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SIMULAID: simulation setup and analysis utilities, written by Mihaly Mezei
Version 02/25/2022; Memory use=1287 Mb; Maximum number of input records=250000
M. Mezei, J. Comp. Chem., Vol 31, 2658-2668 (2010). DOI:10.1002/jcc.21551
NOTE: input prompts showing ? will yield an explanation by typing just a ?
NOTE: input prompts showing + will yield a tip by typing just a +
Conversion files found in directory /simulaid
WARNING: could not determine if this is a cluster headnode
         Functions requiring sizable CPU time should be run on a compute node

SELECT run type:
Print all menu and submenu <F>unctions - - - - - - - - - -  : f
Geometry <O>ptimization (orientation, smallest sphere) [3]  : o
<C>leanup (sort, renumber, regroup, round charges) - - - -  : c
<S>tructure file and type conversions [15] - - - - - - - -  : s
<T>rajectory file and type conversions [4] - - - - - - - -  : t
Atom <N>ame and residue name conversions [4] - - - - - - -  : n
Trajectory - str<U>cture file conversions (pack/unpack) [4] : u
Conformation <E>dit (trans/rot/cent/algn/add/del, etc.) [15]: e
<M>iscellaneous (seq, RTF, UHBD, tors., Amber sum, etc.)[7] : m
<A>nalyze (TRAJELIX, RMSD, H-bonds, CV, etc.) [17] - - - -  : a
Cluste<R> atoms or data defined by a distance matrix [2] -  : r
Make the input <P>redictable - - - - - - - - - - - - - - -  : p
Open <L>ogfile logging the keyboard inputs - - - - - - - -  : l
<Q>uit Simulaid  - - - - - - - - - - - - - - - - - - - - -  : q  f
"Print all menu and submenu functions" selected
  Print all menu and submenu <F>unctions
  Geometry <O>ptimization (orientation, smallest sphere) [3]
    <S>mallest sphere calculation
    O<P>timize orientation in bounding cube/rectangle
    <O>ptimize orientation in a periodic cell
  <C>leanup (sort, renumber, regroup, round charges)
  <S>tructure file and type conversions [15]
    Rearrange a<T>oms in a structure ccording to an RTF file
    Convert structure to <C>harmm CRD format
    Convert structure to <E>xtended Charmm CRD format
    Convert structure to Brookhaven <P>DB format
    Convert structure to C<H>armm PDB format (seg id)
    Convert structure to <M>acromodel dat format
    Convert structure to MMC Monte Car<L>o input
    Convert structure to <G>romos/Gromacs format
    Convert structure to <I>nsightII .car format
    Convert structure to InsightII <N>xyz free format
    Convert structure to InsightII <S>xyz free format
    Convert structure to InsightII sxyz<R>q free form.
    Convert structure to <A>msol 3.5 input format
    Convert structure to Gaussian <O>niom format
    List column ranges for a different structure <F>ormat
  <T>rajectory file and type conversions [4]
    Convert trajectory to <C>harmm format
    Convert trajectory to <A>mber format
    Convert trajectory to <M>acromodel format
    Convert trajectory to <X>cluster format
    <S>eparate GCE MMC trajectory into Amber trajectories
  Atom <N>ame and residue name conversions [4]
    <R>egularizing pdb names
    <U>ndo pdb regularizing (eliminate lead numbers)
    <L>eft-adjust atom names
    Convert to di<F>ferent PDB residue and atomname convention
    Make atom names all <D>ifferent
    Convert <P>DB atm names of the form dHXd to HXdd
  Trajectory - str<U>cture file conversions (pack/unpack) [4]
    <U>npack trajectory into single configurations
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  Unpac<K> configurations into (single) file(s)
  <C>ombine configurations into a trajectory
  Combine PDB file into a set of <M>ODEL/ENDMDL records
Conformation <E>dit (trans/rot/cent/algn/add/del, etc.) [15]
  <E>dit the configuration (delete selected atoms)
    Keep all solute atoms - i.e., drop sol<V>ents (if any)
    Select (keep only one) <C>hain/segment/molecule (id)
    Excise (drop only one) chain/<S>egment/molecule (id)
    Keep only the <B>ackbone
    Keep only the <A>lpha carbons
    Drop aliphatic <H>ydrogens
    Drop al<L> hydrogens
    Select atom range to <K>eep
    Select atom range to <D>rop
    Select <R>esidue index range to keep
    Select r<E>sidue index range to drop
    Select a<T>om names to keep
    Select resid<U>e names to keep
  <R>otate/translate/scale/center/seprate/swap chirality
    <S>hift (translate) the system by an input vector
    Shift the system to a new position of a selected <A>tom
    Shift the system and reset it into a <P>BC cell
    <C>enter the system in a PBC cell
    S<H>ift the center of the system to <0,0,0>
    <R>otate the system by an angle
    Rotate the system based on <B>ond directions
    Sca<L>e the coordinates (change units)
    S<E>parate molecules (for clarity)
    S<W>ap chirality
  Permute the xy<Z> coordinates of a structure
  Modif<Y> the configuration (mutate/add atoms)
    <M>utate an atom
    Add new atom, defined by bond and torsion <A>ngles
    Add new atom, defined by <B>isector of 2 neighbours
    Add new atom, defined by <T>risector of 3 neighbours
    <C>reate bond between two atoms
  Replace coordi<N>ates of a configuration from an other conf.
  <O>verlay structure on a reference structure
  Change a peptide to re<T>ro-inverso
  Replace c<H>arges of a configuration from an other conf.
  Write P<D>B file of the residue trace (alpha carbons)
  Fi<X> water geometry to experimental geometry
  Trim <W>aters outside a simulation cell
  Re<V>erse a previous optimization
  Create full crystal <C>ell from the asymmetric unit
  Create <B>iological oligomers from the asymmetric unit
  Gather all crysta<L> contacts of the asymmetric unit
  Cre<A>te neighboring PBC cells
<M>iscellaneous (seq, RTF, UHBD, tors., Amber sum, etc.)[7]
  <E>xtract sequence
  <C>onvert sequence
  Create a <G>rasp .crg file
  Create a U<H>BD .dat file
  Print neighboring PBC cel<L> centers, cell vertices
  Print a PDB file for a <R>ectangle (box)
  Torsion <I>nput generation
  Create Charmm RT<F> residue record(s)
  Summarize <A>mber energy decomposition tables (csv format)
<A>nalyze (TRAJELIX, RMSD, H-bonds, CV, etc.) [17]
  <G>eometry/topology (links, bond, angle, torsion, etc.)  [4]
    Nei<G>hbor, bondlength, angle, torsion list
    1-<4> neighbour and torsion list
    <F>unctional group and backbone list
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    <B>ond length, angle list and distribution
  <B>ond (salt bridge, hydrogen/hydrophobic) track, corr.  [6]
    <H>ydrogen bond list, time course, and correlation
    Hydro<P>hobic contact list, time course, and correlation
    <S>alt bridge list, time course, and correlation
    Heavy atom VdW <C>ontact search
    M<U>tually proximal contact search
    Hydrogen-bonded <B>ridge search
    Residue-residue bond (HB, SB or HPH) <M>atrix comparison
  Atomic propert<Y> (CV, hydrophobicity, Delphi potential) [3]
    Hydrophobicit<Y> (hydropathy) labeling
    <C>ircular variance labeling
    Delphi <P>otential labeling
  M<O>lecular property (shell vol, rad, com, dipole, axis) [4]
    S<O>lvation shell volume
    Principal axis <D>irections and alignment
    Radius (gyration, hydrodynamic), COM, inert, dipole <M>oment
    Membrane <F>latness calculation
  R<M>SD calculation (1D, 2D RMSD map, 2-traj cross RMSD)  [4]
    <1>-D RMSD and RMSF calculation
    <2>-D RMSD calculation
    <C>ross RMSD map for a trajectory pair
    RMSF <D>ifference calculation
  Meas<U>re distances (atom-atom, residue-residue, etc.)   [8]
    R<E>sidue distance list
    Mo<L>ecule-molecule distance list
    Residue adjacency <M>atrix power analysis
    Track PBC-adj<U>sted distance of two atoms
    Track PBC-adjusted range of sol<V>ent movement
    A<T>om-atom distance distribution
    Atom-atom <S>D matrix from a trajectory
    <C>heck for unphysical distances
    C<O>mpare average residue-residue distance matrices
  Plot PBC cell si<Z>es, volume
  Psi-Phi R<A>machandran and dial plots
  Bond angle statistics d<I>al plots
  <T>orsion angle statistics and dial plots
  Proline <K>ink calculation
  Heli<X> analysis (TRAJELIX)
  <P>seudorotation angle calculation
  D<S>SP secondary structure assignment
  Circular <V>ariance map
  Residue cov/cor matrix (from inp/traj), <N>ormal mode anal.
  Summarize Amber energy <D>ecomposition tables (old format)
  <F>ilter solvents by solute distance and/or CV; by interface
Cluste<R> atoms or data defined by a distance matrix [2]
  Cluster <A>toms of an input structure
  Read the <D>istance matrix of the items to be clustered
Make the input <P>redictable
Open <L>ogfile logging the keyboard inputs

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"Quit Simulaid" selected
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