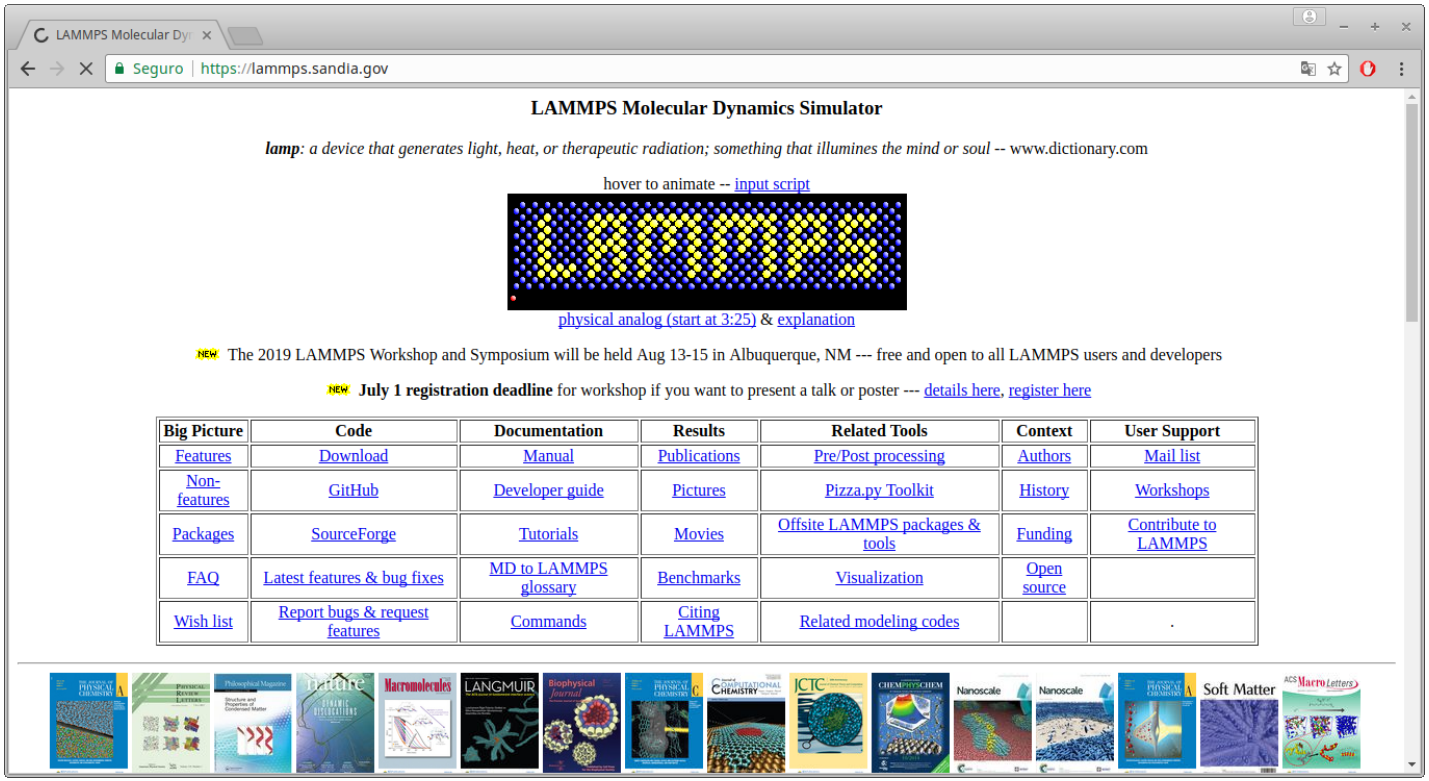
Lo podemos Googlear...



...y nos encontramos con esto!

https://lammps.sandia.g

Seguro | https://lammps.sandia.gov/download.html

LAMMPS website

Download LAMMPS

You can download LAMMPS as a tarball from this page, using the "Download Now" button below.

There are several ways to get the LAMMPS software, either as a tarball, or from an active repository, or in executable form:

- Download a tarball (here or from GitHub)
- Git repository for LAMMPS
- SVN repository for LAMMPS
- Pre-built Linux executables
- Pre-built Mac executables
- Pre-built Windows executables

With source code, you have to build LAMMPS using "cmake" or "make". But you have more flexibility as to what features to include or exclude in the build. If you plan to modify or extend LAMMPS, then you need the source code.

The Install doc page lists what is included in the LAMMPS distribution.

Download a tarball

Select the code you want, click the "**Download Now**" button, and your browser should download a gzipped tar file. Unpack it with the following command, and see the README file to get started.

```
tar -xzvf file.tar.gz
```

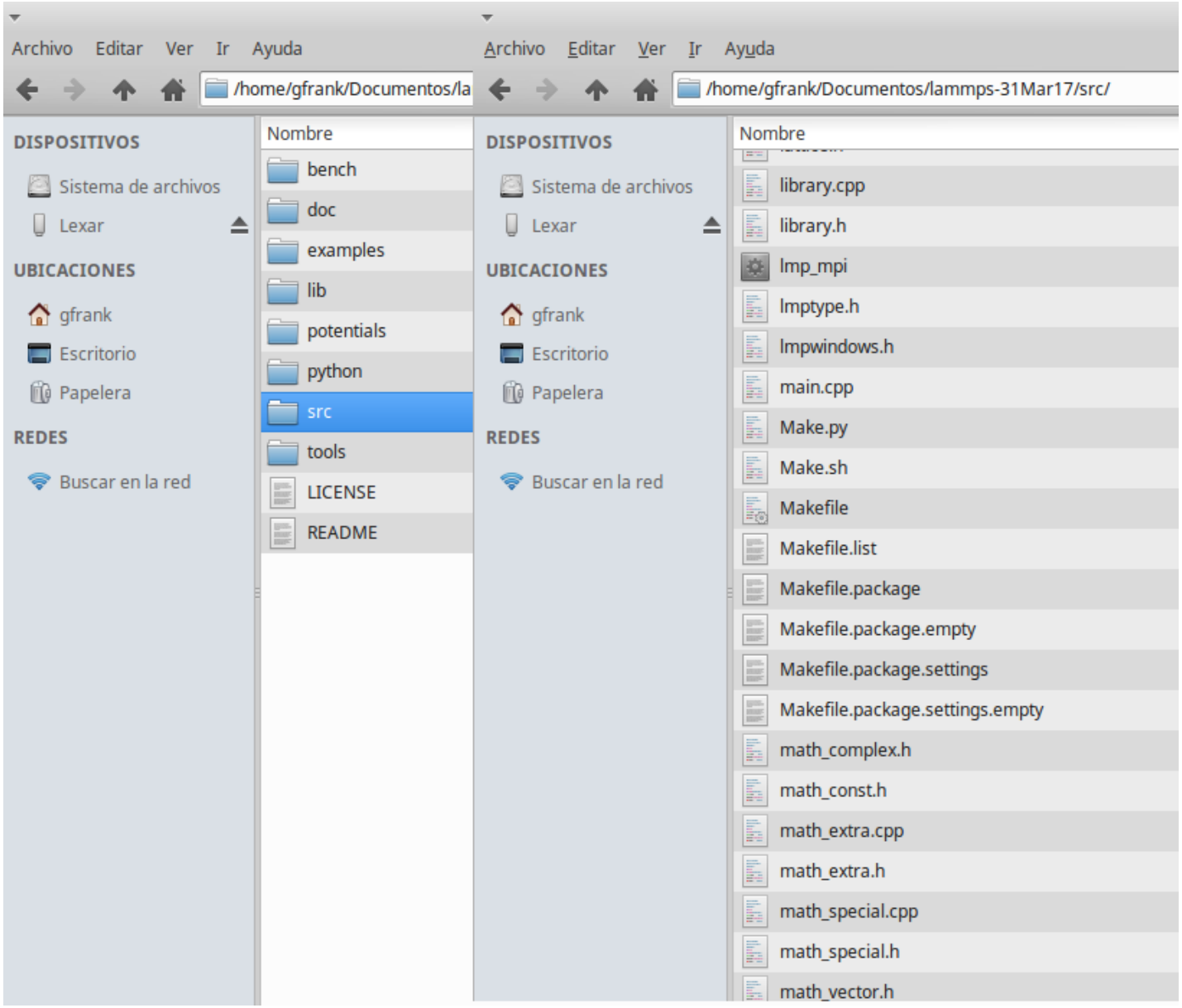
There have been ~316,000 downloads of LAMMPS from Sept 2004 thru Dec 2018.

LAMMPS molecular dynamics package:

- LAMMPS --- Stable version (5 Jun 2019) - Recent C++ version source + doc tarball, GPL license, ~142 Mb. Includes all bug fixes and new features described on this page, up to the date of the most recent stable release.
- LAMMPS --- Development version - Most current C++ version source + doc tarball, GPL license, ~142 Mb. Includes all bug fixes and new features described on this page.
- LAMMPS --- Documentation - Most current C++ version doc tarball, GPL license, ~21 Mb.
- LAMMPS 2001 --- older f90 version source tarball, GPL license, 1.1 Mb, last updated 17 Jan 2005

¡que no es mucha explicación!

Estructura de Lammps



¿Como se usa?

- Hacemos un `make serial` o `make mpi` y se genera el ejecutable `lmp_serial` o bien `lmp_mpi`.
- Escribimos un script y lo corremos...

```
~/lammps-31Mar17/src/lmp_mpi -i myscript.inp
```

- Se generan dos archivos (en principio):

```
myscript.log
myscript.lammpstrj
```

myscript.inp

```
dimension      2
units          lj
lattice        sq 0.1111 origin 0.5 0.5 0.0
region         box block 0 30 0 30 -3 3 units box
create_box     1 box
create_atoms   1 box

mass           1 1.0
velocity       all create 2 87287 dist gaussian
fix            mywalls all wall/region box
               lj126 0.1 0.1 2.5
dump           myexample all image 1
               myexample*.jpg type type
atom_modify     sort 0 0.0

timestep       0.001
fix            1 all nve
thermo         100
run            5000
```

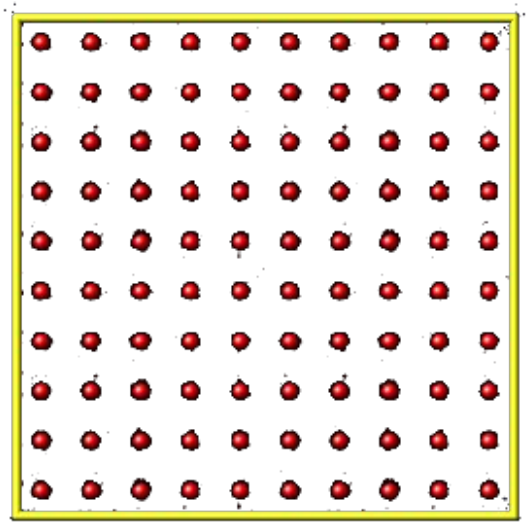
myscript.log

Step	Temp	E_pair	E_mol	TotEng	Press
0	2	0	0	1.98	0.22
100	2	0	0	1.98	0.22
200	2	0	0	1.98	0.22
300	2.0000001	0	0	1.9800001	0.22000001
400	2.0000013	0	0	1.9800013	0.22000015
500	2.000525	0	0	1.9805197	0.22005775
600	2.0003283	0	0	1.980325	0.22003611
700	1.9952534	0	0	1.9753009	0.21947787
800	1.9736402	0	0	1.9539038	0.21710043
900	2.000088	0	0	1.9800871	0.22000968
1000	2.0004502	0	0	1.9804457	0.22004953
1100	2.0010328	0	0	1.9810225	0.22011361
1200	1.996403	0	0	1.976439	0.21960433
1300	2.0000976	0	0	1.9800967	0.22001074
...	...	...	...	...	...

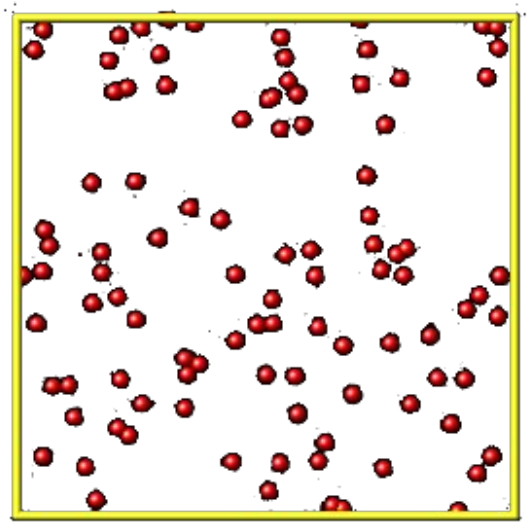
myscript.lammpstrj

```
ITEM: TIMESTEP
0
ITEM: NUMBER OF ATOMS
100
ITEM: BOX BOUNDS pp pp pp
0.0000000000000000e+00 3.0000000000000000e+01
0.0000000000000000e+00 3.0000000000000000e+01
-3.0000000000000000e+00 3.0000000000000000e+00
ITEM: ATOMS id x y vx vy
1 1.50008 1.50008 0.279461 2.62931
2 4.50023 1.50008 -0.146139 -1.78295
3 7.50038 1.50008 -1.12718 -0.235386
4 10.5005 1.50008 1.96689 -1.1713
5 13.5007 1.50008 2.31355 -0.377685
6 16.5008 1.50008 -0.268526 0.687141
7 19.501 1.50008 -0.549147 -1.92898
8 22.5011 1.50008 -1.20579 -0.455545
9 25.5013 1.50008 1.30095 -2.05002
10 28.5014 1.50008 -0.978947 1.67754
.......
```

myscript.jpg



inicial



final

Lammps en múltiples núcleos

- El `script` anterior omite las interacciones entre pares. Esto se incorpora con

```
pair_style lj/cut 2.5
pair_coeff * * 1 1
```

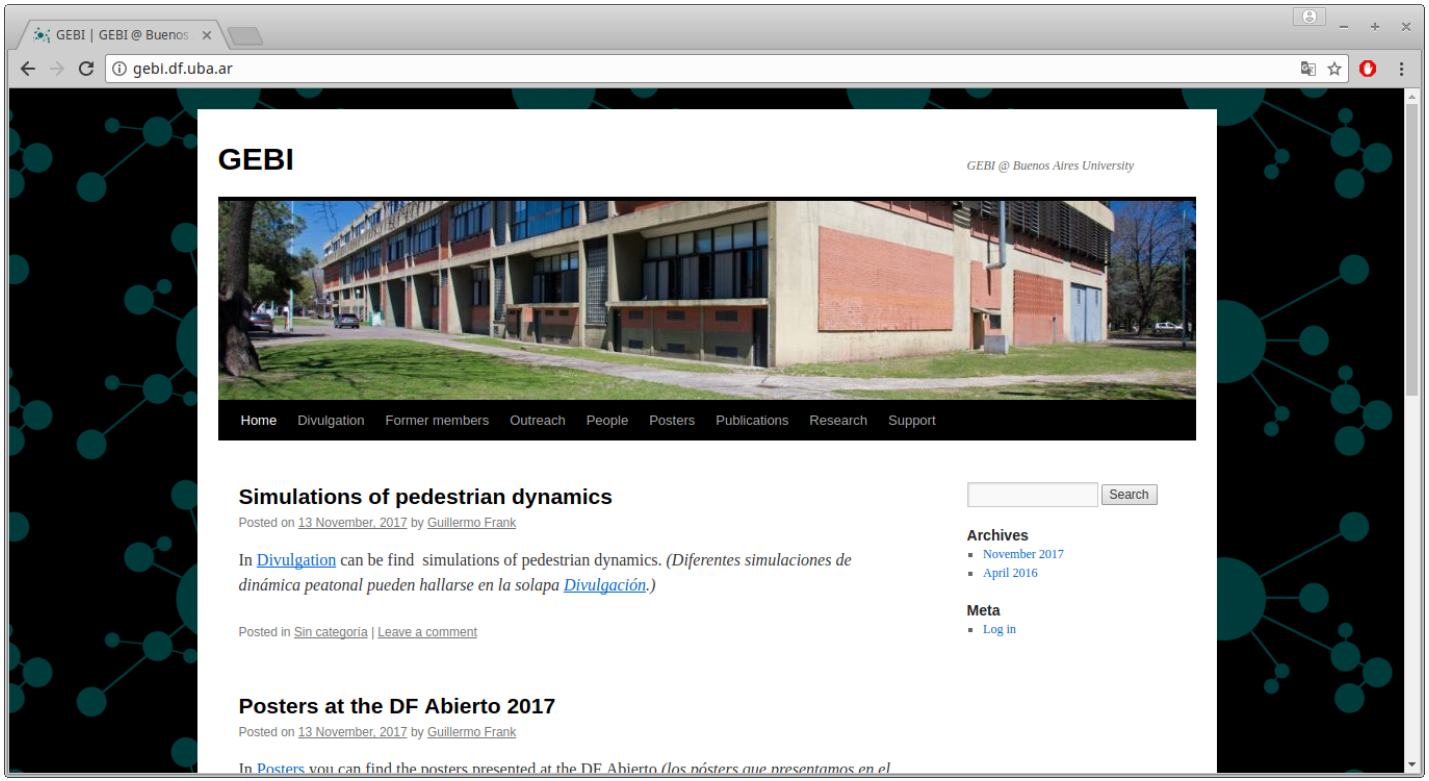
- Para incluir listas de vecinos

```
neighbor 0.3 bin
neigh_modify every 20 delay 0 check no
```

- Para correr con `mpi` (múltiples núcleos)

```
mpirun -np 4 ./lmp_mpi -i /.../myscript.inp
```

Dónde aprender más ...



Dónde aprender más ...