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Workflows for the Simulation of Organic Light-Emitting Diodes

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Description of the Work

The base technology employed, UNICORE 6, is ready to use on high performance computing (HPC) und high throughput computing (HTC) resources required to perform the demanding quantum mechanical calculations in OLED simulations. Based on the UNICORE workflow engine it is possible to assemble complex simulations consisting of several computing steps containing models at different size and time scales. The applications used in the OLED workflows include quantum mechanics models (nanometer scale), atomistic models (micrometer scale), coarse-grained and continuum models (millimeter scale).
The UNICORE 6 Rich Client (URC) offers the concept of GridBeans which allows creating customized user interfaces for the different applications used in the workflow. The GridBeans automatically generate Jobs described in the Job Submission Description Language (JSDL) which is used by UNICORE 6 on the server side for job execution. GridBeans allow creating user interfaces which hide the complexity of a command line application and validate the user input. In the OLED workflow GridBeans are used to parse and visualize computing results. The developed GridBeans will be shared and reused by the project members via a GridBean repository by means of the URC update mechanism.
Multiscale simulations include various individual codes that have different mutually incompatible input and output formats. To this end the Chemical Markup Language (CML) is employed for exchanging atomistic structural data. Additionally an extended version of the OpenMolGrid library provides a parser and writer for input and output files for each supported application. Additional wrappers, located on the server side ensure that the GridBeans interact seamlessly with the software binaries and OpenMolGrid. The wrappers are responsible for creating and validation of the input, for preprocessing, execution of the application, reacting on application failures and converting the output to CML for further usage.

Conclusions

Because the project is based on productively deployed UNICORE services it is easy to run the simulations on various resources, for instance on HPC resources like the ones provided within PRACE (Partnership for advanced computing in Europe) or HTC resources on Grid infrastructures like the European Grid Infrastructure (EGI) or D-Grid. Thus the project provides a significant extension of services of existing e-infrastructures and enables barrier-free access for the user communities.

We demonstrate that the UNICORE middleware offers services and components for setting up an environment for multiscale material simulations and for solution of many challenging requirements for reusability, data handling, security and capacity and capability. As a proof of principle a simple workflow is provided for multiscale modeling and simulation of OLED devices. Future developments will include an improved data model and solution for propagating authorization for restricted software (licensing issues).

Impact

The OLED workflow comprises GridBeans for MOPAC, DEPOSIT and ToFeT and models the hopping transport in disordered organic films containing Alq3 molecules and computes the charge mobility in the film. In the first step of this workflow the spatial structure of Alq3 is optimized using MOPAC and then DEPOSIT is used to generate the film morphology. Then pairs of adjacent sites for the hopping transport model are selected, the local electronic structure of these sites is calculated using MOPAC and parameters for calculation of the local hopping rates are extracted. In the last workflow step the calculated rates enter the kinetic Monte Carlo calculation with ToFeT yielding the charge mobilities.
The main concepts of the project MMM@HPC can be reflected in terms of reusability, data complexity, usability, security as well as capacity and capability. Reusability is realized with GridBeans and workflows. These components are distributed via an update site that is accessible via the Internet. Hence, new workflows can be easily constructed with a set of available GridBeans. Furthermore existing workflows can be adjusted by scientists to their demands.
The problem of heterogeneous data flow in material simulations is approached by the usage of the CML as standardized data format as well as the OpenMolGrid library for parsing application-specific data. This approach yields an open framework that is extendable for further applications.
GridBeans have graphical user interfaces (GUI) which hide the complexity of command line interfaces that are typical for scientific program codes. Users, especially grid newcomers, can use the intuitive URC to obtain access to HPC and grid resources. They need no deep knowledge of specific middleware clients, of grid security mechanism or of operating systems.

URL

https://www.multiscale-modelling.eu

Overview (For the conference guide)

Computational materials science is essential for development of products with novel properties. With the accelerating development cycles of materials, the development of simulation approaches for predictive, de-novo characterization and optimization of materials and device properties emerges as a grand challenge to European Research and Development. A unified multi-disciplinary approach towards the deployment of models, tools, algorithms and simulation and visualization techniques is required to transform isolated solutions for specific problems into comprehensive, industry-ready platforms, which are capable of predicting the properties of complex materials on the basis of their constitutive elements. The project MMM@HPC (Multiscale Materials Modeling on High Performance Computer Architectures) will demonstrate a direct impact towards solving this challenge in the areas of energy storage, e.g. Li ion batteries, and energy conversion, e.g. organic light emitting diodes (OLEDs).

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