# Status of Simulation Laboratories at JSC

In recognition of the extreme software challenges facing its HPC users the Jülich Supercomputing Centre (JSC) has begun to set up a new, high-level support structures: Simulation Laboratories. The JSC blueprint defines a simulation laboratory (SimLab) as a community-oriented research and support team, consisting of a core group located at a supercomputer centre and possibly a number of associated scientists outside. A key requirement for the viability and visibility of the SimLab is that as far as possible, the core team should be hired from the community which it is designed to serve and interact with. In this way, the expertise offered can go far beyond the support of a traditional expert advisor, who might typically be able to perform application performance analysis and bottleneck identification, but would not possess the disciplinary know-how to carry out the necessary code restructuring.

The activities which characterize a simulation laboratory will of course vary depending on the make-up and location of its scientific community, but in general will comprise a combination of specialized and more generic tasks, such as:

- Participation in research projects of the community, including active col laboration with user projects and common publications.

- Development and maintenance of software and databases for the whole community.

- Research and development of computational methods needed by major applications on high-end systems.
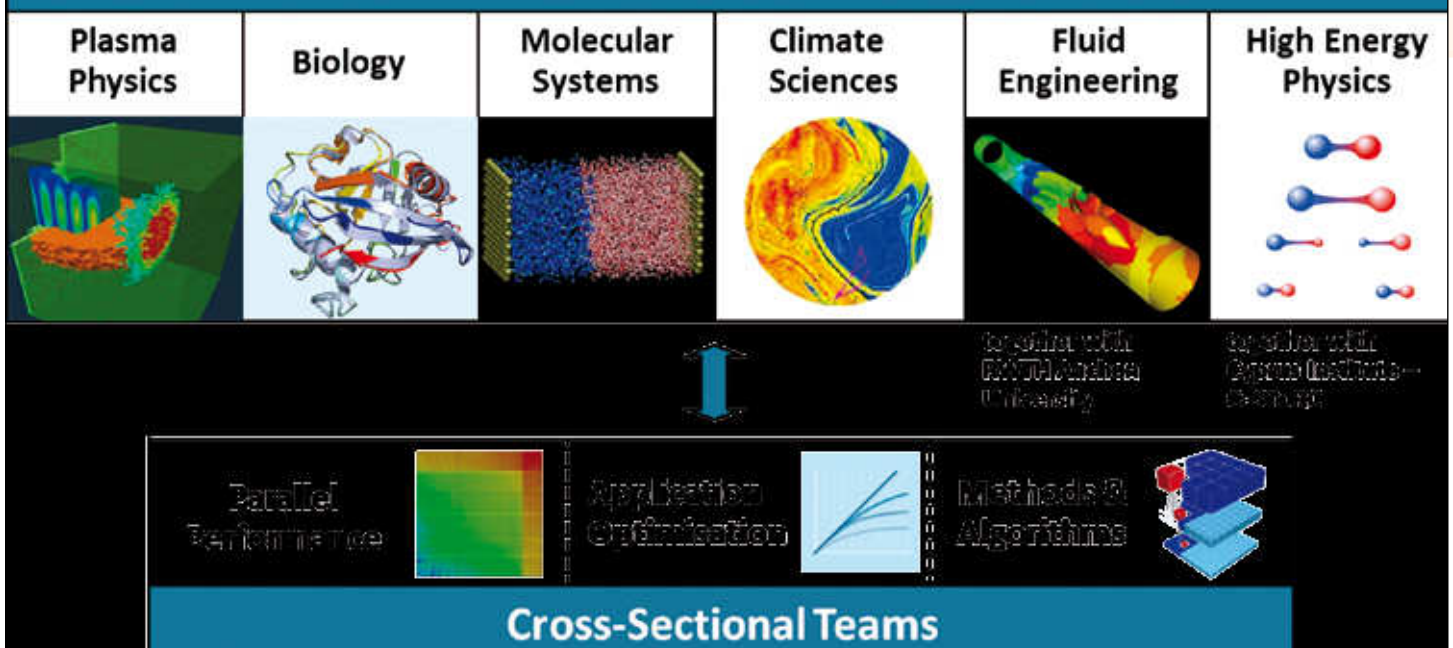
- Performance analysis, diagnosis and adaptation/optimization of software on highly scalable high-end supercomputers.

- Running training courses in computational methods and in efficient usage of high-performance systems.

- Community building measures such as the organization of community-oriented workshops and construction of web-portals.

Three Simulation Labs based on the above blueprint have now been established at JSC in the fields of Computational Biology, Molecular Systems and Plasma Physics, which have already been actively engaged with user groups from their respective communities over the past year. A fourth SimLab in Climate Modelling will come on stream in 2011, and two more in Fluid Engineering and High-Energy Particle Physics are also planned within the next two years. The SimLabs are currently staffed at around 2-3 postdocs with a similar number of PhD and Master students and/or technicians (in software/programming). In addition to the Simulation Laboratories, JSC also houses a number of Cross-Sectional Teams that focus on the development of generic HPC methods and algorithms, programming tools and petabyte data repositories. These complement the work of the Simulation Laboratories by providing first-hand expertise in computer science and numerical mathematics. A short summary of the JSC SimLab profiles can be found at:

http://www.fz-juelich.de/jsc/simlabs

Over the past year, the first three simulation labs at JSC have endeavored to establish themselves as autonomous research and support units. This has involved a range of community engagement activities, including: short visits of scientists to port and analyse applications to the JSC supercomputers; participation in major German and European HPC proposals; and the staging of a joint workshop in June 2010 to promote HPC activities within their respective scientific communities.

As a next logical step to consolidate these initial community-building activities, JSC has issued its first call to current and potential users of the supercomputers in Jülich to apply for high-level support from the Simulation Labs. Specific support actions covered by this call include: restructuring of computational methods needed to exploit highly parallel architectures, performance analysis and scaling improvement of codes/applications, as well as porting of new codes to the Juropa and Jugene systems. In this 6-month pilot phase, work packages will not exceed 2 person-months of SimLab staff resources. Applicants are also expected to contribute an equivalent amount of manpower to the project, particularly where the work involves major code/algorithm redevelopment. In the longer term, it is expected that project proposals will grow in number, duration and complexity, and will therefore inevitably require some form of ranking via an advisory committee.
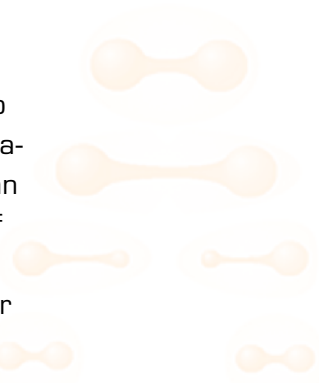
Projects

• Paul Gibbon

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