Simulation labs: A new model for research community support

Dirk Pleiter



ZCUM11, 21 March2011

Concept

- Simulation Laboratory (SL) = Competence centre for a specific research community
 - Performs research and provides support
 - Research staff is part of the community

Tasks

- Development of HPC eco-system tailored for the target research community
- Assist in optimizing use of available compute resources
- Perform large-scale simulations
- Provide field-specific training

Realisation in Germany

- SLs first established at Jülich Supercomputing Centre (JSC)
 - Established SLs: Biology, Plasma Physics, Molecular Systems, Climate Science
 - More SimLabs planned
- SLs have become part of HGF program "Supercomputing"
 - SLs at KIT: NanoMicro, Astro- and Elementary Particles

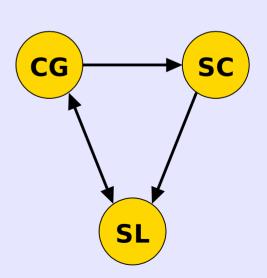
Structure and operation (as proposed by JSC)

Structure

- Minimal SL team size: 1 senior scientist, 1-2 postdocs, PhD & MSc students (+ technical staff)
- Steering Committee (SC) with members from research community (and hosting institution)

Operation

- Community research groups (CG)
 - Make proposals for work program
 - Submit request for support
- SC defines work program



Lattice QCD SL at DESY

- Status: Joined SL for LQCD under discussion
 - Involved institutions: CaSToRC (Cyprus), JSC (Jülich), DESY (Zeuthen)

Tasks:

- Development of algorithms and optimized implementation of application kernels
- Performance benchmarking and analysis
- Analysis and development of HPC architectures
- Data curation
- Training
- Large-scale simulations and LQCD research

Tentative work program

- WP1: Algorithms and Application Kernels
 - Analysis of cache efficiency of kernel implementations
 - Hybrid-parallelization of application program DD-HMC
- WP2: Application Requirements and Performance Analysis
 - Definition and compilation of LQCD benchmark suite
 - Parametric performance model for benchmark suite
- WP3: Analysis and Development of HPC Architectures
 - Technical design studies
- WP4: Data Curation and LatFor Data Grid (LDG)
 - ILDG working groups, LDG operation, VO management
- WP5: Training
 - "Lattice Practices" workshops, summer students