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Prototyping a Competence Center for the Computational Life Science Communities - Experiences from the ScalaLife Project

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Description of the work

The Life Sciences have rapidly become one of the major beneficiaries of the European e- Infrastructures, placing a growing demand on the capabilities of simulation software and on the support services. The ScalaLife project has set to address some of the specific problems associated with this growth, acting along two distinct and complementary directions.

On the one hand, the project is implementing new techniques for efficient small-system parallelization, establishing open software standards for data storage and exchange, and developing new hierarchical approaches. The latter are explicitly based on ensemble and high-throughput computing for new multi-core and streaming/GPU architectures. Automated hierarchical parallelization will be of particular importance for Grid applications with running on many-core and accelerator systems.

On the other hand, the project is committed to the long- term support of the Life Science users and communities, providing both training and expert advice. ScalaLife is documenting and developing training material for the new techniques and data storage formats implemented by the project. The project has created a pilot for a cross-disciplinary Competence Centre, which enables the Life Science community to effectively exploit the key applications developed as part of the project on the existing European e-Infrastructures, including Grid resources provided by EGI.

Link for further information

www.scalalife.eu

Wider impact of this work

The experiences gathered in the development of the ScalaLife Competence Center provide valuable foundations for future efforts to establish similar centers in other areas of computational science. In addition, the center fosters the interactions and exchange of expertise between the HPC and EGI communities.

Printable Summary

Life Science research has become to a large extent dependent on computing resources for simulation and data analysis. Despite the advances in software development, which are pushing Life Science codes towards exascale capabilities, efficient utilization of those resources is often not achieved. Some of the reasons include a lack of HPC awareness and expertise among regular users, a steep learning curve for powerful software features, a lack of documentation of best practices as well as a disconnect between code developers and users.

The ScalaLife project (scalalife.eu) has engaged in prototyping a cross-disciplinary Competence Center as a long-term structure for:

- Maintenance and optimization of key Life Science software
- Provision of training and support infrastructure
- Development of an adequate framework and associated policies to foster collaboration among software developers and users

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