NFDI4Chem, Chemistry Consortium in the NFDI

Activity Update
Report of relevant cross-cutting topics for NFDI4Chem

TA6 – Synergies

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Executive Summary

During the initial phase of the NFDI, several cross-cutting topics have been identified and discussed with different consortia. As a matter of fact, the vision of the NFDI will be shaped by collaborative work on cross-cutting topics among the consortia. This report describes activities of the last year that aim to ensure that NFDI4Chem is involved in all relevant activities of the NFDI and represents the interests of the consortium. NFDI4Chem has been involved in the development process to identify and describe cross-cutting topics during the NFDI's start-up phase. Members of NFDI4Chem are represented in the Task Force Tools subgroups and the first four sections of NFDI e.V., three sections are co-coordinated by NFDI4Chem members. Collaborations with chemistry-related consortia such as NFDI4Ing, NFDI4Cat and NFDI4Health have been established and the first joint events have been hosted. Cross-cutting topics important for NFDI4Chem are actively shaped by two tasks in Task Area 6 and led, among others, to the establishment of the Task Force Tools subgroup AAI. With the sections starting their work, the establishment of working groups and organisation of workshops on the cross-cutting topics training and education, metadata standards and ontologies will start in 2022, to which NFDI4Chem will contribute.

Preceding Activities in 2018 - 2020

From the very beginning of the NFDI, the emerging consortia have identified common areas of interest and discussed the potential of addressing them jointly. This process illustrated at a very early stage the outstanding characteristic of the NFDI, namely how central topics of standardisation and services can be addressed in a cross-disciplinary, collaborative and user-centred way. In the process, 21 consortia agreed in August 2019 on the so-called "Berlin Declaration on NFDI Cross-Cutting Topics". In this declaration the consortia agreed on the general ideas, that the NFDI must build on a cooperative and inclusive effort to foster the FAIR data principles and to pave the way for sharing high-quality research data thus overcoming data interoperability challenges. In this context, a common list of cross-cutting topics was also agreed for the first time, covering (a) Collaborative governance and general framework, (b) Community (user) involvement, (c) Technical infrastructure and concepts, and (d) Legal and ethical aspects.

Following this first agreement representatives of the subject consortia and meanwhile formed cross-cutting initiatives met again in February 2020 to explore joint actions on cross-cutting topics. Their exchange resulted in the publication of the "Leipzig-Berlin-Erklärung zu NFDI-Querschnittsthemen der Infrastrukturentwicklung". The declaration concretised the cross-cutting topics already identified, added some more and outlined ways to address them within the NFDI. Concretely, participants exchanged ideas on the following areas of action: (a) Establishment of a cooperative framework, (b) Incentives for cultural change, (c) Establishment of a common data and services infrastructure, and (d) Legal aspects. Within these areas possible cross-domain services or standardisation efforts relevant for a majority of consortia were discussed. These included the development of a common research data platform, common standards for research data, the operation of IT services and support structures, the sustainable long-term archiving of data, the management of associated research software, and identity & access management (incl. AAI services and rights management). Legal issues like copyright, data protection and data

confidentiality or ownership of digital objects were also addressed. Four model proposals were discussed as possible collaborative approaches to work on cross-cutting topics: 1. Working groups of the NFDI subject consortia, 2. NFDI directorate working groups, 3. Cross-sectional consortia or 4. Funding outside the NFDI. By signing the two previously mentioned declarations, the total of 34 consortia initiatives agreed on the common understanding of the cross-cutting topics and ways to address these within the NFDI.

As a next step the NFDI Directorate organised the first strategy workshop on cross-cutting topics with the nine consortia from the first funding round in August 2020 to enable a deeper systematic understanding. A total of 16 cross-cutting topics with high relevance were selected and organised into the four overarching topic clusters: (a) Technical infrastructure and concepts, (b) Legal and ethical aspects, (c) Community (user) involvement, and (d) Collaborative governance and general framework.

The results of the workshop indicated that none of the discussed cross-cutting topics were completely clear to all consortia and that it is imperative to gain a deeper understanding of the scope and implications of a common approach (e.g., in terms of resource planning) to each topic. It was also agreed that some cross-cutting topics could be addressed by a smaller number of consortia for which these topics are of particular importance, while other topics must be addressed across the board by all consortia. At the same time, it became apparent that some topics can be clearly delineated, while others overlap with other cross-cutting topics, so that it is here that the need for more precise definitions and distinctions becomes most apparent. The still open discussion on which of the topics would be most suitable for processing in a section, working group or task force should be the subject of a follow-up workshop.

NFDI4Chem activities on cross-cutting topics

The coordination of NFDI4Chem's involvement in the cross-cutting topics is managed by Task Area 6 - Synergies. The main goal is to identify cross-cutting activities in the NFDI network relevant to NFDI4Chem and guarantee involvement of our members. These tasks are achieved by close monitoring of cross-consortia activities, participation in corresponding meetings and workshops, and appointment of delegates into the respective working groups and sections of NFDI e.V.. Furthermore TA6 ensures that the results of all cross-cutting activities are efficiently flow back into NFDI4Chem TA's. In our proposal we have already identified cross-cutting topics of outstanding importance for our consortium, to which we want to contribute to the NFDI and sections: a NFDI-wide service catalogue, an AAI service and a legally reliable framework of policies and guidelines for FAIR research data management.

NFDI4Chem was an active part in the identification and elaboration of the cross-cutting topics from the very start. Oliver Koepler and Christoph Steinbeck co-authored both declarations on cross-cutting topics. NFDI4Chem also continuously contributed to the process resulting in the first four NFDI e.V. sections.

NFDI Task Force Tools and their subgroups

Based on the experiences of business operations in the first months, consortia expressed their need to exchange so far gained knowledge and best practises on tools for collaborative work within and between the consortia and to develop common strategies and policies for them. Thus, in the beginning of 2021, the NFDI Task Force Tools was initiated to discuss different tools and technical solutions for e.g. cloud-based document management, code repository, chat, project management tools, helpdesks, authentication and authorisation. In the process, the task force was divided into smaller groups to work on specific issues and to jointly develop solutions. Table 1 shows the representatives of NFDI4Chem in the different subgroups of the Task Force Tools.

Subgroup	NFDI4Chem representative
Rocket.Chat	Christian Popp, Nisha Sharma
AAI & Rights Management	Felix Bach, Michael Klix, Steffen Neumann, Ulrich Weiss
File Sharing Cloud	Oliver Koepler
Project Management	Christian Popp
Helpdesk	Johannes Hunold
Data Management Planning	Daniela Hausen

Table 1: Overview of NFDI4Chem's participation in Task Force Tools.

As an outcome of these activities, a central NFDI Rocket.Chat server has been released to enable communication across all consortia. Rocket.Chat is also used on consortium-owned servers by NFDI4Chem and others for internal communication. The corresponding subgroup provides best practises and hands-on experience. In autumn 2021 several consortia, including NFDI4Chem, agreed to fund a shared enterprise licence of the project management software OpenProject. The evaluation of a joint strategy for the use of a cloud-based file sharing solution is still ongoing to the end of 2021.

NFDI Sections

Following on from the first strategy workshop on cross-cutting topics in Autumn 2020, a follow-up workshop in April 2021 consolidated the topics and prioritised the following four of them:
(Meta)Data, Findability; Terminologies; Provenance
Research Data Commons; Infrastructure / Interoperability / Interfaces
Training & Education
Ethical & Legal Aspects in General / Person-related

Prioritisation based on the relevance of the topic to most of the consortia and whether at least one of the consortia was willing to take a coordination role and become more involved

in that area. The topic of "Ethical and Legal Aspects" had an outstanding role in this discussion. Besides the common legal questions regarding copyright or data ownership it is of utmost importance for some of the consortia dealing with individual related data.

In a third NFDI Strategy Workshop on May 8 2021, the construct of the first four sections was worked out and how they should concretely work on the cross-cutting topics. Following this, the section concepts were developed and presented to the Senate for a decision on the establishment of the section. The Scientific Senate decided in September 2021 to establish the four sections "(Meta)Data, Terminologies and Provenance (Section-Metadata)", "Common Infrastructures (Section-Infra)", "Training & Education (Section-Edutrain)", and "Ethical, Legal & Social Aspects (Section-ELSA)" in order to be able to strategically address the selected cross-cutting topics within the NFDI Network.

The prioritisation of topics and the decision for the first sections were fully supported by NFDI4Chem. Metadata, terminologies, and provenance are of paramount importance to the NFDI4Chem work plan with the development of Minimum Information Standards, the Terminology Service, and the ELNs. The two tasks "Legally reliable framework of policies and guidelines for FAIR research data management" and "Authentication and Authorization Infrastructure'' of Task Area 6 in NFDI4Chem align with goals described in the sections Research Data Commons and Ethical, Legal & Social Aspects. The topics addressed in the section EduTrain are consistent with many of the tasks in Task Area 5 of NFDI4Chem.

Therefore, NFDI4Chem is actively involved in all sections (see Table 2), with NFDI4Chem representatives taking a coordinating role in the three sections "(Meta)daten, Terminologien, Provenienz" and "Training & Education", due to their particular relevance to the chemical community.

Section	NFDI4Chem representative	Institutional affiliation
Common Infrastructures	Felix Bach	KIT - Karlsruhe Institute of Technology
	Matthias Razum	FIZ Karlsruhe - Leibniz Institute for Information Infrastructure
(Meta)daten, Terminologien, Provenienz	Oliver Koepler (Coordination)	TIB - Leibniz Information Centre for Science and Technology
	Johannes Hunold	TIB - Leibniz Information Centre for Science and Technology
	Giacomo Lanza	PTB - Physikalisch-Technische Bundesanstalt
	Steffen Neumann	IPB - Leibniz Institute of Plant Biochemistry
	Christoph Steinbeck	FSU - Friedrich Schiller University Jena

	Sonja Herres-Pawlis (Coordination)	RWTH Aachen University
Training & Education	Ann-Christin Andres	JGU - Johannes Gutenberg University Mainz
	Johannes Liermann	JGU - Johannes Gutenberg University Mainz
	Jochen Ortmeyer	RWTH Aachen University
Ethical, Legal & Social Aspects	Franziska Boehm	KIT - Karlsruhe Institute of Technology
	Thomas Hartmann	FIZ Karlsruhe - Leibniz Institute for Information Infrastructure
	Stephanie von Maltzan	FIZ Karlsruhe - Leibniz Institute for Information Infrastructure

Table 2: Overview of NFDI4Chem's participation in the sections.

Assigned Tasks Cross-Cutting Topics within NFDI4Chem

Two cross-cutting topics were identified early on as particularly relevant for NFDI4Chem development. These are a NFDI-bridging Authentication and Authorization Infrastructure (AAI) for a comfortable and convenient use of NFDI4Chem services and Legal Aspects for numerous questions of data publication and data reuse. Due to their particular importance, these are embedded as dedicated tasks (Task 6.3.2 & 6.3.3) in Task Area 6.

Authentication and Authorization Infrastructure (AAI)

In the spirit of FAIR data principles, access to data and services should be as open and interoperable as possible. Nevertheless, there are several reasons why both resources and services require researchers to sign in. With the many services in the NFDI4Chem, the number of individual, separate logins quickly becomes difficult to manage. This issue is addressed by a NFDI-wide Authentication and Authorisation Infrastructure (AAI).

To begin initial discussions and create a roadmap regarding NFDI-AAI, a corresponding NFDI Task Force subgroup was established in spring 2021. First, the various existing technical approaches were assessed and their usefulness evaluated from the perspectives of NFDI as whole, NFDI4Chem services, and the user perspective. The result of these discussions and evaluation was the preparation of an AAI requirements questionnaire to determine both NFDI4Chem internal and NFDI-wide needs. The results of this survey on AAI experiences and requirements in NFDI services will be available beginning 2022. For the NFDI-AAI and NFDI4Chem requirements analysis, the existing ELIXIR and HIFIS solutions were examined, which are technically very similar to the AARC Blueprint Architecture). The evaluation covered perspectives from different angles. From the perspective of NFDI as a whole, we are looking for an established platform with solid backing, broad buy-in and good sustainability outlook. The choice should be compatible with an envisioned integration into the EOSC ecosystem. It would be great to have the actual operation outsourced to an experienced entity. From the perspective of NFDI4Chem

Services we need AAI that can easily be integrated into the user management of different systems / ELN / repositories. From the user perspective the application of access to a service and subsequently the (single-)sign-on should be intuitive. Planned steps for 2022 are the creation of a AAI Task Force in NFDI4Chem to create roadmap and connect to NFDI-Tools. The results of the AAI survey will be fed into the work of the section Common Infrastructures. Furthermore we plan hands-on using ELIXIR-AAI with OpenID for Rocket.Chat-Service.

Legally reliable framework of policies and guidelines for FAIR research data management

The operation of an infrastructure as the NFDI has to build on rules, to that individual users commit themselves and that are in accordance with German and if possible international legal status quo. It is key to provide a science-friendly legal framework that balances that great variety of interests through guidelines and data policies, terms of use, licensing standards, and data property. We will work on necessary steps to provide a legally reliable framework of policies and guidelines for FAIR RDM for researchers in the NFDI4Chem.

An initial overview of the IP/copyright status of research data in chemistry was elaborated at the Science Data Center MoMaF in cooperation with NFDI4Chem and presented at SaxFDM in February. Following on from this, another corresponding overview was presented by Thomas Hartmann (FIZ Karlsruhe) in March at the E-Science Days 2021 in his lightning talk "Forschungsdaten in den Naturwissenschaften: Eine urheberrechtliche Bestandsaufnahme mit ihren Implikationen für universitäres FDM". In addition to such assessments, the current focus is mainly on the preparation and organisation of a legal aspects workshops series in close collaboration and exchange with our partners (e.g. MoMaF & NFDI4Culture). These workshops, which are tailored to the NFDI4Chem community, will discuss critical issues around the topics copyright and licence models concerning research data; data ownership and scientist personal rights etc. and will answer concrete questions such as "Who owns the data generated during a research project?". These questions have been presented through the use of chart flows. One topic was shortly presented at the consortium meeting 2.0 "Mapping the challenges of data not covered by copyright - a preview". The aim is to raise awareness of these issues among researchers and at the same time to support them in the "legally secure" publication of their work. With the foundation of the section "Ethical, Legal & Social Aspects" in autumn these topics will also be addressed and discussed across consortia on NFDI-wide level. Beyond the preparation of the workshop, an analysis of the Nagoya Protocol has been prepared and presented by means of FAQs and a decision tree. In 2022 we will start with our workshop series "Legal analysis of open questions regarding using, sharing, publishing and archiving data '' covering copyright and licence models, data ownership and scientist personal rights.

Activities with neighbouring, chemistry related consortia

The cooperation of the consortia NFDI4Ing, NFDI4Cat and NFDI4Chem in the fields of metadata, terminologies, standards and ELN has existed since the formation of the consortia and became more concrete with the start of the funding through joint events. Already in July 2020, NFDI4Ing organised a workshop on the interoperability of metadata within the NFDI, to which NFDI4Chem contributed with a presentation. In November 2020,

a joint workshop of experts from the consortia and experts from BASF on ontologies was organised together with the NFDI Directorate to explore collaborations between academia and industry in this field. A joint working group organised a webinar in January 2021 with an introduction to ontologies in science and engineering. The webinar was aimed at interested scientists from the consortia communities. Starting with an introduction to the basics of vocabularies, terminologies and ontologies, practical applications in academic projects and chemical industry were presented. The webinar was followed by an average of 200 participants.

For the development of the NFDI4Chem Terminology Service, a close exchange has grown between the development teams of NFDI4Chem and NFDI4Health. Both consortia are using the code base of the Ontology Lookup Service (OLS) from EBI and are working together on strategies and joint efforts to develop new functionalities.

NFDI Base Services

The need for joint collaboration on cross-cutting topics is formulated by almost all consortia. However, there are not enough resources available in the consortia to work on these topics adequately or even to provide services for the entire NFDI. This has led to the idea of one or more Base Services consortia, which develop services for the entire NFDI along the needs of the subject consortia as described by the cross-topics and moderated by the sections.

The scope and shape of these Base Services consortia is still open to discuss at the time of writing this report. The call for proposals is to be published beginning of 2022. NFDI4Chem is involved in the process of the formation of the Base Services consortia by its representatives in the section and by Christoph Steinbeck as spokesperson of the consortia assembly.

Outlook 2022

The beginning of 2022 will be marked by the start of work in the sections and the launch of concrete work on cross-cutting topics by working groups of the sections. Planning for the continuation of the workshops on metadata and ontologies has already begun. Now that representatives of NFDI4Chem are strategically positioned in the first four NFDI e.V. sections and further Task Forces, TA6 will establish processes for 2022 to ensure the exchange and re-use of work results back into the NFDI4Chem Task Areas. We will continue to monitor the formation of new sections and ensure that NFDI4Chem is represented in them as needed.

For the coming year, we plan to expand joint activities with chemistry-related consortia to include the consortia of the 2nd funding round. In addition to the pursuit of joint workshops and webinars, a main topic under the umbrella of the Section (Meta)data will be the joint development of standards for chemical metadata, data formats, and the alignment of terminologies. After an initial kickoff with the Mathematical Research Data Initiative (MaRDI), we are exploring possible joint activities in the application of mathematical models and methods provided by MaRDI in the field of theoretical and physical chemistry. We intend to deepen joint efforts in software development for the Terminology Service with NFDI4Health and investigate interlinking of infrastructure components. Finally, the start of

the workshop series "Legal analysis of open questions regarding using, sharing, publishing and archiving data" will mark an first milestone on the development of guidelines and policies to support researchers on the publication of research data.

Appendix: Outreach Overview

List of publications (authored or coauthered by NFDI4Chem representives):
- [Berlin Declaration on NFDI Cross-Cutting Topics](#) (22.09.2019)
- [Leipzig-Berlin-Erklärung zu NFDI-Querschnittsthemen der Infrastrukturentwicklung](#) (15.06.2020)
- [NFDI Cross-cutting Topics Workshop Report](#) (11.03.2021)
- [Sektionskonzept Training & Education zur Einrichtung einer Sektion im Verein Nationale Forschungsdateninfrastruktur (NFDI) e.V.](#) (26.10.2021)
- [Sektionskonzept Meta(daten), Terminologien und Provenienz zur Einrichtung einer Sektion im Verein Nationale Forschungsdateninfrastruktur (NFDI) e.V.](#) (29.10.2021)
- [Sektionskonzept "Ethical, Legal & Social Aspects" (section-ELSA)](#) (05.11.2021)
- [Sektionskonzept "Common Infrastructures"](#) (28.10.2021)

List of events 2020 & 2021 (organised, contributed, attended):

Date	Event title	NFDI4Chem partner involved	Kind of contribution
02.-03.07.20	Interoperabilität von Metadaten innerhalb der NFDI – Konsortienübergreifender Metadaten-Workshop	IPB, JGU	contributed with lecture
19.01.21	[Ontologies in Science and Technology – Joint web seminar together with NFDI4Ing and NFDI4Cat](#)	TIB	organised, contributed
18.02.21	An overview about the IP/copyright status of research data in Chemie (elaborated in the Science Data Center MoMaF in Baden-Württemberg, Digital Kitchen von SaxFDM	FIZ Karlsruhe, KIT	contributed
22.-26.02.21	[RDA Deutschland Tagung 2021](#)	TIB	attended, contributed
4.3-5.3.21	Lightning talk "Eine urheberrechtliche Bestandsaufnahme mit ihren Implikationen für universitäres FDM" Tagungsband der E-Science-Tage 2021, coming soon	FIZ Karlsruhe	contributed with lecture
08.07.21	[3. NFDI-Konferenz](#)	TIB	attended
09.-15.08.21	[51st IUPAC General Assembly](#)	TIB	attended & contributed with lecture

01.09.21	GDCh-Wissenschaftsforum Chemie 2021 – NFDI4Chem Session together with NFDI4Cat, FAIRmat, DAPHNE4NFDI & NFDI-MatWerk	FSU, RWTH	organised & contributed with lecture
20.10.21	Kick-off meeting NFDI section "Common Infrastructures"	IPB, KIT	attended
22.11.21	Kick-off meeting NFDI section "Ethical, Legal & Social Aspects"	FIZ	attended & contributed
29.11.21	Kick-off meeting NFDI section "(Meta)daten, Terminologien, Provenienz"	TIB	organised
02.12.21	NFDI4Ing Forum: Electronic lab notebooks (ELNs)	RWTH	contributed with lecture
06.12.21	NFDI InfraTalk: Advancing the usage of Metadata with Electronic Laboratory Notebooks	TIB & KIT	contributed with lecture
08.12.21	NFDI section training & education: Intro to training material repository	RWTH	attended & contributed