

Simulations at the Nanoscale with NAMD

Lab Molecular Dynamics Simulations

NAMD Overview



Jordi Faraudo

jfaraudo@icmab.es

NAMD

Scalable Molecular Dynamics

Free for academics program

NAnoscale Molecular Dynamics- NAMD

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

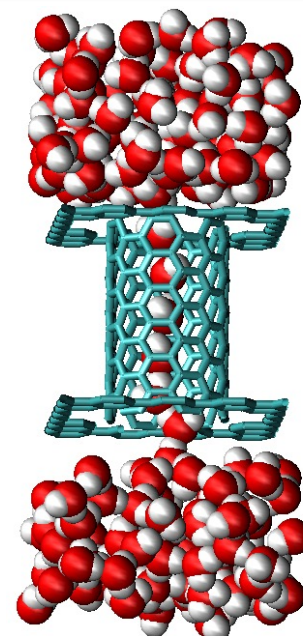
NAMD webpage contains examples of use in Nanoscience

<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

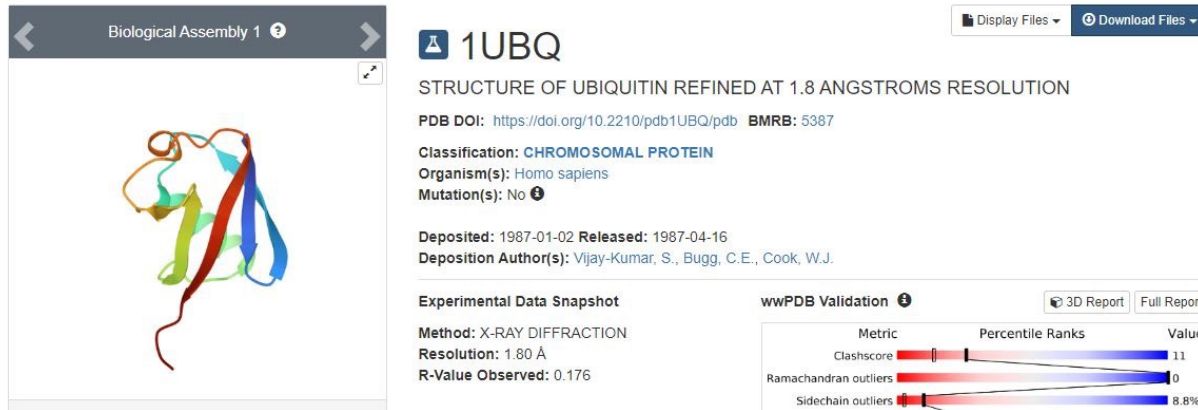


$$\mathbf{F}_i = m_i \mathbf{a}_i \quad \mathbf{a}_i = \frac{d\mathbf{v}_i}{dt} \quad \mathbf{v}_i = \frac{d\mathbf{r}_i}{dt}$$

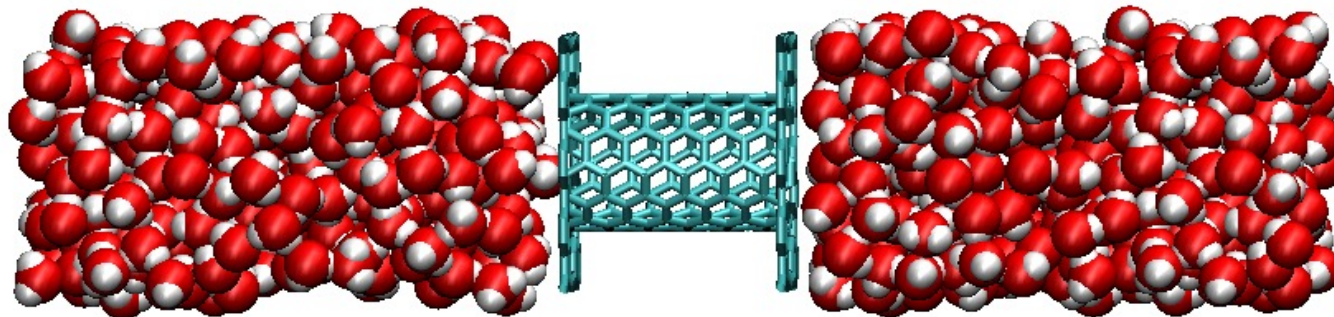
Newton's equations

Examples GitHub

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

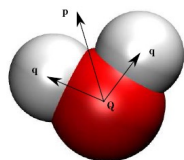
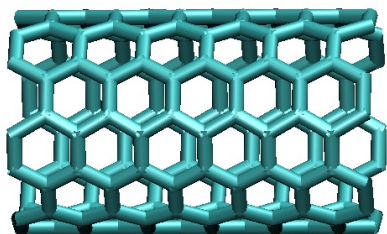


- Starting from structures generated with VMD: Simulation of the flow of water across a carbon nanotube



NAMD Workflow

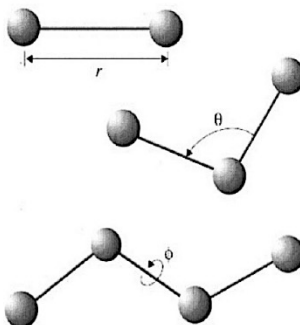
1.- Atomic coordinates (pdb), and topology (psf)



VMD

+

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



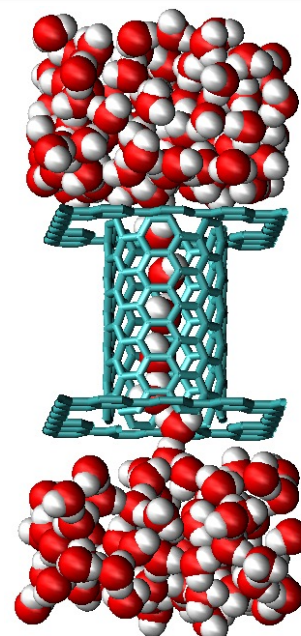
$$U_{total} = U_{vdW} + U_{Coulomb} + \dots$$

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

Force Field:
CHARMM
Files: .inp

+

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

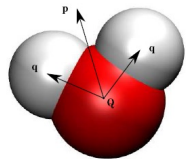
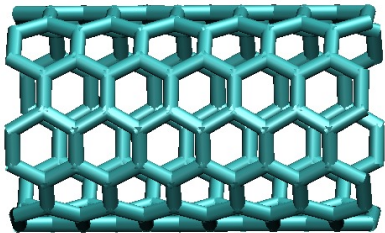


$$\mathbf{F}_i = m_i \mathbf{a}_i \quad \mathbf{a}_i = \frac{d\mathbf{v}_i}{dt} \quad \mathbf{v}_i = \frac{d\mathbf{r}_i}{dt}$$

Newton's equations

NAMD Workflow

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



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 X												
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

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

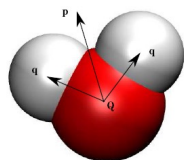
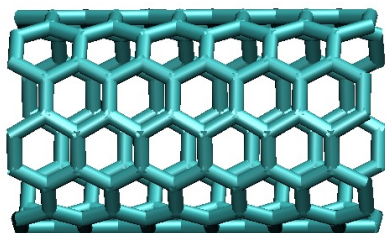
see

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

NAMD Workflow

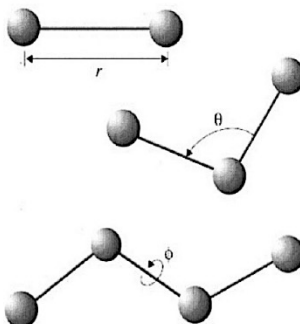
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VMD



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



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

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

*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

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

```
!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

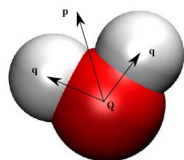
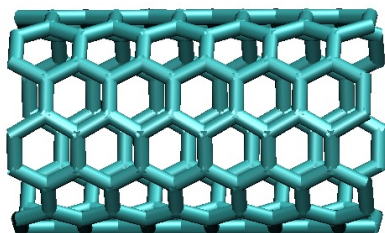
END
```

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MD practical Workflow

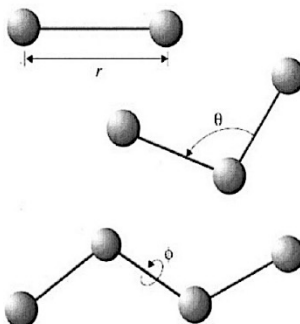
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VMD



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



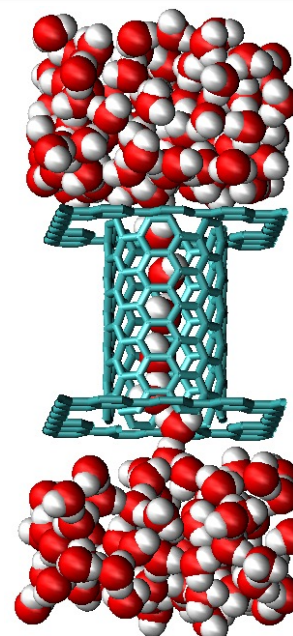
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Newton's equations

Format NAMD script

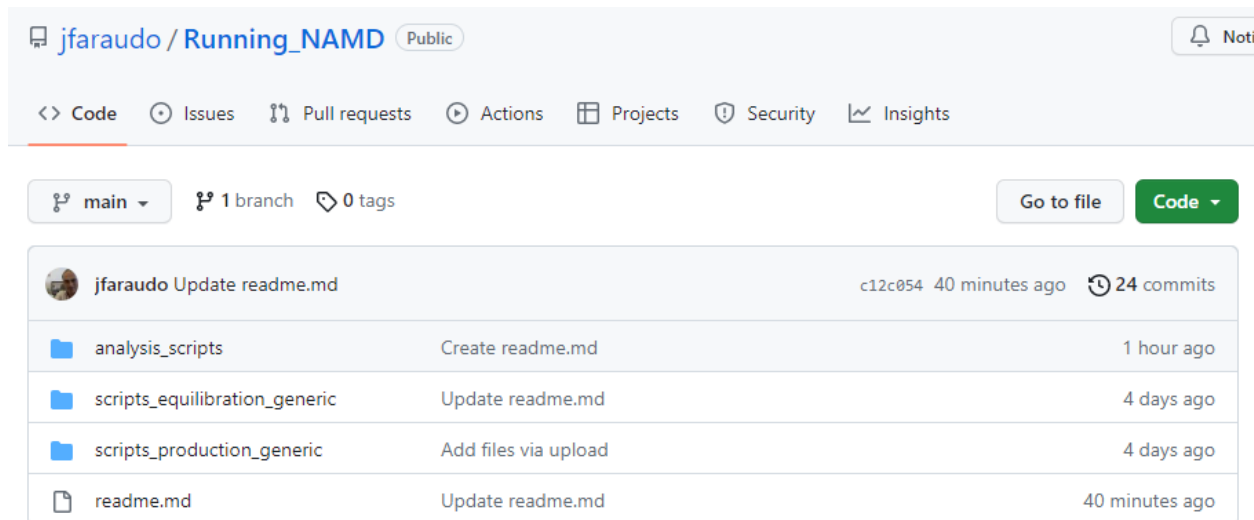
NAMD script

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



The screenshot shows the GitHub repository page for 'jfarauco / Running_NAMD'. The repository is public and has a notification bell icon in the top right. The navigation bar includes links for Code, Issues, Pull requests, Actions, Projects, Security, and Insights. Below the navigation bar, there are buttons for 'main' branch, '1 branch', and '0 tags'. There are also buttons for 'Go to file' and 'Code'. The repository content is displayed in a table with columns for the file/folder name, the commit message, and the commit time.

File/Folder	Commit Message	Commit Time
analysis_scripts	Create readme.md	1 hour ago
scripts_equilibration_generic	Update readme.md	4 days ago
scripts_production_generic	Add files via upload	4 days ago
readme.md	Update readme.md	40 minutes ago

Execute NAMD (Linux)

Check number of processors with lscpu

```
jfaraudo@pcd31b: ~/Research_local
File Edit View Search Terminal Help
(base) jfaraudo@pcd31b:~/Research_local$ lscpu
Architecture:          x86_64
CPU op-mode(s):        32-bit, 64-bit
Byte Order:             Little Endian
CPU(s):                 8
On-line CPU(s) list:   0-7
Thread(s) per core:    2
Core(s) per socket:    4
Socket(s):              1
NUMA node(s):          1
Vendor ID:              GenuineIntel
CPU family:             6
Model:                  85
Model name:             Intel(R) Xeon(R) W-2123 CPU @ 3.60GHz
Stepping:               4
CPU MHz:                1200.002
CPU max MHz:            3900.0000
CPU min MHz:            1200.0000
CpuMIPS:                7200.00
Virtualisation:         VT-x
L1d cache:              32K
L1i cache:              32K
L2 cache:               1024K
L3 cache:               8448K
NUMA node0 CPU(s):     0-7
Flags:                   fpu vme de pse tsc msr pae mce cx8 apic sep mtrr pge mca cmov pat pse36 clflush dts acpi mmx fxsr sse sse2 ss ht tm pbe syscall nx pdpe1gb rdtscp lm constant_tsc art arch_perfmon pebs bts rep_good nopl xtopology nonstop_tsc cpuid aperfmperf pni pclmulqdq dtes64 monitor ds_cpl vmx smx est tm2 ssse3 sdbg fma cx16 xtpr pdcm pcid dca sse4_1 sse4_2 xzavic movbe popcnt tsc_deadline_timer aes xsave avx f16c rdrand lahf_lm abm 3dnowprefetch c
uid fault epb cat l3 cdp l3 invpcid single pti intel ppin ssbd mba ibrs ibpb stibp tpr shadow vmni flexpriority ept vpid fsgsbase tsc_adjust bmi1 hle av
```

run in background using all of them:

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

```
jfaraudo@pcd31b: ~/Cursos/Grau_nano/Curs_2023/Lab10_NAMD/protein_simulation/simulation/MD_1ns
File Edit View Search Terminal Help
(base) jfaraudo@pcd31b:~/Cursos/Grau_nano/Curs_2023/Lab10_NAMD/protein_simulation/simulation/MD_1ns$ nohup namd2 +p8 equilibrationNVT.namd > equilibrationNVT.log &
[1] 26194
(base) jfaraudo@pcd31b:~/Cursos/Grau_nano/Curs_2023/Lab10_NAMD/protein_simulation/simulation/MD_1ns$ nohup: ignoring input and redirecting stderr to stdout
(base) jfaraudo@pcd31b:~/Cursos/Grau_nano/Curs_2023/Lab10_NAMD/protein_simulation/simulation/MD_1ns$ top
```

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

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