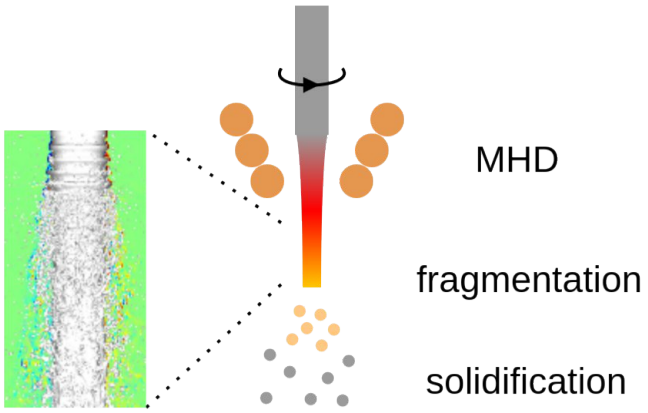
Developing multiphysics VOF DNS for the fragmentation and solidification of low-Prandtl jets

Context and work environment



Context Laser Powder Bed Fusion (LPBF) is an advanced additive manufacturing process, critical from medical implant production to aerospace applications, whose accuracy and relevance ultimately rely on the quality of the metallic powder to be melted. The properties of the material manufactured via LPBF directly depend on the powder flowability, governed by the size and the sphericity of the solid particles. Metallic powders are commonly produced by gas-assisted atomisation of liquid metal jets, but the dispersion of the size and sphericity of the resulting droplets is not sufficiently controlled yet. A better understanding of the balance between interfacial dynamics and the cooling and solidification dynamics is necessary to complement the scarce literature on the fragmentation, cooling, and solidification of liquid metal (low-Prandtl) jets.

The objective of this PhD project is to bridge the gap in simulating the multiphysics of liquid metal jet fragmentation, from the inductive melting of the feedstock to droplet solidification, including primary and secondary atomization as well as heat transfers between the continuous and dispersed phases. The PhD student will conduct numerical investigations on High-Performance Computers (HPC) to run Volume-Of-Fluid (VOF) Direct Numerical Simulations (DNS) and generate data necessary for deciphering the microphysics at play. A specific focus will be put on deriving the droplet statistics (size, velocity, shape, temperature) as well as the scaling laws that govern droplet cooling. Efforts for building numerical solvers able to describe phase change and tackle droplet solidification will be carried out, leveraging and taking part in the community work around the state-of-the-art open-source solver Basilisk.

Team description The PhD will take place within two Tec21 labs located on the Grenoble campus:
- Engineering Science for Material Processes lab (SIMaP), specifically the EPM team, which conducts research on bulk and interfacial liquid metal flows as well as crystal growth and inductive melting,
- Geophysical and Industrial flows lab (LEGI), specifically the EDT team, which has a strong and broad expertise in multiphase and turbulent flows, both experimentally and theoretically,

and will benefit from collaborations with Clélia Couchet (SIMaP, GPM2 team) whose research focuses on the derivation of operating parameters set to produce well-controlled metallic glasses via LPBF. The project will also benefit from the theoretical and numerical expertise of Olga Budenkova (SIMaP) on inductive melting flows and of an experimental liquid metal fragmentation set-up, developed by the PIs with the support of A. El Bakali (lead engineer, SIMaP), that will be used as a benchmark for the numerical developments.

The PhD will be supervised by Romain Vallon (SIMaP), expert in DNS of multiphase flows on HPC and in modelling interfacial flows as well as fluid particle statistics, and Nathanaël Machicoane, expert in imaging techniques and their quantitative processing (e.g., sizing, tracking, and velocimetry), with a strong theoretical background on fragmenting jets, turbulence, and interfacial transfers. This team brings together a wide range of expertise in the physical mechanisms relevant to the fragmentation of liquid metal jets and LPBF powder manufacturing.

This recruitment takes place within the PhD@Tec21 Programme, which is co-funded as part of the Marie Skłodowska-Curie COFUND actions under the grant agreement #101217261. The recruitment process follows a specific selection and evaluation procedure with particular eligibility criteria, all of which are detailed in the applicant guide available on PhD@Tec21 Website.

Mission and main activities

Developing multiphysics VOF DNS for the fragmentation and solidification of low-Prandtl jets

Description of the project:

Direct Numerical Simulations (DNS) will be run on High-Performance Computers (HPC) to explore the fragmentation dynamics of low-Prandtl jets, from the melting of the metal rod to the solidification of the droplets, and assess the influence of the Prandtl and Weber non-dimensional numbers, given by:

$$\mathrm{Pr} = \frac{\nu}{\alpha} = \frac{\text{momentum diffusivity}}{\text{thermal diffusivity}} \quad \text{and} \quad \mathrm{We} = \frac{\rho_g U^2 d}{\gamma} = \frac{\text{inertial force}}{\text{surface tension}}$$

with ρ_g the gas density, d the jet nozzle diameter and U the jet velocity. **The following research axes will be explored:**

1. Characterisation of the jet flow conditions resulting from the inductive melting. The inductive melting flow will be characterised numerically by solving the two-way coupling governing the magnetohydrodynamics (MHD) flow using finite-element Elmer (magnetic field and induced current) and finite-volume OpenFOAM (melting flow) open-source software.

2. Exploration of the cooling dynamics of fragmenting jets. The heat transfer occurring during the jet fragmentation at low-Prandtl number ($\mathrm{Pr} \approx 10^{-1}$), without solidification, will be studied numerically via 3D Volume-Of-Fluid DNS on HPC, using the open-source solvers from the Basilisk community. A statistical analysis will be carried out to characterise the droplet population. This will be complemented by DNS of a fragmenting single droplet to observe the temporal dynamics of cooling and derive the corresponding scaling laws.

3. Development of a numerical framework to model droplet solidification. Dedicated numerical solvers will be developed to run DNS of solidifying droplets in a gas phase. Solvers simulating two-phase front solidification and three-phase flows are available in the Basilisk community and will be taken as a starting point. Based on the solver developments, jet fragmentation DNS with solidification will be computed. The statistical analysis will be repeated and complemented with theoretical work to infer a statistical model for the size and sphericity distribution of the resulting solid particles.

Depending on the candidate's background and specific interests, the PhD may choose to focus more on one or two of those research axes, although all three are important for the project.

Supervisors: Romain Vallon and Nathanaël Machicoane
Research fields: multiphase fluid mechanics, heat transfer, fragmentation, Direct Numerical Simulations
Possible secondments: AIA (RWTH Aachen, Germany), Unit of Processes (KTH, Sweden), Sandvik AB (Sweden)
Doctoral school: I-MEP2 (Engineering - Materials, Mechanics, Environment, Energy, Processes, Production)

Video links for gas atomization (in the lab and on an industry pilot):
https://www.youtube.com/watch?v=EYROdI5eKSk
https://www.youtube.com/watch?v=vklq_1vCktk

Desired profile and expected skills

Education, diplomas

The candidate should have graduated from a MSc (or equivalent) in Applied Science or Engineering with a background in one or more of the following fields: Fluid Dynamics, Physics, Mechanical Engineering or Applied Mathematics. Ideally with knowledge in two-phase flows, heat transfer and /or phase change.

Disciplinary skills, experience

Experience of scientific computing, numerical schemes, large data set analysis and HPC computing will be appreciated. Coding skills without LLMs (large language models) and knowledge of Python are mandatory. Knowledge of C++, bash programming, large data set management and code versioning is a plus. Technical English (speaking, writing and reading skills) are required.

Personal skills

This PhD position requires to be able to work in a group and to have a strong autonomy, solid critical thinking as well as good organisational and interpersonal skills. The candidate will be required to lead numerical investigations, carry out data analysis and manage large set of data rigorously, along with assimilating new knowledge quickly. They should also show perseverance and solid problem-solving skills while scientific curiosity, to make the project moves forward, will be acknowledged and encouraged. Strong communication and reporting skills (written and oral), both on the project's progress and the difficulties encountered, are expected. Being able to disseminate scientific results to a large audience in an educational manner will be appreciated.

Employment benefits and conditions

Université Grenoble Alpes (UGA) is offering a 36-month full-time work contract.
In line with the European Commission rules for Marie Skłodowska-Curie grant holders, the remuneration will consist of a gross monthly salary of 2,669 EUR. The estimated net salary to be perceived by the PhD fellow will be between 2,050 and 2,152 EUR[1].

Benefits include:

- Access to a high-quality work environment, including a personal computer, scientific equipment, HPC clusters, and access to library and shared lab facilities
- Access to high-level scientific and inter-sectoral training through 120 hours of doctoral courses and workshops
- Opportunity for 2-month secondments at an academic institution or industrial partner during the 2nd year of the PhD
- A vast choice of networking events and activities within the PhD@Tec21 Programme and through the international network of MSCA fellows
- Access to the UGA International Student Office, to assist the PhD fellows in searching for accommodation in Grenoble and support with administrative issues including visas, health, bank accounts, etc.
- Visa fees and registration to the UGA Doctoral School are covered by PhD@Tec21
- 45 days of paid holidays
- Sick leave
- Parental leave

General information

Contact for questions related to the position:

PhD@Tec21 Management Board:
guillaume.chambon@univ-grenoble-alpes.fr / amelie.bataille@univ-grenoble-alpes.fr

[1] As an average over the 3 years, depending on French tax regulations. Fellows might benefit from an additional allowance depending on their family situation (74 EUR monthly net allowance)