# EU-DOCS for SmUCS

## CO-SUPERVISED SUBJECT PROPOSAL FOR A DOCTORAL CONTRACT

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| **Title of the thesis project**<br><br>Fast simulation of particle flows for the next generation of green energy systems | |
| **La Rochelle University Research Unit**<br><br>Laboratoire des Sciences de l'Ingénieur pour l'Environnement (LaSIE) | **Partner university**<br>University of Seville (Spain)<br>**Cotutelle research unit:**<br>IMUS (Institute of Mathematics of the University of Seville) |
| **Name of the LRUniv supervisor**<br>Cyrille ALLERY | **Name of the co-supervisor**<br>Samuele RUBINO |
| **Non-academic partner**<br><br>Virtualmechanics S.L. (Seville, Spain) | |
| **Main research field:** Numerical Fluid Mechanics<br><br>**Secondary research field:** Applied Mathematics | |
| **Keywords:** Reduced Order Model, Computational Fluid Dynamics, Multiphase flows, Heat transfer, Mathematical and Numerical Modeling, Green Energy. | |

**Scientific description of the research project**

The simulation of particle flows is generally used in the design and optimization of solar thermal receivers, transport and storage systems, and the corresponding fluidized beds and reactors. These applications usually need numerical simulation technology that allows, with precision and controlled computational cost, to understand their behavior in terms of energy transfer and flow evolution. Therefore, an effort will focus on the simulation of these flows with different computational techniques such as CFD (Computational Fluid Dynamics) or model reduction technique.

The mathematical modelling of the solid phase (e;g particle) is based on kinetic theory of gases, with several approaches. There is a type of alternative models that take into account conservation principles only for the fluid phase. The effect of the particles on the fluid phase is modelled through a special rheology, in which the viscosity depends on the volume fraction of the solid phase. This is the case for example of the SIM model -Shear Induced Model- by Phillips, that we intend to pursue as main objective in the present thesis project.

In the thermal fluidized bed model SIM, the action of particles in a fluid with a suspension at high solid volume fractions is formulated through a variable dynamic viscosity, where the transport velocity is that of the suspension. This model can be extended by adding the energy conservation equation to turbulent thermal flows, which is one of the main scientific challenges we will pursue in this thesis project. On the other hand, it is proposed to model the sub-mesh effects using Variational Multi-Scales (VMS) type models, which will allow the use of coarser meshes and reduce calculation times. The IMUS team has several decades of experience in VMS models and models for turbulent flows.

The proposed numerical model addresses the need to solve efficiently large systems of algebraic equations by iterative methods. Thus, apart from taking advantage of parallel computing environment both at La Rochelle and IMUS, we propose the use of Reduced Order Models (ROMs) to address the design and operational optimization of the fluidized bed thermal system. ROMs achieve reductions of several orders of magnitude in computational times. In the case of turbulent flows, the proportion in the reduction of computational time is typically two orders of magnitude. Techniques such as High Order Singular Value Decomposition (HOSVD), Proper Generalized Decompisition (PGD), or Radial Basis Function (RBF), construct the parametric solution as a tensor function that separates the dependence on the parameters from the dependence on the spatio-temporal variables. Another possible approach is to write the parametric solutions in reduced form and then interpolate (according to the parameter dependence) them using reduced basis interpolation techniques based on geodesics on the Grassmann manifold (such as the Bi-ITSGM method, for example). The IMUS team and LaSIE team have a decade of experience in approximating PDEs and parametric functions by reduced order models. In addition, the IMUS and Virtualmechanics groups are participating in a European project on reduced-order modelling for industrial problems: H2020-ARIA "Accurate Reduced Order Models for Industrial Applications", together with R&D centres and companies such as INRIA (France), SISSA (Italy) and Volkswagen (Germany). Furthemore, in previous work, the LaSIE group, in collaboration with the University of Gdańsk, has investigated the dispersion of solid particles in turbulent flows by means of reduced-order modeling. In that study, a one-way coupling assumption was adopted, whereby the particles were considered to have no feedback effect on the carrier flow. The present objective is to extend this framework to the more complex regime of two-way coupling, in which particle–flow interactions are explicitly accounted for. Such an extension is inherently non-trivial and presents substantial challenges, as only a very limited number of studies addressing this problem are currently available in the literature.

**PhD student profile and skills required**

The candidate must have a strong background in applied mathematics and fluid mechanics. In particular, they should be proficient in numerical methods (finite elements, finite volumes, etc.) and their applications to turbulent flows coupled with heat transfer.

Knowledge in model reduction, machine learning, or multiphase flows would be a valuable asset for undertaking this PhD.

Skills: Numerical and mathematical modelling, fluid mechanics, numerical simulation, turbulent flows, heat transfer, machine learning.

**Scientific alignment with EU-DOCs for SmUCS objectives**

To reduce the impacts of climate change and the dramatic consequences that result from it, it is necessary to decrease the use of fossil fuels and increase the reliance on renewable energies, particularly solar energy. The development of new technologies to enhance solar energy production, transport, and storage is therefore crucial. This thesis work contributes to this endeavor and aligns with SmUCS objectives. Indeed, the aim of the thesis is to develop rapid simulation methods for particle-laden flows, which are fundamental to solar thermal receiver systems and energy storage systems. These simulations will, on the one hand, improve the understanding of their behavior in terms of energy transfer and flow evolution, and, on the other hand, optimize solar energy production and its storage capacity.

**Societal and economic challenges and contributions**

The present research project will contribute to the environment and to the improvement of the quality of life due to its orientation to the next generation of green energy. By achieving the objectives described in this document, we will also contribute to technological innovation, generating new methods for the numerical simulation of fluidization and heat transfer processes, which will drive the development of efficient and precise flow simulation techniques (CFD and reduced order models), and this will allow a deeper understanding of mass and energy transport processes, opening new lines of research in thermodynamics and heat transfer.

**Partnership context**

The thesis will be carried out under a joint supervision agreement between the University of La Rochelle and the University of Seville, in intensive collaboration with the company Virtualmechanics S.L. The PhD student will spend several periods at the company for a total duration of three months. He will spend at least 6 months at University of Sevilla.

**La Rochelle Université:**
The thesis will take place at Laboratoire des Sciences de l'Ingénieur pour l'Environnement (LaSIE), UMR CNRS 7356, La Rochelle Université. (https://lasie.univ-larochelle.fr). The LaSIE brings together a wide range of expertise with integrated approaches from the atomic scale to materials, buildings, and their environments, across different time and spatial scales. It establishes a continuum from the development of mathematical tools to applications, through numerical models, simulations, and experiments. The doctoral student will be affiliated with the M2N team (Mathematical and Numerical Methods for Transfer Phenomena), whose work focuses on the development of mathematical and numerical models in mechanics in general, and transfer phenomena in particular. The researcher contributing to this project is recognized for their work on fluid flow simulation, model reduction (POD, PGD), interpolation of reduced bases, and optimization using reduced-order models.

**University of Seville:**
The thesis will be developed in cotutelle with the "Mathematics" PhD Program of the University of Seville, within the research line "Theoretical and Numerical Analysis of Partial Derivative Equations", to which the proposed director of the thesis from the partner academic side (Samuele Rubino) is assigned. The completion of the thesis will have the material means and administrative support of the IMUS, as well as the supercomputing service of the IMUS. It will be carried out in the scientific environment provided by the Research Group FQM120 of the Junta de Andalucía. Thus, the PhD candidate will complete his training by means of academic courses, seminars and congresses organized at IMUS. In addition, we intend to take advantage of the technology transfer service of IMUS at the time of communicating the project results.

**Virtualmechanics S.L.:**
Virtualmechanics comprises a highly specialized technical team that has extensive knowledge on the different sectors of the industry, such as railway and solar thermal energy industries. The unique Value Proposition is offering VM's clients real results to difficult problems, always adapted to their specific issues. VM achieves these results thanks to data gathering through simulation or experimental measurements offering an effective decision based on objective criteria.

VirtualMech: Technological Expertise in Energy and Transportation

- VirtualMech is a technology-based company with 15 years of experience in the energy and transportation sectors. It specializes in R&D+i and highly specialized engineering for the concentrated solar power (CSP) industry, the broader energy sector, and railway track monitoring systems. The company applies system dynamics modeling and computational fluid dynamics (CFD) tools to these areas to deliver cutting-edge solutions that combine mechanical engineering advancements with interdisciplinary knowledge.

Core Activities

- Energy Industry Solutions: Simulation, analysis, and design of critical components for renewable energy systems, energy storage, and high-temperature technologies, including thermochemical reactors.
- Root Cause Analysis: Investigating failures in critical energy equipment using CFD and FEA simulations.
- Digital Twins: Development of digital replicas for critical components and hybrid renewable plants for electricity, thermal energy, and hydrogen production (multi-generation and multi-demand systems).
- Ad-hoc Software & Hardware Development: Embedded systems for critical operations in energy and transportation sectors.
- Data Science, AI, and Computer Vision: Automated inspection systems using drones and AI-driven tools for solar plants.

R&D Focus Areas

1. Critical Components for CSP and Energy Storage Systems: Next-generation technologies for efficiency and sustainability.
2. Digital Twin Technology: For operations, maintenance, and hybrid plant simulations supporting bankability and control.
3. Advanced CFD Modeling: For complex flows, including turbulence, particle-laden flows, fluidized beds, and multiphase systems with heat transfer.
4. Hybrid Renewable Systems: For heat and cooling generation in industrial settings, urban districts, and large infrastructures.
5. Thermochemical Energy Storage: High-temperature and medium-temperature systems for industrial and process heat applications.
6. Automated Solar Plant Inspections: Leveraging AI, vision systems, and data analytics.

Key Projects and Alliances

- Participation in nationally funded R&D projects such as TRANSFER (renewable energy storage), CERSOL (high-temperature ceramic receivers), and FRESTHER (solar thermal captors).
- Strategic alliances with international companies, including a Memorandum of Understanding (MoU) with SolarDynamics LLC.
- Membership in Protermosolar, Spain's leading CSP industry platform.

Intellectual Property and Innovation

- Holder of patents like a critical metal-ceramic junction system for high-temperature solar receivers, developed in collaboration with Abengoa Solar.
- Additional patents under development, including torque measurement systems for solar collectors.

Academic Contributions

- Over 30 Q1 and Q2 publications and presentations at more than 50 international conferences on topics including computational simulation, CSP technologies, and AI.
- Collaborative research with the University of Seville, resulting in completed and ongoing Ph.D. projects.
- VirtualMech's mission is to bridge science and industry, driving innovation for a sustainable and efficient future in energy and transportation.