



**Laboratoire
Hubert Curien**
UMR • CNRS • 5516 • Saint-Étienne

PhD Fellowship Research Proposal

Multi-scale modeling of ultrafast laser-driven thermofluid flows for nanostructure reshaping

Host Institution: Hubert Curien Laboratory (LabHC) in Saint-Etienne, France.

The Hubert Curien Laboratory is a joint research unit (UMR CNRS 5516) of the Jean Monnet University, Saint-Etienne, the National Research Centre "CNRS" and the Institut d'Optique Graduate School. It is composed of 90 researchers, professors & assistant professors, 25 engineers & administrative staff, and around 110 PhD & post-PhD students. This total of approximately 230 staff makes the Hubert Curien laboratory the most important research structure in Saint-Etienne. Our activities are organized around two scientific departments: Optics, Photonics & Surfaces and Computer Science, Security & Image, and scientific projects are carried out by 7 main teams: Functional Materials and Surfaces, Materials for Optics and Photonics in Extreme Radiative Environments, Laser-Matter Interaction, Photoinduced Reactive Dynamics in Computational Theory, Image Science & Computer Vision, Data Intelligence, and Secure Embedded Systems & Hardware Architectures <https://laboratoirehubertcurien.univ-st-etienne.fr/en/the-lab/edito.html>

Funding: French National Research Agency ANR, ~3500 € gross/month salary, 36-month fellowship

Expected date to start: January 2027

Subject:

Objectives. Within ULTraFlow project (Optimizing Ultrafast Laser-driven Thermofluid Flow for nanofabrication of arbitrary 3D curved nanostructures), PhD fellow will be responsible for developing an efficient computational tool to predict ultrashort laser-induced modifications in surface nanostructures and to identify governing mechanisms at sub-100 nm scales. The project will introduce a new methodology that couples ultrafast near-field absorption, heat transfer and phase transitions, addressing light, heat and energy confinement at the nanoscale, in all-in-one unified multi-physical and multi-scale approach. As a final product, ULTraFlow will deliver novel strategies to control and optimize nanofabrication processes beyond the conventional surface nanostructures, towards structures with irregular 3D nanoscale curvature, that are urgently needed as components for multi-functional metasurfaces, particularly difficult to fabricate or to adjust with conventional methods.

Context. In the era of extreme miniaturization, the continued progress of nanotechnologies requires fabrication approaches capable of controlling matter at ever smaller spatial and temporal scales while remaining scalable and economically viable. Ultrashort lasers, having pulse duration shorter than characteristic scales for heat transport and fluid flow (< 10 picoseconds), can act as an efficient operational and control tool for nanostructure fabrication and reshaping because the laser irradiation provides necessary conditions for light, heat & energy confinement and phase transitions at extreme spatial scales but also an ability to control precisely over the fabrication process by spatio-temporal shaping of the laser beam [1]. This makes it possible to selectively reshape, adjust or fabricate nanostructures with minimal collateral damage to surrounding material. Furthermore, laser-induced optical near-fields of nanostructures can naturally concentrate electromagnetic energy beyond the diffraction limit in specific shapes, fully controllable by key laser parameters, such as laser wavelength, polarization of light, and angle of incidence [2]. Thus, setting a specific optical field distribution allows manipulating the temperature gradients, directed melt flow, and local phase transitions at the nanoscale, that result into permanent modifications after cooling and resolidification on sub-microsecond scales.

Reaching towards ultimate nanoscale features beyond the diffraction limit for visible light (< 250 nm) and with 3D arbitrary designs, however, relies more and more on fundamental understanding and predictive modelling of multi-physical processes at nanoscale. Currently, there is no unified theoretical framework that can rigorously and efficiently couple multi-physics of ultrashort laser-matter interactions on all relevant spatial and temporal scales. Within ULTraFlow project, PhD student will attempt to address the modifications occurring on particularly challenging spatial scales (few tens-few hundred nanometers), incompatible with standard ab initio/atomistic simulations but richer in phenomena than the macroscales, representative in computational fluid dynamics. In particular, the challenge consists in pushing the continuum Navier-Stokes (N-S) equations beyond its validity, requiring corrections for large Knudsen numbers, slip boundary conditions, non-Fourier thermal transport and stochastic models for fluctuating hydrodynamics. These effects are dynamically important for fluids undergoing phase transitions, cavitation, hydrodynamic instabilities, since the nonlinearities can exponentially amplify the relevant nanoscopic forces. The fluctuation effects could be considered as nonlocal corrections within multi-phase N-S model [3], affecting the amplitude and the anisotropy of the effective thermal conduction, shear viscosity and flow rate, all dependent on the size of confinement. These methods were successfully applied to describe phase transitions at nanoscale [3] but haven't been applied yet to complex 3D nanostructure geometries. Another challenge consists in trying to handle highly nonequilibrium multi-phase interfacial dynamics, which requires specific interface tracking methods, such as diffuse-interface (phase-field) [4] that have been routinely applied to describe mixing of two incompressible fluids but rarely for compressible fluid dynamics with embedded equation-of-state. Within this approach, particular attention should be paid to introduce and evaluate interfacial nanoscopic forces, such as surface tension-driven capillary and Marangoni forces, driving reshaping by melt flow at the relevant temporal scales. Finally, a comparative test study will be performed between simulation results provided by both approaches: atomistic molecular dynamics (MD) and extended fluid dynamics, implementing stochastic fluctuations and diffuse-interface tracking at the frontier of particulate and continuous descriptions.

References:

- [1] R. Stoian, & J. Bonse, "Ultrafast laser nanostructuring: the pursuit of extreme scales". Vol. 239, Springer Nature (2023).
- [2] M. Aeschlimann et al., "Adaptive subwavelength control of nano-optical fields". Nature, Vol. 446, 301-304 (2007); S. V. Makarov et al., "Light-Induced Tuning and Reconfiguration of Nanophotonic Structures". Laser Photonics Rev. 11, 1700108 (2017); M. R. Shcherbakov et al., "Nanoscale reshaping of resonant dielectric microstructures by light-driven explosions". Nat. Comm. 14:6688 (2023).
- [3] (1) A. Chaudhri et al., "Modeling multi-phase flow using fluctuating hydrodynamics". Phys. Rev. E 90, 033014 (2014); (2) M. Gallo et al., "A nanoscale view on the origin of boiling and its dynamics". Nat.

Comm. 14, 6428 (2023); (3) J. Schwarz et al., “An OpenFOAM solver for the extended Navier-Stokes equations”. SoftwareX 22, 101378 (2023).

[4] E. M. Adebayo et al., “A review of diffuse interface-capturing methods for compressible multi-phase flows”. Fluids 10, 93 (2025); J. Kim, “A continuous surface tension force formulation for diffuse-interface models”. J. Comput. Phys. 204, 784-804 (2005).

Keywords:

Laser-matter interaction; Multi-physical Modeling; Computational Fluid Dynamics; Molecular Dynamics; Ultrashort Laser; Phase Transitions; Nanofabrication; Nanostructuring

Candidate Profile:

The ideal candidate holds a Master's degree (MSc or equivalent) in Physics, Materials Science, or related fields. The following skills and background are expected:

- Strong knowledge in computational fluid dynamics and thermodynamics
- Experience with programming languages (Python, MATLAB, or C++) and ability to develop and to test its own code involving discretized equations
- Proficiency in written and spoken English
- Background in laser-matter interactions and thermodynamics, basic knowledge of Navier-Stokes equations and finite volume methods, is a plus
- Experience with computational fluid dynamics or atomistic open-source codes/simulations (e. g. OpenFOAM, LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) or others) is a big plus, but not mandatory
- Familiarity with machine learning and parallel programming (OpenMP, MPI, or GPU) is a plus
- Experience in writing/editing/preparing the manuscripts for a publication could be also a plus

The candidate is expected to be motivated to work in a multidisciplinary and international environment, participate, present and describe the research results in national workshops and international conferences, demonstrate initiative and autonomy in order to successfully complete his/her thesis.

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Interested candidates should provide (1) an updated CV with the detailed education background and professional skills, (2) a short motivation letter, (3) a transcript with the detailed courses taken and grades received for a Bachelor's/Master's degrees, (4) 1-2 professional/academic references.
