7/18/2019

Binding Letter of Intent by the Consortium NFDI4MSE for the DFG Call for NFDI Proposals during the Term 2019

List of Abbreviations:

DFG	Deutsche Forschungsgemeinschaft
NFDI	Nationale Forschungsdateninfrastruktur / National Research Data Infrastructure
NFDI4MSE	Consortium National Research Data Infrastructure for Materials Science and Engineering

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1. Type of Notification

This document represents the binding letter of intent as an advance notification as required for proposals in 2019 for participation of the consortium NFDI4MSE within the according NFDI proposal term and deadline October 15, 2019.

2. Formal Details:

Name of the consortium:
National Research Data Infrastructure for Materials Science and Engineering

Acronym of the consortium:
NFDI4MSE

Applicant Institution:
Fraunhofer-Gesellschaft zur Förderung der angewandten Forschung e.V.
Hansastraße 27 c
80686 München
Head of the Institution: Prof. Dr.-Ing. Reimund Neugebauer, President

Spokesperson:

- Prof. Dr. Christoph Eberl
  chris.eberl@iwm.fraunhofer.de
  Deputy Head of the Fraunhofer Institute for Mechanics of Materials, IWM

Co-Applicant Institutions and spokespersons:

- Friedrich-Alexander-Universität Erlangen-Nürnberg
  Prof. Dr. Erik Bitzek
  Martensstr. 5a
  91058 Erlangen

- Karlsruhe Institute of Technology, KIT
  Prof. Dr. Peter Gumbsch
  Straße am Forum 7
  76131 Karlsruhe

- RWTH Aachen
  Prof. Dr. Matthias S. Müller
  Templergraben 55

52062 Aachen

- Saarland University
  Prof. Dr. Frank Mücklich
  Saarbrücken Campus
  66123 Saarbrücken

- Max-Planck-Institut für Eisenforschung GmbH, MPIE
  Prof. Dr. Jörg Neugebauer
  Max-Planck-Straße 1
  40237 Düsseldorf

- FIZ Karlsruhe – Leibniz-Institut für Informationsinfrastruktur GmbH
  Prof. Dr. Harald Sack
  Hermann-von-Helmholtz-Platz 1
  76344 Eggenstein-Leopoldshafen

- Technical University Bergakademie Freiberg
  Prof. Dr. Stefan Sandfeld
  Lampadiusstrasse 4
  09599 Freiberg

- German Research Center for Artificial Intelligence, DFKI
  Prof. Dr. Philipp Slusallek
  Stuhlsatzenhausweg 3
  D-66123 Saarbrücken

- Steinbuch Centre for Computing, Karlsruhe Institute of Technology, KIT
  Prof. Dr. Achim Streit
  Hermann-von-Helmholtz-Platz 1
  76344 Eggenstein-Leopoldshafen

- Fraunhofer Institute for Material and Beam Technology, IWS
  Prof. Dr. Martina Zimmermann
  Winterbergstr. 28
  01277 Dresden

Specifics on the NFDI4MSE Governance and the role of the participants:

The consortium NFDI4SME is committed to leave a maximum of its decision-making power to the scientific community of the materials sciences and engineering (MSE). At the same time, its governance structure has to suit the internal roles as suggested by the DFG guidelines (p. 5), which distinguish the group of project partners into “participants” and “applicant institutions”. Accordingly, the latter are deemed explicitly responsible for specific work areas, while the former ones will primarily apply for funds to assume parts of the overall shared workloads, as e.g. development and implementation of material-sciences specific software. The two roles require the consortium to structure itself in an appropriate way while equally ensuring community empowerment.

With the practical challenges in mind that this project represents, NFDI4MSE intends to shape its internal governance according to these aforementioned conditions. The preliminary composition portrays a two-sided approach, in which the community of the MSE receives budget and program sovereignty in the role of “participants”, ensuring a transparent representation by enabling soft membership borders. Consequently, a number of the MSE stakeholders is assigned particularly to specific task areas, assuming this responsibility, together with the further necessary providers of technical expertise, in the role of “co-applicants”.

These considerations lead to a first governance proposal for this consortium, which is documented more specifically in 5. Annex.

3. Objectives, work program and research environment

Research Area of the proposed consortium (according to the DFG classification system):

This consortium aims to represent the community of research area 43 of the DFG classification system: “Materials Science and Engineering” (MSE).

The Digital Transformation touches core aspects of our scientific way of working in MSE, including technological instrumentation, evaluation strategies and scientific exchange up to the way scientific impact is measured. For smaller or even individual scientific groups it would be quite difficult to make use of all advantages and to tackle all the challenges associated with this transformation. At the same time, the design, processing, characterization and simulation of materials has always required a joint effort of several groups in order to meet the materials complexity. The Digital Transformation is a chance for boosting, structuring and optimizing this exchange, provided transparent communication standards are established. Therefore, such a fundamental transformation naturally has to be addressed through a community effort rather than an individual one.

For this matter and according to its composition, the consortium NFDI4MSE claims to represent the German key stakeholders in the domestic field of the MSE disciplines. The consortium wishes to take up the challenge of initiating the digital transformation in this field, supported by its strong rooting into the scientific community.

Concise Summary of the planned consortium’s main objectives and task areas:

Materials Science and Engineering is a highly interdisciplinary field of research, integrating physics, chemistry, and mechanical, chemical and electrical engineering to develop novel materials, characterize and optimize them, develop processes to manufacture such materials, evaluate their lifetime and develop strategies to maximize the recyclability at the end-of-life. All these aspects are connected with a wide spectrum of data in various formats, which only in combination allow a complete representation of the material and its characteristics.

Special about the plethora of data in material sciences is their inherently multiscale character, capturing various chemical and physical phenomena on different time and length scales. This is reflected by strongly heterogeneous microstructures, which determine the complete mechanical and a substantial fraction of the functional performance. The “microstructure” constitutes of the local chemical composition and the locally changing arrangement of different phases and crystalline areas, which may contain certain crystal defects, which range e.g., from defects at the atomic structure, micron scale phase structures to macroscale pores. Interestingly, any process (e.g., thermal treatment or mechanical loading) applied to a sample or a specimen also changes the materials microstructure in a way that the following processing steps or the resulting behavior depends on the full materials history. As a consequence, the here anticipated materials specific digital data space has to be able to capture the various states of the material on different scales as well as throughout all processes in between. Furthermore, the data space has to capture the various highly complex dependencies between materials properties and the various ingredients of the microstructure (e.g. regions of different chemical composition or crystal structure(Bitzek)). The ultimate objective is the prediction of the correlation of the initial microstructure and the processes applied to the material with the final state of the material and its properties.

Therefore, the NFDI4MSE consortium proposes to set up a digital platform, which will take this complex hierarchical character of materials into account, enabling synergies and reducing the technological barriers among the community. To date, NFDI4MSE has identified **four primary task areas** for proceeding with this goal, each of which are supposed to be addressed by a minimum of **one field expert and one materials scientist** from the group of co-applicants. All the task areas furthermore come with their according objectives, each listed underneath:

- **Task Area Ontologies**

1. Develop and integrate a unified materials ontology, which enables interoperability between heterogeneous materials data, analytics tools and materials models on the different length and time scales characteristic for materials in a flexible and seamless manner.
2. Easily implement ‘private’ materials ontologies for ‘homegrown’ tools and digital workflows supported by a stringent version control and the possibility to suggest or share these ontology branches to partners and the greater community.

- **Task Area Software Development for the MSE**

3. Develop individual digital workflows for experimental and simulation environments based on a seamless integration of available and in-house tools.
4. Enhance elaborated visualization tools as well as materials data analytics tools that reproducibly connect publishable figures with the underlying raw data.
5. Provide advanced data analytics methodologies and integrate machine-learning tools into individual workflows to produce digital materials representations.

- **Task Area Material Data Services**

6. Share and access materials raw data and meta data, based on the FAIR principles[1], to contribute to a comprehensive digital representation of materials and material classes.
7. Set up straightforward data sharing across institutions and disciplines for collaborative projects.
8. Quickly establish local data spaces with integrated data sovereignty (e.g. access management) and a secure authorship (e.g. through cryptography and certification of workflows and data).

- **Task Area Community Interaction**

9. Create online trainings and documentation of ontologies, workflows, software and numerical tools.
10. Create information and course material to help with onboarding of new students and scientists as well as implement it into their teaching.
11. Discover materials specific solutions through an active MSE online community and start new collaborations.

For more information on task area distribution among (Co-) Applicants, refer to the Responsibilities per Task Area (in 5. Annex).

[1] Data ought to be “**F**indable, **A**ccessible, **I**nteroperable and **R**eusable (FAIR) both for machines and for people”, as defined by Wilkinson et al, 2016 [LINK].

Brief description of the proposed use of existing infrastructures, tools and services that are essential in order to fulfil the planned consortium's objectives.

Challenges of digitalization are not unknown to the MSE community, which the consortium NFDI4MSE represents. The discipline has already proceeded with several projects, both of processual and technical nature, promising to smoothen the way into a rather comprehensive approach such as the NFDI aims to become. Some of these ongoing key efforts are stated below.

The availability of platform-independent open-source software solutions for the processing of standardized data defined in the materials data space will enable international visibility. The cross-institutional development of these tools, of related data formats and the sustainable hosting of the source code, of use cases and of accessible documentation is quintessential in order to establish the anticipated standard. Here, both the **Fraunhofer Materials Data Space** and the **Industrial Data Space** initiatives work on comprehensive data standards for multi-stakeholder environments and provide useful starting infrastructures that NFDI4MSE can build upon.

From July 2019 on the **platform "MaterialDigital" and its associated consortium**, which overlaps with NFDI4MSE, will start to work on pilot projects for developing a materials centered data space based on examples from science and industry.

The **Rheinisch-Westfälische Technische Hochschule Aachen** (RWTH) and the **Karlsruhe Institute of Technology** (KIT) with its Steinbuch Centre for Computing (SCC) are experienced **providers of research data management services and infrastructure**. E.g. SCC is a partner in MoMaf (Science Data Center for Molecular Material Sciences), EUDAT, EOSC and coordinator of the Helmholtz Data Federation.Tightly connected to the aspect of tools and infrastructures are a number of existing approaches to unify materials data platforms and foster interaction among the field of material scientists. These use cases could serve as prototypes, for NFDI4MSE to build up on:

At the University of Stuttgart projects in the context of the Open Software and Data Hub (OpenDASH) there is currently an approach being set up within the **Cluster of Excellence Data-Integrated Simulation Science (SimTech, EXC2075),** which could serve as an initial point of departure.

The **Cluster of Excellence *liv*MatS at the University of Freiburg** will implement an ontology based graph database as a common data space bridging the gap between several disciplines of the social and natural sciences. The tools and data space architecture from NFDI4MSE will foster the highly interdisciplinary research within *liv*MatS by enabling continuous digital workflows and enhance the collaboration within the shared labs and workspaces.

The **Cluster of Excellence "3D Matter Made to Order"** initiative of **KIT and the University of Heidelberg** pursues a highly interdisciplinary approach combining natural and engineering sciences. The planned research cluster concentrates on three-dimensional additive manufacturing techniques, from the molecular level to macroscopic dimensions. The tools and data space architecture from NFDI4MSE will accelerate the development of efficient digital workflows of the cluster and vice versa.

Through its **Cluster of Excellence Engineering of Advanced Materials (EAM)** the Friedrich-Alexander-University (FAU) Erlangen-Nurnberg was able to establish several interdisciplinary research centers. This includes, e.g., the Center for Nanoanalyis and Electron Microscopy (CENEM) or the Central Institute for Scientific Computing (ZISC), where the dataspace architecture, tools, workflows and ontology could be tested in an interdisciplinary framework while combining MSE with chemical engineering.

The international research training group **DFG-GRK2078 CoDiCoFRP** at KIT establishes digital twins for complex processing routes for fiber reinforced polymer structures by knowledge and ontology based approaches. Research-oriented modules are set up for BSc and MSc students to become familiar with ontology-based approaches in materials modeling.

The research training groups mentioned above will provide excellent opportunities to train the next generation of material scientists in the use of the concepts and tools developed in NFDI4MSE.

Also FAU's **joint Collaborative Research Center SFB/TR103 "From Atoms to Turbine Blades" together with the RU Bochum** already tracks their samples life from casting through processing, testing and characterization and accumulates and integrates experimental data and scales and combines it with scale-bridging modelling. It will serve as a test-bed for the software tools and workflows developed in the NFDI4MSE.The **Rhineland-Palatinate Priority Research Topic "Advanced Materials Engineering" (AME) at TU Kaiserslautern (TUK)** bundles TUK's materials related research activities in an interdisciplinary platform with participating scientists from materials science and engineering, production and process engineering, physics and informatics. In the upcoming years, AME will serve as TUK's key platform on digital data representation and processing in materials related research.

Interfaces to other proposed NFDI consortia: Brief description of existing agreements for collaboration and/or plans for future collaboration.

The consortium NFDI4MSE has already started to interact with the consortia **FAIRmat, NFDI4Ing** and **MaRDI.** Furthermore, NFDI4MSE is looking forward to discuss the necessary interfaces to **NFDI4Chem, NFDI4Physics** and the **Nanosafety** consortium**,** as well as smaller consortia like **DAPHNE.** NFDI4MSE follows closely as their programs, goals and strategies develop.

In case of the topically closely related consortia (FAIRmat and NFDI4Ing) it is planned to particularly consider the scientific and technological overlap regions in discussions and joint activities. Especially concerning the development of a common ontology requires experts on both sides understanding the semantics and grammar as well as the culture to prevent misunderstandings. For example, the databases for the physical properties of individual phases that are handled by **FAIRmat** can be combined with ontologies, processing history and microstructure information that NFDI4MSE takes care of in order to achieve a complete digital representation of materials. Furthermore, it is planned, to organize joint workshops on ontology and their implementation. Another planned workshop topic is training regarding data handling and data analysis. While this is clearly a common theme for almost all NFDI consortia, synergies between consortia can be fostered best if the underlying scientific work is related, which is particularly the case for the consortia mentioned above.

Furthermore, NFDI4MSE will collaborate with the consortium **MaRDI** regarding the development and usage of representations of mathematical objects. This holds in particular in context of mathematical multi-scale modelling and as a foundation for the ontologies developed at NFDI4MSE. **MaRDI** will connect experimental and simulation data of real materials from NFDI4MSE with mathematical models and metadata in order to established confirmable workflows. Ideally, this will take place for use cases that build upon best practice examples from NFDI4MSE.

NFDI4MSE has furthermore agreed to work hand in hand with **NFDI4Ing** regarding cross-cutting topics and community outreach. For example, the software architecture jointly envisioned by **NFDI4Ing** and NFDI4MSE combines the efforts for international data spaces while mutually ensuring FAIR Data Principles. It therefore provides researchers with best practices for collaboration and data management and thus contributes to the NFDI vision.

Finally, NFDI4MSE has been working with the **Nanosafety** consortium, which covers a relevant and growing field between life science, materials science and engineering as well as chemistry. This highly interdisciplinary extent requires tight interaction of different experts to understand the complex interactions.

4. Cross-cutting topics

Please identify crosscutting topics that are relevant for your consortium and that need to be designed and developed by several or all NFDI consortia:

In accordance with the extent of the NFDI project, there is a number of working areas, which will have to be covered by several consortia equally. Since each of the individual consortia will need to focus primarily on their technical context rather than on processual details, it appears useful to identify overlapping interdependencies and possible synergies among them. Planning and implementing shared methods according to joint approaches does not only promise decreased workloads in comparison to individual solutions, but also leaves easier interfaces for the future integration and sharing of consortia's outputs, like e.g. products, infrastructures and processes. Such cjompatibilities will also play a strong role for the long-term sustainable maintenance of the newly created infrastructures. First and perhaps foremost of these efforts will be the mutual challenge of managing data. This aspect includes, e.g., ensuring data security and sovereignty, guaranteeing fair authorship or finding ways to store interdisciplinary ontologies. Since the data format will determine the necessary software architecture and vice versa, the latter will play a role within these considerations, as well. With the progression of software planning and implementation, also physical issues of the platform will increase in relevance, including joint management of servers and internal processes. Further primarily collective requirements involve legal questions, as e.g. defining the corporate entity of the newly created organizations and constituting their rights and sanctioning management both internally and externally. Finally, all NFDI consortia will have to invest effort into community development, including both hard aspects like educational material about the newly created tools and soft aspects like cultural change and acceptance.

Please indicate which of these crosscutting topics your consortium could contribute to and how:

In following the joint objectives stated above, the consortium NFDI4MSE considers itself generally well positioned and open for collaboration of any kind. The background in materials science and engineering results in a strong expertise of NFDI4MSE in the hierarchical structuring of data and sophisticated dependencies in databases and between various partners. This gives the consortium the capability of managing, scaling and integrating locally stored object-oriented data.

Furthermore, due to the consortium's strong partnerships with data and computing centers, including the Rheinisch-Westfälische Technische Hochschule Aachen (RWTH), the German Research Institute for Artificial Intelligence (DFKI) and the Karlsruhe Institute of Technology (KIT) there are experts and capacities for a variety of technical challenges at the consortium's disposal. This allows NFDI4MSE to act not only from the scientific view of Material Science and Engineering but also from the perspective of the necessary aforementioned infrastructure, software architecture and development and state-of-the-art computer sciences including Artificial Intelligence and Machine Learning methods.

In total, among the variety of NFDI consortia, NFDI4MSE could thus generally serve as a technical advisor in the field of data management and processing, which, according to the considerations above, plays one central role within the NFDI's intentions.

5. Annex

List of all NFDI4MSE (co-)spokespersons and participants, including with whom the former collaborated closely during the last three years:

Title	**First Name**	**Family Name**	**Institution**	**(Co-)Applicants' close Collaborations (due by August, 16th 2019)**
Prof. Dr.	Hannah	Bast	Uni Freiburg	
Prof. Dr.	Tilmann	Beck	TU Kaiserslautern	
Prof. Dr.	Erik	Bitzek	FAU Erlangen	
Prof. Dr.	Thomas	Böhlke	KIT	
Prof. Dr.	Stefan	Diebels	Uni Saarbrücken	
Prof. Dr.	Karsten	Durst	TU Darmstadt	
Prof. Dr.	Chris	Eberl	Fraunhofer IWM	
Dr.	Felix	Fritzen	Universität Stuttgart	
Prof. Dr.	Peter	Gumbsch	Fraunhofer IWM	
Prof. Dr.	Nina	Gunkelmann	TU Clausthal	
Prof. Dr.	Alexander	Hartmaier	Ruhr-Universität Bochum	
Dr.	Ulrich	Herb	SULB, Uni Saarland	
Dr.	Tilmann	Hickel	MPIE	
Dr.	Erica	Lilleodden	HZG	
Prof. Dr.	Joachim	Mayer	RWTH Aachen	
Prof. Dr.	Frank	Mücklich	Uni Saarbrücken	
Prof. Dr.	Matthias S.	Müller	RWTH Aachen	
Prof. Dr.	Jörg	Neugebauer	MPIE	
Prof. Dr.	Ulrich	Panne	BAM	
Prof. Dr.	Harald	Sack	FIZ Karlsruhe	
Prof. Dr.	Stefan	Sandfeld	TU Freiberg	
Prof. Dr.	Hans J.	Seifert	KIT	
Prof. Dr.	Philipp	Slusallek	DFKI, Uni Saarland	
Prof. Dr.	Achim	Streit	KIT	
Prof. Dr.	Thomas	Speck	Uni Freiburg	
Prof. Dr.	Ralf	Wehrspohn	Fraunhofer IMWS	
Prof. Dr.	Stefan	Weihe	MPA Stuttgart	
Prof. Dr.	Stephan	Wulfinghoff	Kiel University	
Prof. Dr.	Martina	Zimmermann	TU Dresden	

Preliminary Governance Structure of NFDI4MSE:

This consortium proposes a shared approach for assuming responsibilities among the two stakeholder groups (“Participants” and “Applicant Institutions”). A possible strucuture would be the formal appointment of both materials scientists and providers of external expertise, possibly each grouped by two, as co-applicants for each task area. Since one or more institutions may lead task areas, the resulting groups could jointly determine their procedure, ensuring both community participation in formalizing each task area and the technical expertise to implement it.

Since the governance must map both processual and hierarchical structures, this approach would lead to a preliminary design as below.

Clarification of applied expressions:

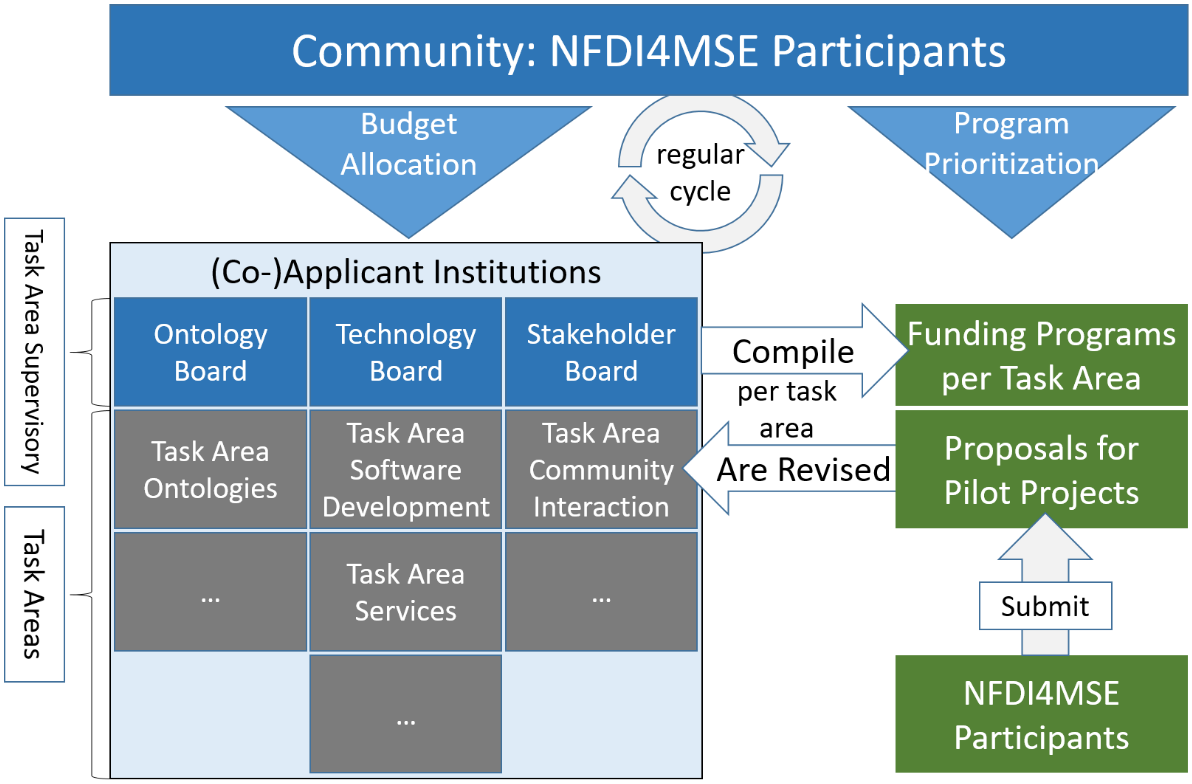
- Community / Participants: The material science community, represented especially by the professional associations and academia. Note that this group works with soft borders, enabling flexible adaption to changes in the group of stakeholders.
- Materials Scientists: Members of NFDI4MSE, which belong to the academic field of material sciences.
- Expertise providers: Members of NFDI4MSE that are unrelated to the material sciences. These experts are supposed to ensure maximum professionalism within the goal implementation.
- Task groups: Responsible for single fields of action (i.e. task areas), each composed of co-applicant institutions from both the groups of material scientists and expertise providers.

Governance Procedure:

The involved community agrees through their representatives about the funding for different task areas for the upcoming budget cycle (of possibly one year). It then passes the budget management competency on to each of the task groups. Task areas and their respective groups are structured internally according to their field of occupation: Ontology building, technology provision and community interaction. The three pillars each carry their own executive board and decision-making responsibilities.

Every academic entity from the group of participants is asked to submit proposals to the appropriate task group for funds to implement pilot projects and software development according its specific solution. Each of the task groups gathers the sum of these proposals over the period of one year. After receiving certainty about its funding for the upcoming cycle as stated above, it has a time to review each of the applicant proposals and develop recommendations according to their practicability, efficiency etc. The task groups then present all of the resulting feasible proposals for their field to the consortium’s community, to which the community holds the responsibility to make a choice according to its priorities.

Schematic Illustration:



Preliminary Responsibilities per Task Area

	Co-Applicants
Task Area **Ontologies**:	Prof. Dr. Stefan Sandfeld, TU Freiberg Prof. Dr. Harald Sack, FIZ Karlsruhe
Task Area **Software Development**:	Prof. Dr. Jörg Neugebauer, MPIE Prof. Dr. Philipp Slusallek, DFKI
Task Area **Services**:	Prof. Dr. Erik Bitzek, FAU Erlangen Prof. Dr. Peter Gumbsch, KIT Prof. Dr. Matthias S. Müller, RWTH Aachen Prof. Dr. Achim Streit, SCC-KIT
Task Area **Community Interaction**:	Prof. Dr. Frank Mücklich, University Saarbrücken Prof. Dr. Martina Zimmermann, TU Dresden