de.NBI Quarterly Newsletter

This de.NBI Quarterly Newsletter in May 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/

Jubilee!!
20th issue
of the
de.NBI Quarterly Newsletter

CONTENT:

EDITORIAL

The corona pandemic not only changed our lives, it also dramatically influenced many activities of the de.NBI network. One of the main activities concerns the organization of training courses almost exclusively carried out as face-to-face events. In 2019, 79 de.NBI training courses were conducted. This number will decrease drastically in 2020 as all de.NBI training courses except two online courses have been cancelled from 25 March 2020 onwards. The network, in particular the SIG 3 training & education, should discuss alternative ways of conducting training events.

The corona crisis also affected the conduct of the de.NBI steering committee meetings. For the past five years, the members of the CCU met every three month at one of the de.NBI Service Centers to discuss and to decide on the future development of the network. The 22nd CCU meeting was planned to take place in Berlin at the end of April 2020. However, since a face-to-face meeting was no longer possible, it was replaced by a video conference which turned out to be quite successful. More than 20 CCU members and guests took part in the video conference and discussed intensively the involvement of the network in current corona research and also questions regarding the sustainable continuation of the network. With a view to the future, the next CCU meeting originally scheduled at Bochum University for end of June, will also be replaced by a video conference.

This de.NBI newsletter also addresses new research activities of de.NBI members. After the worldwide spreading of the SARS-CoV-2 virus, it became obvious that scientists within the de.NBI network immediately responded by switching their research focus to corona and COVID-19 topics. Altogether, 26 de.NBI projects dealing with corona research have been reported by group leaders. Obviously, the de.NBI network has great potential to contribute to new research challenges. In particular, two de.NBI infrastructures, namely the Galaxy platform and the de.NBI Cloud play a major role in carrying out corona related research.

Finally, another important development is the interchange of the two leading positions of the German ELIXIR node. From 1 June 2020 on, the Head of Node and the deputy will swap their positions. Andreas Tauch will become head of ELIXIR Germany, and Alfred Pühler will act as his deputy. Since both of them were already deeply involved in establishing the German ELIXIR node, the transition should be a smooth one.

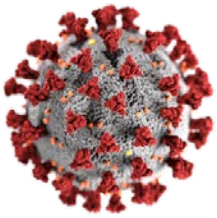
A. Pühler
(de.NBI coordinator)

PARTICIPATION OF THE de.NBI IN RESEARCH PROJECTS TO FIGHT THE PANDEMIC TRIGGERED BY SARS-CoV-2

The current corona pandemic is a major challenge for our society and therefore requires special attention by the established scientific structures. It is important to advance molecular biological research of corona viruses, especially of SARS-CoV-2, and to investigate both medical and epidemiological aspects of the infection process in COVID-19. These research areas generate large amounts of data requiring intensive bioinformatic analysis. Here, the German Network for Bioinformatics Infrastructure (de.NBI), which is funded by the BMBF, is obliged to provide a wide collection of analysis programs and the compute capacities of the de.NBI Cloud infrastructure. Both, analysis programs and compute capacities can be used free of charge by all researchers in the life sciences. In addition, working groups of the de.NBI are directly involved in corona research projects. A survey among the de.NBI project leaders resulted in a list of 26 projects which are classified into six categories (see box). The projects demonstrate the important role of the de.NBI infrastructure for the current coronavirus research.

Classification of de.NBI corona research projects

- Sequence variants and geographical distribution of the SARS-CoV-2 virus
- Interactions of the SARS-CoV-2 virus with human cells
- Analysis of the COVID-19 disease
- Development of drugs for SARS-CoV-2 infections
- Support for classical epidemiological studies
- Tool development to analyze COVID-19 related data



Source: CDC/ Alissa Eckert, MS; Dan Higgins, MAM

The corona related de.NBI projects are presented on the de.NBI webpage: https://www.denbi.de/covid-19.

ELIXIR-DE PARTICIPATES IN ELIXIR'S RESPONSE TO COVID-19

Last week, an ELIXIR paper was published in the European Journal of Human Genetics (EJHG). The article highlights **ELIXIR's response against COVID-19, connecting data, tools and people across Europe**. The authors, N. Blomberg and K. Lauer, showcase the COVID-19 work of the ELIXIR Nodes and link it to the Interconnected European Data Spaces.

ELIXIR-DE provisions to the corona response are included in the linked interactive map on the ELIXIR Website.

Full quotation: Blomberg, N., Lauer, K.B. *Connecting data, tools and people across Europe: ELIXIR's response to the COVID-19 pandemic*. Eur J Hum Genet (2020). https://doi.org/10.1038/s41431-020-0637-5

Further reading on ELIXIR approaches at: https://elixir-europe.org/services/covid-19

EXCHANGE OF HEAD OF NODE AND DEPUTY POSITIONS OF ELIXIR-DE

Germany is member of the international organization ELIXIR since August 2016 when the Federal Ministry of Education and Research (BMBF) signed the so-called ELIXIR consortium agreement. The German ELIXIR Node ELIXIR-DE has been established to organize the cooperation with ELIXIR. Basic activities of ELIXIR-DE are provided by de.NBI groups and are financially supported by the BMBF. The ELIXIR-DE node is chaired by the Head of Node (HoN) and the deputy who are appointed by the BMBF. Since its foundation, ELIXIR-DE has been headed by Alfred Pühler (HoN) and Andreas Tauch (deputy). Effective from **1 June 2020** onwards, there will be an exchange between these two functions: A. Tauch will be the new HoN and A. Pühler will act as deputy. This swap was announced during the 22nd CCU meeting and later approved by the BMBF. It is the right time for this change since ELIXIR-DE, the German ELIXIR node, became legally independent of de.NBI with its own Central Coordinating Unit (CCU) which will be installed on 30 June 2020.

Andreas Tauch
HoN of ELIXIR-DE

elixir GERMANY

Alfred Pühler
Deputy HoN of ELIXIR-DE

TOBY HODGES APPOINTED TrC DEPUTY OF ELIXIR GERMANY

Toby Hodges from HD-HuB Heidelberg (EMBL) has recently been elected by the Central Coordination Unit (CCU) of de.NBI as deputy of the ELIXIR Germany Training Coordinator (TrC).

Photo: T. Hodges

Toby Hodges is managing the EMBL Bio-IT project, building and supporting the bioinformatics community at EMBL Heidelberg. Apart from this, he has organized and delivered more than 50 internal and external training courses and workshops since June 2015, teaching bioinformatics and computational research skills. Toby is an active contributor to several open source projects and communities, including "The Carpentries". Here, he is working as an Instructor Trainer, providing online and in-person training in methods for teaching computing to those who wish to obtain certification as Carpentries Instructors.

ELIXIR training is organized through the Training Platform, a European network of experts in their scientific domains and in adult education. 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 strategy across Europe.

More information at: https://www.denbi.de/elixir-germany

TEN SIMPLE RULES FOR MAKING TRAINING MATERIALS FAIR

The FAIR training group within the ELIXIR Training Platform has formulated ten recommendations to be considered for the development of findable, accessible, interoperable, reusable (FAIR) electronic training materials.

The publication comes timely with the actual pressure due to the corona pandemic to replace F2F training events by virtual formats. These rules may guide the development.

Full quotation: Garcia L, Batut B, Burke ML, Kuzak M, Psomopoulos F, Arcila R, et al. (2020) *Ten simple rules for making training materials FAIR*. PLoS Comput Biol 16(5): e1007854. https://doi.org/10.1371/journal.pcbi.1007854

Ten simple rules for making training materials FAIR. *Illustration from Luc Wiegers and Celia van Gelder: https://doi.org/10.5281/zenodo.3593257. https://doi.org/10.1371/journal.pcbi.1007854.g001*

de.NBI CLOUD/TRYGGVE POSITION PAPER ON PROCESSING SENSITIVE DATA IN THE CLOUD

Representatives of the **de.NBI Cloud** group started a joint collaboration with the **NeIC Tryggve** (https://neic.no/tryggve/), the Nordic collaboration for sensitive data funded by NeIC (Nordic e-Infrastructure Collaboration) and ELIXIR nodes of participating countries. Since dealing with sensitive data is a challenge for the de.NBI Cloud providers, joining forces at the European level is of strong interest.

In the aftermath of a joint workshop on 29 October 2019 at Stockholm Arlanda airport the groups elaborated the position paper: **Common cross-border approach for processing sensitive data based on the e-infrastructure from NeIC Tryggve and de.NBI Cloud** that has been released in April 2020.

The paper provides a background on the infrastructure required for the trusted transfer, storage, access and processing of sensitive data across (federated) service providers. It explains the type of the planned collaboration of German de.NBI Cloud and Nordic NeIC Tryggve and, as a proposed follow-up to Tryggve, the NeIC Heilsa consortium. The focus area of the collaboration is technical interoperability of federated services in the context of legal, operational, and semantic requirements, as well as standards for processing biomedical sensitive data in compliance with the GDPR and according to high IT security.

Find the position paper at: https://www.denbi.de/news/865-de-nbi-cloud-tryggve-position-paper

EMBL HEIDELBERG JOINS THE de.NBI CLOUD FEDERATION

Following approval of the demands for cloud locations in October 2020, the CCU has voted by circulation on 03.03.20 for the inclusion of the EMBL cloud in Heidelberg as an associated federated de.NBI Cloud site.

With EMBL, de.NBI Cloud will now expand on experience in the bioimaging sector. Bioimaging informatics is a fast growing research field where data does increase in size and complexity. New imaging technologies like electron cryo-microscopy and super-resolved fluorescence microscopy provoke a large number of scientists in Germany in need for expertise in processing, analysis and exchange in data.

de.NBI Cloud currently consists of six cloud sites and represents a federation of OpenStack based cloud sites that are unified to one de.NBI Cloud platform. Administrators and developers of the cloud sites are working together on different topics, like information security or the possible application of new cloud based technologies on bioinformatic use cases. Through this collaboration, the de.NBI Cloud team offers for about three years computational resources for life scientists in Germany and is capable of offering support and consulting for researchers to run their applications at scale.

EMBL Heidelberg already has a lot of expertise in cloud-related projects such as the “Helix Nebula” initiative which is a partnership between industry, space and science in the field of cloud computing. By this extension the de.NBI Cloud will get additional 2600 cores and 24 TB of RAM and additional GPUs on the long term. The de.NBI Cloud site at EMBL will provide besides OpenStack a Kubernetes installation which is considered as the best-suited solution in the cloud-based bioimaging field. We welcome EMBL as part of the de.NBI Cloud and look forward to a successful future collaboration.

NEW ASSOCIATED de.NBI PARTNER: THILO MUTH @ BAM

Photo: T. Muth

In April 2020, the CCU approved the application of Dr. Thilo Muth to become an Associated Partner of the de.NBI. Thilo Muth is head of the section eScience at the Bundesanstalt für Materialforschung und -prüfung (BAM) in Berlin. The BAM is a scientific and technical Federal institute with responsibility to the Federal Ministry for Economic Affairs and Energy. It tests, researches and advises to protect people, the environment and material goods. The BAM section eScience coordinates and advises the management and the divisions of BAM on scientific issues regarding digitalization in all fields of research.

Thilo Muth was previously active as team head of the ’Computational Proteomics’ Unit of the Robert Koch Institute (RKI Berlin). He is still collaborating with the de.NBI partner project ’MetaProtServ‘ of Dirk Benndorf and Gunter Saake from University Magdeburg and with Stephan Fuchs from Robert Koch Institute (RKI Wernigerode) who was affiliated to the de.NBI consortium in January 2020 (see Quarterly Newsletter Issue 1/20). Thilo Muth will contribute to the metaproteomics services of de.NBI by supporting the further development of a cloud-based version of the Prophane platform and the technical coupling of Prophane to the MetaProteomeAnalyzer (MPA). He will also participate in training courses in metaproteome analysis. With the successive association of both, Stephan Fuchs and Thilo Muth, the de.NBI consortium has substantially strengthened its activities in metaproteomics services and training.

Find the tools: MetaProteomeAnalyzer (MPA) Software (http://www.mpa.ovgu.de) and Prophane analysis software (http://www.prophane.de).

NEWS FROM THE de.NBI OFFICE

Vera Ortseifen started her new position as **ELIXIR Germany Node Coordinator** at the beginning of March 2020. She follows Rabeaa Alkhateeb in this function.

Vera finished her PhD in the field of Industrial Biotechnology in 2016. Her main research focus was on proteomics. From 2016-2019 she worked as a PostDoc with the phytopathogen *Xanthomonas campestris* and gained knowledge in different fields of systems biology.

In her new role as Node Coordinator, Vera is responsible for the coordination of all activities in the German ELIXIR Node. Furthermore, she supports the Head of Node and corresponds with the ELIXIR Hub.

We welcome Vera in our team and look forward to a successful cooperation!

UPDATE OF THE de.NBI CLOUD FLYER

The update of the de.NBI Cloud Flyer is out! Detailed information on the basic project types OpenStack and Simple VM as well as the Cloud-services and applications have been included. Specialized hardware like high memory nodes, GPU nodes and FPGA as well as Hosted Databases have been included.

For printed version, please write to contact@denbi.de

Download at: https://www.denbi.de/images/Downloads/deNBI_cloud_flyer_cmyk_print_V_02.pdf

de.NBI AT THE JOINT ANNUAL MEETING 2020 VAAM AND DGHM

The joint annual meeting of the Association for General and Applied Microbiology (VAAM) and German Society for Hygiene and Microbiology (DGHM) is one of the largest conferences in Germany for microbiology and biotechnology. This year's VAAM conference took place from 8-11 March at the University of Leipzig with more than 1000 participants accompanied by an industrial exhibition with about 70 companies. The looming pandemic reduced the number of participants and several lectures were held remotely. The de.NBI network appeared as one of the premium supporters at this year's conference. At the booth we introduced bioinformatics solutions to microbiologists to exploit their own data more effectively through applying tools, bioinformatics training, standards and compute services provided by de.NBI. Diverse aspects of microbiology were discussed during the four days of the meeting, beginning from big data in microbiology and microbial ecology, to microbial biotechnology and infection control and prevention. The first plenary session on the second conference day was dedicated to big data. Our de.NBI colleague Rolf Backofen from the RNA Bioinformatics Center (RBC) in Freiburg introduced the microbiologists into "High-Throughput Analysis with the European Galaxy Server (usegalaxy.eu)". Furthermore, our colleagues from the Bielefeld-Gießen Resource Center for Microbial Bioinformatics (BiGi), Jochen Blom and Oliver Schwengers, presented bioinformatic solutions for research data originating from bacterial organisms by introducing the tools Edgar and ASA³P in the poster session and oral presentation, respectively. In addition, a newly scheduled session was dedicated to the ongoing COVID-19 pandemic covering general information about coronaviruses and the developments of the outbreak in Wuhan.

The conference program is available at: https://www.dghm-vaam.de/fileadmin/congress/media/dghmvaam2020/druckelemente/DGHMVAAM2020_Programme.pdf

RECENT UPDATES OF de.NBI SERVICES

New versions of various de.NBI services and tools have been released in the last months accompanied by respective publications:

- **BacDive: The bacterial diversity metadatabase was updated with the** full integration of the taxonomic data from sister database LPSN (https://lpsn.dsmz.de/) and significant improvement of links to external databases, e.g. ChEBI, BRENDA, ENA & SILVA. Find BacDive at https://www.denbi.de/services/347-bacdive-the-bacterial-diversity-metadatabase-focuses-providing-organism-linked-information-covering-the-multifarious-aspects-of-bacterial-biodiversity

- **Proteins Plus:** The webserver for protein and ligand structures has been augmented with new tools published as *ProteinsPlus: interactive analysis of protein–ligand binding interfaces,* K Schöning-Stierand, K Diedrich, R Fährrolfes, F Flachsenberg, A Meyder, E Nittinger, R Steinegger, M Rarey, Nucleic Acids Research, gkaa235, https://doi.org/10.1093/nar/gkaa235. Find the service at: https://www.denbi.de/services/348-proteinsplus-a-web-portal-for-protein-structure-based-life-science-research

- **Crop Analysis Tools Suite (CATS):** A new publication on the module **BRIDGE,** a data warehouse and exploratory data analysis tool for genebank genomics of barley has been provisionally accepted. *BRIDGE – A visual analytics web tool for barley genebank genomics* , P König, S Beier, M Basterrechea, D Schüler, D Arend, M Mascher, N Stein, U Scholz and M Lange, Front. Plant Sci.|doi: 10.3389/fpls.2020.00701. Find CATS at https://www.denbi.de/services/503-crop-analysis-tools-suite

de.NBI @ CONFERENCES

de.NBI supported conferences in the near future

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

This year's conference is organized by a committee from Frankfurt, Mainz and Bingen. Due to the corona pandemic the conference will be held virtually. The first day will be dedicated to a number of workshops.
de.NBI Partners will teach the 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

General information and registration at: https://gcb2020.de/

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.
Due the corona pandemic and the social distancing measures in effect since 25 March 2020, the majority of de.NBI training courses had to be cancelled or postponed. The network is currently discussing and developing alternative forms of training.

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

Overview of upcoming de.NBI events

Date	Event	City	Organizer
15 May 2020	de.NBI Online Data Clinic - May 2020	online	CIBI/MASH
22-26 Jun 2020	Machine Learning using Galaxy	online	RBC
25 Jun 2020	Deploying Web Services for COVID-19 Research in the de.NBI Cloud	online	HD-HuB
30 Jun 2020	23. CCU Meeting	online	CAU
14 Sep 2020	OpenMS at the German Conference for Bioinformatics (GCB)	online	CIBI
14 Sep 2020	BioC++ - solving daily bioinformatic tasks with C++ efficiently	online	CIBI
14 Sep 2020	ProteinsPlus at the German Conference for Bioinformatics (GCB)	online	BioData
23 Oct 2020	24. CCU Meeting	Freiburg	CAU, RBC
15-19 Mar 2021	de.NBI Spring School 2021 - Metagenomics (postponed de.NBI Summer School 2020)	Gießen	BiGi et al.

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

IMPRESSUM

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