XDMF and ParaView: checkpointing format

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21. March 2018

Content

The problem of double data

If we want to save our computation for checkpointing + visualisation:

```
1  import dolfin as d
2  mesh = d.UnitSquareMesh(3, 3)
3  V = d.FunctionSpace(mesh, "CG", 1)
4  u = d.Function(V)
5
6  # Save for vizualization
7  with d.XDMFFile("viz_file.xdmf") as outfile:
8      outfile.write(u)
9
10 # Save for reading back
11 with d.HDF5File("read_file.h5") as outfile:
12     outfile.write(u, "name")
```

The problem of double data

`XDMFFile.write()`

- values at vertices are saved
- could be visualised in ParaView
- could NOT be read back to DOLFIN
- produces (binary) *.h5 and (xml) *.xdmf

`HDF5File.write()`

- values of degrees of freedom and dofmap is saved
- could NOT be visualised in ParaView
- could be read back to DOLFIN
- produces (binary) *.h5

Who are we?

FEniCS users!

What do we want?

Checkpoint and visualise the same file!

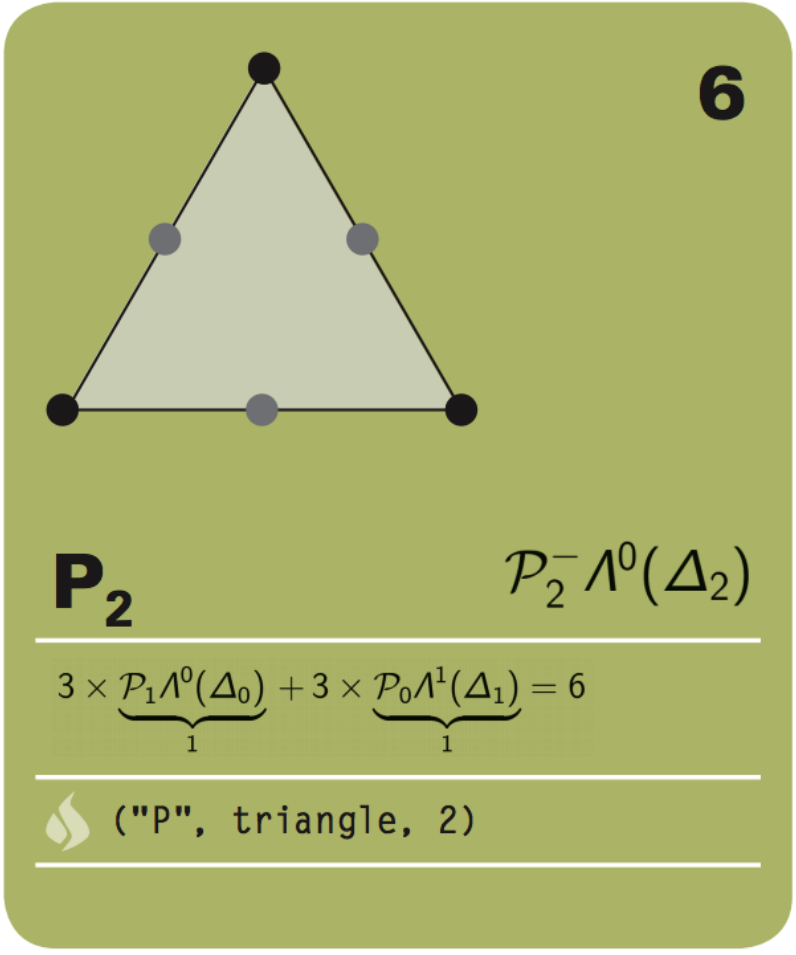
What is a (FEM) function in DOLFIN?

```
1  class dolfin::Function
2  {
3  ...
4  // The function space
5  std::shared_ptr<const FunctionSpace> _function_space;
6  // The vector of expansion coefficients (local)
7  std::shared_ptr<GenericVector> _vector;
8  ...
9  }
```

$$u_h = \sum_{i=1}^{n} U_i \phi_i$$

Periodic table of FEM, meaning of DOFs

- FEniCS mostly used for **iso-** and **super-parametric** ”elements”



FIAT: FInite element Automatic Tabulator

The FInite element Automatic Tabulator FIAT supports generation instances of the Lagrange elements on lines, triangles, and tetrah generating arbitrary order instances of Jacobi-type quadrature rul shapes. Further, H(div) and H(curl) conforming finite element spac Raviart-Thomas, Brezzi-Douglas-Marini and Nedelec are supporte tetrahedra. Upcoming versions will also support Hermite and nonc

FIAT is part of the FEniCS Project.

For more information, visit http://www.fenicsproject.org

Documentation

Documentation can be viewed at http://fenics-fiat.readthedocs.or

docs passing

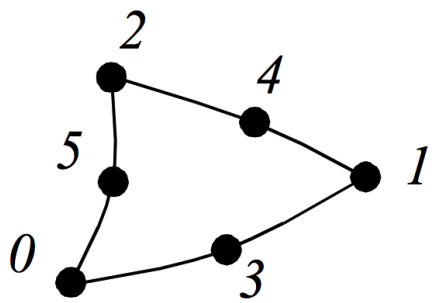
Automated Testing

We use Bitbucket Pipelines and Atlassian Bamboo to perform autc

Builds Passing Bamboo Build Status

How is (FEM) function represented in VTK?

- specification in `www.vtk.org/VTK/img/file-formats.pdf` and `https://www.kitware.com/products/books/VTKTextbook.pdf`
- VTK ONLY for **iso-parametric** ”elements”



`VTK_QUADRATIC_TRIANGLE (=22)`

```
/**
 * @class   vtkBiQuadraticTriangle
 * @brief   cell represents a parabolic,
 *
 * vtkBiQuadraticTriangle is a concrete
 * represent a two-dimensional, 7-node,
 * interpolation is the standard finite
 * shape function. The cell includes thr
 * triangle vertices and a center node.
 * point ids (0-2,3-6) where id #3 is th
 * (0,1); id #4 is the midedge node betw
 * midedge node between points (2,0). id
```

How is data (function) represented in XDMF?

- specification at `http://www.xdmf.org/index.php/XDMF_Model_and_Format`
- library at `https://gitlab.kitware.com/xdmf/xdmf`
- almost the same as VTK
- XDMF = better structured, XML wrapped VTK

Motivation, what users complained about?

The problem, technically speaking

Solution

Examples

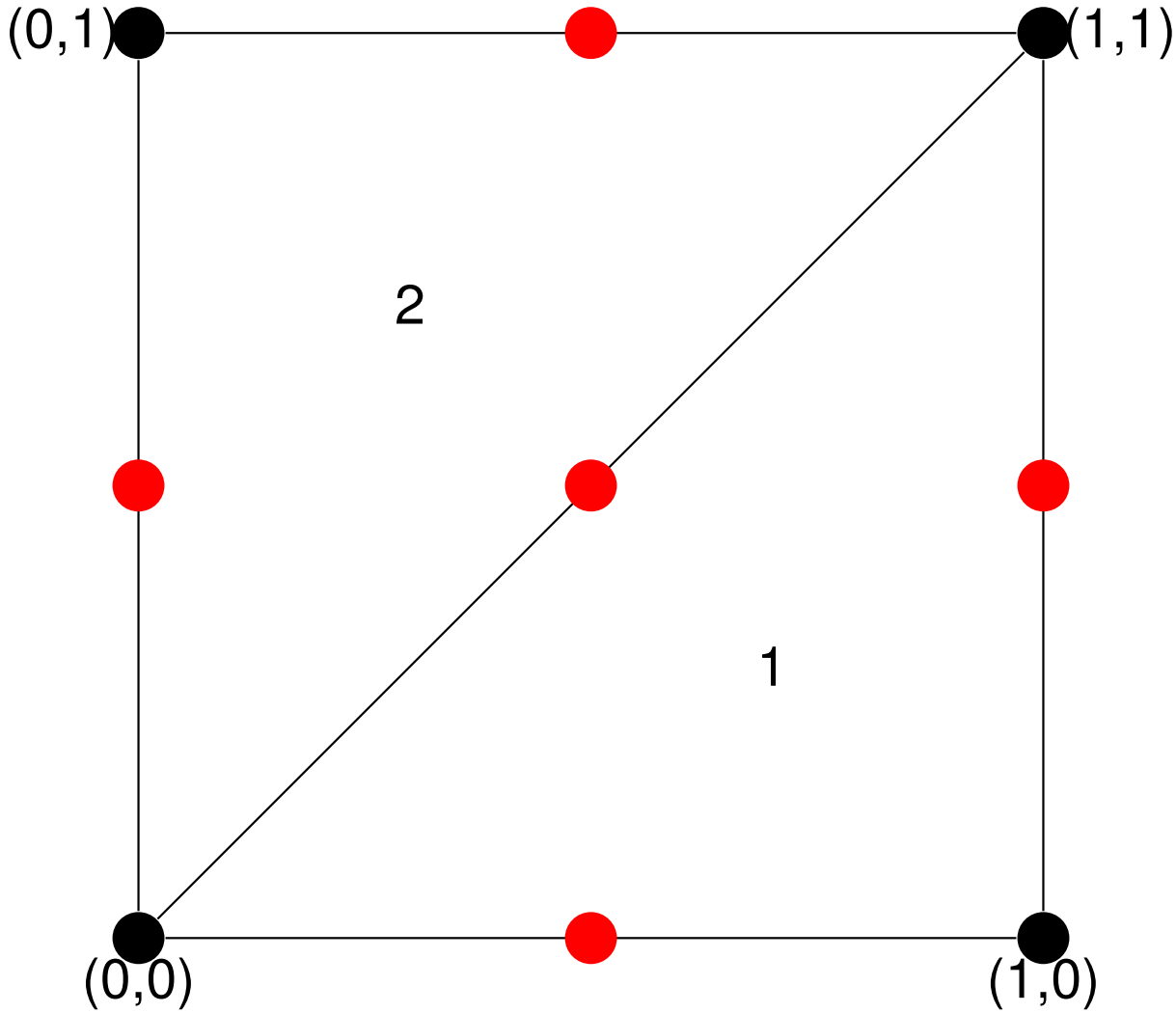
Summary and future work

NEW ”FiniteElementFunction” in XDMF

```
<Attribute
    ItemType="FiniteElementFunction"
    ElementFamily="CG"
    ElementDegree="1"
    ElementCell="triangle"
    Name="u"
    Center="Other"
    AttributeType="Scalar">

    <DataItem Dimensions="8 3"
        NumberType="UInt" Format="XML">
        <!-- Cell-wise degrees of freedom map -->
    </DataItem>

    <DataItem Dimensions="9 1"
        NumberType="Float" Format="XML">
        <!-- Expansion coefficients / values of degrees of freedom -->
    </DataItem>
</Attribute>
```

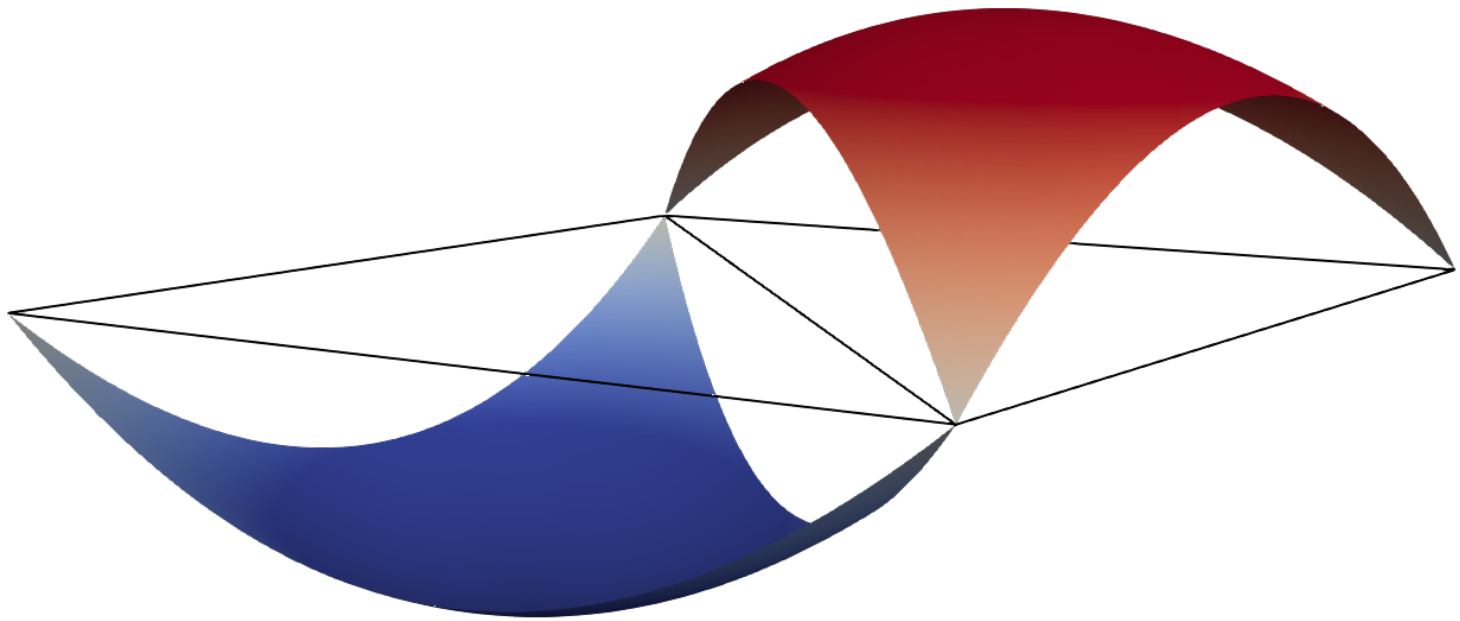

(0,1)
(1,1)
2
1
(0,0)
(1,0)

```
<Attribute ItemType="FiniteElementFunction"
    ElementFamily="DG" ElementDegree="2"
    ElementCell="triangle" Name="u"
    Center="Other" AttributeType="Scalar">

    <DataItem Dimensions="2 6"
        NumberType="UInt" Format="XML">
    1 0 2 3 4 5
    7 6 8 9 10 11
    </DataItem>

    <DataItem Dimensions="2 6"
        NumberType="Float" Format="XML">
    0.0 0.0 0.0 0.2 0.2 0.2
    0.0 0.0 0.0 -0.2 -0.2 -0.2
    </DataItem>
</Attribute>
```

ParaView

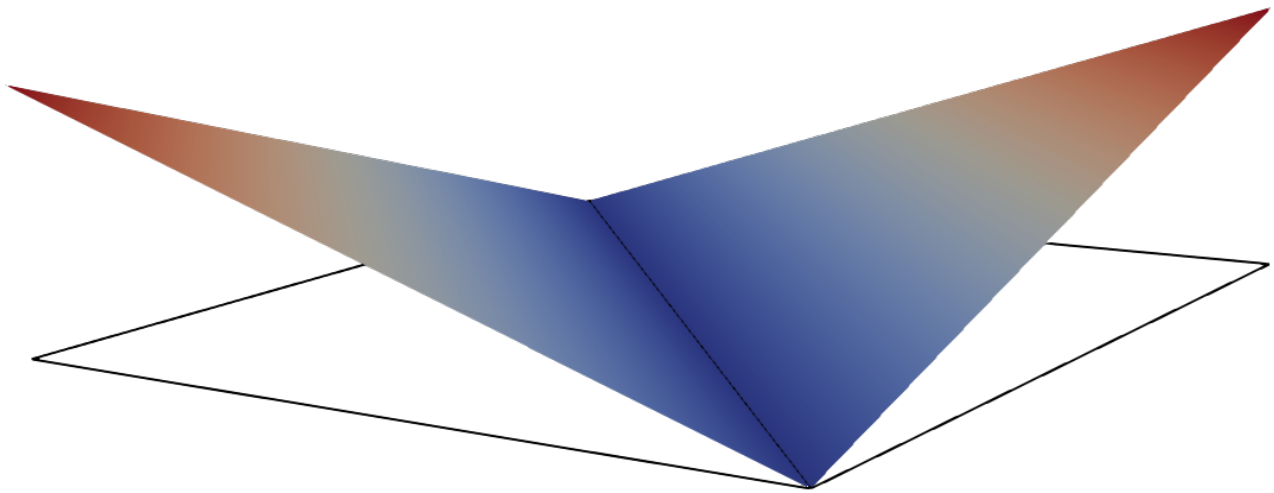


```
<Attribute ItemType="FiniteElementFunction"
    ElementFamily="CG" ElementDegree="5"
    ElementCell="triangle" Name="u"
    Center="Other" AttributeType="Scalar">

    <DataItem Dimensions="2 21"
        NumberType="UInt" Format="XML">
    1 21 2 ...
    1 0 2 ...
    </DataItem>

    <DataItem Dimensions="2 18"
        NumberType="Float" Format="XML">
    0.2 0.0 0.0 ...
    x x 0.2 ...
    </DataItem>
</Attribute>
```

ParaView



Methods for new functionality

- in DOLFIN $\geq$ 2017.2.0 new functionality exposed in *XDMFFile.write_checkpoint()* and *XDMFFile.read_checkpoint()*
- release candidate ParaView $\geq$ 5.5.0

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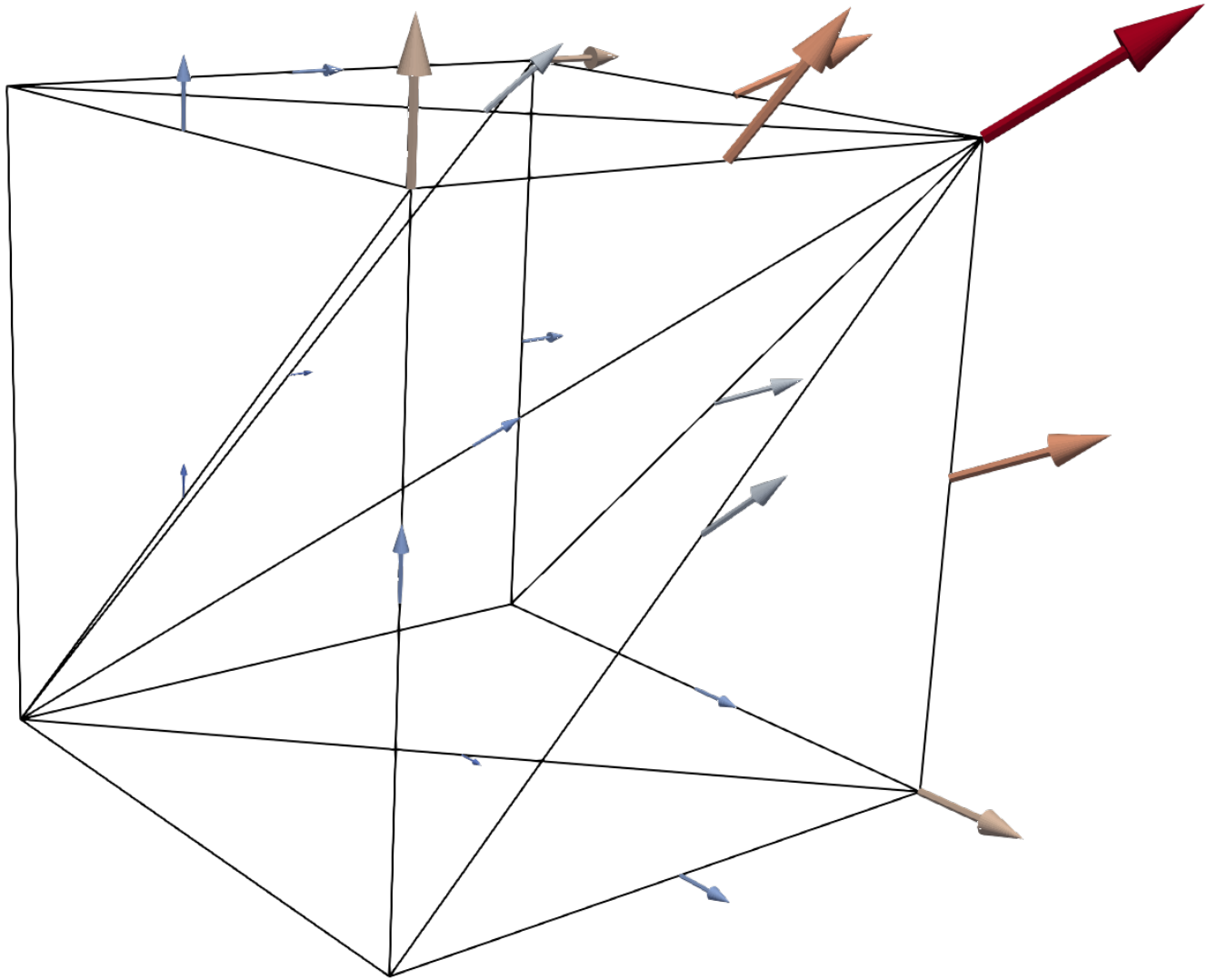
Summary and future work

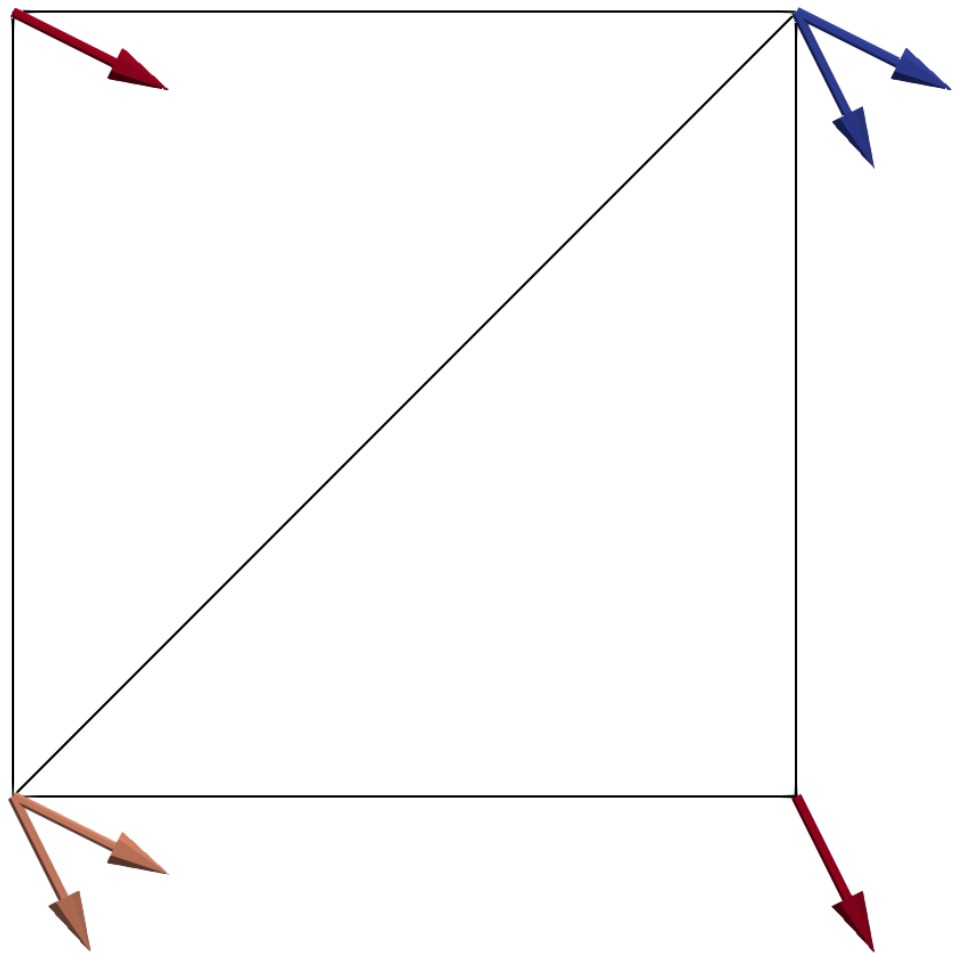

```
1  import dolfin as d
2
3  mesh = d.UnitCubeMesh(1, 1, 1)
4  V = d.VectorFunctionSpace(mesh, "CG", 2)
5
6  u = d.interpolate(d.Expression(
7      ("x[0]*x[1]",
8       "x[1]*x[2]",
9       "x[2]*x[0]"), degree=2), V)
10
11 with d.XDMFFile("ex2_vcg2_3d.xdmf") as outfile:
12     outfile.write_checkpoint(u, "u")
```

ParaView



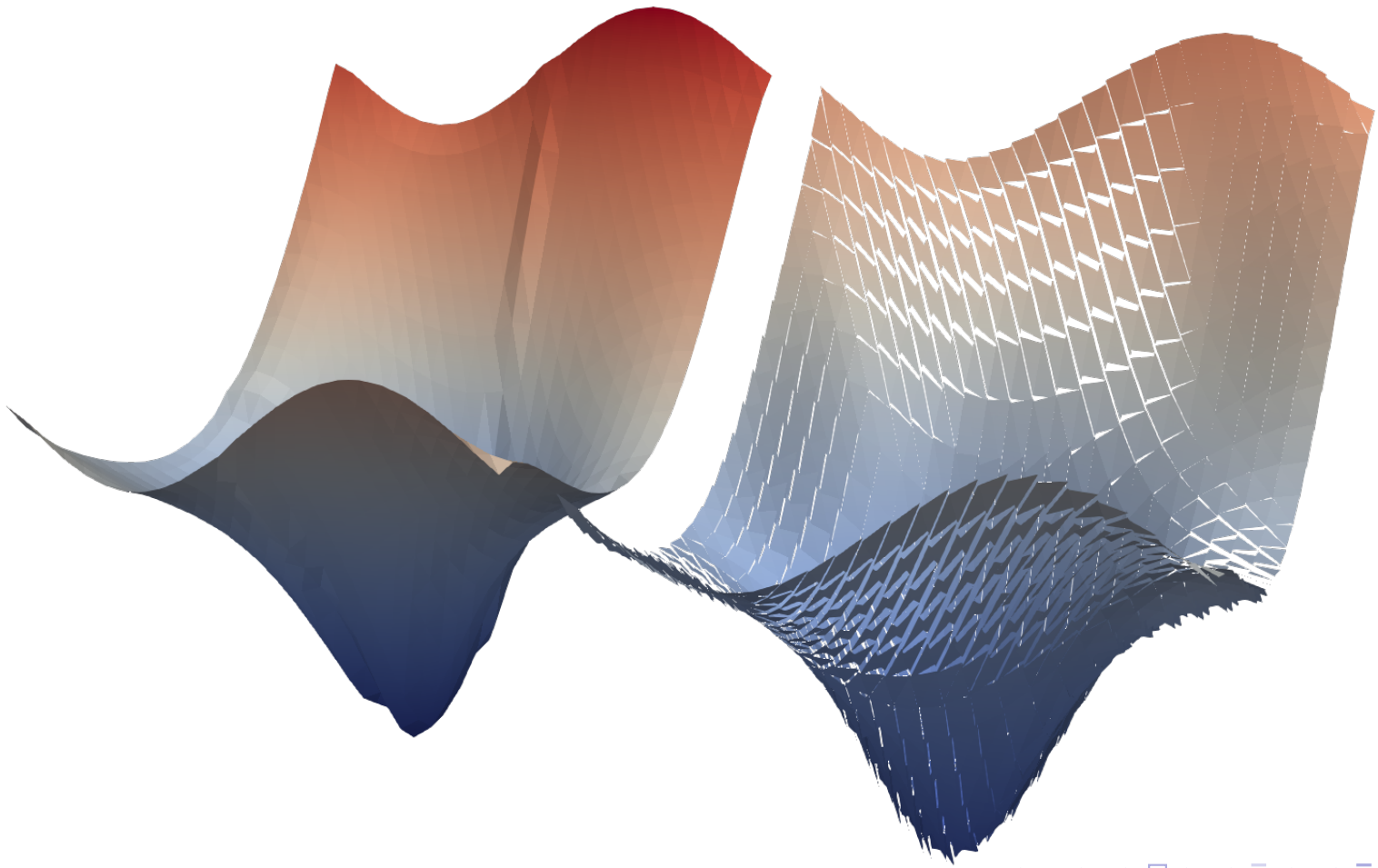

```
1  import dolfin as d
2
3  mesh = d.UnitSquareMesh(1, 1)
4  V = d.FunctionSpace(mesh, "RT", 1)
5
6  u = d.project(d.Expression(
7      ("x[1]", "-x[0]"), degree=1), V)
8
9  with d.XDMFFile("ex3_rt1_2d.xdmf") as outfile:
10     outfile.write_checkpoint(u, "u")
```

ParaView



mpirun -n 4 python3 demo_dg-poisson.py

`XDMFFile.write()` vs. `XDMFFile.write_checkpoint()`



Is done:

- new FiniteElementFunction attribute to XDMF
- XDMF to VTK tweaked to understand FEM function description
- write_checkpoint and read_checkpoint methods in DOLFIN/DOLFINX

Future work:

- add tesselation for higher-order elements
- Crouzeix-Raviart, BDM, RT, ...
- optimisation
- mixed-cell topologies - GSoC 2018 student?


WHEN YOU IMPLEMENT
NEW STUFF TO DOLFIN...
... AND THEY
KEEP IT IN DOLFINX
imgflip.com