

3D visualization in Jupyter Notebooks



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- by thinking constantly about it

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Overview

Basic technologies A quick overview

Some new visualization packages Different goals, different API flavours

A suggestion for FEniCS Supporting lots of visualization packages

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Cahn-Hilliard equation

The Cahn-Hillard equation is a parabolic equation and is typically used to model phase separation in binary mixtures. It involves first-order time derivatives, and second- and fourth-order spatial derivatives. The equation reads:

$$\begin{split} &\frac{\partial c}{\partial t} - \nabla \cdot M(\nabla(\frac{df}{dc} - \lambda \nabla^2 c)) = 0 \quad \text{in } \Omega, \\ &M\left(\nabla\left(\frac{df}{dc} - \lambda \nabla^2 c\right)\right) \cdot n = 0 \quad \text{on } \partial\Omega, \\ &M2\nabla c \cdot n = 0 \quad \text{on } \partial\Omega. \end{split}$$

The implementation

1 [2]:	<pre>mesh = UnitSquareMesh(96, 96) P1 = FiniteElement("Lagrange", mesh.ufl_cell(), 1) ME = FunctionSpace(mesh, P1*P1)</pre>
[9]:	mesh
ıt [9] :	
[5]:	<pre># Weak statement of the equations L0 = c'q'dx - c0'q'dx + dt*dot[grad(mu_mid), grad(q)]*dx L1 = muv*dx - dfdc'v'dx - lmbda'dot[grad(c), grad(v))*dx L = l0 + L1</pre>

In [7]:	t = 0.0; T = 50*dt	
	while (t < T):	
	t += dt	
	$u\theta$, $vector()[:] = u$, $vector()$	
	solver_solve(problem, u_vector())	

In [8]: plot(u.split()[0])





A quick overview of core tech for 3D visualization in notebooks

Jupyter Notebook ecosystem

- Notebook cell outputs can contain arbitrary HTML and Javascript
- Ipywidgets provides generic GUI widgets for notebooks

3D web technologies

- At the core is WebGL, a somewhat limited and slightly high level OpenGL
- Three.js library handles some tedious parts, adds abstractions, scenegraph

import ipyvolume.pylab as p3

p3.clear()
quiver = p3.quiver(x, y, z, vx, vy, vz, size=2, size_
p3.show()

Quite a few visualization tools have added web versions lately

Paraview web

- Visualizer, ArcticViewer
- vtk-js to replace Three.js







Other

- MayaVi
- VisPy
- ipyvolume

Packages developed by or contributed to by OpenDreamKit

Pythreejs is a wrapper for Three.js based on ipywidgets

Compose scenegraph in Python, render with Three.js

- Exposes many of the Three.js classes as ipywidgets
- Objects include camera, lights, basic shapes such as spheres and boxes, text, and also custom triangle meshes
- Great for semi-interactive 3D illustrations and animations
- Not really a scientific visualization library
- Not created by ODK but currently being updated on ODK time



Scivijs is a lightweight Paraview like visualization pipeline written in Javascript

Could be suitable for FEniCS:

- Interactive inspection of functions inline in a notebook (cutplanes, isosurfaces, and more)
- Jupyter widget under development
- Proof of concept FEniCS -> Scivijs exists
- No demo to show right now

K3D aims for a simple 3D plotting interface

positions = boundary.coordinates()
triangles = boundary.cells()
vertexmap = boundary.entity map(0).array()
scalars = u.compute_vertex_values()
scalars = scalars[vertexmap]

Scale and compute colors
scalar_range = (scalars.min(), scalars.max())
print(scalar_range)

scalars[:] = 0
scalar_range = (0,1)

Plot as surface mesh

K3D.mesh(positions, triangles, vertex scalars=scalars, color_range=scalar_range, color_map=K3D.basic_color_maps.CoolWarm)

(0.54881163609402639, 1.0)



Can be suitable for many basic FEniCS plotting needs

- Scatter plots
- Glyphs (quiver)
- Surfaces in 3D
- Under development now at University of Silesia, good time to request features!
- (Missing better figures because of time...)

figs = []



Unray (unreleased) provides volume rendering of tetrahedral meshes

Pipeline overview

- Upload cells, coordinates, vertex values of functions as numpy arrays
- Data uploaded to GPU textures via Three.js
- Surface of each tetrahedron rasterized as a triangle strip using instanced rendering





Unray can be quite fast for anything that can render in WebGL shaders

Framework in place for

- Passing function data on each tetrahedron to shader
- Computing depth of tetrahedron
- Tested with decent performance with 4 million tetrahedral cells



My suggestion: FEniCS should make it easier to get data that users can feed into plotting libraries, instead of hiding it in plot(...)

Some things are easy to use

- mesh.cells() and mesh.coordinates()
- BoundaryMesh, could be simplified
- MeshFunction.array()
- function.compute_vertex_values()

Other nice-to-haves

- function.compute_dg_vertex_values()
- function.compute_cell_values()
- Functionality such as probes and slices from fenicstools should be in dolfin
- A more consistent interface for all of the above

Another idea is to make a small set of functions to package fenics objects into a generic simple format for visualization

This could be just arrays

- points, vectors = make_glyphs(func)
- points, scalars = make_scatter(func)
- triangles, points, values = make_surface(func)
- (above a very simplified version)

Or some vega-like format

- data = { "f": f.compute_vertex_values(), ... }
- enc = { "colors": { "field": "f", "range": [0,1] }, ... }
- plot("glyphs", data=data, encoding=enc)

What do you want from visualization tools in notebooks?

Let me know during the breaks, or at martinal@simula.no!

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