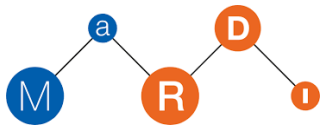
A FAIR File Format

Antony Della Vecchia

Technische Universität Berlin

2023-03-14



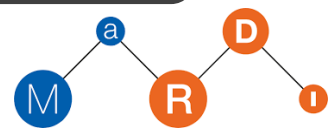
The MaRDI Computer Algebra Team

TU Berlin

- Antony Della Vecchia – data formats
- Michael Joswig
- Lars Kastner – guidelines for reproducibility

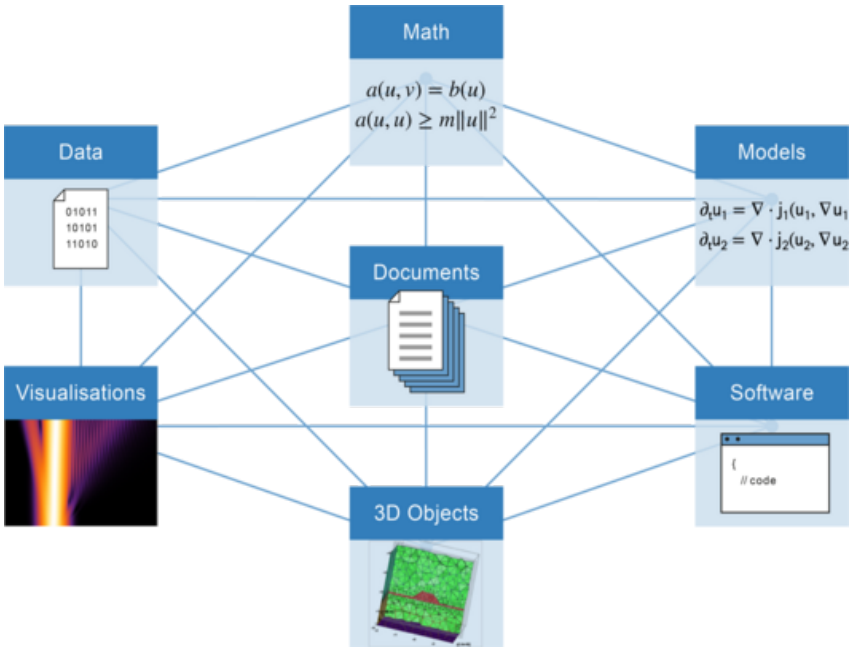
TU Kaiserslautern

- Wolfram Decker
- Claus Fieker
- Jeroen Hanselman – technical peer review
- Max Horn



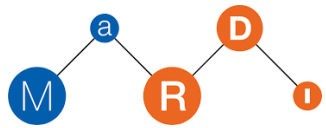
Building an Infrastructure

- 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.



Why Files?

- People often have a preferred software system.



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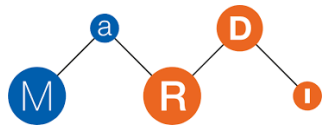

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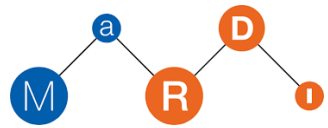

Why Files?

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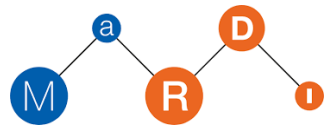
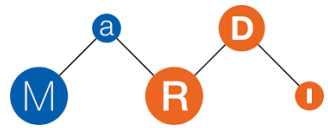
- Computations can be expensive.
- Verification of results is at most as computationally expensive.
- Software changes often.



Storing Mathematical Data

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



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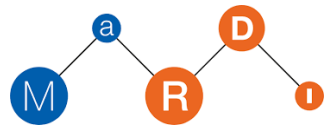

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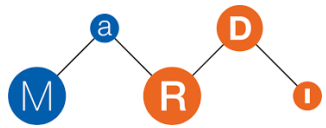
$$p(x, y, z) = xy - z^2$$



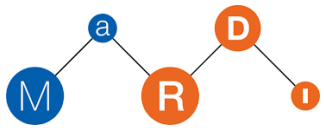
Storing Mathematical Data

- It's common to have multiple perspectives on an object in mathematics.
- While storing mathematical data a choice of perspective must me made.

Say we want to store:

$$p(x, y, z) = xy - z^2$$

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

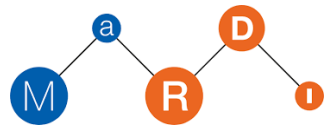


Storing LPs

```
MINIMIZE
  obj: +2 x1 +3 x2 +1
Subject To
  ie0: +1 x1 >= -1
  ie1: -1 x1 >= -1
  ie2: +1 x2 >= -1
  ie3: -1 x2 >= -1
BOUNDS
  x1 free
  x2 free
END
```

```
* 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
    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
```

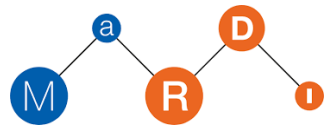
- LPs heavily used in industry.
- Industry natural define standards.
- The LP file format, the MPS file format.



The Polymake File Format

```
<?xml version="1.0" encoding="utf-8"?>
<?pm chk="56e977e8"?>
<object name="square" type="polytope::Polytope&lt;Rational&gt;"
        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&lt;Rational,NonSymmetric&gt;">
    <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.



The Polymake File Format


```
{
  "_attrs": {
    "FACETS": {
      "_type": "SparseMatrix<Rational, NonSymmetric>"
    }
  },
  "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,
  "FACETS": [{ "1": "1" }, { "0": "1/3", "1": "-1"},
             { "2": "1" }, { "0": "1/3", "2": "-1" },
             {     "cols": 3    }],
  "_type": "polytope::Polytope<Rational>",
  "VOLUME": "1/9"
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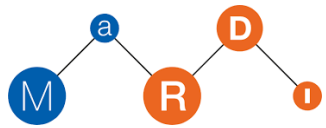
- Currently using JSON.



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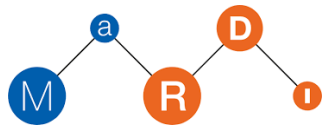

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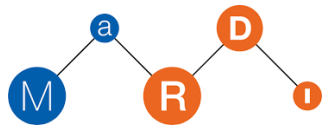
- Extensible, tree structure.



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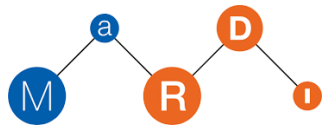
- Extensible, tree structure.
- Has a Schema.



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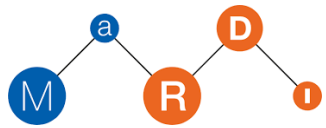

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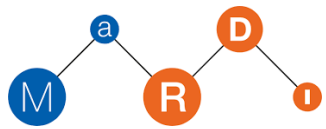
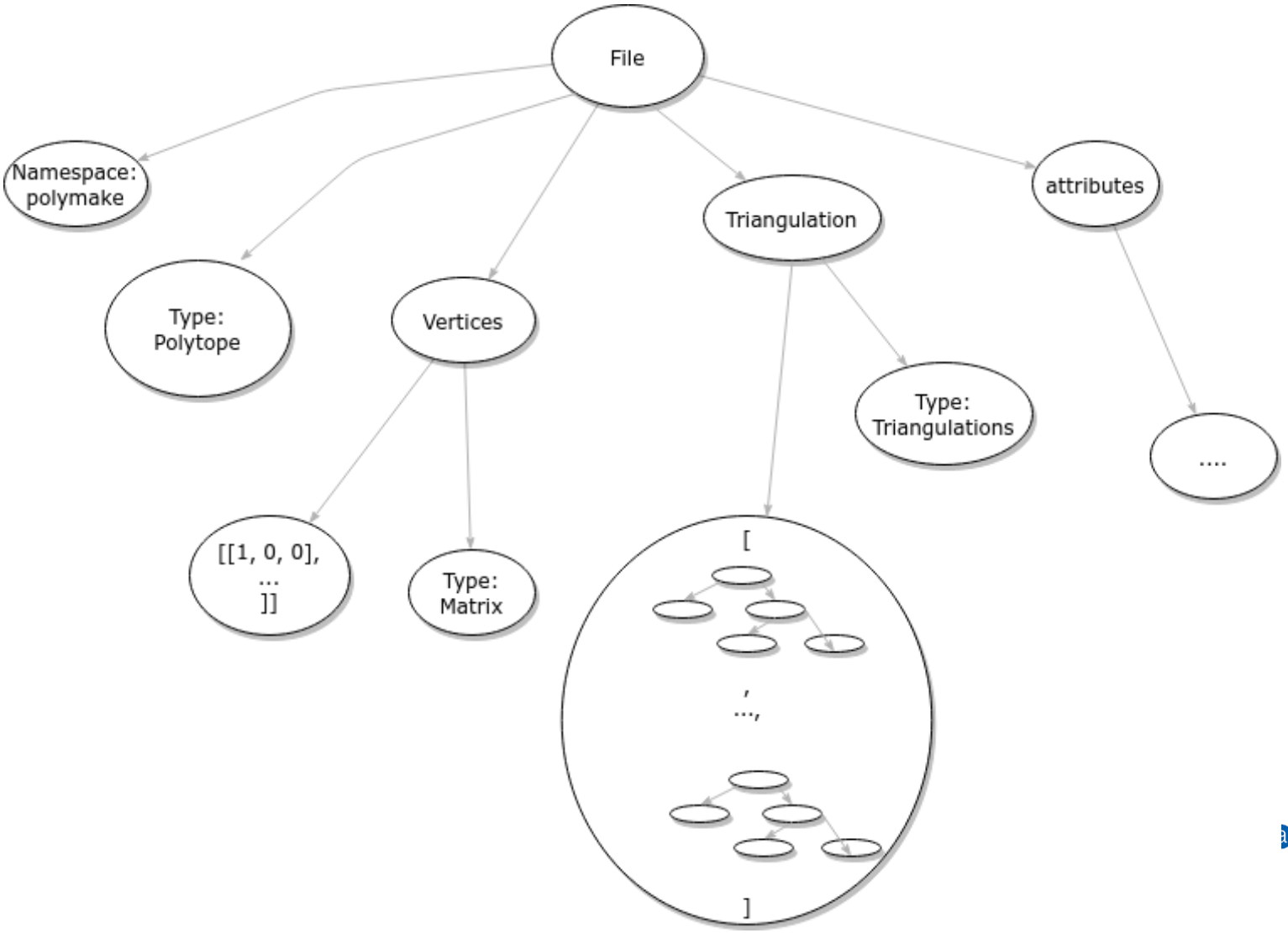
- Extensible, tree structure.
- Has a Schema.
- Older formats will be upgraded on load.
- Can be loaded into OSCAR and SAGE.

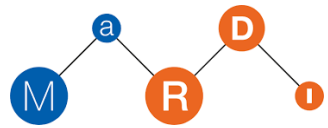


Tree Structure



Schemata

- A schema defines a general structure for data so that it can be interpreted by software.



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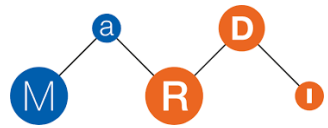

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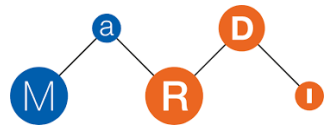
- Is possible to define recursive structure.



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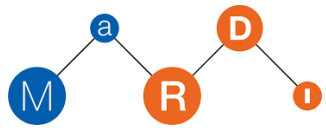

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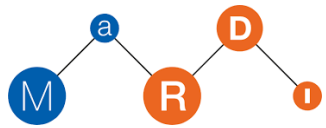
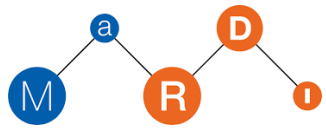
- Can be generated from software.
- Schemata allow data to be validated without being read into software.



Schemata

- A schema defines a general structure for data so that it can be interpreted by software.
- Schema languages.
- Is possible to define recursive structure.
- Can be generated from software.
- Schemata allow data to be validated without being read into software.
- Adds structure to document based databases.



On Going Work


```
{
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    "Oscar": [ ...
    ]
  },
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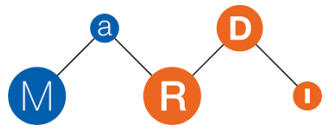
  "data": {
    "terms": [
      {
        "coeff": "1",
        "exponent": {
          "type": "Vector",
          "data": {
            "vector": [ "1", "1", "0" ],
            "entry_type": "Base.Int"
          }
        }
      },
      {
        "coeff": "-1",
        "exponent": {
          "type": "Vector",
          "data": {
            "vector": [ "0", "0", "2" ],
            "entry_type": "Base.Int"
          }
        }
      }
    ],
    "parent": {
      "type": "QQMPolyRing",
      "data": {
        "base_ring": { "type": "QQField"     },
        "symbols": {
          "type": "Vector",
          "data": {
            "vector": [ "x", "y", "z" ],
            "entry_type": "Symbol"
          }
        }
      }
    }
  }
}
```


- Prototyping in OSCAR.



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{
  "_ns": {
    "Oscar": [ ...
    ]
  },
  "type": "QQMPolyRingElem",
  "data": {
    "terms": [
      {
        "coeff": "1",
        "exponent": {
          "type": "Vector",
          "data": {
            "vector": [ "1", "1", "0" ],
            "entry_type": "Base.Int"
          }
        }
      },
      {
        "coeff": "-1",
        "exponent": {
          "type": "Vector",
          "data": {
            "vector": [ "0", "0", "2" ],
            "entry_type": "Base.Int"
          }
        }
      }
    ],
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      "type": "QQMPolyRing",
      "data": {
        "base_ring": { "type": "QQField"     },
        "symbols": {
          "type": "Vector",
          "data": {
            "vector": [ "x", "y", "z" ],
            "entry_type": "Symbol"
          }
        }
      }
    }
  }
}
```
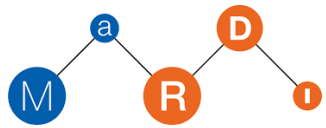


- Prototyping in OSCAR.
- Aim to be software independant.



On Going Work


```
{
  "_ns": {
    "Oscar": [ ...
    ]
  },
  "type": "QQMPolyRingElem",
  "data": {
    "terms": [
      {
        "coeff": "1",
        "exponent": {
          "type": "Vector",
          "data": {
            "vector": [ "1", "1", "0" ],
            "entry_type": "Base.Int"
          }
        }
      },
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        "coeff": "-1",
        "exponent": {
          "type": "Vector",
          "data": {
            "vector": [ "0", "0", "2" ],
            "entry_type": "Base.Int"
          }
        }
      }
    ],
    "parent": {
      "type": "QQMPolyRing",
      "data": {
        "base_ring": { "type": "QQField"     },
        "symbols": {
          "type": "Vector",
          "data": {
            "vector": [ "x", "y", "z" ],
            "entry_type": "Symbol"
          }
        }
      }
    }
  }
}
```
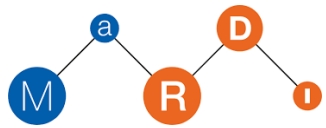


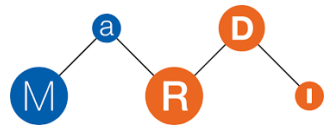
- Prototyping in OSCAR.
- Aim to be software independant.
- Functionality for storing most types in OSCAR.



On Going Work

```
{
  "_ns": {
    "Oscar": [ ...
    ]
  },
  "type": "QQMPolyRingElem",
  "data": {
    "terms": [
      {
        "coeff": "1",
        "exponent": {
          "type": "Vector",
          "data": {
            "vector": [ "1", "1", "0" ],
            "entry_type": "Base.Int"
          }
        }
      },
      {
        "coeff": "-1",
        "exponent": {
          "type": "Vector",
          "data": {
            "vector": [ "0", "0", "2" ],
            "entry_type": "Base.Int"
          }
        }
      }
    ],
    "parent": {
      "type": "QQMPolyRing",
      "data": {
        "base_ring": { "type": "QQField"     },
        "symbols": {
          "type": "Vector",
          "data": {
            "vector": [ "x", "y", "z" ],
            "entry_type": "Symbol"
          }
        }
      }
    }
  }
}
```

- Prototyping in OSCAR.
- Aim to be software independant.
- Functionality for storing most types in OSCAR.
- Julia package for small databases.



References

Thank You!

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