Title: development of an open source software for the multiscale orchestration of computational oncology simulations

Tutor: Prof Marco Viceconti - https://www.unibo.it/sitoweb/marco.viceconti/

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Research Project

In 2017 the European Commission called for proposals on the topic “In-silico trials for developing and assessing biomedical products”; one of the projects funded, PRIMAGE, which will start on December 1st, 2018, aims to develop in silico trials technologies to test the efficacy of new anti-tumour therapies. To predict the response of a new anti-cancer agent over a representative clinical population is a very complex endeavour, which requires a detailed model of the biochemical mechanism of action of the new drug on the cancer cells, another model that describes how this effect modulates the cell-to-cell and the cell-to-tissue interaction and signalling, and another model that can predict the overall growth of the tumour mass over time, its vascularisation, and its cellularity. As each of these models is defined at radically different space-time scales, their coupling is complex and involves an advanced orchestration to build a multiscale simulation.

This problem has been approached in different ways in the past by Prof Viceconti’s team and by other research groups, but all solutions so far have been not entirely satisfactory. The main problem is that the software stack to handle this orchestration becomes rapidly very large and complex (thus difficult to maintain), and strongly dependent on implementations of the models being orchestrated; as in most projects these are being developed in parallel, this create some serious difficulties.

In PRIMAGE we intend to tackle a completely different approach loosely inspired by the High Level Architecture approach standardised by IEEE Std 1516-2010, and popular especially in the context of defence research. We intend to develop a very simple and easy to maintain architecture that orchestrate the models by controlling their data flow, centralising in a database all intermediate data objects, so as to explore possible speed-up strategies based on pre-computation, interpolation, and surrogate modelling methods. The result will be an open source software tool that should make much easier for research groups around the world to design and deploy complex multiscale orchestrations, that execute efficiently and flexibly in different execution environments.

Under the guidance of Prof Marco Viceconti, one of the top experts of in silico trials and biomedical multiscale modelling worldwide, the post holder, a researcher with documented experience in software development in Python, will design and develop this orchestration framework, and use it to deploy a large scale multiscale simulation that orchestrate models developed by specialists at partners ANSYS, UNIVERSITY OF SARAGOZA, UNIVERSITY OF SHEFFIELD, and CHEMOTARGETS, which will be tested as in silico trial solution.

The research contract (Assegno di Ricerca), has an annual salary before taxes of € 26,174.00. While the initial contract is for 12 months, if successful the post holder contract will be extended until the end of the project, in November 2022.

The ideal candidate for this position holds a degree in computer science, math, physics, or engineering, documented experience in software development in Python, good spoken and written English, and one or more of the following skills:

- Familiarity with computational science & engineering software development
- Familiarity with computational biomedicine software development
- Previous experience with model orchestration and/or multiscale modelling
- Previous experience with database software development, NoSQL databases, blockchain public ledgers, surrogate modelling, and/or machine learning
- Previous experience with Open Source projects management