MD projections: PLUMED GUI & MDTraj

Toni Giorgino
National Research Council of Italy
toni.giorgino@cnr.it
www.giorginolab.it

GitHub
@giorginolab

Thesis projects available

github.com/giorginolab/
MD-Trajectory-Tutorial-UniPD-2022

University of Padova c/o Prof. Fuxreiter
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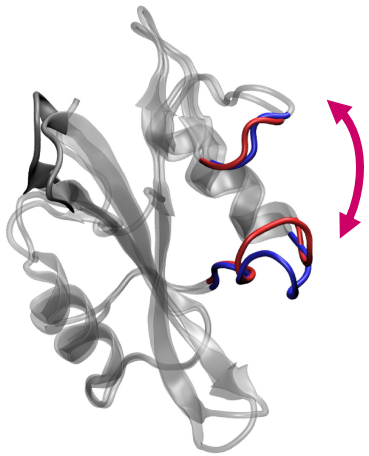
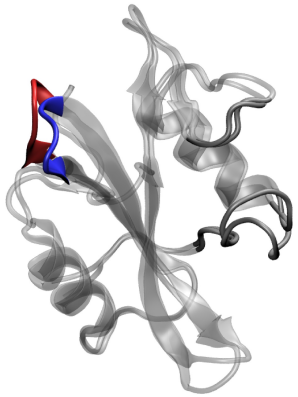
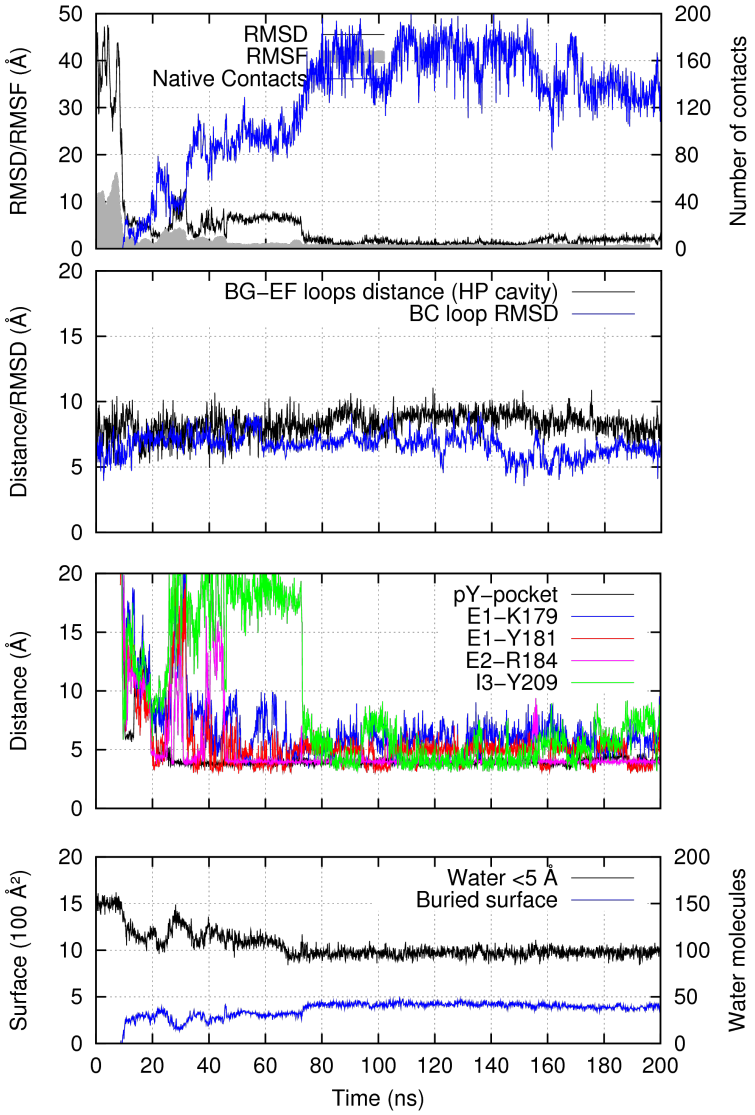
Part I – PLUMED & PLUMED-GUI

Part II – Python + MDTraj

Rationale for a Plumed-GUI







- Local RMSD
- Contacts
- Native contacts
- Hydration
- …

All of them seem good ideas… until you try them

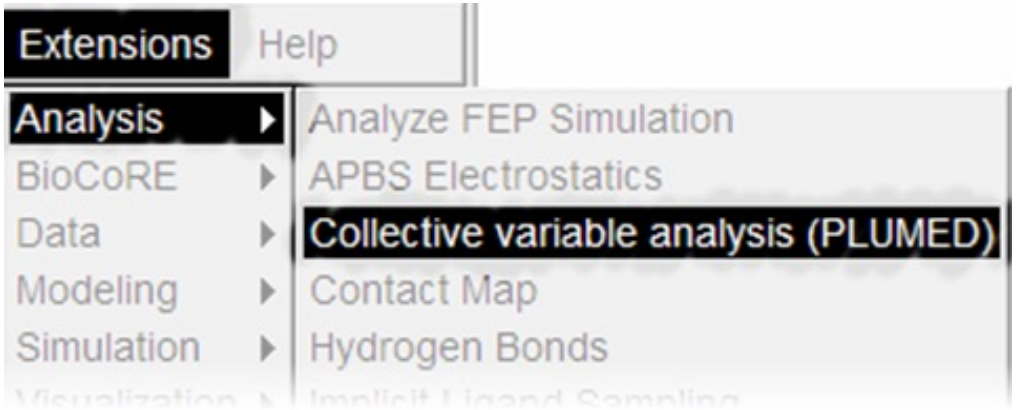
Giorgino et al., JCTC 2012

Managed if we had…

1. A common, *concise* language to define all observables

PLUMED

2. An interface to quickly code, click, and check



Generalized forces in biased sampling

$$f(\mathbf{x}) = f(\mathbf{x}_1, \ldots, \mathbf{x}_n)$$

A collective variable (CV)

$$V(\mathbf{x}) = V_1(f(\mathbf{x}))$$

Bias potential depending on $\mathbf{x}$ only through CV

$$\mathbf{F}(\mathbf{x}) = -\nabla_{\mathbf{x}} V_1(f(\mathbf{x})) = -\frac{\partial V_1(f)}{\partial f} \nabla_{\mathbf{x}} f(\mathbf{x})$$

Bias force

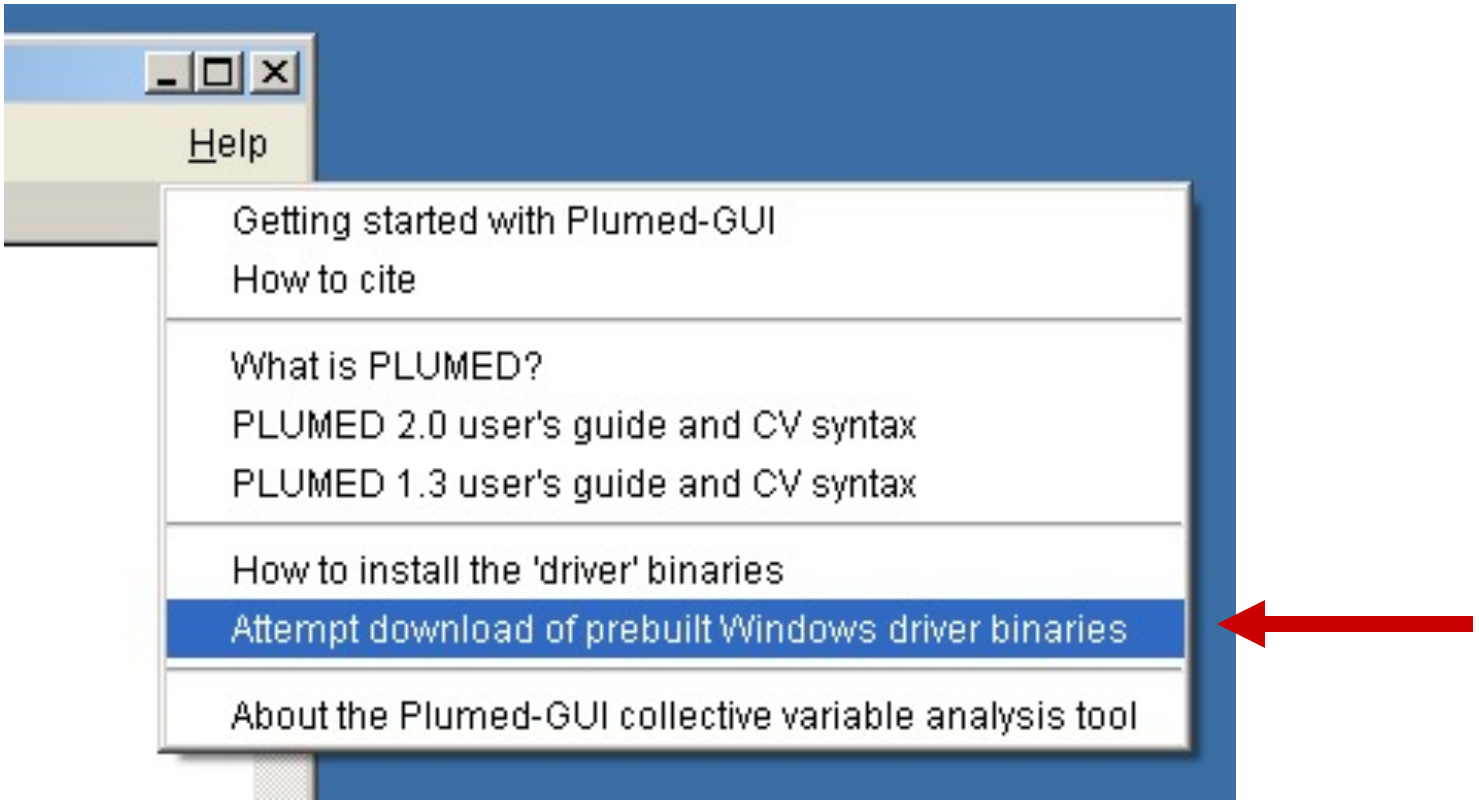
Generalized force

CV gradient

- **Assumptions**
  - Mostly dealing with timeseries, $x_i(t)$
  - Analyze existing trajectories → *driver*
- **Enter PLUMED**
  - Replaces scripting with homogeneous one-liners
  - Speeds up *clue-analysis-result*
- **Desiderata**
  - Syntax mnemonics, manual lookup
  - Symbolic atom selections
  - Immediate visualization

Need *driver* and/or *plumed* in path

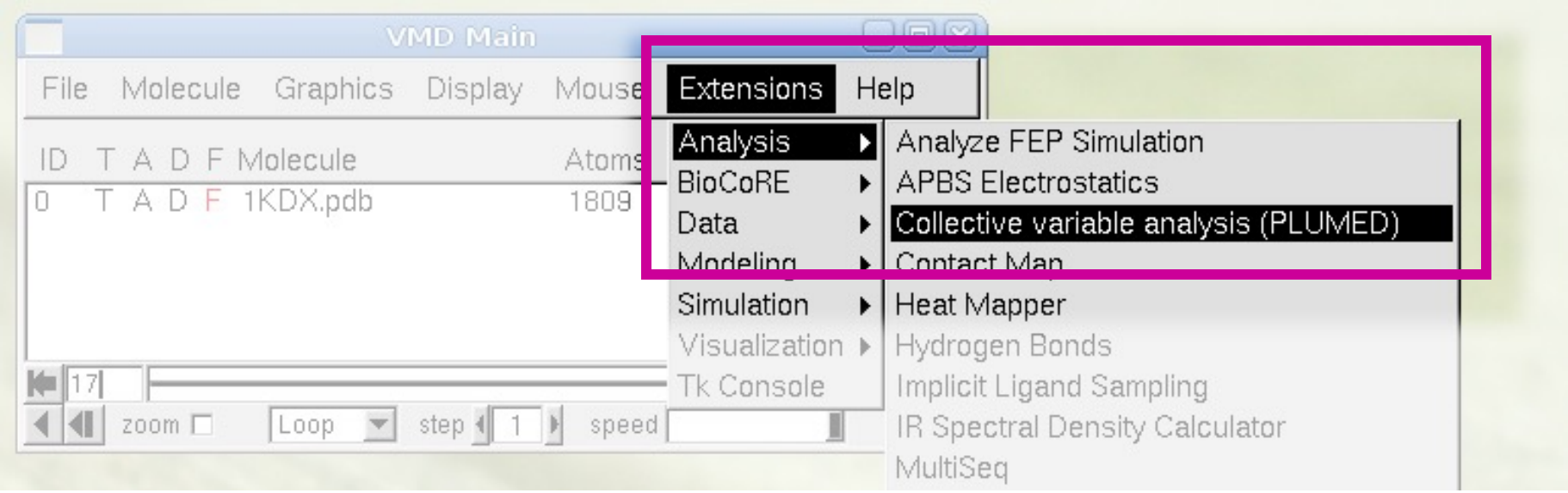
- **Linux** and **OSX**: supported by PLUMED 2.x's *configure*
- **Windows:** "auto-install" gets both 1.3 & 2.0 (cross-compiling 2.x is also easy)



Plumed-GUI objectives

1. Provide mnemonics for CVs (and options)
   - "How was it called…?"
2. Help with the generation of non-trivial CVs
   - "Oh no, I need to redo that Z_PATH reference…"
3. Show the results *fast*
   - "Show me! Now!"

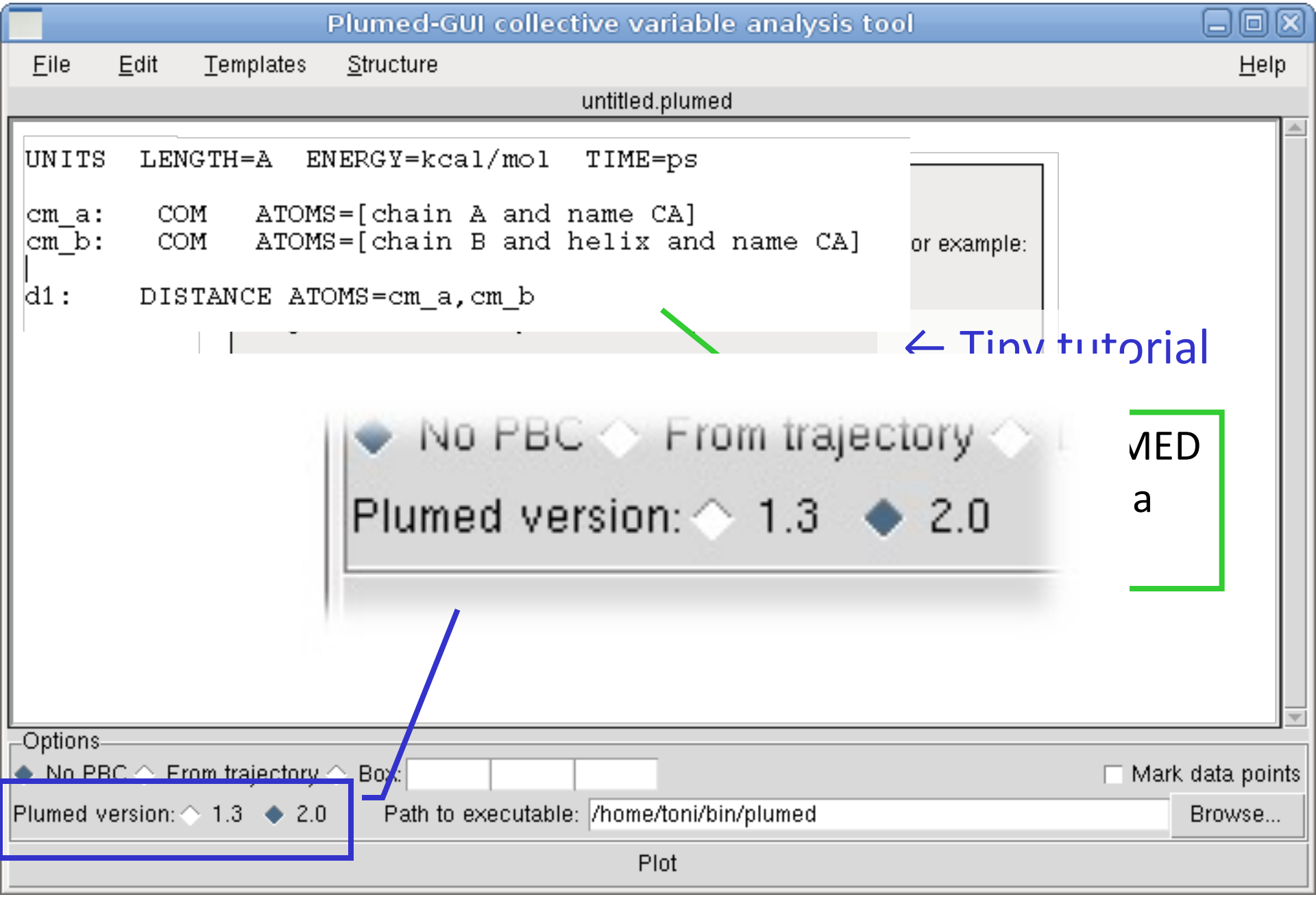
VMD > Extensions > Analysis > CV



GitHub

- tonigi/vmd_plumed

How does it look like?


Plumed-GUI collective variable analysis tool
File
Edit
Templates
Structure
Help
untitled.plumed
UNITS LENGTH=A ENERGY=kcal/mol TIME=ps
cm_a: COM ATOMS=[chain A and name CA]
cm_b: COM ATOMS=[chain B and helix and name CA]
d1: DISTANCE ATOMS=cm_a,cm_b
or example:
← Tiny tutorial
No PBC
From trajectory
Plumed version:
1.3
2.0
MED
a
Options
No PBC
From trajectory
Box:
Mark data points
Plumed version:
1.3
2.0
Path to executable:
/home/toni/bin/plumed
Browse...
Plot

Basics

- **File** and **Edit** menus: like a text editor
  - You write a ".plumed" file (unsubstituted brackets)
- **Free text**: syntax-agnostic
  - Only square brackets are parsed into atom lists
  - Custom PLUMED CVs are totally fine
- To get the script *after* substitutions:
  - **File → Export** ("META_INP", with comments)

Syntax-agnostic editor

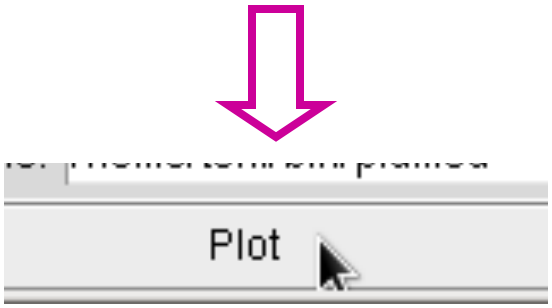
Enter actions as usual…

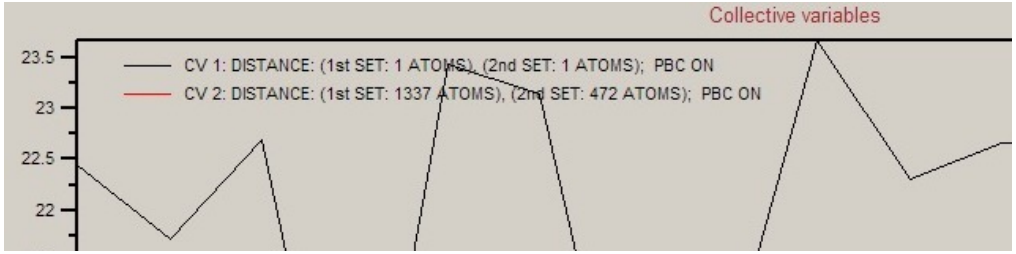
```
nc: COORDINATION GROUPA=kidCA GROUPB=kixCA …
```

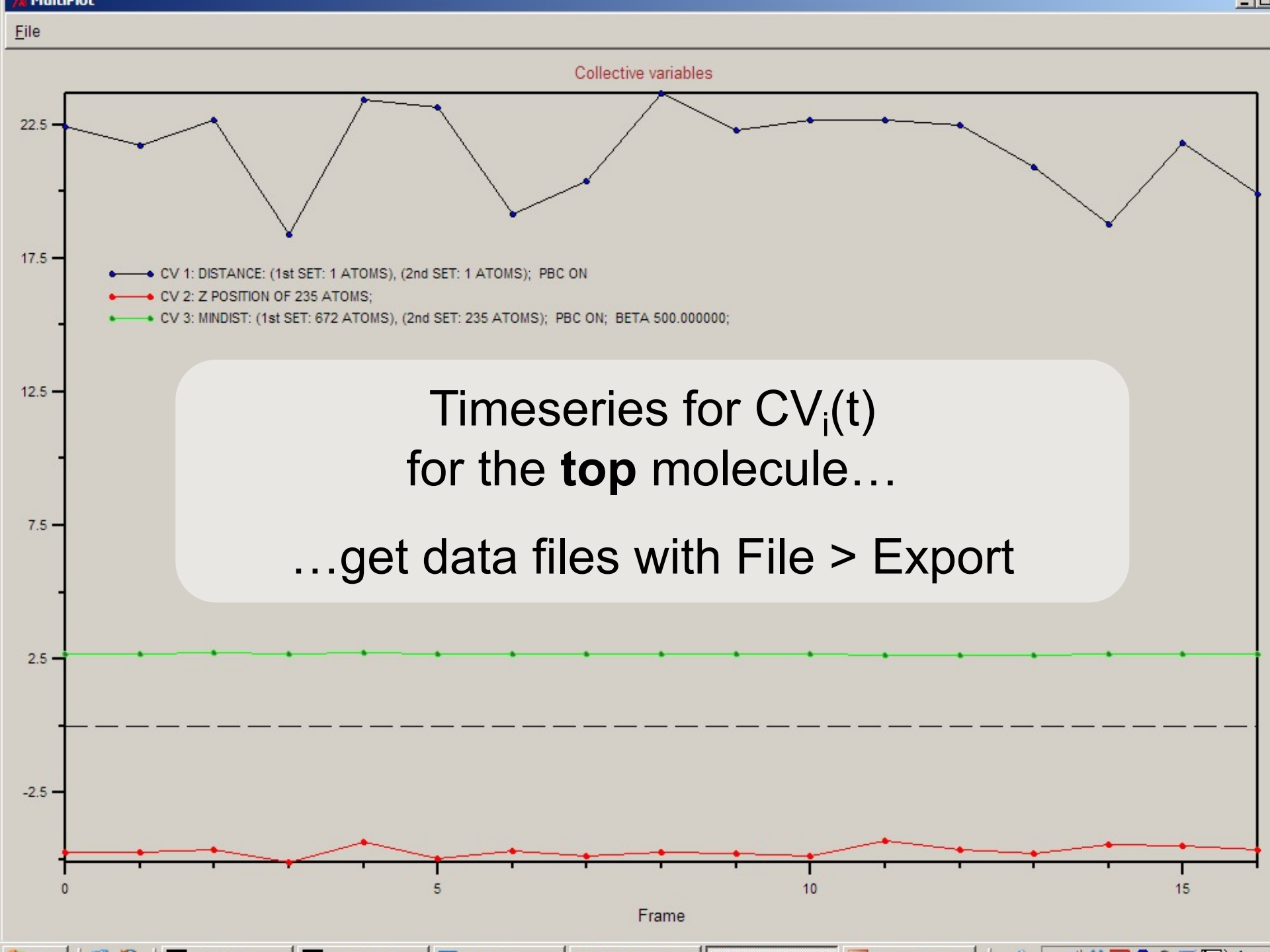
…symbolic atom selections allowed in [·]

```
kixCA:    GROUP ATOMS=[chain A and name CA]
```

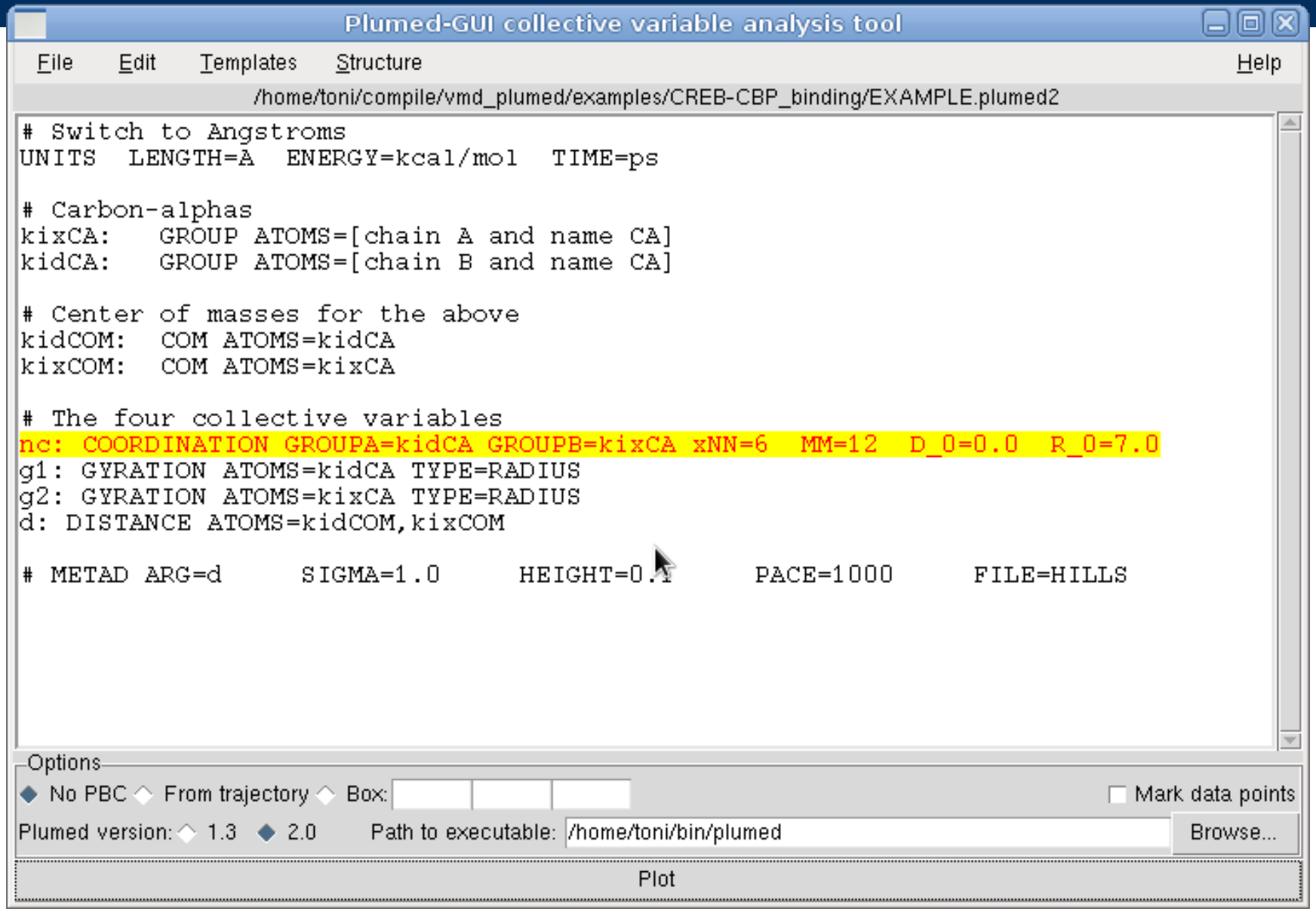
→ 45,66,78,99,… (Transparently)






File
Collective variables
22.5
17.5
12.5
7.5
2.5
-2.5
CV 1: DISTANCE: (1st SET: 1 ATOMS), (2nd SET: 1 ATOMS); PBC ON
CV 2: Z POSITION OF 235 ATOMS;
CV 3: MINDIST: (1st SET: 672 ATOMS), (2nd SET: 235 ATOMS); PBC ON; BETA 500.000000;
Timeseries for $CV_i(t)$
for the **top** molecule…
…get data files with File > Export
0
5
10
15
Frame

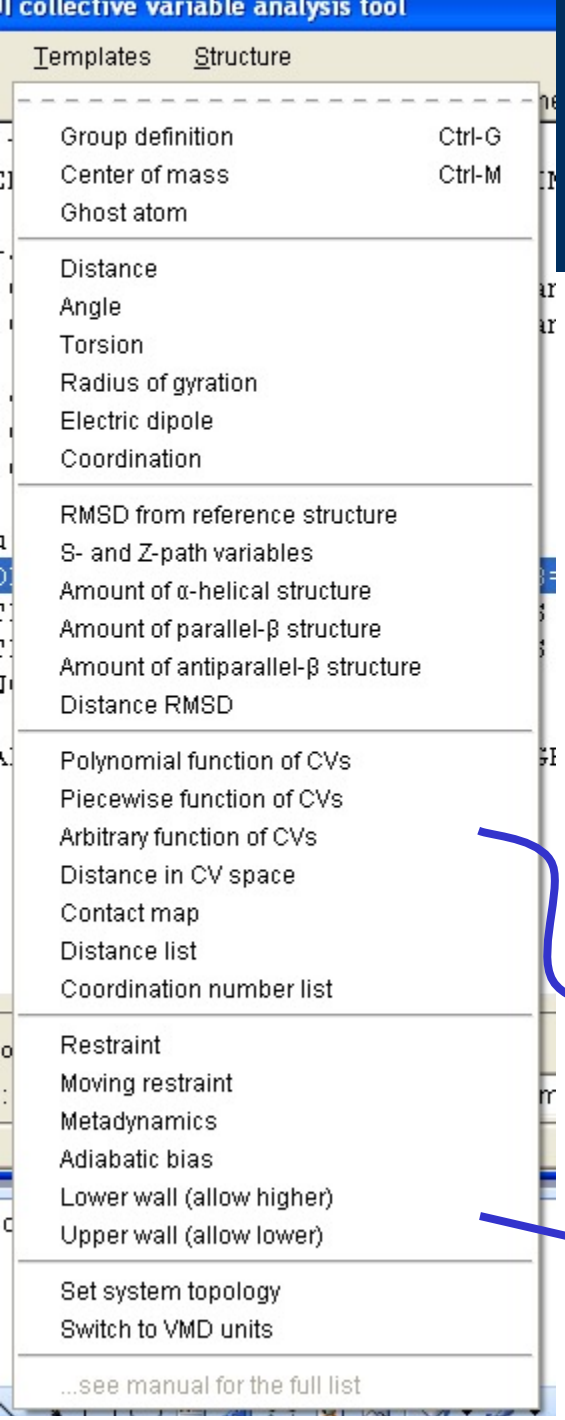
Error highlighting (…sometimes)



Behind the scenes…

- The current trajectory is saved
- Bracketed **[…]** atom selections expand according to the **top** molecule's topology
- Masses and charges → β/occupancy
- *"plumed driver"* is invoked
- ☹ → Errors appear in console
- ☺ → COLVAR is parsed and plotted

Assisted editing



Templates menu

"What was the that CV named again?"

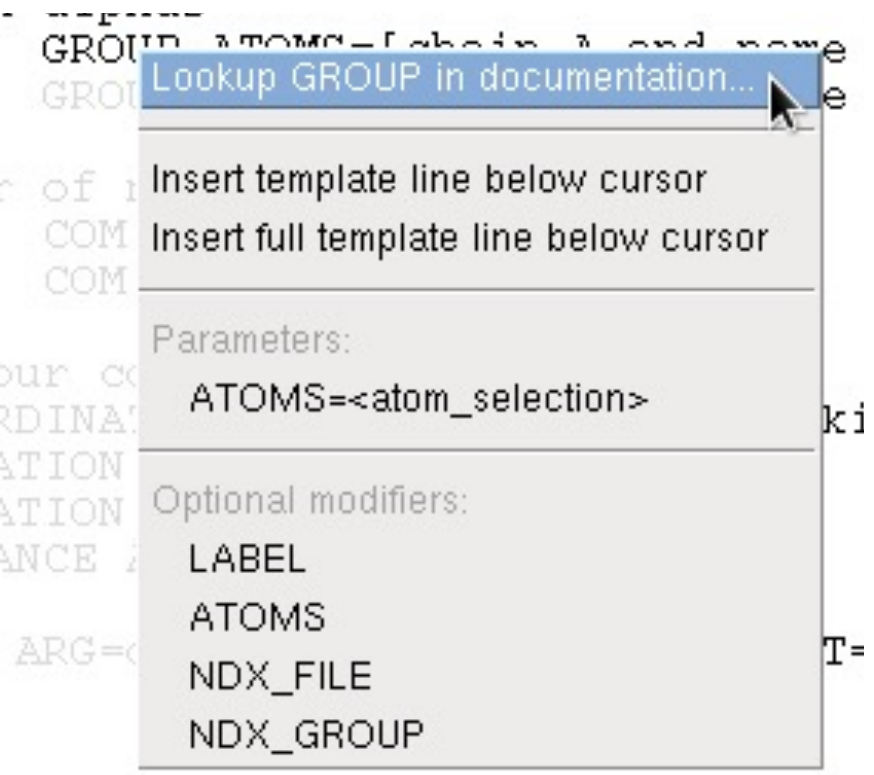
Insert a definition at the cursor

```
kixCA:    GROUP ATOMS=[…]
```

```
PARABETARMSD RESIDUES=<…> TYPE=DRMSD
R_0= D_0=0.0 NN=8 MM=12 STYLE=all
```

```
LOWER_WALLS ARG=      AT=      KAPPA=
OFFSET=0.0   EXP=2.0   EPS=1.0
```

Right-click on action: context-sensitive

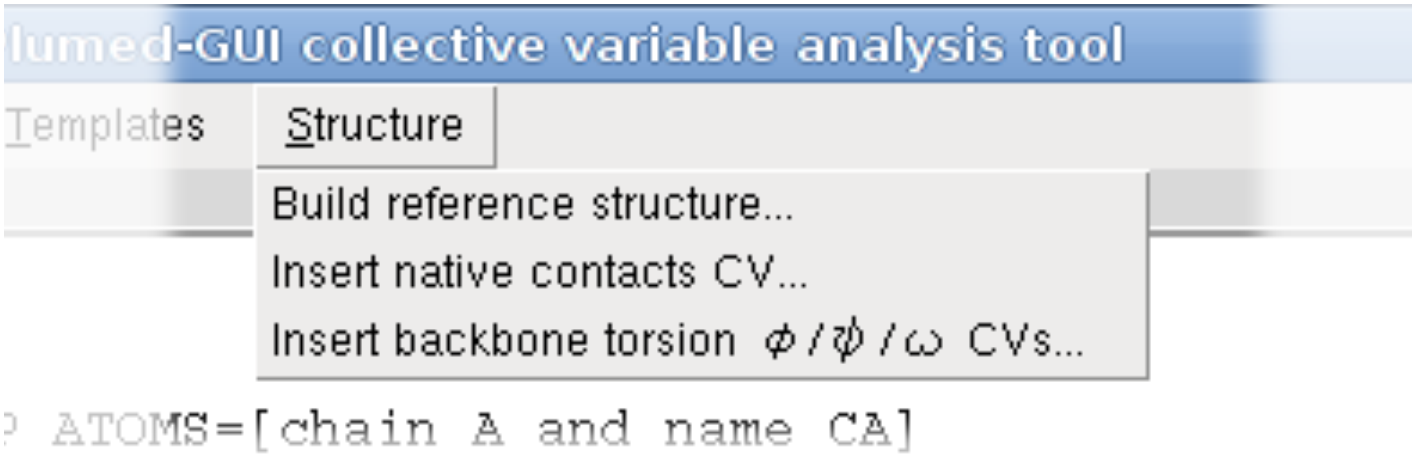


- Doxygen-generated pages are one click away
- If you know the action: insert the template
- Mandatory/optional parameters listed
- Autogenerated with the *gentemplate* tool

```
DISTANCE ATOMS=<atom_selection> [LABEL] [NUMERICAL_DERIVATIVES] [NOPBC] [ATOMS
```

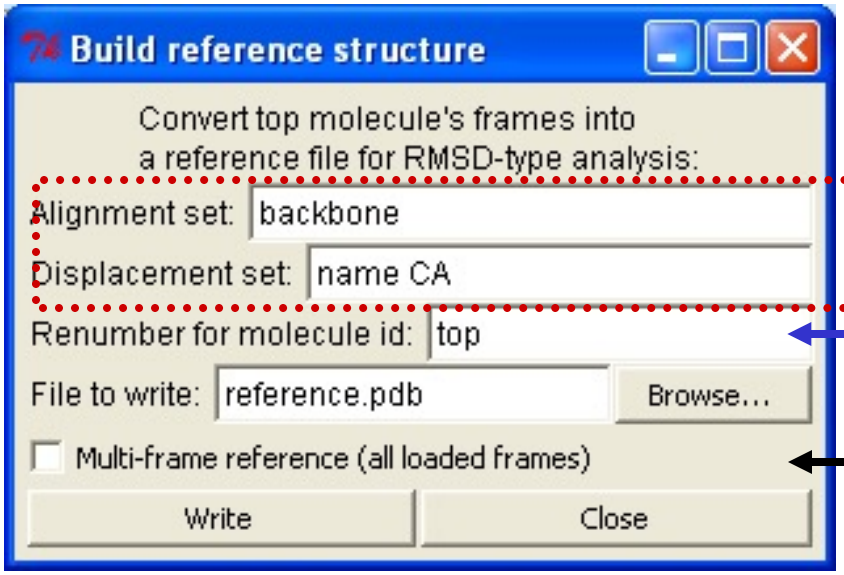
Structure menu

- Simplify preparation of non-trivial CVs
  - More-than-one liners, external files, etc.



Structure → Build reference structure

PDBs for PATHMSD



Source: current frame, top molecule

Target: molecule ID

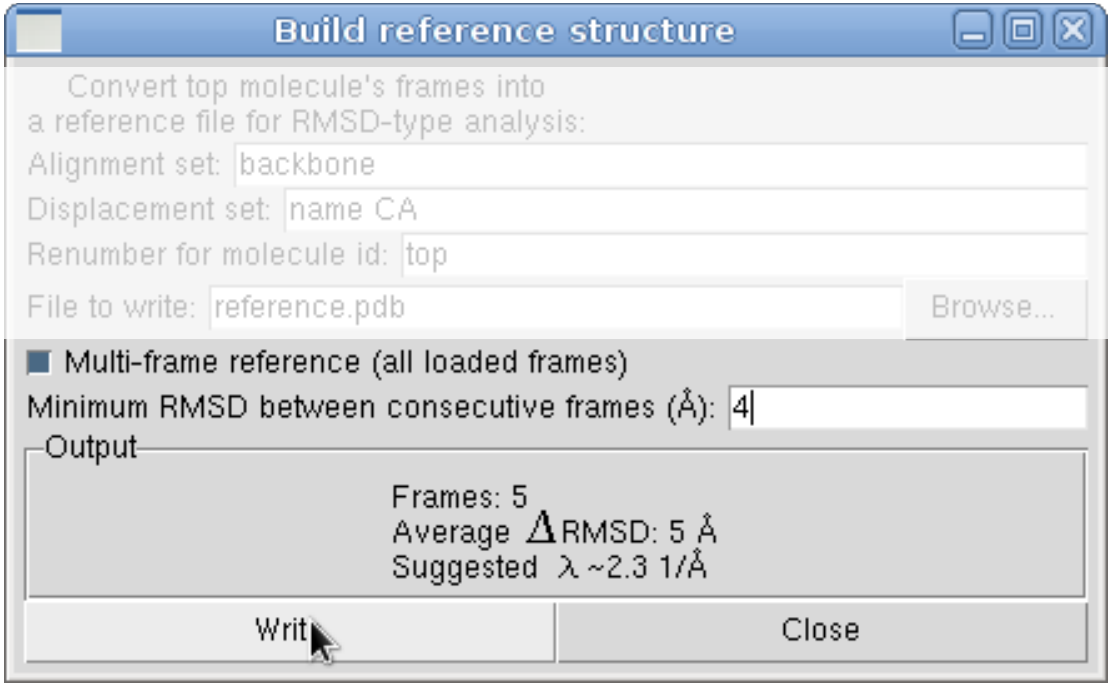
Plumed 2.x allows multi-frame references

Extracts the **current frame** of the **top molecule** (**source**)

Pseudo-PDB numbered for the molecule in the **target box**

Deals with PDB subsetting, fields and parsing quirks

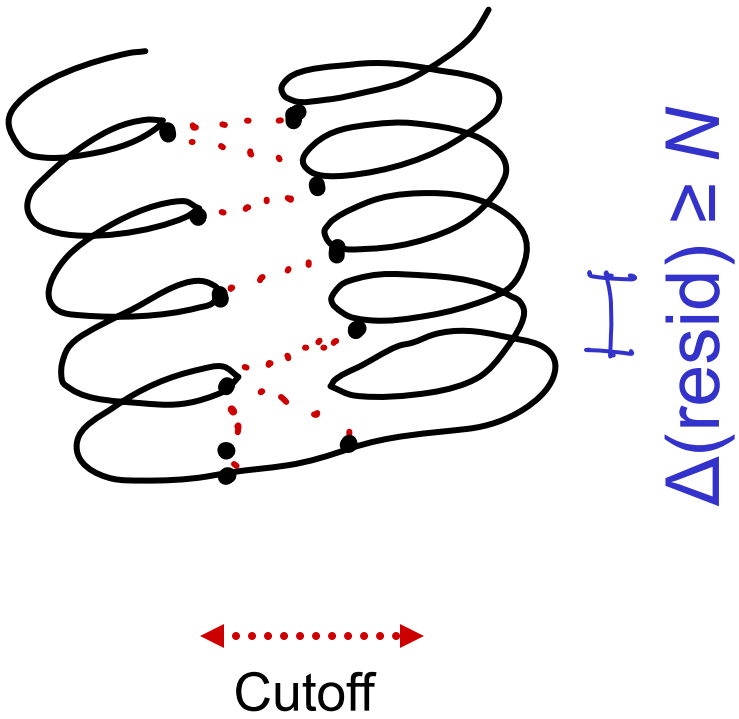
What's next: λ and subsetting



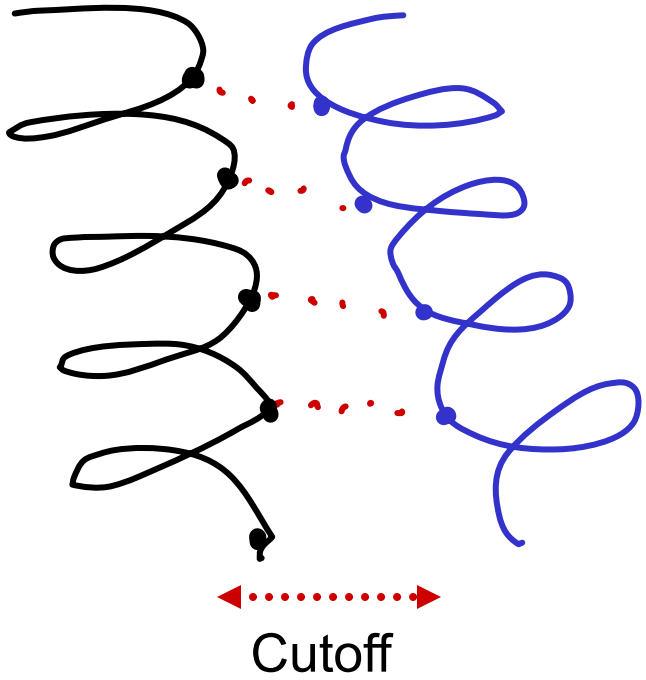
- Subset trajectory so that RMSD(i→i+1) is approximately constant, suggest λ
- Contact maps (suggestions welcome)

Number of native contacts

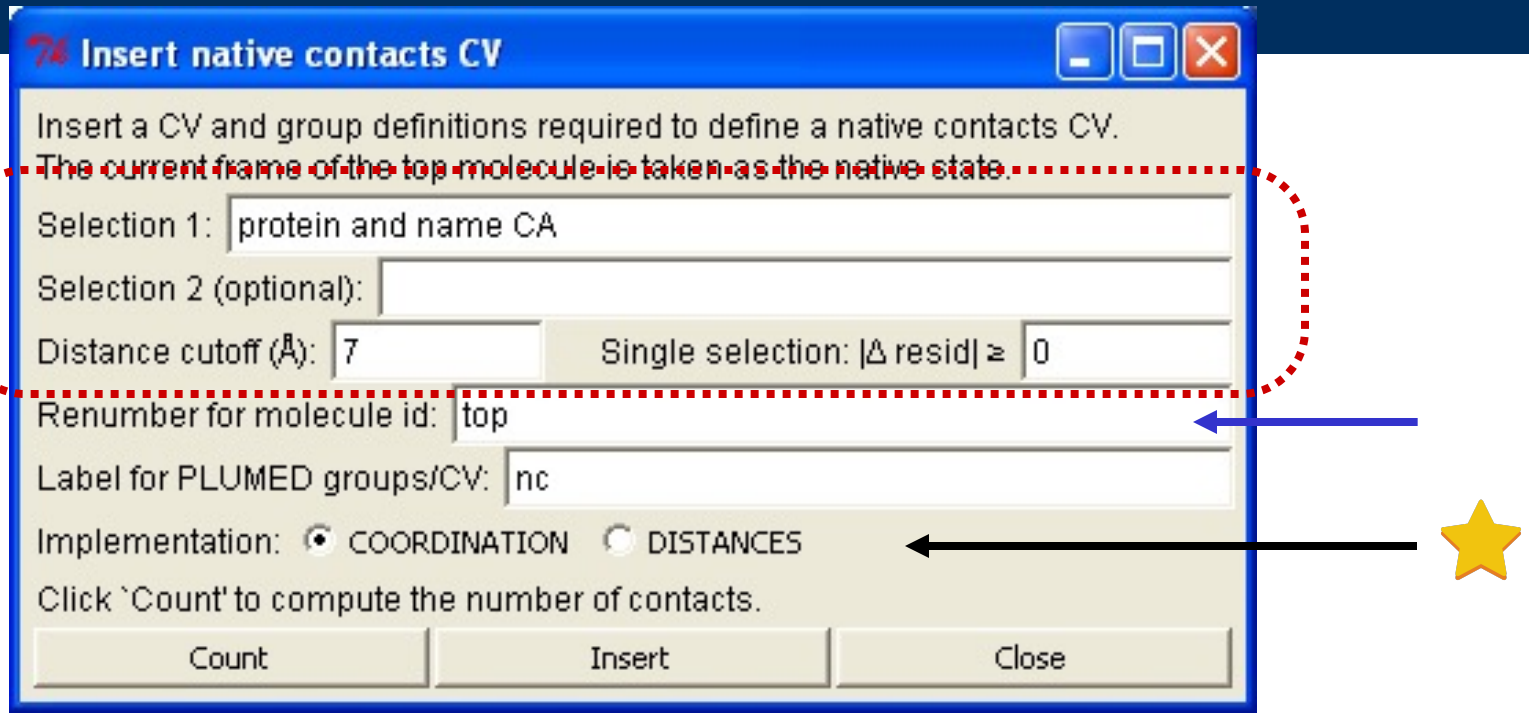
Intramolecular
(one atom set)



Intermolecular
(two atom sets)



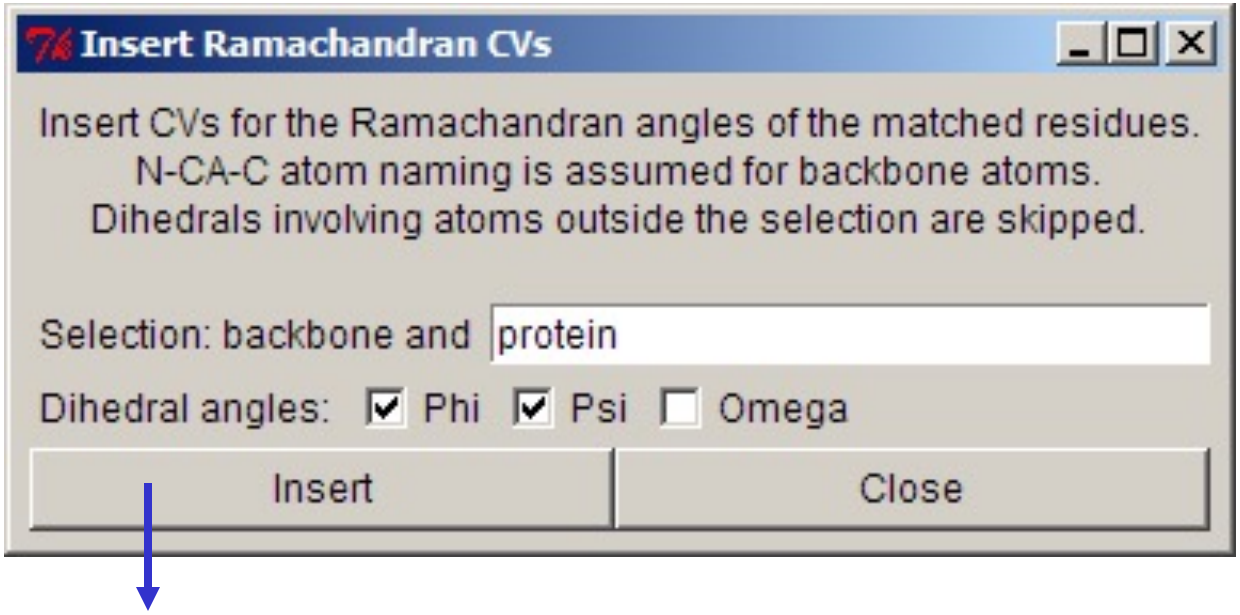
Structure → Insert native contacts CV



- Enumerate **native pairs** in the **current frame** of the **top molecule** (**source**)
- Lists are renumbered for the molecule in the **target box**

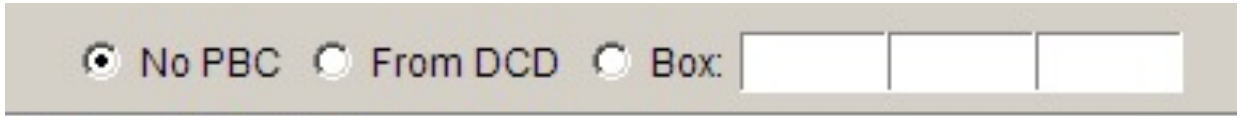
```
co: COORDINATION PAIR GROUPA=nc_a GROUPB=nc_b ... # or
di: DISTANCES LESS_THAN={RATIONAL R_0=0.5 D_0=7} ATOMS1=914,849
```

Structure → Insert ϕ/ψ/ω



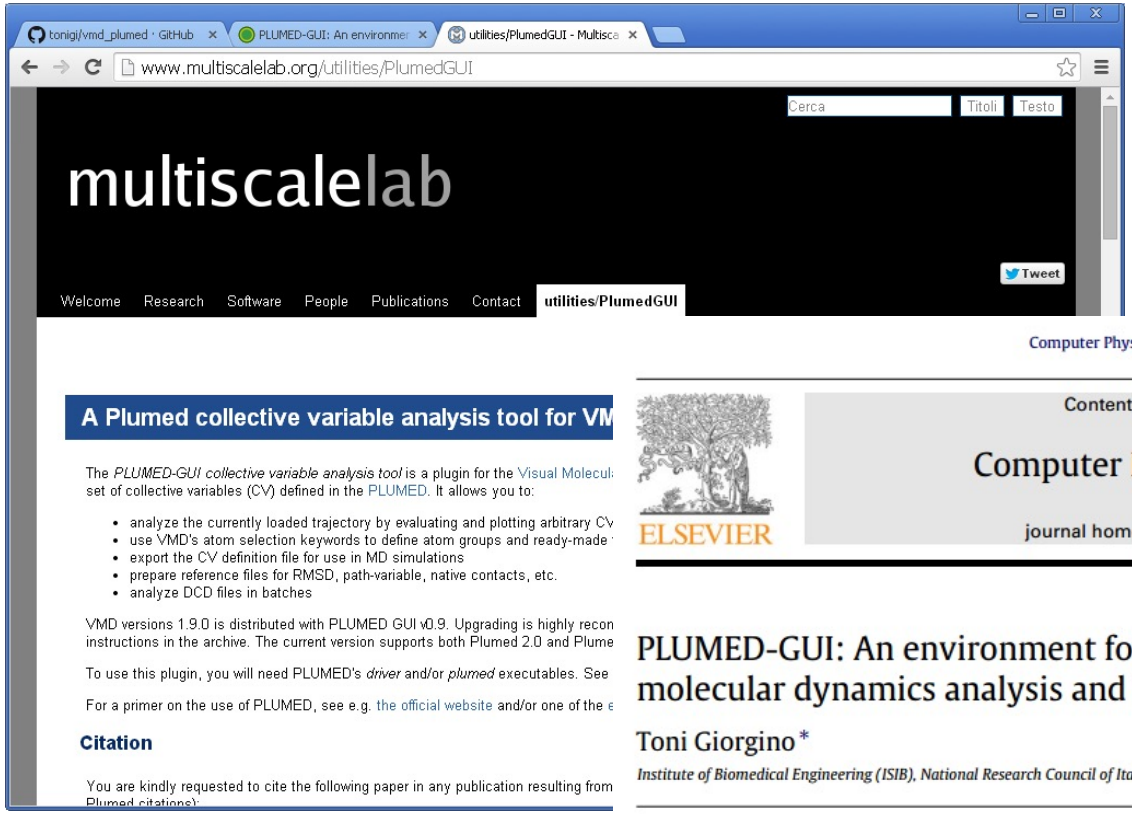

```
TORSION ATOMS=1,2,3,8   LABEL=GLY586_PSI
TORSION ATOMS=3,8,9,10  LABEL=VAL587_PHI
TORSION ATOMS=8,9,10,24 LABEL=VAL587_PSI
…
```

Periodic boundary conditions



- Time-varying cell are now allowed
  - Be mindful of VMD limitation on cell's orientation

Documentation



← Short

www.multiscalelab.org/
/utilities/PlumedGUI

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PLUMED-GUI: An environment for the interactive development of molecular dynamics analysis and biasing scripts☆

Toni Giorgino*

Institute of Biomedical Engineering (ISIB), National Research Council of Italy (CNR), Corso Stati Uniti 4, I-35127 Padua, Italy

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ABSTRACT

PLUMED-GUI is an interactive environment to develop and test complex PLUMED scripts within the Visual Molecular Dynamics (VMD) environment. Computational biophysicists can take advantage of both PLUMED's rich syntax to define collective variables (CVs) and VMD's chemically-aware atom selection language, while working within a natural point-and-click interface. Pre-defined templates and syntax mnemonics facilitate the definition of well-known reaction coordinates. Complex CVs, e.g. involving reference snapshots used for RMSD or native contacts calculations, can be built through dialogs that provide a synoptic view of the available options. Scripts can be either exported for use in simulation programs, or evaluated on the currently loaded molecular trajectories. Script development takes place without leaving VMD, thus enabling an incremental try–see–modify development model for molecular metrics.

Long →

doi:10.1016/j.cpc.2013.11.019
arxiv:1312.3190

Part II – Python + MDTraj

See the online notebook