PYTHON FOR STRUCTURAL BIOINFORMATICS

Sophie COON
and
Michel SANNER

The Scripps Research Institute
La Jolla, California

SCHEDULE

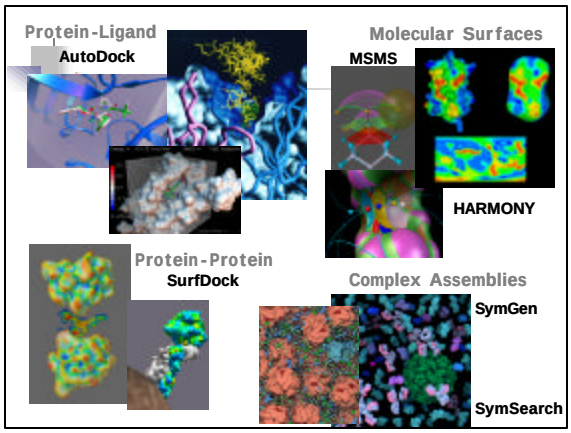
- I - Fundamentals
  - Code development strategies, Python
- II - PMV
  - Fundamentals, main commands
- III - From building blocks to applications
  - MolKit, DejaVu, ViewerFramework, ...
  - Putting it all together
  - Writing a simple command
- Conclusion

I - Fundamentals

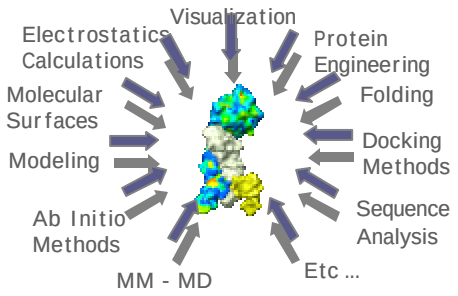
- Code development strategies
- Python primer

I - Fundamentals

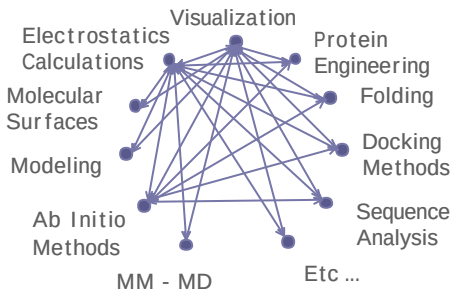
- Code development strategies
  - The challenge
  - Traditional solution
  - Our solution



The challenge

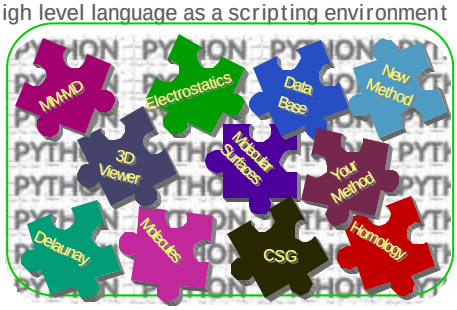


"Traditional" solution

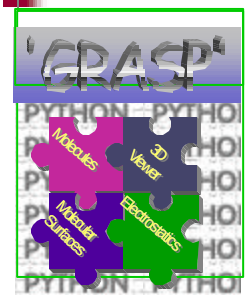


Our solution

High level language as a scripting environment



Writing an application



- High level coding
- Code re-use
- Extensible

Why Python ?

Our language needed :	Not met by :
Object-Oriented	Tcl, Perl, C, ...
Advanced data structures	Tcl, Perl
Powerful data-parallel arrays	Tcl
Readability and modularity	Perl
High-level	C, C++, Fortran
Platform independence	C, C++, Java, ...
Interpreted	C, C++, Java, ...

Python based molecular software

- Chimera : UCSF - Computer Graphics Lab.
  http://www.cdl.ucsf.edu/chimera
- MMTK : CNRS - Institut de Biologie Structurale
  http://starship.python.net/crew/hinsen/mmtk.html
- Pymol : Delano Scientific.
  http://www.pymol.org
- PyDayLight : Daylight Chemical Information Systems, Inc.
  http://starship.python.net/crew/dalke/PyDaylight/
- MDTools : UIUC - Theoretical Biophysics Group.
  http://www.ks.uiuc.edu/~jim/mdtools/
- ...

I - Fundamentals

- Python primer
  - Python installation
  - Language characteristics
  - Basics
  - Standard library
  - Extending Python
  - Numeric extension

Python installation

1- Open the demoNPACI folder on your desktop

2- Double click on  icon to start the installation of Python.

3- Follow the installation instructions:

- Use default settings for steps 1 through 5
- Step 6 Install Tcl/Tk : YES
- Use default settings for the remaining steps.

4- In C:\Program Files\Python:

Double click → starts a Python interpreter

Language characteristics

- Interpreted, high level, object-oriented
- Flexible and extensible
- Introspection, self-documenting
- Platform independent
- Open-source
- Rapidly gaining acceptance

Basics

```
>>> a = 2            # integer
>>> b = 7.5          # float
>>> c = 'hello'      # string
>>> d = " World!"    # string too
>>> # this is a comment
>>> print c+d
>>> print "sum :", a+b
```

- No Memory allocation
- No variable declaration
- simple and intuitive

List - mutable sequences

lst contains:

```
>>> lst = [2, 1,'hello']          → [2, 1,'hello']
>>> lst.append(5)                 → [2, 1, 'hello', 5]
>>> lst.remove(1)                 → [2,'hello',5]
>>> lst.insert(1,'Paul')          → [2,'Paul','hello',5]
>>> lst.sort( )                   → [2,5,'Paul','hello']
```

Tuple - immutable sequences

tup contains:

```
>>> tup = (1,2,'spam')            → (1, 2, 'spam')
# automatic packing and unpacking
>>> tup = 1,2, 'spam'             → (1, 2, 'spam')
>>> a,b,c = tup
>>> print a, b, c                 → 1 2 'spam'
# correct singleton syntax
>>> tup = (1,)                    → (1,)
>>> tup[0] = 6  # ERROR : cannot assign value in a immutable sequence !
```

Sequences indexing and slicing

```
>>> lst = [1,'b',6,'a',8,'e']
```

0	1	2	3	4	5
1	'b'	6	'a'	8	'e'
-6	-5	-4	-3	-2	-1

- Indexing : lst[i]

```
>>> lst[4]
>>> lst[-2]
```

0	1	2	3	4	5
1	'b'	6	'a'	8	'e'
-6	-5	-4	-3	-2	-1

i

- Slicing : lst[from:to]

```
>>> lst[2:4]
>>> lst[2:-2]
>>> lst[-4:-2]
```

0	1	2	3	4	5
1	'b'	6	'a'	8	'e'
-6	-5	-4	-3	-2	-1

Exercise

In the Python interpreter:

1- Create a list l1 containing the following elements: 1, 2.6, 'b', 7, 9, 'z'

2- Assign a new value to the 3rd element of l1?

3- If l2 = l1[1:-2] guess the elements contained in l2.

Solution

```
>>> l1 = [1, 2.6, 'b', 7, 9, 'z']
>>> l1[2] = 'new'
>>> print l1
[1,2.6,'new', 7, 9, 'z']
>>> l2 = [1:-2]
>>> print l2
[2.6,'new', 7]
```

Dictionary

dict = { ~~key1 : value1~~, key2 : value2, ...}

item1

```
>>> dict = { 'Marc':25, 30 : 'Jim' }
>>> dict[5.7] = 'joe'                    ▸ { 'Marc':25, 30:'Jim', 5.7: 'joe'}
# Accessing the information
>>> dict.items()                         ▸ [('Marc',25), (30,' Jim'), (5.7,'joe')]
>>> dict.values()                        ▸ [ 25,'Jim', 'joe']
>>> dict.keys()                          ▸ ['Marc', 30, 5.7]
>>> dict.has_key('Marc')                 ▸ True
```

Control flow

- While :

```
>>> b = 0
>>> while b < 5:
...         print b; b=b+1
0 1 2 3 4
```

- If :

```
>>> q = 'Please Enter a number'
>>> x = int( raw_input (q) )
>>> if x == 0:
...       print 'x equals 0'
... elif x < 0:
...       print ' x is negative'
... else:
...       print 'x is positive'
```

- For, range(), break, continue :

```
>>> seq = range(-3, 4, 1)
>>> print seq
[-3,-2,-1,0,1,2,3]
>>> for s in seq:
...       if s < 0:
...             continue
...       else:
...             print s
0,1,2,3
```

Functions and arguments

Positional arguments (required)

```
def func( a, b, n1=10, n2='hello' ):
```

Function name — Named arguments (optional)

Argument matching:

```
>>> func( 2, 'string', 3.14 )
>>> func( 7.2,  'string',  n2=15)
>>> func( 'hello', 2 , 5, 'bye')
>>> func( n1 = 5 )
>>> func( n1=12, 3.14 )
```

	a	b	n1	n2
	2	'string'	3.14	'hello'
	7.2	'string'	10	15
	'hello'	2	5	'bye'

ERROR: missing argument
ERROR: positional argument after named argument

Functions - Arbitrary arguments

```
def func( *args, **kw):
```

Tuple of positional arguments — Dictionary of named arguments

Argument matching:

```
>>> func( 2, 'string' , n1 = 5, n2 = 'a' )
```

	args	kw
	(2,'string')	{'n1' : 5, 'n2' : 'a' }

Combining the two argument passing methods

```
>>> def func( a, b, f=10, *args, **kw):
```

Classes - basics

```
class Rectangle:
    def __init__(self, width, length): # Constructor
        self.w = width                 # instance attribute
        self.l = length                # instance attribute

# call the constructor to create an instance
rect1 = Rectangle( 5, 6 )
# create another instance
rect2 = Rectangle( 4, 2 )
# access instance's attributes
print rect1.w, rect1.h  -> 5 6
print rect2.w, rect2.h  -> 4 2
```

Classes - methods

```
class Rectangle:
    def __init__(self, width, length): # Constructor
        self.w = width                 # instance attribute
        self.l = length                # instance attribute
    def area(self):                    # method area
        return self.w * self.l

# call the constructor to create an instance
rect1 = Rectangle( 5, 6 )
rect2 = Rectangle( 4, 2 )
# calling a method
print rect1.area( )                    -> 30
print rect1.area( ) + rect2.area( )    -> 38
```

Classes - overwriting operators

```
class Rectangle:
    def __init__(self, width, length): # Constructor
        self.w = width                 # instance attribute
        self.l = length                # instance attribute
    def __add__(self, right):          # defines rect1+rect2
    def __mult__(self, right):         # defines rect1*rect2
    def __repr__(self ):               # defines print(rect1)
    def __call__(self, *args, **kw):   # define rect1('hello')
    etc ...
```

Modules

The file MyModule.py contains:

```
def func1(b):
    print 'You called func1 with b = ',b
```

```
>>> import MyModule
>>> dir(MyModule)
['__builtins__','__doc__','__file__','__name__',func1]
>>> MyModule.func1(10)
You called func1 with b = 10
```

```
>>> from MyModule import func1
>>> func1(10)
You called func1 with b = 10
```

```
>>> from MyModule import *
>>> func1(10)
You called func1 with b = 10
```

Exercise

1- Open in emacs the file myModule.py located in the demo folder.

2- Extend the class Rectangle with a method to compute the perimeter.

3- Start a Python interpreter. Import the class Rectangle from the package myModule.

4- Create an instance rect1 of that class.

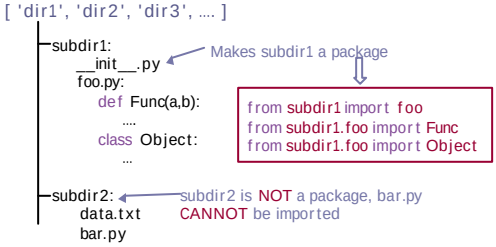
Solution

```
class Rectangle:
    def __init__(self, width, length): # Constructor
        self.w = width                 # instance attribute
        self.l = length                # instance attribute
    def area(self):                    # method area
        return self.w * self.l
    def perimeter(self):               # method perimeter
        return 2*(self.w + self.l)
```

```
>>> from MyModule import Rectangle     #  importing the class Rectangle
>>> rect1 = Rectangle(7,3)             # creating an object rect1
>>> per = rect1.perimeter()            # calling the new method.
>>> print per
```

Packages - organizing modules

```
>>> import sys
>>> print sys.path   # print the Python path
[ 'dir1', 'dir2', 'dir3', .... ]
```



Standard libraries

sys, os, string, math, cgi, commands, shelve etc...

Example:

```
>>> import sys
>>> path = sys.path
>>> print path[:3]
[ ' ', 'C:\\Program Files\\Python', ' C:\\ Program
   Files\\Python\\Lib\\plat-win']
```

Extending Python

Add functionality to Python

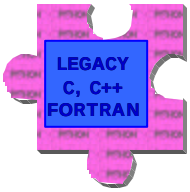
Gaining access to legacy code

Extending PYTHON

Implement

Platform independent
Portability

Wrap



Platform dependent
speed

Wrapping C code

MyLib.h

SWIG

```
extern int fact(int i);
```

MyLib.a

```
/* Compute factorial of n */
int fact(int n) {
  if (n<=1) return 1;
  else return n*fact(n-1);}
```

```
#include "MyLib.h"
...
PyObject *fact_w(PyObject *obj)
{
  int n = PyGetInt(obj);
  int res = fact(n);
  PyObject *Pyres = PyMakeInt(res)
  return Pyres;
}
...
```

MyLibModule.so

```
>>> import MyLib
>>> a = 5
>>> MyLib.fact(a)
```

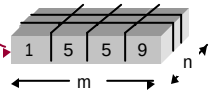
Numeric extension

Efficient storage and manipulation of large arrays of data.

Concepts

In C :

PyArrayObject
void *data
int *shape
char typecode



In Python:

```
import Numeric
ar = Numeric.array( [(1,5,5,9),
                     (-2,3,4,26),
                     (1, 2, 3, 7) ])
print ar.shape          → (3,4)
print ar.typecode()     → 'l'
print ar.iscontiguous() → '1'
```

Reshaping

```
>>> B = Numeric.array([ [1,2,3],[4,5,6] ])
```

$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$ — Numeric.reshape(B,(3,2)) → $\begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix}$

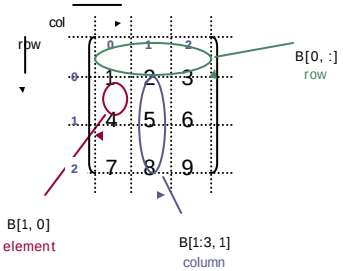
shape (2, 3) → (3, 2)

$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$ — Numeric.reshape(B,(-1,)) → $\begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 \end{bmatrix}$

shape (2,3) → (6,1) or (6,)

Indexing & Slicing

```
>>> B = Numeric.array( [ [1,2,3],[4,5,6],[7,8,9] ])
```



Element-wise operations

Element-wise operation at C speed !

$$\begin{bmatrix}1\\2\\3\end{bmatrix} \text{ bop } \begin{bmatrix}4\\5\\6\end{bmatrix} = \begin{bmatrix}1 \text{ bop } 4\\2 \text{ bop } 5\\3 \text{ bop } 6\end{bmatrix} \qquad \text{uop } \begin{bmatrix}1\\2\\3\end{bmatrix} = \begin{bmatrix}\text{uop } 1\\\text{uop } 2\\\text{uop } 3\end{bmatrix}$$

$$\begin{bmatrix}1\\2\\3\end{bmatrix} \text{ bop } 2 \text{ same as } \begin{bmatrix}1\\2\\3\end{bmatrix} \text{ bop } \begin{bmatrix}2\end{bmatrix} = \begin{bmatrix}1 \text{ bop } 2\\2 \text{ bop } 2\\3 \text{ bop } 2\end{bmatrix}$$

$$\begin{bmatrix}1\\2\\3\end{bmatrix} \text{ bop } \begin{bmatrix}4\\5\end{bmatrix}$$

binary operators (bop) : +, x, /, - ,% , power ...
unary operators (uop) : sin, cos, sqrt ...

Universal functions.

The most common Numeric universal functions:

take,transpose, repeat, choose, ravel, nonzero,where, compress, diagonal, trace, searchsorted, sort, argsort, argmax, fromstring, dot, matrixmultiply, clip,indices, swapaxes, concatenate, innerproduct, array_repr, array_str, resize,diagonal, repeat, convolve, where, identity, sum, cumsum , product,cumproduct, alltrue, sometrue.....

II - PMV

- Fundamentals
- Commands
- Specialized extension: ADT

Installing PMV

1- Open the demoNPACI folder on your desktop.

2- Double click on  icon to install PMV.
setup

3- Open the demo directory and double click on  to start PMV.
pmv

An extensible and customizable application.

- Load commands on the fly : loadCommand & loadModule commands.
  - Loading the readPDB commands and the displayCommands module.
    - File -> loadCommand -> fileCommands -> readPDB
    - File -> loadModule -> displayCommands -> Load Module
  - Exercise:
    - 1- Load the "deleteMol" command from the deleteCommands module.
    - 2- Load the "colorCommands" module.

Basic interaction with the viewer

Action	Mouse button	Modifier
Rotation	Right	
Scaling	Right	Alt
XY Translation	Right	Control
Z Translation	Right	Shift
Picking	Left	

An extensible and customizable application.

- Define Commands to be applied to molecule when loaded: onAddObjectCommand
  - Loading a molecule displayed as lines.

    File -> OnAddObjectCommand -> buildBondsByDistance -> displayLines -> Dismisss

  ! The order in which the commands are selected is the order in which the commands are applied to the molecule.

    File -> Read PDB -> 1crn.pdb -> Open
  - Exercise:

    Load a new molecule to be displayed as cpk and colored by residue type.

An extensible and customizable application

- User preferences:
  - SetUserPreference command.

    Set for the current session

    Made as default for the following sessions
- Customization of the GUI
  - Customize command.

An extensible and customizable application.

- User specific customization files .pmvrc:

  1- Open the .pmvrc in emacs

  Right click on the .pmvrc file and send to 'emacs'

  2- Start a customized Pmv session:

  Double click on the  icon to start a new Pmv session.

  3- Load molecules:

  Load the protease displayed as lines.

  Load the indinavir displayed as cpk and colored by atom type.

Working with PMV

- Interactive Commands:
  - Bind a Command to a mouse picking event.
  - For applying the same command to multiple subsets of atoms.

Altering the representation of subsets of atoms:

ICOM -> displaySticksAndBalls -> ICOM level -> Residue

Working with PMV

- Undo Command:
  - Undo commands stack
  - User preference to set the number of undo.
  - The “Delete Molecule” command voids the undo stack.

File -> Undo “last command executed”

Working with PMV

- “Regular Commands”:
  - Define the current selection:
  - Apply multiple commands to the same current selection.
- Current selection
  - homogeneous
  - empty -> everything is selected

Working with PMV

- Create a selection of Atoms:
  ICOM -> select -> Atom -> pick and drag select in the viewer.
- Change to a selection of Residues:
  Icom level Residue.
- Save the current selection as a set:
  Select -> Save current selection as a set -> set1 -> OK -> Clear selection.

Working with PMV.

- Retrieve the saved selection:
  Select -> Select a set -> set1 -> OK
- Color the selection by atom type and display as sticks and balls.
  Color -> by Atom Type -> lines -> OK
  Un/Display -> sticks and balls -> OK

Surfaces, Ribbons, etc...

- Compute the molecular surface of the protease and alter its representation:
  Clear Selection
  File -> Load Module -> msmsCommands -> Dismiss
  Select -> Select From String -> Molecule List … -> protease -> Select -> Dismiss
  Compute -> Msms For Molecule -> density = 2.0 -> OK
  Color -> by Residue Type -> Rasmol -> msms -> OK
  Clear selection.

  And more ….

Working with PMV at a higher level

- Exercise:

Represent the protease with a standard Ribbon diagram colored by chains.

And more ....

Cool stuffs ...

- Color the surface of the ligand by the closest distance to protease.
- Magic lens.

Application design features

- Dynamic loading of commands
- Python shell for scripting
- Dual interaction mode (GUI/Shell)
- Lightweight commands: Macros
- Command logging
- Dynamic commands (introspection)
- User-preferences / customization

Application design features (cont'd)

- Load multiple molecules
- Hierarchical representation of molecules
- Create/Select homogeneous sets
- Current selection concept
- Commands apply to current selection
- Interactive commands

II - PMV

- Commands
  - Create, delete, write molecules
  - Selection
  - Basic representations and coloring
  - Advanced representations
  - Editing molecules
  - ...

Create, delete, write molecules

- Create:
  - PDBReader
  - Mol2Reader
  - PDBQReader
  - PDBQSReader
  - PQRReader
  - GeneralReader
- Delete
  - deleteMol
- Write
  - PDBWriter

Selection

- From string
- By picking
  - molecule, chain, residue, atom
- By distance
- Displayed lines or cpk
- Invert selection
- On chain
- ...

Basic representations and coloring

- Color geometries by:
  - atom type
  - residue type
    - shapely, Rasmol, N to C
  - chains
  - molecules
  - properties
  - secondary structure type
  - ...
- Display by:
  - lines
  - cpk
  - sticks and balls
  - ...
- Label:
  - by properties

Advanced representations

- MSMS molecular surface
  - compute & display :
    - MSMSMol
    - MSMSSel
- CA trace:
  - compute
  - extrude
  - display
- Spline:
  - compute
  - display
- Secondary Structure:
  - get SS information:
    - from file
    - from stride
  - extrude
    - default (rectangle, circle)
    - circle
    - rectangle
    - ellipse
    - ...
  - display

Editing molecules

- AIDE Module:

(pyBabel reimplementation of some of the Babel v1.6 functionalities)

  - atom type assignment
  - gasteiger charges calculation
  - atom type conversion
  - rings detection
  - bond order assignment
  - aromaticity detection
  - hydrogen atoms addition

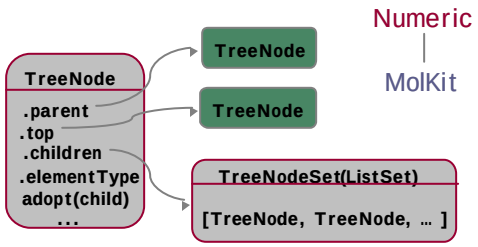
III - From Building Blocks to applications

- MolKit
- DejaVu
- ViewerFramework
- Putting it all together
- Writing a simple command

III - From Building Blocks to applications

- MolKit
  - Hierachical data-structure
  - TreeNodes and TreeNodeSets
  - Derived classes
  - Parsers
  - Examples

Hierachical data-structure



Hierachical structure (cont'd)

- building trees by adoption

```
parent = TreeNode()
child = TreeNode()
parent.adopt(child)
```

- TreeNodeSet slicing and indexing

```
node.children[5]
node.children[10:25]
```

- multi-level hierachy

```
node.children[0].children[-1]
```

- dynamic adding of new members

```
node = TreeNode()
node.newMember = myvalue
```

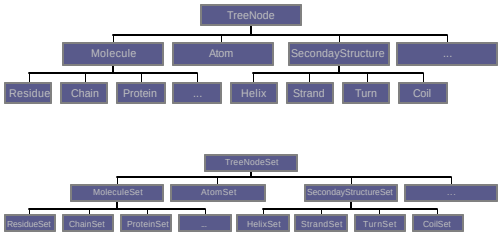
- shortcut to access children's members

```
print node.children.name
['NoName', 'NoName', 'NoName',...]
```

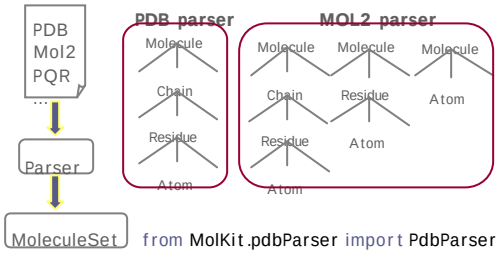
TreeNode, TreeNodeSet

- TreeNodeSet:
  - Boolean operation
  - uniq( )
  - split( )
  - sort( )
  - NodesFromName( )
  - findChildrenOfType( )
  - findParentOfType( )
  - …
- TreeNode:
  - adopt( ) / remove( )
  - full_name( )
  - NodeFromName( )
  - split( ) / merge( )
  - getParentOfType( )
  - findType( )
  - compare( )
  - assignUniqIndex( )
  - isAbove( ) / isBelow( )
  - …

TreeNode and TreeNodeSet specialization



Parsers




```
from MolKit.pdbParser import PdbParser
parser = PdbParser('1crn.pdb')
mols = parser.parse( )
```

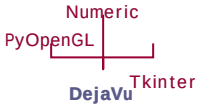
Examples

```
>>> from MolKit import Read
>>> molecules = Read('./1crn.pdb')
>>> mol = molecules[0]            # Read returns a ProteinSet

>>> print mol.chains.residues.name
>>> print mol.chains.residues.atoms[20:85].full_name()

>>> from MolKit.molecule import Atom
>>> allAtoms = mol.findType(Atom)
>>> set1 = allAtoms.get(lambda x: x.temperatureFactor >20)

>>> allResidues = allAtoms.parent.uniq()
>>> import Numeric
>>> for r in allResidues:
...     coords = r.atoms.coords
...     r.geomCenter = Numeric.sum(coords) / len(coords)
```

III - From Building Blocks to applications

- DejaVu
  - Overview
  - Features
  - Geometries
  - DejaVu and MolKit

Overview



DEMO

```
from DejaVu import Viewer
vi = Viewer( )
from DejaVu.Spheres import Spheres
centers = =[[0,0,0],[3,0,0],[0,3,0]]
s = Spheres('sph', centers = centers)
s.Set(quality=10)
vi.AddObject (s)
```

Demo Code

```
>>> from DejaVu import Viewer
>>> vi = Viewer( )
>>> from DejaVu.Spheres import Spheres
>>> centers = =[[0,0,0],[3,0,0],[0,3,0]]
>>> s = Spheres('sph', centers = centers)
>>> s.Set(quality=10)
>>> vi.AddObject(s)
```

Features

- OpenGL Lighting and Material model
- Object hierarchy with transformation and rendering properties inheritance
- Arbitrary clipping planes
- Material editor
- DepthCueing (fog), global anti-aliasing
- glSscissors/magic lens
- Multi-level picking
- Extensible set of geometries

Geometries

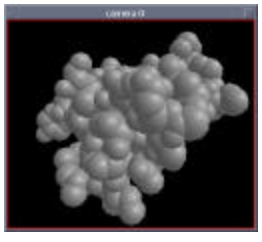
Geom

- PolyLine
- Points
- Spheres
- Labels
- Arc3D...

IndexedGeoms

- IndexedPolyLines
- IndexedPolygoms
- Triangle_Strip
- Quad_Strip
- Cylinders ....

DejaVu and MolKit



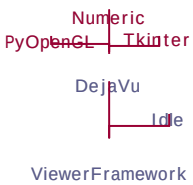
Demo Code

```
>>> from MolKit import Read
>>> molecules = Read('./1crn.pdb')
>>> mol = molecules[0]   # Read returns a ProteinSet
>>> coords = mol.chains.residues.atoms.coords
>>> radii = mol.defaultRadii()
>>> sph = Spheres('sph', centers = coords, radii = radii,
                  quality=10)
>>> vi.AddObject(sph)
```

III - From Building Blocks to applications

- ViewerFramework
  - Overview
  - Design features
  - Implementation

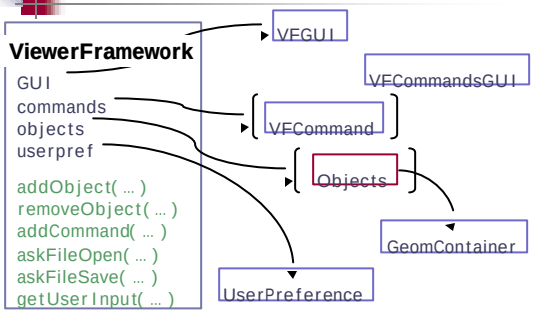
Overview



Design features

- Dynamic loading of commands
- Python shell for scripting
- Dual interaction mode (GUI/Shell)
- Support for command:
  - development, logging, GUI, dependencies
- Lightweight commands: Macros
- Dynamic commands (introspection)
- Extensible set of commands

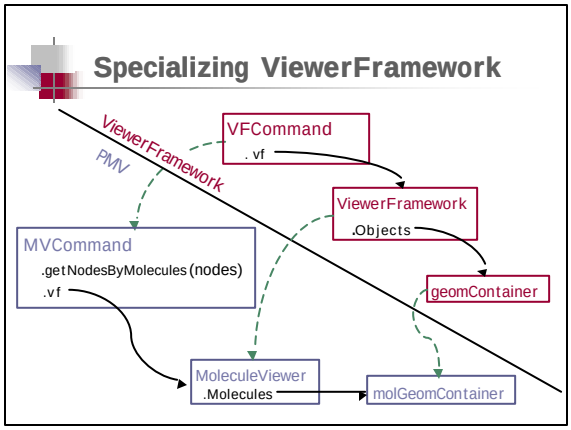
Implementation



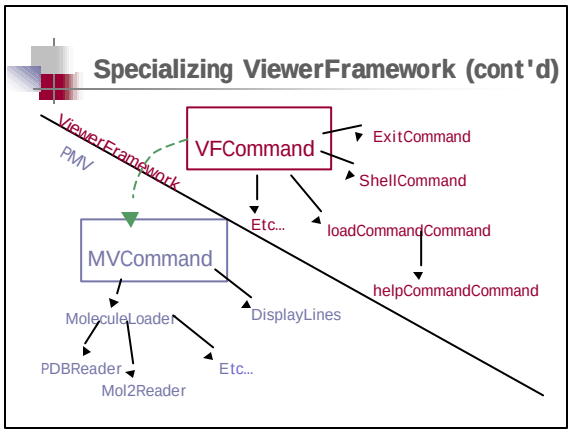
III - From Building Blocks to applications

- Putting it all together:
  - Specializing ViewerFramework
  - MolKit in PMV
  - DejaVu in PMV

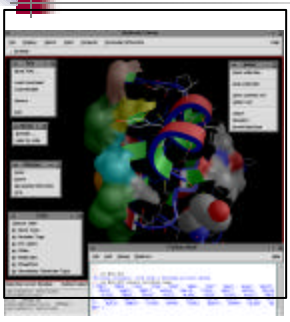
Specializing ViewerFramework

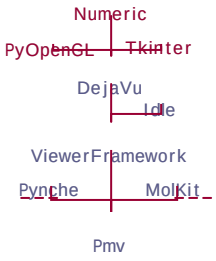


Specializing ViewerFramework (cont'd)



PMV Architecture





MolKit in PMV

```
>>> print mv.Mols
<MoleculeSet instance> holding 2 Protein

>>> mv.Mols[0]
<Protein instance>1crn with 1 MolKit.protein.Chain

>>> from MolKit.protein import Residue
>>> residues = mv.Mols.findType(Residue)
>>> residues
<ResidueSet instance> holding 154 Residue

>>> residues.myIndex = range(len(residues))
>>> residues[1:10].myIndex
[1,2,3,4,5,6,7,8,9]
```

DejaVu in PMV

```
>>> # access to DejaVu features from the pyShell

>>> vi = mv.GUI.VIEWER
>>> camera = vi.cameras[0]
>>> camera.Set( color=(1.,1.,1.) )
>>> vi.Redraw()

>>> # show the Viewer's original GUI
>>> vi.GUI.root.deiconify( )

>>> # hide the Viewer's original GUI
>>> vi.GUI.root.withdraw( )
```

III - From Building Blocks to applications

- Writing a simple command
  - MVCommand overview
  - Subclassing MVCommand
  - Loading the command

MVCommand overview

```
class MyCommand(MVCommand):
    def guiCallback(self, *args, **kw):
        apply( self.doitWrapper, args, kw)

    def doitWrapper(self, *args, **kw):
        self.beforeDoit()
        self.vf.tryto(apply(self.doit,args,kw))
        self.afterDoit()

    def doit(self, *args, **kw):
        pass
```

```
    def __call__(self, *args, **kw):
        apply( self.doitWrapper, args, kw)
```

Subclassing MVCommand

```
from Pmv.mvCommand import MVCommand
class MyReader(MVCommand):
    def guiCallback(self):
        fTypes = [( 'PDB file','*.pdb'), ('PDBQ file','*.pdbq'),
                  ( 'MOL2 file','*.mol2')]
        filename = self.vf.askFileOpen(types= fTypes,
                                       title='Choose molecule file')
        val['redraw']=1
        mol = apply(self.doitWrapper, (filename, ), val)
        return mol
    def __call__(self, filename, **kw):
        if not kw.has_key('redraw'): kw['redraw']=1
        apply(self.doitWrapper, (filename, ) , kw)
    def doit (self, filename):
        from MolKit import Read
        molecules = Read(filename)
        for mol in molecules:  self.vf.addMolecule(mol)
```

Loading the command

Instance of a Command

```
mv.addCommand( MyCommand(),
               'myCommand',
               MyCommandGUI )
```

Command name in PMV.

Instance of a CommandGUI : describes the GUI associated with a command (radiobutton, checkbutton, menu entry ...)

Example

```
>>> from Pmv.myCmd import MyReader
>>> from ViewerFramework.VFCommand import CommandGUI
>>> # Create a menu entry GUI for the command MyReader
>>> MyReaderGUI = CommandGUI()
>>> # Add the GUI to the menuRoot in the File menu
>>> MyReaderGUI.addMenuCommand('menuRoot', 'File',
                               'Read File ...',index=0)
>>> # add the command with its associated GUI, and name to PMV
>>> mv.addCommand(MyReader(),'myread', MyReaderGUI)
```

DEMO

Conclusion

- Validity of the approach
- Python
- Availability
- Future directions

Validity of the approach

- Set of components
  - extensible
  - inter-operable
  - **re-usable**
  - short development cycle
- User base expanding beyond our lab.
- Components re-use outside the field of structural biology

Python

- Appropriate language for this approach
  - modularity, extensibility, dynamic loading, object-oriented, virtually on any platform, many extensions from third party
- Rapidly growing community of programmers using Python for biological applications
- Short comings
  - reference counting, distribution mechanism, no strong typing

Availability

- Modularity enables fine grain licensing schemes (a la carte)
- Core modules are freely available
- Online Download site:
  http://www.scripps.edu/~sanner/Python

Future directions

- Add support for editing molecular structures (i.e. mutations, deletion, addition)
- Interface with MMTK, Tinker, ...
- Enhance documentation and tutorials
- Setup a CVS server for programmers wanting to help !
- Too many to list ....

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