

JSCNews

Jülich
Supercomputing
Centre

No. 230 • April 2015

Neutron-Proton Mass Difference Calculated Using JUQUEEN and JUROPA

In a recent paper published in the 27 March 2015 issue of Science, physicists from Budapest, Marseille, Wuppertal, and Jülich calculated the neutron-proton mass difference using the JUQUEEN and JUROPA supercomputers at JSC. This work was described as a 'landmark calculation' by Nobel laureate Frank Wilczek.

The mass difference results from two counteracting effects: for equal light quark masses, electrodynamics renders the proton slightly heavier due to the energy stored in the electromagnetic field that surrounds it. Differences in the light quark masses, conversely, increase the neutron mass, since the neutron contains two of the heavier down-quarks compared to one in the case of the proton. The interplay of these effects has significant implications for the stability of matter: if the neutron-proton mass splitting only differed slightly from the value found in nature, the universe as we know it could not exist.

Due to the complicated non-linear interaction between quarks and gluons, combined with the long-range nature of the electromagnetic interaction, this mass difference could not, until now, be calculated from the underlying theory, the Standard Model of elementary particle physics. Through a combination of new algorithms, analytical calculations and simulations on JUQUEEN and JUROPA, with contributions from machines at HLRS, LRZ, and IDRIS in France, the authors made 'breakthrough progress',

according to Wilczek, some 80 years after the discovery of the neutron and 40 years after the first formulation of the theory.

The Science article is available at <http://dx.doi.org/10.1126/science.1257050>, and Wilczek's comment at <http://dx.doi.org/10.1038/nature14381>. (Contact: Dr. Stefan Krieg, s.krieg@fz-juelich.de)

Update on the JURECA Time Plan

In JSC News No. 228, JSC announced its plan to replace the JUROPA system by a petascale successor system named JURECA. JSC and the vendor T-Platforms are now starting to install the first stage of the JURECA system, which is set to take over from JUROPA at the end of June. This first stage of JURECA will equal JUROPA in available computing power and will provide users with a production environment while the JUROPA cluster is dismantled and the remaining JURECA racks are installed.

A short service interruption, however, is necessary during the switch from JUROPA to JURECA in order to synchronize the home file system data between Lustre and GPFS. As communicated to all JUROPA users in March, JSC is automatically copying the user data from the Lustre home file systems on JUROPA to the centre-wide GPFS home file system that will be used on JURECA. The transfer of data from the Lustre to the GPFS work file system is the users' responsibility and all data that is not transferred before the end of life of JUROPA

Forschungszentrum Jülich GmbH
in der Helmholtz-Gemeinschaft
Jülich Supercomputing Centre
52425 Jülich | Germany

Phone +49 2461 61-6402

jsc@fz-juelich.de
www.fz-juelich.de/jsc

will be irretrievably lost. All JUROPA users are therefore kindly asked to start migrating their data as soon as possible. JSC will inform JUROPA users about the exact time plan through the 'message of the day', e-mail and on <http://www.fz-juelich.de/ias/jsc/jureca>.

(Contact: Dr. Dorian Krause, d.krause@fz-juelich.de)

4th PRACE Implementation Phase Project

PRACE-4IP is the fourth project in a series of PRACE implementation phase projects. The project is funded in the H2020 framework programme and started on 1 February 2015. Like its predecessors, PRACE-4IP is coordinated by Forschungszentrum Jülich. It has a budget of nearly € 16.5 million, a duration of 27 months and 26 partners. The project will support the transition from the initial five-year period (2010-2015) of the Research Infrastructure established by the Partnership for Advanced Computing in Europe (PRACE) to the next period, known as PRACE 2.0.

Over 250 researchers from 49 organisations (including third parties) in 25 countries will assist the PRACE Research Infrastructure and support PRACE users. PRACE-4IP will enable application codes for PRACE leadership platforms and prepare for future systems by investigating new programming tools and developing suitable benchmarks. The project will also continue and extend the highly visible training events including the PRACE Advanced Training Centres (PATCs). In order to support a balanced eco-system of HPC resources for Europe's researchers, the project will work on improving PRACE operations and prototyping new services. Links will be established to other e-infrastructures and the future Centres of Excellence, and the existing international collaborations will be extended. PRACE-4IP will expand its market watch and evaluation based on user requirements, study best practices for energy efficiency and lower environmental impact throughout the life cycle of large HPC infrastructures and define best practices for prototype planning and evaluation. The project will continue to organize well-known events like PRACEdays, Summer of HPC or the International HPC Summer School in order to promote and support innovative scientific approaches in modelling, simulation and data analysis. The PRACE-4IP kick-off meeting will be held at the Technical University of Ostrava, Czech Republic from 28-29 April 2015.

(Contact: Dr. Florian Berberich, f.berberich@fz-juelich.de)

Retrospective of the Jülich CECAM School on Computational Sciences

From 23-27 March the Jülich CECAM School on Computational Trends in Solvation and Transport in Liquids was held at JSC (<http://www.fz-juelich.de/stl-2015>). 43 students, postdocs and senior scientists from eight countries participated in the school. The 23 lecturers from Europe and

overseas were highly respected scientists who presented the latest research developments in the fields of soft matter physics and solvation chemistry together with a broad overview of the field.

The topics of the school were grouped into several blocks, covering atomistic methods, coarse-grain and continuum methods, hybrid methods, mesoscale fluid methods as well as numerical methods and hardware. As a complement to the topical lectures, a practical aspect of the school was a hands-on session for computing on graphical processing units (GPU), providing a code-oriented approach for first steps in GPU computing. The lecture notes (IAS series vol. 28) are available online as a pdf version at <http://www.fz-juelich.de/ias/jsc/ias-series>.

To stimulate discussion between participants and lecturers, four evening events were organized, comprising a get-together during the first evening, two poster sessions and an excursion. The positive feedback from participants and lecturers provides strong motivation for organizing further schools oriented to computational science on a similar basis. (Contact: Dr. G. Sutmann, g.sutmann@fz-juelich.de)

Former JSC Summer Student Among Finalists of BGCE Best Student Paper Prize

Every two years the Society for Industrial and Applied Mathematics (SIAM) organizes its premier conference in Computational Science and Engineering (CSE). It has become an established tradition of the CSE conference to host the awards ceremony of the Bavarian Graduate School of Computational Engineering's Student Paper Prize for outstanding student work in the field of Computational Science and Engineering. Since 2007, at every conference eight student finalists have been chosen by expert reviewers and invited to the awards ceremony. This year, a former student of the JSC Guest Student Programme (GSP), Marija Kranjcevic, was among the finalists of the Student Prize.

Marija is a Master's student in Applied Mathematics at the University of Zagreb. She participated in the JSC GSP in summer 2014, working on the shared memory parallelization of the Chebyshev Accelerated Subspace iteration Eigensolver (ChASE) developed within the SimLab 'ab initio'. She reported on the work she carried on during the summer programme in a paper which was recognized for its outstanding quality and excellence. As one of the eight selected finalists, Marija was invited to give a talk on her work on ChASE to this year's CSE conference, which was held from 13 to 18 March in Salt Lake City, Utah. The fact that she was among the BGCE finalists testifies to the exceptional quality and high standards of the JSC summer programme.

(Contact: Dr. Edoardo Di Napoli, e.di.napoli@fz-juelich.de)