Python for scientific algorithm development

Fernando Perez
Applied Mathematics
CU Boulder

Scipy'06 – Caltech
August 17 2006

A recent quote

I will, in fact, claim that the difference between a bad programmer and a good one is whether he considers his code or his data structures more important. Bad programmers worry about the code.

Good programmers worry about data structures and their relationships.

-- Linus Torvalds

Initial remarks

- Does anyone have my USB drive from the tutorial?
- I gambled on the audience: more scientists new to python than experts on the language.
- I'll try to keep it interesting for the experts.
- Light on the math/physics, used mostly for illustration purposes. Talk to me if you care.
- $$$: DARPA, DOE.
- Collaborators:
  - Gregory Beylkin (CU Boulder)
  - Martin Mohlenkamp (Ohio Univ.)
  - Robert Harrison, George Fann (ORNL)

Modern algorithms:
There is more to life than arrays

Today's scientific software needs:

- Complex data structures
- To work at a high level of abstraction
- to handle mixed data (genetic sequences, time-tagged data, information from databases...). *It's not just floating-point.*
- Interact with other external systems (web, hardware, software subsystems, ...)

Q: how can we write better scientific software, and do it faster?

A: I don't know...

But I think that Python can help

Word counting:
The power of good data types

Dictionaries: flexible, efficient and powerful hash tables

Strings: lots of useful methods.

```
def word_freqs(text):
    """Return a dictionary of word frequencies for the
  given text."""

    freqs = {}
    for word in text.split():
        freqs.setdefault(word,0)
        freqs[word] += 1
    return freqs
```

Lightweight and expressive

```
class Tree:
    """A binary tree class."""
    def __init__(self, label, left=None, right=None):
        self.label = label
        self.left = left
        self.right = right

def inorder(t):
    """Return the leaves of t in left-right order."""
    if t:
        for node in inorder(t.left):
            yield node
        yield t.label
        for node in inorder(t.right):
            yield node
```

Interactive

Explore ideas, data with your fingers

vs

Other good things...

- Choose your code style. Write
  - standalone all-global scripts, or...
  - procedural code, or ...
  - Object Oriented libraries (with a simple object model compared to C++), or...
  - in a functional style.

  Choose the code that best fits your brain or the problem.
- Reuse your existing code (Fortran, C/C++).
- Uniformity (functions are first-class objects).
- Optimize only what *really* needs speed.

A mathematical problem:

Accurate, adaptive, fast algorithms for:

$$g = T f \Leftrightarrow g(x) = \int K(x-y) f(y) d^n y$$

where n=2,3,...,6. (Integral formulations are nice...)

- Electrostatics (Poisson's equation)
- Electrodynamics (Helmholtz)
- Quantum mechanics (Schrodinger – Lippman-Schwinger)
- Lots more...

Yes, this is 'just' a matrix-vector product.

What do you need?

$$g(x) = \int K(x-y)\, f(y)\, d^n y$$

Operators:
- Sparse
- Good scaling with *n*

Functions:
- Adaptively represented
- Compatible with op. rep.

Some ideas (I won't go into the details):

- Gaussian expansions for the kernel *K(x-y)*
- Multiwavelets (think tensor products of Legendre polynomials)
- Adaptive 2-*n* trees for function decomposition

What do you want from your code?

- Make functions easily:

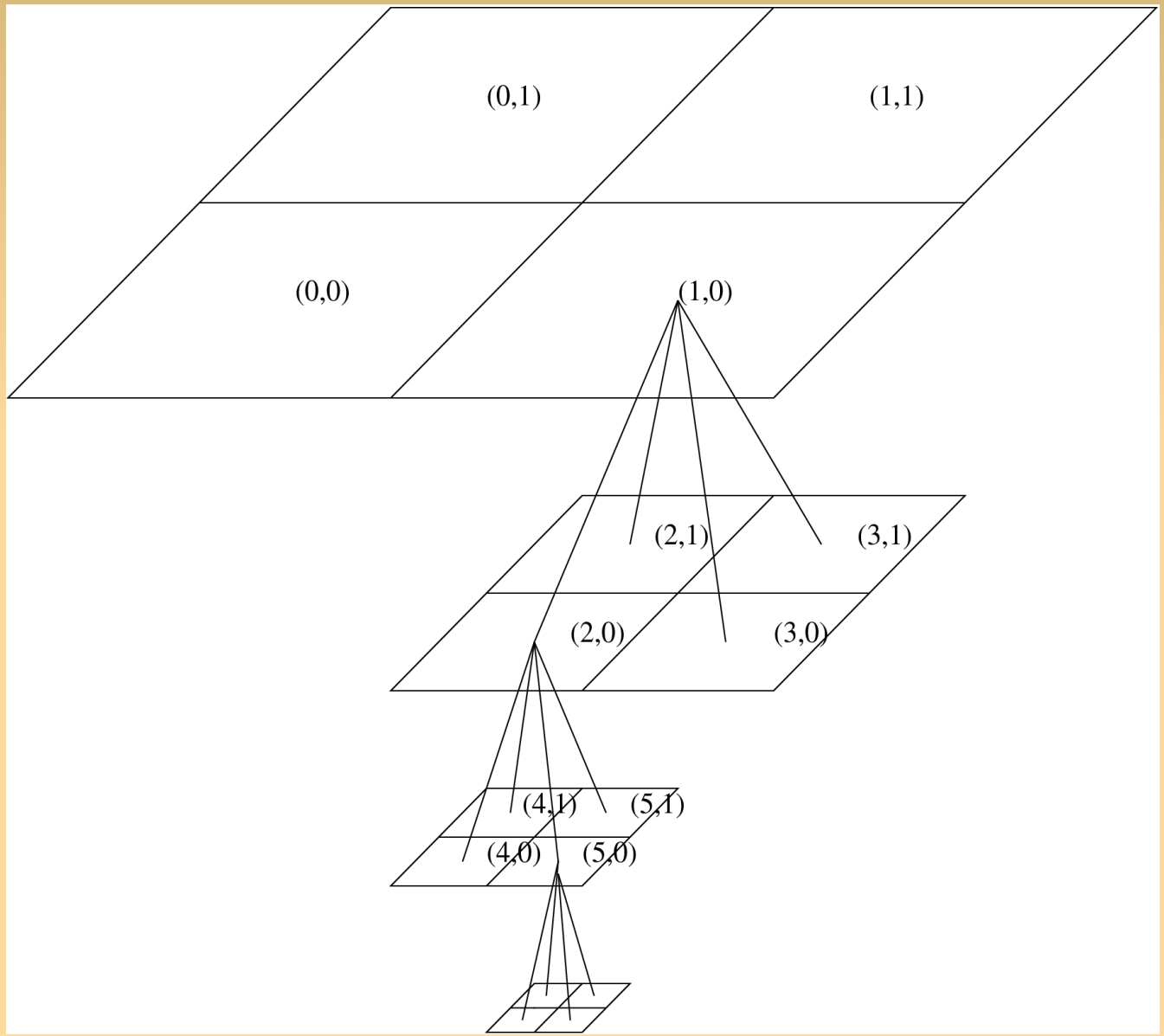
```
f = from_snippet(nnod=6,ndim=2,cutoff=1e-6,1.0,
                 'return sin(x)*cos(y)')
```

- Write code that reads like math (see demo):

$$h(x)=g(x)-f(x)$$

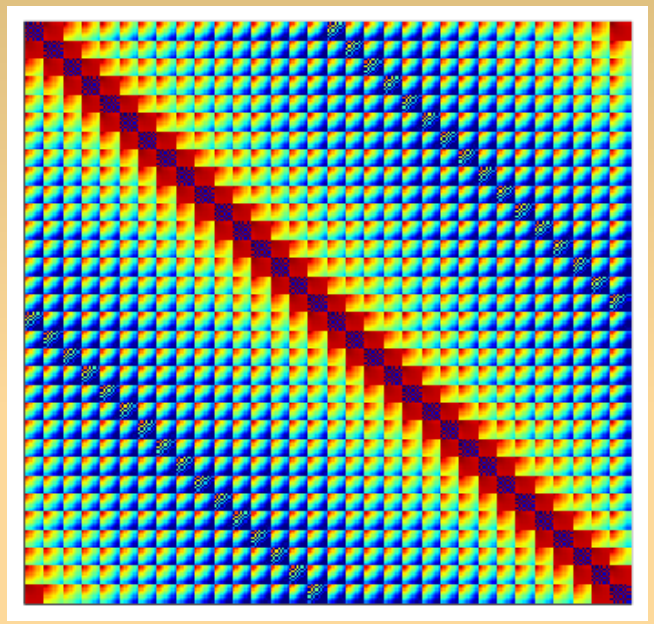
- How do we do this?
  - scipy's weave.inline
  - dictionaries
  - easy but powerful string handling
  - in-process calling of multiple different libraries (even written in different languages)

Functions: simple adaptive decompositions



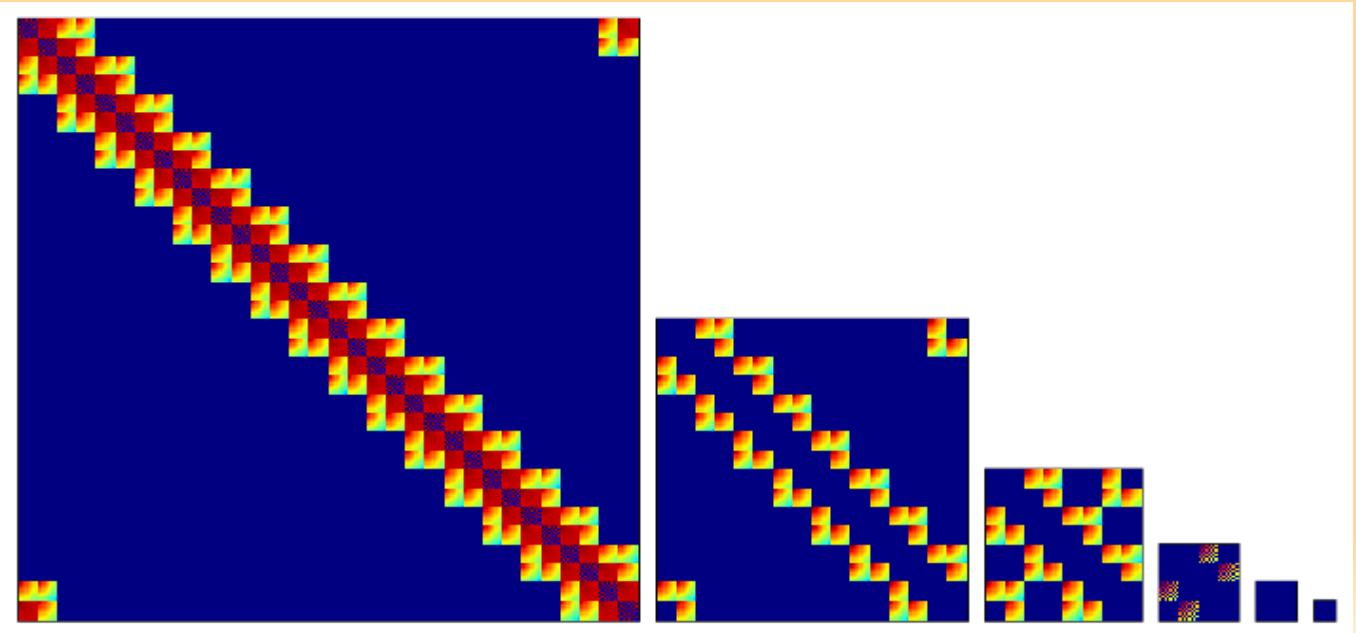
Operators: sparsity and high order methods

Multiwavelets (illustrated for d=1):



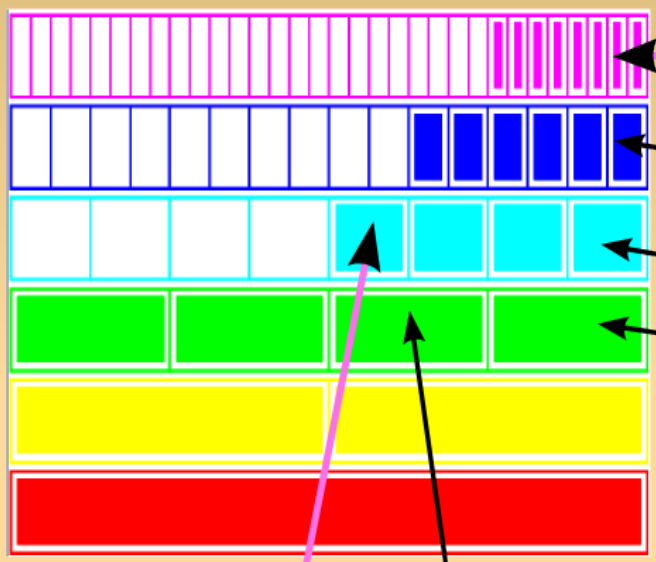
from this

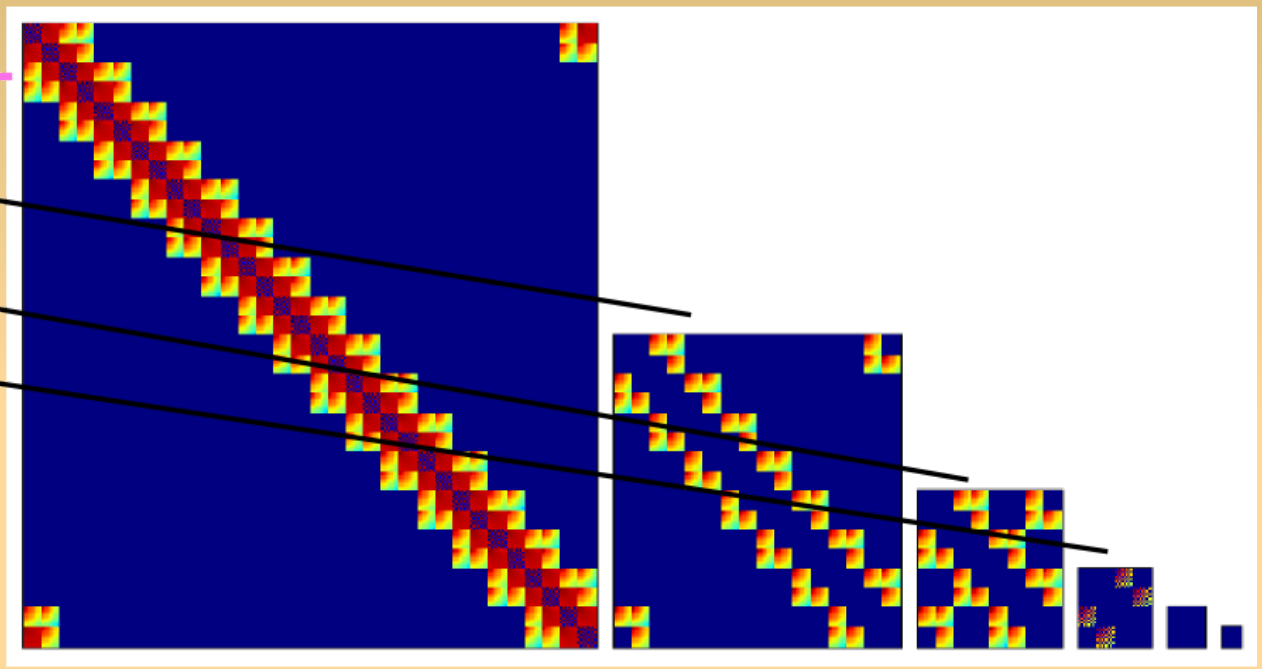
to this



Putting it all together (see code)

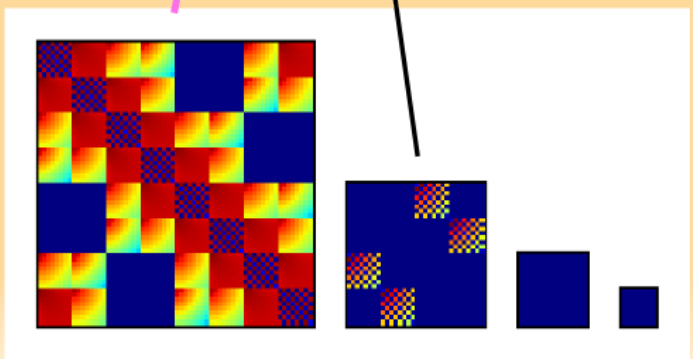
Redundant tree of input
(output skeleton)





Terminal

Non-terminal



The Hydrogen ground state

Plain old Schrodinger

$$H\psi = E\psi \Leftrightarrow [-\frac{1}{2}\nabla^2 - \frac{1}{r}]\psi = E\psi$$

can be written as

$$\phi = -2G_\mu V\phi \Leftrightarrow -2(-\nabla^2 + \mu^2 I)^{-1} V\phi$$

and at

$$\mu = \sqrt{-2E} \Rightarrow \psi = \phi$$

We can try to solve this by iterating to a fixed point:

1) Initialize all variables

2) Compute $\phi_{new} = -2G_\mu V\phi_{old}$

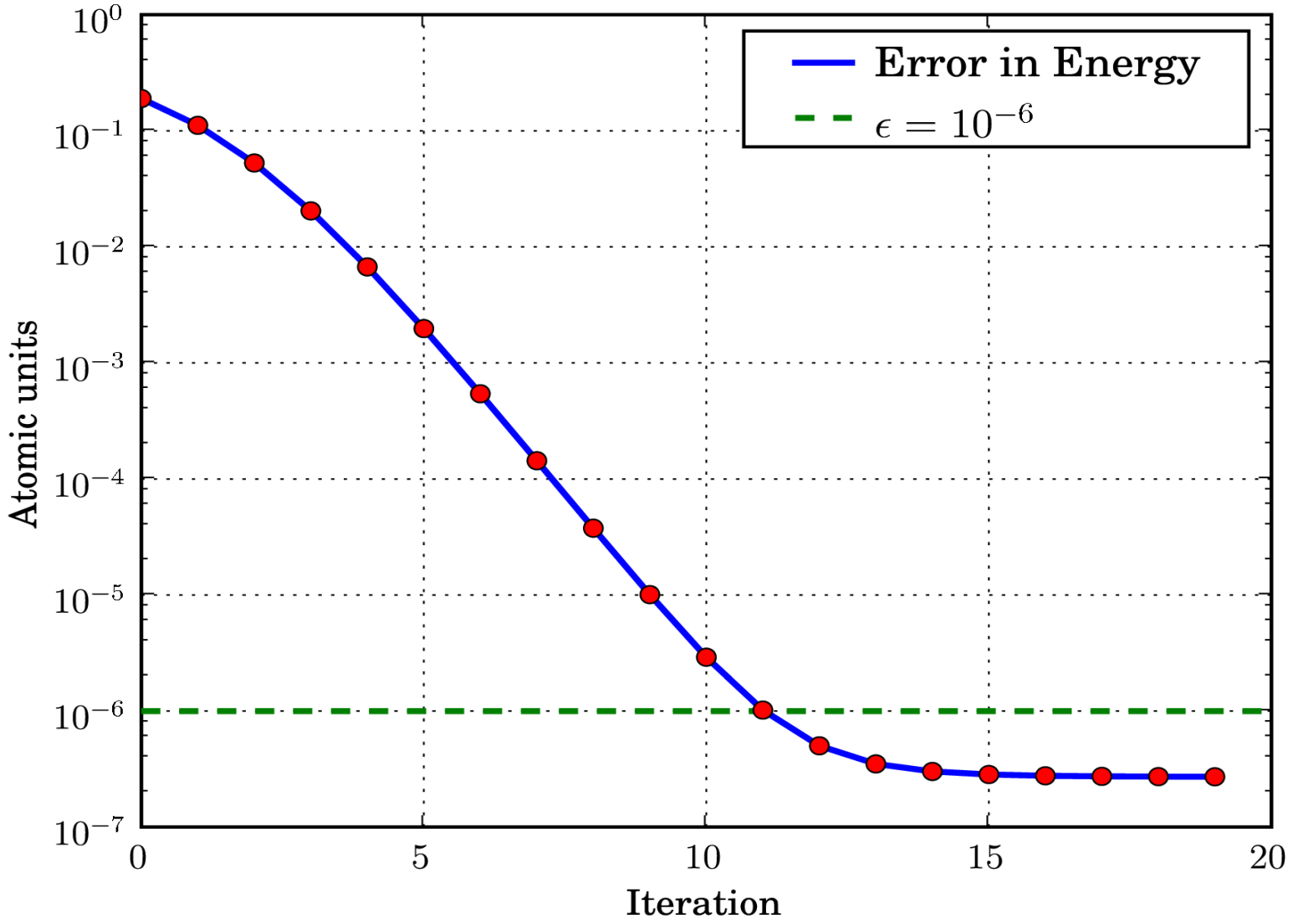
3) New Energy, new mu, repeat: $E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \Rightarrow \mu = \sqrt{-2E}$

The solution code

```
# Green's function iteration for the ground-state
# of the Hydrogen atom
# Initialize:
# V   = potential (1/r)
# psi = guess wavefunction
# G   = Bound-state Helmholtz operator

for n in range(num_iterations):
    # Apply the Greens' function with current value of mu
    psi = -2*G(V*psi)
    # Computation of energy as E = <psi|H|psi>/<psi|psi>
    E = ( (-1/2.)*psi.weak_laplacian(psi) +
          V.innerproduct(psi*psi) ) / psi.norm_l2()**2
    # Update the operator to new value of mu
    G.mu = sqrt(-2*E)
    # Prepare wavefunction for next iteration
    psi.normalize()
```

Green's function iteration: convergence



A brief summary

- Write code that reads like the science you care about.
  - Python offers a lot of tricks to let you do that.
- Express new ideas and algorithms as simply as possible.
- Put as many tools to explore your data as you can
  - You debug with the same methods you produce plots for a paper.
- Take advantage of excellent libraries.
- `f2py`, `weave.inline` (and `.blitz`), `ctypes`, `pyrex`, ... are *very* easy to use.
- Have fun coding science!