Forschungszentrum Jülich's NO_x Plotter

Traffic emissions of nitrogen oxides are the main reason for high NO_2 concentrations in German cities. JSC and IEK-8 have released a new web tool to evaluate NO_2 levels at German air quality monitoring sites and estimate the required traffic reduction to meet air quality targets in cases where the legal limits are exceeded. The tool at https://nox-plotter.fz-juelich.de asks for a place or street name and presents the user with a list of air quality monitoring stations within a selected search radius. After a station has been selected, a series of plots can be generated showing the development of annual mean NO_2 concentrations at this station over the past 10 years, the necessary reduction in the NO_2 concentration, and the estimated emission reduction. The tool has been accessed by several thousand users a day. Shortly after its release, it had to be modified to enable it to cope with such a high number of requests. The data for this tool originate from the German Environment Agency (UBA) and are stored several times a day in the Tropospheric Ozone Assessment Report (TOAR) database, which is hosted at JSC. The Earth System Data Exploration team is working on the further development of this database and is looking into further applications for scientific and general use. Deep learning techniques are being applied to the TOAR data within the ERC project IntelliAQ.

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HPC Optimisation and Scaling Workshop

To help make the most effective use of JSC supercomputing systems, the HPC Optimisation and Scaling Workshop from 18 to 22 February combined training from Intel and JSC in the use of their parallel application performance analysis tools with the opportunity to execute large-scale runs and measurements to validate correctness and investigate and improve scaling. Over twenty participants (often working in teams of two to four) were supported by a comparable number of JSC employees from the Simulation Laboratories and Cross-Sectional Teams, three instructors from Intel, and additional HPC systems support staff assisting in the background. JUWELS and JURECA (cluster and booster parts) had reservations each day to run executions with large numbers of compute nodes. These were progressively released when no longer required to minimize service disruption.

Participants were encouraged to provide their codes with test cases and/or execution measurements for auditing in advance of the workshop. Preliminary analyses of several codes were briefly presented at the start of the workshop and incorporated into plans developed during the workshop. Assessments are continuing in most cases.

Three codes which effectively employed multi-threading combined with MPI were readily scaled to run successfully with up to 2048 compute nodes of JUWELS, and two codes using only MPI (and no threading) were tuned to use 1024 compute nodes. Large-scale modular supercomputing combining JURECA cluster and booster nodes was also demonstrated. Other code teams focused on optimizing memory access and vectorization. The workshop participants were very grateful for the opportunity and assistance provided.

In the course of this thorough exercising of system hardware and software, a variety of issues were encountered, not all of which could be resolved during the workshop but are still actively being addressed. Usage of the supercomputing systems will thereby be improved, allowing the solution of larger computational problems and a more efficient use of resources.

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CECAM Events 2019 at Jülich

Within the context of CECAM activities, Forschungszentrum Jülich organizes and runs a number of events per year, mainly focused on scientific computing in the fields of electronic structure, materials science, soft matter, or biophysics. This year, there are two central events and a follow-up workshop planned at Jülich.

The International Guest Student Programme on Scientific Computing runs from 5 August to 11 October, where undergraduate students from international universities

come to work at JSC upon application. JSC offers about 12 students the possibility to work in direct contact with scientific groups at JSC on specific topics in the fields of scientific computing, data analysis, or visualization.

The tutorial “Picking flowers: Hands-on FLEUR” will take place on 9–13 September. It is run by Stefan Blügel’s group (PGI-1/IAS-1) and provides an introduction to the electronic structure code FLEUR, which was developed at Jülich and is part of the code suite of the European Centre of Excellence MAX.

Another event is devoted to a follow-up workshop on “Load Balancing for Particle Simulation Codes”, which is co-organized by the Centre of Excellence E-CAM. The first workshop was held last year in September, and discussed general topics and requirements of various community codes. The next workshop in the series will discuss further developments and will also consider implementations in selected particle simulation codes. A date for the workshop has not yet been set. Anyone interested should contact local organizer Godehard Sutmann.

A further event scheduled for 2020 is part of the approved CECAM calendar: the multi-node international symposium “Ions, membrane and channels: Multiscale simulations from quantum to coarse-grain” in Paris co-organized by Jülich. It will celebrate the 80th birthday of Mike Klein, a pioneering scientist in the field of the computer simulation of condensed molecular systems.

Furthermore, CECAM will celebrate its 50th anniversary this year and several special events have been planned to mark it. A one-day symposium will take place on 8 April at the CECAM node in Paris, where CECAM was founded by Carl Moser as a European centre for discussing, teaching, and promoting computer simulation methods in the fields of electronic structure and molecular systems. A larger conference is planned at the current CECAM head-quarters in Lausanne on 9-12 September (see https://cecam50.cecam.org/).

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New Map of the Sky Published

LOFAR is an enormous European network of radio telescopes, which are connected to each other via a high-speed fibre-optic network and whose measuring signals are combined into a single signal. High-performance supercomputers convert 100,000 individual antennae into a virtual antenna dish with a diameter of 1,900 km. LOFAR operates in previously largely unexplored frequency ranges of approximately 10–80 MHz and 110–240 MHz. It is headed by the ASTRON research institution in the Netherlands and is considered to be the world’s leading telescope of its kind. There are six measurement stations in Germany, which are operated by different scientific institutions. One of these is located to the southeast of the campus of Forschungszentrum Jülich and is run by JSC together with the University of Bochum.

LOFAR produces enormous amounts of data, which need to be transferred, stored, and analysed. JSC is one of the three data centres in the project and is home to roughly 15 petabytes of data. This is almost half of all the LOFAR data, one of the largest astronomical data collections in the world. The data are stored in a distributed storage system based on dCache software. Processing these gigantic data sets is a great challenge. While positioned in the middle of a multi 10 GBit/s star-network topology, JSC furthermore coordinates the German LOFAR network activities for the observation data as well as the LOFAR archive data through modern JSC-operated DWDM (dense wavelength division multiplexing) connections. Over the last few years, the LOFAR data have become by far the biggest fraction of community-data transferred via the JSC-managed networks in and out of Forschungs-zentrum Jülich.

An international team of more than 200 astronomers from 18 countries recently published the first map produced by a radio sky survey with previously unprecedented sensi-tivity using the LOFAR radio telescope. The map reveals hundreds of thousands of unknown galaxies and sheds new light on research fields such as black holes, interstellar magnetic fields, and galaxy clusters. A special issue of the scientific journal Astronomy & Astrophysics is dedicated to the first 26 articles describing the results.

The creation of radio sky maps at low frequencies demands both considerable telescope and computation time as well as large teams to analyse the data. What would have taken centuries on conventional computers was achieved within one year thanks to the use of innovative algorithms and extremely powerful computers. Part of this work was done at JSC, where huge amounts of data were transformed into high-quality images, making use of JURECA and later of JUWELS.

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Events

Programming with C++
Instructor: Dr. Sandipan Mohanty, JSC
Date: 6-9 May 2019, 09:00-16:30
Venue: Jülich Supercomputing Centre, Computer Lab 2
http://fz-juelich.de/ias/jsc/2019/cplusplus

From zero to hero, Part I: Understanding and fixing on-core performance bottlenecks
Instructors: Andreas Beckmann, Dr. Ivo Kabadshow, JSC
Date: 14-15 May 2019, 09:00-16:30
Venue: Jülich Supercomputing Centre, Computer Lab 1
http://fz-juelich.de/ias/jsc/2019/zero2hero-1

Introduction to the usage and programming of supercomputer resources in Jülich
Instructors: Representatives of Atos, Intel and ParTec, JSC staff members
Date: 20-21 May 2019, begin on 20 May at 13:00
Venue: Jülich Supercomputing Centre, Lecture Hall
http://fz-juelich.de/ias/jsc/2019/sc-may

For further events, talks, and training courses, please visit:
http://fz-juelich.de/ias/jsc/events