

JÜLICH SUPERCOMPUTING CENTRE

CROSS-SECTIONAL TEAM MATHEMATICAL METHODS AND ALGORITHMS



Algorithms and Software for CS&E

Fast Multipole Method

- Porting to GPUs
- Introducing of I-dynamics
- Part of the DFG project GROMEX (SPPEXA)

Parallel-in-time integration algorithms

- Up to 448K cores on an IBM Blue Gene/Q with a full space-time parallel multigrid solver
- Part of the BMBF project ParaPhase
- · Fault-tolerant parallel-in-time integration techniques

Mathematical morphology for color images Mathematical modeling software

Models and Simulations

CFD

 Massively parallel gas turbine simulations with OpenFOAM on JURECA

FEM

- Simulation of the Second Bosphorus Bridge
- Seismic analysis for asynchronous and multi-support excitations

Numerical Linear Algebra

- · Solving large-scale eigenvalue problems
- Performance analysis of mathematical libraries (ScaLAPACK, ELPA, Elemental)
- · Numerical kernels for hybrid systems
- Mathematical analysis of parallel-in-time integration methods using multigrid techniques

Cooperation with SimLabs

Molecular Systems

- ScaFaCos library: Parallelization of FMM
- Large-scale parallel-in-time MD simulations

Neuroscience

- Determination and correction of optical distortion
- Parallelization of Polarized Light Imaging workflow
- Processing images with a total amount of 1 PB/brain

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