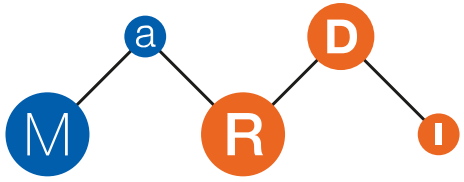


Scientific Computing

MaRDI TA2: Research Data and Reproducibility in Scientific Computing

Peter Benner, Christian Himpe, **Kathryn Lund**, Saksham Malhotra, Tim Mitchell, Jens Saak, Malte Speidel, Alexander Stage

Computational Reproducibility Seminar of the Swiss Reproducibility Network
November 15, 2023

MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

Outline

Scientific computing within MaRDI

M 2.3 — MaRDIMark

Model Order Reduction Wiki (MORWiki)

Model Order Reduction Benchmarker (MORB)

Analyzing a Collection of Collections (MathBench)

Outline

Scientific computing within MaRDI
MaRDI — THE Mathematical Research Data Initiative
Overview of Task Area 2 (TA2)

M 2.3 — MaRDIMark

Model Order Reduction Wiki (MORWiki)

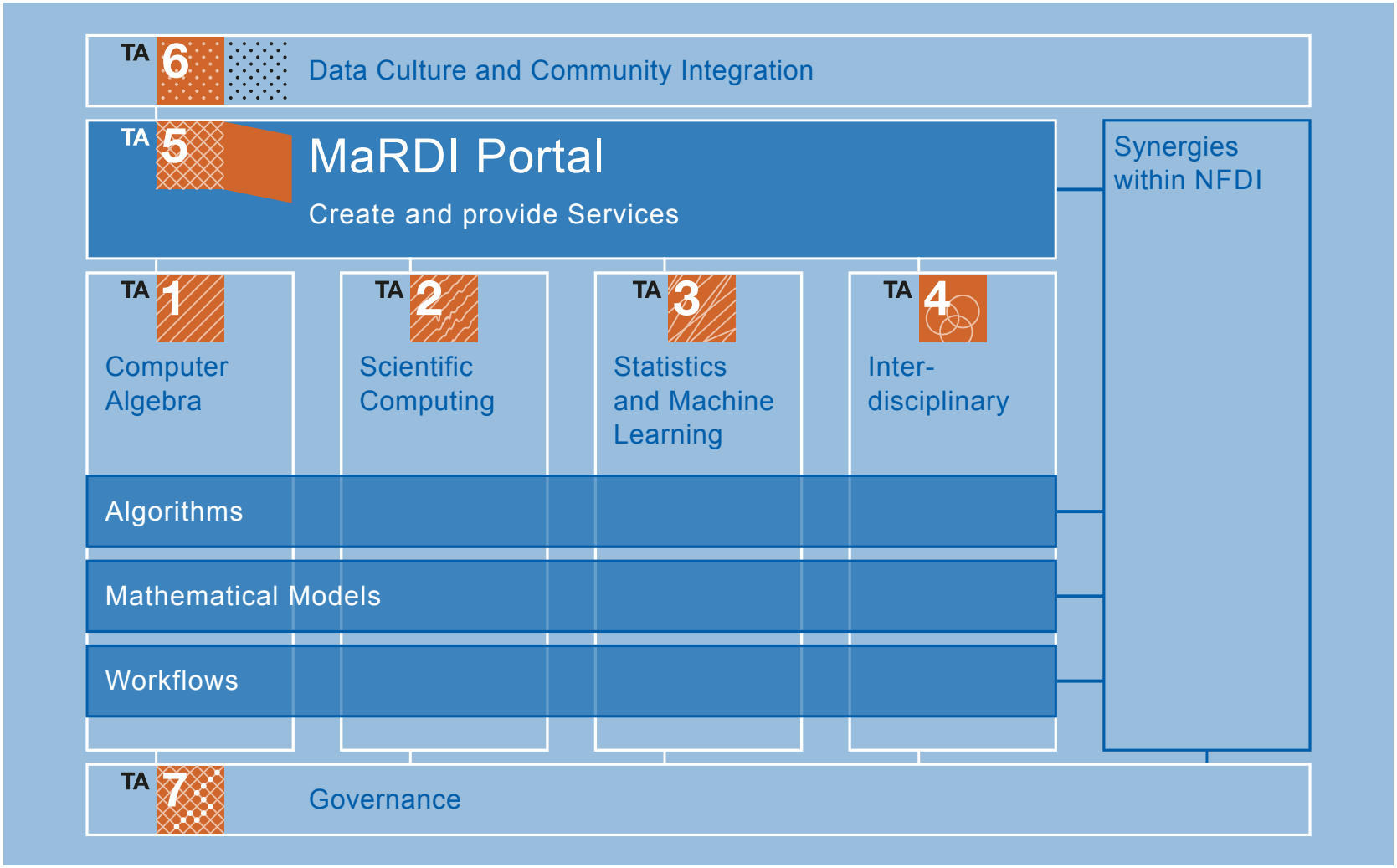
Model Order Reduction Benchmarker (MORB)

Analyzing a Collection of Collections (MathBench)

MaRDI — THE Mathematical Research Data Initiative

- 1 out of 27 NFDI consortia
- the one consortium of mathematics
- 16 institutions and partners
- kick-off November 2021
- 28 (full-time equivalent) employees
- funding over a period of five years

TA2 within MaRDI



MaRDI Task Area 2: Measures and major objectives

Objects / Data

problem
input
model
benchmark
algorithm
output
solution
visualization
.....

M1 Knowledge Graph of Numerical Algorithms

M2 Open Interfaces for Scientific Computing

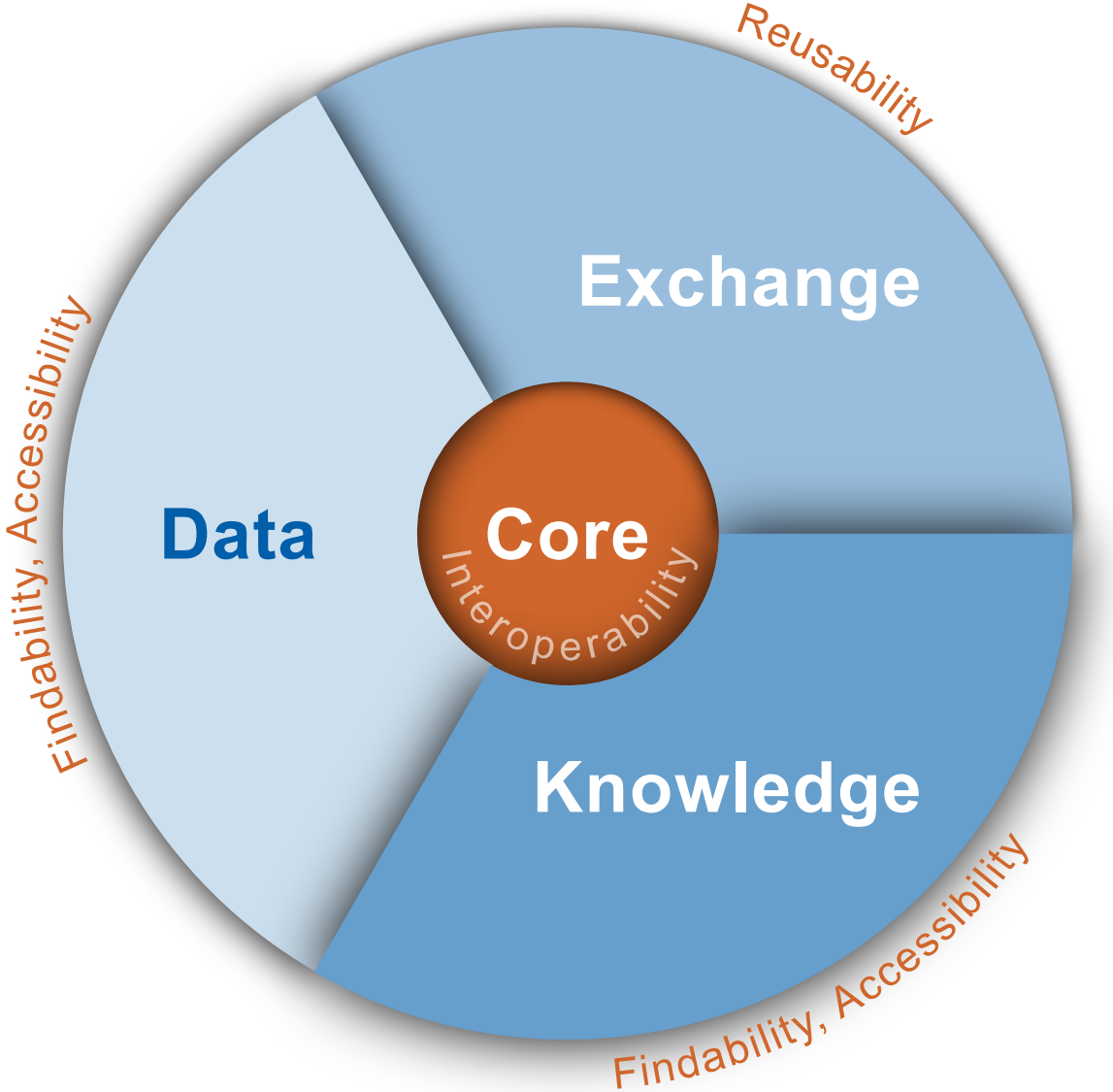
M3 Benchmark Framework

M4 Description and Design of FAIR CSE workflows

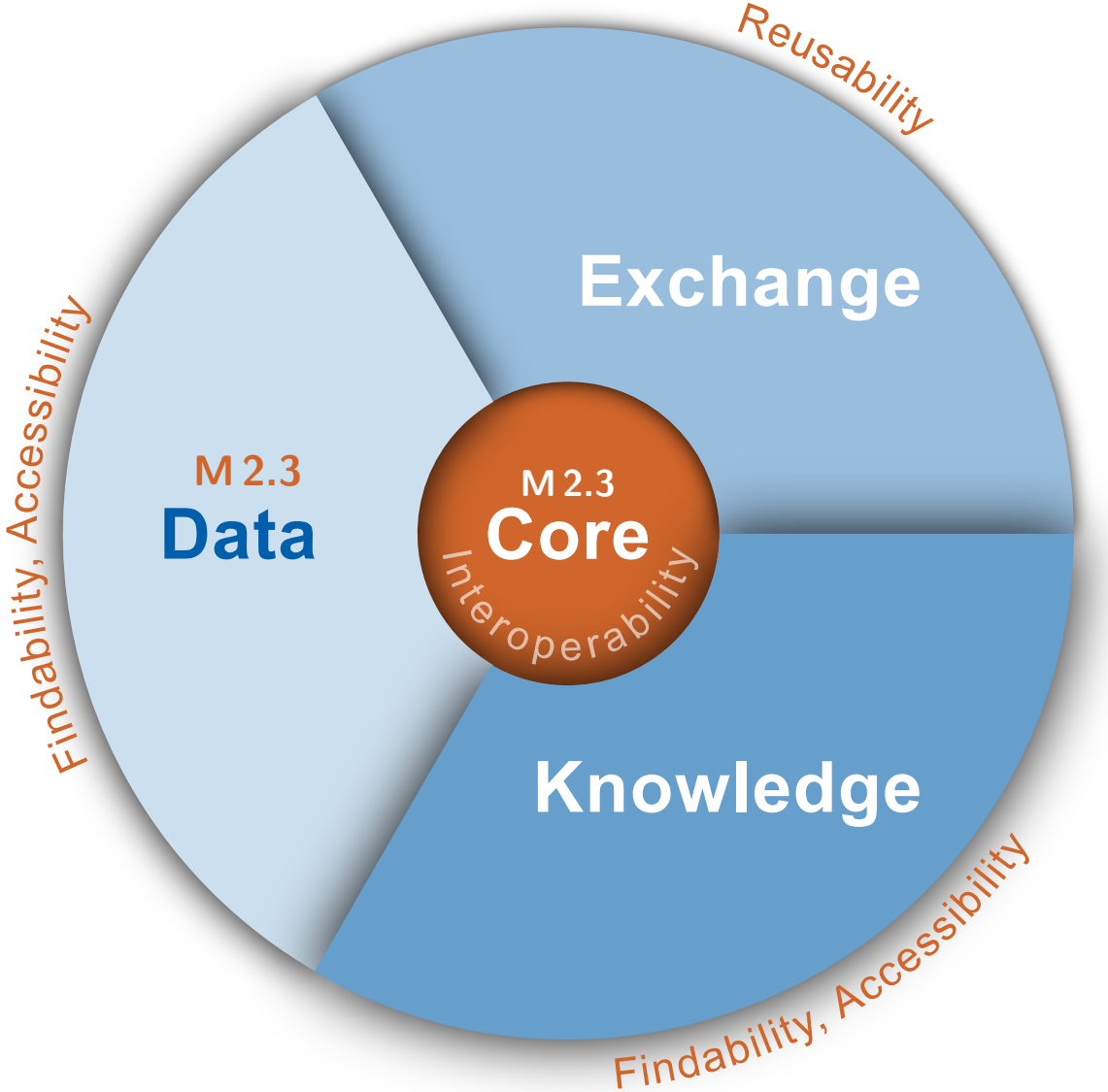
TA2 Objectives

- Verified research data in scientific computing and its fields of application
- FAIR principles for computer-based experiments and the entailing data
- Ontology of mathematical objects
- Confirmable workflows for trustworthy computations
- Dissemination of numerical methods and algorithms

MaRDI Layer structure



MaRDI Layer structure



Interplay with other Consortia

case studies with other disciplines

nfdi4chem

NFDI4Cat
NFDI for Catalysis-Related Sciences

NFDI4 DataScience

NFDI4ing

NFDI MatWerk

nfdi culture

MaRDI

NFDI Neuroscience

PUNCH 4NFDI

NFDI×CS

BERD @NFDI

Outline

Scientific computing within MaRDI

M 2.3 — MaRDIMark

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M 2.3 — MaRDIMark

A general-purpose benchmarking framework for comparing implementations of algorithms using problems native to a community

Aims:

- **Generic, extensible toolkit**
- **Language-agnostic interoperability**
- **Fair comparison among different implementations of algorithms (e.g., from different libraries, packages, toolboxes, etc.)**
- **Flexible (community-driven) performance measures**

M 2.3 — MaRDIMark

Main Elements

Problems	Methods	Driver	Analysis	Explorer
data, metadata	code, executable, metadata	interfaces, parameters	performance measures	distillation, result browser
X2: Data	X2: Data	X1: Core	X2: Data	X4: Knowledge

Tasks

- Assembly of domain-independent specifications
- Database of curated benchmarks
- Result data (schemes, amounts, formats, raw or analyzed?)
- Classification, visualization?

Connections

- Uses knowledge graph (M 2.1)
- Uses open interfaces (M 2.2)
- Uses confirmable workflows (M 2.4)
- Has high synergetic potential (TA3)
- Integrates into MaRDI Portal (TA5)

M 2.3 — MaRDIMark

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M 2.3 — MaRDIMark

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Outline

Scientific computing within MaRDI

M 2.3 — MaRDIMark

Model Order Reduction Wiki (MORWiki)

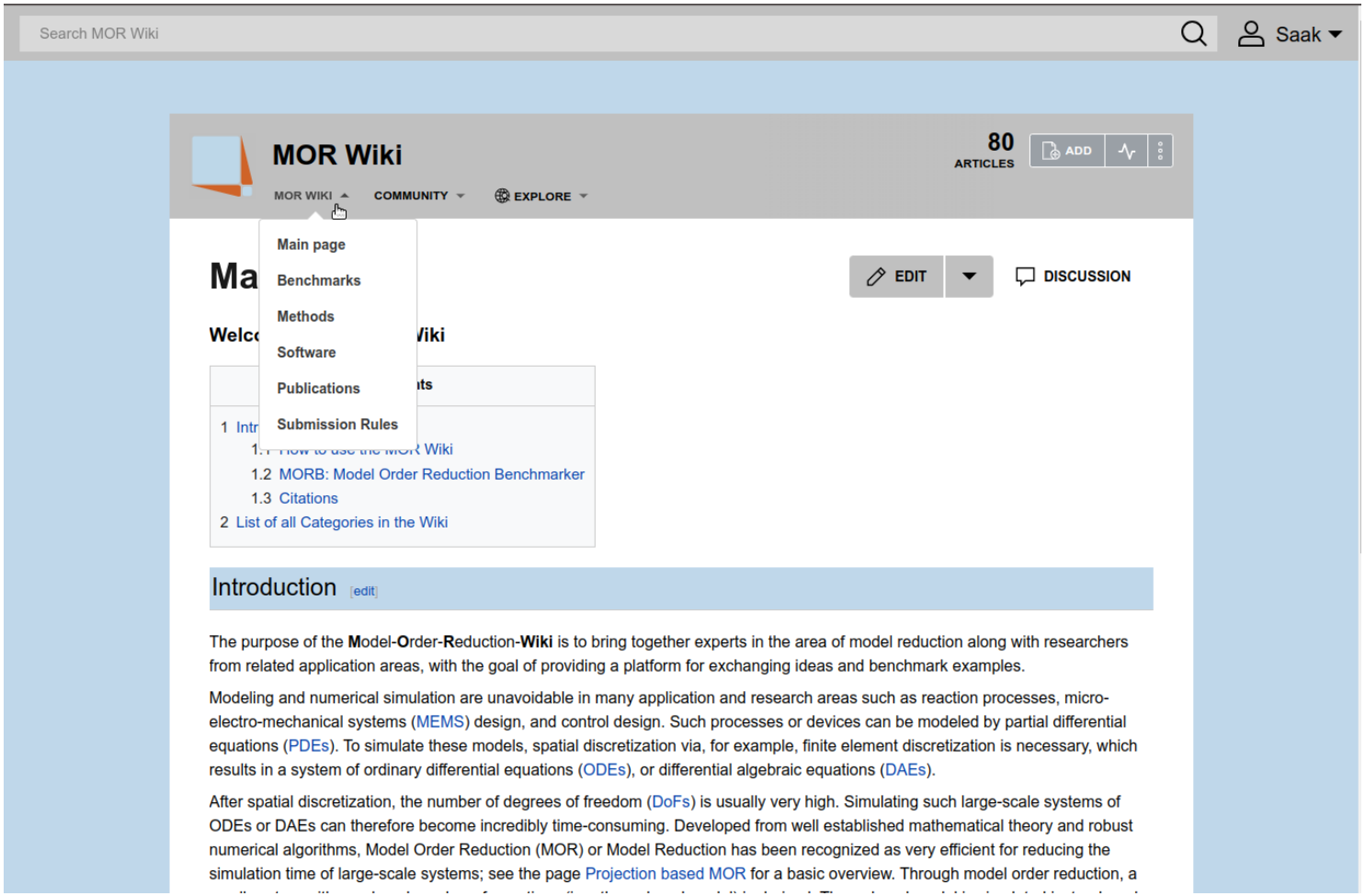
- A community platform as a prototype for a curated benchmark collection
- Tasks and challenges

Model Order Reduction Benchmarker (MORB)

Analyzing a Collection of Collections (MathBench)

Model Order Reduction Wiki (MORWiki)

A community platform as a prototype for a curated benchmark collection



http://modelreduction.org

Model Order Reduction Wiki (MORWiki)

A community platform as a prototype for a curated benchmark collection

Services provided

- Descriptions of basic MOR methods
- Collection of curated benchmark examples
- Description and comparison of available MOR software
- MOR literature aggregation and BibTeX data
- Compilation of community events

Lessons learned

- Encourage community engagement via low contribution barrier:
  - Easy access
  - Simple formats
  - Small rule-sets
- Ensure content licensing and create proper citation culture
- Incentivize users for their contributions

Model Order Reduction Wiki (MORWiki)

Tasks and challenges

Licensing

- Old benchmark models without licenses
  - SLICOT Collection collected 2002–2006
  - Oberwolfach Collection circa 2005
- Benchmark descriptions and illustrations in the wiki

Assembling metadata

- Classic data properties (creators, editors, etc.)
- Mathematical properties of
  - the systems modeled by the benchmark data
  - the numerical data itself (e.g., matrix sparsity, symmetry, condition number, etc.)

Outline

Scientific computing within MaRDI

M 2.3 — MaRDIMark

Model Order Reduction Wiki (MORWiki)

Model Order Reduction Benchmarker (MORB)
MORB 0.1 — benchmarking stable LTI Systems in MATLAB

Analyzing a Collection of Collections (MathBench)

Model Order Reduction Benchmarker (MORB)

MORB 0.1 — benchmarking stable LTI Systems in MATLAB

Linear Time-Invariant (LTI) System

$$E\dot{x}(t) = Ax(t) + Bu(t), \qquad y(t) = Cx(t) + Du(t). \quad \Leftrightarrow \quad H(s) = C(sE - A)^{-1}B$$

Why so restrictive at the moment?

- Most MORWiki benchmarks are LTI or parametric LTI
- Most MOR software for LTI systems is written in MATLAB
- Simple proof-of-concept to get feedback on

Model Order Reduction Benchmarker (MORB)

MORB 0.1 — benchmarking stable LTI Systems in MATLAB

Challenges

- Ensuring all benchmark data is encoded uniformly (.mat, v7.3)
- Calling external software as “black boxes” and without unnecessary overhead
- Determining what counts as a unique implementation of an algorithm (“algorithm isotope”)
- Finding subroutines that compute measures (e.g., error, speed, etc.) efficiently and accurately

Model Order Reduction Benchmarker (MORB)

MORB 0.1 — benchmarking stable LTI Systems in MATLAB

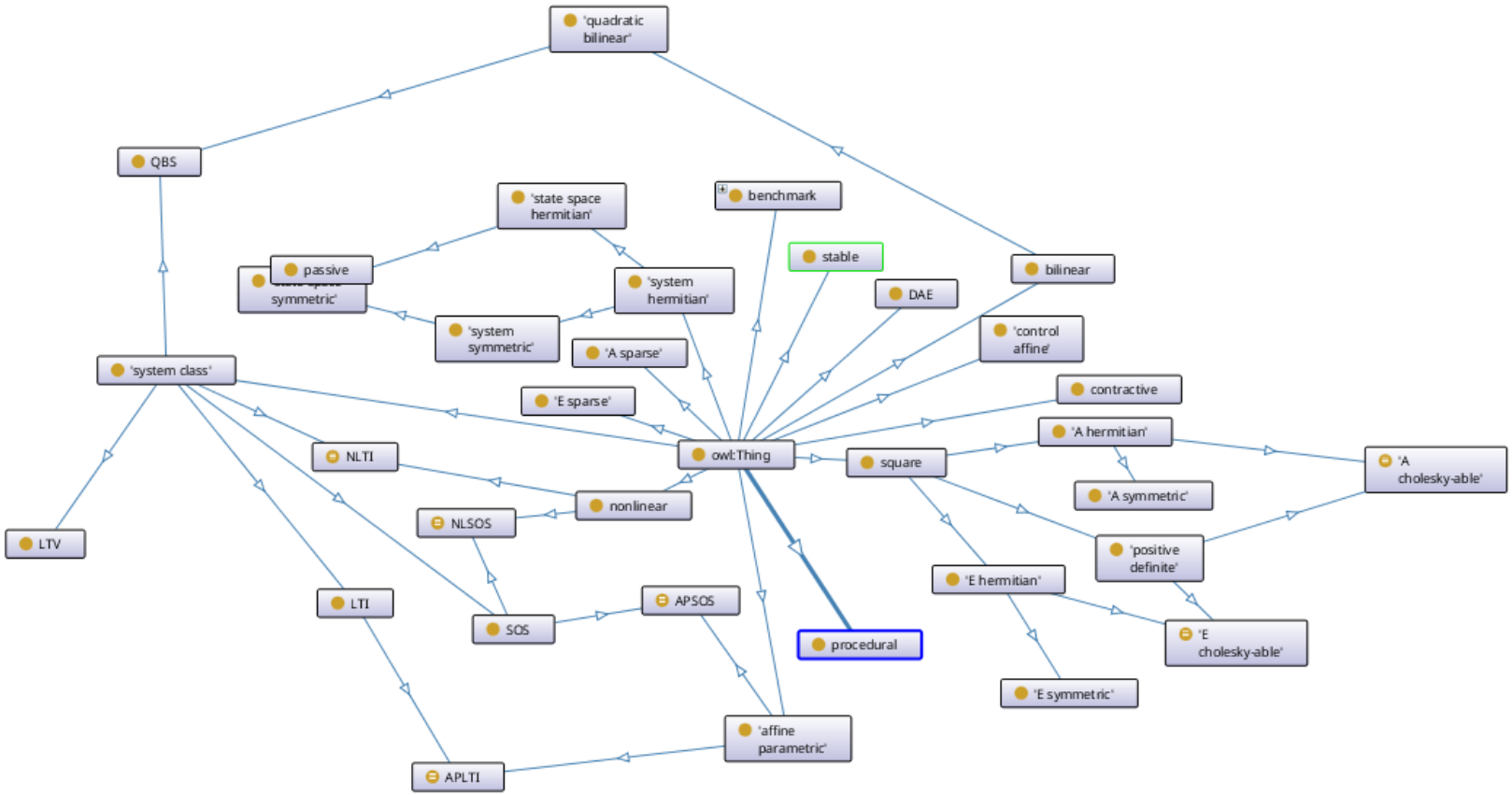
Mostly completed tasks

- Automated computation of mathematical metadata
  - Still ongoing for large systems (symmetry, stability, passivity, contractivity, etc.)
- Database of benchmark-metadata
  - Interns (A. Stage and M. Speidel) worked on MORBO (MORB Ontology) and search interface
- Balanced Truncation (BT) algorithm isotopes for Control Systems Toolbox, M-M.E.S.S., MORLAB, and pyMOR

Model Order Reduction Benchmarker (MORB)

MORB 0.1 — benchmarking stable LTI Systems in MATLAB

MORBO (MORB Ontology)



Model Order Reduction Benchmarker (MORB)

MORB 0.1 — benchmarking stable LTI Systems in MATLAB

MORB search tool / database

filename	MORWikiPageName	directory	MORWikiLink	nStates	nInputs	nOutputs	components	nParameters	systemClass	isDAE	daeDiffIndex	isSquare	isStateSpaceSymm	isSysSym m	isPassive	isContractive	isStable	nUnstabPoles	isASymm	isACholAble	isASparse	nnzA	condA
linear1DBeam_n14m1q1	Linear 1D Bear	oberwolfach	https://morwiki.mj	14	1	1	B, C, E, K, M	0	LTI-SOS			1	0	1					NaN	NaN	NaN	NaN	NaN
nonlinearHeatTransfer_n1	Nonlinear Heat	oberwolfach	https://morwiki.mj	15	2	2	A, B, C, E	0	LTI-FOS	0	0	1	0	0			0	15	1	1	1	43	4.80E+02
nonlinearHeatTransfer_n1	Nonlinear Heat	oberwolfach	https://morwiki.mj	15	2	2	A, B, C, E, F, f	0	NLTI-FOS			1	NaN	NaN					1	1	1	43	4.80E+02
linear1DBeam_n18m1q1	Linear 1D Bear	oberwolfach	https://morwiki.mj	18	1	1	B, C, E, K, M	0	LTI-SOS			1	0	1					NaN	NaN	NaN	NaN	NaN
electrostaticBeam_n38m1	Electrostatic Be	oberwolfach	https://morwiki.mj	38	1	1	B, C, E, F, K, M, f	0	NLTI-SOS			1	NaN	NaN					NaN	NaN	NaN	NaN	NaN
buildingModel_n48m1q1	Building Model	slicot	https://morwiki.mj	48	1	1	A, B, C	0	LTI-FOS	0	0	1	0	1	0	0	1	0	0	0	1	1176	1.23E+04
newEngland_n66m1q1	Power System	power_system	https://morwiki.mj	66	1	1	A, B, C	0	LTI-FOS	0	0	1	0	1	0	0	0	1	0	0	0	NaN	3.03E+11
convectionReaction_n84r	Convection Rea	slicot	https://morwiki.mj	84	1	1	A, B, C	0	LTI-FOS	0	0	1	0	1	0	0	0	1	0	0	1	382	7.36E+00
orrSommerfeld_n100m1q	Orr-Sommerfeld	slicot	https://morwiki.mj	100	1	1	A, B, C	0	LTI-FOS	0	0	1	0	1	0	0	1	0	0	0	1	10000	7.36E+02
cdPlayer_n120m2q2	CD Player	slicot	https://morwiki.mj	120	2	2	A, B, C	0	LTI-FOS	0	0	1	0	0	0	0	1	0	0	0	1	240	1.81E+04
heatEquation_n200m1q1	Heat Equation	slicot	https://morwiki.mj	200	1	1	A, B, C, E	0	LTI-FOS	0	0	1	0	1			0	4	1	0	1	598	6.51E+03
random_n200m1q1	Random	slicot	https://morwiki.mj	200	1	1	A, B, C	0	LTI-FOS	0	0	1	0	1	0	0	1	0	0	0	1	2132	3.00E+03
transmissionLines_n256n	Transmission L	slicot	https://morwiki.mj	256	2	2	A, B, C, E	0	LTI-FOS	0	1	1	0						1	1	0	256	2.22E+05
iss_n270m3q3	International Sp	slicot	https://morwiki.mj	270	3	3	A, B, C	0	LTI-FOS	0	0	1	0	0	0	0	1	0	0	0	1	405	9.68E+03
rclCircuitEquations_n306	RCL Circuit Eq	oberwolfach	https://morwiki.mj	306	2	2	A, B, C, E	0	LTI-FOS	1		1	0				0	168	0	0	1	696	Inf
clampedBeam_n348m1q	Clamped Beam	slicot	https://morwiki.mj	348	1	1	A, B, C	0	LTI-FOS	0	0	1	0	1	0	0	1	0	0	0	1	60726	3.74E+07
electrostaticBeam_n398n	Electrostatic Be	oberwolfach	https://morwiki.mj	398	1	1	B, C, E, F, K, M, f	0	NLTI-SOS			1	NaN	NaN					NaN	NaN	NaN	NaN	NaN
nonlinearHeatTransfer_n4	Nonlinear Heat	oberwolfach	https://morwiki.mj	410	2	2	A, B, C, E, F, f	0	NLTI-FOS			1	NaN	NaN					1	1	1	1228	3.37E+05
peecModel_n480m1q1	PEEC Model (S	slicot	https://morwiki.mj	480	1	1	A, B, C, E	0	LTI-FOS	1		1	0	1			0	264	1	0	1	1346	1.85E+14
mna_n578m9q9	Modified Nodal	slicot	https://morwiki.mj	578	9	9	A, B, C, E	0	LTI-FOS	1		1	0				0	290	0	0	1	1694	2.63E+09
earthAtmosphere_n598m	Earth Atmosph	slicot	https://morwiki.mj	598	1	1	A, B, C	0	LTI-FOS	0	0	1	0	1	0	0	1	0	0	0	0	357406	1.60E+02
mna_n980m4q4	Modified Nodal	slicot	https://morwiki.mj	980	4	4	A, B, C, E	0	LTI-FOS	1		1	0				0	258	0	0	1	2872	6.03E+07
penzlFOM_n1006m1q1	Penzl's FOM	slicot	https://morwiki.mj	1006	1	1	A, B, C	0	LTI-FOS	0	0	1	0	1			0	258	0	0	1	1012	1.00E+03
steelProfile_n1357m7q6	Steel Profile	oberwolfach	https://morwiki.mj	1357	7	6	A, B, C, E	0	LTI-FOS	0	0	0	0	0			1	0	1	0	1	8985	2.23E+04
iss_n1412m3q3	International Sp	slicot	https://morwiki.mj	1412	3	3	A, B, C	0	LTI-FOS	0	0	1	0	0			1	0	0	0	1	2118	7.75E+01
peekInductor_n1434m1q1	Peek Inductor	oberwolfach	https://morwiki.mj	1434	1	1	A, B, C, E	0	LTI-FOS	0	0	1	0	1			1	0	1	0	1	18228	1.47E+06
transmissionLines_n1600	Transmission L	misc	https://morwiki.mj	1600	14	14	A, B, C, E	0	LTI-FOS	0	1	1	0						0	0	1	5280	Inf
tunableOpticalFilter_n166	Tunable Optica	oberwolfach	https://morwiki.mj	1668	1	5	A, B, C, E	0	LTI-FOS	0	0	0	0	0			1	0	1	0	1	10750	7.23E+04
rclCircuitEquations_n184	RCL Circuit Eq	oberwolfach	https://morwiki.mj	1841	16	16	A, B, C, E	0	LTI-FOS	1		1	0	1			0	945	0	0	1	5881	4.04E+07
circularPiston_n2025m1q	Circular Piston	oberwolfach	https://morwiki.mj	2025	1	2025	B, C, E, K, M	0	LTI-SOS			0	0	0					NaN	NaN	NaN	NaN	NaN
transmissionLines_n2624	Transmission L	misc	https://morwiki.mj	2624	30	30	A, B, C, E	0	LTI-FOS	0	1	1	0						0	0	1	8640	Inf
thermalModel_n4257m1q	Thermal Model	oberwolfach	https://morwiki.mj	4257	1	7	A, B, C, E	3	AP-LTI-FOS	0	1	0	0	0									
micropyrosThruster_n425	Micropyros Thr	oberwolfach	https://morwiki.mj	4257	1	7	A, B, C, E	0	LTI-FOS	0	0	0	0	0			1	0	1	0	1	37465	2.52E+16

Model Order Reduction Benchmarker (MORB)

MORB 0.1 — benchmarking stable LTI Systems in MATLAB

MORB test and algorithm configuration

```
"newEngland_n66m1q1":
    {
    "alg_iso":
        {
        "bt":
            {
            "cst":
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                "tol": 1E-6
                },
                {
                "tol": 1E-12
                }],
            "emgr": null,
            "mess":
                [{
                "max_order": 100,
                "tol": 1E-6
                },
                {
                "tol": 1E-12
                }],
            "morlab":
                {
                "tol": 1E-6
                },
            "pymor":
                {
                "tol": 1E-6
                }
            },
        "bg":
            {
            "emgr": null,
            "mess": null
            }
        },
    "meas_opt":
        {
```

```
    "meas_opt":
        {
        "norm_id": ["l0","l1","l2","linf","h2"],
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            "MaxPoints":500
            },
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            "MaxPoints":500
            },
        "ml_frobeniusplot":
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            "ShowPlot": 0,
            "MaxPoints": 500
            }
        },
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        "ShowPlot": 0,
        "MaxPoints": 500
        },
    "plot_opt":
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        "save_eps": true,
        "save_fig": true
        },
    "report_opt":
        {"tol": 1E-6,
        "max_order": 100}
        },
```

Model Order Reduction Benchmarker (MORB)

MORB 0.1 — benchmarking stable LTI Systems in MATLAB

MORB reports

- Measures: timings and error
- Plots: error, Bode diagrams, sigma plot, and Frobenius plot
- TeX report: autogenerated with specifications, simple formatting, and system info
- End product: PDF that can be easily shared with colleagues

Model Order Reduction Benchmarker (MORB)

MORB 0.1 — benchmarking stable LTI Systems in MATLAB

Ongoing and future tasks

- Upload standardized benchmark data to Zenodo with correct licenses
- Integrate MORBO with existing ontologies from MaRDI collaborators (MaRDIPortal, AlgoData, etc.)
- Publish MORB search tool in MORWiki
- Refactor MORB 0.1 in python and implement more algorithms
- Solicit feedback from the community

Outline

Scientific computing within MaRDI

M 2.3 — MaRDIMark

Model Order Reduction Wiki (MORWiki)

Model Order Reduction Benchmarker (MORB)

Analyzing a Collection of Collections (MathBench)

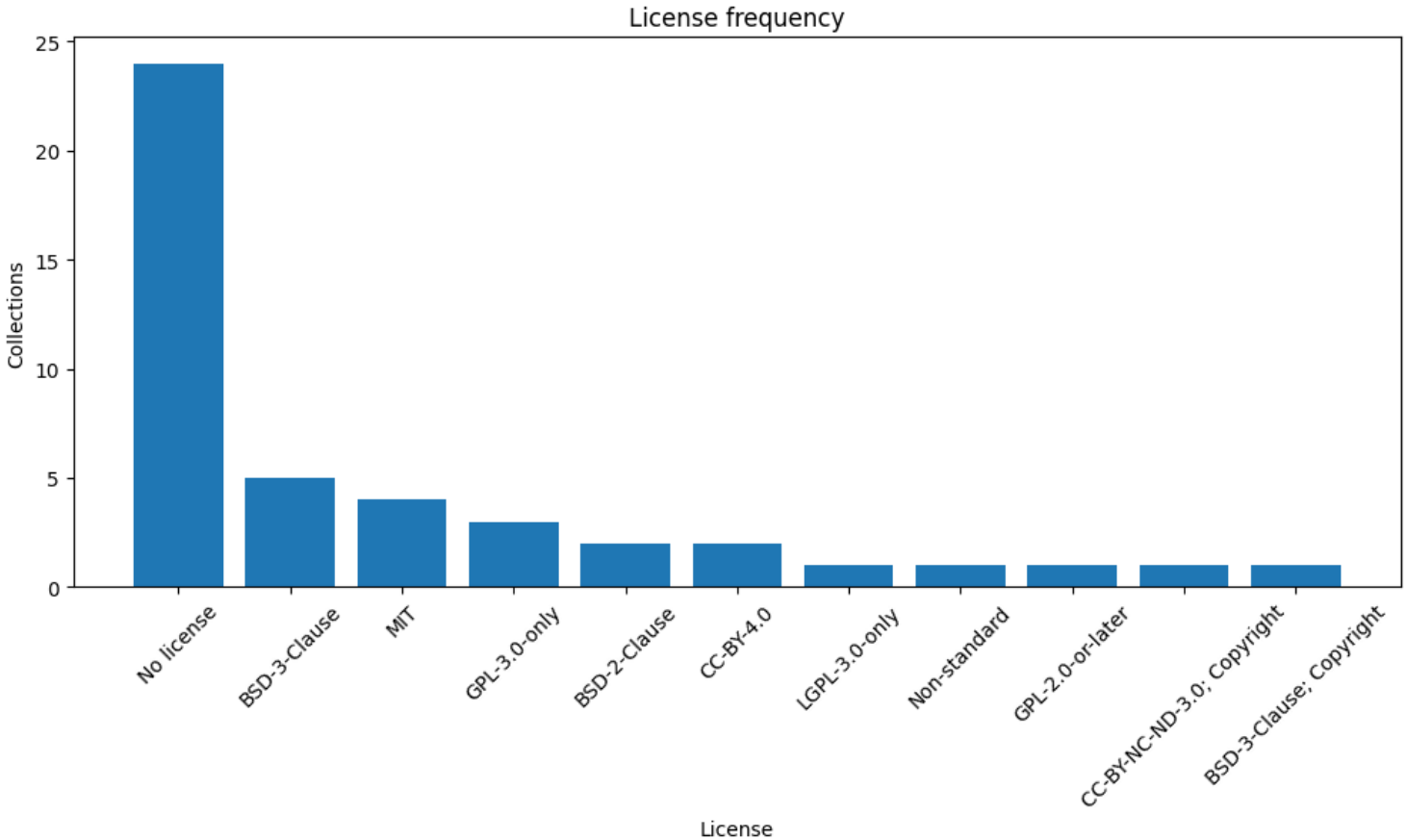
Analyzing a Collection of Collections (MathBench)

Research Question

What is the state of affairs in mathematical data collections?

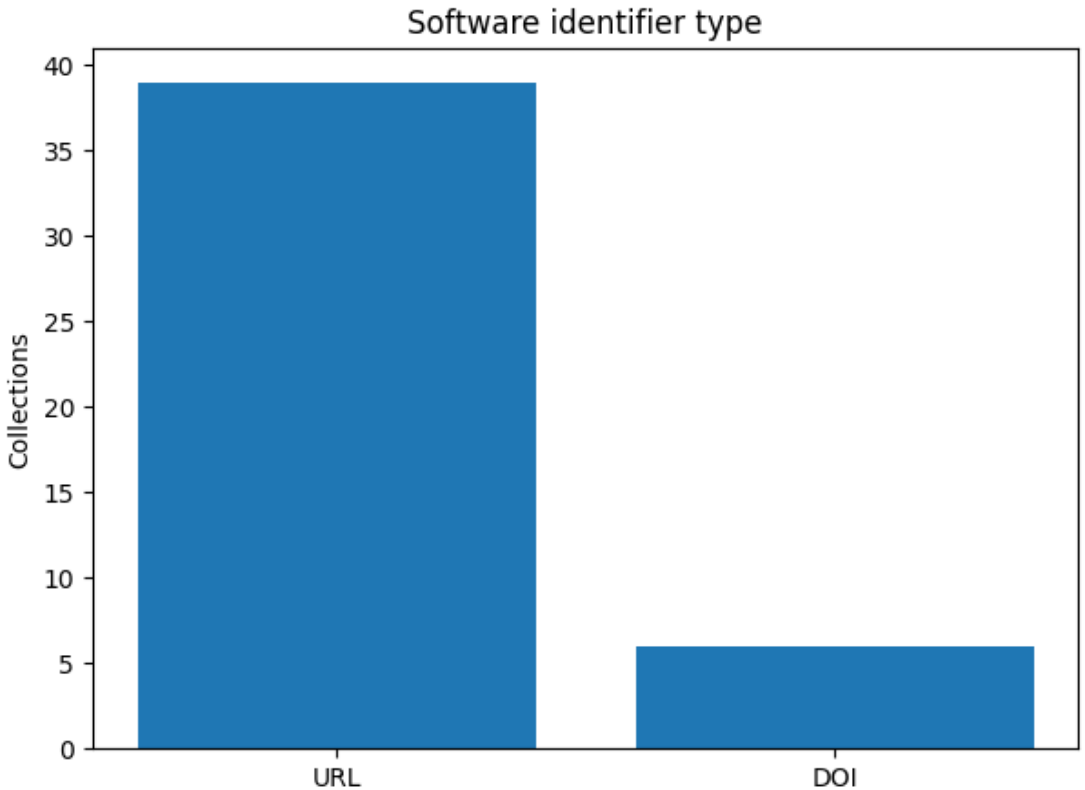
Analyzing a Collection of Collections (MathBench)

Licenses Used



Analyzing a Collection of Collections (MathBench)

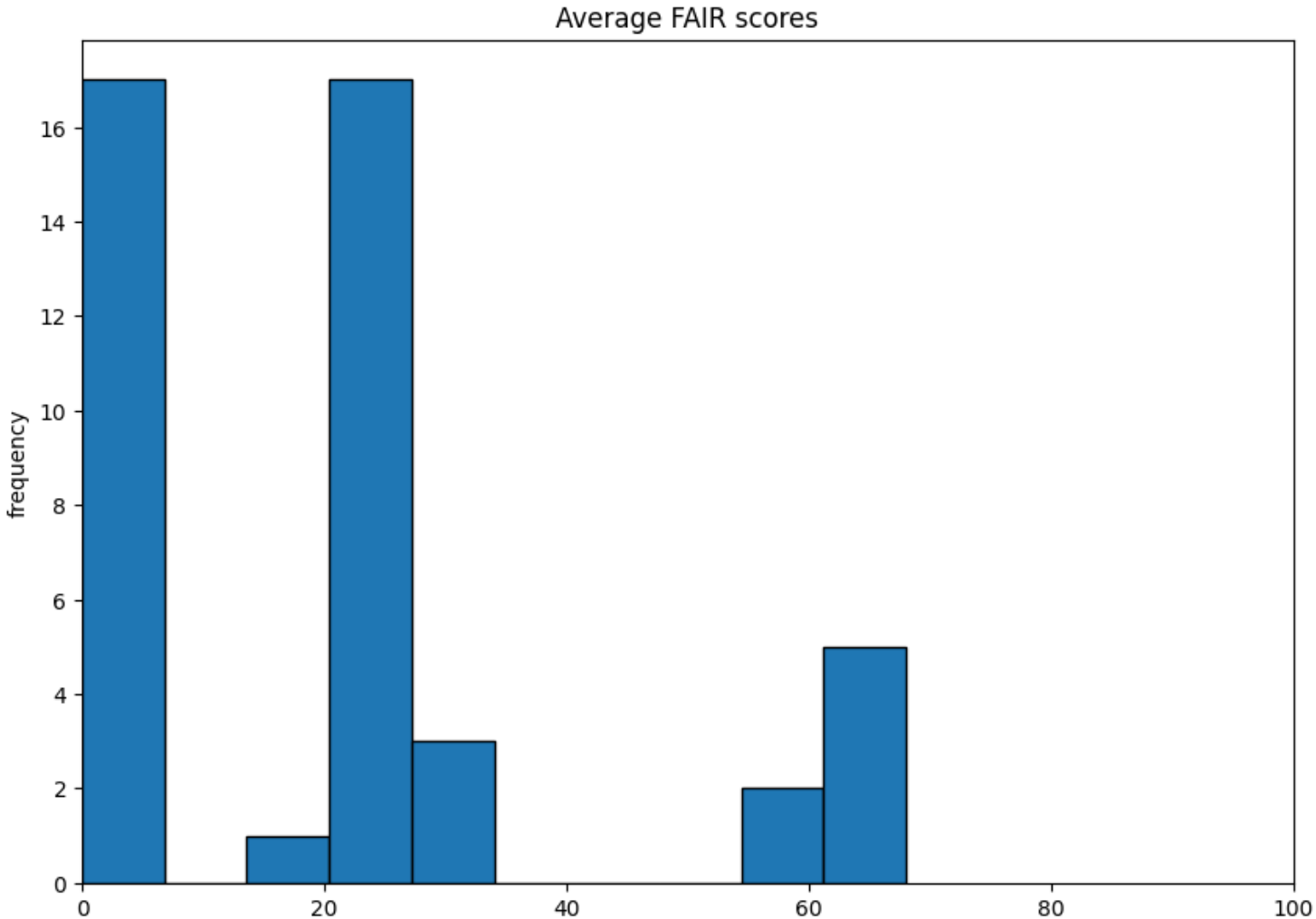
Dataset Identifiers



Analyzing a Collection of Collections (MathBench)

FAIR Scores (Homepages)

scores generated using `https://www.f-uji.net/`



Analyzing a Collection of Collections (MathBench)

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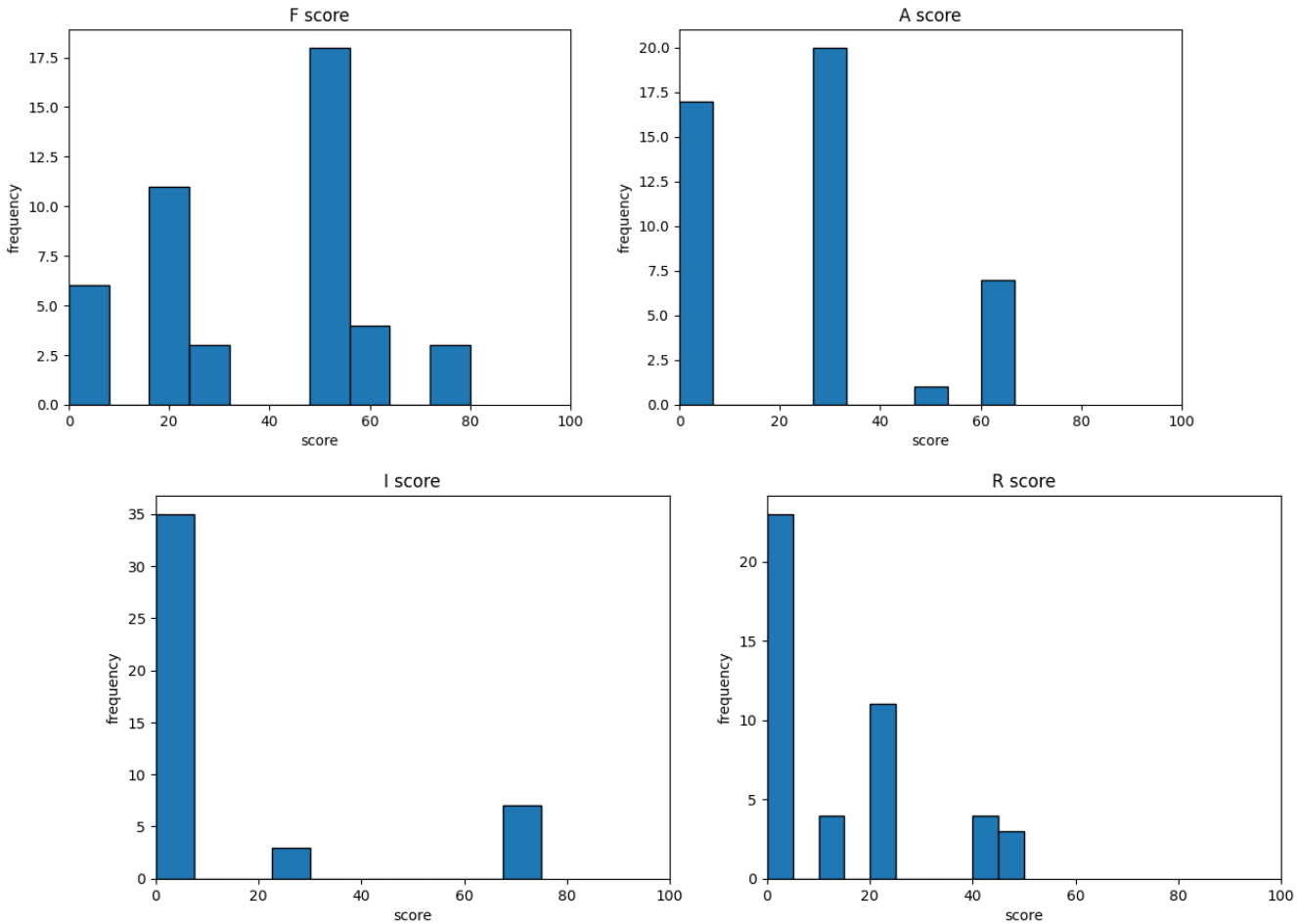
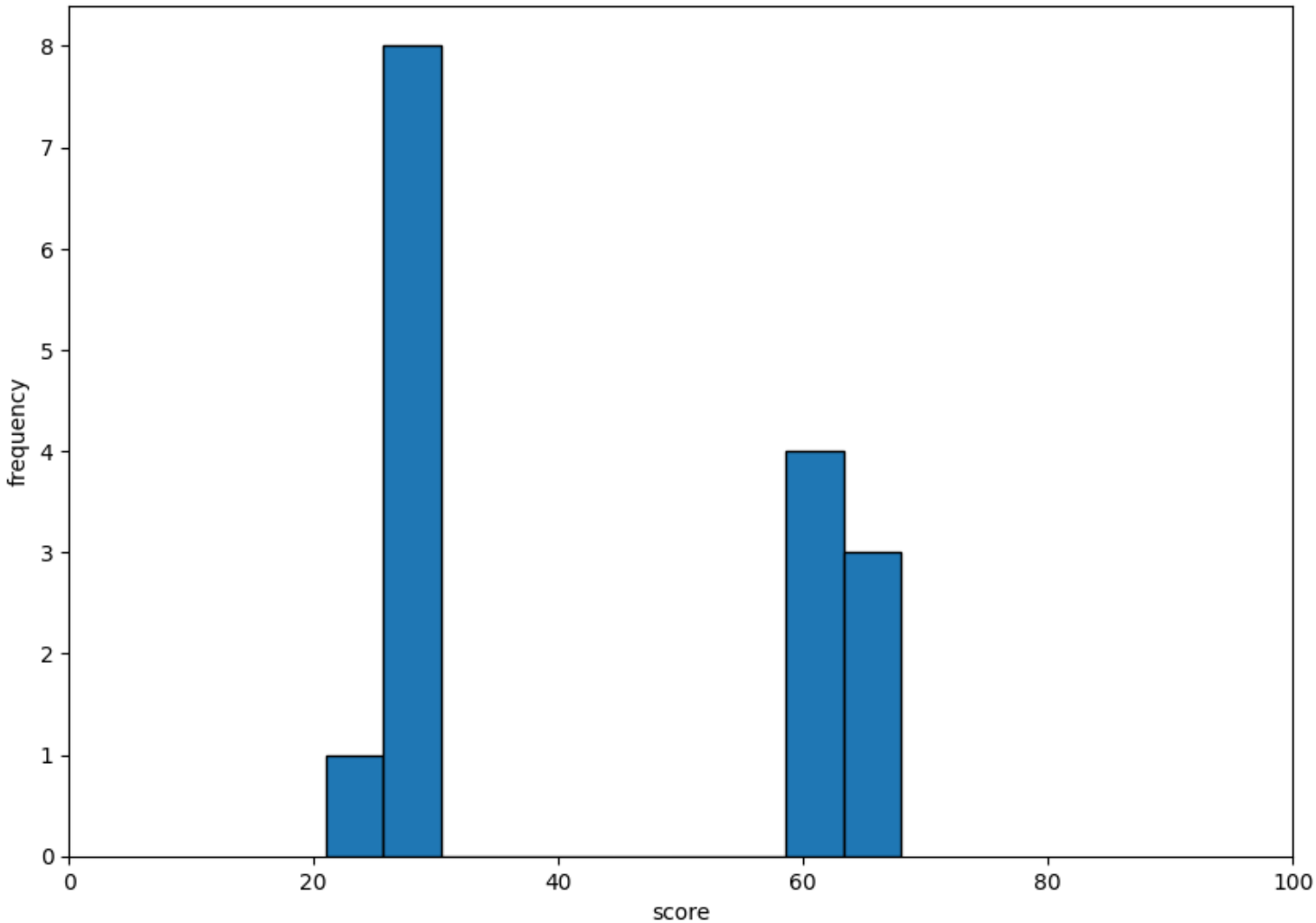


Analyzing a Collection of Collections (MathBench)

FAIR Scores (GitHub & Zenodo)

scores generated using `https://www.f-uji.net/`



Analyzing a Collection of Collections (MathBench)

FAIR Scores (GitHub & Zenodo)

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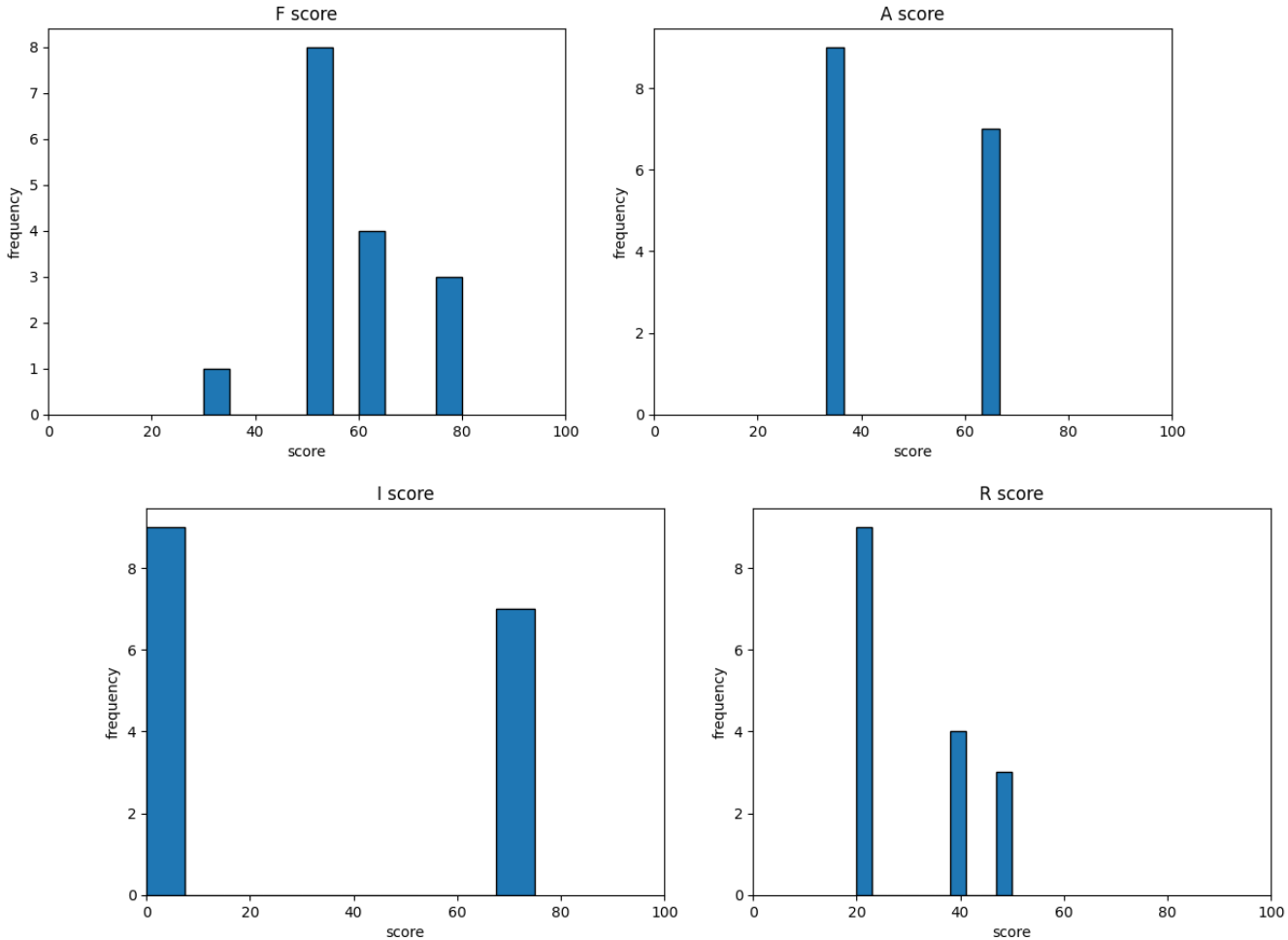
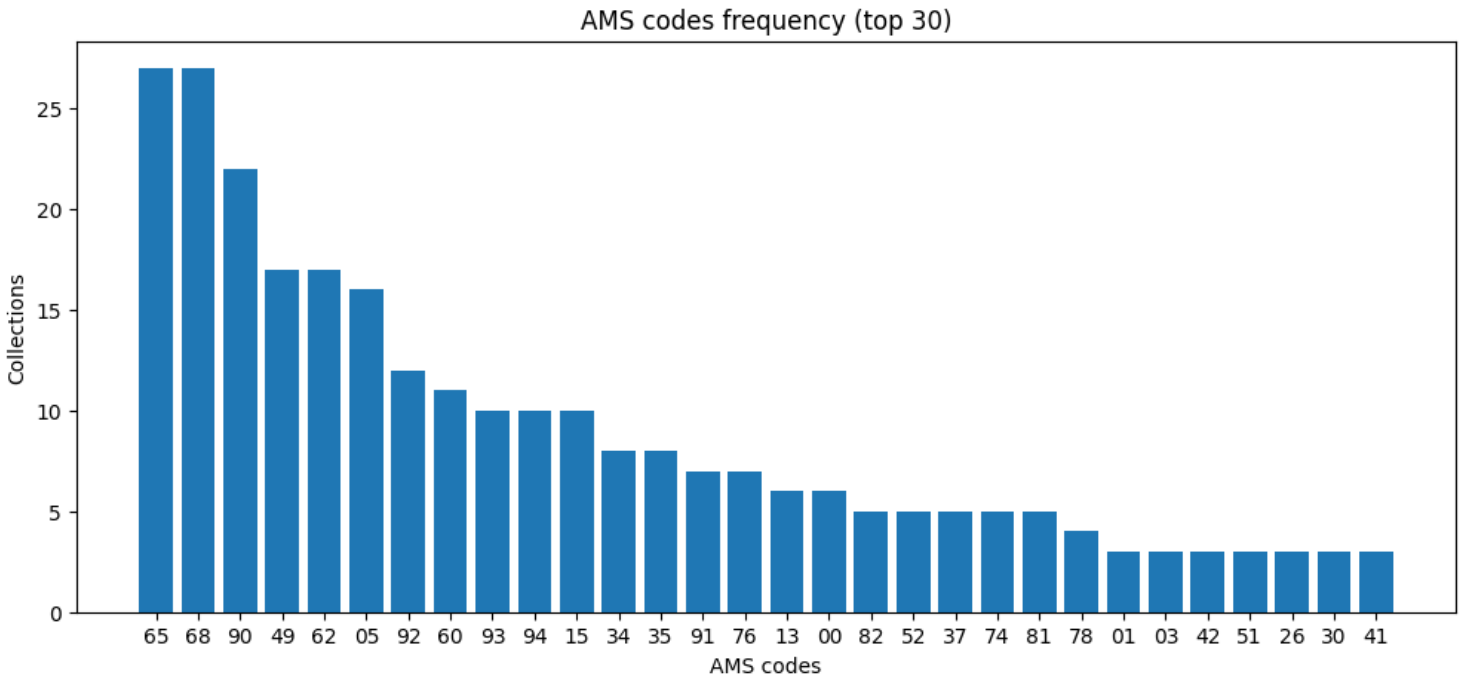


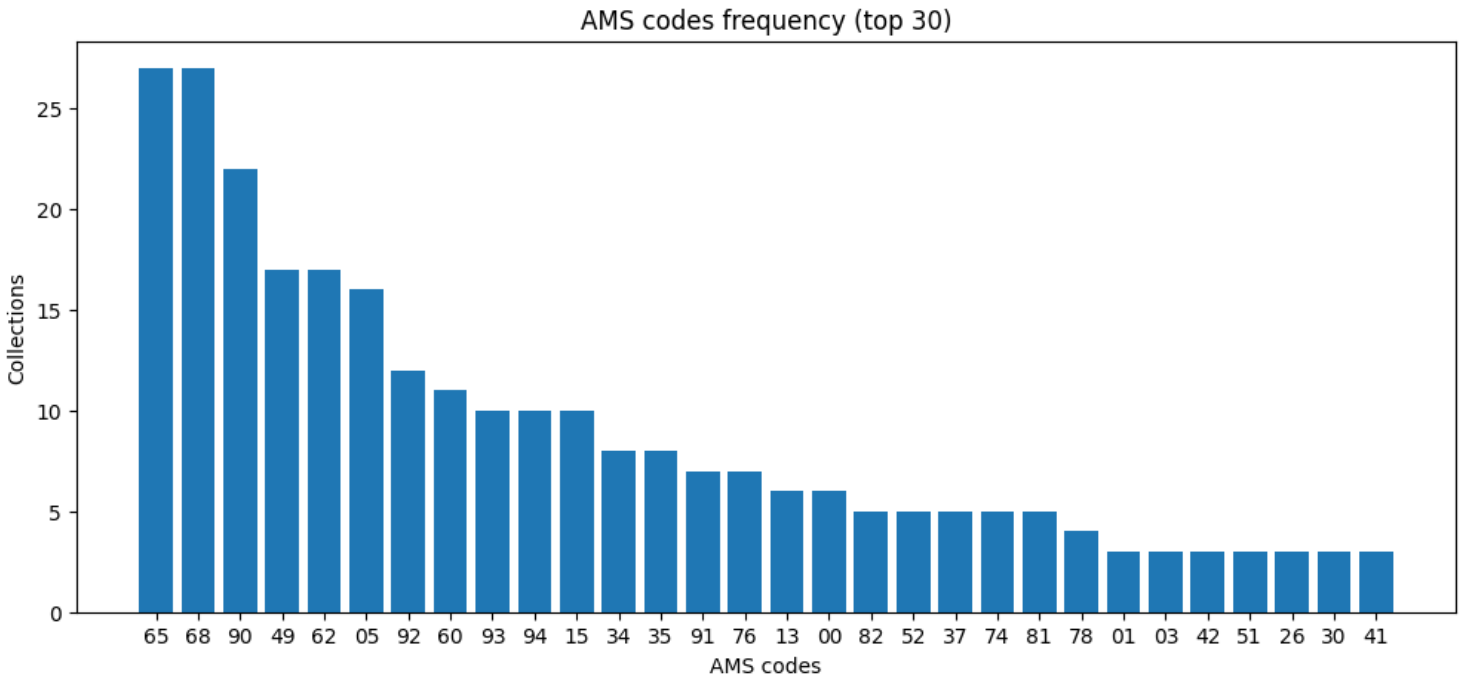
Analyzing a Collection of Collections (MathBench)

Mathematical Subject Classification 2020



Analyzing a Collection of Collections (MathBench)

Mathematical Subject Classification 2020



65 Numerical analysis
68 Computer science
90 Operations research, mathematical programming
30 Functions of a complex variable
41 Approximations and expansions

MaRDI TA2 Team

Jens Saak

Dmitry Kabanov

Kathryn Lund

Mario Ohlberger

Stephan Rave

Peter Benner

Frank Wübbeling

Pavan Veluvali

Jan Heiland