PRACE: how an european research infrastructure supports the graphene community

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SUMMARY

PRACE (Partnership for Advanced Computing in Europe) is a pan European research infrastructure spanning over 25 countries which aims to offers to European scientists access to world-class resources and services in HPC (High Performance Computing) and advanced numerical simulation. Established since April 2010 with a seat in Brussels (Belgium), PRACE is providing in 2014 a unique computing capacity of more than 15 Petaflops across 6 complementary supercomputers based in France, Germany, Italy and Spain.

By offering this unique aggregated computing power and services upon a single peer-review based on scientific excellence, PRACE is allowing its scientific and industrial users to have access to similar capacities and services like their competitors in USA, China, Japan or Russia. Since this level of resources and diversity of HPC architectures was clearly unreachable for any single European country, THE rationale of PRACE was to unite efforts from European countries in order to sustain scientific and industrial competitiveness of Europe.

Since mid 2010 PRACE has been able to allocate close to 7 billion cpu core hours on 259 research projects, allowing major breakthroughs in climate modelling, astrophysics, chemistry, materials, biology and medicine or combustion to name a few.

The study of graphene-based materials and other families of two-dimensional materials crucially demands for advanced simulation techniques to explore realistic models of materials of technology and industrial relevance. To that end, beyond the development of suitable numerical approaches for studying large-scale models, the access, implementation and use of high-performance computing has become a strategic value for Europe.

In this talk, the European High Performance Computing infrastructure (PRACE) will be briefly presented, and illustrated with an undergoing scientific project focused on simulation of Hall Kubo conductivity in graphene-based materials. The scalability and performance of supercomputers will be shown on a concrete study of quantum Hall effect in structurally and chemically disordered graphene, with new physics revealed thanks to such computing resources, and out of reach otherwise.