-Silicate-Hydrate (C-S-H), the main phase of hydrated cement.

3. Investigating the role of interlayer water and interfacial adsorbed water at grain surfaces of C-S-H in the dehydration process at high temperatures.

Methodology

The research will employ molecular simulations to provide inputs for a mesoscale model, bridging the gap between molecular and continuum modeling. This integrated approach is essential for capturing the multiscale hierarchical nature of the C-S-H gel and its porosity network. Molecular simulations will offer critical insights that conventional experimental techniques cannot provide, informing macroscopic constitutive relationships and overcoming the limitations of numerical continuum-based models.

Duration and localisation

The duration of this Ph.D. program is three years, starting in the fall of 2024 and will be based at the 3SR laboratory in Grenoble.

Collaboration and Funding

This Ph.D. position is part of the broader project funded by the financial support of the French National Research Agency (ANR) via the project ANR "MULTI-FIRE" (See Figure 1). The research will be conducted in the 3SR laboratory, which has acquired strong expertise in advanced experimental techniques such as neutron and X-ray imaging. These techniques are essential for understanding the micro-scale mechanisms underlying spalling. Our research team combines simultaneous Neutron and X-ray Tomography (See Next) developed at Institut Laue-Langevin (ILL). This infrastructure enables us to validate and improve our model's predictions at the local scale by comparing entire 5D fields (3D+time+X-ray/neutrons).

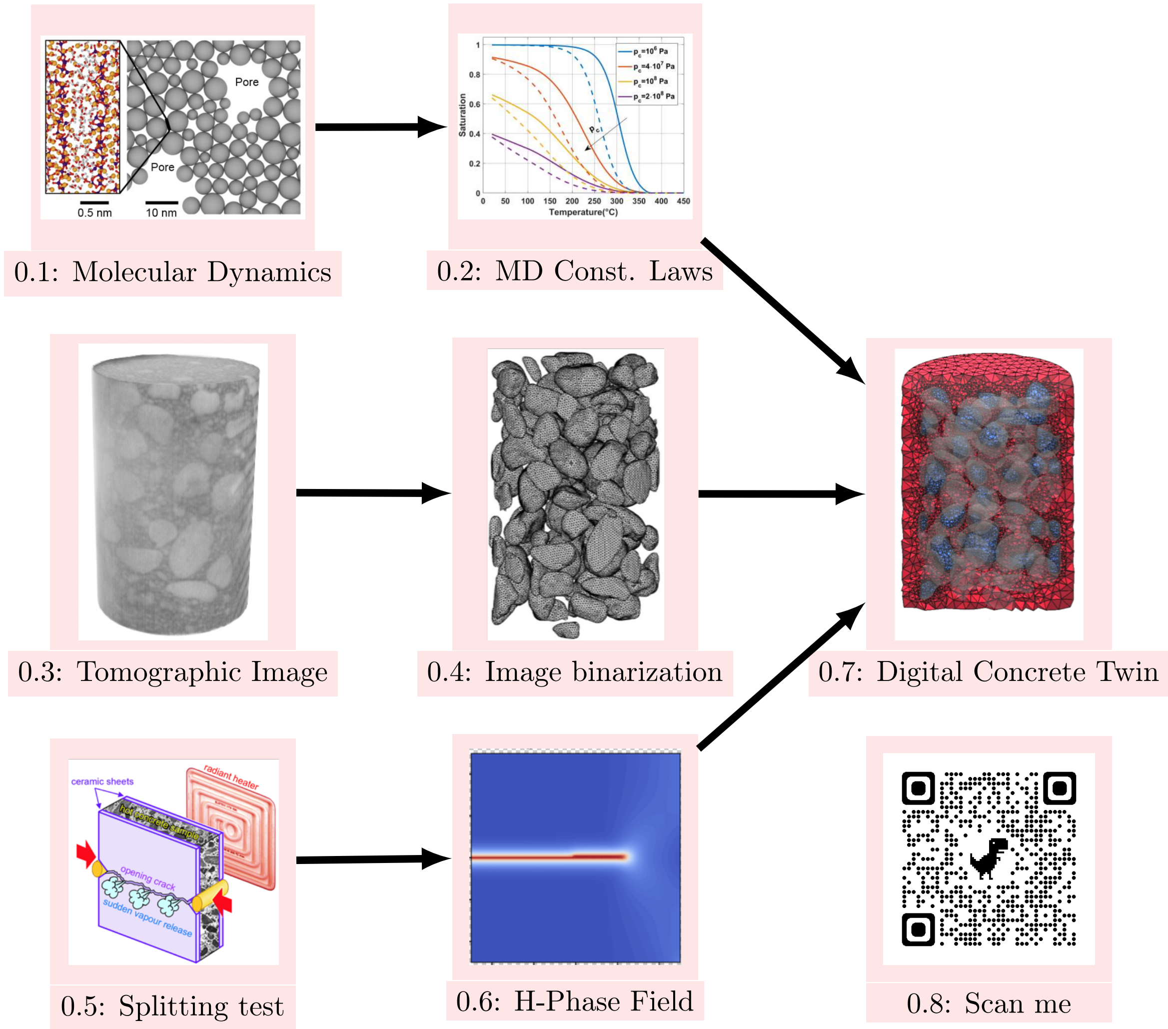

Figure 1: General scheme of the "MULTI-FIRE" project (QR code loads a Youtube movie)

Requirements

Candidates with a Master's degree in Physics, Materials Science, or a related field are encouraged to apply. While a background in molecular modeling and simulations is appreciated, it is not mandatory. The key requirement is a strong motivation to learn and a keen interest in investigating the physics of materials under extreme conditions.

Why Join Us

Engage in a project characterized by a multifaceted approach, incorporating both experimental and modeling components across various scales—from nano to material. The initiative is enriched by the wealth of information facilitated by cutting-edge technological advancements. The project benefits from a diverse range of expertise, spanning from experimental proficiency including high temperature In-Situ SEM Micro-mechanical testing to thermo-hydro-mechanical modeling of concrete at high temperatures incorporating molecular simulations and upscaling approaches.

The 3SR laboratory, with the support of the Université Grenoble Alpes, has developed a unique instrument named NeXT (Neutron and X-ray Tomograph), relying on the world's highest cold neutron flux provided by the Institut Laue-Langevin (ILL). This groundbreaking setup is crucial for capturing inherently rapid processes with meticulous spatio-temporal detail. Beyond the unique imaging apparatus, the group has developed in-situ testing equipment and image analysis protocols, enabling the quantification of fundamental processes.

Application Process

Interested candidates are invited to submit their CV, a cover letter detailing their research interests and relevant experience, and contact information for two referees to Dr. Majdouline Laanaiya - majdouline.laanaiya@univ-grenoble-alpes.fr or/and Pr. Stefano Dal Pont - stefano.dalpont@univ-grenoble-alpes.fr **before March 31st, 2024**. Interviews will be scheduled shortly thereafter.