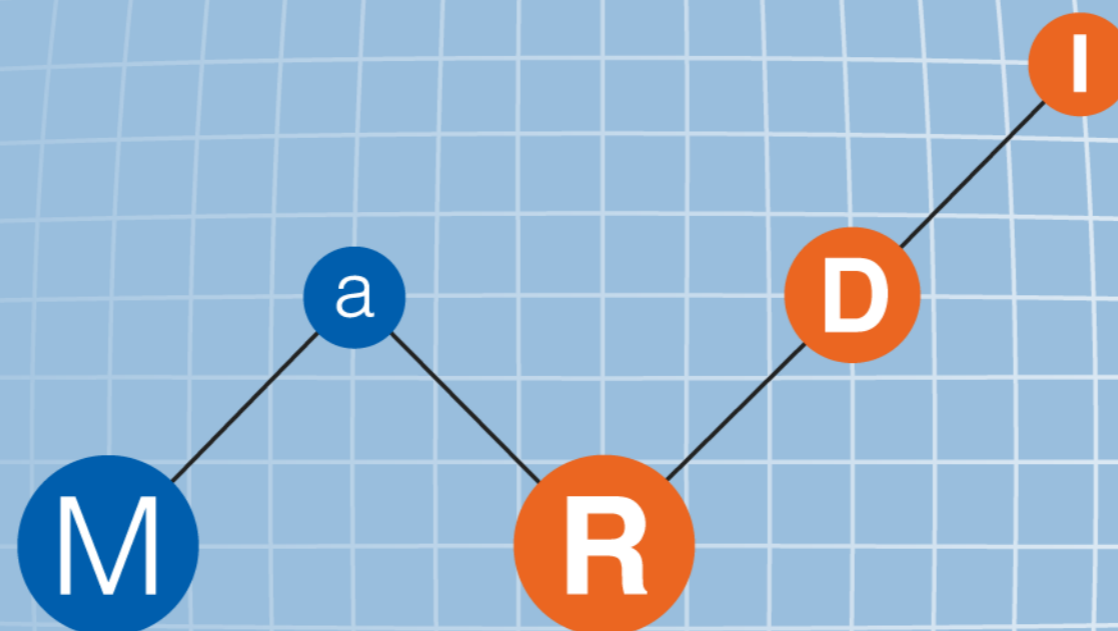


# MaRDI - The Mathematical Research Data Initiative

*within the NFDI*

Towards a  
Data Culture  
for Mathematics  
and Its Users



@mardi4nfdi

Minisymposium „Ready for MaRDI,  
am I a digital mathematician?“

Thomas Koprucki and Karsten Tabelow

WIAS, Weierstrass Institute for Applied Analysis and Stochastics



### Periodic Table of Finite Simple Groups

1																				$C_2$
$Alt_5$	$A_1(7)$	$A_n$	$B_n$	$C_n$	$D_n$	$F_4$	$G_2$							$B_3(2)$	$C_3(3)$	$D_4(2)$	${}^2D_4(2)$	${}^2A_2(3)$		$C_3$
$Alt_6$	$A_1(8)$				$E_{6,7,8}$									$B_2(4)$	$C_3(5)$	$D_4(3)$	${}^2D_4(3)$	${}^2A_2(4)$		$C_5$
$Alt_7$	$A_1(11)$	$E_6(2)$	$E_7(2)$	$E_8(2)$	$F_4(2)$	$G_2(2)$	${}^3D_4(2)$	${}^2E_6(2)$	${}^2B_2(8)$	${}^2F_4(2)'$	${}^2G_2(27)$			$B_3(2)$	$C_4(3)$	$D_5(2)$	${}^2D_5(2)$	${}^2A_2(5)$		$C_7$
$Alt_8$	$A_1(13)$	$E_6(3)$	$E_7(3)$	$E_8(3)$	$F_4(3)$	$G_2(3)$	${}^3D_4(3)$	${}^2E_6(3)$	${}^2B_2(32)$	${}^2F_4(8)$	${}^2G_2(243)$			$B_2(5)$	$C_3(7)$	$D_4(5)$	${}^2D_4(4)$	${}^2A_3(3)$		$C_{11}$
$Alt_n$	$A_1(q)$	$E_6(q)$	$E_7(q)$	$E_8(q)$	$F_4(q)$	$G_2(q)$	${}^3D_4(q)$	${}^2E_6(q)$	${}^2B_2(q)$	${}^2F_4(q)$	${}^2G_2(q)$			$B_n(q)$	$B_n(q)$	$D_n(q)$	${}^2D_n(q)$	${}^2A_n(q)$		$C_p$

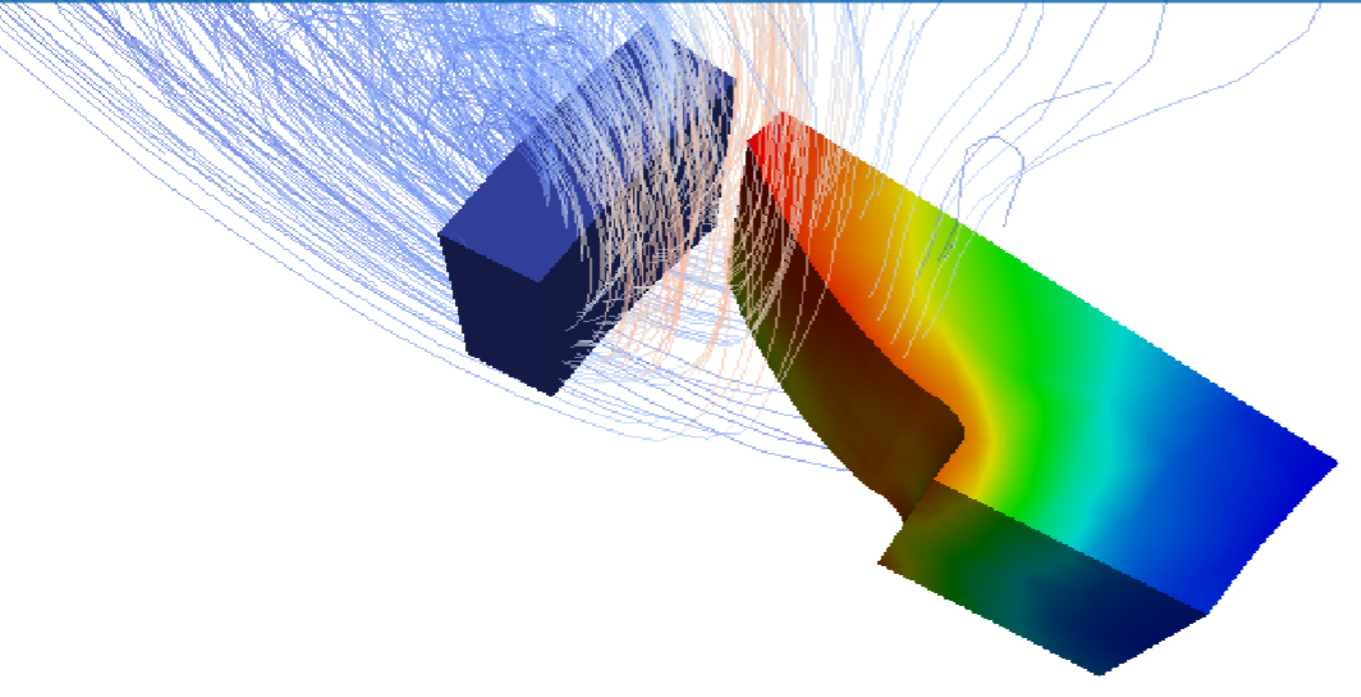
<ul style="list-style-type: none"> <li>Alternating Groups</li> <li>Classical Groups</li> <li>Chevalley Groups</li> <li>Classical Steinberg Groups</li> </ul>	<ul style="list-style-type: none"> <li>Suzuki Groups</li> <li>Ree and Tits Groups</li> <li>Sporadic Simple Groups</li> <li>Cyclic Groups</li> </ul>
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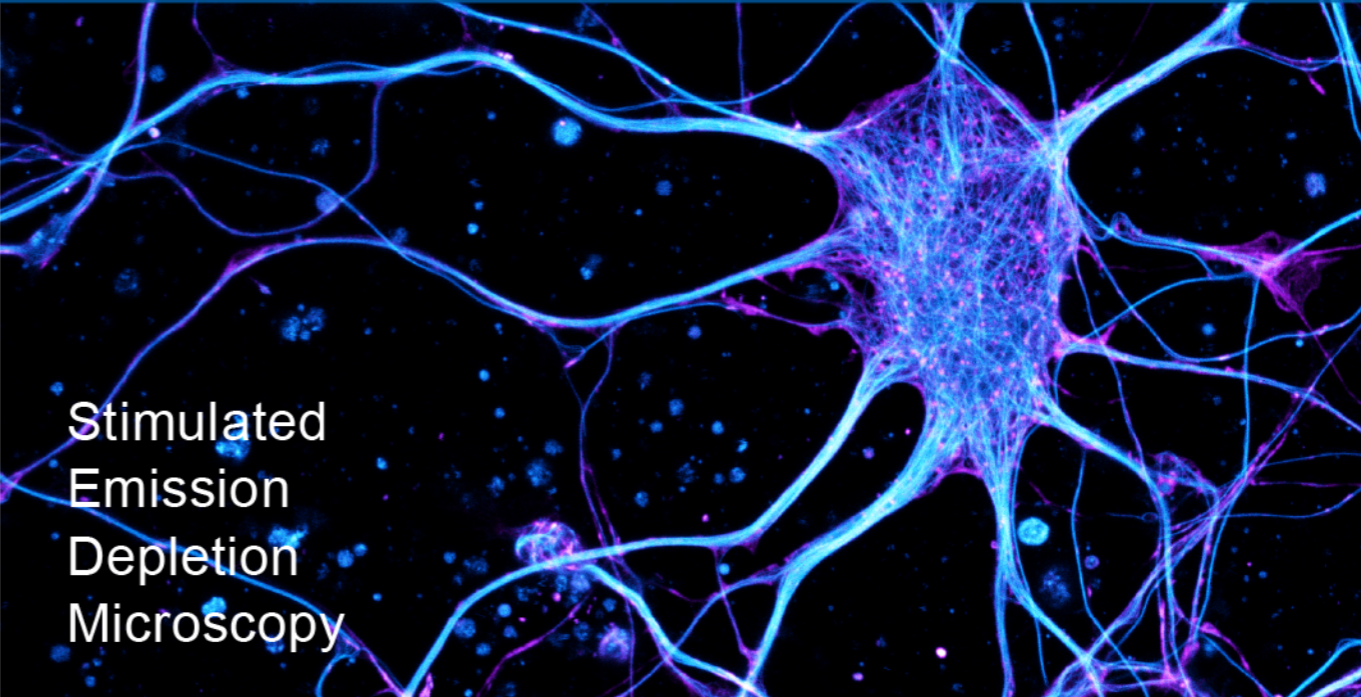
$M_{11}$	$M_{12}$	$M_{22}$	$M_{23}$	$M_{24}$	$J_1$	$J_2$	$J_3$	$J_4$	HS	McL	He	Ru
Suz	O'N	Co <sub>3</sub>	Co <sub>2</sub>	Co <sub>1</sub>	HN	Ly	Th	Fi <sub>22</sub>	Fi <sub>23</sub>	Fi <sub>24</sub>	B	M

(Original table by Ivan Adonis 2012)

## Model-Based Simulation



## Learning From Data



Stimulated Emission Depletion Microscopy

\* Images: WIAS; K. Jansen and E. Katrukha, Kapitein Lab, Molecular and Cellular Biophysics, Utrecht University, NL (STED)

## Confirmability

Kepler's conjecture:  
The art of packing oranges



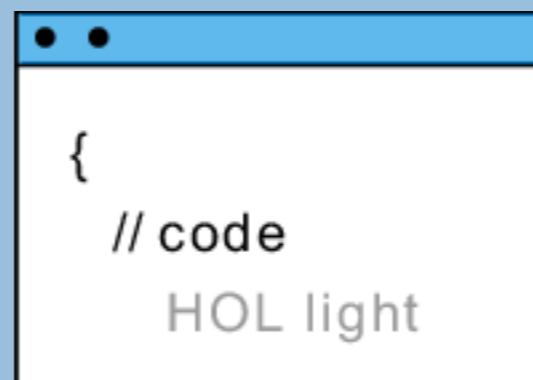
### Proof by T. Hales

Ann. Math. 162 (2005),  
1065–1185



### Formal Verification

Based on computer code



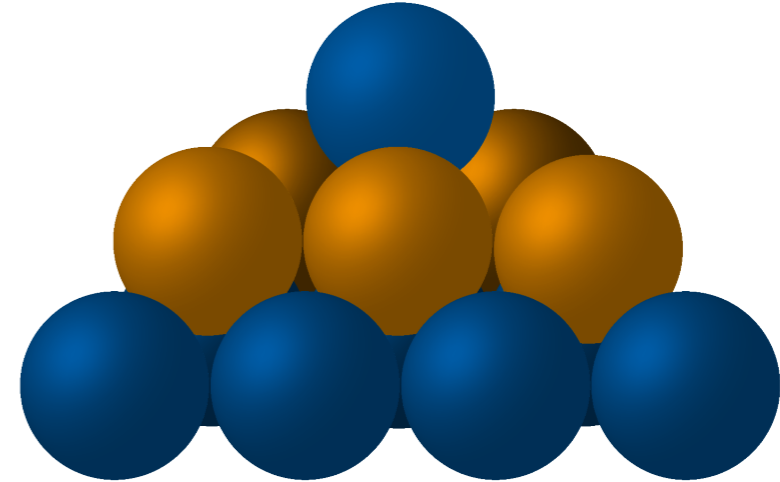
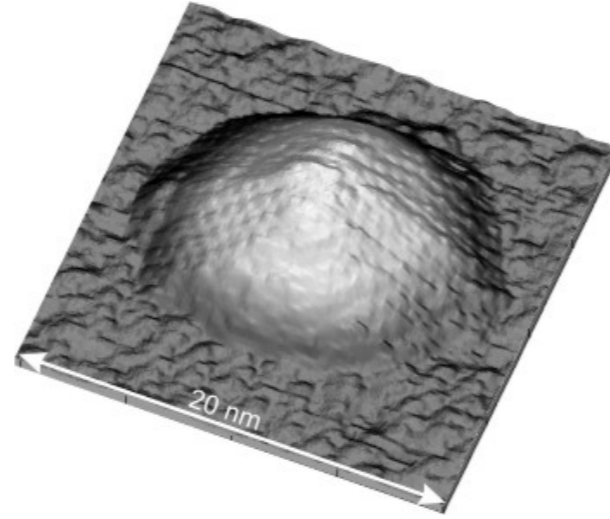
### Verified Proof

Not accessible to classical  
peer-review



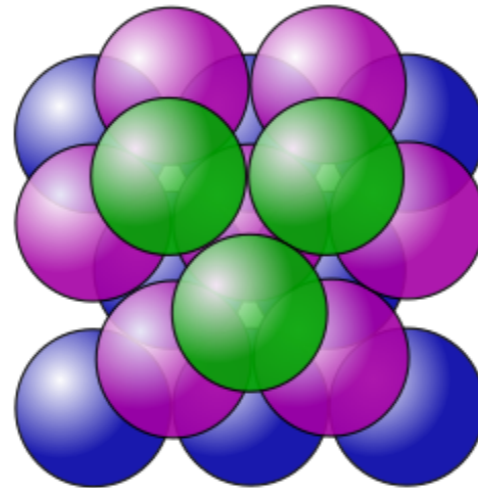
## Confirmability

Kepler's conjecture:  
The art of packing oranges

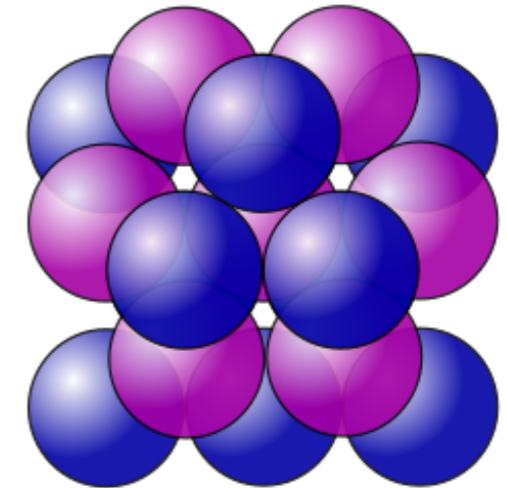


Two important  
Crystallographic  
Lattices

Face centered cubic lattice



Hexagonal closed package



Optimal solutions

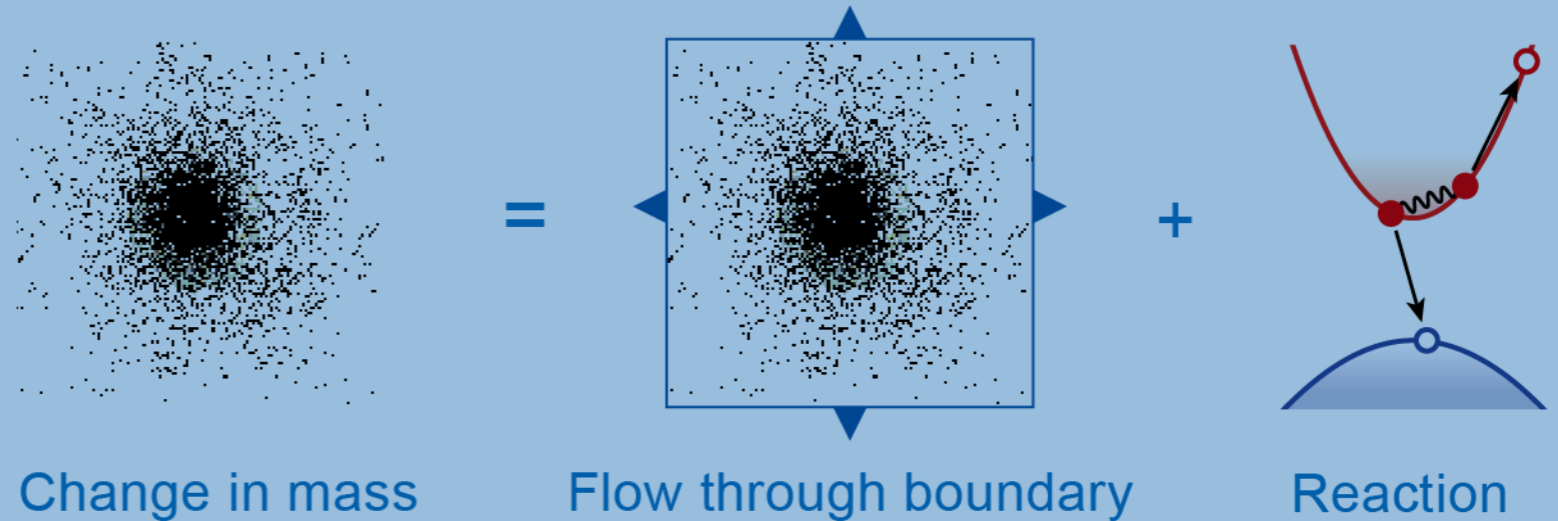
# Mathematical Models

## Reaction-Diffusion Systems

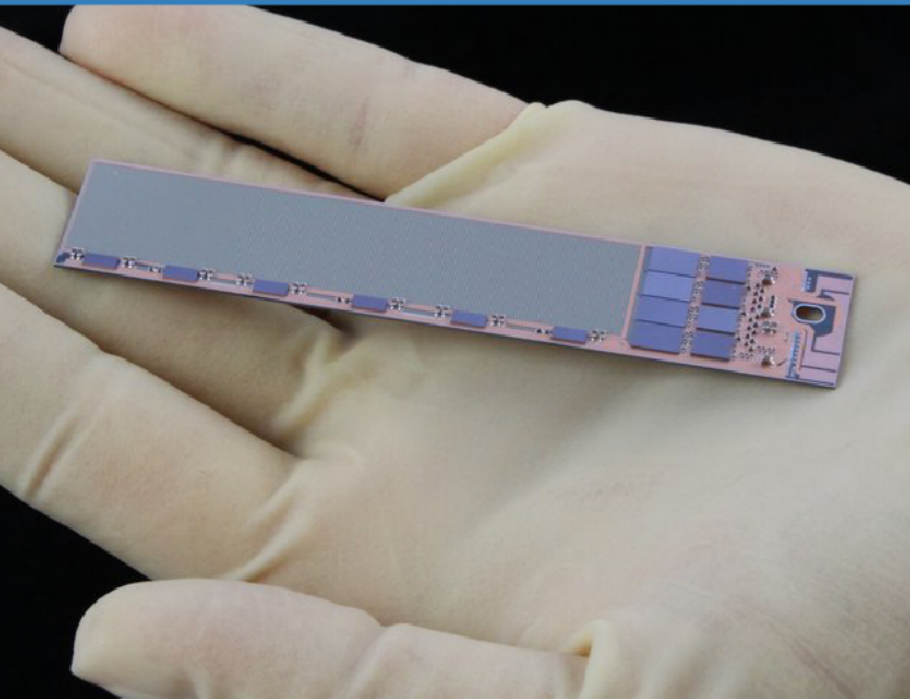
- Drift-diffusion equations
- Poisson-Nernst-Planck model
- van Roosbroeck system
- Semiconductor equation

$$\partial_t u_1 = \nabla \cdot j_1(u_1, \nabla u_1) + r_1(u_1, u_2)$$

$$\partial_t u_2 = \nabla \cdot j_2(u_2, \nabla u_2) + r_2(u_1, u_2)$$



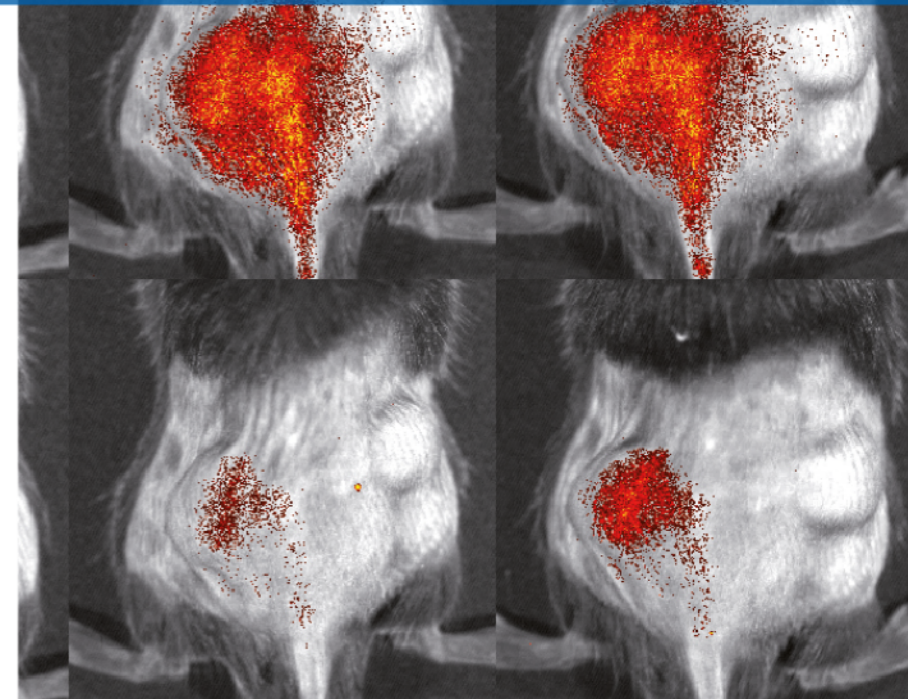
## Detectors

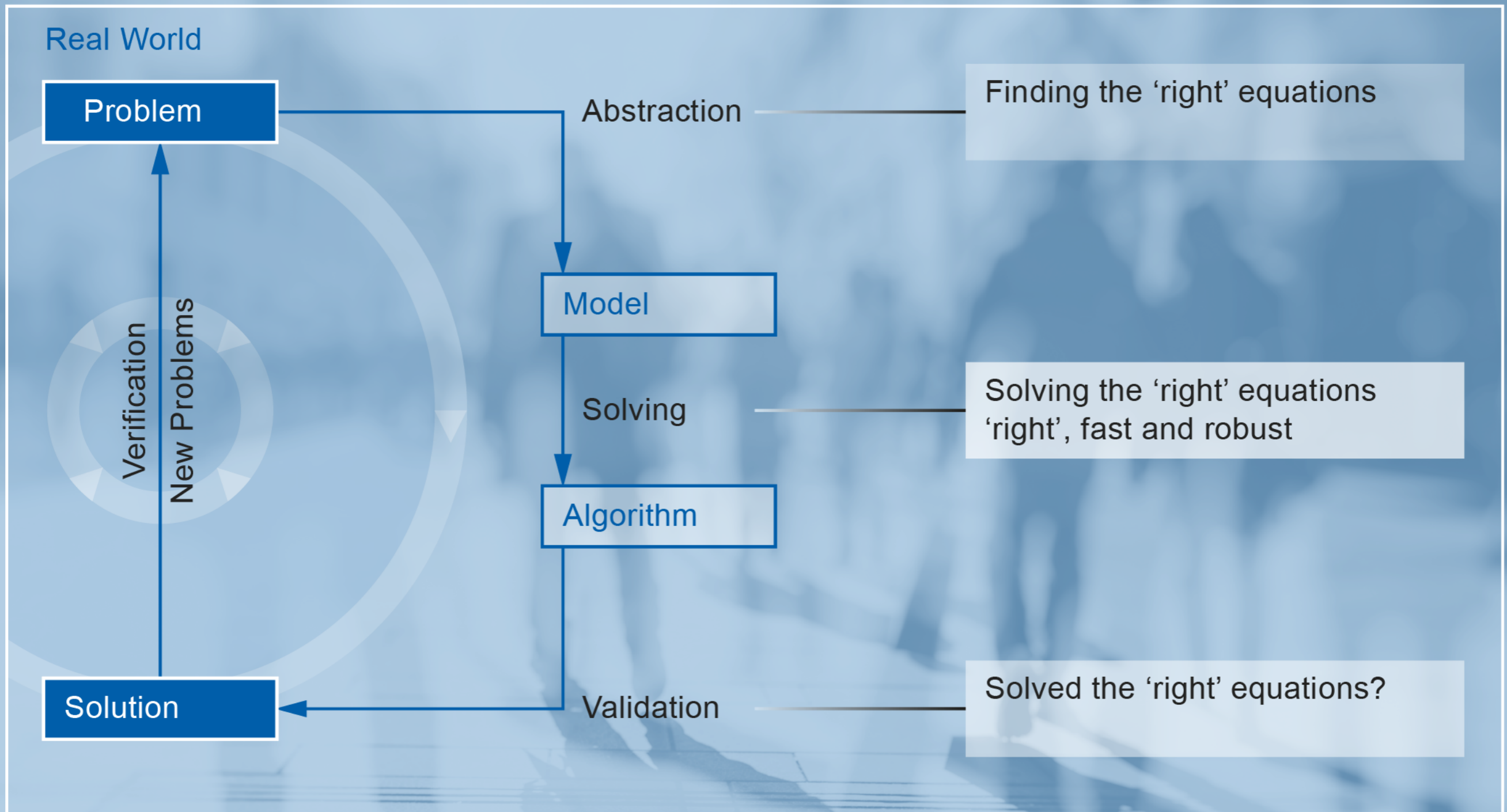


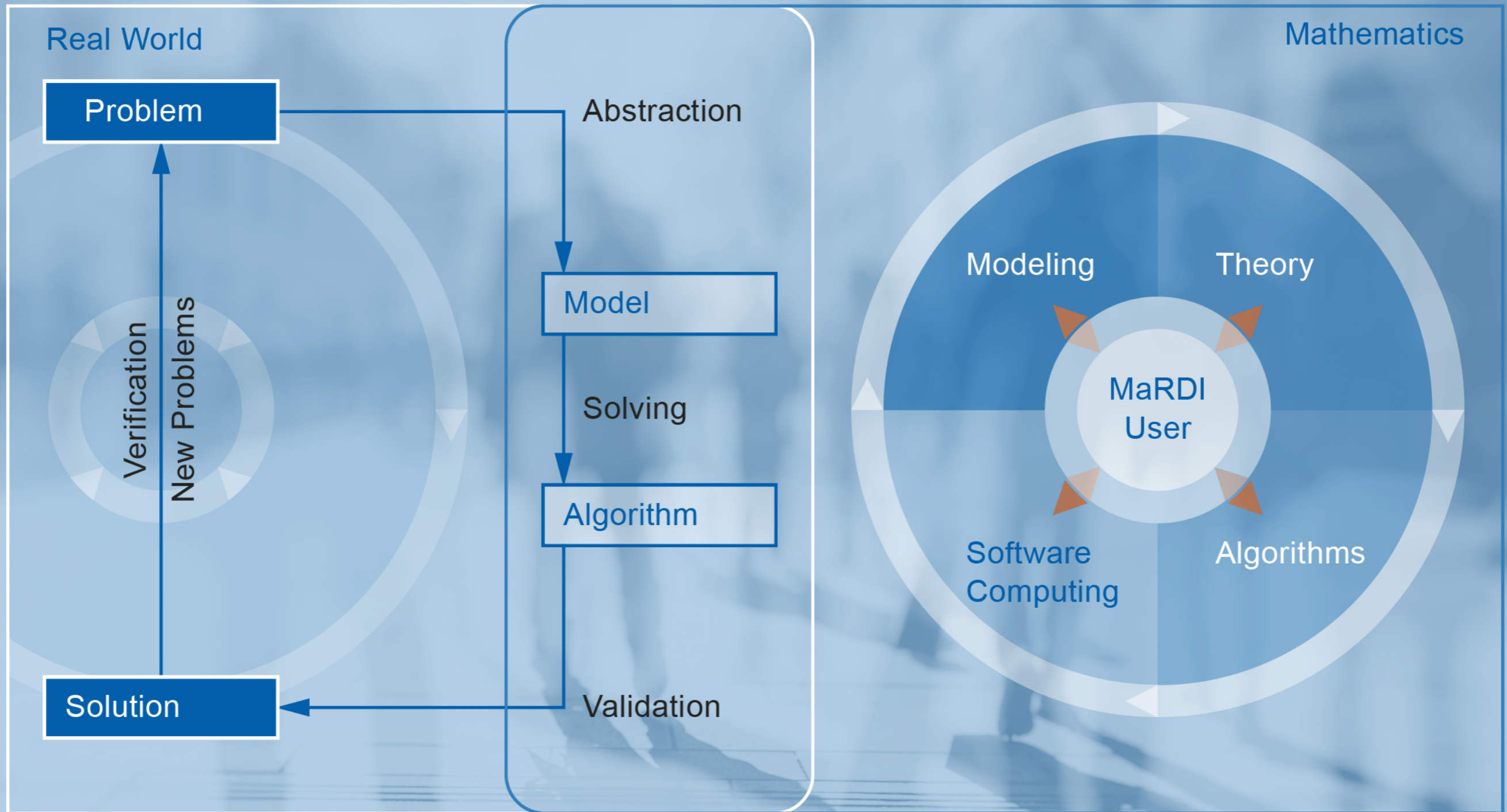
## Batteries



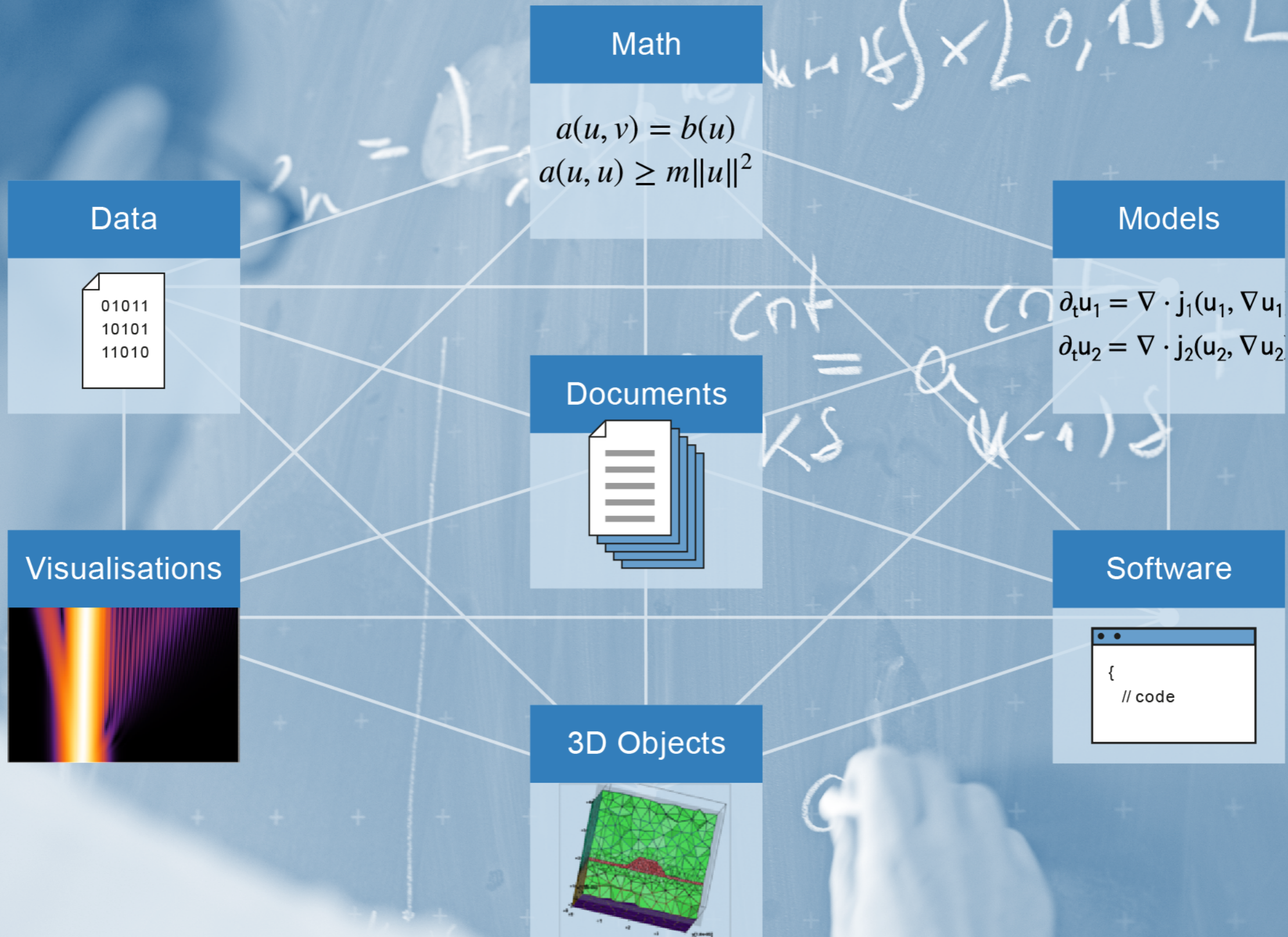
## Cells





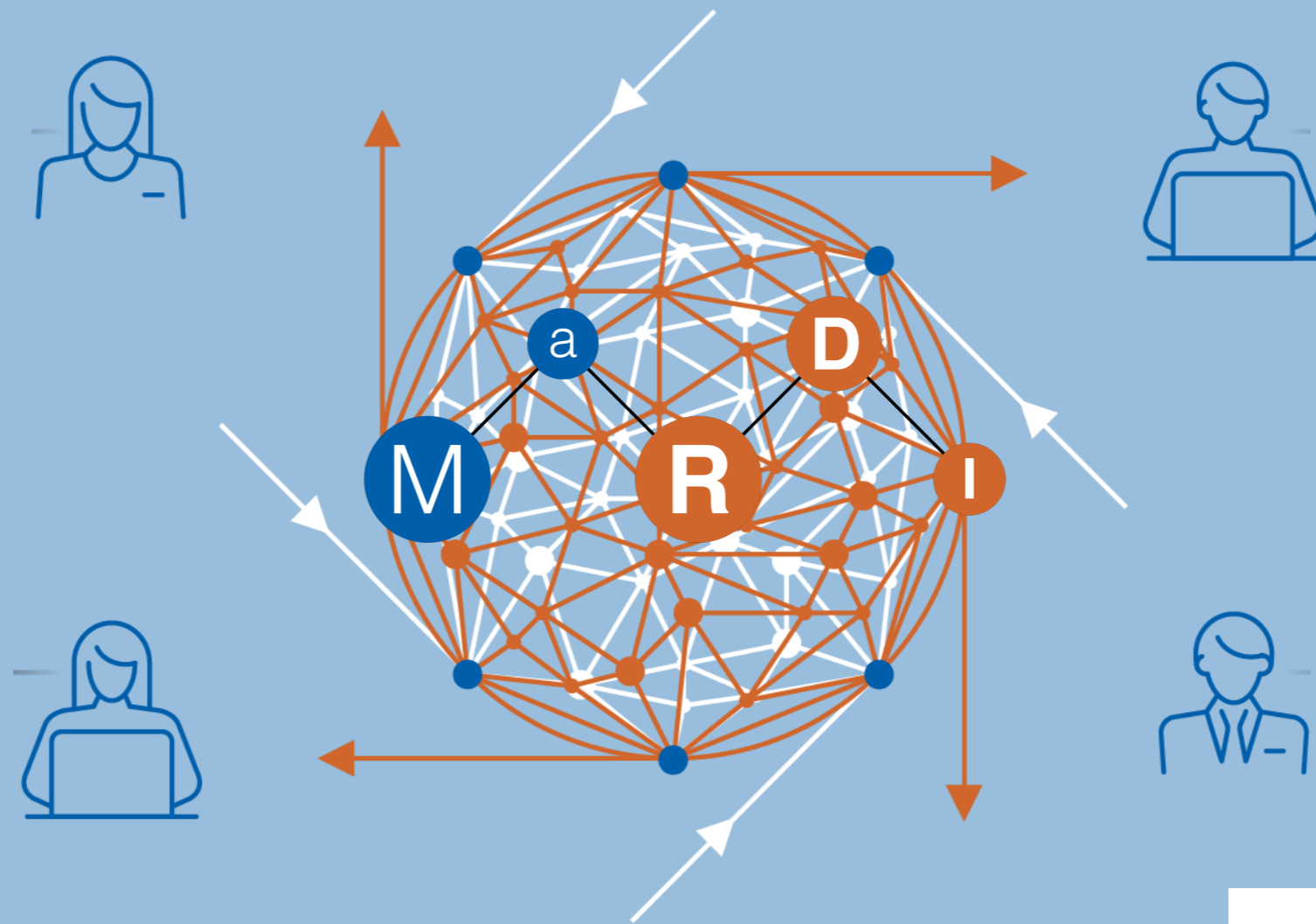


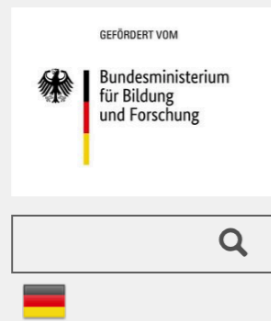
# Mathematical Research Data





# Supporting Mathematical Research by a Research Data Infrastructure





- FAIR research data infrastructure
- 30 consortia, all disciplines
- 3 calls (`19, `20, `21)

## Nationale Forschungsdateninfrastruktur

Die Nationale Forschungsdateninfrastruktur und das NFDI-Direktorat befinden sich momentan im Aufbau.

In der Nationalen Forschungsdateninfrastruktur (NFDI) sollen die wertvollen Datenbestände von Wissenschaft und Forschung für das gesamte deutsche Wissenschaftssystem systematisch erschlossen, vernetzt und nachhaltig sowie qualitativ nutzbar gemacht werden. Bislang sind sie zumeist dezentral, projektbezogen oder auf Zeit verfügbar. Bund und Länder werden die NFDI gemeinsam fördern und mit diesem digitalen Wissensspeicher eine unverzichtbare Voraussetzung für neue Forschungsfragen, Erkenntnisse und Innovationen schaffen.

[mehr erfahren](#)



Prof. Dr. York Sure-Vetter  
Director

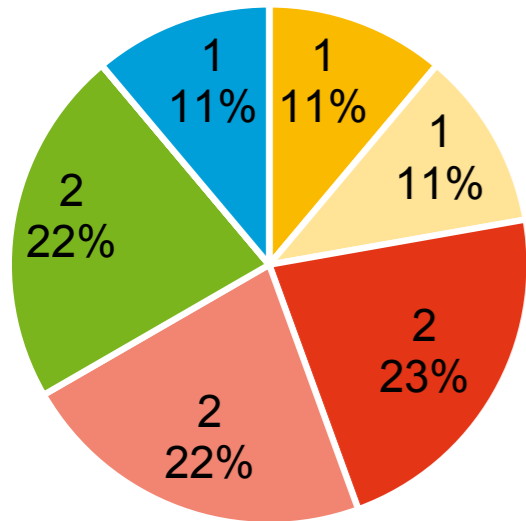
Informationen zum Ausschreibungs-,  
Auswahl- und Begutachtungsverfahren:



Deutsche Forschungsgemeinschaft (DFG):  
<https://www.dfg.de/foerderung/programme/nfdi/>

Runde 1

startet  
October 2020

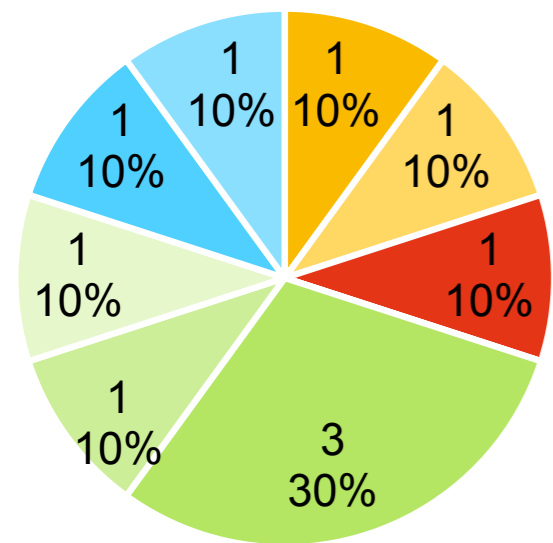


Runde 1 und 2



Runde 2

starting  
October 2021



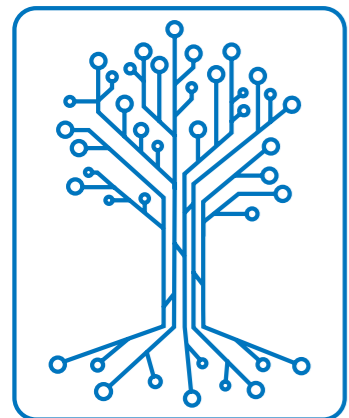
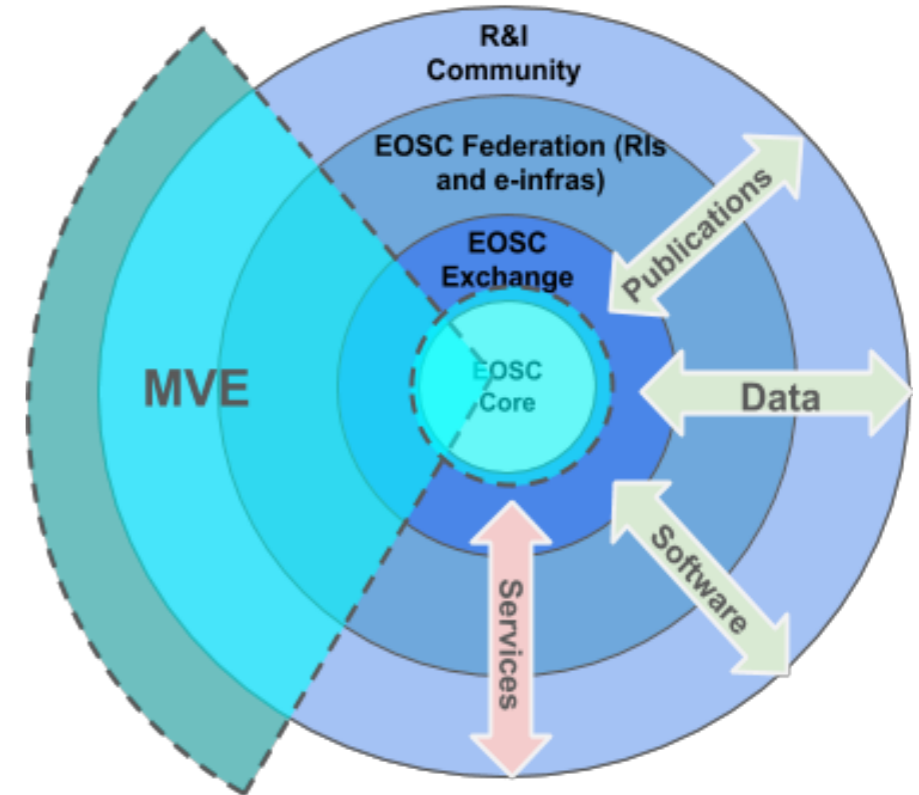
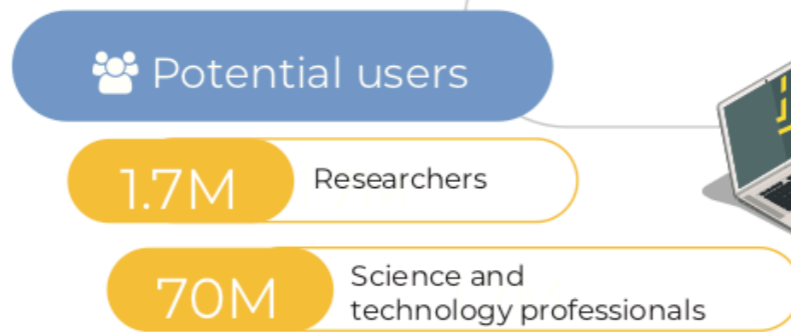
- Geisteswissenschaften
- Sozial- und Verhaltenswissenschaften
- Biologie
- Medizin
- Chemie
- Physik
- Mathematik
- Geowissenschaften
- Maschinenbau und Produktionstechnik
- Materialwissenschaft und Werkstofftechnik
- Informatik, System- und Elektrotechnik

# European Open Science Cloud (EOSC) and GAIA-X



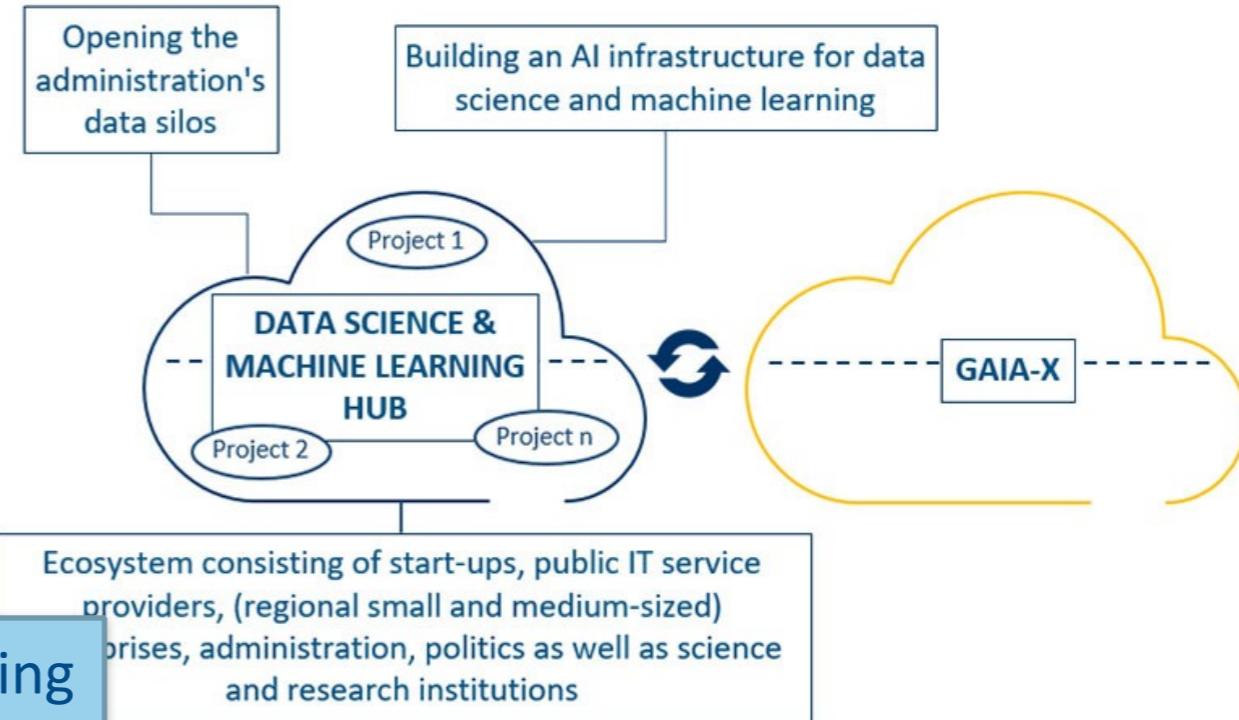
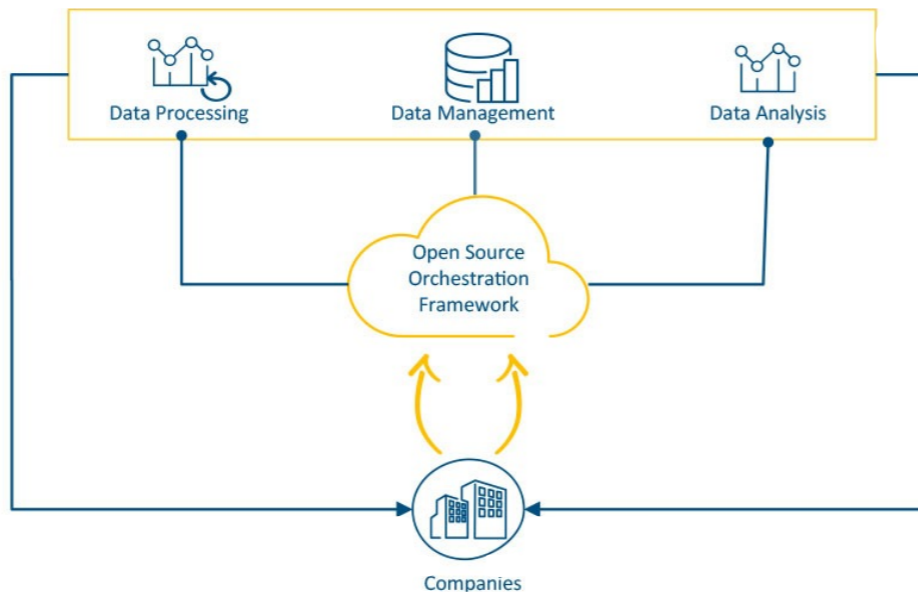
## EUROPEAN OPEN SCIENCE CLOUD

- started 2015, launched 2018
- secretariat est. 2020



## GAIA-X

started 2020



FAIR-Data-Spaces: 6.3 M€ BMBF funding for cooperation with NFDI (Jun 2021)

# NFDI

Findable

F



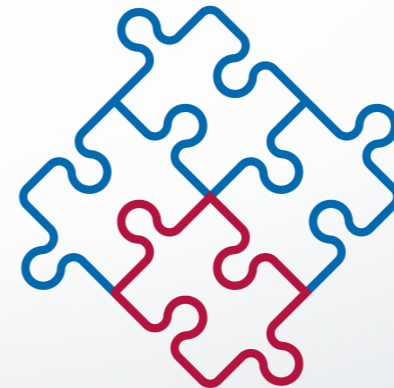
Accessible

A



Interoperable

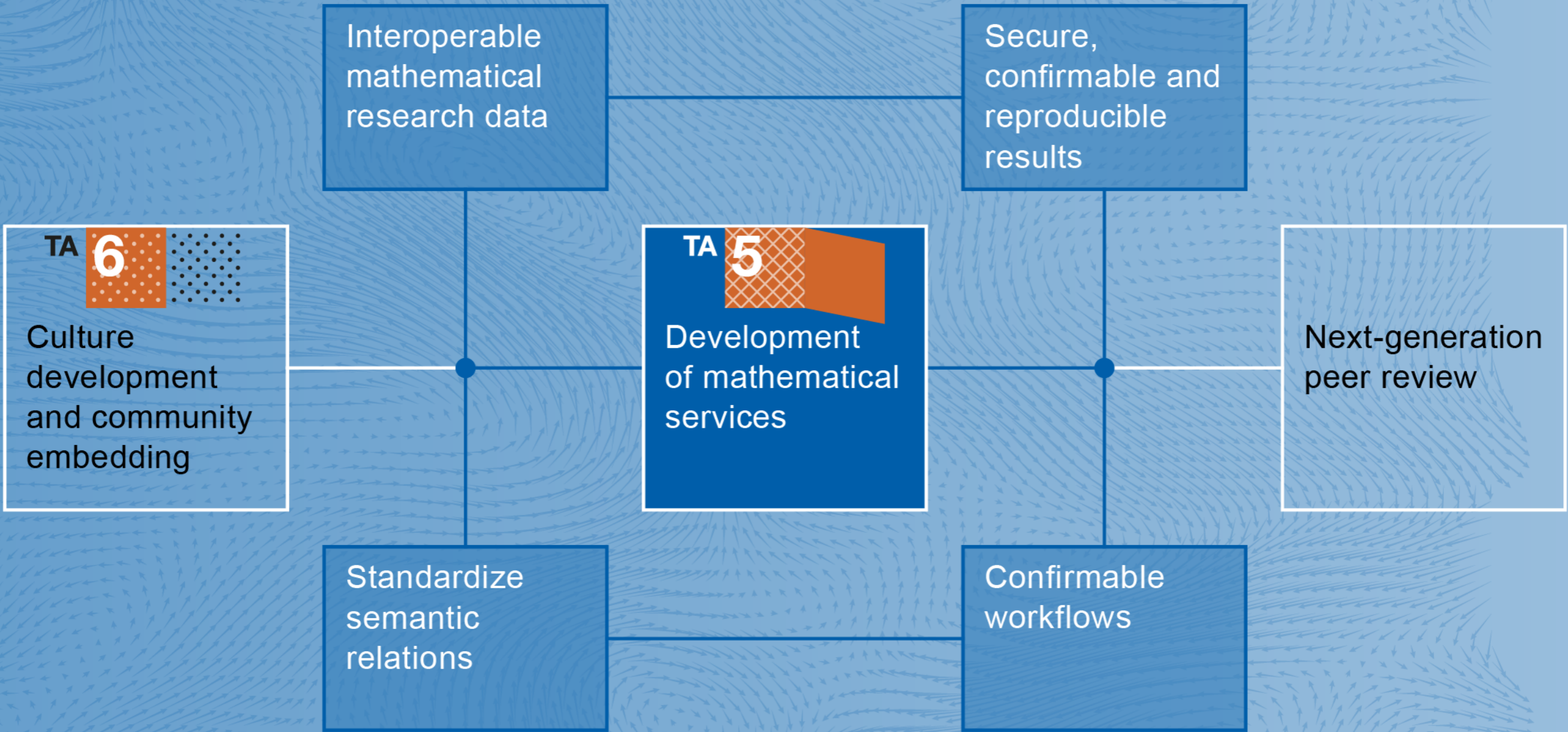
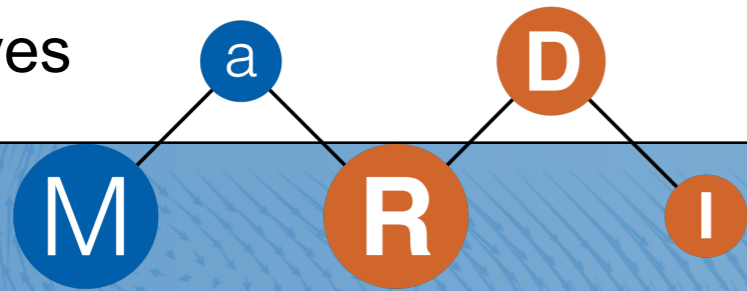
I



Re-usable

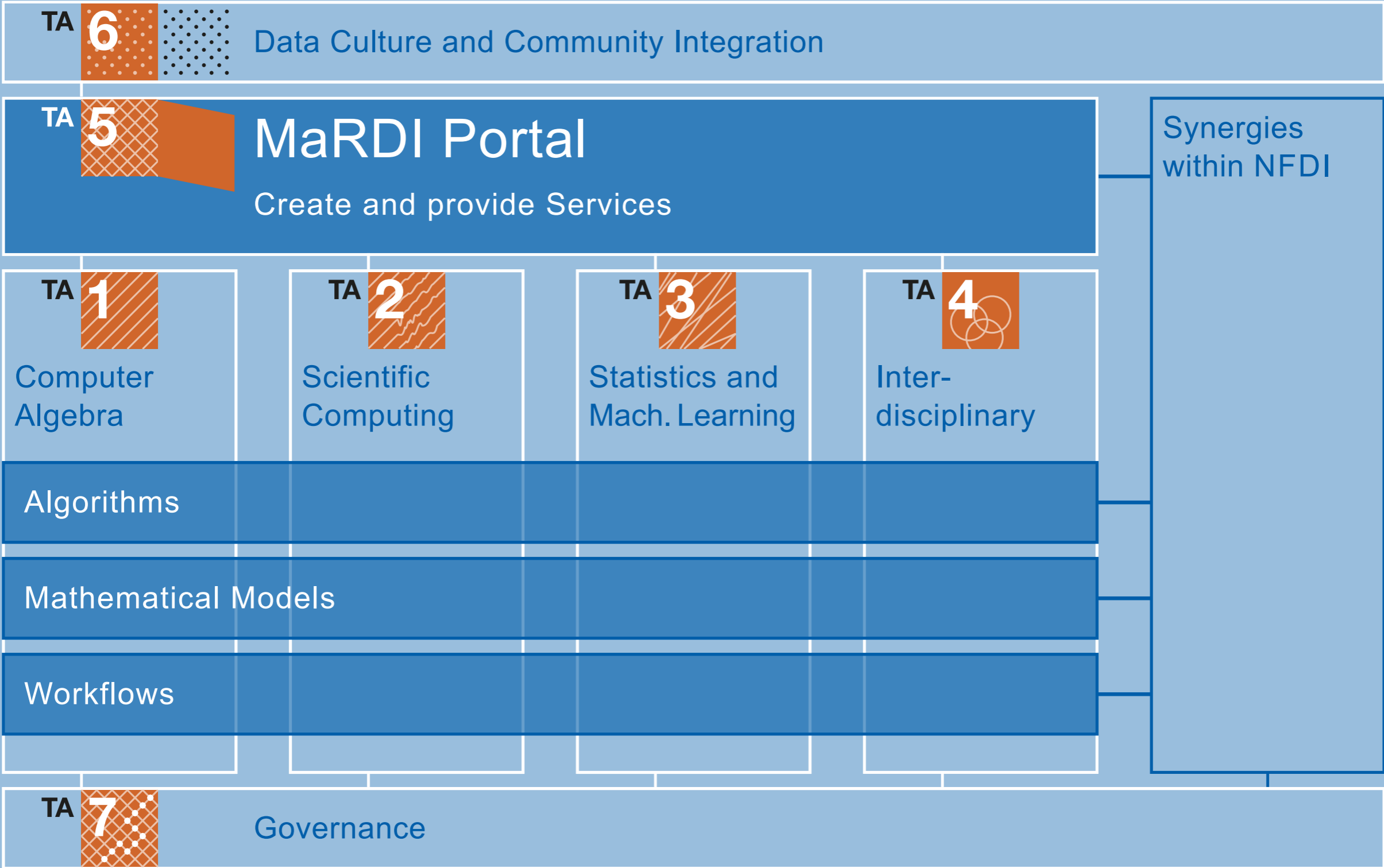
R



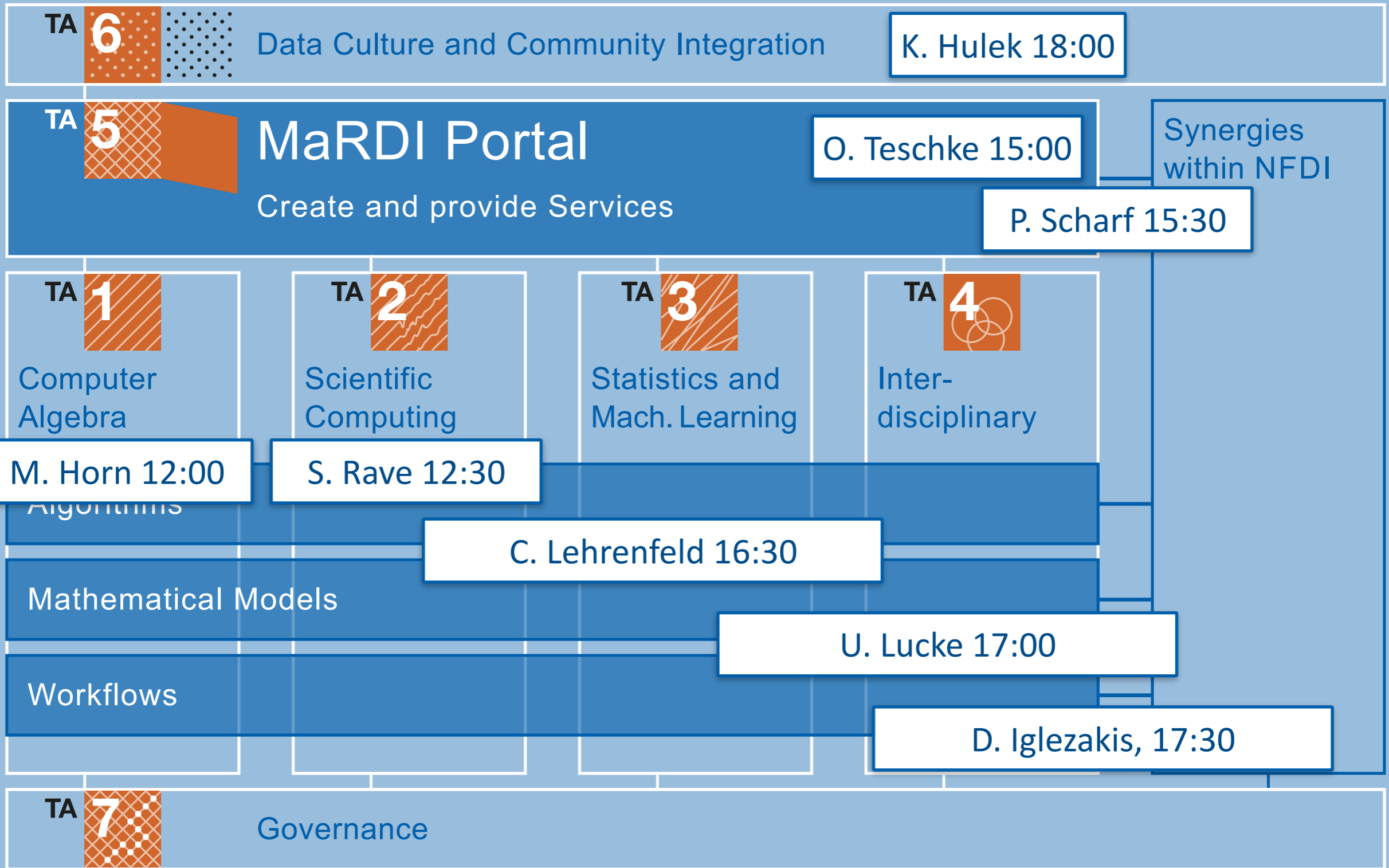


FAIR mathematical research data and confirmable workflows as a foundation for future mathematics-driven research

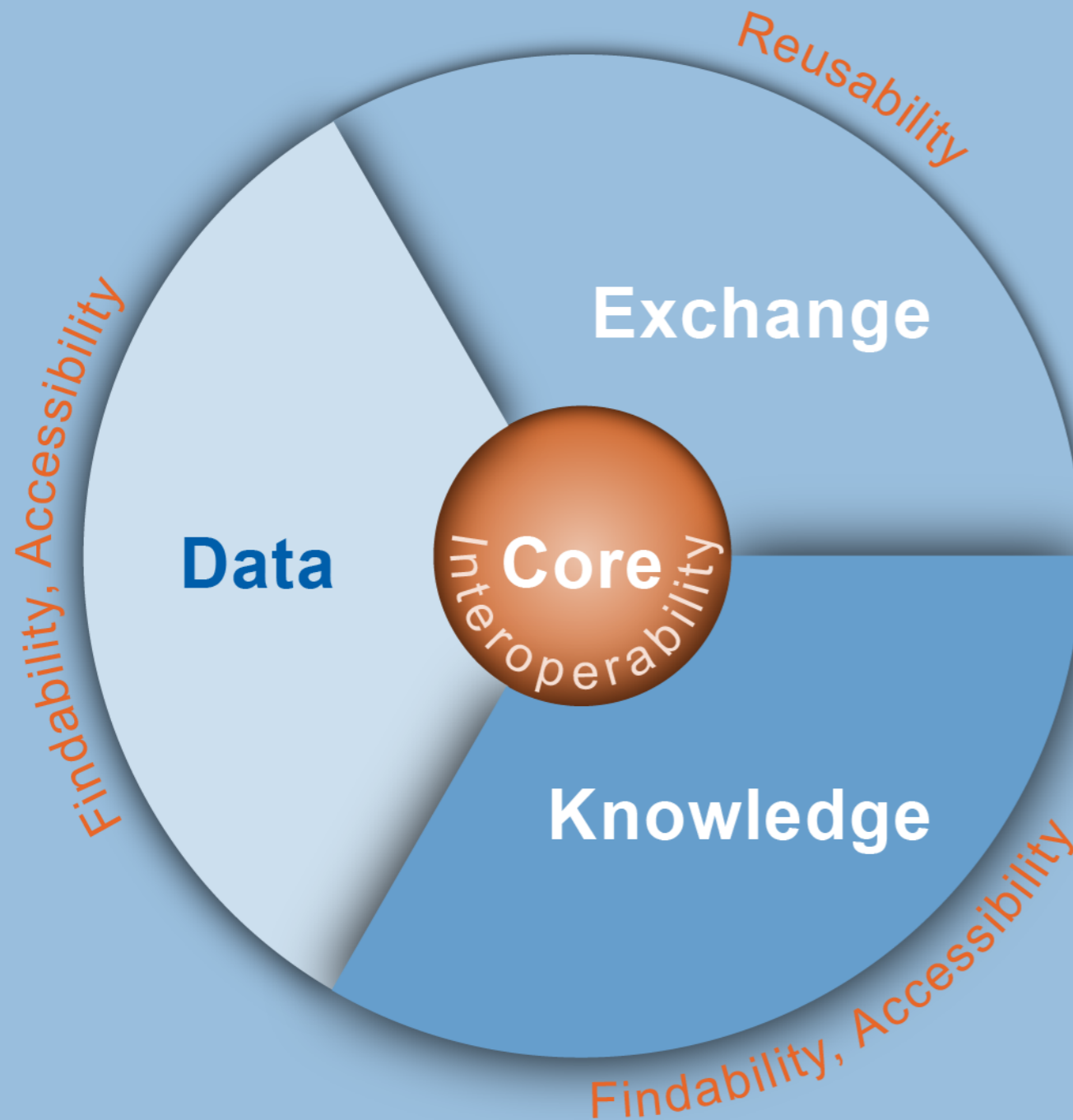
# Task Areas



# Task Areas







## Example: Linear Solver $Ax=b$

### X1: Core

- Data structures for matrices and vectors
- Representation formats
- Exchange formats
- Application programming interfaces (APIs)

### X2: Data

- Test cases (matrices, solutions)
- Matrix properties (meta-data)
- Persistent identifiers (PIDs)

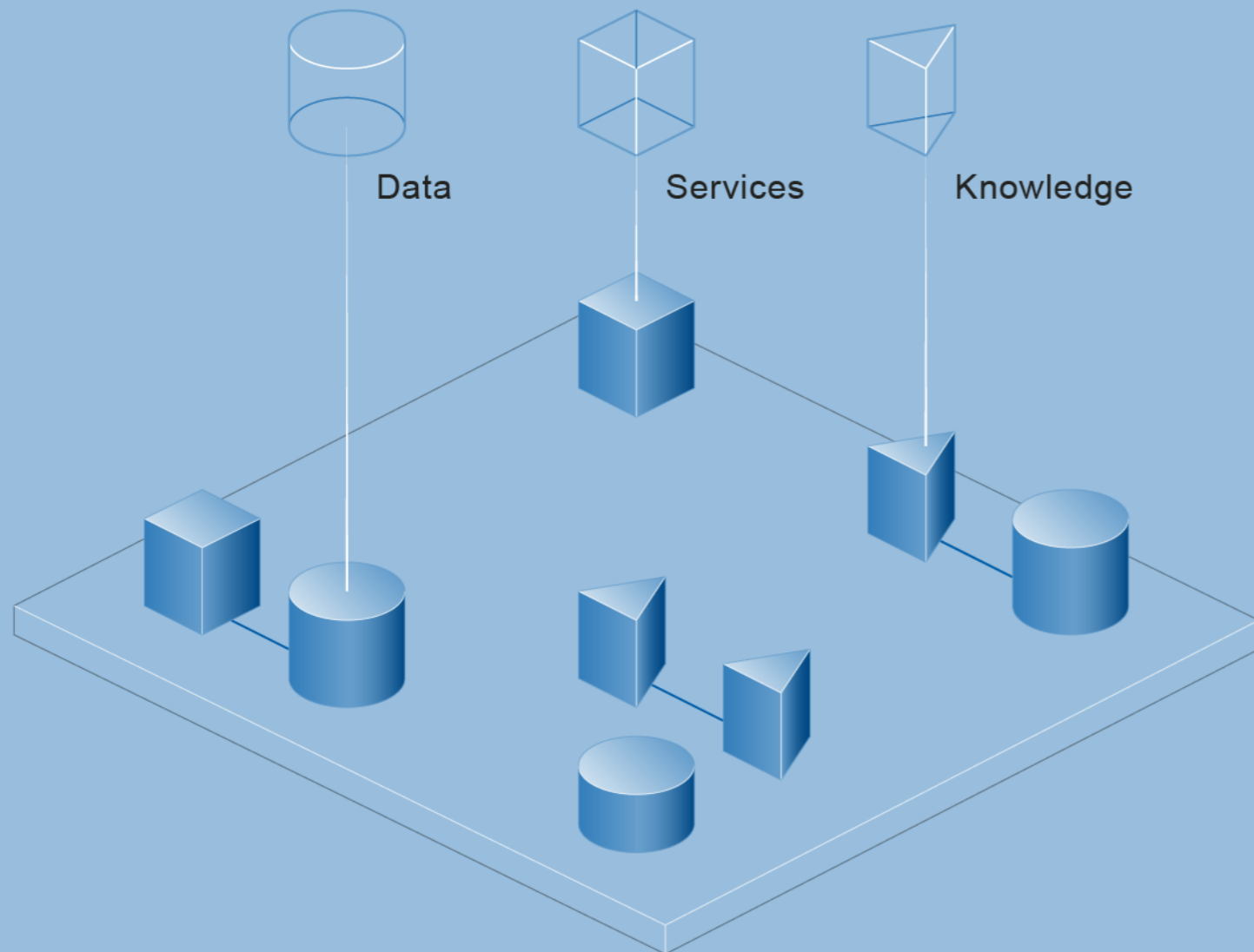
### X3: Exchange

- Benchmark framework
- Pre-defined software environments
- Workflows, continuous-benchmarking

### X4: Knowledge

- Ontology of linear problems and solvers
- Link to algorithms, publications software and test-data

# Existing MaRDI Services



## Examples for Services

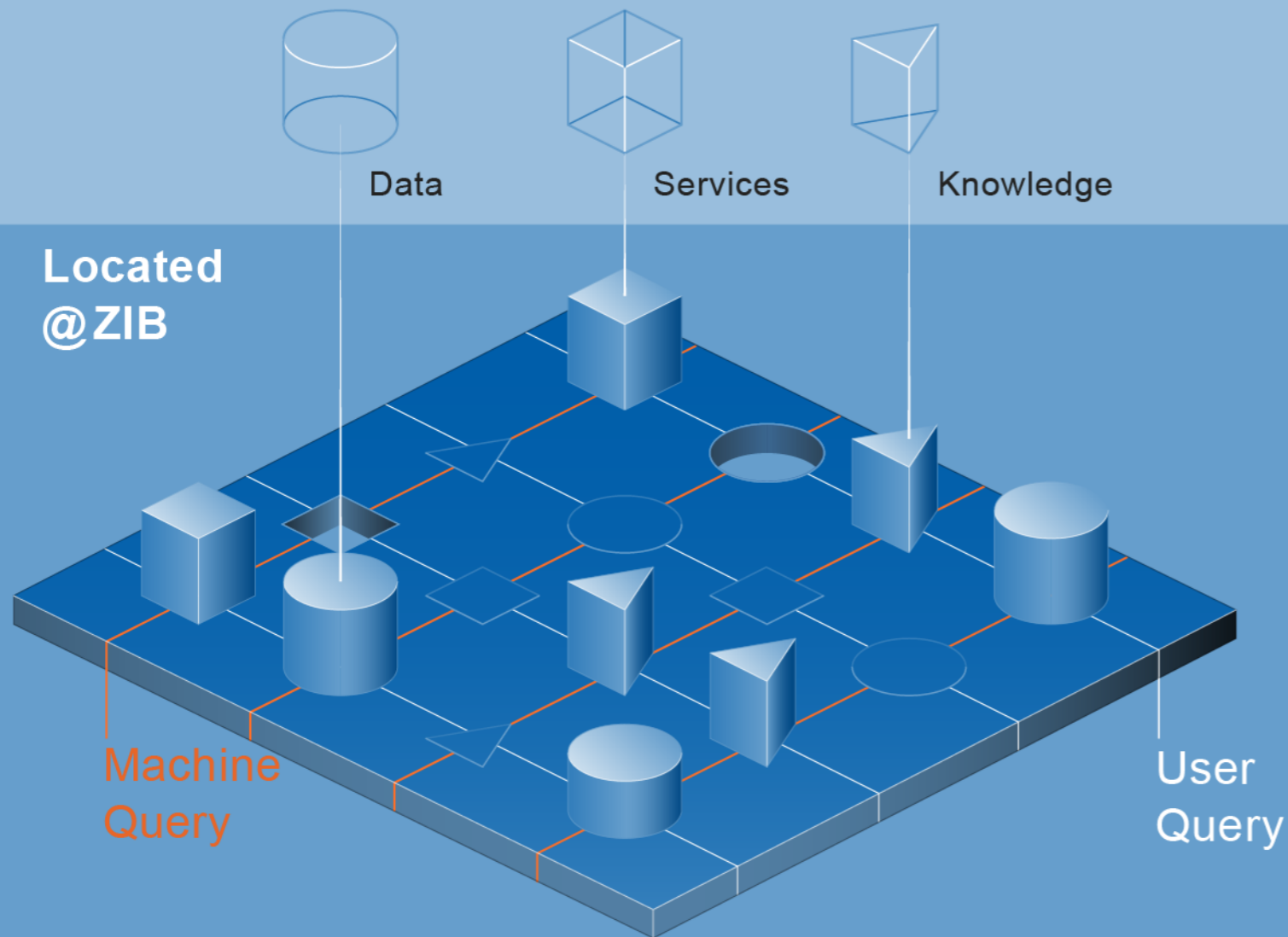
- OpenML
- MORwiki
- polyDB & SmallGrp

## Examples for Infrastructures

- zbMATH & swMATH
- Encyclopedia of Mathematics
- RADAR

# Integration of Federated Services into MaRDI Portal

Located@Provider-Site



## Examples for Services

- OpenML
- MORwiki
- polyDB & SmallGrp

## Examples for Infrastructures

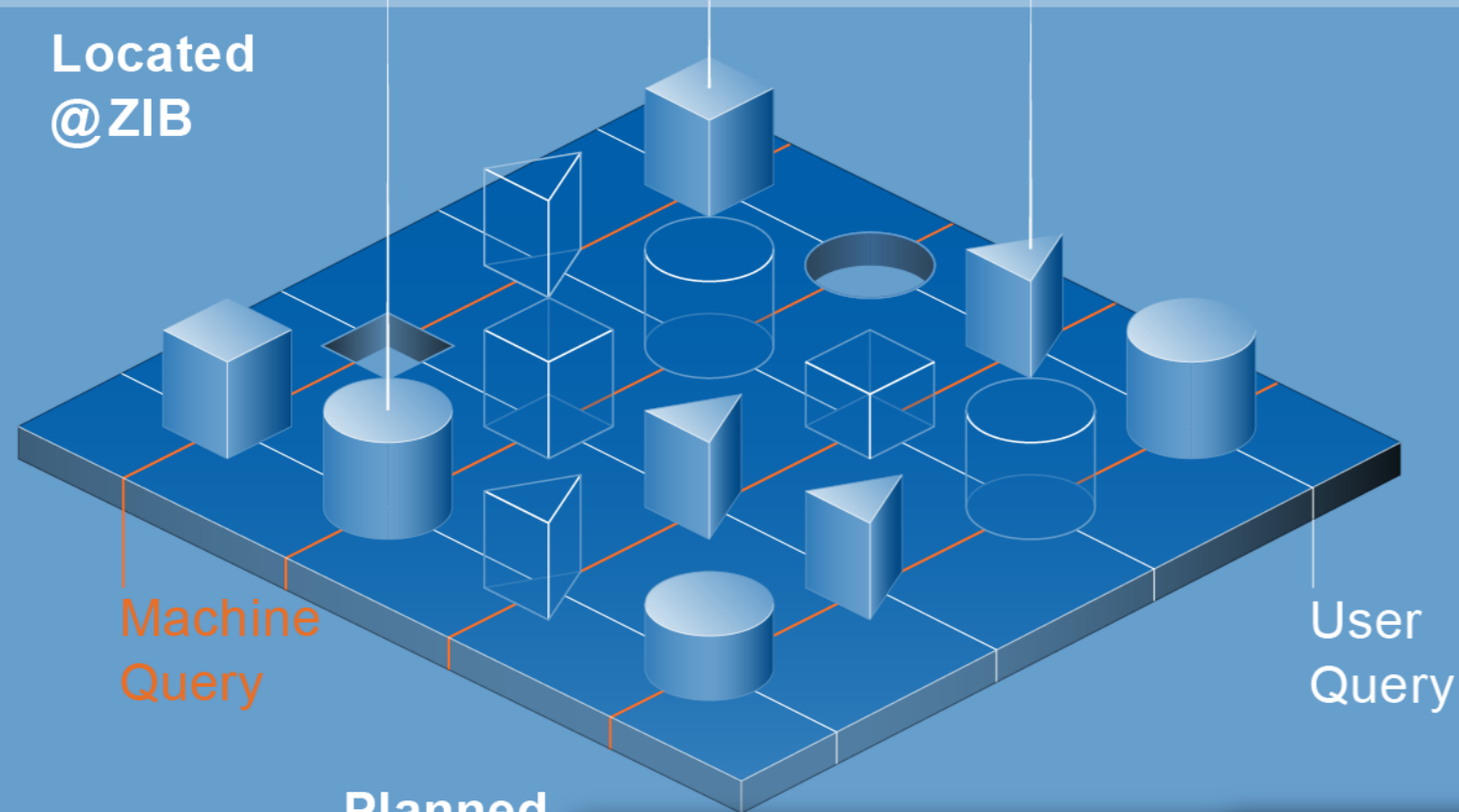
- zbMATH & swMATH
- Encyclopedia of Mathematics
- RADAR

# Value-Chain for New Services for Data, Research and Knowledge

Located @ Provider-Site



Located @ZIB



## Examples for Services

- OpenML
- MORwiki
- polyDB & SmallGrp

## Examples for Infrastructures

- zbMATH & swMATH
- Encyclopedia of Mathematics
- RADAR

## Planned Services:

### Data

- Repositories for Computer Algebra
- Library of Benchmark Data
- Persistent Identifier Registry

### Research

- Benchmark Framework
- Library of Statistical Analysis
- Workflow and Data Certification Service

### Knowledge

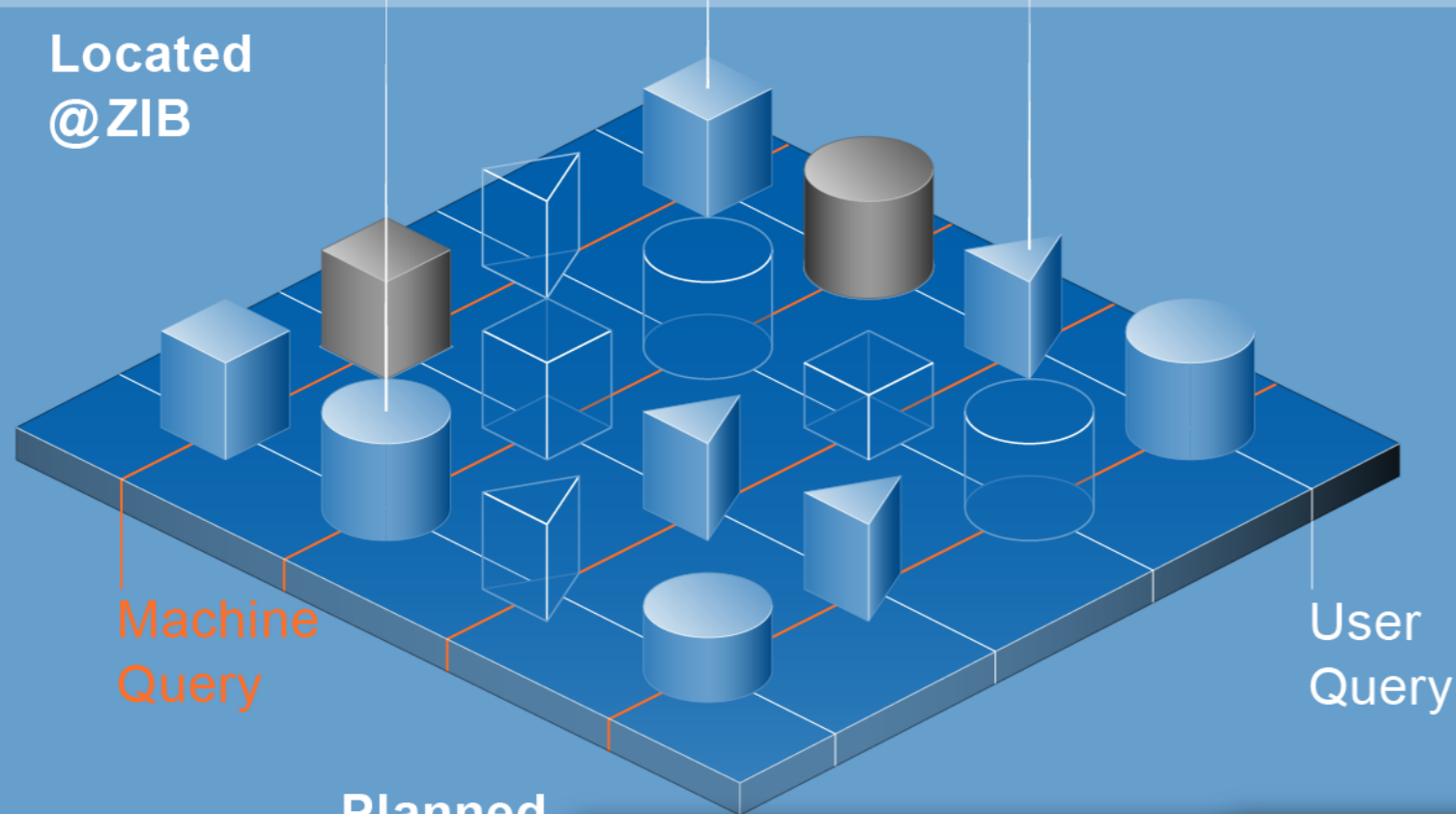
- Knowledge Graph of Numerical Algorithms
- Knowledge Graph for Modeling and Simulation
- Terminology Service

# Value-Chain for Integration With External Services

Located @ Provider-Site



Located @ ZIB



Planned Services:

## Data

- Repositories for Computer Algebra
- Library of Benchmark Data
- Persistent Identifier Registry

## Research

- Benchmark Framework
- Library of Statistical Analysis
- Workflow and Data Certification Service

## Knowledge

- Knowledge Graph of Numerical Algorithms
- Knowledge Graph for Modeling and Simulation
- Terminology Service

External

- OpenAIRE
- Zenodo
- DLMF

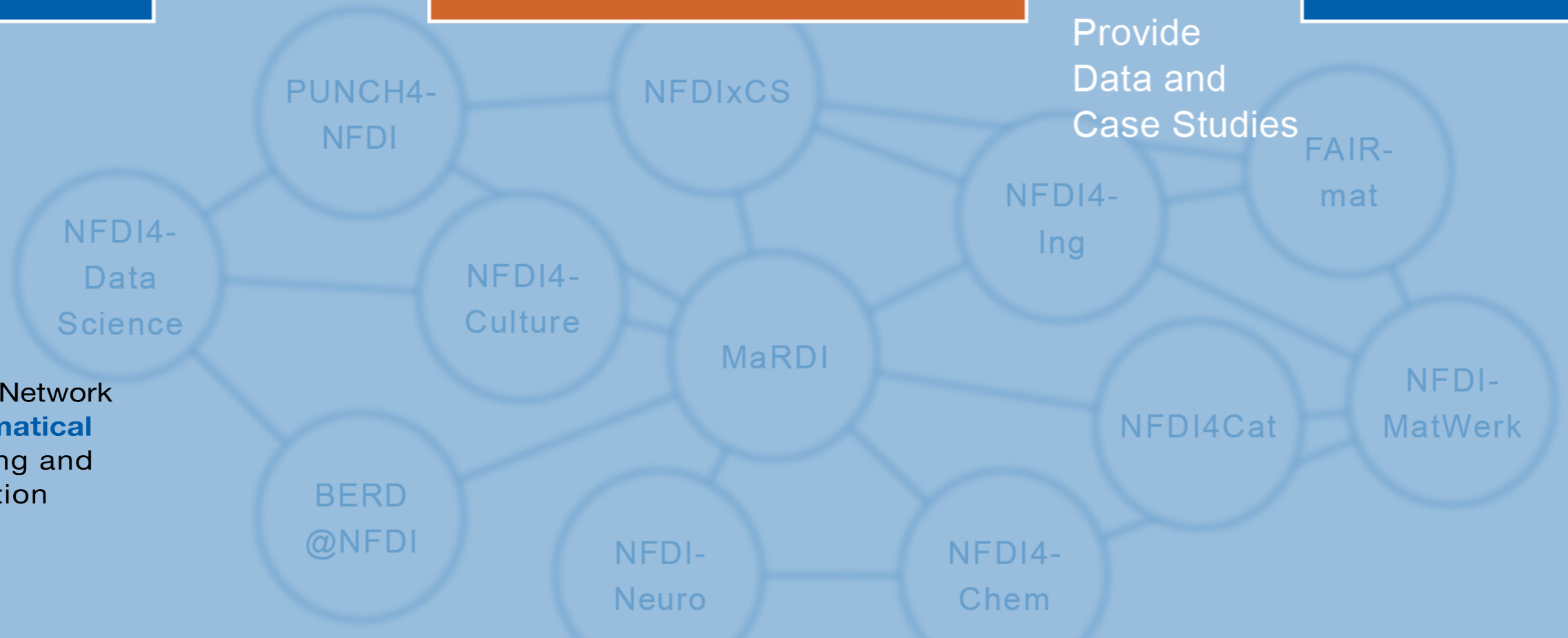
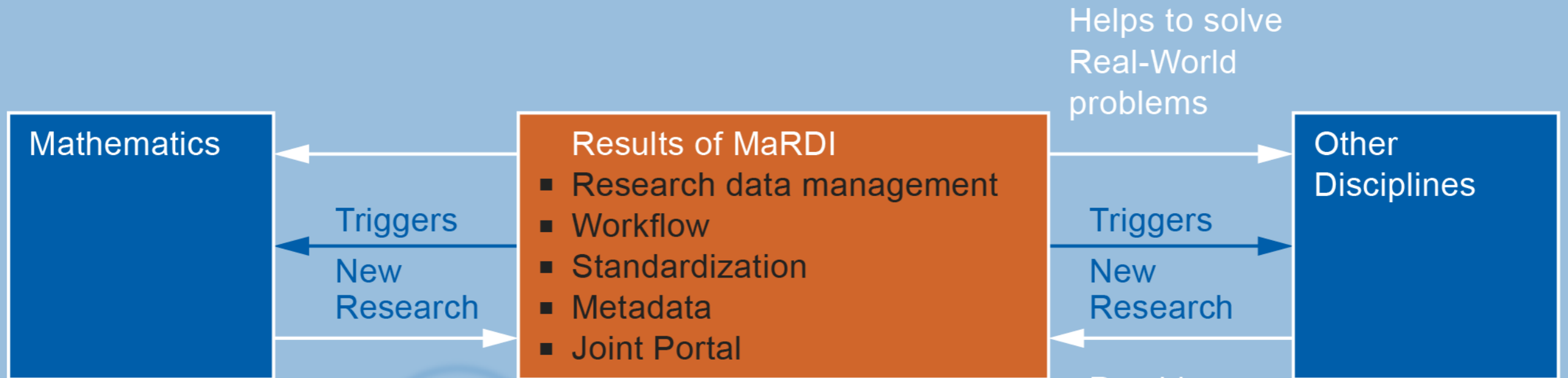
Examples for Services

- OpenML
- MORwiki
- polyDB & SmallGrp

Examples for Infrastructures

- zbMATH & swMATH
- Encyclopedia of Mathematics
- RADAR

# MaRDI for Other Disciplines



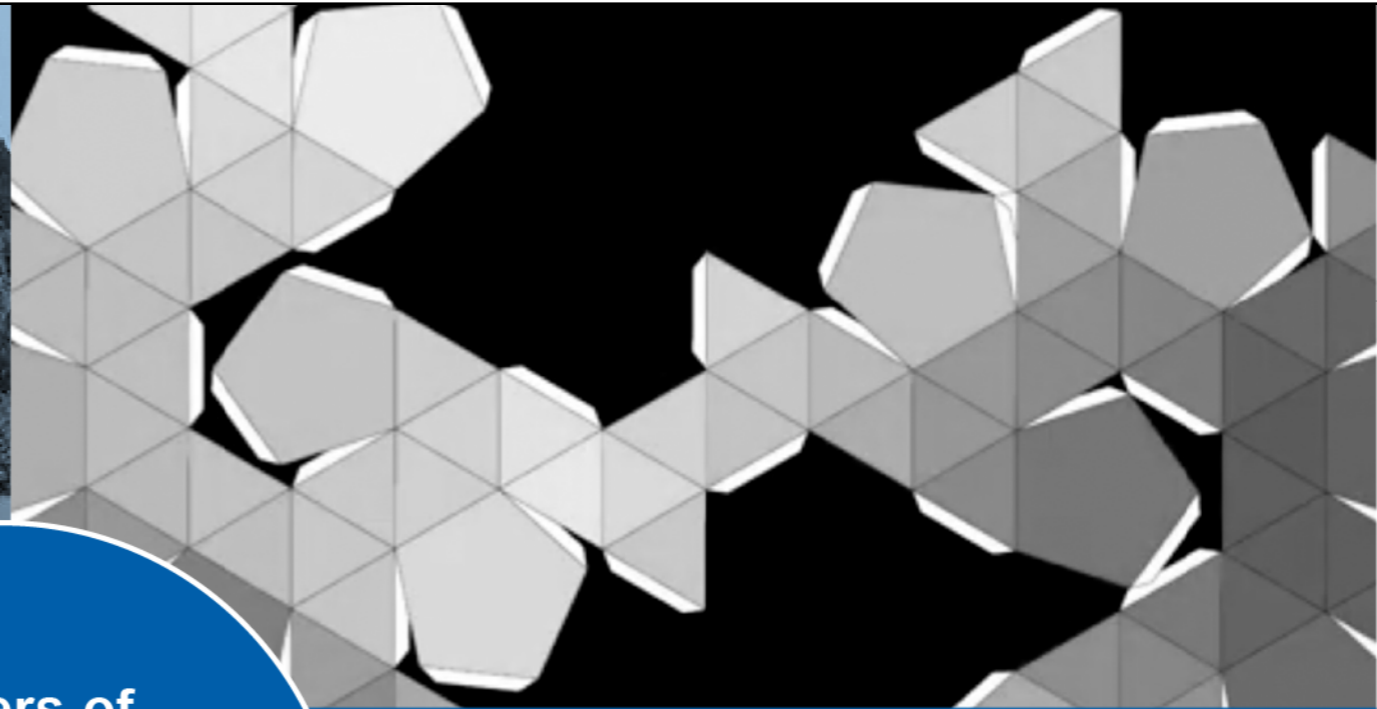
Leibniz Network  
**Mathematical**  
Modeling and  
Simulation





MFO

Clusters of  
Excellence



DMV

EMS

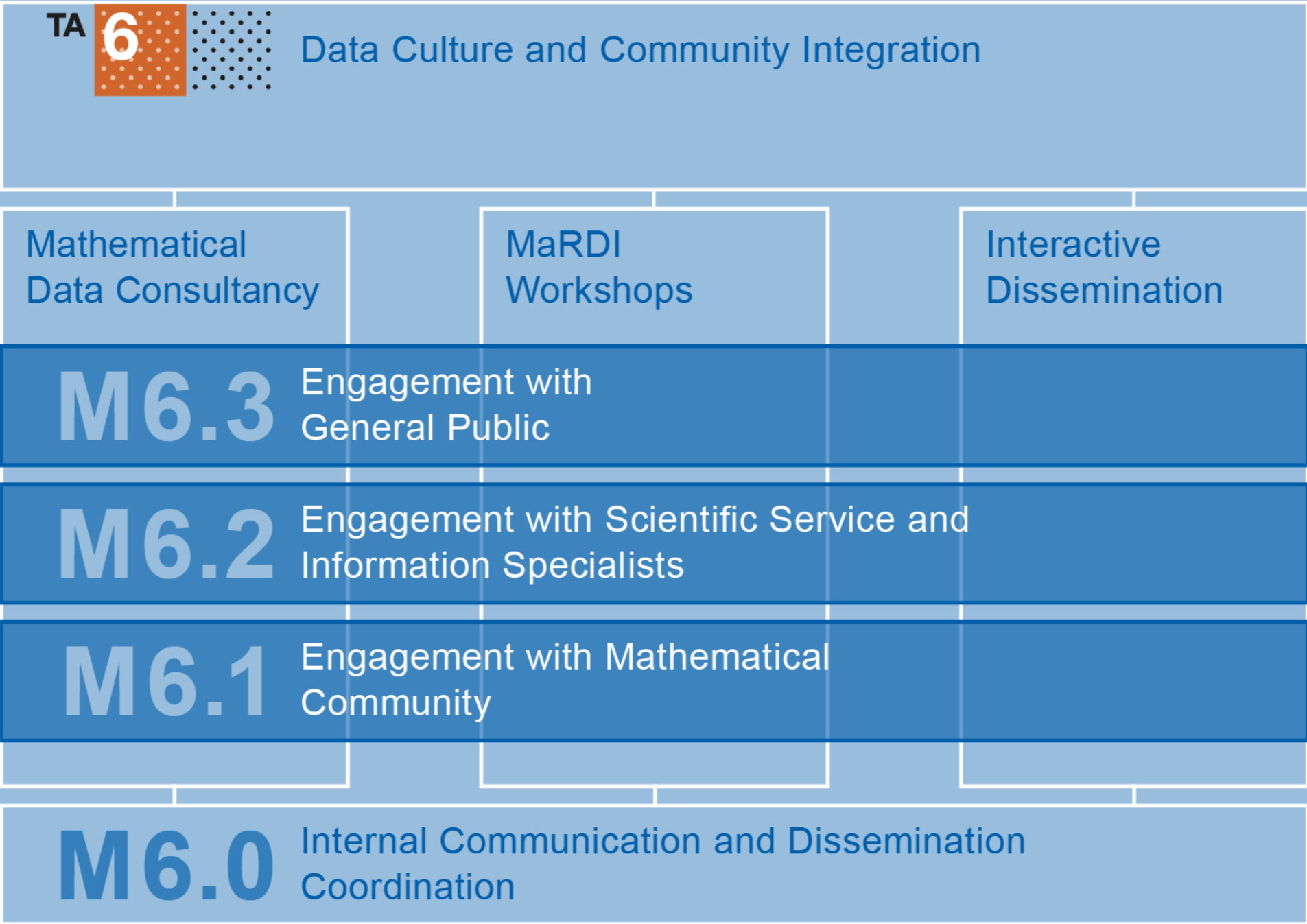
Research and  
Infrastructure  
Projects

GAMM/GOR



The Mathematics Community Publisher







# Consortium and Competencies

Mathematics  
Cross-Disciplinary  
Infrastructure  
Providers

## Clusters of Excellence

- SimTech
- Mathematics Münster
- MATH+
- STRUCTURES

## Scientific Associations and Societies

- DMV
- GAMM
- GOR
- EMS
- FhG IUK

IMAGINARY  
open mathematics

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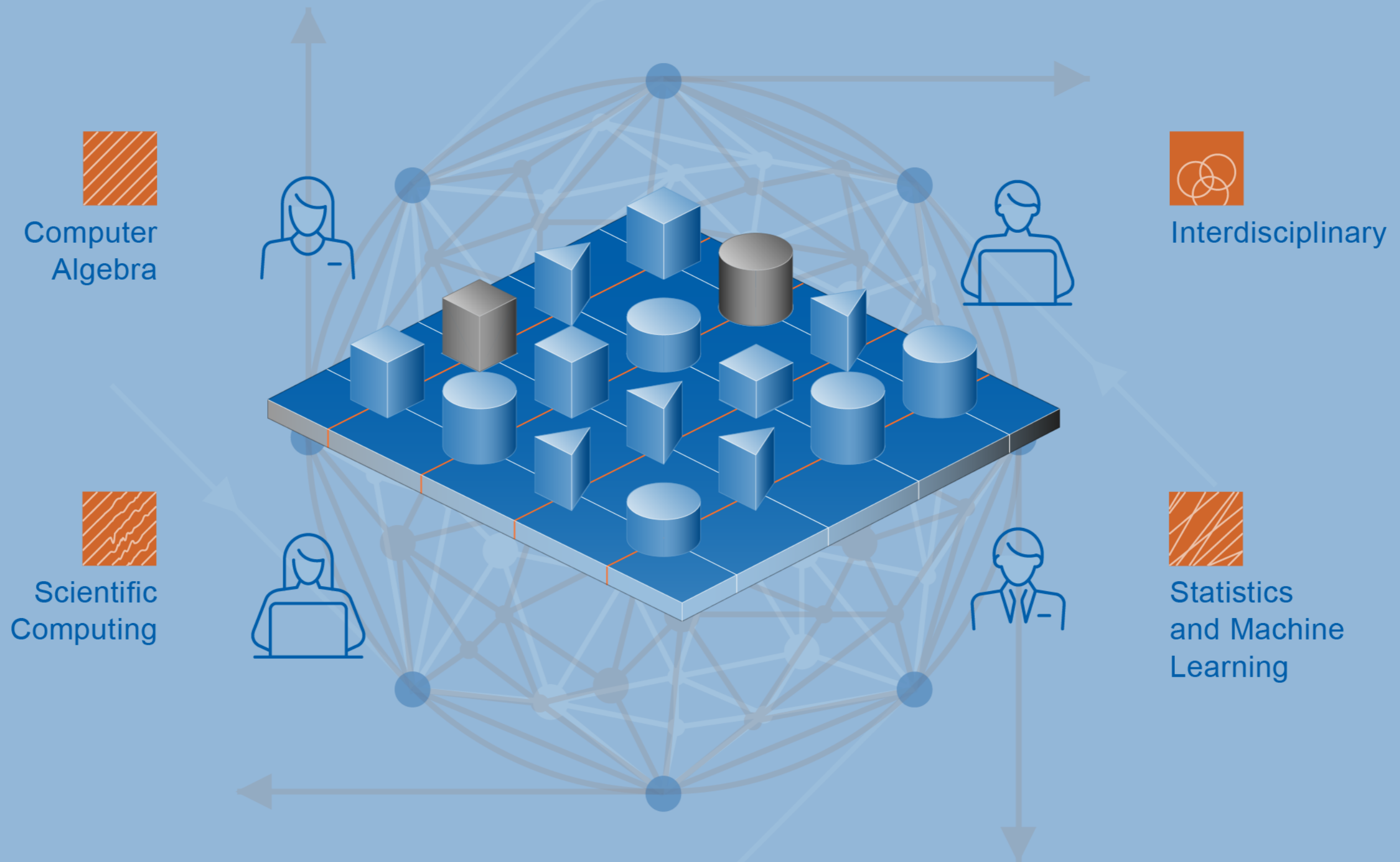
- **WIAS**
- ZIB
- MPI DCTS Magdeburg
- FIZ Karlsruhe
- MPI MIS Leipzig
- Fraunhofer ITWM
- MFO

- TU Berlin
- FU Berlin
- U Stuttgart
- LMU München
- TU München
- WWU Münster
- TU Kaiserslautern

Leibniz Network  
**Mathematical**  
Modeling and  
Simulation

**M** | **S**

# An Infrastructure for Mathematics-Driven Research of Tomorrow



# An Infrastructure for Mathematics-Driven Research of Tomorrow

  
Computer  
Algebra

  
Interdisciplinary

  
Scientific  
Computing

  
Statistics  
and Machine  
Learning

We are starting October 2021!

MaRDI Kick-off Meeting: 2.-4.11.2021

# Towards a Data Culture for Mathematics and Its Users

FAIR mathematical research data and confirmable workflows as a foundation for future mathematics-driven research

