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Multiscale materials modelling on High Performance Computer Architectures

DELIVERABLE D7.2

Help desk and consulting service

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Version history

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2	2012-06-06	S. Widmaier	I. Kondov	Inserted the portion about nanomatch	Draft	
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4	2012-06-08	W. Wenzel	I. Kondov	Minor corrections	Draft	
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1 Introduction

Following the provision of low-level services in WP4 and technological developments (development of GridBeans and development and validation of Workflows in WP8 the upcoming milestones of the MMM@HPC project can be grouped into two major groups: Proof-of-principle Simulations (WP9-WP12) and Community Building (WP2, WP3, and WP7). The support activities are part of the community building.

Providing support already in the early phase of the project is essential for the successful transfer of the implemented solutions to other partners and further users. The support activities are dependent on the progress in technological development work packages and closely related to documentation and training activities. The novelty of our concept consists in addressing the needs not only of the end user of the simulation services but also developers on different levels. These target groups, their needs and the related tasks are described in the next section.

2 Target user groups for the support

The user support activity (WP7) takes into account different target groups whose requests necessitate systematic support:

Developers of application interfaces and wrappers

This support includes helping project partners as well as enthusiastic non-members to develop GridBeans and application wrappers. The persons are usually developers of the individual application code that is to be integrated using the GridBean technology. They have the necessary expertise on the HPC level and also grid computing. Thus the support effort was more concentrated on the complex setup of numerous tools and services in a sandbox. For this purpose a special platform (MMM@HPC Development Toolkit) has been developed and provided by KIT. The toolkit is documented in D5.2 “External developer manuals” and the work done for the development of the toolkit is described in more detail in D7.3 “User support”. The development toolkit has proven very successful as it has been used by several partners (CSC, CEA, STFC and UPA) boosting the development of several GridBeans. The support provides constant expert-level help using this toolkit and further services such as the MMM@HPC Update Site, and the developer’s software repositories.

Developers of workflows (workflow designers)

This is a support provided to scientists constructing workflow models for different applications. These developers are usually unaware of the complexity of the grid, however, have knowledge on the physics and computer simulations. The support for this group thus consists of help in giving directions to documentation, download services, service registries in personal consultations, phone calls, email communication and video conferences.

The support work for developers of interfaces and workflow designers is highly non-trivial and required substantial efforts. Several personal consultations with duration of 3-5 days have been organized during the project: An expert from KIT has visited developers in Mons, Espoo and Grenoble, and two developers from CEA and STFC have visited the expert at KIT in the past. Further two support meetings are planned at KIT (with visits from UPA and from CEA).

End users

This target group includes industrial users or experimentalists with little or no experience in HPC, Grid computing or theoretical modelling and computer simulation. The support for this audience consists in giving directions to end-user documentation, helping in registration for the services and managing grid certificates, installing the UNICORE client and running pre-defined workflows. The support for end users is directly related to the consulting service (see Section 4).

The concept and general actions performed for user support have been outlined in Deliverable D7.3 “User Support”. The help desk and the consulting service are important part of the user support plan of the project and underpin the research activities in WP8-WP12 ensuring rapid uptake of the applications, technologies and tools in these activities.

3 Help desk

For support requests from all three different target groups a central place to go is the help desk. The help desk processes requests from all three groups and the different request often have different priority. This is why the help desk starts to process the requests with prioritizing and categorizing the requests (called tickets). Because there are well established help desk instances that implement these functionalities we reused such existing solutions, in particular the NGI-DE help system basing in the GGUS system, see below. As an alternative the support is also provided using simple technical solutions such as email distribution lists (support@multiscale-modelling.eu) on which experts for the different target groups are registered.

We concentrated our effort on the processing of support requests (see Deliverable D7.3 “User support”) and less on the implementation and maintenance of a help desk because of reuse of good existing technical solution.

Support unit in NGI-DE

For the resources provided via KIT the project has obtained a support unit (as 2nd level VO support) in the GGUS system. The system is accessible under <https://helpdesk.ngi-de.eu>. Using this infrastructure we can perform our community user support. There we should also submit our requests to provider of grid resources and services. Temporarily, all support requests (tickets) which are categorized to m3hpc are forwarded to the mailing list support@multiscale-modelling.eu. Tickets regarding underlying infrastructure, such as computing and storage resources and grid-middleware services are forwarded to the centre provider of the respective resource and services. Later, this mailing list should be used to transport notification on all support requests to the project partners. Experts from our consortium, who wish providing support within our project, can apply to become support staff under <https://helpdesk.ngi-de.eu>. The email address is used only to send notifications and quick links and the actual support is done under <https://helpdesk.ngi-de.eu>.

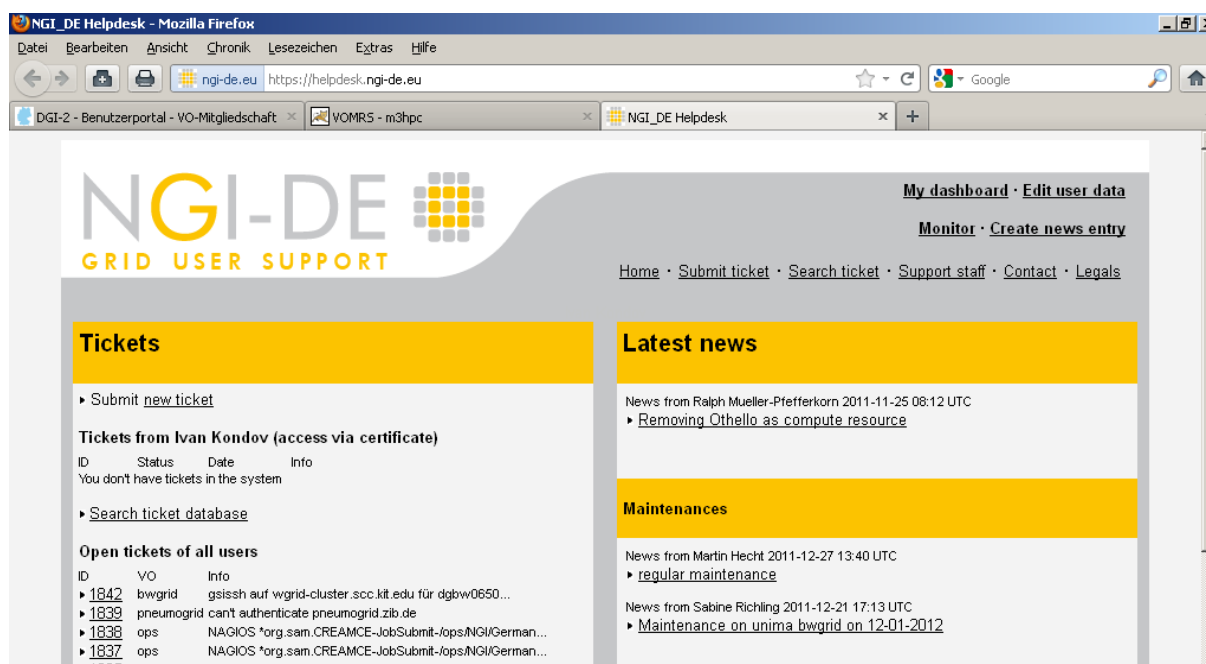


Figure 1: MMM@HPC helpdesk created basing on the Global Grid User Support (GGUS) system

How project members and further users get support

Experimental groups and industrial partner groups, but also code developers are encouraged to benefit from the support portal. They can submit their request quickly and easily following the link “Submit ticket”. The requesting person should specify the issue in such a way that it can be categorized and assigned appropriately to MMM@HPC support by the help desk staff. The portal can be used also for any other support requests, e.g. regarding computing resources, access issues etc. In the latter cases the tickets are assigned to the provider of resources but not to the support unit of MMM@HPC.

How project members provide support

Experts from the MMM@HPC consortium, who wish providing support within the project, should do the following two steps:

1. Apply to become support staff under <https://helpdesk.ngi-de.eu>. On the portal they should navigate through the link “Support Staff” (see **Fehler! Verweisquelle konnte nicht gefunden werden.**) and follow the instructions. They should specify the name of the support unit “m3hpc” as they fill in the forms.
2. Send an e-mail message to coordinator@multiscale-modelling.eu requesting the membership in the e-mail distribution list support@multiscale-modelling.eu. The email address support@multiscale-modelling.eu is used to send notifications and quick links and the actual support is done under <https://helpdesk.ngi-de.eu>.

4 Consulting Service

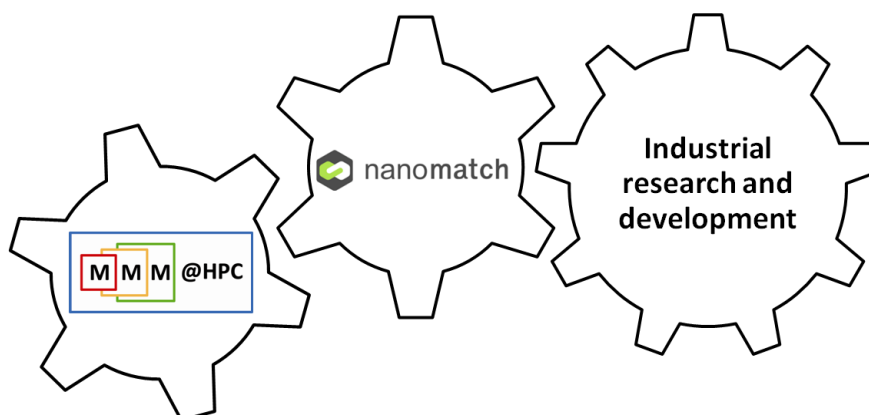
Providing a solution for a consulting service is one of the major tasks in the community support activities of the MMM@HPC project. The industrial materials research lacks the resources and the expertise to maintain and operate the simulation services provided by the MMM@HPC project. The consulting service will bridge the gap between simulation services developed and the industrial customer. On the other hand, reliable underlying commercial grid and cloud services will ensure the technical operation of the simulation services beyond the MMM@HPC project life-time.

Recently, the project partner KIT has done substantial efforts to deploy the consulting service via a spin-off company Nanomatch located in Karlsruhe, Germany. The site KIT in Karlsruhe as part of the NanoValley (<http://www.nanovalley.eu/en>) is the optimal location for the consulting service providing unique opportunities for technology transfer not only to large companies but also to small and medium enterprises. On the other hand, the co-location of the MMM@HPC team at KIT with the staff of Nanomatch has additional benefits, for example low cost and low administrative effort for transfer, immediate communications and team exchange.

Nanomatch (<http://www.nanomatch.de>) will be a spin-off company from KIT and the Helmholtz-Association. The expertise of Nanomatch is industry-scale computational screening and computer simulations targeting high-performance materials for the field of organic electronics. Basing on highly efficient simulation methods the company Nanomatch offers simulation solution services predominantly for the growing markets of organic electronics. The objective of Nanomatch is to accelerate the company internal and cross-industry development plans of the Nanomatch customers through the integration of materials simulations in their development process in order to reduce the development costs, to achieve improved products and shorter time-to-market.

Nanomatch employs different algorithms to predict the morphology of arbitrary organic materials and amorphous material compositions, such as doped organic semi-conductors, solvent inclusions and host-guest systems. The resulting structural information allows the characterization of the molecular and electronic interactions by quantum chemical methods. As a consequence the functionalities of a material that are essentially defined by the molecular and electronic interactions can be optimized in the simulation process without the need for experimentally derived parameters.

Nanomatch targets customers in the field of materials chemistry, nanotechnology and organic electronics. The search and optimization of new high-performance chemicals especially in the field of organic electronics is a task for chemical and electronic industries that will be successively supported by computational approaches.



Nanomatch had developed experience with simulating molecular nanostructures in fields very common with the applications addressed in the MMM@HPC project: optimization of crystalline and amorphous layers in organic light-emitting diodes (OLEDs), organic solar cells and other application areas such as energy storage systems, or surface coatings. This has been done predominantly using the simulation tool SiMona developed previously.

The simulation services developed by MMM@HPC are currently being adopted in Nanomatch as a powerful tool to extend the spectrum of services provided by the company. In particular, the OLED simulation workflow which has been released by the MMM@HPC project will be applied as tool for high-performance materials screening enabling developers to generate arbitrary material compositions such as doped organic semiconductors, matrix and additives, including i.e. dipolar and metal-organic molecules explicitly. The measures started in the early 2012 and included presentations of the simulation services, internal tutorials and trainings, discussions of the objectives of the consulting service.

After the life-time of the MMM@HPC project the company Nanomatch will continue to support the industrial users in using the developed simulation services. The users can send request either directly to the company support contact or use the help desk established within the MMM@HPC project (see Section 3).

Links:

http://www.kit.edu/visit/pi_2011_6983.php

<http://www.oled-info.com/simona-new-oled-optimization-software-enable-cheaper-oleds-soon>