Confirmable Workflows in Computer Algebra

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2025-03-31 Computer Algebra, Number Theory and More
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MaRDI

- **Ma**thematical **R**esearch **D**ata **I**nitiative
- Funded by DFG Project number 460135501
- `https://www.mardi4nfdi.de`
- 7 Task Areas, Task Area 1: Computer Algebra
- Strong focus on reproducibility of computer experiments.
- Whitepaper on data management [Con23].

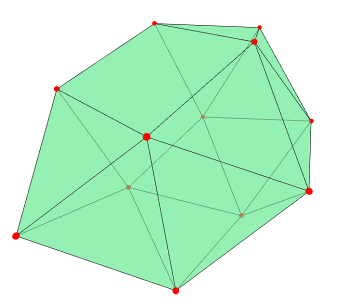
Can I have this data?

full, correspond to those tropical hypersurfaces which are smooth. For the first time, we computed the full triangulations of $3 \cdot \Delta_3$, and these classify the smooth tropical cubics in 3-space [18, §4.5].

Theorem 19. *There are exactly* 21 125 102 *orbits of regular and full triangulations of* $3 \cdot \Delta_3$ *with respect to the natural action of the symmetric group of degree four. Out of these,* 14 373 645 *are unimodular.*

This is the largest experiment that we completed so far. The computation took about four days on the Intel Xeon E5-2630 v2 cluster with 40 threads.

How can I make such a picture?



What is this data?


```
{"_ns":
   {"Oscar":["https://github.com/oscar-system/Oscar.jl","1.4.0-DEV-
         ae6f43fc584f54039ec05dcd40b94c1c3779c412"]},
   "_type":"PermGroup",
   "data":{
      "degree":"17",
      "gens":[
         ["6","15","9","2","4","13","11","1","7","14","8","3","5","12","10"],
         ["16","3","2","5","4","7","6","9","8","11","10","13","12","15","14","1"],
         ["7","13","10","11","12","6","1","14","9","3","4","5","2","8"],
         ["1","3","2","9","7","8","5","6","4","14","13","15","11","10","12","17","16"]
      ]
   },
   "attrs":{},
   "id":"ab806634-cc8b-4be1-b1b6-7016698a7373"
}
```

MaRDI TA1: Computer Algebra

Software and data are part of mathematics. This has consequences for the publication process:

- There should be guidelines on what to do with software and data.
- Software and data should also be reviewed.
- We need data formats and data bases.
- Software is special, since programming languages and dependencies move very fast.

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But why is this an issue?

Reproducibility in Mathematics

Technical reviews at ANTS and LuCaNT

Jeroen Hanselman performed technical reviews of papers at NT conferences [Han25].

Results before review:

	Ran	Correct	Ran and Correct
Pieces of Software	41	35	30
Percentage of Total[2]	69.5%	59.3%	50.8%

Results after review:

	Ran	Correct	Ran and Correct
Pieces of Software	32	29	27
Percentage of Total[4]	91.4%	82.8%	77.1%

Note that these are computational conferences!

Three studies

- Victoria Stodden et al.: **Enabling the Verification of Computational Results: An Empirical Evaluation of Computational Reproducibility** (2018) [SKB18]
  - 306 papers from the Journal of Computational Physics surveyed. More than half of the results were *impossible* to reproduce.

Reproducibility in Mathematics

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- Daniel Mietchen; Sheeba Samuel: **Computational reproducibility of Jupyter notebooks from biomedical publications** (2022) [SM22]
  - Of more than 10 000 Jupyter notebooks from biomedical publications 4 000 selected for an automated reproducibility check. Of these 10% could be rerun, 6% resulted in the recorded results.

FAIR

The FAIR principles

- **Findable** A researcher who does not know about your data, but is working on something related to your data, can **F**ind it.
- **Accessible** A researcher who knows about your data can **A**ccess it, ideally in some standardized way, say web portal.
- **Interoperable** Different systems and applications can **I**nteract with your data, integrating it with other datasets and tools in a meaningful way.
- **Reusable** A researcher can **R**epurpose your data for new analyses or projects, ensuring that your data remains valuable over time.

These principles also affect metadata.

MaRDI TA1: Computer Algebra

What do we contribute?

- Guidelines for RDM. [Con23]
- FAIR file format for computer algebra. [DJL24]
- Predefined software environments. [Kau24]
- Technical reviews. [Han25]

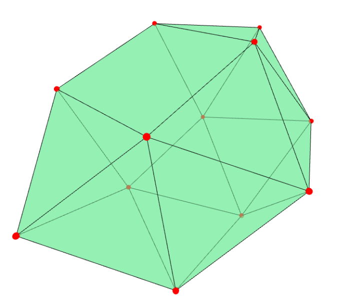
The `mrdi` file format

A FAIR file format

- File format developed in MaRDI for mathematical data. [DJL24]
- Based on JSON.
- First implementation of file format in `OSCAR`.
- Many data types of `OSCAR` (and `Julia`) can already be serialized and deserialized in this format.
- Work in progress for reading this file format in CoCoA, Magma, and Sage.

A Johnson solid

Sphenomegacorona



https://zenodo.org/records/10729583

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MATH+ The Berlin Mathematics Research Center MATH+

Published February 29, 2024 | Version v1

Dataset Open

Exact Johnson Solids

Geiselmann, Zoe[1]; Jordan, Alexej[1]; Joswig, Michael[2]; Sturmfels, Bernd; Panizzut, Marta; Röhrig, Olivia[1]

Show affiliations

This collection contains vertex, facet, and incidence data for each of the 92 Johnson solids. A Johnson solid is a 3-dimensional convex polytope, where each facet is a regular polygon. The latter definition generalizes the Platonic and the Archimedean solids. Here we consider proper Johnson solids only, i.e., we ignore the Platonic and Archimedean solids.

The data can be loaded with the julia package OSCAR, but can also be read elsewhere due to its FAIR file format. The coefficients are described either as rational numbers or as elements of an embedded number field to enable efficient algebraically exact computations. Additionally, the dataset offers approximations of the values as floating point numbers. A sample script for accessing the data from outside of OSCAR is included. Further information can be taken from the README file.

A Johnson solid

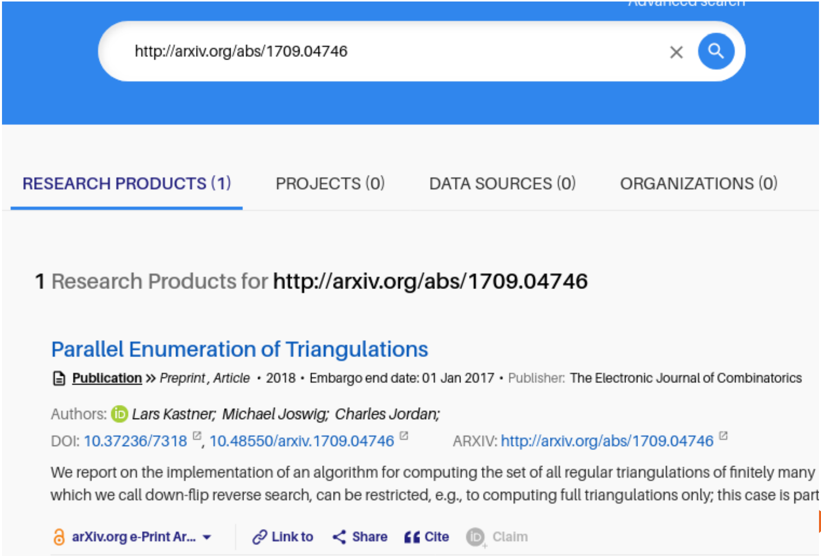
```
{
  "_ns": {
    "Oscar": [
      "https://github.com/oscar-system/Oscar.jl"
            ,
      "1.1.0-DEV-393962
            ae3172ace5e2d4c50ef17cb8ee89828d1e"
    ]
  },
  "_type": {
    "name": "Polyhedron",
    "params": "a65b5810-9f39-4bfe-8e4d-9
          f5bf89e63b3"
  },
  "data": { [...]
        "VERTICES": {
          "name": "MatElem",
          "params": "73744d5a-9d44-49f6-a4d5-
                d9e74803139e"
        }, [...]
    "data": "VERTICES" : [[ ... some coordinates
          ... ]]
  },
```

```
{
  "_refs": { [...]
    "a65b5810-9f39-4bfe-8e4d-9f5bf89e63b3": {
      "_type": "EmbeddedNumField",
      "data": {
        "num_field": "eea1dea1-bd4c-4869-bece-
              bbf412869a55",
        "embedding": "1d972617-9785-4f3d-8769-02
              ecd7fedc25"
      }
    },
    "73744d5a-9d44-49f6-a4d5-d9e74803139e": {
      "_type": "MatSpace",
      "data": {
        "base_ring": "a65b5810-9f39-4bfe-8e4d-9
              f5bf89e63b3",
        "ncols": "4",
        "nrows": "12"
      }
    },
    [...]
```

Zenodo

- Launched in 2013, relaunched in 2015.
- OpenAIRE (Open Access Infrastructure for Research in Europe) indexes Zenodo.
- Operated by CERN.
- Up to 50GB per dataset.
- Provides DOI to dataset and BibTeX export for citation.
- Can integrate github repositories.
- **This is where the metadata magic happens!**

Zenodo and OpenAire



Zenodo and OpenAire

arXiv.org e-Print Ar... View all 3 versions

parallel enumeration of triangulations

Publication » *Preprint*, *Article* • 13 Jul 2018 • Embargo end date: 01 Jan 2017 • Publisher: The Electronic Journal of C

Authors: *Lars Kastner; Michael Joswig; Charles Jordan;*

DOI: 10.37236/7318, 10.48550/arxiv.1709.04746 ARXIV: http://arxiv.org/abs/1709.04746

Summary Subjects Related research (2) Metrics

Abstract
We report on the implementation of an algorithm for computing the set of all regular triangulations of
restricted, e.g., to computing full triangulations only; this case is particularly relevant for tropical geomet
many cores. Our implementation allows to compute the triangulations of much larger point sets than befo

Zenodo and OpenAire

parallel enumeration of triangulations

Summary | Subjects | Related research (2) | Metrics

2 Research Products, Page 1 of 1

Regular full triangulations of the 3-dilated 3-simplex

Research Data • 2024 • Harvested • IsSupplementedBy

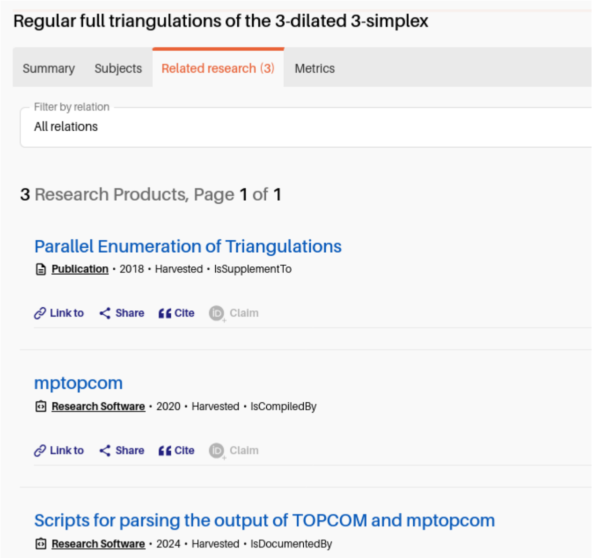
Link to Share Cite Claim

Regular unimodular triangulations of the 3-dilated 3-simplex

Research Data • 2024 • Harvested • IsSupplementedBy

Link to Share Cite Claim

Zenodo and OpenAire



Other repositories and databases

Community databases

- The L-functions and modular forms database
  `https://www.lmfdb.org/`
- Graded Ring Database `http://www.grdb.co.uk/`
- polyDB `https://polydb.org/`
- Mathematical Research Data Repository
  `https://mathrepo.mis.mpg.de/`
- Specially taylored to target audience, i.e. nice web interface, API
- Better findability within specific mathematical community
- Use both Zenodo and specific databse

MaPS

MaRDI packaging system

- Light-weight containerization building on existing Linux tools
- For packaging dependencies of software
- Can be installed via Linux package managers
- Currently used for the technical reviews of LuCaNT
- `https://github.com/aaruni96/maps`

MaPS

MaRDI packaging system

Deploy OSCAR

Once MaPS is running deploy and run OSCAR.

```
$ python src/maps -d org.oscar_system.oscar/x86_64/latest
$ python src/maps -r org.oscar_system.oscar/x86_64/latest
```

This will launch a shell inside the OSCAR runtime. Then simply launch julia inside the runtime.

```
root@runtime:~# julia
```

```
tester@virtbuntu: ~
tester@virtbuntu:~$ sudo apt install maps
[sudo] password for tester:
Reading package lists... Done
Building dependency tree... Done
Reading state information... Done
The following additional packages will be installed:
```

Reproducibility of computer experiments

The OSCAR book

- Consists of 19 chapters.
- Every chapter contains code.
- How can we make sure that the code keeps working?
- How can we guarantee that the output in the book is the same as in OSCAR 1.0?

OscarBookExamples.jl

OscarBookExamples

Build Status

To test some parts of the book please try the following:

Clone this repository, the oscar-book repository and a create a checkout of the Oscar.jl repo on the `backports-release-1.0` branch.

```
$ julia-1.10
               _
   _       _ _(_)_     |  Documentation: https://docs.julialang.org
  (_)     | (_) (_)    |
   _ _   _| |_  __ _   |  Type "?" for help, "]?" for Pkg help.
  | | | | | | |/ _` |  |
  | | |_| | | | (_| |  |  Version 1.10.1 (2024-02-13)
 _/ |\__'_|_|_|\__'_|  |  Official https://julialang.org/ release
|__/                   |
```

OscarBookExamples.jl

- Collects the code from the `OSCAR` book.
- Runs it with the current master of `OSCAR` (other branches are possible).
- Compares output, detects errors.
- Can automatically fix the code in the book.

OscarBookExamples.jl

Oscar.jl / test / book / cornerstones / polyhedral-geometry /

lkastner and benlorenz Add tests of book chapter to CI. (#3588)

Name	Last commit message
..	
auxiliary_code	Add tests of book chapter to CI. (#3588)
D222Computation.jlcon	Add tests of book chapter to CI. (#3588)
Explosion.jlcon	Add tests of book chapter to CI. (#3588)
GKZ_orbits.jlcon	Add tests of book chapter to CI. (#3588)
GT_character.jlcon	Add tests of book chapter to CI. (#3588)
GelfandTsetlinEx.jlcon	Add tests of book chapter to CI. (#3588)
SecondaryPolytope.jlcon	Add tests of book chapter to CI. (#3588)
ch-benchmark.jlcon	Add tests of book chapter to CI. (#3588)
dodecahedron.jlcon	Add tests of book chapter to CI. (#3588)

OscarBookExamples.jl

- 90% of examples give different output than recorded in the book.
- 70% resulted in errors.
- Managed to bring these numbers down to 0 with `OSCAR` 1.0.
- Input is intended to keep working with `OSCAR` 1.x, output allowed to change for ¿1.0.
- Guidelines collected in book chapter [JKL25].

In an ideal world

- Your software comes with a container that packages all dependencies.
- Your data comes with documentation such that any mathematician is able to write a parser.
- Your software, data, and article are all linked by appropriate metadata.
- Reproducing your results happens with by running a single script.

Summary

Rules of thumb

- Upload your software to GitHub
- Upload your data to Zenodo
- Upload your paper to the ArXiv

There are many more details to pay attention to, e.g. licenses, see [Con23].

Summary

Rules of thumb

- Upload your software to GitHub
  - Sign the repo up for tracking by Zenodo
  - Ideally, add CI
- Upload your data to Zenodo
  - Link your GitHub repo
  - Link your ArXiv article
- Upload your paper to the ArXiv
  - Cite your data on Zenodo
  - Cite your GitHub repo or its Zenodo copy

There are many more details to pay attention to, e.g. licenses, see [Con23].

The end

Thank you!

[Con23] The MaRDI Consortium. *Research Data Management Planning in Mathematics*. Oct. 2023. DOI: 10.5281/zenodo.10018246.

[DJL24] Antony Della Vecchia, Michael Joswig, and Benjamin Lorenz. “A FAIR File Format for Mathematical Software”. In: *Mathematical Software – ICMS 2024*. Ed. by Kevin Buzzard et al. Cham: Springer Nature Switzerland, 2024, pp. 234–244.

[Gei+24] Zoe Geiselmann et al. *Exact Johnson Solids*. Zenodo, Mar. 2024. DOI: 10.5281/zenodo.10729583.

[Han25] Jeroen Hanselman. *Guidelines for writing and reviewing software in computer algebra*. 2025. arXiv: 2503.01541 [math.HO].

[JKL25] Michael Joswig, Lars Kastner, and Benjamin Lorenz. “Confirmable Workflows”. In: *The Computer Algebra System OSCAR: Algorithms and Examples*. Ed. by Wolfram Decker et al. Cham: Springer Nature Switzerland, 2025, pp. 473–491. DOI: 10.1007/978-3-031-62127-7_19.

[Kau24] Aaruni Kaushik. “Predefined software environment runtimes as a measure for reproducibility”. English. In: *Mathematical software – ICMS 2024. 8th international conference, Durham, UK, July 22–25, 2024. Proceedings*. Cham: Springer, 2024, pp. 245–253. DOI: 10.1007/978-3-031-64529-7_26.

[Rie+22] Christian Riedel et al. “Including Data Management in Research Culture Increases the Reproducibility of Scientific Results”. In: *GI-Jahrestagung*. 2022.

[SKB18] Victoria Stodden, Matthew S. Krafczyk, and Adhithya Bhaskar. “Enabling the Verification of Computational Results: An Empirical Evaluation of Computational Reproducibility”. In: *Proceedings of the First International Workshop on Practical Reproducible Evaluation of Computer Systems*. P-RECS'18. Tempe, AZ, USA: Association for Computing Machinery, 2018. DOI: 10.1145/3214239.3214242.

[SM22] Sheeba Samuel and Daniel Mietchen. *Computational reproducibility of Jupyter notebooks from biomedical publications*. 2022. arXiv: 2209.04308 [cs.CE].