Xplor-NIH: Recent Developments

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outline

1. description, history
2. Scripting Languages: XPLOR, Python, TCL
   - Introduction to Python
3. Potential terms available from Python
4. IVM: dynamics and minimization in internal coordinates
5. Parallel determination of multiple structures
   - Using the Biowulf cluster
6. VMD molecular graphics interface
7. line-by-line analysis of an Xplor-NIH Python script

goal of this class:
Xplor-NIH's Python interface will be introduced, described in enough detail such that scripts can be understood, and modified.

What is Xplor-NIH?

Biomolecular structure determination/manipulation

- Determine structure using minimization protocols based on molecular dynamics/ simulated annealing.

- Potential energy terms:
  - terms based on input from NMR (and X-ray) experiments: NOE, dipolar coupling, chemical shift data, etc.
  - other potential terms enforce reasonable covalent geometry (bonds and angles).
  - knowledge-based potential terms incorporate info from structure database.

- includes: program, topology, covalent parameters , potential energy parameters, databases for knowledge-based potentials.
  [in the future: protocols.]

Automatic NOE Assignment:
John K's MARVIN/PASD auto-assignment facility.

Description

Source code of Xplor-NIH:

- original XPLOR Fortran source, with contributions from many groups.
- current work uses C++ for compute-intensive work.
- scripts and much code are written in Python, TCL scripting languanges.
- SWIG used to “glue” scripting languanges to C++.

What Xplor-NIH is not

Not general purpose molecular dynamics engine. Major deficiency: no Ewald summation for long-range electrostatic potentials. Use CHARMM, Amber, Gromacs, or NAMD.

Crystallography tools are dated. CNS X-ray facilities are more up-to-date.
But, CNS no longer under development, and its NMR facilities are dated.
$\rightarrow$ use Xplor-NIH for NMR structure determination.

Not an NMR spectrum analysis tool.
[future: tighter integration with tools such as NMRWish.]

Scripting Languages- three choices

scripting language:

- flexible interpreted language
- used to input filenames, parameters, protocols
- flexible enough to program non compute-intensive logic
- relatively user-friendly

XPLOR language:

strong point:

selection language quite powerful.

weaknesses:

String, Math support problematic.

no support for functions/subroutines.

Parser is hand-coded in Fortran: difficult to update.

NOTE: all old XPLOR scripts should run unchanged in Xplor-NIH.

general purpose scripting languages: Python and TCL

- excellent string support.
- languages have functions and modules: can be used to better encapsulate protocols (e.g. call a function to perform simulated annealing.)
- well known: these languages are useful for other computing needs: replacements for AWK, shell scripting, etc.
- Facilitate interaction, tighter coupling with other tools.
  - NMRWish has a TCL interface.
  - pyMol has a Python interface.
  - VMD has TCL and Python interfaces.

separate processing of input files (assignment tables) is unnecessary: can all be done using Xplor-NIH.

New development in C++: scripting interfaces (semi-)automatically generated using a tool called SWIG.

Introduction to Python

assignment and strings

```
a = 'a string'   # <- pound char introduces a comment
a = "a string"   # ' and " chars have same functionality
```

multiline strings - use three ' or " characters

```
a = '''a multiline
string'''
```

raw strings - special characters are not translated

```
a = r'strange characters: \%~!'  # introduced by an r
```

C-style string formatting - uses the % operator

```
s = "a float: %5.2f   an integer: %d" % (3.14159, 42)
print s
a float:  3.14   an integer: 42
```

lists and tuples

```
l = [1,2,3]           #create a list
a = l[1]              #indexed from 0 (l = 2)
l[2] = 42             # l is now [1,2,42]
t = (1,2,3)           #create a tuple (read-only list)
a = t[1]              # a = 2
t[2] = 42             # ERROR!
```

Introduction to Python

calling functions

```
bigger = max(4,5)  # max is a built-in function
```

defining functions - whitespace scoping

```
def sum(a,b):
    "return the sum of a and b"    # comment string
    retVal = a+b                   # note indentation
    return retVal

print sum(42,1)                    #un-indented line: not in function
43
```

loops - the for statement

```
for cnt in range(0,3):
    cnt += 10
    print cnt
10
11
12
```

Introduction to Python

Python is modular

most functions live in separate namespaces called modules

The import statement - loading modules

```
import sys          #import module sys
sys.exit(0)         #call the function exit in module sys
```

or:

```
from sys import exit  #import exit function from sys into current scope
exit(0)               #don't need to prepend sys.
```

Introduction to Python

In Python objects are everywhere.

Objects: calling methods

```
file = open("filename")    #open is built-in function returning an object
contents = file.read()     #read is a method of this object
                           # returns a string containing file contents
dir(file)                  # list all methods of file
['__class__', '__delattr__', '__doc__', '__getattribute__',
  '__hash__', '__init__', '__iter__', '__new__', '__reduce__',
  '__repr__', '__setattr__', '__str__', 'close', 'closed', 'fileno',
  'flush', 'isatty', 'mode', 'name', 'read', 'readinto', 'readline',
  'readlines', 'seek', 'softspace', 'tell', 'truncate', 'write',
  'writelines', 'xreadlines']
```

Introduction to Python

Tools for List Processing:

map - convert one list to another list:

```
map(int, ['1','2','3'])   # apply int() function to list of strings
\begin{pythout}
[1, 2, 3]
\end{pythout}

\pause

lambda - a simple function with no name
\begin{python}
twoTimes=lambda x: 2*x  # define twoTimes to be a lambda function
twoTimes(3)
6
```

lambdas are useful when used with map:

```
map(lambda c: 2*int(c), ['1','2','3'])  # convert string list to ints
                                        # with multiplication
[2, 4, 6]
```

Introduction to Python

interactive help functionality: `dir()` is your friend!

```
import sys
dir(sys)    #lists names in module sys
dir()       # list names in current (global) namespace
dir(1)      # list of methods of an integer object
```

the help function

```
import ivm
help( ivm )         #help on the ivm module
help(open)          # help on the built-in function open
```

browse the Xplor-NIH python library on your local workstation:

from the command-line:

```
% xplor -py -pydoc -g
```

Python in Xplor-NIH

current status: low-level functionality (similar to that of XPLOR script) implemented.

mostly implemented: high-level wrapper functions which will encode default values, and hide complexity.

future: develop repository of still-higher level protocols to further simplify structure determination.

stability: Python interface fairly stable. Small changes possible.

Accessing Xplor-NIH's Python interpreter

from the command-line: use the -py flag:

```
% xplor -py

                       XPLOR-NIH version 2.9.8

 C.D. Schwieters, J.J.  Kuszewski,       based on X-PLOR 3.851 by A.T. Brunger
 N. Tjandra, and G.M. Clore
 J. Magn. Res., 160, 66-74 (2003).       http://nmr.cit.nih.gov/xplor-nih

python>
```

or the pyXplor executable - a bit quieter- and can be used as a complete replacement for the python command:

```
% pyXplor

python>
```

or as an extension to an external Python interpreter:

```
% ( eval `xplor -csh-env` ; python)

Python 2.3.3 (#1, Feb 11 2004, 14:56:19)
[GCC 3.2.3] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>> import xplorNIH
>>> execfile('script.py')
```

accessing Python from XPLOR: PYTHon command

```
X-PLOR>python           !NOTE: can’t be used inside an XPLOR loop!
python> print ’hello world!’
hello world!
python> python_end()
X-PLOR>
```

for a single line: CPYThon command

```
X-PLOR>cpython "print ’hello world!’"   !can be used in a loop
hello world!
X-PLOR>
```

using XPLOR, TCL from Python

to call the XPLOR interpreter from Python

```
xplor.command('''struct @1gb1.psf end
                 coor @1gb1.pdb''')
```

`xplor` is a built-in module - no need to import it

to call the TCL interpreter from Python

```
from tclInterp import TCLInterp               #import function
tcl = TCLInterp()                             #create TCLInterp object
tcl.command('xplorSim setRandomSeed 778') #initialize random seed
```

Atom Selections in Python

use the XPLOR atom selection language.

```
from atomSel import AtomSel
sel = AtomSel('''resid 22:30 and
                 (name CA or name C or name N)''')
print sel.string()          #AtomSel objs remember their selection string
resid 22:30 and
                 (name CA or name C or name N)
```

AtomSel objects can be used as lists of Atom objects

```
print len(sel)             # prints number of atoms in sel
for atom in sel:           # iterate through atoms in sel
   print atom.string(), atom.pos()
```

prints a string identifying the atom, and its position.

Using potential terms in Python

available potential terms in the following modules:

1. rdcPot - dipolar coupling
2. csaPot - Chemical Shift Anisotropy
3. noePot - NOE distance restraints
4. jCoupPot - ^{3}J-coupling
5. prePot - Paramagnetic relaxation enhancement
6. xplorPot - use XPLOR potential terms
7. potList - a collection of potential terms

all potential objects have the following methods:

instanceName()	-	name given by user
potName()	-	name of potential term, e.g. "RDCPot"
scale()	-	scale factor or weight
setScale(val)	-	set this weight
calcEnergy()	-	calculate and return term's energy

residual dipolar coupling potential

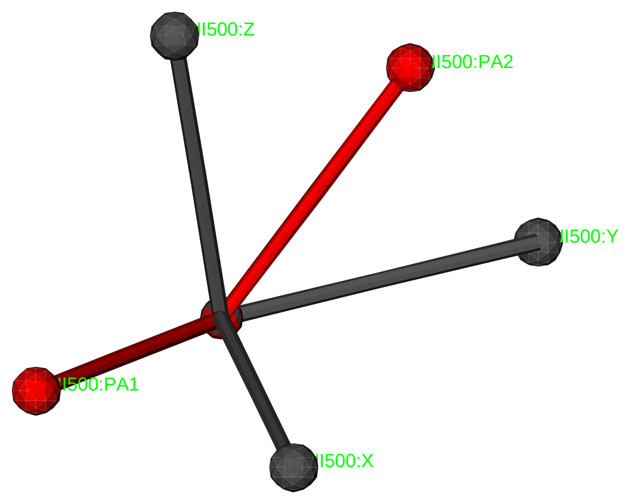
Provides orientational information relative to axis fixed in molecule frame.

$$\delta_{\text{calc}} = D_a[(3u_z^2 - 1) + \frac{3}{2}R(u_x^2 - u_y^2)] ,$$

u_x, u_y, u_z- projection of bond vector onto axes of tensor describing orientation. D_a, R- measure of axial and rhombic tensor components.

rdcPot (in Python)

- tensor orientation encoded in four axis atoms
- allows Da, R to vary: values encoded using extra atoms.
- reads both SANI and DIPO XPLOR assignment tables.
- allows multiple assignments for bond-vector atoms - for averaging.
- allows ignoring sign of D_a (optional)
- can (optionally) include distance dependence: $D_a \propto 1/r^3$.



How to use the rdcPot potential

```
from varTensorTools import create_VarTensor, calcTensor
btensor = create_VarTensor('phage')   #create a tensor object

btensor.setDa(7.8)          #set initial tensor Da, rhombicity
btensor.setRh(0.3)
btensor.setFreedom('varyDa, varyRh') #allow Da, Rh to vary

from rdcPotTools import create_RDCPot
rdcNH = create_RDCPot("NH",oTensor=btensor,file='NH.tbl')

calcTensor(btensor)         #calc tensor parameters from current structure
```

NOTE: no need to have psf files or coordinates for axis/parameter atoms- this is automatic.

analysis, accessing potential values:

```
print rdcNH.instanceName()                # prints 'NH'
print rdcNH.potName()                     # prints 'RDCPot'
print rdcNH.rms(), rdcNH.violations()     # calculates and prints rms, violations
print btensor.Da(), btensor.Rh()          # prints these tensor quantities
rdcNH.setThreshold(0)                     # violation threshold
print rdcNH.showViolations()              # print out list of violated terms
from rdcPotTools import Rfactor
print Rfactor(rdcNH)                      # calculate and print a quality factor
```

RDCPot: additional details

using multiple media:

```
btensor=create_VarTensor('bicelle')
rdcNH_2 = create_RDCPot("NH_2",tensor=btensor,file='NH_2.tbl')
#[ set initial tensor parameters ]
btensor.setFreedom('fixAxisTo phage') #orientation same as phage
                                      #Da, Rh vary
```

multiple expts. single medium:

```
rdcCAHA = create_RDCPot("CAHA",oTensor=ptensor,file='CAHA.tbl')
```

`rdcCAHA` is a new potential term using the same alignment tensor as `rdcNH`.

Scaling convention: scale factor of non-NH terms is determined using the experimental error relative to the NH term:

```
scale_toNH(rdcCAHA,'CAHA')   #rescales RDC prefactor relative to NH
scale = (5/2)**2
      #  ^ inverse error in expt. measurement relative to that for NH
rdcCAHA.setScale( scale )
```

Chemical Shift Anisotropy potential

Provides additional orientational information from the full chemical shift tensor.

$$\Delta\delta = \sum_{i,j} A_i \sigma_j \cos^2(\theta_{i,j})$$

A_i - a principal moment of the orientation tensor
σ_j - a principal moment of the CSA tensor
$\theta_{i,j}$ - angle between the i^{th} orientation tensor principal axis and the j^{th} CSA tensor principal axis.

How to use the csaPot potential

```
from csaPotTools import create_CSAPot
csaP = create_CSAPot(name,oTensor=tensor,file='csaP.tbl')

csaP.setDaScale( scaleToRDCnormalization )
csaP.setScale( forceConstant )
calcTensor(tensor)          #use if the structure is approximately correct
```

NOTE: `create_CSAPot` determines the atom type involved and uses built-in values for the chemical shift tensor. Alternate values can be specified by modifying csaPotTools.csaData.

NOE potential term

most commonly used effective NOE distance (sum averaging):

$$R = (\sum_{ij} |q_i - q_j|^{-6})^{-1/6}$$

Python potential in module noePot

- reads XPLOR-style NOE tables.
- potential object has methods to set averaging type, potential type, etc.

creating an NOEPot object:

```
from noePot import NOEPot
noe = NOEPot('noe', open('noe_all.tbl').read() )
```

analysis:

```
print noe.rms()
noe.setThreshold( 0.1 )          # violation threshold
print noe.violations()           # number of violations
print noe.showViolations()
```

J-coupling potential

$$^{3}J = A\cos^2(\theta+\theta^*) + B\cos(\theta+\theta^*) + C,$$

θ is a torsion angle.
A, B, C and θ^* are set using the COEF statement in the j-coupling assignment table (or using object methods).

Use in Python

```
from jCoupPot import JCoupPot
Jhnha = JCoupPot('hnha',open('jna_coup.tbl').read())
jCoup.setA(15.3)                   #set Karplus relationship parameters
jCoup.setB(-6.1)
jCoup.setC(1.6)
jCoup.setPhase(0)
```

analysis:

```
print Jhnha.rms()
print Jhnha.violations()
print Jhnha.showViolations()
```

using XPLOR potentials

Example using a Radius of Gyration (COLLapse) potential

```
import protocol
from xplorPot import XplorPot
protocol.initCollapse('resid 3:72')     #specify globular portion
rGyr = XplorPot('COLL')
xplor.command('collapse scale 0.1 end') #manipulate in XPLOR interface
```

accessing associated values

```
print rGyr.calcEnergy().energy      #term's energy
print rGyr.potName()                # 'XplorPot'
print rGyr.instanceName()           # 'COLL'
```

all other access/analysis done from XPLOR interface.

Commonly used XPLOR terms: VDW, BOND, ANGL, IMPR, RAMA, HBDA, CDHI

collections of potentials - PotList

potential terms which is a collection of Pots:

```
from potList import PotList
pots = PotList()
pots.append(noe); pots.append(Jhnha); pots.append(rGyr)
pots.calcEnergy().energy                              # total energy
```

nested PotLists:

```
rdcs = PotList('rdcs')                    #convenient to collect like terms
rdcs.append( rdcNH ); rdcs.append( rdcNH_2 )
pots.append( rdcs )
for pot in pots:                          #pots looks like a list
    print pot.instanceName()
noe
hnha
COLL
rdcs
```

The IVM (internal variable module)

Used for dynamics and minimization

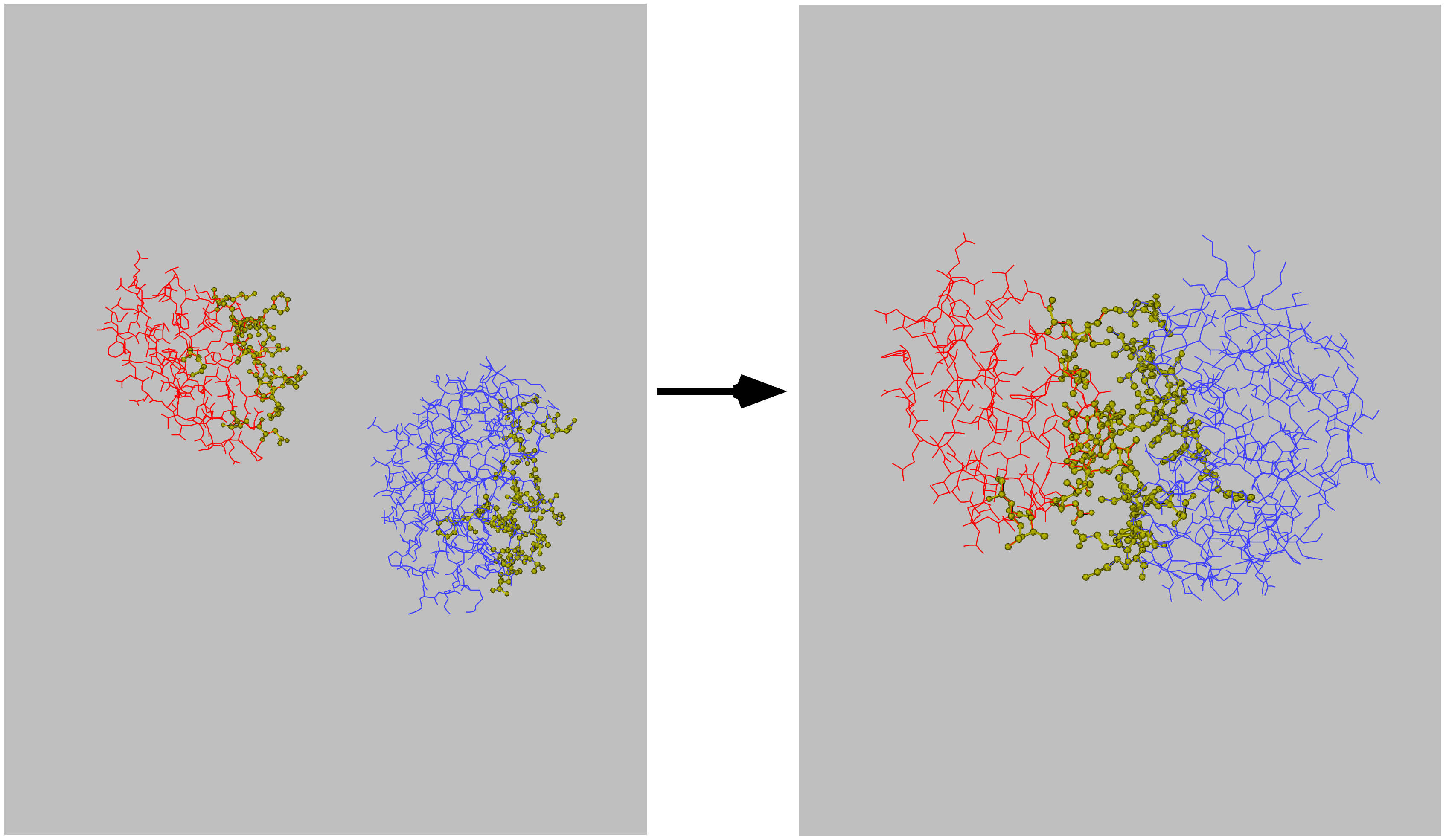
in biomolecular NMR structure determination, many internal coordinates are known or presumed to take usual values:

- bond lengths, angles.
- aromatic amino acid sidechain regions
- nucleic acid base regions
- non-interfacial regions of protein and nucleic acid complexes (component structures may be known- only interface needs to be determined)

Can we take advantage of this knowledge (find the minima more efficiently)?

- can take larger MD timesteps (without high freq bond stretching)
- configuration space to search is smaller:
  $N_{\text{torsion angles}} \sim 1/3 N_{\text{Cartesian coordinates}}$

Hierarchical Refinement of the Enzyme II/ HPr complex



active degrees of freedom are displayed in yellow.

MD in internal coordinates is nontrivial

Consider Newton's equation:

$$F = Ma$$

for MD, we need a, the acceleration in internal coordinates, given forces F.

Problems:

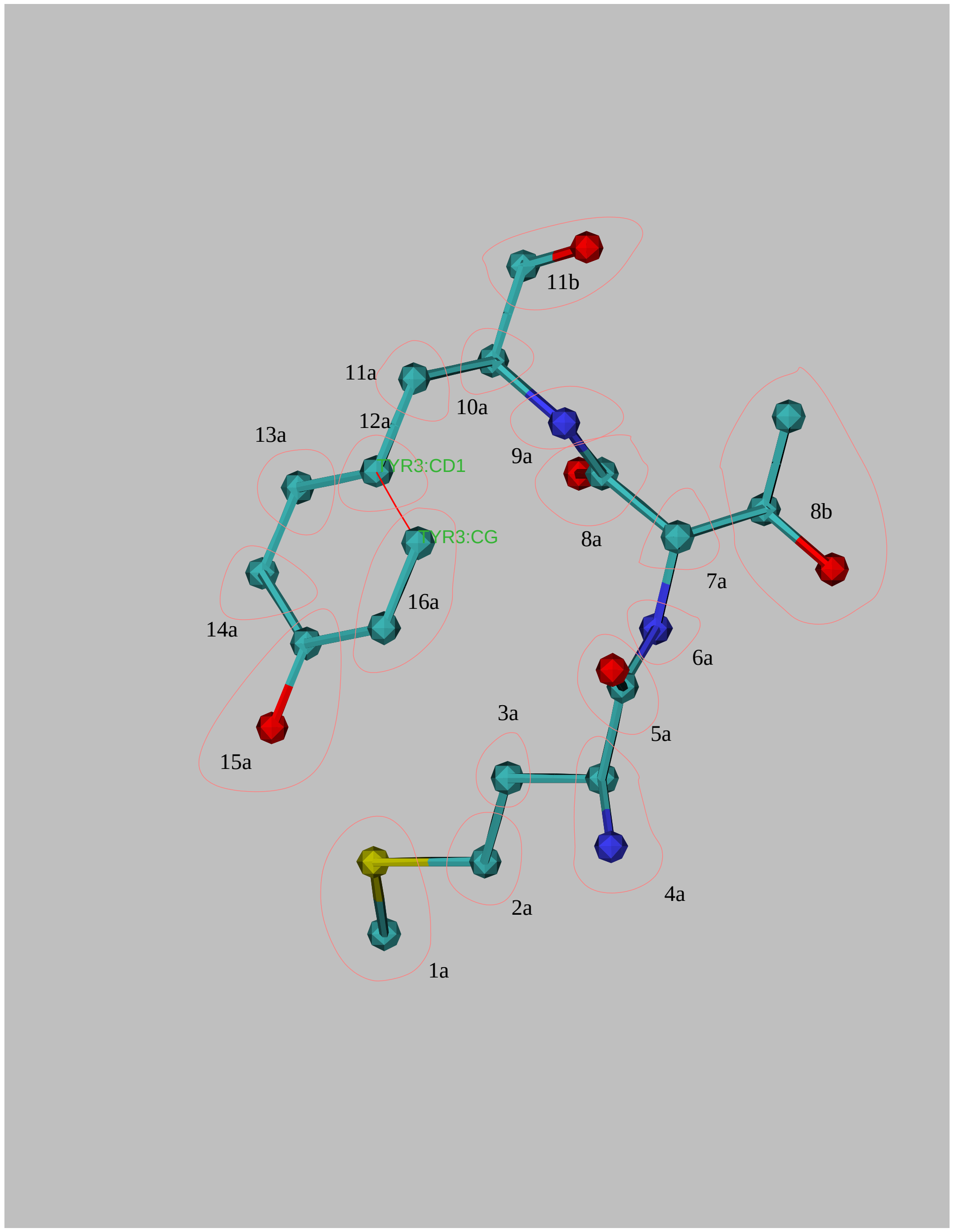
- express forces in internal coordinates
- solve the equation for a.

In Cartesian coordinates a is (vector of) atomic accelerations. M is diagonal.

In internal coordinates M is full and varies as a function of time: solving for a scales as $N^3_{\text{internal coordinates}}$.

Solution: comes to us from the robotics community. Involves clever solution of Newton's equation: The molecule is decomposed into a tree structure, a is solved for by iterating from trunk to branches, and backwards.

Tree Structure of a Molecule



atoms are placed in rigid bodies, fixed with respect to each other.

between the rigid bodies are “hinges” which allow appropriate motion

rings and other closed loops are broken- replaced with a bond.

Topology Setup

torsion angle dynamics with fixed region:

```
from ivm import IVM
integrator = IVM()                                #create an IVM object
integrator.fix( AtomSel("resid 100:120") )        # these atoms are fixed
                                                  # relative to each other

import protocol
protocol.torsionTopology(integrator)              # group rigid sidechain regions
                                                  # break proline rings
                                                  # group and setup all remaining
                                                  #  degrees of freedom for
                                                  #  torsion angle dynamics
```

RDC topology setup - for tensor atoms

tensor axis should rotate only - not translate.

only single dof of D_a and Rh parameter atoms is significant.

```
from varTensorTools import topologySetup
topologySetup(integrator,listOfVarTensors)    #call before protocol.torsionTopology()
```

IVM Implementation details:

other coordinates also possible: e.g. mixing Cartesian, rigid body and torsion angle motions.

convenient features:

- variable-size timestep algorithm
- will also perform minimization
- facility to constrain bonds which cause loops in tree.

full example script in eginputs/protG/anneal.py of the Xplor-NIH distribution.

dynamics with variable timestep

```
import protocol
bathTemp=2000
protocol.initDynamics(ivm=integrator,       #note: keyword arguments
                      bathTemp=bathTemp,
                      finalTime=1,          # will use variable timestep al
                      printInterval=10,     # print info every ten steps
                      potList=pots)

integrator.run()          #perform dynamics
```

parallel computation of multiple structures

computation of multiple structures with different initial velocities and/or coordinates: gives idea of precision of NMR structure.

```
xplor -parallel -machines <machine file>
```

convenient Xplor-NIH parallelization

- spawns multiple versions of xplor on multiple machines via ssh or rsh.
- structure and log files collected in the current local directory.

requirements:

- ability to login to remote nodes via ssh or rsh, without password
- shared filesystem which looks the same to each node

following environment variables set: `XPLOR_NUM_PROCESSES`, `XPLOR_PROCESS`

example script skeleton

```
from simulationTools import StructureLoop
from pdbTool import PDBTool

def calcOneStructure( structData ):
    # [ get initial coordinates, randomize velocities ]
    # [ high temp dynamics ]
    # [ cooling loop ]
    # [ final minimization ]
    # [ analysis ]
    structData.pdbFile().write()  #write out a structure

simWorld.setRandomSeed( 785 )
outPDBFilename = 'SCRIPT_STRUCTURE.sa'
#SCRIPT -> replaced with the name of the input script (e.g. 'anneal.py')
#STRUCTURE -> replaced with the number of the current structure

StructureLoop(numStructures=100,
              pdbTemplate=outPDBFilename,
              structLoopAction=calcOneStructure).run()
```

`StructureLoop` transparently takes care of parallelization.

Using Biowulf

how to get a Biowulf account:
`http://biowulf.nih.gov/user_guide.html#account`

on Biowulf, compute jobs are managed using the PBS queuing system:
`http://biowulf.nih.gov/user_guide.html#q`

submit jobs using `qsub`:

```
qsub -l nodes=4 xplor.pbs
```

note that each node has two CPUs.

example Biowulf PBS script:
`http://nmr.cit.nih.gov/xplor-nih/nih/xplor.pbs`

Refinement against an ensemble

```
esim = EnsembleSimulation('ensemble',3)  #creates a 3-membered ensemble
```

creates two extra copies of the current atom positions, velocities, *etc*.

Ensemble members don't interact, except with explicit potential terms.

Energy terms:
AvePot- average over the ensemble with no intra-ensemble interactions.

```
from avePot import AvePot
aveBond=AvePot(XplorPot,'bond') # ensemble averaged bond energy
```

aveBond's energy is $\langle E_{\mathrm{BOND}} \rangle$ averaged over the ensemble.

Refinement against an ensemble

most NMR observables must be averaged appropriately- AvePot is not appropriate.

For example, the appropriate RDC value is $\langle\delta_{\text{calc}}\rangle$ averaged over the ensemble. The resulting energy is then $E(\langle\delta_{\text{calc}}\rangle)$.

Energy terms which are ensemble aware: rdcPot, csaPot, noePot, jCoupPot, potList.

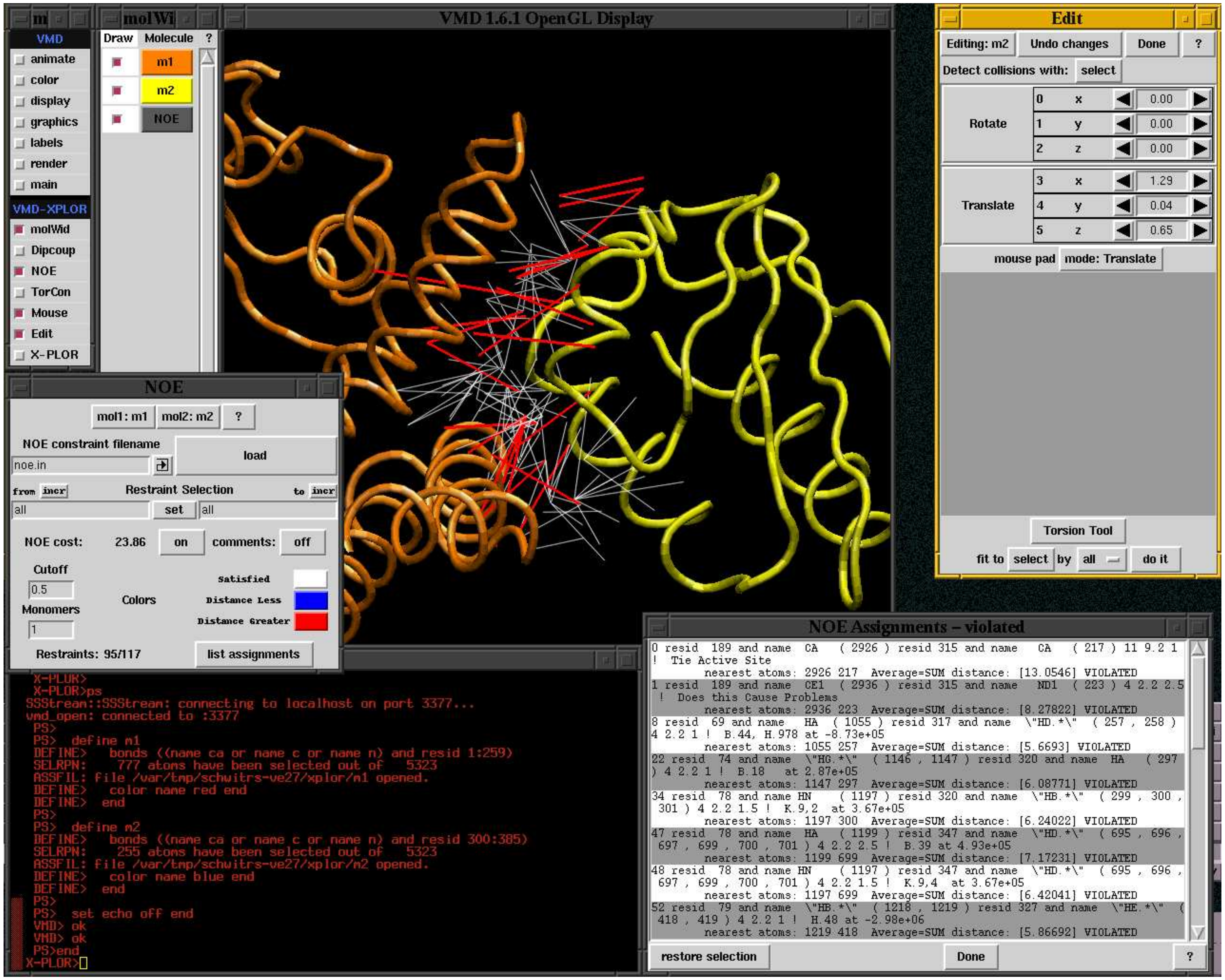
New potential term: NCSPot - restrains atom positions within an ensemble - so members don't drift too far apart.

Example: restrain the positions of C_α atoms to be the same in all members of the ensemble.

```
ncs = NCSPot("ncs","name CA") # create term
ncs.setScale( 100.0 )
ncs.setPotType( "square" )    # harmonic potential has a flat region
ncs.setTol( 0.3 )             # 1/2-width of flat region
```

Feature: ensemble calculations can be parallelized by specifying the `-num_threads` option to the `xplor` script.

VMD interface



Editing: m2

Detect collisions with: select

Rotate: 0 x 0.00; 1 y 0.00; 2 z 0.00

Translate: 3 x 1.29; 4 y 0.04; 5 z 0.65

mode: Translate

NOE constraint filename: noe.in

Restraint Selection: from all; to all

NOE cost: 23.86 on

comments: off

Cutoff: 0.5

Monomers: 1

Satisfied ⬜

Distance Less 🟦

Distance Greater 🟥

Restraints: 95/117

```
  X-PLOR>
  X-PLOR>ps
 SSStream::SSStream: connecting to localhost on port 3377...
 vmd_open: connected to :3377
  PS>
  PS>  define m1
  DEFINE>   bonds ((name ca or name c or name n) and resid 1:259)
  SELRPN:    777 atoms have been selected out of   5323
  ASSFIL: file /var/tmp/schwitrs-ve27/xplor/m1 opened.
  DEFINE>   color name red end
  DEFINE>  end
  PS>
  PS>  define m2
  DEFINE>   bonds ((name ca or name c or name n) and resid 300:385)
  SELRPN:    255 atoms have been selected out of   5323
  ASSFIL: file /var/tmp/schwitrs-ve27/xplor/m2 opened.
  DEFINE>   color name blue end
  DEFINE>  end
  PS>
  PS>  set echo off end
  VMD> ok
  VMD> ok
  PS>end
 X-PLOR>
```

```
0 resid  189 and name  CA   ( 2926 ) resid 315 and name   CA   ( 217 ) 11 9.2 1
!  Tie Active Site
        nearest atoms: 2926 217  Average=SUM distance: [13.0546] VIOLATED
1 resid  189 and name  CE1  ( 2936 ) resid 315 and name   ND1  ( 223 ) 4 2.2 2.5
 !  Does this Cause Problems
        nearest atoms: 2936 223  Average=SUM distance: [8.27822] VIOLATED
8 resid  69 and name   HA  ( 1055 ) resid 317 and name  \"HD.*\"  ( 257 , 258 )
4 2.2 1 !  B.44, H.978 at -8.73e+05
        nearest atoms: 1055 257  Average=SUM distance: [5.6693] VIOLATED
22 resid  74 and name  \"HG.*\"  ( 1146 , 1147 ) resid 320 and name  HA   ( 297
) 4 2.2 1 !  B.18   at 2.87e+05
        nearest atoms: 1147 297  Average=SUM distance: [6.08771] VIOLATED
34 resid  78 and name HN    ( 1197 ) resid 320 and name  \"HB.*\"  ( 299 , 300 ,
 301 ) 4 2.2 1.5 !  K.9,2  at 3.67e+05
        nearest atoms: 1197 300  Average=SUM distance: [6.24022] VIOLATED
47 resid  78 and name  HA   ( 1199 ) resid 347 and name  \"HD.*\"  ( 695 , 696 ,
 697 , 699 , 700 , 701 ) 4 2.2 2.5 !  B.39 at 4.93e+05
        nearest atoms: 1199 699  Average=SUM distance: [7.17231] VIOLATED
48 resid  78 and name HN    ( 1197 ) resid 347 and name  \"HD.*\"  ( 695 , 696 ,
 697 , 699 , 700 , 701 ) 4 2.2 1.5 !  K.9,4  at 3.67e+05
        nearest atoms: 1197 699  Average=SUM distance: [6.42041] VIOLATED
52 resid  79 and name  \"HB.*\"  ( 1218 , 1219 ) resid 327 and name  \"HE.*\"  (
 418 , 419 ) 4 2.2 1 !  H.48 at -2.98e+06
        nearest atoms: 1219 418  Average=SUM distance: [5.86692] VIOLATED
```

vmd-xplor screenshot

Use VMD-XPLOR to

- visualize molecular structures
- visualize restraint info
- manually edit structures

command-line invocation of separate Xplor-NIH and VMD-XPLOR jobs:

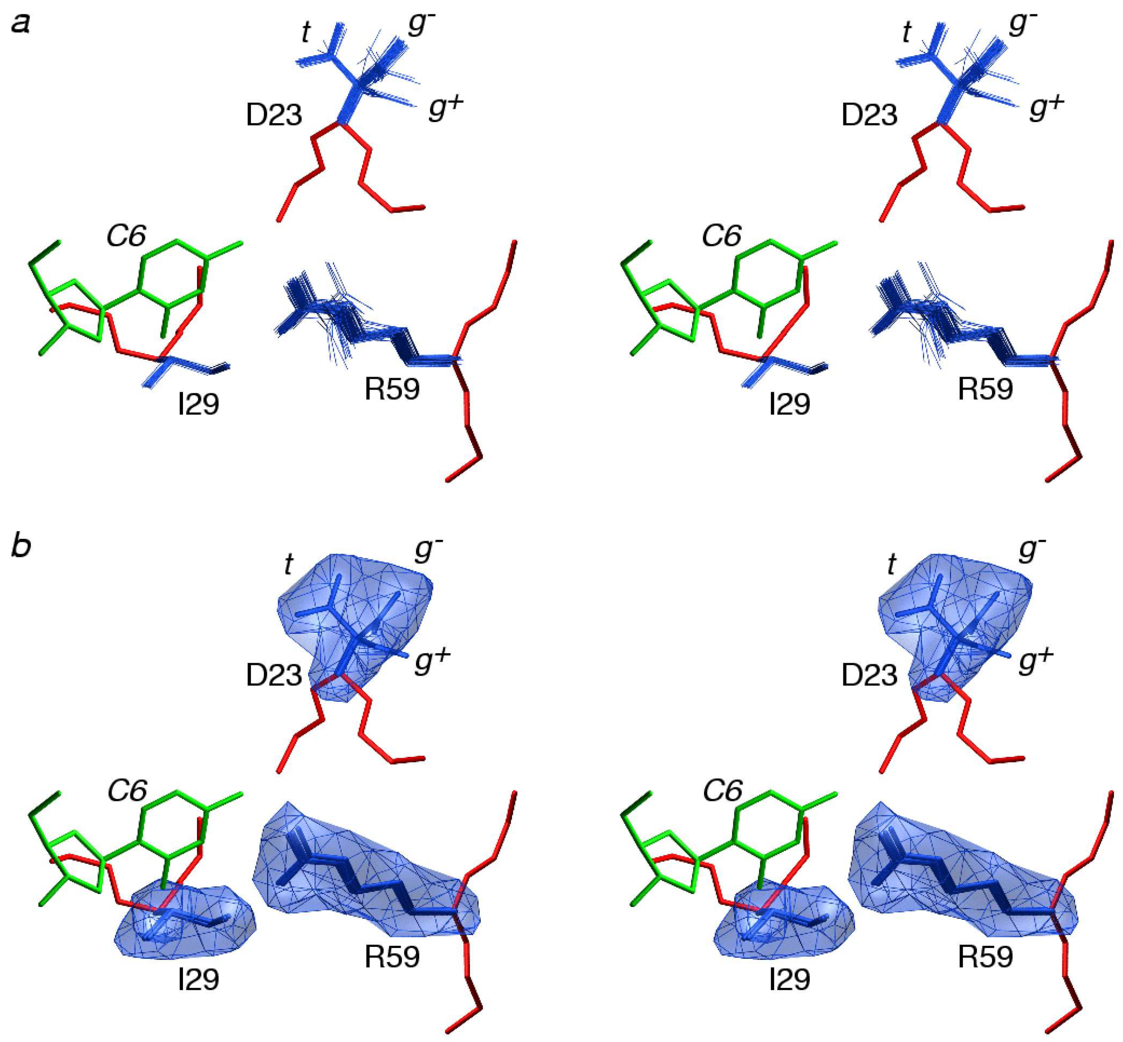
```
% vmd-xplor -port 3359 -noxplor
% xplor -port 3359 -py
```

Xplor-NIH snippet to draw bonds between backbone atoms, and labels:

```
import vmdInter

vmd = VMDInter()
x = vmd.makeObj("x")
x.bonds( AtomSel("name ca or name c or name n") )
label = vmd.makeObj("label")
label.labels( AtomSel("name ca") )
```

Graphical Representation of ensembles



intelligently convert ensemble of structures into a probability distribution.

Convenience Scripts

pdb2psf - generate a psf from a PDB file. Convenient when working from the PDB database.

```
% pdb2psf 1gb1.pdb
```

creates 1gb1.psf.
Please send us pdb files which fail.

seq2psf - generate a psf file from primary sequence.

```
% seq2psf -segname PROT -startresid 300 -protein protG.seq
```

creates protG.psf with segid PROT starting with residue id 300.

Putting it together: a full script

Full script for refining protein G from a random extended chain, using NOEs, RDCs, Jcoup data.

`http://nmr.cit.nih.gov/xplor-nih/doc/current/python/anneal.py.html`

Also available in the Xplor-NIH distribution in as eginput/protG/anneal.py

Where to go for help

online:

`http://nmr.cit.nih.gov/xplor-nih/`	-	home page
xplor-nih@nmr.cit.nih.gov	-	mailing list
`http://nmr.cit.nih.gov/xplor-nih/faq.html`	-	FAQ
`http://nmr.cit.nih.gov/xplor-nih/doc/current/`	-	current Documentation including XPLOR manual

subdirectories within the xplor distribution:

eginputs	-	newer complete example scripts
tutorial	-	respository of XPLOR scripts
helplib	-	help files
helplib/faq	-	frequently asked questions

Python:
M. Lutz and D. Ascher, "Learning Python, 2th Edition" (O'Reilly, 2004); `http://python.org`

TCL:
J.K. Ousterhout "TCL and the TK Toolkit" (Addison Wesley, 1994); `http://www.tcl.tk`

Please complain! and suggest!