

The High-Q Club

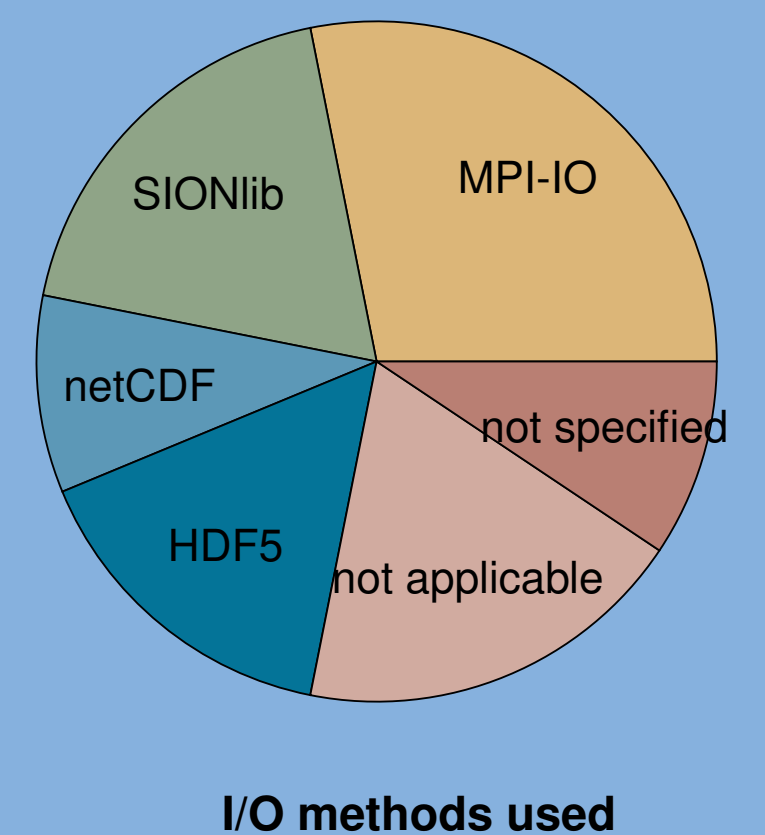
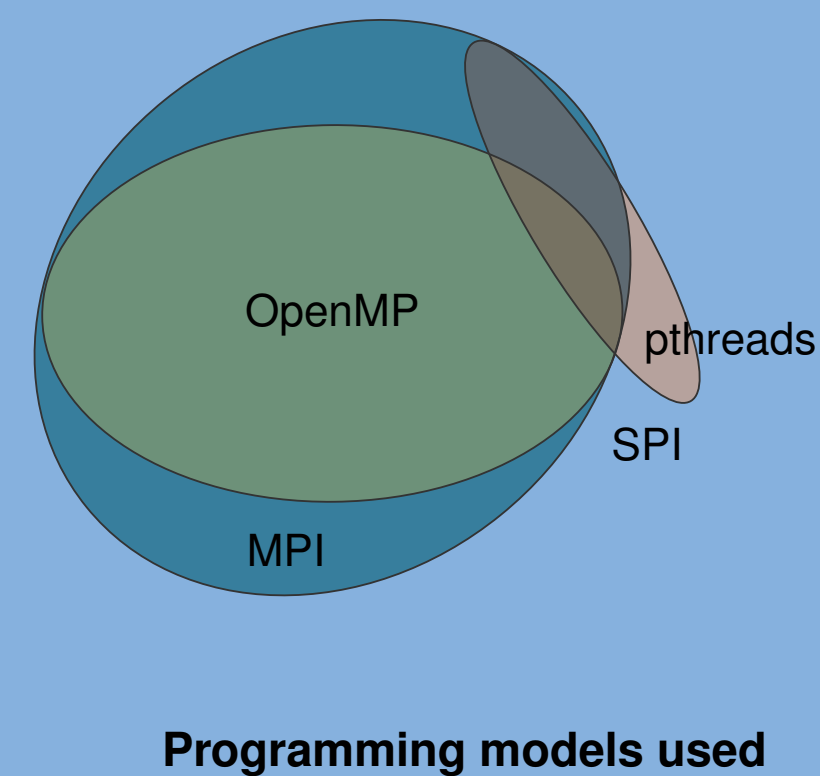
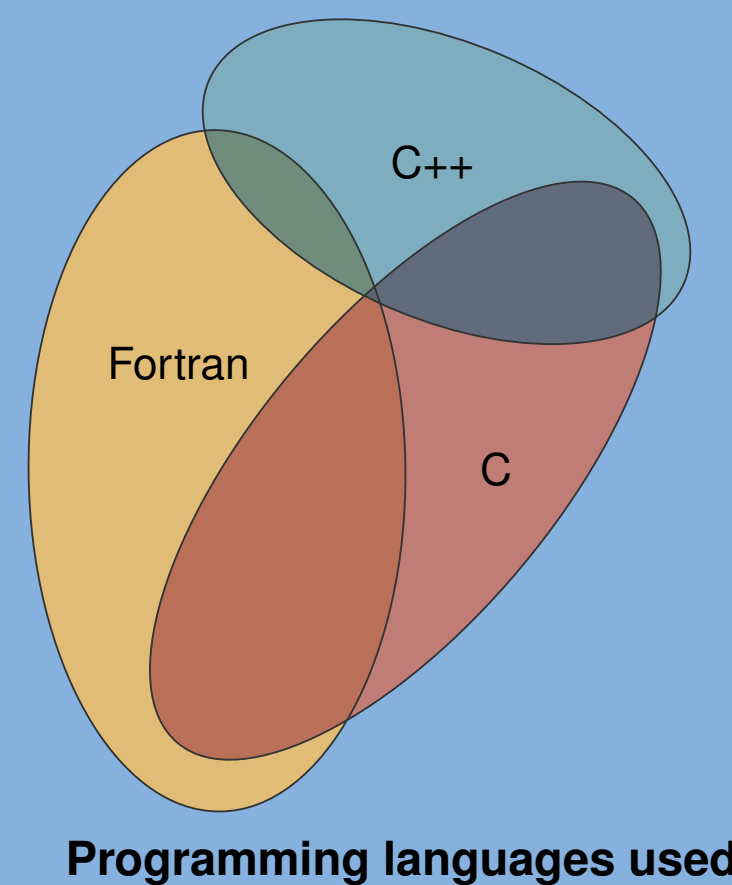
Applications scaling to the full JUQUEEN system with 458 752 cores and over 1.8M threads

Dirk Brömmel, Wolfgang Frings, and Brian J. N. Wylie | Jülich Supercomputing Centre | Forschungszentrum Jülich GmbH

Contact: {d.broemmel, w.frings, b.wylie}@fz-juelich.de | **DOI:** 10.14529/jsfi180104 | **Website:** www.fz-juelich.de/ias/jsc/high-q-club



- Showcase of 32 application codes demonstrating extreme scalability from diverse fields and global developer community
- Based on effective use of full JUQUEEN IBM Blue Gene/Q system (installed spring 2012, decommissioned spring 2018)
- 28 racks, 28 672 processors, 458 752 cores, 1 835 008 threads (16 GiB memory/processor, 5D torus network, GPFS filesystem)
- Membership supported by 3 Extreme Scaling Workshops, JSC Simulation Laboratories and Cross-Sectional Teams
- Application benefits extended beyond BG/Q to other HPC leadership computer systems
- Potential insight for expected future exa-scale applications
- Reference basis for successor activity



Lessons

- Compute node memory and file I/O are common constraints
- Need effective parallel I/O solutions for metadata and bandwidth, such as SIONlib
- Standard programming languages and MPI combined with multi-threading suffice
- Optimised libraries developed for efficient mesh partitioning and non-blocking 3D FFTs
- Tuning often required as directed by tools such as Scalasca

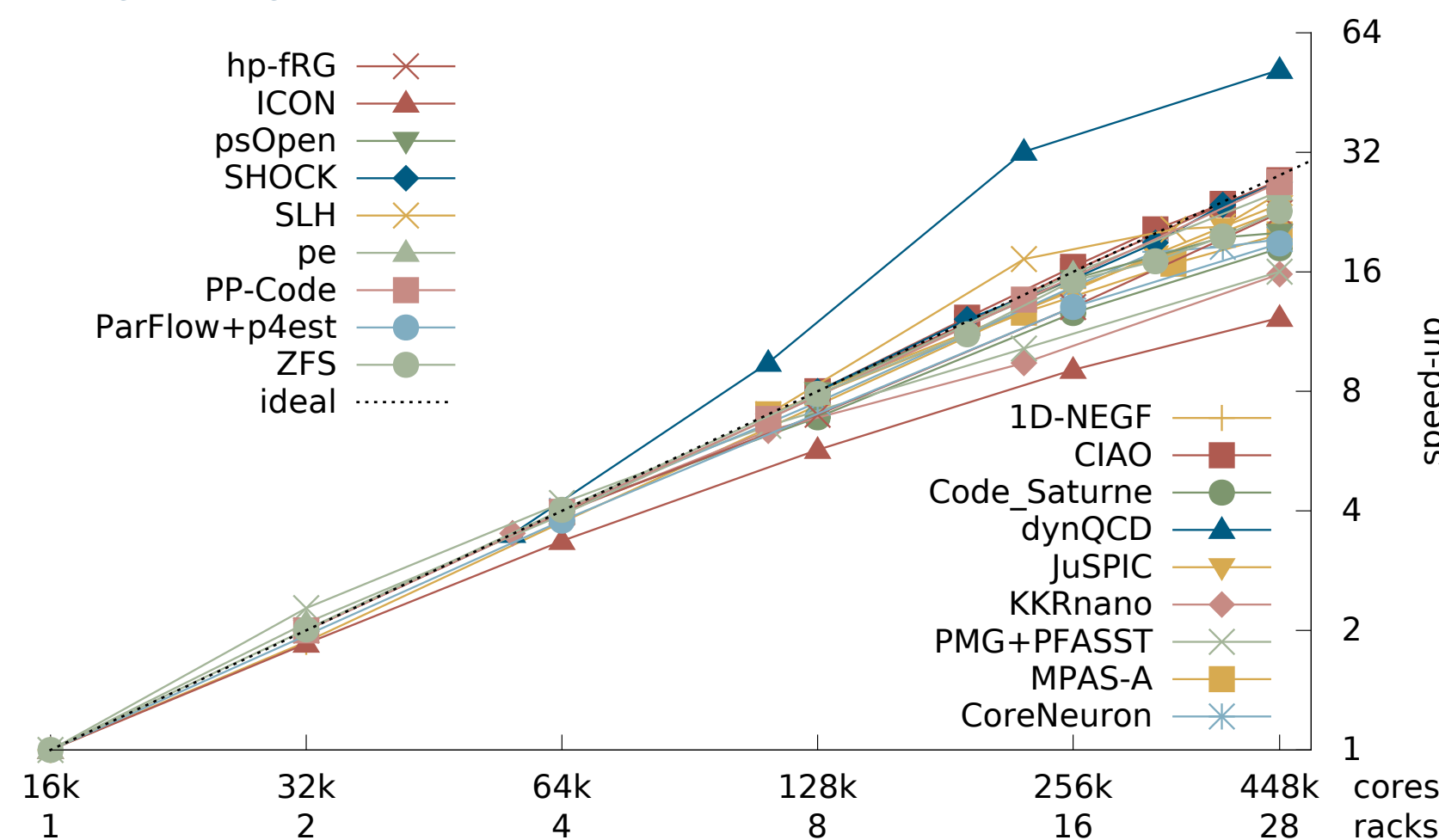
Application characteristics

- Fortran, C & C++ languages all used, and often combined
- MPI usage ubiquitous, mostly with OpenMP and/or pthreads mixed-mode combination more memory-efficient
- Additionally used hardware threads benefitted most codes
- SIONlib, MPI-IO & HDF5 equally prevalent for file I/O (often data synthesised or writing disabled as workarounds)

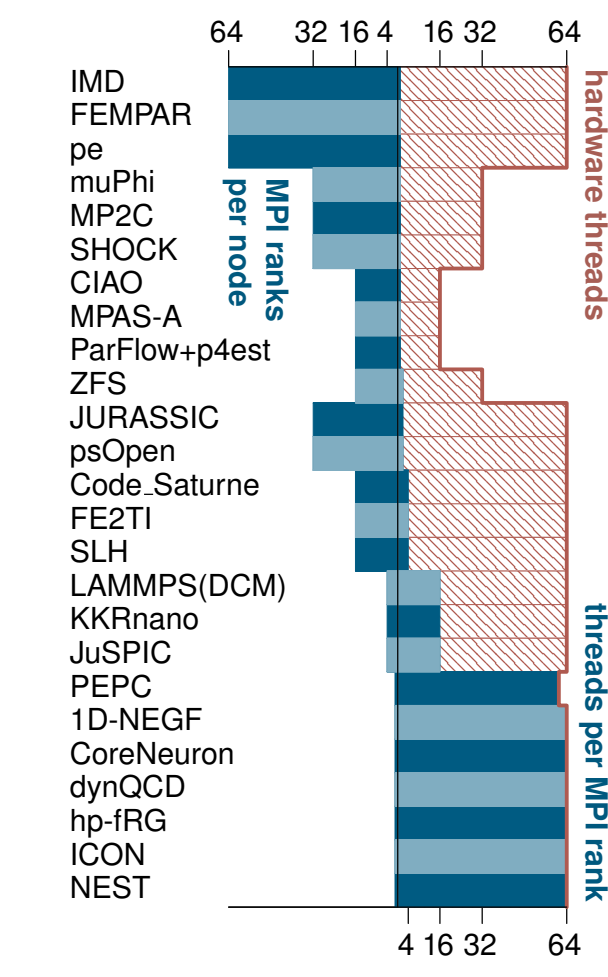
Scaling performance

- Weak scaling is easiest: 12 codes with scaling efficiency over 80%
- Strong scaling is much more challenging: 10 codes maintained normalised scaling efficiency over 80% (compute node memory requirements can limit baseline to quarter of machine)
- Cache benefits and machine topology can be important

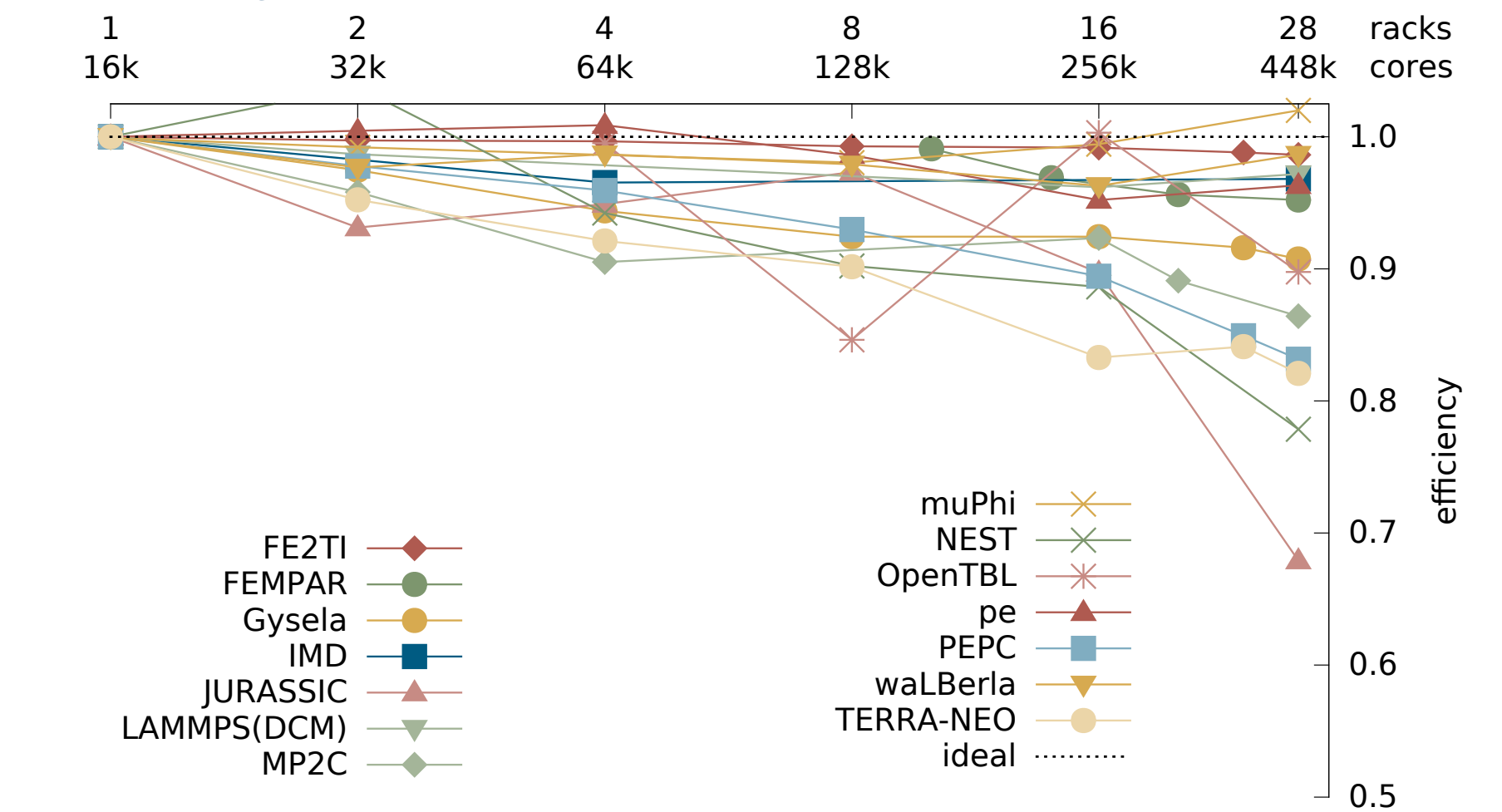
Strong scaling



Hardware threads



Weak scaling



High-Q Club codes

- 1D-NEGF** (JSC SimLab Quantum Materials) 1D Non-Equilibrium Green's Functions framework for transport phenomena
- CIAO** (RWTH ITV) multiphysics, multiscale NS solver for turbulent reacting flows in complex geometries
- Code_Saturne** (EDF & STFC Daresbury Laboratory) multiphysics simulation of the Navier-Stokes equations
- CoreNeuron** (EPFL Blue Brain Project) simulation of electrical activity of neuronal networks including morphologically detailed neurons
- dynQCD** (JSC SimLab Nuclear and Particle Physics & Bergische Universität Wuppertal) lattice quantum chromodynamics with dynamical fermions
- FE2TI** (Universität Köln & TUB Freiberg) scale-bridging incorporating micro-mechanics in macroscopic simulations of multi-phase steels
- FEMPAR** (UPC-CIMNE) massively-parallel finite-element simulation of multi-physics problems governed by PDEs
- Gysela** (CEA-IRFM Cadarache) gyrokinetic semi-Lagrangian code for plasma turbulence simulations
- hp-fRG** (JSC) hierarchically parallelised functional renormalisation group calculations
- ICON** (DKRZ & JSC SimLab Climate Science) icosahedral non-hydrostatic atmospheric model
- 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
- LAMMPS(DCM)** (RWTH AICES) molecular dynamics simulation with dynamic cutoff method for arbitrarily large interfacial systems
- MP2C** (JSC SimLab Molecular Systems) massively-parallel multi-particle collision dynamics for soft matter physics and mesoscopic hydrodynamics
- MPAS-A** (KIT & NCAR) multi-scale non-hydrostatic atmospheric model for global, convection-resolving climate simulations
- μφ (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
- ParFlow+p4est** (FZJ IBG-3, Colorado School of Mines, LLNL & Universität Bonn) high resolution parallel simulation of variably saturated flow

- pe** (Universität Erlangen-Nürnberg) physics engine framework for simulations of rigid bodies with arbitrary shapes
- 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
- psOpen** (RWTH ITV, JARA & CNRS CORIA) highly-resolved direct numerical simulation of fine-scale turbulence
- Seven-League Hydro** (Heidelberg Institute for Theoretical Studies) all Mach number fluid dynamics in astrophysics
- SHOCK** (RWTH Shock Wave Laboratory) structured high-order finite-difference kernel for compressible flows
- 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
- ZFS** (RWTH AIA & JARA SimLab Fluids & Solids) Computational fluid dynamics, computational aeroacoustics, conjugate heat transfer, particulate flows

Programming language and model I/O