High-Q en route to exascale

Scaling applications to the full JUQUEEN system with 458 752 cores and over 1.8M threads

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JUQUEEN Porting & Tuning and Extreme Scaling Workshops, 2–6 February 2015

- **7 teams invited to (im)prove their application scalability with 30 hours of dedicated access to the entire JUQUEEN system**
- **Expert assistance provided by JSC Simulation Laboratories (SimLabs) and Cross-sectional teams, with IBM and JUQUEEN technical support**
- **All 7 teams within 24 hours successfully ran their codes using the full system, preparing for entry to the High-Q Club**
- **Additional experience gained about effectively exploiting extremely scalable computer systems**

CoreNEURON (F. Delalondre & A. Ovcharenko, EPFL Blue Brain Project) simulation of electrical activity of neuronal networks including morphologically detailed neurons

FE2TI (M. Lanser, Universität Köln & O. Rheinbach, TUB Freiberg) scale-bridging incorporating micro-mechanics in macroscopic simulations of multi-phase steels

FEMPAR (A. Martín, UPC-CIMNE) massively-parallel finite-element simulation of multi-physics problems governed by PDEs

ICON (T. Jahns, DKRZ & C. Meyer, JSC SimLab Climate Science) icosahedral non-hydrostatic atmospheric model

MPAS-A (D. Heinzeller, KIT) multi-scale non-hydrostatic atmospheric model for global, convection-resolving climate simulations

psOpen (M. Gauding, RWTH-ITV Inst. for Combustion Technology & J.-H. Göbbert, JARA) direct numerical simulation of fine-scale turbulence

SHOCK (M. Gageik, RWTH Shock Wave Laboratory) structured high-order finite-difference kernel for compressible flows

JUQUEEN

IBM BlueGene/Q with **28 racks**, 28 672 nodes.
Each 1.6 GHz PowerPC A2 compute **node** has:

- 16 cores with 64 hardware threads
- 16 GB memory, 32 MB L2 Cache

In total 458 752 cores with 1 835 008 threads.
Aggregate I/O bandwidth 200 GB/s to GPFS.

Impediments to large-scale executions

File I/O Large machine runs often require parallel I/O, but which is no guarantee of success: SHOCK and CoreNEURON had to limit or disable I/O. ICON, MPAS-A, and psOpen employ PIO/NetCDF, HDF5 or pNetCDF to read in up to 1.2 TB of data. An exception are codes making use of SIONlib, which is developed by JSC to address I/O scalability. Examples using SIONlib are High-Q members KKRnano, MP2C, and muPhi.

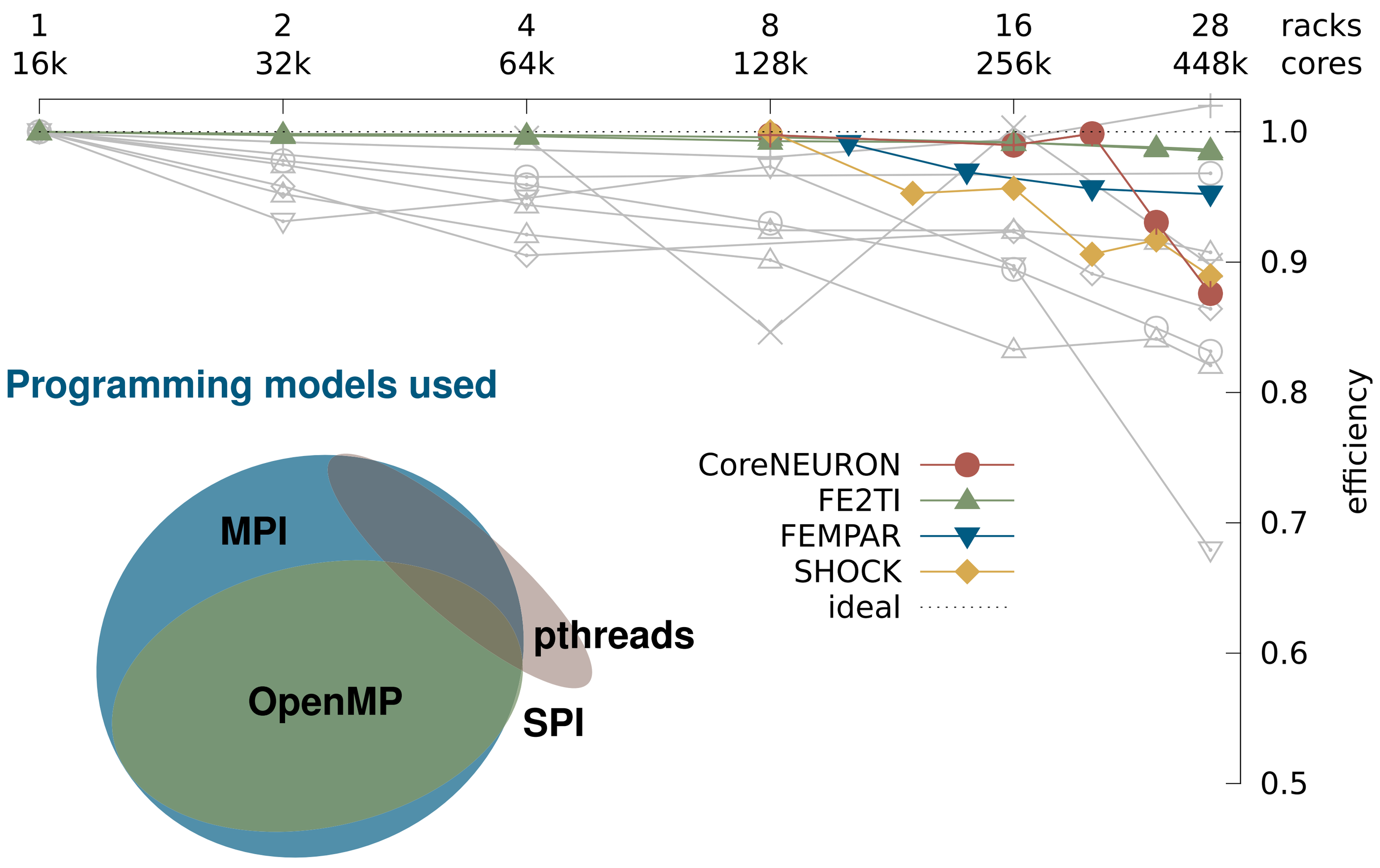
Memory The limited amount of memory available per node provides constraints not only for strong scaling runs: After tuning the problem size CoreNEURON was able to use 15.9 GB (99%) of the available RAM, FEMPAR had to trade memory for MPI against prohibitive MPI execution times, and MPAS-A was limited to 16 MPI ranks per node to fit in 1 GB per process.

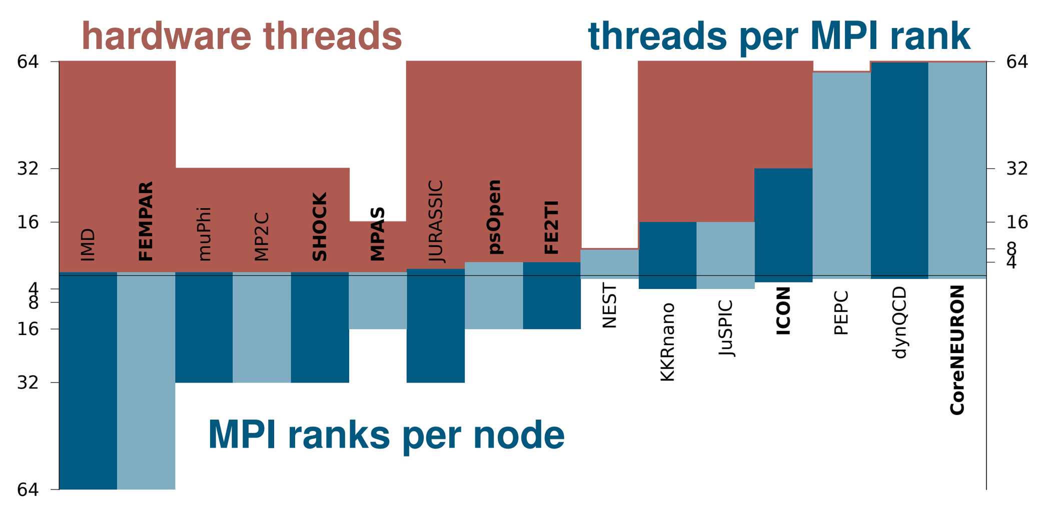
Results

On the right is a selection of results from the High-Q Club and Extreme Scaling Workshop:

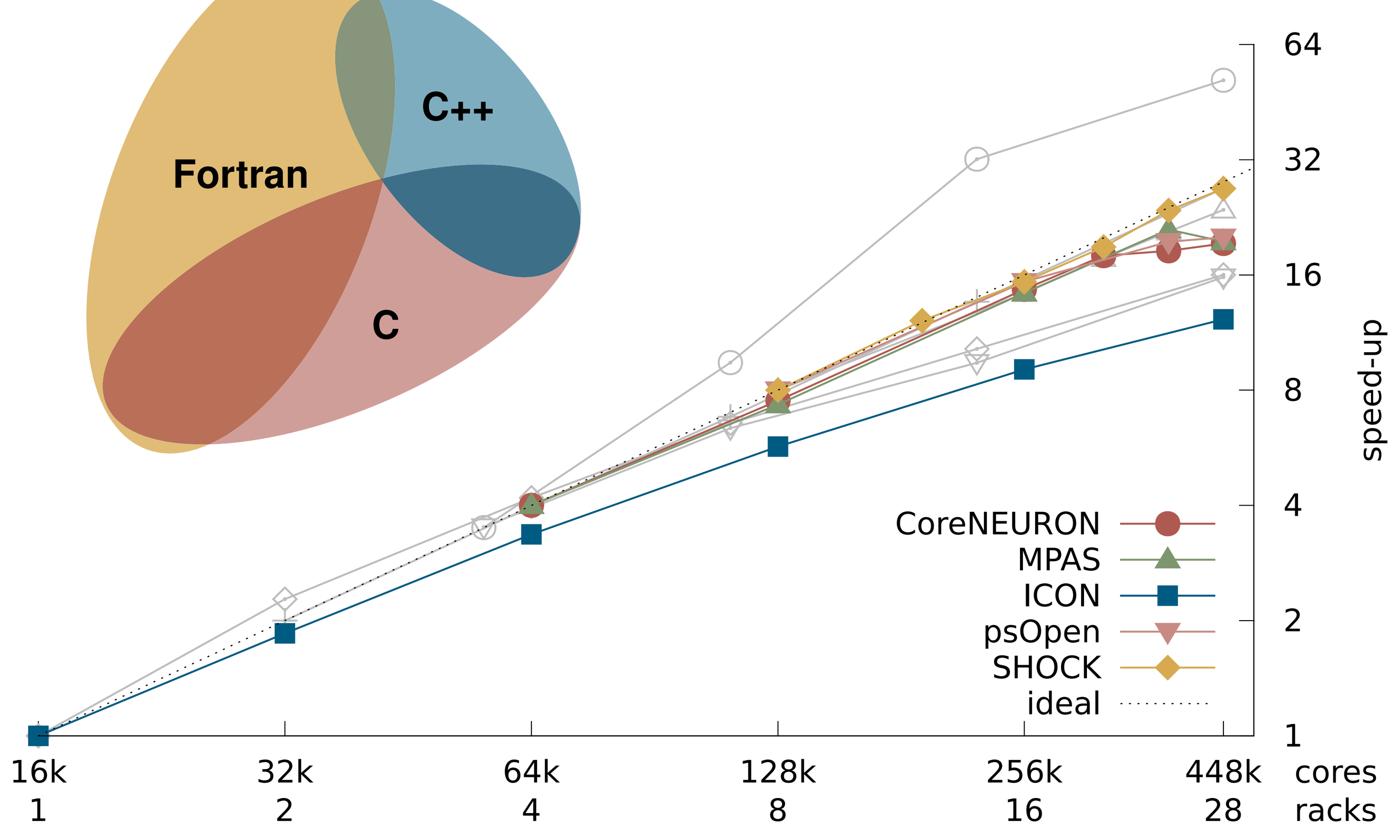
- Weak and strong scaling graphs summarise some of the submitted performance data. (For reference, High-Q club codes grey and unlabelled.)
- Venn set diagrams with statistics about the programming models and languages used by the codes provide the colour key to the code listing. While all 3 programming languages are roughly equally popular, mixed-mode programming combining MPI and multi-threading dominates.
- A bar chart shows the breadth of MPI process / thread combinations used and the extent of oversubscription of cores to fully exploit the hardware capabilities.
- More results can be found in the technical report **FZJ-JSC-IB-2015-01**

Weak scaling





Programming languages used



Strong scaling

High-Q Club Codes

dynQCD (JSC SimLab Nuclear and Particle Physics & Bergische Universität Wuppertal) lattice quantum chromodynamics with dynamical fermions

Gysela (CEA-IRFM Cadarache) gyrokinetic semi-Lagrangian code for plasma turbulence simulations

IMD (Ruhr-Universität Bochum & JSC SimLab Molecular Systems) classical molecular dynamics simulations

JURASSIC (JSC SimLab Climate Science) solver for infrared radiative transfer in the Earth's atmosphere

JuSPIC (JSC SimLab Plasma Physics) fully relativistic particle-in-cell code, plasma physics simulations, laser-plasma interaction

KKRnano (FZJ-IAS) Korringa-Kohn-Rostoker Green function code for quantum description of nano-materials in all-electron density-functional calculations

MP2C (JSC SimLab Molecular Systems) massively-parallel multi-particle collision dynamics for soft matter physics and mesoscopic hydrodynamics

$\mu\phi$ (muPhi) (Universität Heidelberg) modelling and simulation of water flow and solute transport in porous media, algebraic multi-grid solver

Musubi (Universität Siegen) multi-component Lattice Boltzmann solver for flow simulations

NEST (FZJ/INM-6 & IAS-6) large-scale simulations of biological neuronal networks

OpenTBL (Universidad Politécnica de Madrid) direct numerical simulation of turbulent flows

PEPC (JSC SimLab Plasma Physics) tree code for *N*-body simulations, beam-plasma interaction, vortex dynamics, gravitational interaction, MD simulations

PMG+PFASST (LBNL, Universität Wuppertal, USI & JSC) space-time parallel solver for systems of ODEs with linear stiff terms, e.g. from lines discretisations of PDEs

PP-Code (University of Copenhagen) simulations of relativistic and non-relativistic astrophysical plasmas

TERRA-NEO (Universität Erlangen-Nürnberg, LMU & TUM) modeling and simulation of earth mantle dynamics

waLBerla (Universität Erlangen-Nürnberg) Lattice-Boltzmann method for the simulation of fluid scenarios

Programming Model
and Language

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