


Lo podemos Googlear...

LAMMPS Molecular Dynamics Simulator

lamp: a device that generates light, heat, or therapeutic radiation; something that illumines the mind or soul -- www.dictionary.com

hover to animate -- [input script](#)




[physical analog \(start at 3:25\)](#) & [explanation](#)

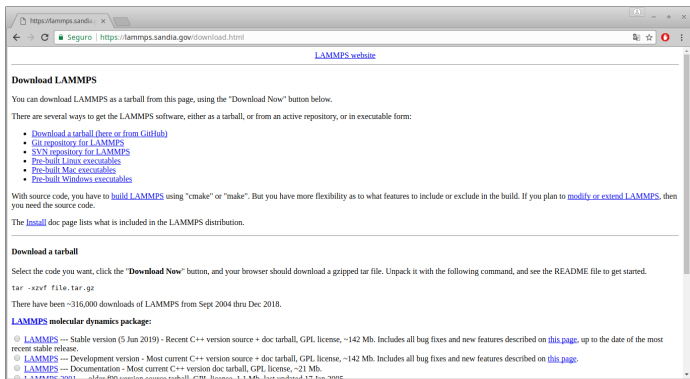
NEW The 2019 LAMMPS Workshop and Symposium will be held Aug 13-15 in Albuquerque, NM --- free and open to all LAMMPS users and developers

NEW July 1 registration deadline for workshop if you want to present a talk or poster --- [details here](#), [register here](#)

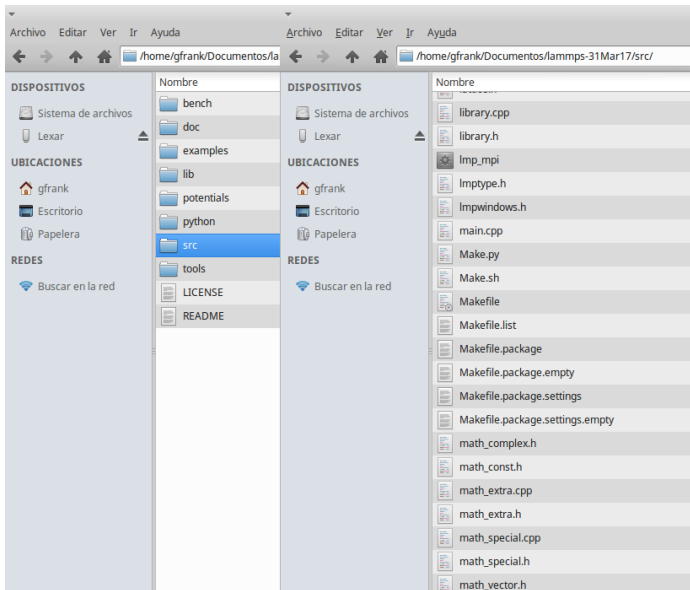
Big Picture	Code	Documentation	Results	Related Tools	Context	User Support
Features	Download	Manual	Publications	Pre-Post processing	Authors	Mail list
Non-features	GitHub	Developer guide	Pictures	Pizza.py Toolkit	History	Workshops
Packages	SourceForge	Tutorials	Movies	Offsite LAMMPS packages & tools	Funding	Contribute to LAMMPS
FAQ	Latest features & bug fixes	MD to LAMMPS glossary	Benchmarks	Visualization	Open source	
Wish list	Report bugs & request features	Commands	Citing LAMMPS	Related modeling codes		



...y nos encontramos con esto!



Estructura de Lammmps



¿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
```

mymscript.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

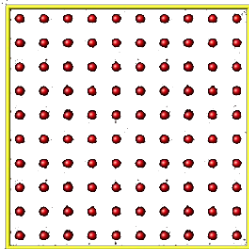
7 19.501 1.50008 -0.549147 -1.92898

8 22.5011 1.50008 -1.20579 -0.455545

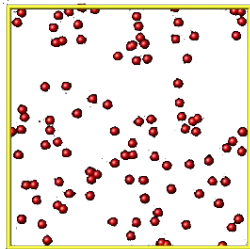
9 25.5013 1.50008 1.30095 -2.05002

10 28.5014 1.50008 -0.978947 1.67754

.....



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
```

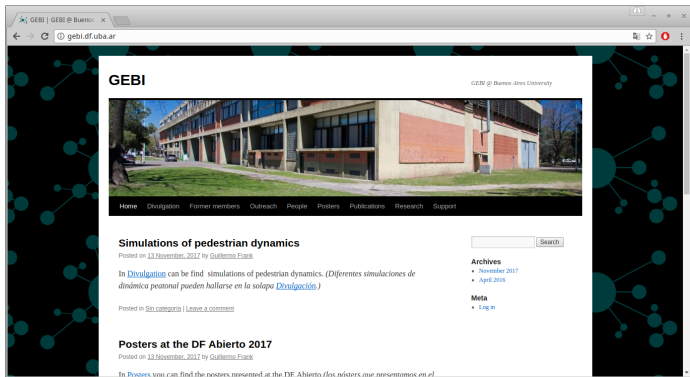
- Para incluir listas de vecinos

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

- Para correr con `mpi` (múltiples núcleos)

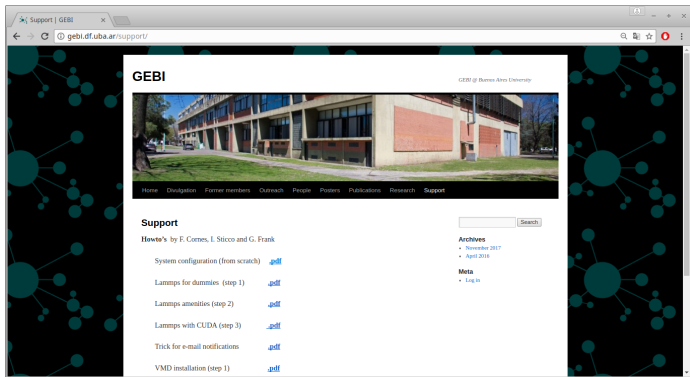
```
mpirun -np 4 ./lmp_mpi -i ../../myscript.inp
```

Dónde aprender más ...



The screenshot shows a web browser window with the address bar displaying "gebi.df.uba.ar". The website has a dark blue header with the "GEBI" logo on the left and "GEBI @ Ramon Abreu University" on the right. Below the header is a navigation bar with links: Home, Divulgation, Former members, Outreach, People, Posters, Publications, Research, and Support. A large photograph of a modern building with a red brick facade and large windows is featured in the center. Below the photo, the section "Simulations of pedestrian dynamics" is highlighted, with a sub-header "Posted on 13 November 2017 by Guillermo Fraile". The text below states: "In [Divulgation](#) can be find simulations of pedestrian dynamics. (Diferentes simulaciones de dinámica peatonal pueden hallarse en la solapa [Divulgación](#).)". To the right of this text is a search bar with a "Search" button. Below the search bar, there are two sections: "Archives" with links for "November 2017" and "April 2016", and "Meta" with a link for "Log in". At the bottom, the section "Posters at the DF Abierto 2017" is shown, with a sub-header "Posted on 13 November 2017 by Guillermo Fraile". The text below states: "In [Posters](#) you can find the posters presented at the DF Abierto (los posters que presentamos en el

Dónde aprender más ...



The screenshot shows a web browser window with the address bar displaying "gebi.df.uba.ar/support/". The page title is "Support | GEBI". The main content area features a large photograph of a modern building with a red brick facade and large windows. Below the photo is a navigation menu with links: Home, Divulgation, Former members, Outreach, People, Posters, Publications, Research, and Support. The "Support" section is highlighted. It includes a search bar and a list of links to PDF documents: "Howto's by F. Cornes, I. Sticco and G. Frank", "System configuration (from scratch)", "Lammps for dummies (step 1)", "Lammps amenities (step 2)", "Lammps with CUDA (step 3)", "Trick for e-mail notifications", and "VMD installation (step 1)". On the right side, there are sections for "Archives" (November 2017, April 2016) and "Meta" (Log in).

Support | GEBI

gebi.df.uba.ar/support/

GEBI

GEBI @ Buenos Aires University

Home Divulgation Former members Outreach People Posters Publications Research Support

Support

Howto's by F. Cornes, I. Sticco and G. Frank

System configuration (from scratch) [.pdf](#)

Lammps for dummies (step 1) [.pdf](#)

Lammps amenities (step 2) [.pdf](#)

Lammps with CUDA (step 3) [.pdf](#)

Trick for e-mail notifications [.pdf](#)

VMD installation (step 1) [.pdf](#)

Archives

- November 2017
- April 2016

Meta

- Log in