Integrated Services for Multiscale Materials Modelling and Simulation

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Computational materials science is essential for development of products with novel properties such as catalysts, semiconductors, and polymers. Nevertheless, next generation materials, especially nano-structured materials, exhibit pronounced complexity and include building blocks on several length scales. Thus, the physical models and the simulation protocols employ many different well established methods and specific codes to treat the steps in these protocols. However, the lack of integration of these individual codes, the increasing complexity of models and the high demand for distributed HPC resources reduces industrial usability of the methods. In addition, joint effort of groups providing expertise for all different methods is needed. These aspects are treated within the project MMM@HPC [1] which brings together scientists from industry and academia into a unified community which is able to use the e-infrastructure to solve modern real-life problems.

We will give an overview of our methodology and applications to provide adequate solutions for the following requirements:

- Reusable interfaces and workflows. To this end, we adopted GridBeans [2] which is a modern technology to create application interfaces for use in grid middleware, such as UNICORE 6 [3]. Every GridBean provides a graphical user interface and can be readily included into different workflows without further modifications. Moreover, the workflows created for one specific task can be reused in other simulations with minor parametric modifications (See Figure 1).

- Dataflows. In the field of materials modelling a variety of data formats are used and virtually every individual code has its own non-standard input and output formats. Thus, we aim to enhance data interoperability of individual GridBeans employing the Chemical Mark-up Language (CML) standard and work together with experienced developers from other projects, currently from UNICORE and OpenMolGrid [4].

- Solutions for licensing issues. Some of the codes used in the community are provided under non-free (proprietary) licenses. To treat this aspect we are working on a solution based on the Virtual Organization Membership Service (VOMS) and UNICORE.

- Capacity (high throughput) and capability (high performance) computing: The applications addressed in the community are particularly demanding with regard to computing and storage resources. This is why the scalable deployment of the application services requires linking to HPC and distributed resources.

All these user requirements pose a great challenge for both code developers and providers of e-infrastructures. The application protocols are mapped onto scientific workflows and the application interfaces are able to exchange input/output data using data formats like CML. The platform of our choice is the UNICORE middleware that is broadly and productively deployed in different grid infrastructures such as D-Grid, NGI-DE, DEISA and PRACE.

We demonstrate the functionalities of the developed tools considering key applications, including de-novo modelling and simulation of whole devices, such as organic electronics, molecular electronics, carbon nano-device and Li-Ion batteries. In this specific contribution we exploit a multiscale model for devices such as light-emitting diodes (OLEDs, see Figure 2).

References

[1] Project MMM@HPC: Multiscale Materials Modelling on High Performance Computer Architectures, Available online under www.multiscale-modelling.eu.

[2] R. Ratering, A. Lukichev, M. Riedel, D. Mallmann, A. Vanni, C. Cacciari, S. Lanzarini, K. Benedyczak, M. Borcz, R. Kluszcynski, P. Bala, G. Ohme, "GridBeans: Support e-Science and Grid Applications", Proceedings of the Second IEEE International Conference on e-Science and Grid Computing (e-Science'06), p. 45, IEEE 2006.

[3] A. Streit, P. Bala, A. Beck-Ratzka, K. Benedyczak, S. Bergmann, R. Breu, J. Daivandy, B. Demuth, A. Eifer, A. Giesler, B. Hagemeier, S. Holl, V. Huber, N. Lamla, D. Mallmann, A. Memon, M. Memon, M. Rambadt, M. Riedel, M. Romberg, B. Schuller, T. Schlauch, A. Schreiber, T. Soddemann, and W. Ziegler, UNICORE 6 — Recent and Future Advancements}, Ann. Telecommun. 65, 757-762, 2010.

[4] S. Sild, U. Maran, M. Romberg, B. Schuller, E. Benfenati, OpenMolGRID: Using Automated Workflows in GRID Computing Environment. In Advances in Grid Computing - EGC 2005, P. M. A. Sloot et al (Eds.), LNCS 3470, 464-473, Springer 2005.

[5] J. J. Kwiatkowski, J. Nelson, H. Li, J. L. Bredas, W. Wenzel, and C. Lennartz, Simulating charge transport in tris(8-hydroxyquinoline) aluminium (Alq3), Phys. Chem. Chem. Phys., 10, 1852-1858, 2008.

Figures

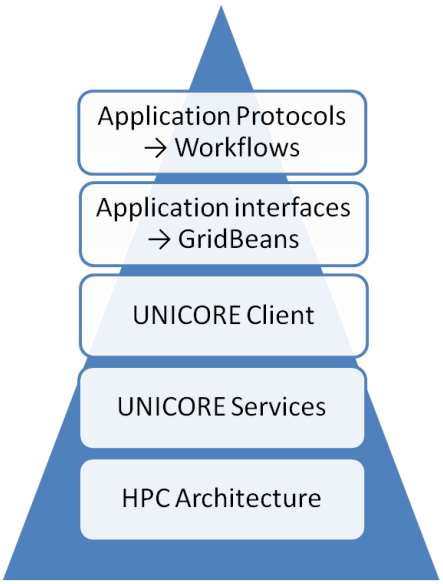

Figure 1: Our integration approach allows the seamless access both to HPC resources, such as massively parallel supercomputers, and to computing grids for capacity processing, employing the middleware UNICORE.

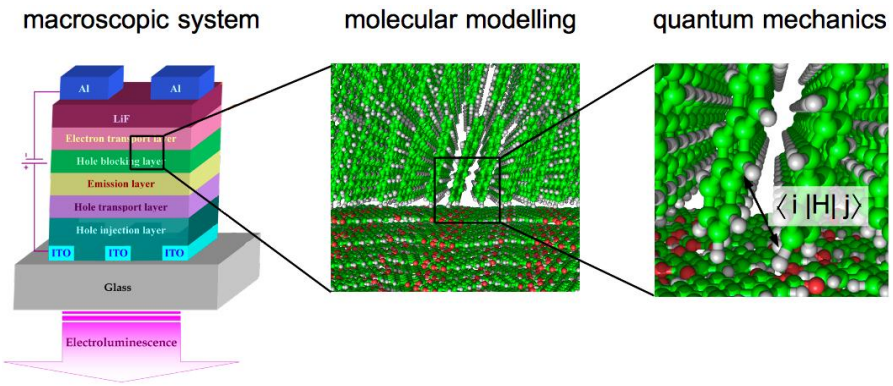

Figure 2: OLED Simulations require in addition to the three scales sketched here, simulation modules to generate the morphologies and charge-transport codes. A single simulation thus requires integration of five complex, but existing software solutions.