TCL VMD SCRIPT TO ANALYSE TRAJECTORY and Can be UTILIZED as CUSTAMIZED COMMANDS in VMD

VERSION : analysis_script_V 1.0

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Step 1 : SOURCE analysis.tcl in VMD Tk console
Step 2 : Command_name {Arguments}

After Sourcing analysis.tcl script in VMD console, type following
my_commands show : List out all available commands from this script.
--help command_name : Shows the details of command ,with examples.

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TIP OF THE DAY :

Keep this analysis.tcl script in a adirectory called vmd_tcl_scripts/
Mention its path in vmd startup file ~/.vmdrc

eg. source /home/anjibabu/vmd_tcl_scripts/analysis.tcl

That's it, here after when ever you open VMD automatically analysis.tcl will be excecuted.
So, U can start using these commands as default commands.
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Following analysis can be done by using this script :

Alignment
RMSD
Distance btw two atoms
Measure Angle
Measure Dihedral
Contact map
Print Interactions within given cutoff
Print No. of waters within given cutoff
Print No. of HBonds within given cutoff
Print residue names and resid for given sel
Molecule details (No of frames, No of atoms, No of waters, Box size)
On pbc_box and off Pbc_box and prints box size
save_pdb
save_image : Renders image using Tachyon
save_movie : creates a movie for given frames (gif file) other formats will be updated soon.
save_coordinates
--help : which gives details of command
my_commands show : shows avalilable commands

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Future updates:
save_view : saves the visivilization of current vmd
Ramachandran plot
HB plot
PBC Wrapping
delete_frame : Deletes the frames for given intial and final frames
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AVAILABLE COMMANDS AND DETAILS :
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1. Command Name : my_commands show
   PURPOSE   : Shows all available commands written in this script
   USAGE&example : my_commands show
   Here you have to use "show" as fixed argument to see commands list.

2.Command name   : --help
   PURPOSE   : Prints the details of any mentioned command
   USAGE   : --help command_name
   EXAMPLE   : --help distance
   EXAMPLE 2   : --help angle
   Prints the details of commands distance and angle.

3.Command Name   : save_pdb
  PURPOSE   : Writes pdb file for given options
  USAGE   : save_pdb {atomselection} {start_frame} {end_frame} {stride} {molid} {filename}
  EXAMPLE   : save_pdb "protein" 5 100 5 top file.pdb
  It will write file.pdb for "protein" from frame 5 to 100 by skipping every 5 frames.

4.Command Name   : align
  PURPOSE   : To align two molecule for given molids
  USAGE   : align {molid1} {molid2}
  EXAMPLE   : align top 1

5.Command Name   : rmsd
  PURPOSE   : Measures Avg.RMSD & std for given selections
  USAGE   : rmsd "sel1" "molid1" "sel2" "molid2"
  EXAMPLE   : rmsd "backbone" 0 "backbone" 1
  OUTPUT   : Generates data into a file "RMSD.dat".
  (IF both the molids are same , RMSD will be calculated by taking zeroth frame as reference)

6. Command Name : distance
   PURPOSE   : Measures Avg Distance & std for any given 2 atoms
   USAGE   : distance sel1 sel2
   EXAMPLE   : distance "serial 3418" "serial 3415"
   OUTPUT   : Generates data into a file "DISTANCE.dat"

7. Command Name : angle
   PURPOSE   : Measures Avg. angle & std for any given 3 atoms
   USAGE   : angle "sel1" "sel2" "sel3"
   EXAMPLE   : angle "serial 3418" "serial 3415" "serial 3395"
   OUTPUT   : Generates data into file " ANGLE.dat ".

8. Command Name : dihedral
   PURPOSE   : Measures Avg Dihedral angle & std for any given 4 atoms
   USAGE   : dihedral sel1 sel2 sel3 sel4
   EXAMPLE   : dihedral "serial 3418" "serial 3415" "serial 3412" "serial 3395"
   EXAMPLE   : dihedral "index 3417" "index 3414" "index 3411" "index 3394"
   OUTPUT   : Generates data into a file " DIHEDRAL.dat ".

9. Command Name : show_residues
   PURPOSE   : Prints RESID and corresponding RESNAME for given selection and for given frames

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   USAGE         : show_residues sel molid <initial frame>  <final frame>
   EXAMPLE       : show_residues "resid 170 to 180" top 0 5
   EXAMPLE1      : show_residues "(not resname WAT) and within 3 of resid 235" 0
5 10
   EXAMPLE2      : show_residues "protein and hydrophobic " top 1 0
   EXAMPLE3      : show_residues "protein and basic" top
    " In Example3 frame numbers are optional ,
      if you omits frame numbers it prints all basic residues from zeroth frame"
   OUTPUT        : Generates data into a file  "RESNAMES.dat ".


10.Command Name  : details
   PURPOSE       : Prints required molecular details for given molid
   USAGE         : details molid
   EXAMPLE       : details 1
   EXAMPLE1      : details top


 11.Command Name : count_waters
    PURPOSE      : Prints Avg. No of waters of entire trajectory or for selcted
frames
                   which are present around given selection
    USAGE        : count_waters "sel" molid start_frame end_frame
    EXAMPLE      : count_waters "within 5 of resid 235" 0 5 10
    OUTPUT       : Generates data into a file "NO-OF-WATERS.dat".


12.Command Name  : pbc_box
   PURPOSE       : Sets BOX ON or OFF or shows the size of PBC BOX
   USAGE         : pbc_box {choice}
   ARGUMENTS     : on, off, size
   EXAMPLE       : pbc_box on
   ( It will ON the pbc box for current top molecule)
   EXAMPLE1      : pbc_box off
   ( It will off the PBC box )
   EXAMPLE2      : pbc_box size
   ( It  prints the size of BOX (values) on Tk console)


13.Command Name  : show_interactions
   PURPOSE       : Prints Interactions between given two selections within given
DISTANCE cutoff
   USAGE         : show_interactions sel1 sel2 cutoff <start frame> <end frame>
   EXAMPLE       : show_interactions "protein" "resid 143" 3.0 5 10
   (It prints all interactions within cutoff of 3.0 (A) between protein and
resid 143 of all atoms )
    OUTPUT FORMAT:indexA residA resnameA(typeA)---indexB residB
resnameB(typeB) :  Distance
   ARGUMENTS     :
      sel1       : Any given  atom selction
      sel2       : Any given atom selction
      cutoff     : distance cutoff
      start frame: Starting frame , from here start analysing
      end frame  : Final framme , It stops here
   OUTPUT        : Stores all the information in "INTERACTIONS.dat" file


14.Command Name  : contact_map
   PURPOSE       :  Measures all the contacts between given two selections and
                    Prints 1 (one) if contact is below cutoff , 0 (zero)
otherwise
   USAGE         : contact_map " sel1"  "sel2"  cutoff startframe endframe
   Example       : contact_map "resid 1 to 50 and name CA" "resid 51 to 100 and
name CA" 6.0 0 10
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   OUTPUT        : Stores all data in "CONTACT_MAP.dat" file.
   OUTPUT FORMAT : RESID_A  RESID_B 1/0 DISTANCE

   PLOTTING DATA : gnuplot >>  splot "CONTACT_MAP.dat" u 1:2:3 w p notitle
                   gnuplot >>  set view 0,0,1
                   gnuplot >>  replot
   It generates a beautiful CONTACT MAP 3D image.


15.Command Name   : count_hbonds
   PURPOSE        : Prints AVG No. of HBonds b/w given DONOR and ACCEPTOR
selections
                     and given distance_cutoff & angle_cutoff .
   USAGE          : count_hbonds "Donor_sel1"  "Acceptor_sel2"  distance_cutoff
angle_cutoff
   EXAMPLE        : count_hbonds "protein and name N" "protein and name O" 3.0
30
   OUTPUT         : Stores data in file "HBONDS_COUNT.dat".
   (Which contains Frame vs No.of Hbonds ,You can plot this data as Frames v/s
No. of Hbonds)
   NOTE           : It assumes that molis as "top" or zero. It prints AVG HBONDS
per FRAME.


16.Command Name   : show_hbonds
   PURPOSE        : Prints the all HBonds b/w given DONOR & ACCEPTOR selections
for
                    given distance & angle cutoff.
   USAGE          : show_hbonds  "D_sel1" "A_sel2" dist_cutoff angle_cutoff
<startframe> <endframe>
   EXAMPLE        : show_hbonds "protein and name N" "protein and name O" 3.0 30
5 10
   OUTPUT         : Stores all HBONDS data in HBONDS.dat.
   OUTPUT FORMAT  : indexD residD resnameD(type)-- indexA residA
resnameA(type)-- Distance
   (Prints and Stores data for every Frame )
   NOTE           : Always Atomselctons should be DONOR and ACCEPTOR , (not
ACCEPTOR and DONOR)


 17.Command Name  :  HB_occupancy
    PURPOSE       :  Prints only the HBONDS occupancy for given selctions for
selected frames
    USAGE         :  HB_occupancy "D_sel1" "A_sel2" dist_cutoff angle_cutoff
<startframe> <endframe>
    EXAMPLE       :  HB_occupancy "protein" "resid 147" 3.0 30 0 20
    OUTPUT FORMAT :  RESID_D  RESNAME_D --  RESID_A  RESNAME_A    ---OCUPANCY
(%)
    EXAMPLE       :  140  LYS -- 147 ARG  --- 80.00 %   (Pints for all selected
frames)
    ARGUMENTS     :
     SELECTION1   : MUST BE ANY DONOR SELECTION
     SELECTION2   : MUST BE ANY ACCEPTOR SELECTION
     CUTOFF       : Distance cutoff to measure HBonds
     ANGLEE_CUTOFF: Angle cutoff to measure HBonds
     START_FRAME  : Starting Frame Number
     END_FRAME    : End Frame Number


18.Command Name   : save_image
   PURPOSE        : Renders a high quality image using Tachyon for currently
active frame.
   UASAGE         : save_image {molid} filename
   EXAMPLE        : save_image top my_image
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(extension of file not required)
OUTPUT FILES : filename.dat , filename.dat.tga, filename.dat.jpg
Above example produces my_image.dat , my_image.dat.tga, & my_image.dat.jpg.

19.Command Name : save_movie
PURPOSE : GENERATES A MOVIE IN GIF FORMAT FOR GIVEN MOLID & FOR SELECTED FRAMES
USAGE : save_movie molid filename <start frame> <end frame>
(no extension of filename is required)
EXAMPLE1 : save_movie top my_protein 0 20
EXAMPLE2 : save_movie 1 drug_protein 20 40
EXAMPLE3 : save_movie top my_protein
EXAMPLE4 : save_movie 1 drug_protein 30
OUTPUT : Example1 Genarates "my_protein.gif" file from zeroth frame to 20th frame.
: Example2 generates "drug_protien.gif" file from 20th frame to 40th frame.
: Example3 generates "my_protein.gif" file from zeroth frame to end frame .
: Example4 generates "drug_protein.gif" file from 30th frame to end frame.

NOTE : Other Movie formats will be updated soon.

20.Command Name : save_coordinates
PURPOSE : Saves coordinates for given arguments
USAGE : save_coordinates "Sel" {molid} {filename} {filetype} {start_frame} {end_frame} {stride}
EXAMPLE : save_coordinates "protein" top my_protien.mol2 mol2 5 30 5

ARGUMENTS :
AtomselectioN: Any given slection
Start frame : From which frame to save coordinates
End frame : To which frame to save coordinates
Stride : After how many frames you want save (skipping)"
molid : Which molecule you want save
Filename : Filename with extension
EXAMPLE : protein.mol2, protein.xyz, protein.gro, protein.dcd.....etc.
Filetype : Which format you want to save.

Available Filetypes : ABINIT , bgf, binpos, crd, crdbox, dcd, gro, trr, js, lammpstrj, mol2, namdbin, pdb, pqr, rst7,POSCAR, xbgf, xyz, dtr, m"ae, dms, hoomd .

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" yad bhavam tad bhavati " means "you become whatever you think"

----from vedas