From mathematics to a nice figure in a \LaTeX{} document: a post-processing chain

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Autrans, 26-30 Septembre 2011,
École d’été Masse de données : structuration, visualisation
A post-processing chain

Little physics problem

Numerical scheme to find an approximation

Approximation of the solution

Analytical solution

Solution evaluation

Python/numpy
C/F90/MPI/HDF5...

The answer in a nice pdf

nice eps figure with label

svg figure

nice eps figure

latex

inkscape

VisIt/paraview

Matthieu Haefele (HLST IPP)  From mathematics to a nice figure in a LaTeX document
def myfunction(foo, bar=3):
    " This function computes something useful "
    print "I was called with ", foo, bar
    pi = 3.14
    for i in range(11):
        if i % 2 == 0:
            # Writes pi * i = XX
            print "pi *", i, "=", i * pi
        else:
            # Writes i * pi = XX
            print i, "*pi =", i * pi

myfunction("superstring")
Main Python packages to do numerics

- numpy: implementation of n-d arrays
- matplotlib/pylab: 1D, 2D graphics
- scipy: package based on numpy that solves different dedicated problems
- h5py: Python bindings for the HDF5 library
- f2py, swig: tools to automate the creation of Python bindings from C/F90 codes
- ...
import numpy
import h5py

tab = numpy.zeros((22, 20), dtype=numpy.int32)
f = h5py.File('myfile.hdf5', 'w')
f['MyDataset'] = tab

tab = numpy.ones((8, 8), dtype=numpy.int32)
f['MyDataset'][3:11, 2:10] = tab
f.close()
Gnuplot

- open source software
- can produce 2D and 3D plots
- analytic or numeric functions
Using gnuplot interactively

```
set xrange [0:4*3.14159]
plot sin(x), sin(x-3.14159/2), "data.txt" u 1:2 w l
pause -1
```

- $x \in [0 : 4\pi]$
- plot on the same figure:
  - $\sin(x)$
  - $\sin(x - \frac{\pi}{2})$
  - The second column of the file named data.txt, and plot with lines (w l)
- `pause -1` means: do not close the window before I hit the Enter key
Using gnuplot non interactively

```plaintext
set terminal svg
set output "myfig.svg"
set xrange [0:4*3.14159]

plot sin(x), sin(x-3.14159/2), "data.txt" u 1:2 w l
```

- Same figure
- A svg file is created instead of opening a window
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From mathematics to a nice figure in a LaTeX document
Inkscape software

- Free and open source software
- Vector graphics edition/creation
- Standard Vector Graphics format based (SVG), the W3C standard
- Similar capacities as Illustrator, Freehand, CorelDraw or Xara X
Raster is an array of dots that “appear” to be shapes

- Pro: With sufficient resolution can be photo-realistic
- Con: Takes up lots of space even for simple geometric representations
- Con: Difficult to split into component pieces for further editing

Vector is real 2D shapes

- Pro: Geometric representations scalable to any resolution
- Pro: Easy to edit component pieces
- Con: Difficult to do photo-realistic images at small file sizes
A post-processing chain

1. Little physics problem
   - pencil and paper

2. Numerical scheme to find an approximation
   - Python/numpy
   - C/F90/MPi/HDF5...

3. Approximation of the solution

4. Solution evaluation
   - Python/numpy

5. Solution

6. Approximation of the solution
   - Python/pylab
   - C/F90/MPi/HDF5...

7. The answer in a nice pdf
   - latex

8. nice eps figure with label
   - inkscape

9. svg figure

10. nice eps figure

11. latex

12. VisIt/paraview

From mathematics to a nice figure in a LaTeX document
Let us consider the following magnetic diffusion equation

\[
\frac{\partial B_y(x, t)}{\partial t} = \eta \nabla^2 B_y(x, t)
\]

with an initial discontinuous field given by

\[
B_y(x, 0) = \begin{cases} 
B_0 & \text{for } x > 0 \\
-B_0 & \text{for } x < 0 
\end{cases}
\]

Please find the analytical solution and produce a \LaTeX generated pdf file containing figures that illustrates this diffusion.
The analytical solution is

$$B_y(x, t) = B_0 \text{erf}(\xi)$$

with $\xi = x/\sqrt{4\eta t}$ and the error function

$$\text{erf}(\xi) = \frac{2}{\pi^{1/2}} \int_0^\xi e^{-u^2} du$$

Illustration with $\eta = 1$ and $B_0 = 2$
Part of the process in numerical science

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