

de.NBI Quarterly Newsletter

This de.NBI Quarterly Newsletter in **November 2020** informs about current developments and recent events in the BMBF project **German Network for Bioinformatics Infrastructure - de.NBI**.

Further information at: <https://www.denbi.de/>

de.NBI Industrial Forum 1st Annual Meeting on 26 Nov 2020

The de.NBI Industrial Forum was founded with a kick-off meeting last year in Berlin. So far 34 companies are members of the de.NBI Industrial Forum (<https://www.denbi.de/industrial-forum>), including members from Austria, Luxembourg and Switzerland.

The first Annual Meeting of the de.NBI Industrial Forum will take place as an online event on 26 November 2020. Although this meeting will be more condensed compared to the kick-off meeting last year, the program of the meeting offers a wide range of topics, e.g., highlights of the de.NBI network, but also recent developments in the interaction of the de.NBI Industrial Forum with the de.NBI network. In particular, the further development of the de.NBI cloud the Galaxy platform as well as the contribution of the de.NBI network to COVID-19 research will be presented as highlights. The intense interaction in the field of plant bioinformatics between academia and industry will then be described. Furthermore, two companies will present their software solutions, which are available free of charge as de.NBI Industrial Forum services (<https://www.denbi.de/industrial-forum/industrial-forum-services>).

Find program and registration at: <https://www.denbi.de/events/977-online-jahrestagung-des-de-nbi-industrieforums:-2020>


**Online-Jahrestagung des
de.NBI-Industrieforums**

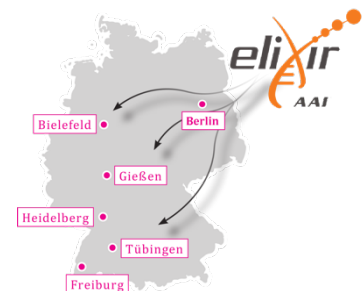
26 November 2020

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Further Growth of the de.NBI Cloud thanks to significant financial Support by the BMBF

The de.NBI Cloud is organized as a federation with locations at the universities of Bielefeld, Freiburg, Gießen, Heidelberg and Tübingen, also with installations at the EMBL in Heidelberg, as well as at the Berlin Institute for Health Research (BIH) of the Charité. Since 2016 the Federal Ministry of Education and Research (BMBF) supports infrastructure and staff of the de.NBI Cloud. These efforts are complemented by the hosting research institutions with personnel for operating the infrastructure. In the recent years, the extension of the de.NBI Cloud included compute and storage infrastructure, but also IT security measures and ISO certification. This year, the de.NBI Cloud again receives a substantial funding of 12.6 million Euros for an urgently needed expansion of hardware to meet the growing demand of life science research in current and upcoming projects. Meanwhile, the de.NBI Cloud counts more than 1100 researchers making use of the compute facilities in more than 360 life sciences projects.



The federated de.NBI Cloud provides actually approx. 25,000 cores, 230 TB RAM and 40 PB storage capacity. The cloud portal represents the central access point to the federated de.NBI Cloud platform. The whole system is accessible through single sign-on based on the ELIXIR Authentication and Authorization Infrastructure (ELIXIR-AAI). The de.NBI Cloud is the

largest scientific cloud in Germany and one of the leading European academic clouds in life sciences.

More information on the de.NBI cloud: <https://www.cloud.denbi.de>

High-Tech Forum Discussion Paper "Bio-IT Innovations" highlights the Role of de.NBI for bio-based Innovations

The High-Tech Forum is the central committee, which advises the German Federal Government on implementing its High-Tech Strategy 2025. The forum publishes discussion papers on previously identified topics. One of these publications deals with "Bio-IT innovations – the convergence of life sciences and information technologies". The paper focuses on the importance of Bio-IT innovations presenting innovation potentials as well as significant international developments. Finally, the High-Tech Forum suggested to establish an ambitious Bio-IT research center, which should be built on the achievements of the de.NBI network, bundling and making available relevant software, methods and data inventories in Germany and Europe.

In the meantime, the discussion paper was commented by Alfred Pühler, Vera Ortseifen and Andreas Tauch. The comments underlined the importance of the de.NBI infrastructure for the proposed Bio-IT center, in particular the established federated cloud together with the German ELIXIR node should be decisive building blocks in the development of a future-oriented Bio-IT institute. In a next step the recommendations including the comments were presented to the round table of State Secretaries for the High-Tech Strategy 2025.

For more information please visit: www.hightech-forum.de



New chairs for SIG 2 Service & Service Monitoring

The Special Interest Group 2 - Service & Service Monitoring handles one of the de.NBI core tasks, which are defined as provision of service, training and compute capacities to life scientists. After 5 ½ years of activity as the chair of this group, Frank Oliver Glöckner (BioData, Jacobs University Bremen and AWI Bemerhaven) stepped down from his function. The CCU would like to express its sincere thanks to Frank Oliver Glöckner for his commitment in building up the SIG and his long-term pioneering work.



Uwe Scholz
SIG 2 chair

SIG 2
Service &
Service Monitoring



Michael Turewicz
SIG 2 co-chair

Now, in its 24th meeting on 23 October 2020, the CCU has elected the previous co-chair Uwe Scholz, IPK Gatersleben, as the new chairperson and Michael Turewicz, Ruhr University Bochum, as his deputy. Both have been active in this group since the beginning and will ensure a continuous development of the service topic in the next phases of the de.NBI. One of the future challenges will be the collection of performance data for the services. The new leads will be assisted by Manuel Wittchen from the de.NBI Administration Office.

Renato Alves appointed Deputy TrC of ELIXIR Germany



Renato Alves from EMBL Heidelberg has been elected by the ELIXIR Germany CCU as ELIXIR Germany Deputy Training Coordinator (Deputy TrC). He already joined the ELIXIR Training Platform representing an international network of training experts that spans all ELIXIR member states. The Training Platform aims to strengthen national training programs and to empower life sciences researchers to use Elixir's bioinformatic services and tools. The members of the ELIXIR Training Platform meet regularly to share information and expertise and to coordinate and lead the implementation of the ELIXIR training program. The national team for training coordination of the German ELIXIR Node is completed by the TrC Daniel Wibberg (ELIXIR Administration Office, Bielefeld University) and the Deputy TrC Bérénice Batut from University of Freiburg.



Find information on ELIXIR Germany here: <https://www.denbi.de/elixir-de>

New tool simplifies Submission of SARS-CoV-2 Data to open Databases

ELIXIR Belgium and ELIXIR Germany (de.NBI) help researchers share FAIR COVID-19 data. ELIXIR Belgium, in collaboration with ELIXIR Germany and the European COVID-19 Data Platform, have developed a tool to simplify the submission of viral sequencing data to the European Nucleotide Archive (ENA), an ELIXIR Core Data Resource providing open access to nucleotide sequences. The new submission tool offers an easy-to-use interface, guides researchers through the submission process and verifies the data format and description.



Find more information and the tool at: <https://elixir-europe.org/news/ENA-new-tool-COVID-19-data>

3rd de.NBI Cloud User Meeting - revisited

The 3rd de.NBI Cloud User Meeting took place from 8 -14 October 2020 as an online conference. The organizational structure consisted of a daily lecture illustrating cloud use cases followed by one or two workshops to actively foster know-how on the software used for cloud deployment. The scope of the meeting covered interesting topics for beginners such as virtualization but also key elements for software engineers and administrators such as orchestration with Kubernetes.



**CLOUD
USER
MEETING
ONLINE 2020**

Almost 60 participants attended the 5-day meeting. Starting off with an introduction to the de.NBI Cloud, the presentation sessions provided insights in capabilities of the de.NBI Cloud and use cases regarding human genome assembly, image annotation and microbial community proteomics.

The workshop program featured use cases, best practices, and detailed hands-on lessons to learn and actively engage in the cloud environment. Beyond a UNIX introduction for new cloud users, the sessions included practical exercises on BioConda/Biocontainers, BibiGrid and Ansible, introductions to Terraform and Kubernetes, as well as in-depth views on OpenStack, Snakemake, and Web Services. All workshops were conducted by experts from the de.NBI Cloud locations Bielefeld, Berlin, Gießen, Freiburg, and Tübingen thus ensuring a direct communication between the user community and the de.NBI Cloud environment.

We appreciated the interest in the de.NBI Cloud and its projects and hope that all attendees enjoyed the first ever virtual Cloud User Meeting. The next de.NBI Cloud Meeting will take place in Fall 2021.

Find the program at: <https://cloud.denbi.de/3rd-de-nbi-cloud-user-meeting/>

1000th User of the de.NBI Cloud



We are pleased to announce that Prof Dr Nico Pfeifer is our 1000th registered de.NBI Cloud user. Prof Pfeifer leads the Methods in Medical Informatics group in Tübingen and he registered in August this year in order to apply for resources that are needed in the frame of a master's project. The main part of the thesis is to extend the idea of the weighted elastic net method that was introduced by his group at ISMB in 2019 [1]. The project is based on the SimpleVM project type that the de.NBI Cloud offers to allow easy access to cloud resources including GPUs. With these resources the python-based machine learning library PyTorch can be used to speed up the computation on multiple GPUs.

On average the de.NBI Cloud access committee approves 4-5 new projects per week. This shows the high demand for computational resources in the German life sciences community. It is also proof of the high level of acceptance of the cloud that has now been achieved. Furthermore, there are already 146 publications that acknowledge the use of the de.NBI cloud.

As a new trend we observe more and more projects, which allocate compute resources for training and educational purposes for university courses.

[1] <https://academic.oup.com/bioinformatics/article/35/14/i154/5529259>

Apply for de.NBI cloud resources at: <https://cloud.denbi.de>

de.NBI Brochure “Data Analysis for Insights into complex Biological Systems”

Early February 2020, the de.NBI Administration Office presented the brochure entitled “Von der Datenanalyse zum Verstehen komplexer biologischer Systeme”, which was launched to mark the occasion of the 5-year anniversary of the de.NBI network. The brochure reports on the research activities of the de.NBI as a national bioinformatics infrastructure and provides solid information about recent progress in the field of big data analysis in life sciences. To target predominantly national life scientists and interested public, the brochure was initially published in German language and was well received within the scientific community.

Now the English translation is available, which illustrates the work of the de.NBI for an international audience. In particular, the ELIXIR and European Life Sciences communities should be addressed.

Find the full version at: https://www.denbi.de/images/Downloads/deNBI_Highlight_Brochure_English.pdf



Recent Updates of de.NBI Services

New features or versions of various de.NBI services and tools have been released in the last months:

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OpenMS 2.6.0 released, contains numerous adaptors, new features, and fixes. OpenMS is a flexible code-base that can be tailored to many different applications ranging from the standard label free analysis to top down, metabolomics, crosslinking or DIA. Find the service at: <https://www.denbi.de/services/369-openms>


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BacDive has a great new feature: A summary at the top of the page, which shows the most important data for a microbe in a short sentence, followed by a couple of keywords. Find the service at: <https://www.denbi.de/services/347-bacdive>


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e!DAL-PGP: Plant genomics & Phenomics Research Data Repository. High-throughput plant genomics and phenomics technologies are producing research data in abundance, the storage of which is not covered by established core databases. e!DAL-PGP provides a FAIR solution as illustrated in a new publication by: D Arend, P König, A Junker, U Scholz, M Lange, *The on-premise data sharing infrastructure e!DAL: Foster FAIR data for faster data acquisition*, GigaScience, Volume 9, Issue 10, October 2020, g107, <https://doi.org/10.1093/gigascience/giaa107>. Find the service at: <https://www.denbi.de/services/513-e-dal-pgp>



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MeDeCom is a computational method for decomposition of heterogeneous DNA methylomes. New publication by M Scherer, PV Nazarov, R Toth, S Sahay, T Kaoma, V Maurer, C Plass, T Lengauer, J Walter, P Lutsik, *Reference-free deconvolution, visualization and interpretation of complex DNA methylation data using DecompPipeline, MeDeCom and Fac-torViz*. Nat Protoc 15, 3240–3263 (2020). <https://doi.org/10.1038/s41596-020-0369-6>. Find the service at: <https://www.denbi.de/services/915-medecom>
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SeqAn 3.0.2 is released. The new release of the modern CPP library for sequence analysis has been amended with some great new features and also a lot of usability improvements. Find the service at: <https://seqan.de/seqan-3-0-2-release/>


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SILVAngs has been updated to run with SILVA release 138.1 by default. Older releases of SILVA are still available for projects that have already been analysed. For new projects, only SILVA release 138.1 is available. Find the service at: <https://www.denbi.de/services/344-silvangs>


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UseGalaxy.eu: The latest factsheet (Oct 2020) names 20.000 registered users and >180 hands-on tutorials. Find the figures at: <https://github.com/usegalaxy-eu/branding/blob/master/factsheet/factsheet.png>


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LipidCreator: LipidCreator is a lipid building block-based workbench and knowledge base for the semi-automatic generation of targeted lipidomics mass spectrometry assays and in silico spectral libraries. The Publication on the tool is out: B Peng, D Kopczynski, BS Pratt et al. *LipidCreator workbench to probe the lipidomic landscape*. Nat Commun 11, 2057 (2020). <https://doi.org/10.1038/s41467-020-15960-z>. Find the press release at: <https://www.isas.de/news/die-software-lipid-creator-unterstuetzt-die-diagnose-und-prognose-von-krankheiten>. Find the tool at: <https://www.denbi.de/services/340-lipidcreator>



Recent Publications by de.NBI partners:

-  F Heigwer, M Boutros. (2021) **Cloud-Based Design of Short Guide RNA (sgRNA) Libraries for CRISPR Experiments**. In: Fulga T.A., Knapp D.J.H.F., Ferry Q.R.V. (eds) CRISPR Guide RNA Design. Methods in Molecular Biology, vol 2162. Humana, New York, NY. https://doi.org/10.1007/978-1-0716-0687-2_1
-  W de Koning, M Miladi, S Hiltmann, A Heikema, JP Hays, S Flemming, M van den Beek, DA Mustafa, Backofen R, Grüning B, Stubbs AP, **NanoGalaxy: Nanopore long-read sequencing data analysis in Galaxy**, GigaScience, Volume 9, Issue 10, October 2020, g1005, <https://doi.org/10.1093/gigascience/giaa105>
-  B Serrano-Solano, A Erxleben, C Gallardo-Alba, H Rasche, S Hiltmann, M Föll, M Fahrner, MJ Dunning, M Schulz, B Scholtz, D Clements, A Nekrutenko, B Batut, B Grüning. **Fostering Accessible Online Education Using Galaxy as an e-learning Platform**. Preprints 2020, 2020090457, doi: [10.20944/preprints202009.0457.v1](https://doi.org/10.20944/preprints202009.0457.v1).
-  H Rasche, B Grüning, **Training Infrastructure as a Service**, bioRxiv 2020.08.23.263509; doi: <https://doi.org/10.1101/2020.08.23.263509>
-  D Baker, M van den Beek, D Blankenberg, D Bouvier, J Chilton, N Coraor, F Coppens, I Eguinoa, S Gladman, B Grüning, N Keener, D Larivière, A Lonie, S Kosakovsky Pong, W Maier, A Nekrutenko, J Taylor, S Weaver. (2020) **No more business as usual: Agile and effective responses to emerging pathogen threats require open data and open analytics**. PLoS Pathog 16(8): e1008643. <https://doi.org/10.1371/journal.ppat.1008643>
-  S Trump, S Lukassen, MS Anker, RL Chua, J Liebig, L Thürmann, VM Corman, M Binder, J Loske, C Klasa, TG Krieger, BP Hennig, M Messingschlager, F Pott, J Kazmierski, S Twardziok, JP Albrecht, J Eils, S Hadzibegovic, A Lena, B Heidecker, C Goffinet, F Kurth, M Witzentrath, MT Völker, SD Müller, UG Liebert, N Ishaque, L Kaderali, LE Sander, S Laudi, C Drosten, R Eils, C Conrad, U Landmesser, I Lehmann. **Delayed viral clearance and exacerbated airway hyperinflammation in hypertensive COVID-19 patients**. medRxiv 2020.09.22.20199471; doi: <https://doi.org/10.1101/2020.09.22.20199471>

de.NBI @ CONFERENCES

de.NBI CAU members have recently present the network at:



GCB 2020 – German Conference on Bioinformatics, 14-17 September 2020 – Virtual Conference

The GCB is the annual conference devoted to all areas of bioinformatics in Germany. The de.NBI network had the opportunity to virtually introduce its excellent bioinformatics service, training and cloud resources to the life sciences community. This year, the focus of the conference was set on medical research, in particular the need to advance the molecular biological and bioinformatics research on coronaviruses, especially SARS-CoV-2. The first day was dedicated to a number of workshops with de.NBI partners organizing the following tutorials:

- BioC++ - solving daily bioinformatic tasks with C++ efficiently; R. Rahn, S. Mehringer, M. Ehrhardt, FU Berlin
- Protein Structure Fundamentals: Searching – Analyzing – Modelling; K. Schöning-Stierand, M. Rarey, Uni Hamburg

The keynote lecture within the session RNA/Single cell analysis was held by Gene Myers (MPI Dresden), who presented the newest research in the field of high-fidelity genome sequencing, K-mer counting, and padded minimizers.

Find general information at: <https://gcb2020.de/>



de.NBI supported conferences in the near future



e:Med Kick-off Meeting on Systems Medicine, 24-25 Nov 2020

The de.NBI office will be presented with a virtual booth to inform the newly formed e:Med consortium about the offers of the de.NBI Network, especially the de.NBI Cloud

General information at: <https://www.sys-med.de/de/meeting/emed-kick-off-2020/>



Goes virtual...

November 24-25, 2020

e:Med Kick-off Meeting on Systems Medicine

UPCOMING EVENTS

The calendar lists the de.NBI training courses and events scheduled in the next months. All courses are accessible via the de.NBI web page. The network is continuously developing alternative forms of training. Have also a look into our online

training library, which is continuously expanded.

Under the actual conditions, please consult the de.NBI training program for updates.



Overview of upcoming de.NBI events



Date	Event	City	Organizer
19 Nov 2020	de.NBI – e!DAL-PGP training course – Sharing and Publishing Comprehensive Plant Research Data	Online	GCBN
20 Nov 2020	de.NBI Crop Analysis Tool Suite (Part II) training course – Working with repetitive sequences	Online	GCBN
23 Nov 2020	Introduction to the Cloud for Proteomics Analyses	Online	BioInfra.Prot
24 Nov 2020	de.NBI Crop Analysis Tool Suite (Part III) training course – Explore barley diversity	Online	GCBN
30 Nov-4 Dec 2020	de.NBI - CeBiTec Nanopore Workshop 2020 - Best Practice and SARS-CoV-2 applications	Online	BiGi, CAU, Ce-BiTec
7 Dec 2020	Data visualization using R	Online	BioInfra.Prot /LIFS
25 Nov 2020	1st Annual Meeting of the de.NBI Industrial Forum	Online	CAU
21. Jan 2021	25. CCU Meeting	Online	CAU
26-28 Jan 2021	Data Carpentry Workshop 2021	Online	HD-HuB
15-19 Mar 2021	de.NBI Spring School 2021 - Metagenomics will be postponed	Gießen	BiGi et al.

Further information at: <http://www.denbi.de/training>

IMPRESSUM

RESPONSIBLE FOR CONTENTS

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