

programming models currently in use in HPC.

The software products are accompanied by training and support offerings through the Virtual Institute–High Productivity Supercomputing (VI-HPS [8]), and will be maintained and adapted to emerging HPC architectures and programming paradigms beyond the lifetime of the Score-E project itself.

Besides the evident economic and environmental benefits in terms of energy, Score-E will also empower the optimized programs to unlock new scientific and commercial potentials.

The academic project partners in LMAC are the Jülich Supercomputing Centre, the German Research School for Simulation Sciences, RWTH Aachen University, TU Dresden and TU Munich. The industrial partner GNS mbH, a private company that specializes in services related to metal forming simulations, such as mesh generation for complex structures and finite element analyses, coordinates the project.

In addition, the University of Oregon, an associated partner, complements the Score-E objectives with corresponding extensions to the performance tool TAU. Further associated partners are Engys UG, who specializes in the application, support and development of Open Source Computational Fluid Dynamics (CFD) software and Munters Euroform which its expertise in engineering droplet separation systems for various industrial purposes.

For more information see:
<http://www.vi-hps.org/projects/score-e>
 and <http://www.score-p.org>

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References

- [1] Bischof, C., an Mey, D., Iwainsky, C. Brainware for green HPC Computer Science–Research and Development, 27(4):227–233, 2012.
- [2] <http://scalasca.org/>
- [3] <http://www.vampir.eu/>
- [4] <http://www.lrr.in.tum.de/~periscop/>
- [5] <https://www.cs.uoregon.edu/research/tau/home.php>
- [6] <http://www.score-p.org>
- [7] http://www.fz-juelich.de/ias/jsc/EN/Expertise/Support/Software/SIONlib/_node.html
- [8] <http://www.vi-hps.org>

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UNICORE 7 Released

The UNICORE middleware suite is well-established as one of the major solutions for building federations and e-infra-structures, with a history going back to 1996 [1]. It is in worldwide use in HPC oriented infrastructures, for example PRACE, the US-project XSEDE [2] and in national grid initiatives such as PL-Grid. This spring, UNICORE 7 was released, which is the first major release since UNICORE 6.0 in August 2007. It is no paradigm change as was the change from UNICORE 5 to UNICORE 6. Instead, UNICORE 7 is built on the same ideas and principles as UNICORE 6, and the two versions are compatible. We decided to make this a major release due to a number of improvements that serve to put the software on an updated technological basis.

As the most prominent change, we updated the internal web services stack to use the Apache CXF framework [3], which is the most advanced and mature Java services stack available today. This allows to build both WS/SOAP services as are currently used in UNICORE and RESTful services that will become more and more important in the future.

As the major new feature, we have added the possibility to deploy and run UNICORE in a way that end-users do not need certificates, using the Unity group management and federated identity solution [4]. Instead of using X.509 certificates to identify themselves, UNICORE clients request a signed Security Assertion Markup Language (SAML) [5] document from the Unity

service, which is validated by the UNICORE services to assert the user's identity. Nevertheless, the strong client authentication based on X.509 certificates is still available and will continue to be supported in future releases.

Apart from the enhanced web services container and improved security stack, there are a number of other new features. For example, a new data-oriented processing feature allows to define data processing via user-defined rules. Jobs can be restarted easily, and data staging now supports wildcards.

Several changes have been made to improve the performance of UNICORE 7. For example, security sessions have been introduced to reduce the amount of XML data transferred between client and server, also reducing the CPU time required to process the XML messages. Several new batch operations have been added, for example allowing to delete multiple files or to check the status of many jobs using a single request/reply web service call. In data staging, the transfer of directories or multiple files has been optimized. Now, multiple files can be transferred in a single session, greatly using the overhead. This works especially well in conjunction with the UFTP high-performance data transfer protocol.

Together with the UNICORE 7.0 release, a first version of the new UNICORE Portal component was made available. This serves the increasing demand of users and infrastructure operators for a web-based access to UNICORE

resources. Compared to desktop clients, no installation on end user machines is required, and updates and fixes can be made available much easier. The UNICORE Portal was developed in a highly modular and customizable fashion, and allows deployers to disable unneeded functionality and to extend the portal with customized components, for example for user authentication. The underlying technology is Java, using Vaadin [6], an open-source web framework which allows for a rich user experience comparable to desktop clients.

Special care has been taken to allow integrating the Portal with different user authentication methods. The user can authenticate via X.509 certificate in the browser, or via the Unity identity management service, which allows also username/password authentication. Other methods such as authentication

via Kerberos are possible, too, since the security subsystem is extensible.

The Portal currently offers access to the most important UNICORE features, which is job submission and monitoring, data access and transfer, and access to a subset of workflow features.

The screenshot (Fig. 1) shows the data browser view, which is a two-window component inspired by tools such as Norton Commander. It allows to manage data on both UNICORE storages and the end user's local filesystem. Data can be uploaded to, downloaded from or transferred between UNICORE servers in a very simple way. The user's local file system is made accessible using a Java applet.

UNICORE 7 is a major step forward in many respects, and we expect it will

be quickly and widely deployed by our users in PRACE, XSEDE, national infrastructures such as PL-Grid, and others.

A particularly interesting new deployment of UNICORE is under development in the FET-Flagship „Human Brain Project“, where UNICORE will form the basis for the HPC platform, which will combine High-Performance Computing and scalable storage into a future exascale platform for simulating the human brain. The Human Brain project is expected to bring new requirements, such as interactive supercomputing, large user federations, and others. UNICORE is well-placed to take on these requirements. A strong focus of further development will be put on the UNICORE portal, where we plan to add support for some of the more advanced UNICORE features such as metadata management. Customization of the portal for specific use cases and applications will play a big role, e.g. through the development of an application integration layer. Last not least, we will work on adding social features and “teamwork” functions, leveraging the group membership management capabilities of the Unity system to allow simple sharing of task definitions or data files, as well as receiving notifications about activities of group members.

References

[1] Streit, A. et.al. annals of telecommunications 65, pp. 757-762, 2010

[2] UNICORE in XSEDE- <https://www.xsede.org/software/unicore>

[3] Apache CXF-<http://cxf.apache.org>

[4] Unity identity management solution- <http://www.unity-idm.eu>

[5] SAML-http://en.wikipedia.org/wiki/Security_Assertion_Markup_Language

[6] Vaadin web application framework- <http://vaadin.com>

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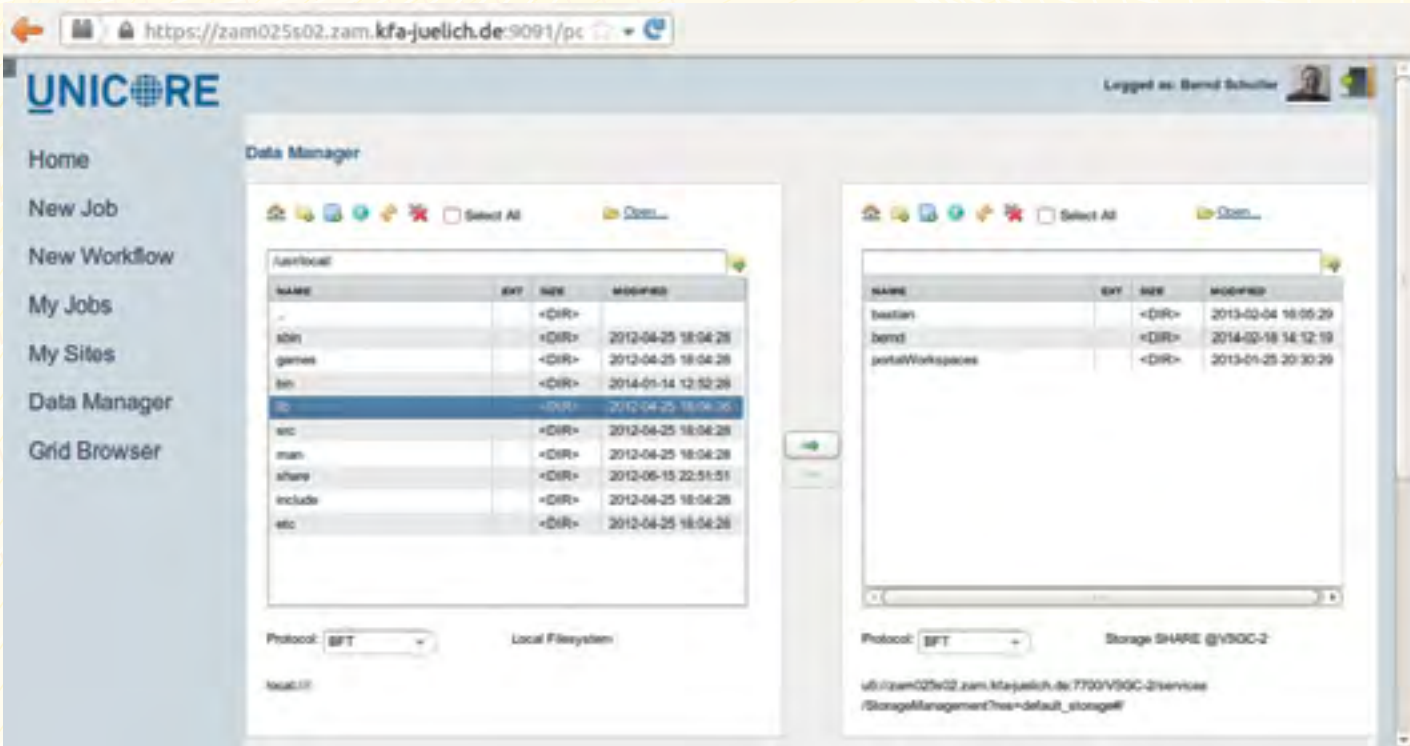


Figure 1: Screenshot of the data browser view in the UNICORE Portal