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Science Gateways for the Broader Take-up of Distributed Computing Infrastructures

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Accessing Distributed Computing Infrastructures (DCI) such as resources of computational Grids has long been regarded as the privilege of the knowledgeable few. Early adoption of these technologies required significant patience due to the instability of the infrastructure and the ever-changing nature of middleware and low level tools. Early adopters of DCIs also required low level technical knowledge and understanding of distributed computing paradigms. As a result the take up of Grid infrastructures has been relatively low. While some researchers published significant results using large amount of computational power, the majority of scientists found it too complex and too difficult to engage with. Although cloud computing technologies address some of these problems, the utilisation of vast amount of resources to solve computation and data intensive tasks still stayed well beyond the computational knowledge of a typical domain scientist, such us a biologist or a chemist.

Science gateways offer the potential to significantly change this trend and open the utilisation of DCIs to a much larger audience. Low level command line interfaces will always be mastered by a knowledgeable minority offering them greater flexibility and the ability to solve a larger variety of problems. The price for this flexibility is the requirement for low level scripting and programming, and using command line interfaces. On the other hand, a much larger user community can be targeted with simple high level graphical user interfaces that allow them to run experiments on massive computing and data resources. The complexity of the infrastructure can be completely hidden from the end-user by a tailored science gateway interface. While this interface can be simple and easy to use it will always come with the price of losing some of the flexibility and extendibility. However, there are many typical application areas of DCIs where this flexibility is less required. In these user scenarios Grid and cloud computing infrastructures can be opened to a brand new and much broader audience than before.

Interest in and work on science gateways have accelerated in the past few years. Several projects and initiatives have been started worldwide to develop generic science gateway frameworks and customised gateways for diverse user communities. For example, more than thirty science gateways are now listed on the XSEDE (Extreme Science and Engineering Digital Environment) gateways page [1], while the EGI (European Grid Infrastructure) Applications Database has recently introduced its new science gateway

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category that already lists nearly forty entries [2]. Most of the large funded projects in various disciplines are now creating their own customized gateway solutions based on widely used gateway frameworks or by developing their own custom solutions.

One of the prime events of the gateway developer and user communities has been the International Workshop for Science Gateways (IWSG) [3]. IWSG, with slightly different names and themes have been running since 2009, and provided a constantly growing platform to present the latest results of gateway frameworks and custom science gateway solutions. The idea of this current Special Issue of the Journal of Grid Computing on Science Gateways has risen during the organization of IWSG-Life 2011. As the title suggests that workshop has been organized specifically around the life sciences theme. Participants of the workshop have been specifically encouraged to submit papers for this special issue. However, several other submissions have also been received via the open call. Besides the life sciences topic, that still dominates the papers, science gateway related work from other disciplines has also been accepted and encouraged.

This special issue includes nine papers giving a representative and wide overview of science gateway related work, especially in Europe and in the United States. The first four papers describe science gateway development frameworks and environments, including WS-PGRADE (Z. Farkas et al.), the Vine Toolkit (P. Grabowski et al), the DARE framework (Yaakoub El Khamra et al), and the TRENCADIS technology (J. D. Segrelles Quilis et al.) that are widely utilised by several user communities. Besides the generic technological overview examples for science gateway instances built on top of the frameworks are also provided. These gateway technologies are generic and have applications in various disciplines beyond life sciences too.

The second part of the special issue is dedicated to the description and evaluation of experiences when building or utilising customised science gateways by various user communities. All of the included examples are from the life sciences domain. However, the experiences gained are typically more generic and well recommended to gateway developers in different application areas too. The DECIDE gateway (Ardizzone et al.) supports the medical community in its daily duties of patients' examination and diagnosis, the Charite Grid portal (J Wu et al.) has portlets for brain image processing, and the e-BioInfra Gateway (S. Shahand et al.) performs large scale data analysis experiments. A.M.J.J Bonvin et al. introduce a large set of individual gateways to streamline and automate the analysis of Nuclear Magnetic Resonance (NMR) and Small Angle X-Ray scattering (SAXS) imaging data. Finally, S. Gesing et al. concentrate on the security aspects of the MoSGrid (Molecular Simulation Grid) gateway for structural bioinformatics, molecular modelling, and quantum chemistry.

This special issue is recommended to computer scientists who are developing or extending generic science gateway frameworks that can be utilised in multiple application domains. This issue is also a good starting point for domain specific application and gateway developers who build custom science gateways for their communities. Finally, users of distributed computing infrastructures will find these papers useful to get new ideas and to learn best practices and experiences when utilising large computational and data resources in a user friendly manner.

References

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