

HPC-based prediction of the optical properties of dyes

Fortissimo Experiment Facts:

- Segment: Pharmaceutical Engineering
- Application Domain: Molecular Simulation
- Application: Perturbed Matrix Method (PMM)



The Company

Scriba Nanotechnologie is an SME active in the fields of smart packaging, health and machine vision. In particular, Scriba is involved in the development of time temperature integrators (TTIs) which are devices for recording the thermal history of goods. Placed close to perishable products, they can be used to monitor the thermal history of packaging and storage conditions. Such devices address an important aspect of cold chain logistics in a world where production is global. Cold chain logistics are also addressed by regulators because the quality of products and goods is greatly affected by the thermal history across the distribution chain.

This Fortissimo experiment addresses the prediction of the optical properties of dyes. It uses molecular dynamics to simulate dyes used in the manufacture of innovative TTIs. Simulations reduce the time to customise these devices, thus lowering the overall cost of traceability systems. Molecular dynamics-based simulations are known to be well suited to HPC systems, since existing algorithms have been optimized to obtain a very high performance. The objective of this experiment is to develop an effective Cloud-based-HPC system for the modelling of potential dyes for the manufacture of TTIs.

The Challenge

The challenge faced by this experiment is to use HPC to simulate candidate dyes, based on molecular dynamics, to be used in the fabrication of innovative TTIs. Customization of temperature and time of integration is fundamental to optimize the data provided by the smart sensor and its integration into the production line, without slowing down the rates of production and distribution. This requires a multidisciplinary approach using molecular dynamics-based simulations of dyes in the fabrication of innovative TTIs. The aim is to reduce the time required for customisation of TTIs, lowering the overall cost of traceability systems proposed to manufacturers. The goal is to develop a new tool for cold chain logistics which enhances both packaging technology and the availability of relevant logistical data.

The Solution

The experiment has addressed the determination of the physical properties of dyes suitable for use in the productions of TTIs. A computational pipeline for the simulation of optical properties of dyes in different environments has been set up. A cloud-based web portal has been developed, to manage the simulation of the optical properties of dyes. This portal has been specifically designed for a user with no expertise in simulation. The complexity of the simulation is hidden from the user, who needs only select the material of interest and the experimental conditions to be simulated. Default options are presented to help the user proceed through the steps in the simulation and, most importantly, to optimise the balance between computational cost and the reliability of the simulation.

The Benefits

Through the use of the advanced simulation package Scriba expects to see a saving of €90K per simulation in the first year of use, with further savings of €70K in subsequent years. This can be broken down as savings in personnel costs of €45K, in infrastructure costs of €10K,



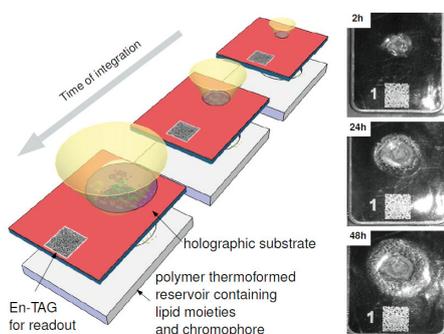
Fortissimo Experiment Partners:

- Scriba Nanotechnologie (End-user)
- CINECA (HPC Expert and HPC provider)
- UNIVAQ and UNIMORE (Domain Experts)

More Information:

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in material costs, including computing costs, of €25K and optical readout and further development of €15K in the first year. Scriba estimates that it will be involved in ~ 6 simulations per year resulting in an annual saving of ~€400K.

CINECA expects to see an increase in HPC cycle sales due to the use of the simulation package. It also plans to use the success of this experiment to target SMEs in the European market having the need for high-fidelity chemical and molecular dynamics simulations needs. The target is to acquire two customers of this type per year in each of the following three years. UNIMORE and UNIVAQ expect to see an increase in their consultancy business as a result of this successful experiment. Both partners will be further involved in the enhancement of the software, operating as external consultants. The value of the external consultancy to the two domain experts is estimated to be ~€10K per year each. The number of potential users to run simulations explicitly for the development of temperature sensors is about 5 and for the design of optical (bio)sensors about 100.

Scriba will make available the developed virtual tool in the Fortissimo marketplace, subject to appropriate terms and conditions.

The Fortissimo Project

Fortissimo is a collaborative project that enables European SMEs to be more competitive globally through the use of simulation services running on a High Performance Computing cloud infrastructure. The project is coordinated by the University of Edinburgh and involves 123 partners including Manufacturing Companies, Application Developers, Domain Experts, IT Solution Providers and HPC Cloud Service Providers from 14 countries. These partners are engaged in 53 experiments (case studies) where business relevant simulations of industrial processes are implemented and evaluated. The project is funded by the European Commission within the 7th Framework Programme and is part of the I4MS Initiative.

I4MS Fortissimo is part of I4MS ICT Innovation for Manufacturing SMEs: www.i4ms.eu



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