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   - Traditional approaches
   - Python?

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   - EEG analysis for epilepsy
   - Multiwavelets
   - PMV: molecular structures
   - MayaVi: customizable data visualization
   - SAGE: System for Algebra and Geometry Experimentation
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   - Development in Python
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FORTRAN, C and C++

Caveat: C++ suffers less from some of these problems, but it has other issues.

- Tools from a time when CPU time was more expensive than human time.
- Low-level:
  - Primitive data types (no good strings, sets, hash tables, ...).
  - Slow edit/compile/test cycle.
- Clumsy access to visualization, quick profiling, text processing, ...
- No interactive facilities - scientific work is inherently exploratory.
- Object Orientation?
  - Not a silver bullet, but a very good model for many scientific codes.
  - Non-existent in (old) FORTRAN & C, difficult and subtle in C++.

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- They deliver excellent performance.
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  - Great interactivity, visualization, and extensive libraries.
  - Unpleasant languages for large-scale programs and non-numerical tasks.
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  - Often considered ‘prototyping’ tools: this leads to a lot of code rewriting.
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Python is growing in scientific computing
Entire May/June 2007 issue of CiSE devoted to Python
Python in this context

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- Interactive interpreter provided.
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- Extremely readable syntax ("executable pseudo-code").
- Simple: non-professional programmers can become (and remain) proficient with a very small effort (c.f. C++).
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Data analysis for epilepsy surgery
Isolating the origin of drug-resistant epileptic seizures which require surgery.

John Hunter, Department of Pediatric Neurology, University of Chicago.
Electrode location in 3D, combined with MRI data
Full reconstruction of electrode location
Correlation analysis of seizure data
Final location of epileptic foci for surgery
Adaptive, multiwavelet algorithms for integral operators


- Fast application of integral kernels. (Partial Differential Equations)
- Implementation went from 1 to 3 dimensions directly (extremely unusual).
- A clean Object Oriented design: the code reads like the underlying math.
- Very good performance, thanks to NumPy, F2PY and weave.
Structural Bio-Informatics

Michel F. Sanner, Molecular Biology Department, The Scripps Research Institute, La Jolla, California. http://www.scripps.edu/~sanner

Applications:

- PMV: Visualization and analysis of biological molecules
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- Heavy lifting of OpenGL-based rendering: VTK (a C++ library).
- A very good example of how to properly use Python:
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  - Python: very easy to modify, even by adding at runtime user-defined modules which populate the GUI automatically.
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The punchline: fully programmable visualization, with builtin access to all kinds of numerical (and other) libraries from within the viz tool.
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FluidLab: a MayaVi based CFD visualization tool

Volumetric rendering with FluidLab
SAGE: open source mathematics

```python
show(graphs.CubeGraph(5).plot3d())
```

```python
show(graphs.CubeGraph(6).plot3d())
```

```python
show(plot(sin(x^2)+x, -pi, pi, hue=0.7, thickness=3))
```
IPython
Extensible interactive environment with parallel computing support

1. **A better Python shell**: object introspection, system access, ’magic’ command system for adding functionality when working interactively, . . .

2. **An embeddable interpreter**: useful for debugging and for mixing batch-processing with interactive work.

3. **A flexible component**: you can use it as the base environment for other systems with Python as the underlying language. It is very configurable in this direction.

4. **A system for interactive control of distributed/parallel computing systems.**

5. **An interactive component** we can plug into GUIs, browser-based shells, etc.
IPython: IDL-like interactive use

In [1]: import math, numpy
In [2]: from scipy.integrate import quad
In [3]: from scipy.special import j0
In [4]: def j01(x):
   ...:     """Integral form of J_0(x)"""
   ...:     def integrand(phi):
   ...:         return math.cos(x*math.sin(phi))
   ...:     return (1.0/math.pi)*quad(integrand, 0, math.pi)[0]

In [5]: x = numpy.linspace(0, 20, 200) # sample grid: 200 points between 0 and 20
In [6]: y = j0(x) # sample J0 at all values of x
In [7]: xl = x[::10] # subsample the original grid every 10th point
In [8]: yl = map(j01, xl) # evaluate the integral form at all points in xl
In [9]: # Make a plot with these values (the ; suppresses output)
In [10]: plot(x, y, label="$J_0(x)$");
In [11]: plot(xl, yl, 'ro', label="$\int_0^\infty \cos(x \sin \phi) d\phi$");
In [12]: axhline(0, color='green', label="nolegend");
In [13]: title('Verify $J_0(x) = \frac{1}{\pi} \int_0^\infty \cos(x \sin \phi) d\phi$');
In [14]: xlabel('5x5');
In [15]: legend();
In [16]: matplotlib.pyplot.figure.Figure instance at 0x4630042c
IPython: interactive control of VTK visualizations

In [1]: from enthought.tvtk.tools import mlab
In [2]: from scipy import *
In [3]: def f(x, y):
    ...:     return sin(x+y) + sin(2*x-y) + cos(3*x+4*y)
    ...:
In [4]: x = linspace(-5.0, 5.0, 200)
In [5]: y = linspace(-5.0, 5.0, 200)
In [6]: fig = mlab.figure()
In [7]: surf = mlab.SurfRegular(x, y, f)
In [8]: fig.add(surf)
In [9]:
IPython’s future
A 2-process kernel

Work with Brian Granger (Tech-X, Boulder) and Benjamin Ragan-Kelley (U. C. Berkeley physics).

Why do we need this?

- The Python VM has a global lock (the Global Interpreter Lock – GIL).
- It protects the global state of the interpreter
  - Only one thread can execute Python code at the same time.
  - No Python variables may be modified without holding the GIL.
- Python *does* have threads: they work well for non-CPU bound tasks.
- **BUT**
  - Extensions (C, Fortran) can fully block the VM.
  - And poof goes all hope of the ability to control a cluster.
A 2-process kernel on the network

The "IPython VM"

- Kernel Controller
  - Non-blocking
  - World-visible

Kernel Engine

MAY BLOCK!

Twisted

Networks
Distributed/parallel computing

- Think of Python as ’the CPU’
- But these souped-up kernels let you talk to it conveniently.
import numpy, Ngl, Nio
dirc = Ngl.pynglpath("data")
cfile = Nio.open_file(dirc + "/cdf/seam.nc")
lon = numpy.ravel(cfile.variables["lon2d"][:, :, :])
lat = numpy.ravel(cfile.variables["lat2d"][:, :, :])
ps = numpy.ravel(cfile.variables["ps"][0, :, :])/100.
rlist = Ngl.Resources()
rlist.wkColorMap = "BlAqGrYeOrReVi200"
wks_type = "ps"
wks = Ngl.open_wks(wks_type,"seam",rlist)
resources = Ngl.Resources()
resources.sfXArray = lon
resources.sfYArray = lat
map = Ngl.contour_map(wks, ps, resources)
Ngl.end()
HOMME grid: Surface pressure w/smoothing
A few other projects
Python is becoming very popular in many different scientific areas

- **PyDAP**: Python implementation of the OpenDAP protocols (client and server).
- **PyTables**: HDF-5 read-write support with excellent performance.
- **PyTrilinos**: Python interface to Sandia’s Trilinos parallel solvers. Coupled with IPython, they can be used interactively.
- **PyRAF**: Hubble Space Telescope interface to IRAF, a standard in astronomical image processing.
- **VPython**: easy, real-time 3D programming (Carnegie Mellon, used for an introductory mechanics course).
- **Galaxy**: integrated access to multiple tools in genomics research. Very impressive.
Outline

1. Scientific Computing
   - Traditional approaches
   - Python?

2. Interlude: Python in the real world
   - EEG analysis for epilepsy
   - Multiwavelets
   - PMV: molecular structures
   - MayaVi: customizable data visualization
   - SAGE: System for Algebra and Geometry Experimentation
   - IPython
   - PyNGL

3. Python and Scientific Computing
   - Basic features
   - Development in Python
Basic Python features

Meaningful indentation, self-documenting, interactive language

- Examples below: IPython (enhanced interactive environment)
- Exploratory, incremental development, with live debugging on exceptions.
- Direct access to the filesystem and OS.

```python
In [8]: def hypot(a,b):
    ...:     "Return the length of the hypotenuse."
    ...:     return sqrt(a**2+b**2)
In [9]: pdoc hypot
Return the length of the hypotenuse.
In [10]: pdef hypot
hypot(a, b)
In [12]: cd talks/figs/
/home/fperez/talks/figs
In [13]: ls
cise_cover.jpg kernel2p.eps ...
```
Dictionaries (C-implemented, well optimized hash tables)

- Perfect for building complex, sparse data structures

In [21]:
```python
dct={'k1':'v1',(3,4):cos,'nest':{1:2}}
```

In [22]:
```python
dct.keys(), dct.values()
```

Out[22]:
```python
(['k1', 'nested', (3, 4)], ['v1', {1: 2}, <built-in function cos>])
```

In [23]:
```python
dct[3,4](pi)
```

Out[23]:
```python
-1.0
```

Easy access to C/C++ (via SciPy’s weave.inline) and FORTRAN (f2py)

In [26]:
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code='std::cout < < "a is: " < < a < < std::endl;'
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In [27]:
```python
a='Hello world'
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In [28]:
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inline(code,['a'])
```

a is: Hello world

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a=99
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a is: 99
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Pros

A general programming language: **this is a feature!**

- Free, open source, extremely portable: from the OLPC or a cellphone (Nokia) to a supercomputer.
- Networking, text processing, XML parsing, database access, etc.
- Integrated support for testing (`unittest`, `doctest`)
- Automatic API documentation tools are standard (`doxygen`).
- Supports all major GUI toolkits.
- Extremely expressive for complex algorithms.

There are still rough edges!

- Installation, deployment: harder than needed (but improving rapidly).
- No good, single-point of entry integrated help system.
- Lots of good documentation, but scattered all over.
- Funding agency support for infrastructure work is difficult to get.
Python compared to IDL, Matlab, etc.

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A different model of development

Global optimization is the root of all evil

Never write `main()` in C anymore: you are optimizing globally!

- Prototype the code in Python.
- Wrap existing libraries for Python access and reuse them (Numeric, LAPACK, VTK, ...)
- Identify remaining hot spots via profiling.
- Rewrite only the code for those hot spots in C/C++/FORTRAN.

The resulting code will be production-ready: no throw-away codes.

- Make your code available as a library for interactive use.
- Integrate plotting, visualization, logging, ..., into your objects.

Apply this to existing codes

- Break them into a library core and control layers.
- Wrap the libraries and expose them to Python.
- Write all new control as quick, light Python scripts.
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Summary

- **Python**
  - An excellent language for scientific computing development.
  - Scales from interactive exploration to full-blown production codes.
  - Accessible to scientists who are not professional programmers.

- **Outlook**
  - NumPy, SciPy, matplotlib, IPython, MayaVi, ... are moving forward and improving.
  - Major DOE, NSF, NIH projects are adopting it as a core technology.
  - Yearly conference at Caltech (just finished) growing.
  - These projects are all Open Source: if you find a flaw, a bug, or a missing feature, *jump on board!*
  - There are still many rough edges to which various projects can contribute.
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An overview of Python’s features
A readable, eclectic collection of the best features from many languages.

Data types

- **Arbitrary length integers**
  
  ```
  In [1]: 2**64
  Out[1]: 18446744073709551616L
  ```

- **Floats (standard C doubles) and complex numbers**
  
  ```
  In [4]: 1j**2
  Out[4]: (-1+0j)
  ```

- **Strings**
  
  ```
  In [6]: 'hello world'.upper()
  Out[6]: 'HELLO WORLD'
  ```

- **Lists (arbitrarily nested, variable length)**
  
  ```
  In [9]: [99,'hello',1j,[{'sublist'},99]].count(99)
  Out[9]: 2
  ```
Data types (cont)

- **Dictionaries (C-implemented, well optimized hash tables)**

  In [21]:
  ```python
dct={'k1':'v1','v2',2,(3,4):math.cos,'nest':{1:2}}
  ```

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dct.keys()
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  In [24]:
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dct[3,4](math.pi)
  ```

  Out[24]:
  ```python
-1.0
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Strongly, but dynamically typed

- One of its major strengths: extreme flexibility.

- Slow: everything is checked at runtime.

  ```python
  for x in range(10):
    print x**2  # x and ** are checked every time!
  ```
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Interactive

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Clean object system

With multiple inheritance and operator overloading:

```python
In [12]: class simple:
   ....:     def __add__(self, other):
   ....:         print 'Me plus something else:', other
In [13]: a = simple()
In [14]: a + 34
Me plus something else: 34
```
Python Basics (3)

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def compose(f, g):
    return lambda x: f(g(x))
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Elegant, simple and expressive: quicksort in 3 lines (Nathan Gray)

```python
def qsort(L):
    if len(L) <= 1: return L
    return qsort([lt for lt in L[1:] if lt < L[0]]) + \
    [L[0]] + qsort([ge for ge in L[1:] if ge >= L[0]])
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