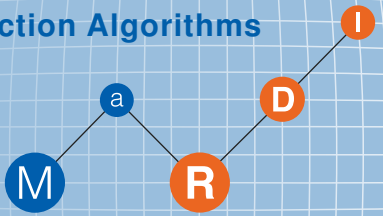
MaRDI
Mathematical Research Data Initiative

FAIR Benchmarking of Model Reduction Algorithms



Reisensburg Workshop on Nonlinear and Structure-Preserving Model Reduction
January 20–22, 2025

Peter Benner, Kathryn Lund, Ashwin Nayak, Jens Saak
Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany

Reproducibility Crisis

- First mentions around the turn of the millennium
- Initially discovered in medicine, psychology and biology
- Now relevant in all disciplines
- Presents itself in various forms

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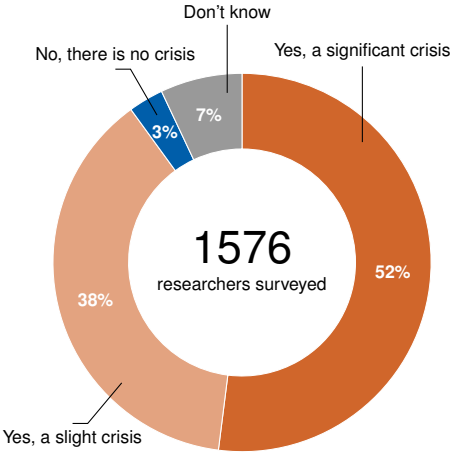

Baker, M. 1,500 scientists lift the lid on reproducibility. *Nature* **533**, 452–454 (2016). https://doi.org/10.1038/533452a

Reproducibility Crisis

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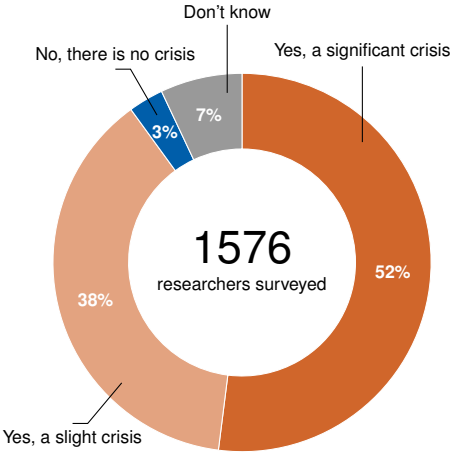
- More than 70% of researchers have tried and failed to reproduce another scientist's experiments.
- More than 50% have failed to reproduce their own experiments.
- The majority replied that there is a significant reproducibility crisis!



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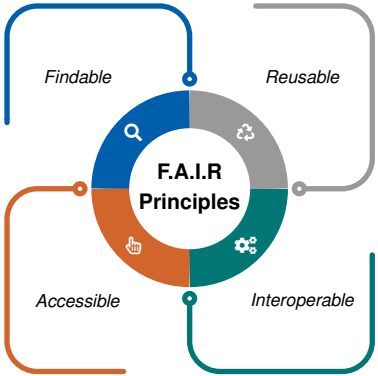
FAIR Principles

- Unique and persistent identifier (e.g. DOI)
- Rich metadata (machine-readable)
- Indexed in a searchable resource



- Documentation and precise attributes
- Proper licensing
- Detailed provenance
- Adhere to community standards

- Accessible via standard protocols
- Transparent access
- Accessible metadata

- Standardized language for knowledge representation
- Vocabularies and ontologies
- References to other data

https://www.go-fair.org/fair-principles/

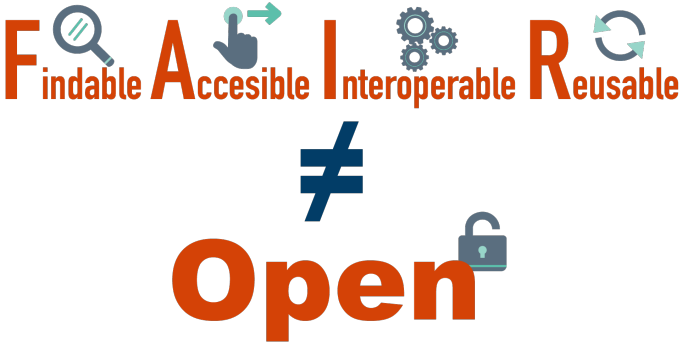


Image from https://libraries.mit.edu/news/data-necessarily/31452/

- 26 consortia across the disciplines
- Base4NFDI alliance for basic services
- 90 million € annual budget
- Organized as “eingetragener Verein”
- Members are most participating institutions

- 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

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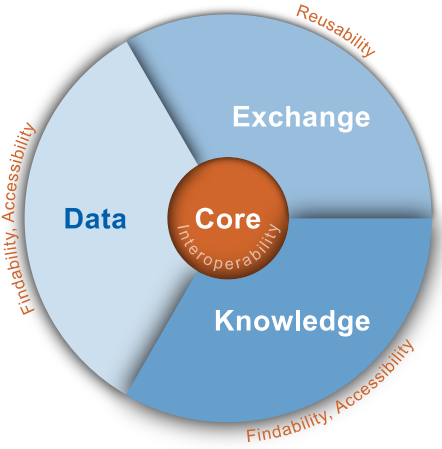
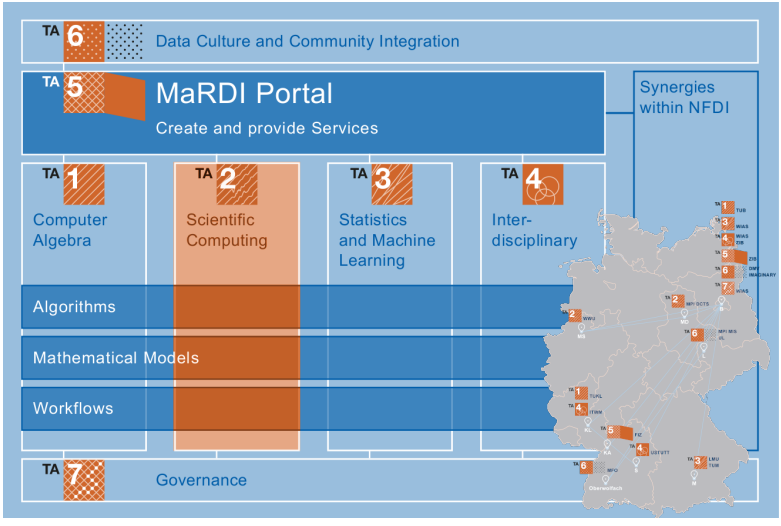
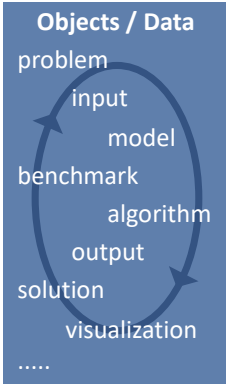



TA 6
Data Culture and Community Integration
TA 5
MaRDI Portal
Create and provide Services
Synergies within NFDI
TA 1
Computer Algebra
TA 2
Scientific Computing
TA 3
Statistics and Machine Learning
TA 4
Inter-disciplinary
Algorithms
Mathematical Models
Workflows
TA 7
Governance



M1 Knowledge Graph of Numerical Algorithms

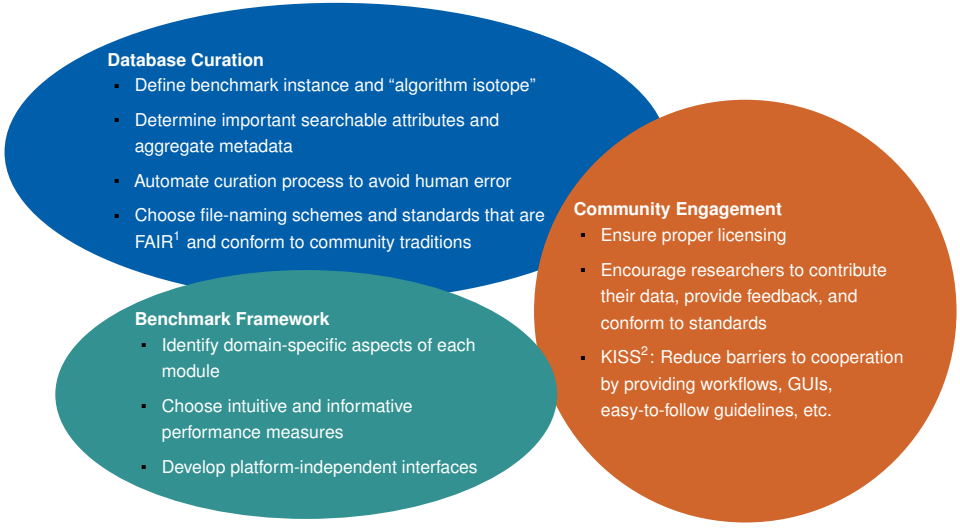
M2 Open Interfaces for Scientific Computing

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

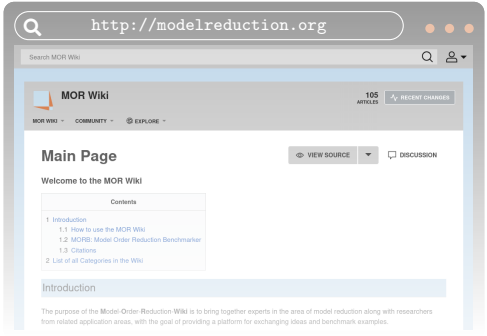


[1] https://www.go-fair.org/fair-principles/ [2] Keep It Simple, Silly https://en.wikipedia.org/wiki/KISS_principle

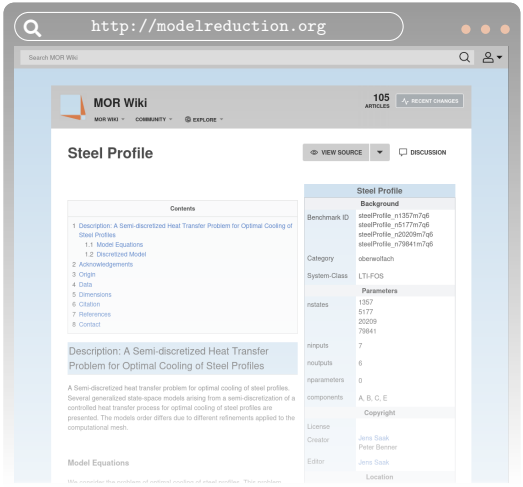
MORWiki: A community platform for curated benchmark collection

- Description of basic MOR methods.
- Collection of curated benchmark examples.
- Detailed description and comparison of available MOR techniques.
- Aggregate MOR literature and BibTeX data.

- Encourage community engagement lowering contribution barrier
- Ensure proper content licensing
- Ensure proper citation and references



- A semi-discretized heat transfer problem for optimal cooling of steel profiles.
- The models order differs due to four different refinements applied to the computational mesh.
- Uses ALBERTA based FEM descretization with P1 elements.
- This benchmark is part of the Oberwolfach Benchmark Collection, #38881.



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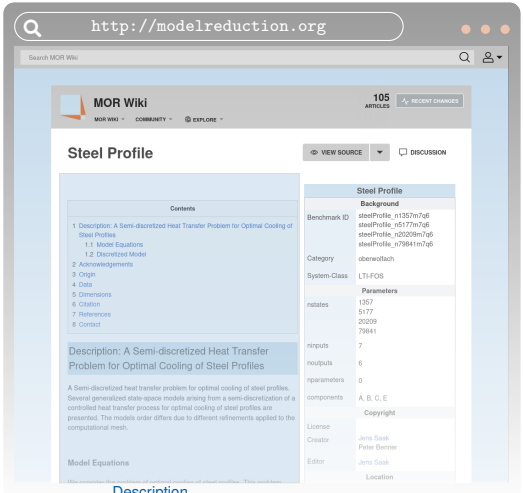

Description

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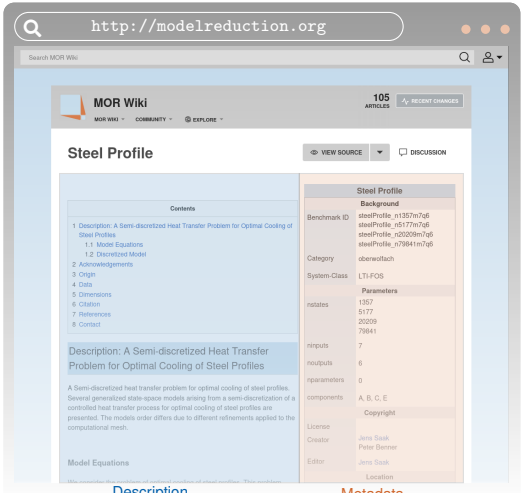
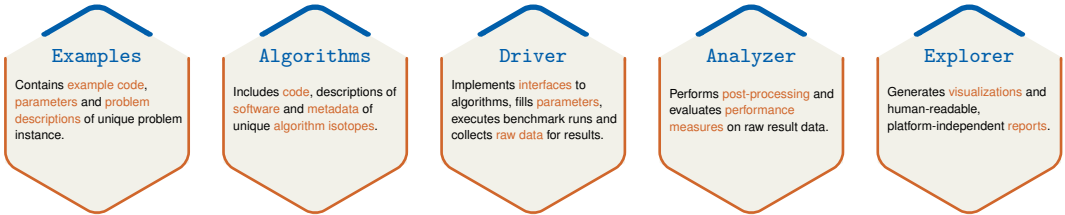


- Generic extensible toolkit specification
- Language agnostic interoperability
- FAIR comparison among different algorithm implementations
- Flexible performance measures
- Versatile visualizations of results

- Connect with Knowledge graphs
- Use open interfaces
- Confirmable workflows
- Integrate into MaRDI portal



A generic, extensible benchmark framework specification

MORB: Model Order Reduction Benchmarker

- A MaRDIMark implementation for Model Order Reduction community.
- Simple proof-of-concept to get feedback.
- Serve as a template for other mathematical communities.
- Focus on Linear Time-Invariant, First-Order Systems (LTI-FOS).

Linear Time-Invariant (LTI) System

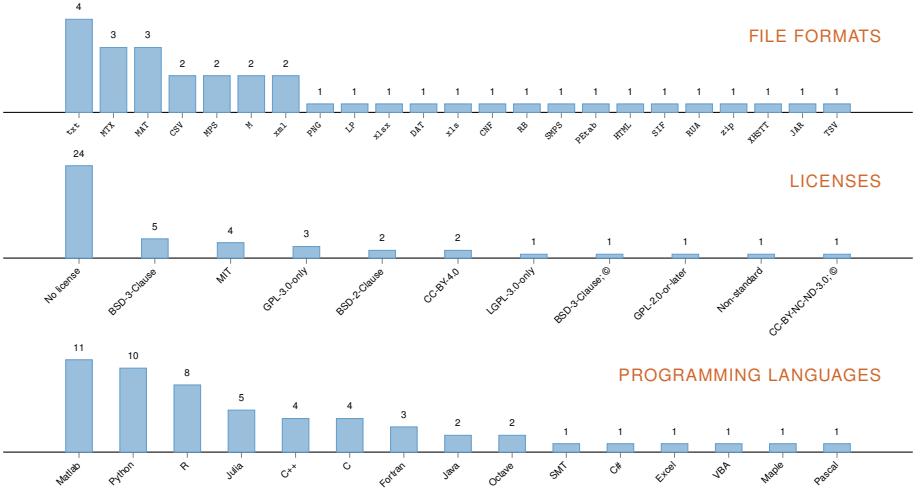
$$\begin{aligned} E\dot{x}(t) &= Ax(t) + Bu(t), \\ y(t) &= Cx(t) + Du(t). \end{aligned} \quad \Leftrightarrow \quad H(s) = C(sE - A)^{-1}B$$

Challenges

- Ensuring benchmark data is encoded uniformly (`.mat`, `v7.3`)
- Calling external software as “black box”-es and without unnecessary overhead
- Distinguish unique implementation of an algorithm (“algorithm isotope”)
- Find subroutines that compute measures (e.g. error, speed etc.) efficiently and accurately.

filename	MORWikiPageName	directory	MORWikiLink	nStates	nInputs	nOutputs	components	nParameters	systemClass	isDAE	daeDiffIndex	isSquare	isStateSpaceSymm	isSysSym	isPassive	isContractive	isStable	nUnstabPoles	isASymm	isAcholAble	isASparse	nnzA	condA
linear1DBeam_n14m1q1	Linear 1D Bear	oberwolfach	https://morwiki.mi	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.mi	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.mi	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.mi	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.mi	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.mi	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.mi	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_n84	Convection Rea	slicot	https://morwiki.mi	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
ornSommerfeld_n100m1q	Orn-Sommerfeld	slicot	https://morwiki.mi	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_n120n2q2	CD Player	slicot	https://morwiki.mi	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.mi	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.mi	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_n256r	Transmission L	slicot	https://morwiki.mi	256	2	2	A, B, C, E	0	LTI-FOS	0	1	1	0	1					1	1	0	256	2.22E+05
iss_n270m3q3	International Sp	slicot	https://morwiki.mi	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.mi	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.mi	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_n396m	Electrostatic Be	oberwolfach	https://morwiki.mi	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.mi	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	slicot	https://morwiki.mi	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.mi	578	9	9	A, B, C, E	0	LTI-FOS	1		1	0				0	290	0	0	1	1694	2.83E+09
earthAtmosphere_n598m	Earth Atmosph	slicot	https://morwiki.mi	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.mi	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.mi	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.mi	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.mi	1412	3	3	A, B, C	0	LTI-FOS	0	0	1	0	0			1	0	0	0	1	2118	7.75E+01
peekInductor_n1434m1q	Peek Inductor	oberwolfach	https://morwiki.mi	1434	1	1	A, B, C, E	0	LTI-FOS	0	0	1	0	1			1	0	1	0	1	16228	1.47E+06
transmissionLines_n1600	Transmission L	misc	https://morwiki.mi	1600	14	14	A, B, C, E	0	LTI-FOS	0	1	1	0	1					0	0	1	5280	Inf
tunableOpticalFilter_n166	Tunable Optica	oberwolfach	https://morwiki.mi	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.mi	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.mi	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.mi	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.mi	4257	1	7	A, B, C, E	3	AP-LTI-FOS	0	1	0	0	0									
micropyrosThruster_n425	Micropyros Thr	oberwolfach	https://morwiki.mi	4257	1	7	A, B, C, E	0	LTI-FOS	0	0	0	0	0			1	0	1	0	1	37465	2.52E+16

Collection and classification of benchmarks


FILE FORMATS
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RB
SMPS
PSz.ab
html
SIF
RUA
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No license
BSD-3-Clause
MIT
GPL-3.0-only
BSD-2-Clause
CC-BY-4.0
LGPL-3.0-only
BSD-3-Clause; ©
GPL-2.0-or-later
Non-standard
CC-BY-NC-ND-3.0; ©
PROGRAMMING LANGUAGES
11
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C#
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VBA
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      "pymor": [
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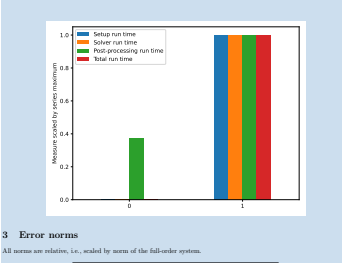
         }
      ]
   }
}
```

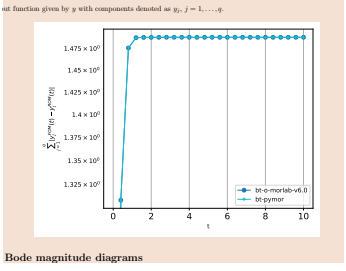
JSON-based readable input files

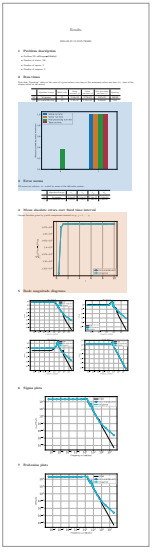
```python
from morb.driver import Benchmark
import morb.analyzer
import morb.explorer.plot
import morb.explorer.report

# Set up problem and algo_isos
prob_id = 'newEngland_n66m1q1'
algo_iso_json = f'configs/{prob_id}.json'

# Run benchmark and compute measures
benchmark = Benchmark(prob_id, algo_iso_json).run()
measures = morb.analyzer.calc_meas(benchmark)

# Generate all plots
morb.explorer.plot.make_all_plots(measures)

# Generate report
morb.explorer.report.make_tex(measures)
```

Python-based easy-to-use interface

- Measures: Timings and Error
- Plots: Error, Bode Plots, Sigma plot and Frobenius plot.
- TEX Report: autogenerated with specifications, simple formatting and system information.
- PDF Report: Easily distributed and viewed.







Closing Remarks

Takeaways

- Ensure content licensing and proper citation culture.
- Lower barriers for contributors.
- Lower turn-around times to reproduce results.

How can you contribute?

- Most MORWiki benchmarks are LTI or parametric LTI — Add more benchmark cases
- Log and improve accessibility to software metadata.
- Clear definitions and distinctions of performance measures.
- Develop FAIR software with a fair comparison and proper credits.

MaRDI TA2 Team

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Stephan Rave

Pavan Veluvali

Peter Benner

Jan Heiland

Maximilian Bindhak

Interplay with other Consortia

FAIRmat