Simulations at the Nanoscale with NAMD

Lab Molecular Dynamics Simulations

NAMD Overview

ICMAB
INSTITUT DE CIÈNCIA DE MATERIALS DE BARCELONA
EXCELENCIA SEVERO OCHOA
CSIC
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NAMD

Scalable Molecular Dynamics

Free for academics program
NAnoscale Molecular Dynamics- NAMD

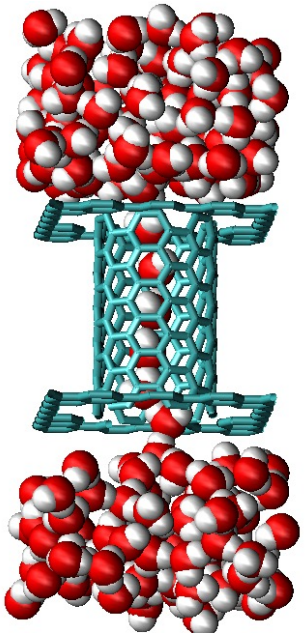
J. Comp. Chem., 26:1781-1802, 2005.

NAMD webpage contains examples of use in Nanoscience

http://www.ks.uiuc.edu/Research/Categories/Nano/all.cgi

and useful tutorials for self-learning
http://www.ks.uiuc.edu/Training/Tutorials/index-all.html#namd

Molecular Dynamics: simulation of the motion of atoms based on Physics

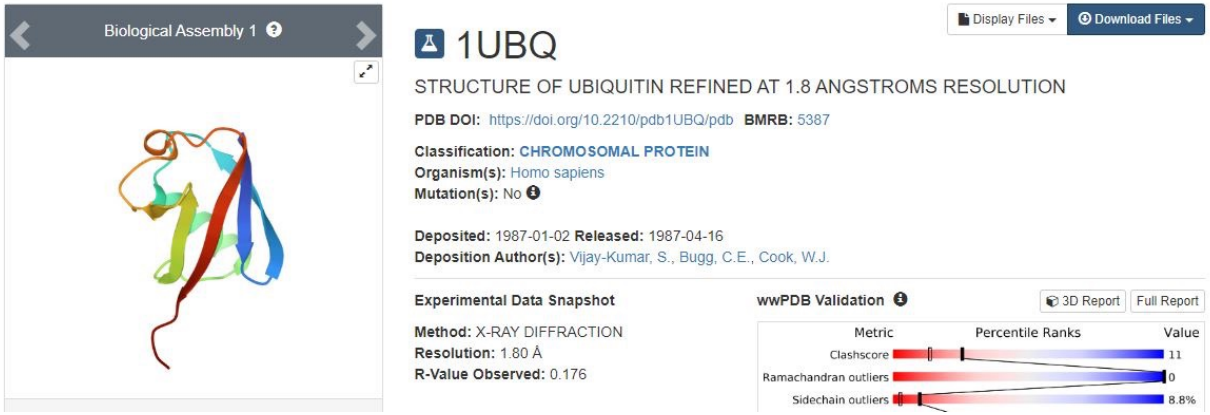


$$F_i = m_i a_i \qquad a_i = \frac{dv_i}{dt} \qquad v_i = \frac{dr_i}{dt}$$

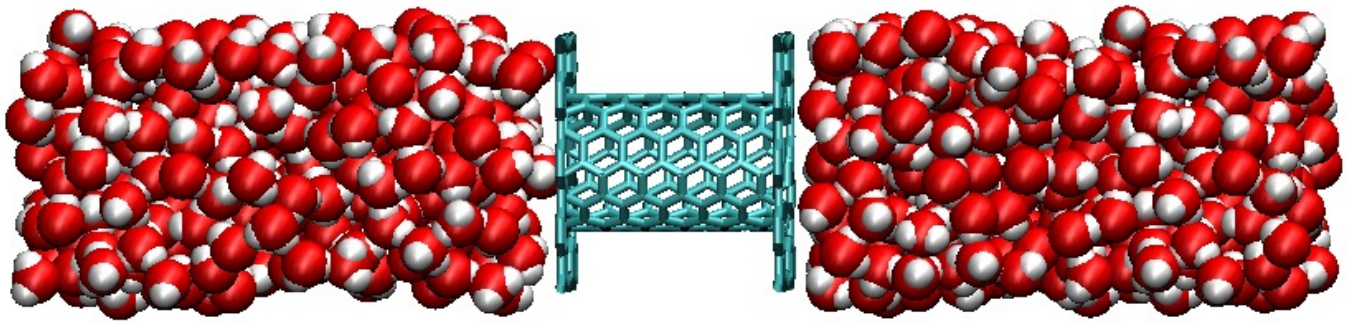
Newton's equations

Examples GitHub

-Starting from experimental structures complemented/modified with VMD: Simulation of 1UBQ protein (complete the structure, add water)

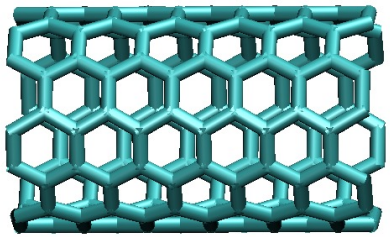


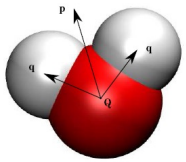
- Starting from structures generated with VMD: Simulation of the flow of water across a carbon nanotube



NAMD Workflow

1.- Atomic coordinates (pdb), and topology (psf)

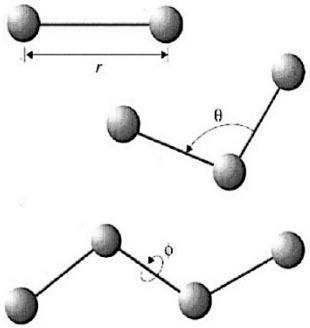




VMD

+

2.- Parameters for force field (interactions) **.inp files**



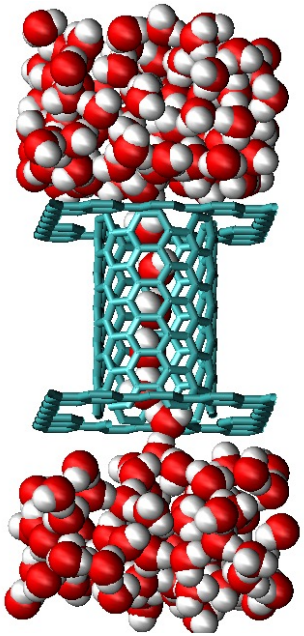
$$U_{total} = U_{vdW} + U_{Coulomb} + \cdots$$

$$\ldots U_{bond} + U_{angle} + U_{dihedral}$$

Force Field:
CHARMM
Files: .inp

+

Molecular Dynamics: simulation of the motion of atoms based on Physics



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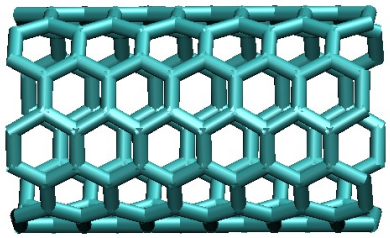

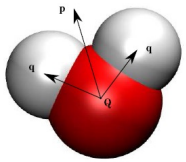

VMD

Input of atomic coordinates for NAMD

ALWAYS PDB format (originally from Protein Data Bank)

Extension: .pdb

<record type> <atom ID> <atom name> <residue name> <residue ID>
< x, y, and z coordinates in Angstrom > <ccupancy> <beta factor> < segment name> <lin

system.pdb

```
CRYST1   17.194   17.018   80.000  90.00  90.00  90.00 P 1           1
ATOM      1   C1  CNT T   1       4.078   0.000  -6.754  1.00  1.00      TUB  C
ATOM      2   C2  CNT T   1       3.832   1.395  -6.754  1.00  1.00      TUB  C
ATOM      3   C3  CNT T   1       3.531   2.039  -5.526  1.00  1.00      TUB  C
ATOM      4   C4  CNT T   1       2.621   3.124  -5.526  1.00  1.00      TUB  C
ATOM      5   C5  CNT T   1       2.039   3.531  -6.754  1.00  1.00      TUB  C
ATOM      6   C6  CNT T   1       0.708   4.016  -6.754  1.00  1.00      TUB  C
ATOM      7   C7  CNT T   1       0.000   4.078  -5.526  1.00  1.00      TUB  C
ATOM      8   C8  CNT T   1      -1.395   3.832  -5.526  1.00  1.00      TUB  C
ATOM      9   C9  CNT T   1      -2.039   3.531  -6.754  1.00  1.00      TUB  C
ATOM     10   C10 CNT T   1      -3.124   2.621  -6.754  1.00  1.00      TUB  C
ATOM   1858  OH2 TIP3W9096      -5.682   5.688  28.813  1.00  0.00      WT2  O
ATOM   1859  H1  TIP3W9096      -6.442   5.905  29.336  1.00  0.00      WT2  H
ATOM   1860  H2  TIP3W9096      -5.878   4.824  28.431  1.00  0.00      WT2  H
ATOM   1861  OH2 TIP3W9226      -0.019  -7.677  31.770  1.00  0.00      WT2  O
ATOM   1862  H1  TIP3W9226      -0.669  -7.979  31.113  1.00  0.00      WT2  H
ATOM   1863  H2  TIP3W9226      -0.034  -6.708  31.754  1.00  0.00      WT2  H
ATOM   1864  OH2 TIP3W9241      -1.310   1.663  39.234  1.00  0.00      WT2  O
ATOM   1865  H1  TIP3W9241      -1.966   0.964  39.496  1.00  0.00      WT2  H
ATOM   1866  H2  TIP3W9241      -0.478   1.160  39.271  1.00  0.00      WT2  H
END
```

see

https://www.ks.uiuc.edu/Training/Tutorials/namd/namd-tutorial-unix-html/node22.html

Input of topology data for NAMD

Structure data File **Extension:** .psf

A first section with: atom ID, segment name, residue ID, residue name, atom name, type, charge and mass, and an unused field with 0.

Second section with molecular topology: bonds, angles, dihedrals

```
PSF CMAP

       6 !NTITLE
 REMARKS original generated structure x-plor psf file
 REMARKS 2 patches were applied to the molecule.
 REMARKS topology top_all27_prot_lipid.inp
 REMARKS segment U { first NTER; last CTER; auto angles dihedrals }
 REMARKS defaultpatch NTER U:1
 REMARKS defaultpatch CTER U:76

    1231 !NATOM
       1 U    1    MET  N    NH3   -0.300000       14.0070           0
       2 U    1    MET  HT1  HC     0.330000        1.0080           0
       3 U    1    MET  HT2  HC     0.330000        1.0080           0
       4 U    1    MET  HT3  HC     0.330000        1.0080           0
       5 U    1    MET  CA   CT1    0.210000       12.0110           0
       6 U    1    MET  HA   HB     0.100000        1.0080           0
       7 U    1    MET  CB   CT2   -0.180000       12.0110           0
```

```
1237 !NBOND: bonds
   1       5       2       1       3       1       4       1
   5       6       7       5       7       8       7       9
  10       7      10      11      10      12      13      10
```

see

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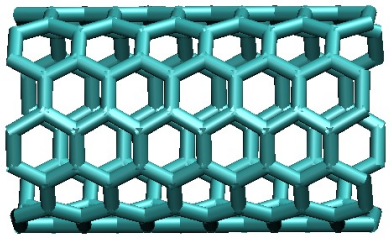

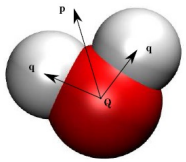

VMD

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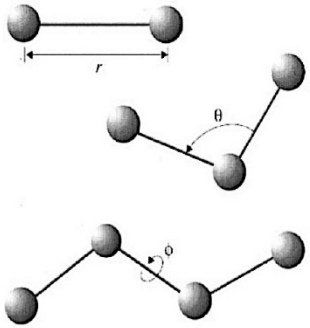

$$U_{total} = U_{vdW} + U_{Coulomb} + \cdots$$

$$\ldots U_{bond} + U_{angle} + U_{dihedral}$$

Force Field:
CHARMM
Files: .inp

Format atomic interaction Force Field

Force Field File **Extension:** .inp .rtf

Header with each interaction potential (equation and units)
Atom types and values of parameters of the interaction potential

Sections with intramolecular parameters (bonds, angles, dihedrals) and Lennard-Jones intermolecular forces

```
BONDS
!V(bond) = Kb(b - b0)**2
!
!atom type Kb          b0
CA   CA    305.000     1.3750

ANGLES
!V(angle) = Ktheta(Theta - Theta0)**2
!V(Urey-Bradley) = Kub(S - S0)**2
!
!atom types     Ktheta    Theta0   Kub      S0
CA   CA   CA    40.000    120.00   35.00    2.41620
```

Force Field files available from

http://mackerell.umaryland.edu/charmm_ff.shtml

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```
!V(Lennard-Jones) = Eps,i,j[(Rmin,i,j/ri,j)**12 - 2(Rmin,i,j/ri,j)**6]
!
!atom  ignored    epsilon      Rmin/2
CA     0.000000  -0.070000     1.992400

HBOND CUTHB 0.5

END
```

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MD practical Workflow

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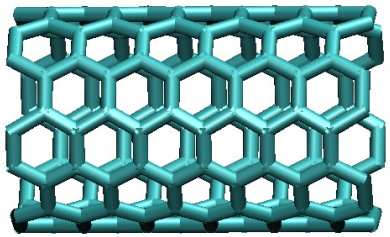

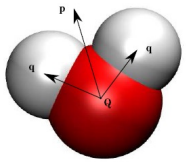

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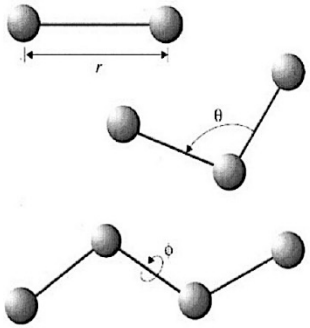

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Force Field:
CHARMM
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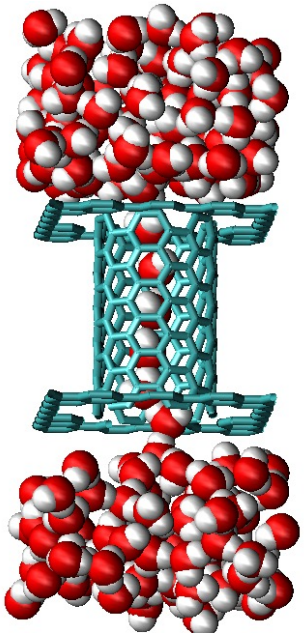

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Newton's equations

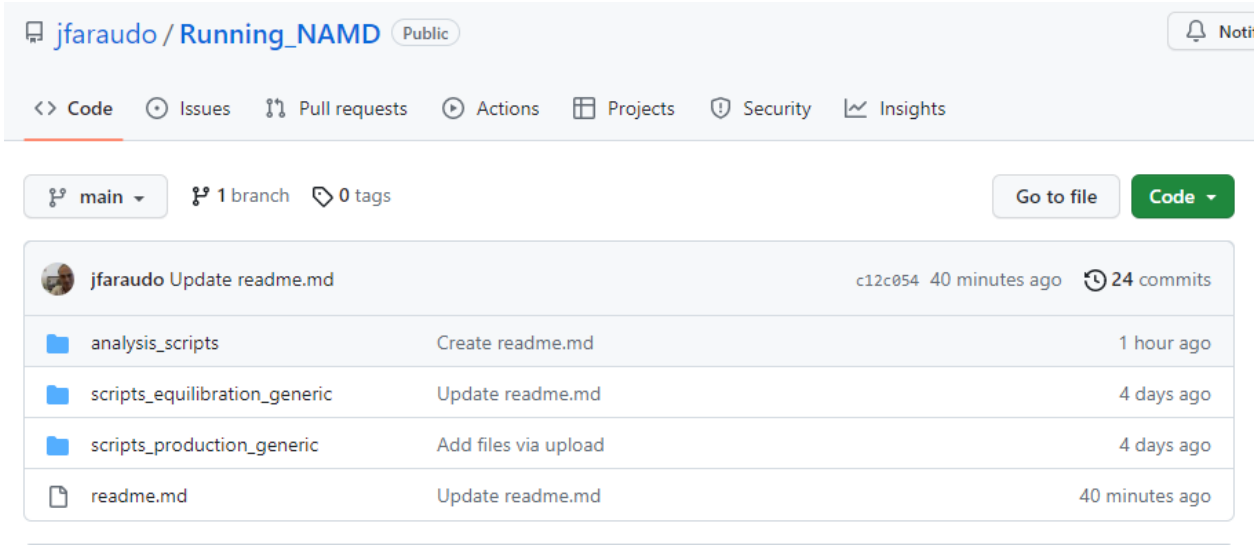
Format NAMD script

NAMD script **Extension:** .namd .conf

Many details including:

- Input/output files
- Time step and details of Integration eqs. of motion
- Thermostats and barostats
- External fields or external forces
- Maintain selection of atoms at fixed positions
- Specification on frequency to save data

LOOK TO THE SAMPLE SCRIPTS PROVIDED AT GitHub

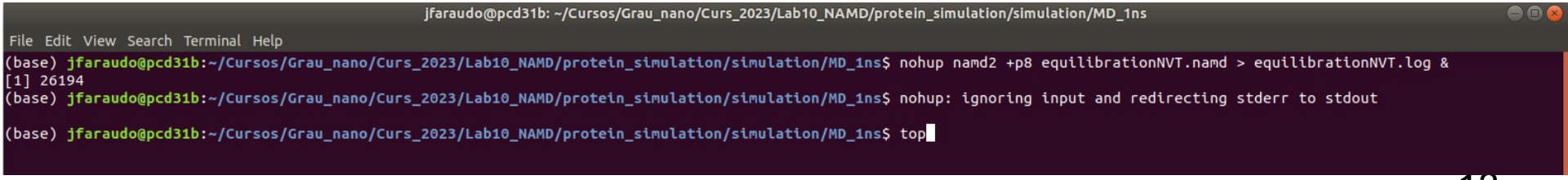


Execute NAMD (Linux)

Check number of processors with lscpu

run in background using all of them:

nohup namd2 +p8 myfilename.namd > myfilename.log &



NAMD: Nonequilibrium simulations

The .namd file can be programmed to add external forces over selected atoms (other features such as move at fixed velocity are also possible)

```
#############################################################
## EXTRA PARAMETERS
#############################################################

tclForces              on

tclForcesScript {
  set cellLengthZ 70.4338967403  ;# The length of the unit
  set LowerBoundary -32.52
  set UpperBoundary 32.52
  set force {0 0 0.4}
  set watIdList {}
  for {set i 277} {$i<1866} {incr i 3} {
    lappend watIdList $i
    addatom $i
  }
  proc calcforces {} {
    global cellLengthZ LowerBoundary UpperBoundary force wa
    loadcoords coorList
    foreach i $watIdList {
      set z [lindex $coorList($i) 2]
      set z [expr $z-round($z/$cellLengthZ)*$cellLengthZ]
      if {$z>$UpperBoundary || $z<$LowerBoundary} {
        addforce $i $force
      }
    }
  }
}
```

Apply F over each molecule in a thin region

$$\Delta p = \frac{N_{molec} F}{A}$$

https://www.ks.uiuc.edu/Training/Tutorials/science/forces/forces-tutorial.pdf