Introduction into Simulations in Internal Coordinates

Command Line Style

ICM Language Reference

ICM Language

- Words: read,write, show, list, display, delete, object, molecule, residue, atom, sequence, alignment, table, … , **list command**
- **Variables and Constants, e.g. A = {1, 2, 3}**
- Built-in functions: **Nof**(a_/*), **Disgeo**(distmat),..
  try **list functions**, or typing function name: **Random**
- **Macros, icm-Function** (**_macro**) (e.g. convert2Dto3D ..)
- Shell-objects, *atom selection language*: (try **selection help**).
  - real, logical, string
  - 3D molecular object (object)
  - sequence (`eg read sequence fasta "a.fa", readUniprot "IL2_HUMAN"`)
  - alignment
  - rarray, iarray, sarray (arrays of reals, integers and strings)
  - parray p stands for pointer
    - Chemicals, slides, images, audio,..
  - **collection (json, xml)**
  - **table** header columns

Selections

Icm> **selection help**

- Syntax: **a_[*<obj>*.]*<mol>*/*<res>*/*<atom>*** Types: *<os>* *<ms>* *<rs>* *<as>* *<vs>*
- *<field>*== [!]*<name_or_pattern>*|*<number>*|*<range>*[,..], e.g. **a_*.!a*/asn**?, 12:14,60
- Object: **a_** (current), **a_*.** (all), ICM CATRACE LAST "<comment_ptn>"
- Molecule: **A**(amino) **B**(bio-unit) **C**<chains> **H**(hetero) **J**<minlen> **K**(linK2ali) **L**(lipid) **M**(metal) **N**(nucl) **P**(uniProt) **Q**(link2seq) **S**(sugar) **TRACE W**(water) **U**(unknown), eg a_!Ca (all except chain 'a')
- Residue: A B|Q<barcode> C<consensus>(X,h,s,p,o,n,a,x,g:gap) D(display,RLD) F<siteType> K(insert.label:22a) S<ss>(_EHB) T(term) U(unk) "seq_pattern"
- Atom: A<alter>|AS C<code> CH<hydration_code> CM (metals) D<display>(ABCDTSVWX) E H HA HD M<mmff> O<n1>:<n2> P(polar) R(aroma) T(tethers) X<0123>(chiral) Z(tZ)
- Variable: v_ (free) or V_ (all) v|V_*/*/<vars> A(angle) B(bondlen) DL F(phase) FC(chiral) H(heavy) M(methyls) P(polarH) T(tors) V(6 positionals)
- Expressions: ! , & , | , <vs> & <as>, <as> & <R_6box>. Reserved: as_graph, as2_graph, as_out, as2_out
- Functions: Acc Atom Deletion Insertion Mol Next Obj Res Sphere Select

Converting to ICM and Linking

- build your system by **convertObject** or
- **build** [string] command or one of the macros
- **build string "o"** # a single atom object
- Learn about icm selections for atoms, residues, molecules, objects and variables (try **selection help**)
- t = Table(residue) # list of aa and termini for **build**
- t = AminoAcids # full list of aa for **modify**
- **build model** <seq> <ms_template> [<ali>]
- build smiles <smiles>
- **modify** and **modifyGroupSmiles** macro
- **link** <ms> <alignment>

Energy terms

- **set terms [only] “vw,14,el,to,hb,sf”**
- **show energy**
- **minimize**
- **montecarlo *<vs>***
  - **mncalls , mncallsMC, temperature, mcShake, …**
- Example: http://xablab.ucsd.edu/folding.icm

Tethers

- A harmonic or bi-quadratic distance restraint between an atom in ICM object and an atom outside that object.
- **tether**: **set , delete , show , display, minimize , tzMethod, tzWeight**
- set term “tz” # to activate

Selftethers

- Does not need an extra object, - memorizes the target coordinate during the **set selftether** [*a_sel*] [*M_xyz*|“box”] command
- selftether : `set , delete, show`
- Need `“ts”` term, can
  - **convert selftether** or **minimize selftether**
- **TOOLS.tsToleranceRadius, TOOLS.tsWeight**
- **TOOLS.tsShape, TOOLS.tsShapeData**

Distance restraints

- **set drestraint** *<i_ty>|<R3_low_up_wt> <as_1> <as_2>* [only]
  - Example: set drestraint a_/24/cb a_/33/ca 2.//4.//1.
- **set drestraint all** *<i_ty> <as_group1> <as_group2>* [only] # restraint between atom groups
- set drestraint *<distpairs> [<os_ICM>] [<i_cntype>|<R3_low_up_wt>]* [only] [find [edit]]
- set drestraint field <distmatrix> [<os_>] [<r_distance_scale_factor>(1.)]
- see also: set drestraint type <i_ty> <w> <low> <upp> [local <r>]

Stack of Conformations

- Stack contains conformations (**conf** in ICM)
  - A vector of all geometrical variables
  - Its energy, comment
  - The number of visits by the search
- ICM terms, commands and variables:
  - **stack** (read,write,show,delete,display,store/load .. *obj* , compress/compare)
  - **conf** (load,store,delete)
  - **Nof**(stack),
  - **mnconf**
  - **minimize stack [selftether]**

Building stack, storing it in object

- **store stack a_** **load conf a_**
- **build loop stack** <rs_loop> [<limit>]
  - icm.lps file (write model)
- montecarlo [append]

Masking and unmasking atoms

- set <selection> on | off , e.g. set a_/52:57 off

Alignment

- ZEGA: zero-end-gap global alignment
- `alignMethod` ("ZEGA" or "H-align")
- `gapFunction` (with H-align), e.g.
- Commands:
  - align sequence
  - Align(..)
  - find database

Abagyan RA, Batalov S
Do aligned sequences share the same fold?
J Mol Biol, 1997 Oct 17, 273, 355-68
http://xablab.ucsd.edu/pdf/97_zega_jmb.pdf

- `write index sequence` *<"file"> #blast*