

DOI-Vergabe für Großgeräte im Journal of Large Scale Research Facilities JLSRF

23. Januar 2016 | Dr. Christoph Holzke, Dr. Claudia Frick, Dr. Bernhard Mittermaier

Das Anliegen

Woher kommen eigentlich die ganzen Daten die nun publiziert werden sollen?

- Von (verschiedenen) Autoren aus (verschiedenen) Forschungseinrichtungen
- Zum Teil aus Experimenten an großen Forschungsgeräten!
- BILDER von Groß(-groß)-geräten (Polarstern, MRT, HPC, Colider, Beamlines)

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.

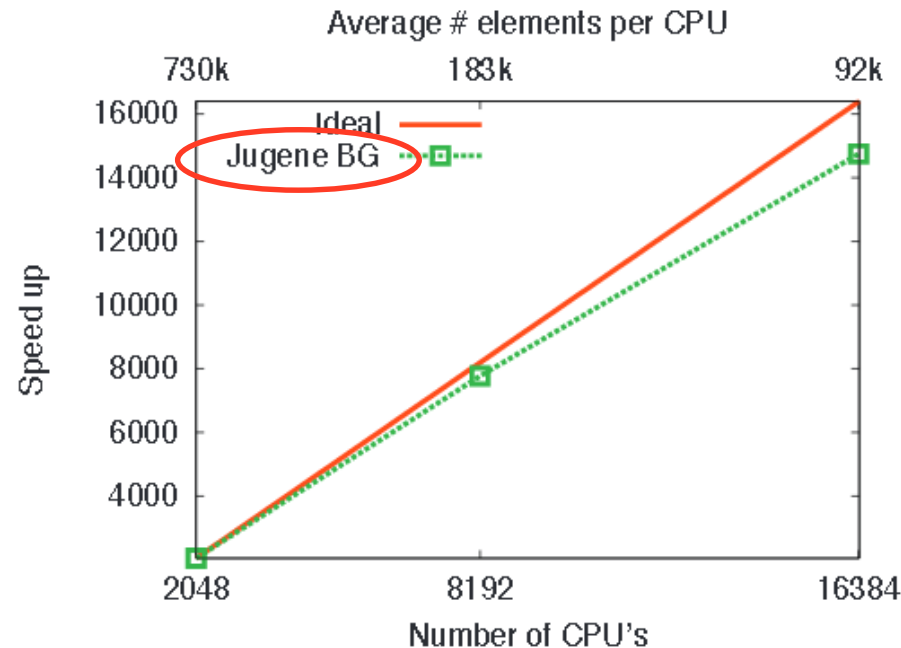


Figure 4 Alya speedup

DOI:10.1016/j.proeng.2013.08.013

Die Fragen

Großgeräte der Helmholtz-Gemeinschaft stehen den wiss. Communities für Experimente zur Verfügung

- Wie und von wem werden die Großgeräte genutzt?
- Welche Anteile haben Eigen- und Fremdnutzung?
- Erfüllt die HGF ihren Auftrag?
- Entwicklung von Experimenten

Das Anliegen

Zunächst auf Helmholtz-Ebene:

- HGF-Kernkompetenz Großgeräte verdeutlichen
- Sichtbarkeit der Geräte erhöhen
- Reputation für die Facilities
- Nachweis der lohnenden Investition

Die Idee: ***Großgeräte zitierbar machen***

Journal für den Nachweis „Großgeräte“

NREX: Neutron reflectometer with X-ray option | Khaydukov | Journal of large-scale research facilities JLSRF - Mozilla Firefox

NREX: Neutron reflectomet... x +

jlsrf.org/index.php/lsf/article/view/30/pdf

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Journal of large-scale research facilities, 1, A38 (2015) <http://dx.doi.org/10.17815/jlsrf-1-30>

Published: 21.12.2015

NREX: Neutron reflectometer with X-ray option

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

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

Published: 01.01.2015

BioDiff: The New Diffractometer for Crystals with Large Unit Cells

Heinz Maier-Leibnitz Zentrum

Instrument Scientists:

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- T. E. Schreder, Jülich Centre for Neutron Science (JCNS) at MLZ, Forschungszentrum Jülich GmbH, Garching, Germany

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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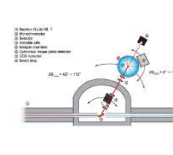


Figure 1: Schematic view of the BioDiff instrument (top) and a picture taken from a similar viewpoint (left). The biological shielding removed (left).

selector. The latter acts as $\lambda/2$ filter. Together with the pyrolytic graphite crystal it forms a monochromator with a $\Delta\lambda/\lambda$ of $\sim 2.5\%$. Before entering the cylindrical drum of the image plate the beam is shaped by variable slits to fit to the sample size.

The beam is equipped with two detectors. The cylindrical image plate detector (400mm in diameter and in height) is covering roughly half of the total 4π solid angle. It can be read out with three resolutions of 125 μm , 250 μm and 500 μm . As an alternative, one can lower the image plate and swing in a neutron sensitive scintillator which is imaged onto a CCD-chip.

A CCD-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 197mm x 197mm and its distance from the sample is 100mm. It can be moved around the sample to achieve 2θ -values between 113° . Additionally, it can be displaced vertically by 100mm. Measuring at several positions, the solid angle coverage achievable with the CCD-detector amounts also to 2π . Performance tests for both detector types showed that the CCD-camera detector is comparable in sensitivity to the image plate detector, but covers only a smaller area (compare Figure 2). However, taking into account 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 detector covers a smaller area.

In the first 18 months of user operation 14 complete data sets of protein and DNA crystals were successfully collected at BioDiff.

Planned instrument development and upgrades

When the crystal has to be taken off the instrument when one wants to tilt it in order to increase the completeness of the data set. This increases the risk to damage the crystal either mechanically using it up when working under cryo-conditions. With a mini kappa goniometer head as shown in Figure 3 this can be avoided and an optimised tilt geometry can be chosen using special strategy. This will help to collect the data more efficiently.

A humidity controlled gas stream can in some cases improve the crystal quality due to hydration and ion procedures with D₂O vapour (already tested at Protein in Martinred). It will also enable variation techniques in low resolution crystallographic applications: e.g. lipids or detergents can be distinguished from the protein in membrane protein crystals. Better Lithium-ceramic flight will help to reduce the background from air scattering of the primary beam. Illumination of the sample crystal with an optical fibre will allow to prepare and maintain intermediate states of photoactive proteins.

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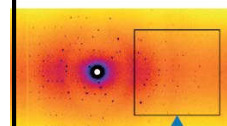


Figure 2: Comparison of the image plate detector (upper part) and the CCD-detector (lower part). The image plate detector (upper part) compared to the same settings for the CCD-detector (lower part).

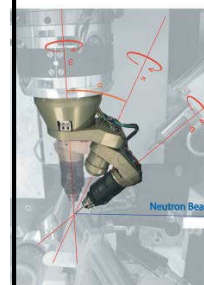


Figure 3: A 3D model of the mini kappa goniometer head, showing the crystal and the neutron beam path. The crystal is taken from Bockhauer, S. and Ravelli, R. B. G. and McCarthy, A. A.

(2013).

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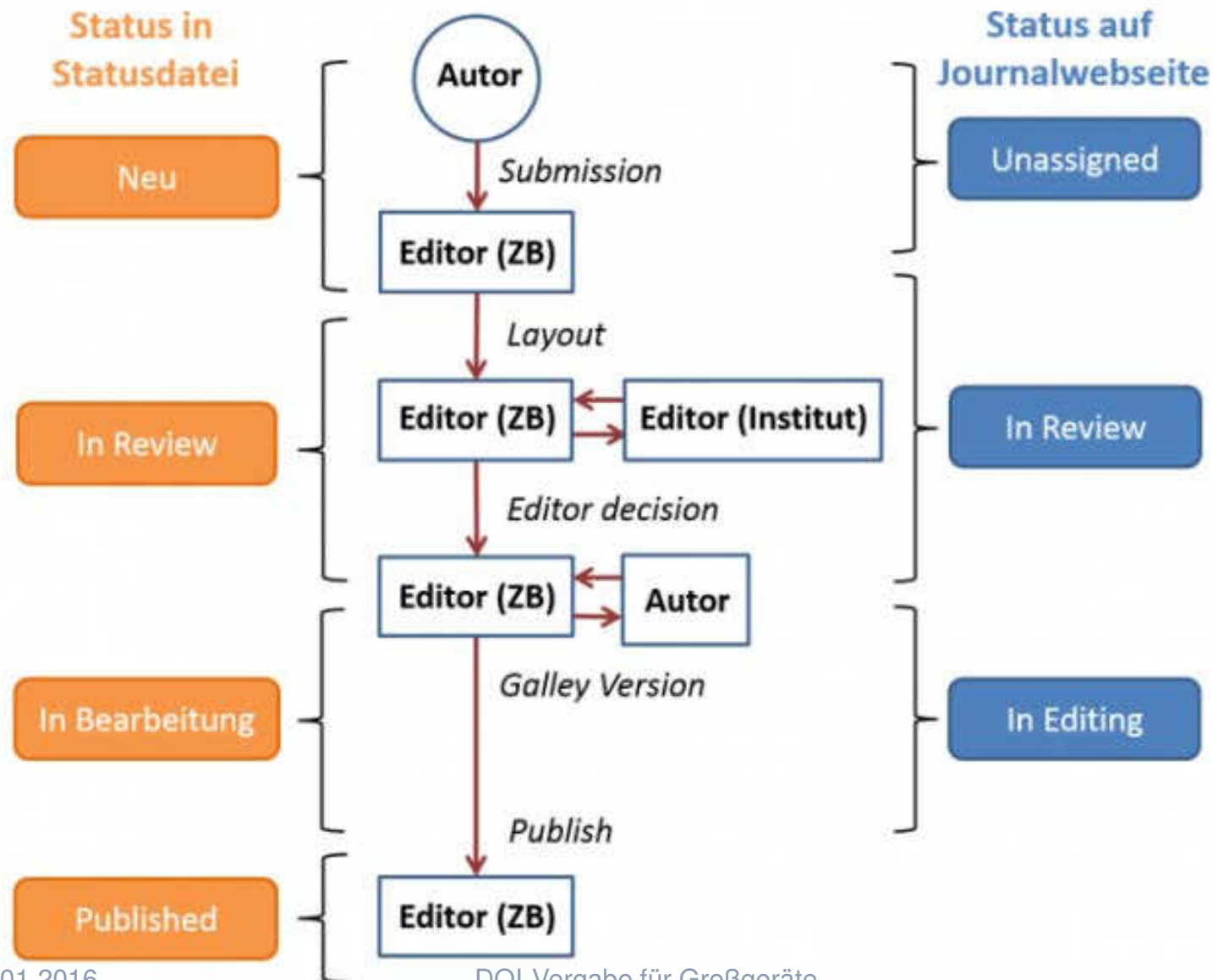
extend the existing wavelength range down to about 1.8 Å utilising a monochromator. This will close the gap to the thermal single crystal application range of BioDiff to medium compound crystals.

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

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

and McCarthy, A. A. (2013). The use of a mini-kappa goniometer head in diffraction experiments. *Acta Crystallographica Section D: Biological Crystallography*. <http://dx.doi.org/10.1107/S0907444913003880>

Publikationsprozess im Journal of large-scale research facilities (JLSRF)





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erstellt	C.frick 12:30, 16. Okt. 2015 (CEST)
geprüft	Ch. Esser 13:57, 22. Okt. 2015 (CEST)
freigegeben	B.mittermaier 14:35, 25. Okt. 2015 (CET)

Inhaltsverzeichnis [Verbergen]

1 Zeitschriften

1.1 Journal of large-scale research facilities (JLSRF)

1.1.1 Relevante Dateien und Adressen

1.1.2 Submission

1.1.3 Status: Neu

1.1.4 Status: In Review

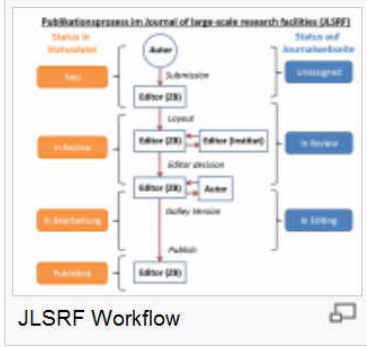
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1.1.6 Status: Published

Zeitschriften

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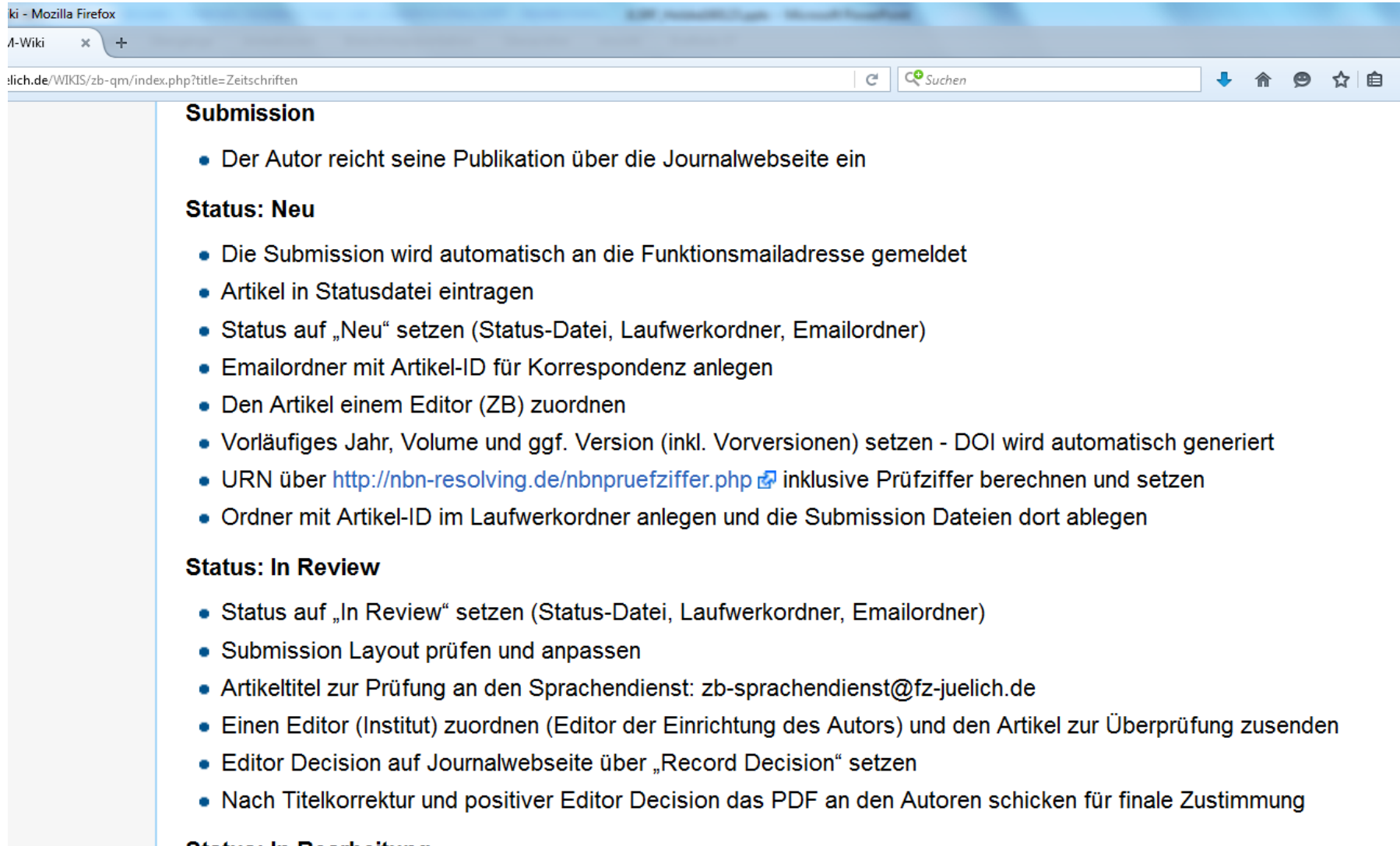
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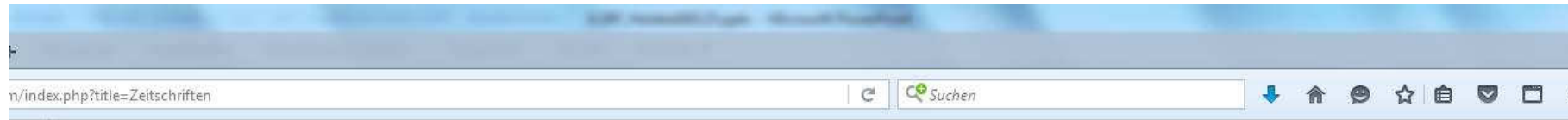
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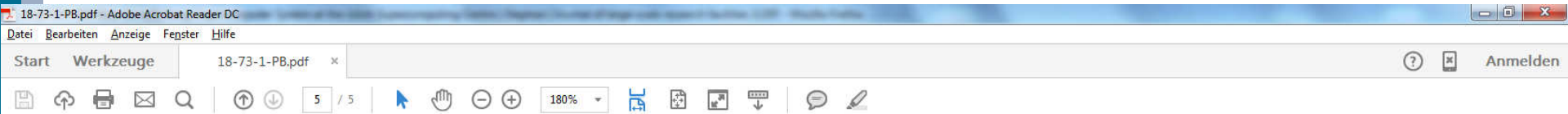
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Vielen Dank für Ihre Aufmerksamkeit!

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Anhang



fraction, coming mainly from the power supplies, is still moved out of the rack by air. Engineered with fewer moving parts and built in redundancy, Blue Gene/Q has proven to be extreme reliable. Designed with a small footprint and low power requirements, Blue Gene/Q was ranked as the number-one most energy-efficient supercomputer in the world by the Green500 in Nov. 2011 (Green500, 2011).

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