

# Increasing the attractiveness of EGI for computational chemistry

*Tuesday, 18 September 2012 15:00 (15 minutes)*

## Description of the work

Virtual Organisations that the EGI community offers in the 'Computational Chemistry and Material Sciences' domain; Identifying key scientific applications that could benefit from resources and services of the National Grid Infrastructures, and assists the integration of these applications with these services through focused technical projects. The work aimed at increasing the number of EGI beneficiaries from the computational chemistry and material sciences domain by improving the portfolio of services that EGI provides for researchers and application developers in this field. The talk will present the achievements of the seconded application expert and the lessons learnt by EGI from this work.

## Wider impact of this work

## Printable Summary

EGLeu as an organisation that coordinates the work of the European Grid Infrastructure community is involved in a number of projects. These projects require on occasion skills and effort beyond which EGLeu has available internally. To respond to these needs, and allow the exchange of experiences between EGLeu and NGI/EIRO staff, EGLeu established a secondment programme that allows technical staff from organisations affiliated to EGLeu as participants or associated participants, to work at EGLeu on these projects. An application expert from the Lithuanian NGI, with scientific background in computational chemistry has been working at EGLeu for three months in 2012 in the secondment programme. Her task involved the review of existing applications, tools and

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**Session Classification:** Experience in community building

**Track Classification:** Community and Co-ordination (Sergio Andreozzi: track leader)