Extreme Scaling of Real World Applications to >130,000 Cores on SuperMUC

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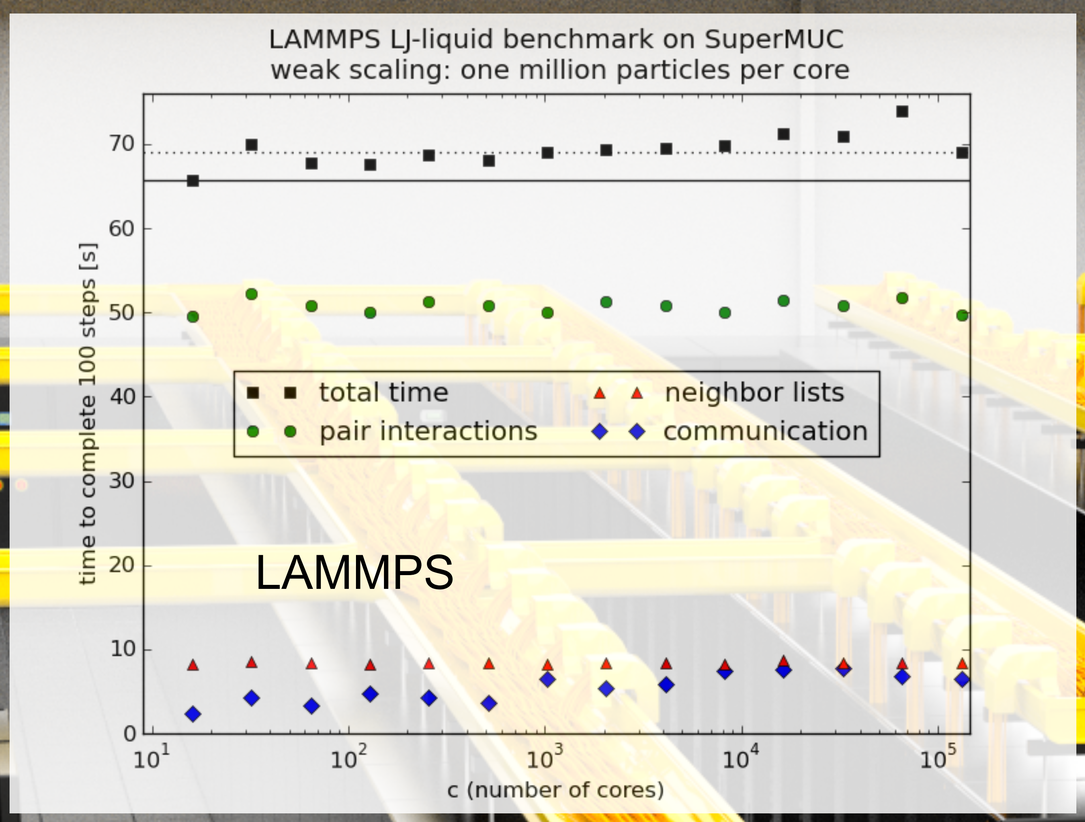
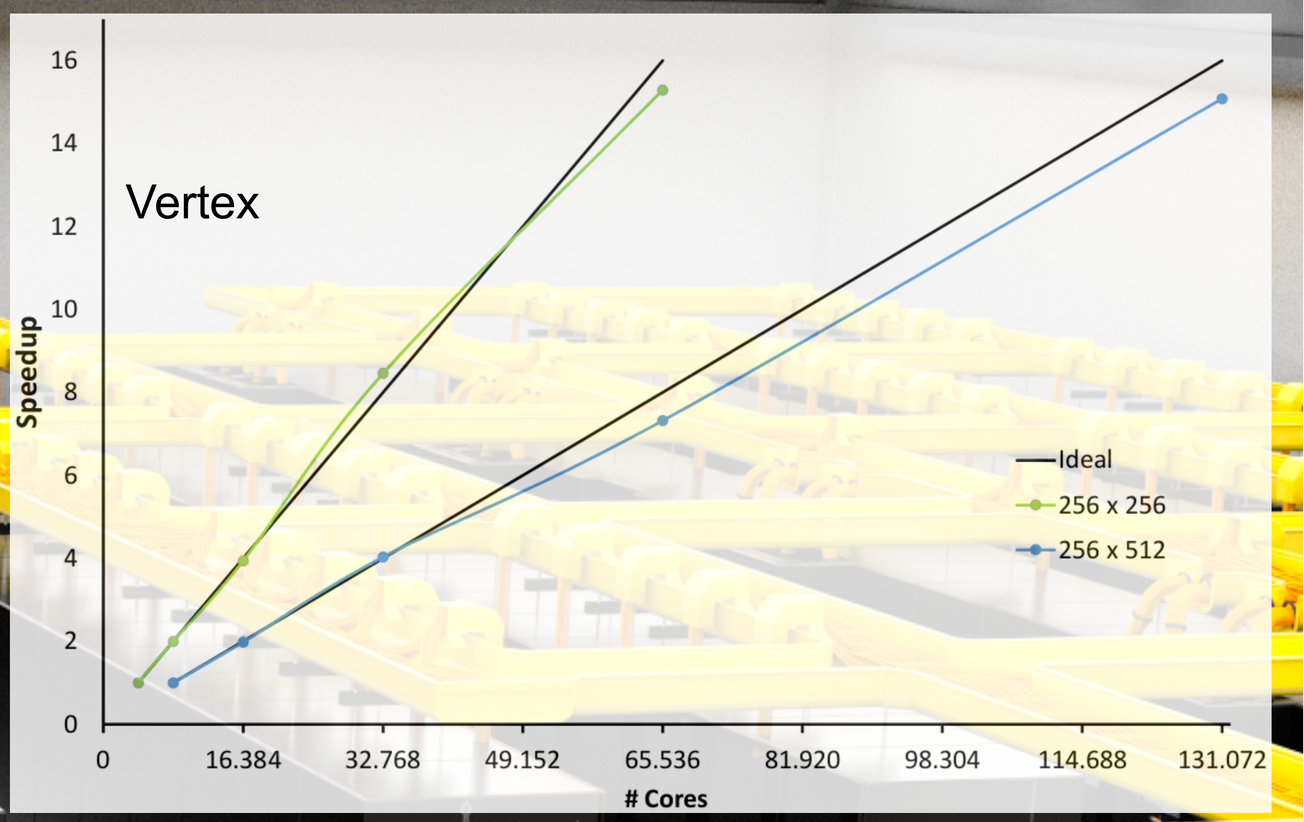
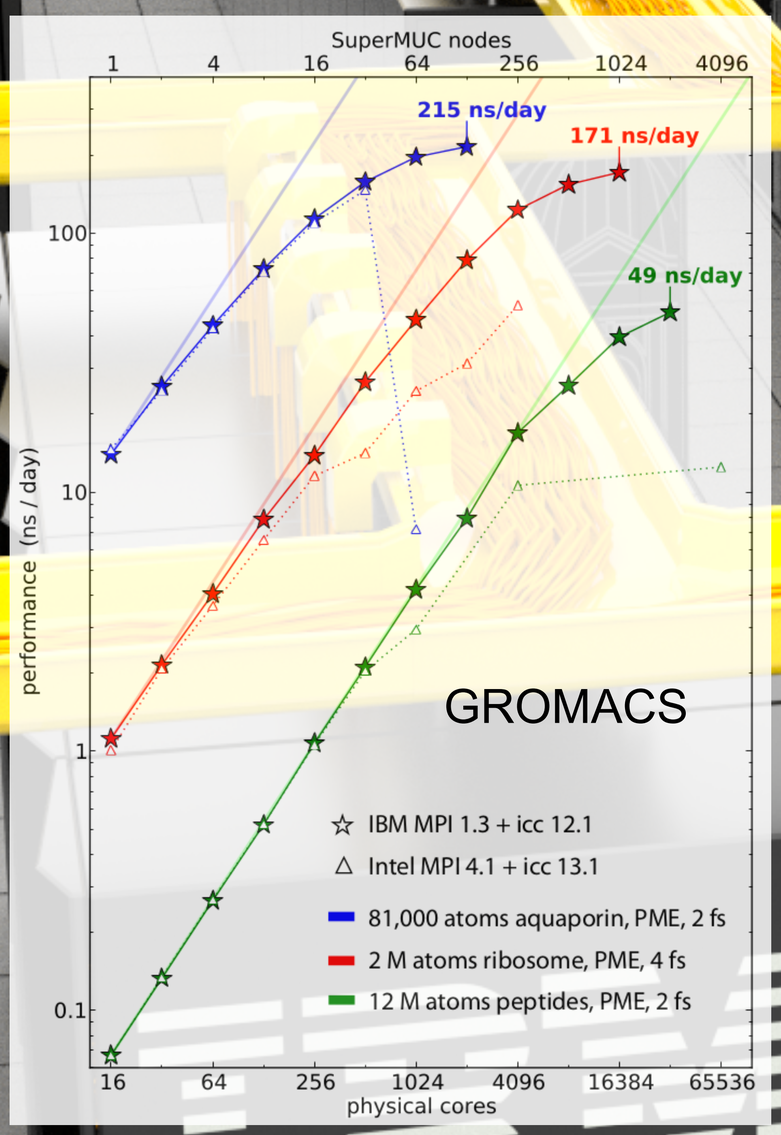
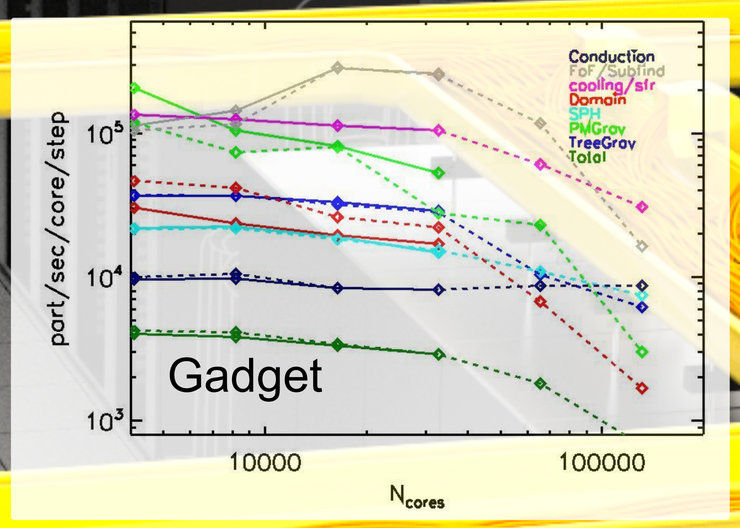
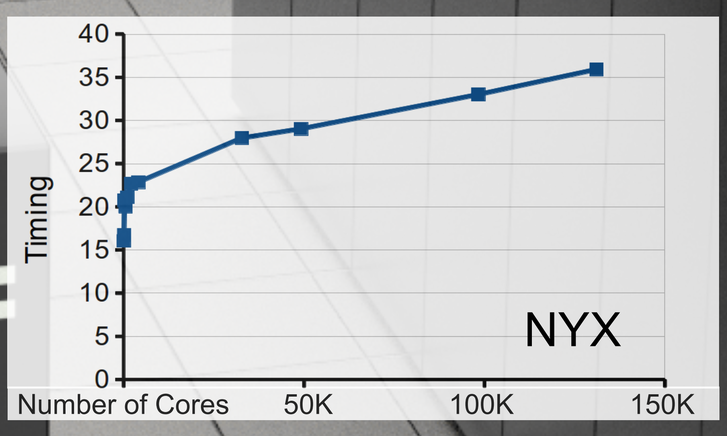
Abstract: In July 2013, the Leibniz Supercomputing Centre (LRZ) held the first workshop to test extreme scaling on SuperMUC, the 3 PFLOP/s system with 147,456 Intel Sandy Bridge CPU cores. Groups from 15 international projects came to the LRZ with codes that had already shown scaling up to 4 islands (32,768 cores). During the workshop, the participants could test the scaling capabilities of their codes on the whole system. Application experts from the LRZ, Intel and IBM were on site to resolve issues and assist in the performance optimization. New techniques like fast startup were successfully tested which helped to reduce the startup time by a factor of 2-3. At the end of the workshop, 6 applications were successfully running on the full machine, while the other 8 applications managed to run on half of the system. All projects were able to generate scaling curves up to 8 or 16 islands. From the preliminary data the following Flops rates have been obtained: 250 TFlop/s for VERTEX on 16 and 223 TFlop/s for Gromacs on 4 islands. The measured Flop rates for the complete application codes correspond to 10% or more of the peak performance of SuperMUC. These results obtained in a short workshop can definitely compete with results reported from other Top10 supercomputers such as the K-computer and the Blue Waters system. They demonstrate the usability of SuperMUC for real world applications. The LRZ is already planning a follow-up workshop where the improvements and feedback from the experts will be tested. For more information, visit us at http://www.lrz.de.











SuperMUC has a theoretical peak performance of 3.185 PFLOP/s. **LINPACK** achieves 161 TFLOP/s on one island, 2.56 PFLOP/s on 16 islands, and 2.897 PFLO/s on 18 islands. The following real world applications ran successfully on SuperMUC (absolute performance numbers are given where available):

BQCD[7]: Hybrid Monte-Carlo program for simulating lattice QCD with dynamical Wilson fermions. BQCD managed to achieve 10TFLOP/s on one island (8192 cores) and 27 TFLOP/s on 16 islands.

CIAO[6]: Second order, semi-implicit finite difference code (combustion research).

Gadget[4]: TreePM-MHD-SPH code (astrophysics).

GROMACS[2]: Molecular dynamics code. GROMACS achieved 98 TFLOP/s on one island, 154 TFLOP/s on two islands and 223 TFLOP/s on four islands.

LAMMPS[3]: Classical molecular dynamics code. LAMMPS achieved 5.6 TFLOP/s on one island and 90 TFLOP/s on 16 islands.

Nyx[1]: N-body and gas dynamics code (astrophysics).

Vertex[5]: Neutrino-radiation hydrodynamics code, simulates from first principles the physical processes during the evolution of a supernova explosion. Vertex achieved 15 TFLOP/s on one island and 250 TFLOP/s on 16 islands.