

Building Software Infrastructure for Research Mathematics

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2024-06-20



Overview

- MaRDI and the FAIR Principles
- Julia and OSCAR
- Serialization and Datasets



The FAIR Guiding Principles for scientific data management and stewardship

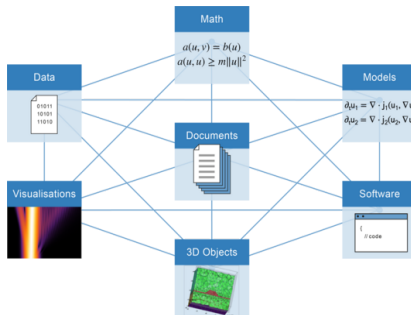
M. Wilkinson et al. 2019

- Findable
- Accessible
- Interoperable
- Reusable



Mathematics Research Data Initiative

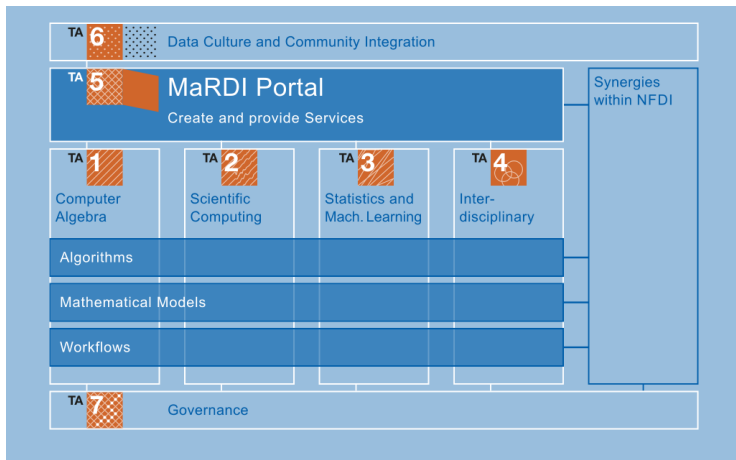
- Develop a mathematical research data infrastructure.
- Set standards for confirmable workflows and certified mathematical research data.
- Provide services to both the mathematical and wider scientific community.



Find the MaRDI proposal here <https://zenodo.org/records/6552436>



MaRDI Task Area Breakdown



Computer Algebra Task Area

Principle Investigators

- Claus Fieker (RPTU Kaiserslautern)
- Michael Joswig (TU Berlin)

On Going Projects

- Confirmable workflows (OSCAR Book) Lars Kastner
- Technical Peer Review (ANTS, LuCANT, MEGA) Jereon Hanselman
- Containerization and environments (MaPS) Aaruni Kaushik
- Serialization and Databases (.mrdr File Format)



Some Key Features of Julia

Reproducibility

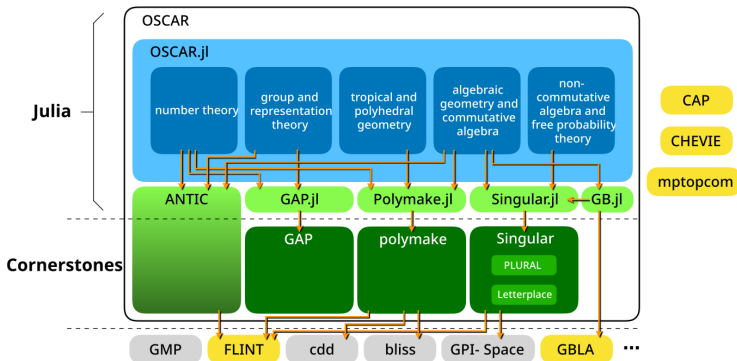
- Built-in package manager.
- Intuitive and user friendly environment functionality.
- Uses git hash when recreating environments.

Interoperability

- Consistent tool for building and wrapping binaries. (Binary builder)
- Excellent Multiple dispatch functionality.



OSCAR



Why Files?

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- Verification of results is at most as computationally expensive.



Serialization

Why Files?

- People often have a preferred software system.
- Computations can be expensive.
- Verification of results is at most as computationally expensive.
- Software changes often.



Storing Mathematical Data

- It's common to have multiple perspectives on an object in mathematics.



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Say we want to store:

$$p = 2y^3z^4 + (a + 3)z^2 + 5ay + 1$$



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Say we want to store:

$$p = 2y^3z^4 + (a + 3)z^2 + 5ay + 1$$

- Some technicalities with the coefficients.
- Is x considered as a coefficient of y ?



History of File Formats

```
* Class:      LP
* Rows:       5
* Columns:    2
* Format:     MPS
*
Name          unnamed#0
ROWS
  N  C0000000
  ...
  G  R0000003
COLUMNS
  x1  C0000000  2      R0000000  1
  x1  R0000001 -1      R0000002  1
  x2  C0000000  3      R0000002  1
  x2  R0000003 -1
RHS
  B  C0000000 -1      R0000000 -1
  B  R0000001 -1      R0000002 -1
  B  R0000003 -1
BOUNDS
FR BND      x1
FR BND      x2
ENDATA
```

- The LP file format and the MPS file format. IBM [1970s] (industry standards)
- Mathematica Notebooks. Wolfram Mathematica [1988]
- OpenMath (tree structure). Mike Dewar [2000]
- IPython 0.12 Interactive Browser Notebooks (Jupyter) [2011]
- polymake File Format. E. Gawrilow, S. Hampe, and M. Joswig [2016]



The Polymake File Format

```
<?xml version="1.0" encoding="utf-8"?>
<?pm chk="56e977e8"?>
<object name="square" type="polytope::Polytope<Rational>;"
  version="3.0"
  xmlns="http://www.math.tu-berlin.de/polymake/#3">
  <description><![CDATA[cube of dimension 2]]></description>
  <property name="VERTICES">
    <m>
      <v>1 0 0</v>
      ...
    </m>
  </property>
  <property name="FACETS"
    type="SparseMatrix<Rational,NonSymmetric>";>
    <m cols="3">
      <v> <e i="1">1</e> </v>
      ...
    </m>
  </property>
  <property name="LINEALITY_SPACE"><m /></property>
  <property name="BOUNDED" value="true" />
  <property name="N_FACETS" value="4" />
  <property name="N_VERTICES" value="4" />
  <property name="VOLUME" value="1/9" />
  <property name="TRIANGULATION">
    <object name="unnamed#0">
      <property name="FACETS">
        <m>
          <v>0 1 2</v>
          <v>1 2 3</v>
        </m>
      </property>
      <property name="F_VECTOR">
        <v>4 5 2</v>
      </property>
    </object>
  </property>
</object>
```

- First version (XML) published in 2016.



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  },
  "VERTICES": [[["1", "0", "0"],
                 ["1", "1/3", "0"],
                 ["1", "0", "1/3"],
                 ["1", "1/3", "1/3"]],
  "CONE_AMBIENT_DIM": 3,
  "N_VERTICES": 4,
  "_ns": {
    "polymake": [
      "https://polymake.org",
      "4.9"
    ]
  },
  "_info": {
    "description": "cube of dimension 2"
  },
  "TRIANGULATION": [{
    "FACETS": [[["0", "1", 2],
                 ["1", 2, 3]],
    "_id": "unnamed#0",
    "F_VECTOR": [4, 5, 2]
  }],
  "N_FACETS": 4,
  "_id": "square",
  "BOUNDED": true,
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- Older formats will be upgraded on load.



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      "https://polymake.org",
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    ]
  },
  "_info": {
    "description": "cube of dimension 2"
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The `mrdi` File Format

2024, joint work with Michael Joswig and Benjamin Lorenz

- JSON based file format.
- Similar to `polymake` format but generalizes to include algebraic data.
- Uses namespaces for semantic separation.
- Uses references stored with UUIDs.
- Prototype developed using `OSCAR`.



Demo

```
julia> using Oscar

julia> F = GF(7)
Prime field of characteristic 7

julia> L, a = finite_field(x^2 + 1)
(Finite field of degree 2 and characteristic 7, o)

julia> Lyz, (y, z) = L[:y, :z]
(Multivariate polynomial ring in 2 variables over L, FqMPolyRingElem[y, z])

julia> p = 2 * z^4 * y^3 + (a + 3) * z^2 + 5 * a * y + 1
2*y^3*z^4 + 5*o*y + (o + 3)*z^2 + 1

julia> q = z^2 + 3 * y
3*y + z^2

julia> save("p.mrdi", p)

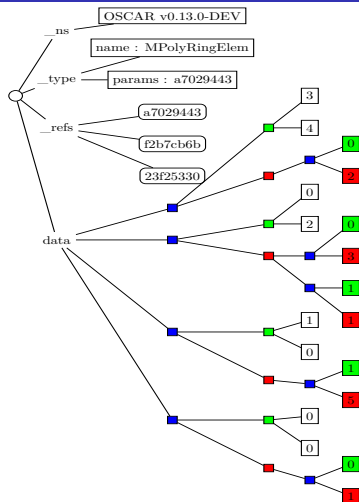
julia> save("q.mrdi", q)

julia> Oscar.reset_global_serializer_state()
Dict{Base.UUID, Any}{}

julia> load("p.mrdi") * load("q.mrdi")
6*y^4*z^4 + 2*y^3*z^6 + o*y^2 + (o + 2)*y*z^2 + 3*y + (o + 3)*z^4 + z^2
```



Tree Structure



$$2y^3z^4$$

$$(a + 3)z^2$$

$$5ay$$

$$1$$



Example File Serialized with OSCAR

```
{
  "_ns": { "Oscar": [ "https://github.com/oscar-system/Oscar.jl", "1.0.0" ] },
  "_type": {
    "name": "MPolyRingElem",
    "params": "869a359a-43d3-43f4-9821-0af9346be019"
  },
  "data": [[["3", "4"], [{"0", "2"}]],
    [{"0", "2"}, [{"0", "3"}, ["1", "1"]]],
    [{"1", "0"}, [{"1", "5"}]],
    [{"0", "0"}, [{"0", "1"}]],
  "_refs": {
    "152ac7bd-e85a-4b36-acc2-743ade2cad4f": {
      "data": { "base_ring": { "data": "7", "_type": "FqField"},
        "symbols": ["x"] },
      "_type": "PolyRing"
    },
    "869a359a-43d3-43f4-9821-0af9346be019": {
      "data": {
        "base_ring": "a8309b96-caec-443c-bedb-e23bb0634c14",
        "symbols": [ "y", "z" ]
      },
      "_type": "MPolyRing" },
    "a8309b96-caec-443c-bedb-e23bb0634c14": {
      "data": {
        "def_pol": {
          "data": [{"0", "1"}, ["2", "1"]],
          "_type": {
            "name": "PolyRingElem",
            "params": "152ac7bd-e85a-4b36-acc2-743ade2cad4f"
          }
        }
      },
      "_type": "FqField"
    }
  }
}
```



Parallelization

```
channels = Oscar.params_channels(Union{Ring, MatSpace})

Qx, x = QQ["x"]
F, a = number_field(x^2 + x + 1)
MR = matrix_space(F, 2, 2)

Oscar.put_params(channels, Qx)
Oscar.put_params(channels, F)
Oscar.put_params(channels, MR)

c = [MR([a^i F(1); a a + 1]) for i in 1:5]
dets = pmap(det, c)
total = reduce(*, dets)
```



Beyond OSCAR (within Julia)

```
struct LabelledPolynomial
    p::MPolyRingElem
    l::String
end

function save_object(s::SerializerState, l_p::LabelledPolynomial)
    save_data_dict(s) do _
        save_typed_object(s, LabelledPolynomial.p, :poly)
        save_object(s, LabelledPolynomial.l, :label)
    end
end

function load_object(s::DeserializerState)
    p = load_typed_object(s, :poly)
    l = load_object(s, String, :label)

    return LabelledPolynomial(p, l)
end
```



Beyond OSCAR (beyond Julia)

Other Implementations

- Magma
- Sage
- CoCoA
- Lean



Johnson Solids

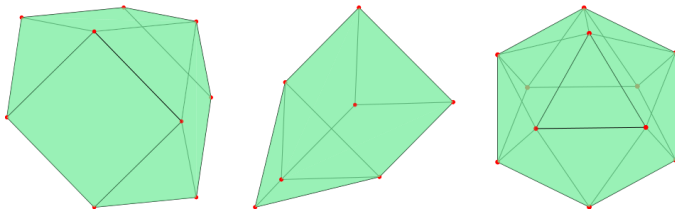


Fig. 4. (a) Triangular cupola, (b) elongated triangular pyramid, (c) gyroelongated pentagonal pyramid

```
> jq '.data.float.VERTICES | length' j3
9
> jq '.data.float.VERTICES | length' j7
7
> jq '.data.float.VERTICES | length' j11
11
```

<https://zenodo.org/records/10729583>



Other datasets

- Surfaces in \mathbb{P}^4
- QSM Models in F-theory
- Small Phylogenetic Tree Website (ongoing work)
- ...



Schema



- A schema defines a structure for data.

Figure: <https://www.pexels.com/photo/plastic-shape-sorter-toy-11030155/>



Schema



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- Schema languages. (RELAX NG [2002], JSON Schema [2022])



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- Is possible to define recursive structure.



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- Schemata allow data to be validated before loading.
- Adds structure to document based databases.
- PolyDB, Paffenholz [2017]



You can find more information here



<https://arxiv.org/abs/2309.00465>

Thank You!

