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APPENDICES

bubble.tcl

```
wrapmode cell
# Two first agruments of calcforces are automatically forwarded
# to it by NAMD. The other 4 arguments match the list of 4 values
# from command tclBCArgs.
foreach { x0 y0 z0 } $bubbleCenter { break }
proc calcforces {step unique Rstart Rtarget Rrate K} {
  global x0 y0 z0  ;# defined in tclBCScript{ ... }
  # increase R, starting from $Rstart, by $Rrate at each step,
  # until it reaches $Rtarget; then keep it constant

  set R [expr $Rstart + $Rrate * $step]
  if { $R > $Rtarget } { set R $Rtarget }

  # get the components of the bubble center vector

  if { $step % 200 == 0} { cleardrops}
  # pick atoms of the given patch one by one
  while { [nextatom]  } {
        set atomid [getid]
        #OXY atom
        if {  $atomid > 4239 && $atomid < 4540 } {
        set rvec [getcoord] ;# get the atom's coordinates
        foreach { x y z } $rvec { break } ;# get components of the vector

   # find the distance between the atom and the bubble center
        # (long lines can be broken by a backslash and continued
        # on the next line)
        #set rho [expr sqrt(($x-$_)*($x-$x0) + ($y-$y0)*($y-$y0) +  #($z-$z0)*($z-$z0))]

        set rho [expr sqrt(($z-$z0)*($z-$z0))]

        # if the atom is inside the sphere, push it away radially
        set roxy [expr $R + 2 ]
         if { $rho > $roxy } {
                #set forceX [expr -1*$K * ($x-$x0) / $rho]
                #set forceY [expr -1*$K * ($y-$y0) / $rho]
                set forceZ [expr -1*$K * ($z-$z0) / $rho]
                addforce "0.0 0.0 $forceZ"
```

```
            } elseif { $rho < $R  } {
            dropatom
           }
   } elseif { $atomid > 4539 && $atomid < 4840  } {
         #nic Atom
         set rvec [getcoord] ;# get the atom's coordinates
         foreach { x y z } $rvec { break } ;

         set rho [expr sqrt(($z-$z0)*($z-$z0))]
         set rnic [expr $R - 2 ]
          if { $rho < $rnic } {
                  #set forceX [expr -1*$K * ($x-$x0) / $rho]
                  #set forceY [expr -1*$K * ($y-$y0) / $rho]
                  set forceZ [expr $K * ($z-$z0) / $rho]
                  addforce "0.0 0.0 $forceZ"
            } elseif { $rho > $R } {
           dropatom
           }
   } else  {
         dropatom ;# no longer consider this atom until "cleardrops"
         }
}
}
```


namd.conf

```
#######################################################
#######################################################
############namd configuration file ################
structure          ./proteininput.psf
coordinates         ./proteininput.pdb
set ctonnb          9
set ctofnb          10
set pairdis         12
set temperature     310
set outputname      proteininput
firsttimestep       0
#############################################################
## SIMULATION PARAMETERS                    ##
```

```
#####################################################################
# Input
paraTypeCharmm          on
parameters              param19-epr.inp
COMmotion               no
temperature             $temperature


# tclBC
tclBC on
tclBCScript {
   set bubbleCenter    "0.0 0.0 0.0 "
   set tclBCScript      bubble.tcl
   source $tclBCScript
}
tclBCArgs {0. 15. .01 5.}


# Force-Field Parameters
exclude                 scaled1-4
1-4scaling              1.0
cutoff                  $ctofnb
nonbondedScaling        1.0
switching               on
switchdist              $ctonnb
pairlistdist            $pairdis
pairlistsPerCycle       2
margin                  0.0

#fixed atom
fixedAtoms on
fixedAtomsForces off
fixedAtomsFile ./proteininputfix.pdb
fixedAtomsCol B

#2nd stcr restraint
extraBonds on
extraBondsFile extrabonds.txt

# Integrator Parameters
timestep                2.0  ;# 2fs/step
```

```
rigidBonds          all  ;# needed for 2fs steps
nonbondedFreq         1
useSettle           on
fullElectFrequency    2
stepspercycle        20

#################################################################
## Boundary Conditions                                         ##
#################################################################
# Periodic Boundary Conditions
cellBasisVector1      100 0   0
cellBasisVector2      0   100 0
cellBasisVector3      0   0   100
cellOrigin          0.00  0.00  3.87
XSTfile             $outputname
XSTfreq              2000
wrapAll             on

#################################################################
## EXECUTION SCRIPT                                            ##
#################################################################
# Output
outputName           $outputname
binaryrestart        yes
restartfreq          1000     ;# 500steps = every 1ps
DCDfreq              500
outputEnergies       500
outputPressure       500
outputtiming         500

# Minimization
minimize             2000
reinitvels          310
run                 50000 ;#1  ns  310K
```

VITA

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EDUCATION

Master Student, Physical Chemistry, Department of Chemistry, Faculty of Science, Chulalongkorn University, 2011-present.

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PRESENTATIONS

Membrane Protein Refolding Simulation by NAMD-PaDSAR: Procedures and Evaluation. Oral presentation at the 39th Congress on Science and Technology of Thailand, BITEC, Bangkok, Thailand. October, 2013.

Evaluation of Membrane Protein Positions in Membrane by Poisson-Boltzman Energy Landscape. Poster presentation at the 10th Thai Summer School on Computational Chemistry, Kasetsart University at Sri-Racha campus, Chonburi, Thailand, October, 2013.

Pseudoatom-Driven Solvent Accessibility Refinement on NAMD: A Preliminary Study. Poster presentation at the 38th Congress on Science and Technology of Thailand, The Empress Convention Halls, Chaing Mai, Thailand. October, 2012.

ADDITIONAL RESEARCH EXPERIENCE

JAIST's ASEAN Short Stay Program in Material Science at Japan Advanced Institute of Science and Technology, Japan. 39 days, October, 2012.