© 2013 FIZ Karlsruhe

io-port 05705895

Saksena, Radhika S.; Boghosian, Bruce; Fazendeiro, Luis; Kenway, Owain A.; Manos, Steven; Mazzeo, Marco D.; Sadiq, S.Kashif; Suter, James L.; Wright, David; Coveney, Peter V.

Real science at the petascale.

Philos. Trans. R. Soc. Lond., Ser. A, Math. Phys. Eng. Sci. 367, No. 1897, 2557-2571 (2009).

Summary: We describe computational science research that uses petascale resources to achieve scientific results at unprecedented scales and resolution. The applications span a wide range of domains, from investigation of fundamental problems in turbulence through computational materials science research to biomedical applications at the forefront of HIV/AIDS research and cerebrovascular haemodynamics. This work was mainly performed on the US TeraGrid 'petascale' resource, Ranger, at Texas Advanced Computing Center, in the first half of 2008 when it was the largest computing system in the world available for open scientific research. We have sought to use this petascale supercomputer optimally across application domains and scales, exploiting the excellent parallel scaling performance found on up to at least 32 768 cores for certain of our codes in the so-called 'capability computing' category as well as high-throughput intermediate-scale jobs for ensemble simulations in the 32-512 core range. Furthermore, this activity provides evidence that conventional parallel programming with MPI should be successful at the petascale in the short to medium term. We also report on the parallel performance of some of our codes on up to 65 636 cores on the IBM Blue Gene/P system at the Argonne Leadership Computing Facility, which has recently been named the fastest supercomputer in the world for open science.

Keywords: petascale computing; parallel and distributed computing; lattice-Boltzmann methods; molecular dynamics; material simulation; computational biomedicine
doi:10.1098/rsta.2009.0049