HELMHOLTZ GEMEINSCHAFT

Open Science

JÜLICH FORSCHUNGSZENTRUM

Das Journal of Large-Scale Research Facilities oder: Wie Großgeräte eine DOI bekommen

Helmholtz Open Science Webinare zu Forschungsdaten
Webinar 26 – 27.04./07.05.15

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Mission der Helmholtz-Gemeinschaft

„Wir erforschen Systeme hoher Komplexität unter Einsatz von Großgeräten und wissenschaftlichen Infrastrukturen gemeinsam mit nationalen und internationalen Partnern.“

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Das Großgerät wird im Abstract genannt …

„ First demonstrations of this setup at the coherence beamline of the PETRA III storage ring yield a highly divergent far-field diffraction pattern, from which the autocorrelation function of the near-field intensity distribution was obtained. “

DOI:10.1063/1.3698119

… oder im Acknowledgment

„And many thanks to the Alfred Wegener Institute for Polar and Marine Research (AWI) for providing the opportunity to join several research cruises across the Atlantic Ocean on RV Polarstern, especially the expeditions ANT-XXIII/10, ANT-XXIV/1, ANT-XXIV/4, ANT-XXV/5 and ANT-XXVI/1.“

doi:10.5194/amt-5-2391-2012

… oder irgendwo

In the finite element context of Alya, the proposed gluing method consists in adding new elements, referred to as extension elements. These elements are assembled *almost* like normal finite elements (during the Assembly task) and do not require any particular treatment. Therefore the gluing method inherits the parallel performance in Alya. Figure 4 shows the speedup obtained on a Blue-Gene Q.

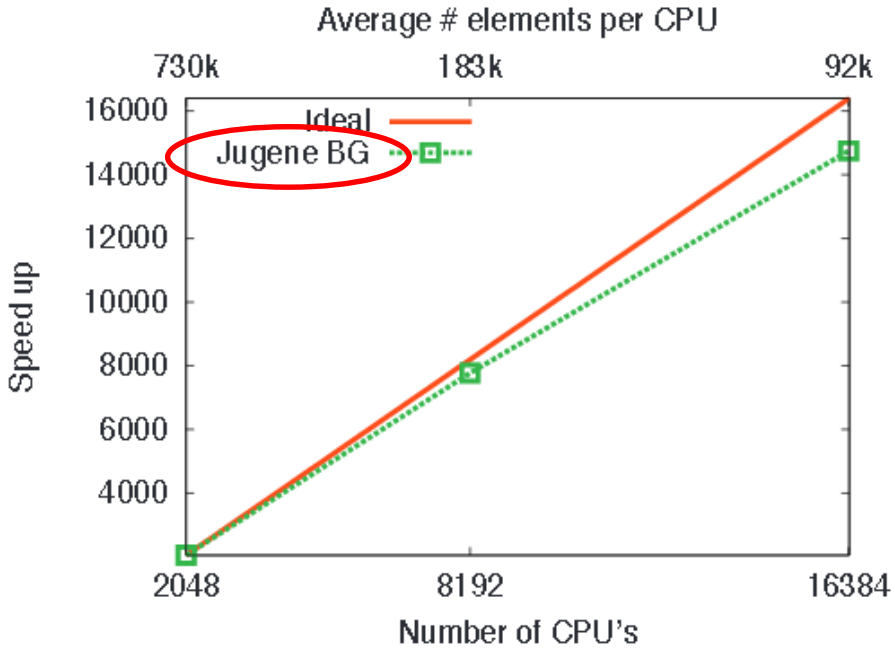


Figure 4 Alya speedup

DOI:10.1016/j.proeng.2013.08.013

… oder gar nicht.

Status quo

1. Die Nennung des Helmholtz-Zentrums / des Großgerätes erfolgt derzeit an unterschiedlichen Stellen in der Publikation (Einleitung, Methodenteil, Acknowledgement) oder sie fehlt ganz.
2. Sie erfolgt nicht auf normierte Weise, weshalb eine Gesamtauswertung (z.B. über eine Suche im Web of Science) praktisch kaum durchführbar ist.

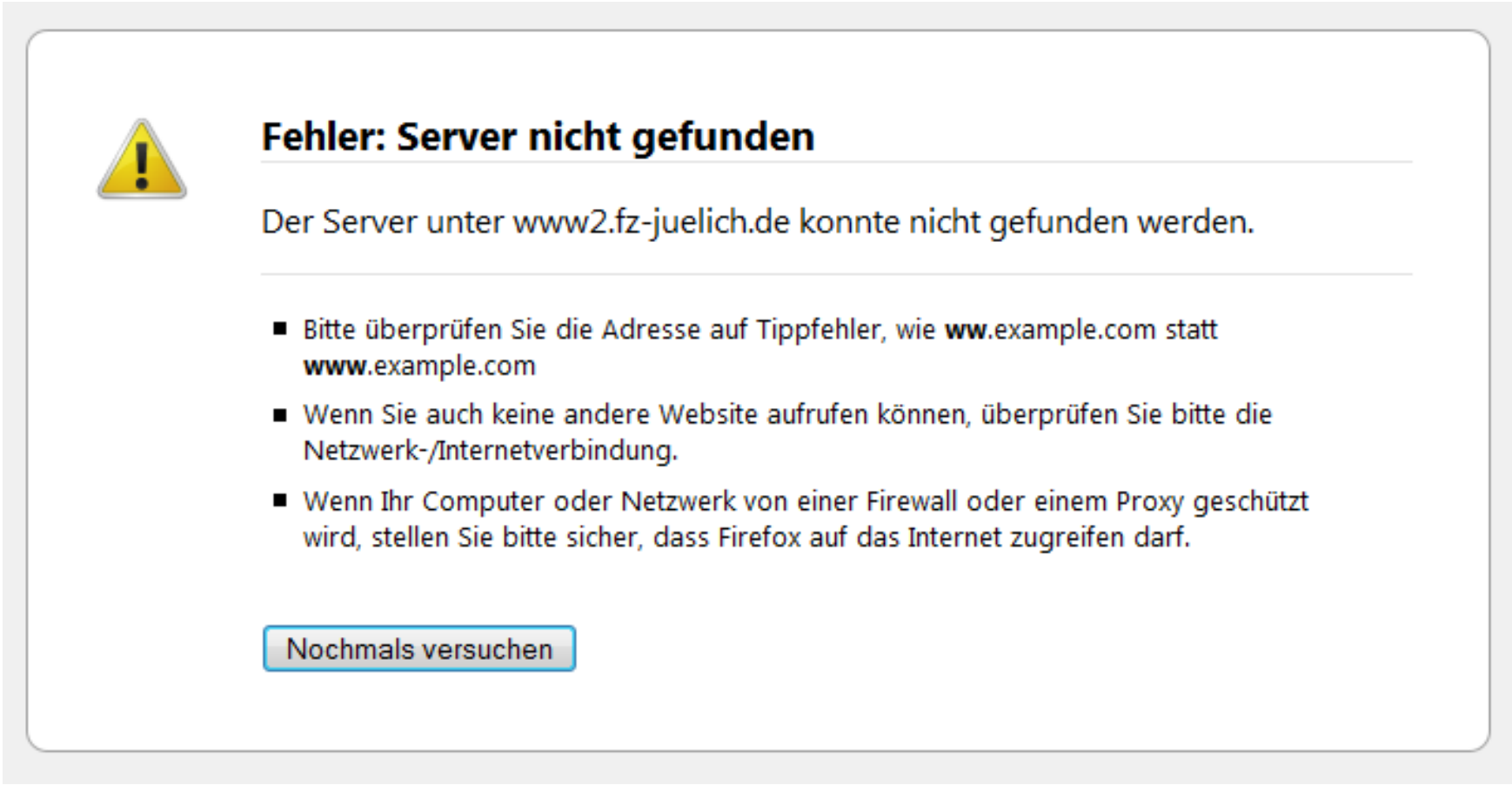
Die Erfolgsbilanz des Helmholtz-Gemeinschaft stellt sich in einer Kernkompetenz schlechter dar als sie ist.

Im Ansatz nicht schlecht

„This work was financially supported both by the PRACE First Implementation Project funded in part by the EUs 7th Framework Programme (FP7/2007–2013) under grant agreement no. RI-261557 and by Science Foundation Ireland (grant 08/HEC/I1450). Benchmarks were carried out on the Jugene [14] machine at Jülich, on Curie [13] at the CEA and on Fermi [15].“

[14] http://www2.fz-juelich.de/jsc/jugene

DOI:10.1016/j.cpc.2013.03.003


Fehler: Server nicht gefunden
Der Server unter www2.fz-juelich.de konnte nicht gefunden werden.
Bitte überprüfen Sie die Adresse auf Tippfehler, wie ww.example.com statt www.example.com
Wenn Sie auch keine andere Website aufrufen können, überprüfen Sie bitte die Netzwerk-/Internetverbindung.
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Nochmals versuchen

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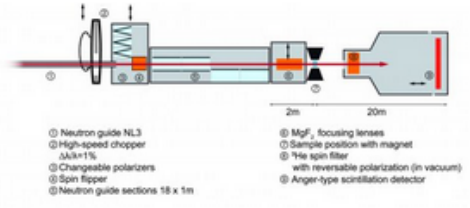
1. Für jedes Großgerät wird eine DOI vergeben („Digital Object identifier“; persistent). Die externen Nutzer sind gehalten (ggf. in einer Benutzungsordnung, in einer Messzeitbewilligung etc.), diese DOI zu zitieren. Dadurch erfolgt die Referenzierung auf das Großgerät stets an der gleichen Stelle (in den Referenzen der Publikation) und in der gleichen Form (über die DOI), was eine Gesamtauswertung möglich macht.
2. Eine DOI muss zu einem Objekt im Internet auflösen. Dieses Objekt ist eine kurze Beschreibung des Großgerätes sein, vgl. z.B. die Instrumentenbeschreibung am MLZ.

KWS-1

Small angle scattering diffractometer



The KWS-1 is dedicated to high resolution measurements due to its 10 % wavelength selector. This property is interesting for highly ordered or highly monodisperse samples. With the foreseen chopper the wavelength uncertainty can be reduced further to ca. 1 %. The scientific background of KWS-1 is placed in magnetic thin films. Magnetic samples will be studied with the full polarization analysis including incident beam polarization and polarization analysis of the scattered neutrons. In front of the collimation, a 3-cavity polarizer with V-shaped mirrors is placed. The full bandwidth of 4.5 to 20 Å will be covered with min. 90 % (95 % typical) polarization. A radio frequency spin flipper allows for changing the polarization. The polarization analysis will be realized with 3He-cells which will be optimized for the used wavelength and scattering angle. Vertical magnets will be provided to render the magnetic field at the sample position. Thin films can be well studied in the grazing incidence geometry – the method is called grazing incidence small angle neutron scattering (GISANS). A newly installed hexapod will allow for positioning the sample with 0.01 mm and 0.01° precision.

Classical soft-matter systems will be investigated on KWS-1 if the resolution is needed. Biological samples can be handled due to the detector distance of ca. 1 m, which will allow for maximal scattering angles of Q = 0.5 $Å^{-1}$.

The MgF_2 lenses are used for the high flux mode with large sample areas, while the resolution stays in the classical SANS range. These enhanced intensities allow for real time measurements in the 1/10 second region (typical 1 s).

Instrument Scientists

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Operated by

Jülich Centre for Neutron Science

Gallery

Lösung

3. Mit Blick auf die Akzeptanz durch die Nutzer und mit Blick auf eine größtmögliche Verbreitung wurde die **Open Access-Zeitschrift „Journal of large-scale research facilities“ (JLSRF)** gegründet, die derartige Dokumente enthält. Die Zentralbibliothek des Forschungszentrums Jülich übernimmt die organisatorische Abwicklung. 

4. Die Beschreibungen werden durch Personen erstellt, die für das jeweilige Großgerät verantwortlich sind. Sie werden als anonyme Werke publiziert, um keine persönlichen Zitierungen zu „erzwingen“:
   Heinz Maier-Leibnitz Zentrum. (2015). BioDiff. *Journal of large-scale research facilities*,1, A7. http://dx.doi.org/10.9999/example-doi.

3. Statt Peer Review findet lediglich ein Editorial Review statt mit Editoren aus den einzelnen Helmholtz-Zentren.

Vorlage

Journal of **large-scale research** facilities

Journal of large-scale research facilities, 1, A1 (2015)

http://dx.doi.org/10.9999/example-doi

Published: 01.01.2015

eine DOI für ein Messgerät

Änderungen etc. behalten die Grund-DOI, z.B. http://dx.doi.org/10.9999/examle-doi-1

Abbreviation and full name of the large-scale research facility as title

Instrument Affiliation

Instrument Scientists:
- J. Doe, Affiliation, Contact Information
- R. Who, Affiliation, Contact Information

Zitieren

Heinz Maier-Leibnitz Zentrum. (2015a). Instrument. *Journal of large-scale research facilities, 1*, A2. http://dx.doi.org/10.9999/example-doi

Heinz Maier-Leibnitz Zentrum. (2015b). Instrument. *Journal of large-scale research facilities, 1*, A5. http://dx.doi.org/10.9999/example-doi

Instrument Affiliation. (2015). Instrument. *Journal of large-scale research facilities, 1*, A10. http://dx.doi.org/10.9999/example-doi

Beispiel

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BioDiff: The New Diffractometer for Crystals with Large Unit Cells

Heinz Maier-Leibnitz Zentrum

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Abstract: The BioDiff diffractometer is a new instrument built at the Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II) in collaboration between the Forschungszentrum Jülich and the FRM II. It is optimised for studies of crystals with large unit cells and its main application lies in the structural analysis of protein crystals, more precisely in the determination of the position of the hydrogen atoms that are easily seen by neutron scattering but are normally not observed by X-ray crystallography. The BioDiff instrument is now in full user operation.

1 Instrument description

Since the human genome has been decoded and sequencing of the genome of other organisms has become a standard procedure the resulting information on the proteins encoded in these genomes can be used to express them in bacterial or yeast based expression systems and thereby study their interplay and function. One of the overall goals is a better understanding of the metabolism of a cell and thereby improving drugs and suppress side effects since they are tailored to attack only the part of the cell metabolism they are supposed to do so. In order to understand the function of a protein the knowledge of its three dimensional structure is a prerequisite. Often intermediate steps in the course of the catalytic process of a protein can be trapped and investigated with structure analysing techniques exhibiting atomic resolution, e.g. with X-ray or neutron diffraction. Here, the instrument BioDiff is able to perform neutron diffraction studies on protein crystals with comparatively large unit cells. The unique feature of BioDiff as compared to comparable instruments (e.g., LADI-III at ILL) is that the incident neutron wavelength can be adapted to the unit cell size of the sample crystal. Figure 1 shows a schematic view of the BioDiff instrument from the top and a corresponding picture when the biological shielding has been partly removed.
By Bragg reflection from a pyrolytic graphite crystal (002-reflection) neutrons are selected from the white spectrum of the neutron guide NL1 and pass through a first boron carbide adjustable slit and

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: Schematic view of the BioDiff instrument (top) and a picture taken from a similar viewpoint e biological shielding removed (left).

selector. The latter acts as $\lambda/2$ filter. Together with the pyrolytic graphite crystal it forms chromator with a $\Delta\lambda/\lambda$ of $\sim 2.5\%$. Before entering the cylindrical drum of the image plate e beam is shaped by variable slits to fit to the sample size.
is equipped with two detectors. The cylindrical image plate detector (400*mm* in diameter and in height) is covering roughly half of the total 4π solid angle. It can be read out with three t resolutions of 125μm, 250μm and 500μm. As an alternative, one can lower the image plate and swing in a neutron sensitive scintillator which is imaged onto a CCDchip.
CD-camera set-up serves as second detector but can also be used for the fast alignment of the crystal with respect to the neutron beam. The size of the scintillator is 197*mm* x 197*mm* and its from the sample is 100*mm*. It can be moved around the sample to achieve 2Θ-values between 13°. Additionally, it can be displaced vertically by 100*mm*. Measuring at several positions, the lid angle coverage achievable with the CCD-detector amounts also to 2π.
nance tests for both detector types showed that the CCD-camera detector is comparable in sen- to the image plate detector, but covers only a smaller area (compare Figure 2). However, taking count the longer readout times of the image plate detector, the CCD-detector is an alternative of strongly scattering crystals. Here, the faster readout of the CCD-chip pays off even if the tector covers a smaller area.
the first 18 months of user operation 14 complete data sets of protein and DNA crystals were fully collected at BioDiff.

anned instrument development and upgrades

moment the crystal has to be taken off the instrument when one wants to tilt it in order to in- he completeness of the data set. This increases the risk to damage the crystal either mechanically ating it up when working under cryo-conditions. With a mini-kappa goniometer head as shown e 3 this can be avoided and an optimised tilt geometry can be chosen using special strategy e. This will help to collect the data more efficiently.
dity controlled gas stream can in some cases improve the crystal quality due to hydration and dation procedures with D_2O vapour (already tested at Proteros in Martinsried). It will also enable t variation techniques in low resolution crystallographic applications: e.g. lipids or detergents n be distinguished from the protein in membrane protein crystals. Better Lithium-ceramic flight ill help to reduce the background from air scattering of the primary beam. Illumination of the crystal with an optical fibre will allow to prepare and maintain intermediate states of photo- active proteins.

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image plate

region of interest shown above recorded with CCD-detector

e image plate detector (upper part) compared to the same settings for

r a variable tilt of the crystal while keeping it in the cold nitrogen gas e taken from Brockhauser, S. and Ravelli, R. B. G. and McCarthy, A. A. (2013).

3

es, 1, A1 (2015) http://dx.doi.org/10.9999/example-doi

tend the existing wavelength range down to about 1.8$\AA$ utilising an monochromator. This will close the gap to the thermal single crystal ng the application range of BioDiff to medium compound crystals.

eration where the protein crystal is typically mounted in a sealed e mother liquor BioDiff offers a standard Oxford Cryosystems 700+ ts in a nitrogen gas stream down to 90K. Additionally, a closed cycle temperatures down to 4K in vacuum for small compound crystals.

e neutron structure analysis of proteins, especially the determination tal fields of interest are:
tonation states of amino acids in the active center)
on shell of proteins
hydrogen bonds
monitor of structural stability/flexibility
roven to produce good quality crystallographic data sets and is now

, and McCarthy, A. A. (2013). The use of a mini-k goniometer head in y diraction experiments. *Acta Crystallographica Section D: Biological* 1251. http://dx.doi.org/10.1107/S0907444913003880

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