EGI Community Forum 2014 - Helsinki

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High Performance Computing for Nanoscale Simulations

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Summary :

Slovak Grid NGI will set up NGI virtual centre of excellence for application development and consultancy to researchers from various application domains to improve their adoption of EGI e-Infrastructure services. Our work has been focused on Grid application activities such as analysis of Case Studies and solving of either ready simulation programs or development of software packages. Researchers and involved research communities have varying requirements on the e-Infrastructure services and resources and so far eleven Case Studies have been worked out in details, all differing in specific scientific demands and nanotechnology applications.

From the selected Case Studies, the Case Study “Nanoscale modelling and structure optimization” which uses OOMF and MagPar simulation SW packages will be presented more in details. New phenomena and exotic magnetic arrangements like vortices or skyrmions are investigated in this Case Study for practical applications like information storage. Simulations of dynamical processes in magnetic devices are quite CPU time consuming and new algorithms are developing for increasing simulations speed and efficiency. Related to this Case Study, the nanotechnology portal is already developed as a pivot step to make easier access for end-users toward high performance applications on Grid.

Description :

Slovak Grid NGI will set up NGI virtual centre of excellence for application development and consultancy to researchers from various application domains to improve their adoption of EGI e-Infrastructure services. The centre will co-operate with similar centres in other NGI's to build human networks which will include experts on grid and cloud infrastructures as well as experts from application domains.

Nanotechnology and advanced materials research is offered as a transformative technology, with the potential to improve every aspect of social, physical, and economic well-being. Presently excellent research is running at Slovak Academy of Sciences in various subfields and research disciplines in nanotechnology, and SAS

provides technology experts operating the infrastructure.

At the moment we have cooperation with several partners abroad. Our work has been focused on Grid application activities such as analysis of whole chosen Case Studies and solving of either ready simulation programs or development of software packages. Researchers and involved research communities have varying requirements on the e-Infrastructure services and resources. So far eleven Case Studies have been worked out in details, all differing in specific scientific demands and nanotechnology applications.

From the selected Case Studies we will give more information about the Case Study "Nanoscale modelling and structure optimization" which uses OOMF and MagPar simulation SW packages. New phenomena and exotic magnetic arrangements like vortices or skyrmions are investigated in this Case Study for practical applications like information storage. Simulations of dynamical processes in magnetic devices are quite CPU time consuming and new algorithms are developing for increasing simulations speed and efficiency. Related to this Case Study, the nanotechnology portal is already developed as a pivot step to make easier access for end-users toward high performance applications on Grid.

Conclusion :

Slovak Grid NGI virtual center of excellence will build upon human capital and expertise in porting applications to HPC clusters, grids and clouds to help researchers from various disciplines to fully utilize potential of EGI and other e-Infrastructures (on national as well as transnational level) to deliver excellent and innovative science.

Scientists currently debate the future impact of nanotechnology that may be able to create many new materials and devices with a vast range of applications, such as in medicine, electronics, biomaterials, energy production as well as in many other areas.

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