



Contribution ID: 28

Type: **Presentation/Paper**

ScalaLife –Providing Scalable Software Services and Expertise to Life Science

Wednesday, 28 March 2012 12:05 (25 minutes)

Impact

The main impact of the ScalaLife project and the Competence Centre will be to break the barriers between hardware, software, and application research; this unified community of computational scientists will be an essential element of underpinning next-generation e-Infrastructures, and have a significant structuring impact on the European Research Area. The infrastructure will provide new users with access to suitable software and test accounts on high-end hardware, application developers will get access to computer science expertise to aid in scaling and optimization, and supercomputer centres or policy-makers will have a natural community partner to define hardware investment needs based on the most important application problems.

URL

<http://www.scalalife.eu>

Overview (For the conference guide)

This submission presents a new EU project, ScalaLife. One of the main goals of the project is to provide a long-term support for the computational life science communities.

Description of the Work

The ScalaLife project addresses the fast growing demand the Life Sciences put on both the capabilities of simulation software and the capacity of e-Infrastructure support services. On the one hand, the project is concerned with the discrepancy between large-system scalability advances made by e-Infrastructure projects such as PRACE and the reality of the typical Life Science application, which is run on small-to-medium systems. Thus, ScalaLife is set to implement new techniques for efficient small-system parallelisation, developing new hierarchical approaches explicitly based on ensemble and high-throughput computing for new multi-core and streaming/GPU architectures, and establishing open software standards for data storage and exchange. On the other hand, the project is committed to supporting the Life Science users and communities, providing both training and expert advice. First, ScalaLife is documenting and developing training for the new techniques implemented in pilot European open-source codes (such as the widely used Gromacs and Dalton), as well as for the new bioinformatics data storage and exchange formats. Second, the project created a pilot for a cross-disciplinary Competence Centre concerned with scalable Life Science software, to enable the community to exploit e-Infrastructures effectively. The Centre provides a training and support infrastructure, and establishes a long-term framework for maintenance and optimisation of Life Science software. ScalaLife is working on the long-term sustainability of the Centre, by developing an adequate framework and associated

policies to foster collaboration with and between users and communities as well as with external projects such as EGI. A clear advantage is the participation of key developers of the pilot software as project members, which ensures a unique position to both determine the specifics of the scalable solutions and to offer optimal software support to the community across many platforms.

Conclusions

Through its centralized services the ScalaLife Competence Center can provide valuable HPC expertise to the EGI Life Science communities.

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Session Classification: Community-tailored Services

Track Classification: Users and communities