TITLE:
MULTISCALE SIMULATION OF GAS PHASE NANOPARTICLE SYNTHESIS PROCESSES WITHIN THE H2020 SIMDOME PROJECT ENVIRONMENT

TUTOR:
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WORKING SITE:
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RESEARCH PROJECT:
The Department of Industrial Engineering (DIN) of the University of Bologna (UNIBO) is coordinating the activities of the H2020 project SimDOME - Digital Ontology-based Modelling Environment for Simulation of materials, approved and financed by the European Commission with a 4.577M€ budget in the framework of the topic H2020-NMBP-TO-IND-2018 DT-NMBP-09-2018: Accelerating the uptake of materials modelling software (IA), starting in the fall 2019 and lasting for four years.

SimDOME aims to develop an industry-ready software framework for materials modelling interoperability, based on EU/EMMC standards on materials modelling, by combining, further developing and adapting existing software developed within previous EU FP7-NMP projects SimPhoNy and MoDeNa, the H2020-NMBP project NanoDome and the FP7 ERC-AdG STRATUS.

SimDOME achieves the highest level of interoperability through the standardization of the material users case (i.e. the material/process to be simulated, according to EMMC definitions) that are provided within the SimDOME framework by means of the European Materials Modelling Ontology (EMMO). User case standardization will allow data communications between software by translating the concept of each specific implementation to the standard unified concepts and interfaces provided by the ontology.

The framework will provide also ready-to-use modules that cover different industrial applications and materials modelling fields spanning through multiple scales. The demonstration of the exploitation potential of the framework will be done within project by testing the SimDOME framework prototype and each integrated modelling software in their respective industrial operational environments (TRL 7) in the fields of gas and liquid phase material synthesis, molecule characterization and chemical kinetics.

ACTIVITY PLAN:
The Research Associate will take part to the activities of UNIBO-DIN in the SimDOME project, focusing on:
- Development of dedicated interface library for CFD codes
- Continuum CFD modeling at reactor scale
- Coupling of CFD models with the mesoscale model
HPC cluster (about 200 computational cores) and Xeon PHI workstations are available fully dedicated to these activities.

**Requirements:**
Applicants must meet the following mandatory **requirements**:
- Experience in CFD modeling
- Experience in scientific computer programming
- Knowledge of C or C++ programming language

Moreover, the following **preferred requirements** will be considered during evaluation of the applicants:
- Experience in plasma modeling
- Linux systems knowledge

**Training Plan:**
A dedicated training plan will be scheduled during the first months of the collaboration in order to overcome the lack of knowledge in one or more of the above-mentioned preferred requirements.

**Relations with other Entities:**
The SimDOME project involves six different academic and industrial partners within EU from Italy, Germany, Belgium and United Kingdom:
- Computational Modelling Cambridge Ltd (UK)
- UMICORE (Belgium)
- POLITO (Italy)
- FRAUNHOFER IWM (Germany)
- NIREOS SRL (Italy)

Relations with US entities are foreseen.

**The Tutor**
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