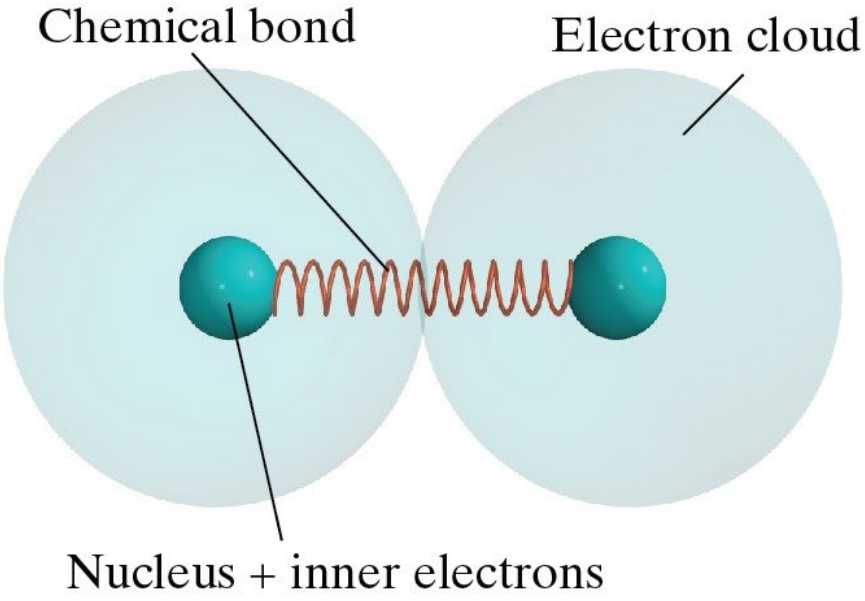
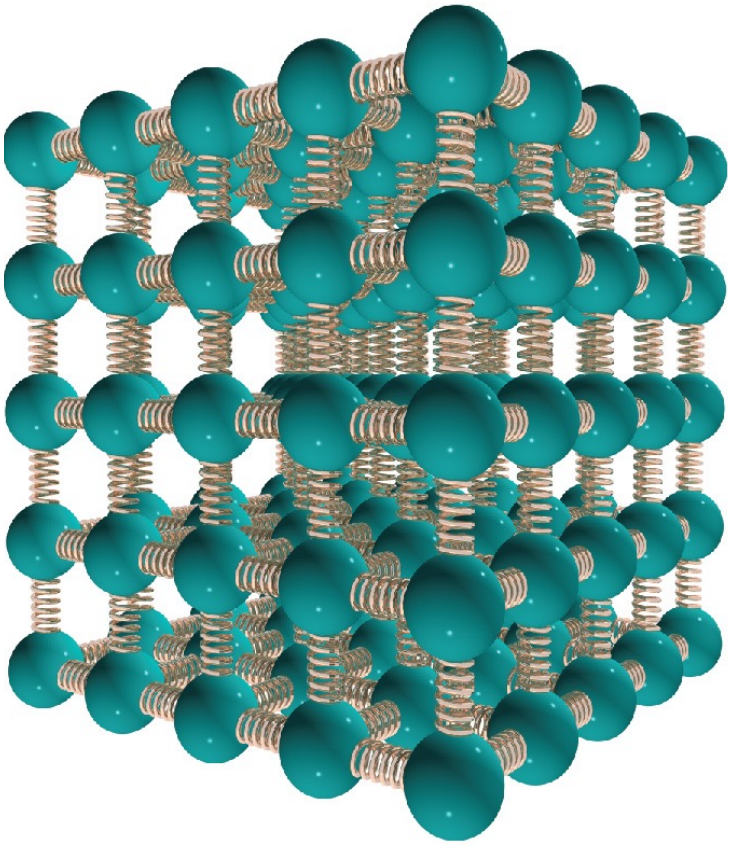
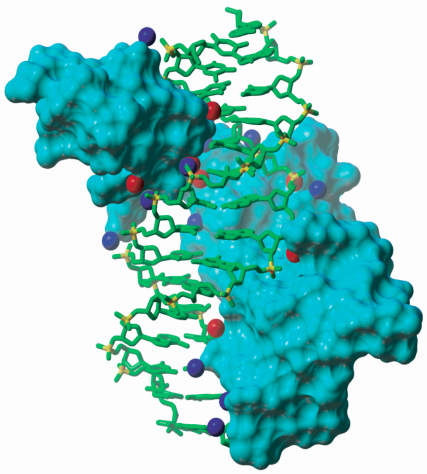
Applications of the Spring Force: molecules

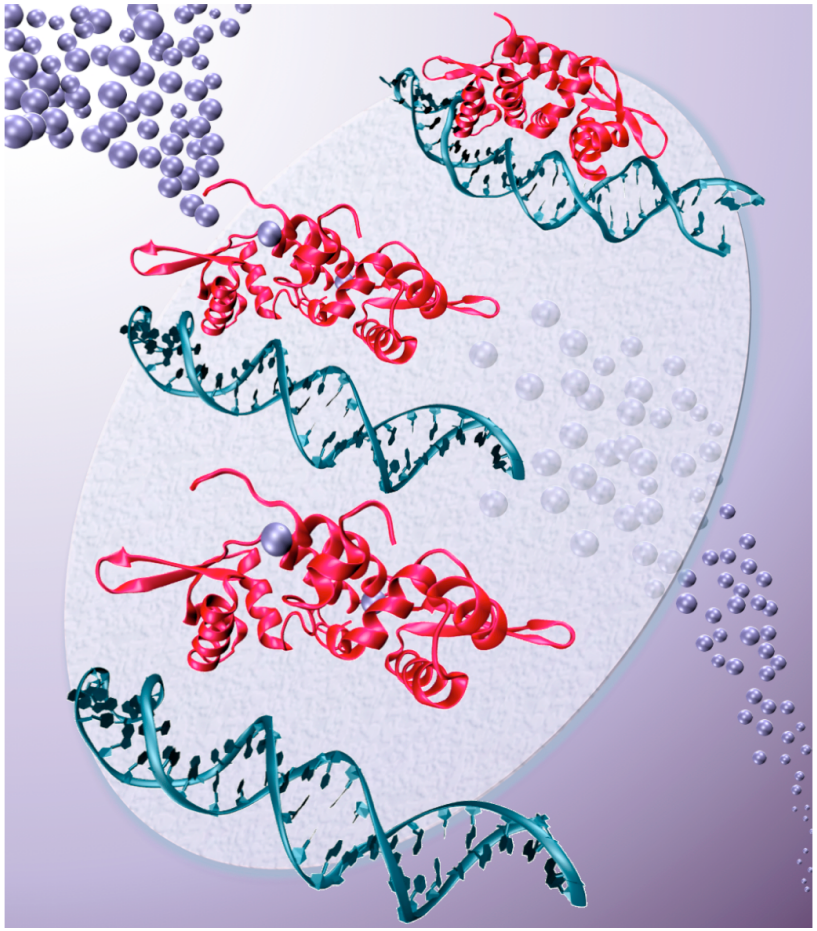
- Atoms interact via the coulomb force
- When atoms are far apart, they are attractive
- When atoms are too close, they are repulsive
- Atoms in a molecule display relative oscillatory motion
- Therefore: the spring force is a good model



- Solids are composed of a large number of atoms in a lattice structure
- Can be modeled as a collection of spring-masses with “spring” or force constants *k*
- Force constants are tabulated for any A-B atom combination and in various liquids, solids
- Used to model structure, dynamics of complex molecules (DNA, …) using computer codes (Amber, CHARMM, …)







Amber Home Page

"insert clever motto here"
(Learn more about real Amber)

AmberTools15 Amber14 GPU info Xeon Phi Info Manuals Tutorials Updates Mail lists Force Fields Contacts Developers

News

New Optimized Amber Certified Systems provide >15% GPU performance boost.

AmberTools15 was released on May 4, 2015

GTX-Titan-X Launched AMBER 14 breaks MD speed record for a single desktop.

New 8 GPU Amber Certified GPU nodes now available with GTX-Titan-Black, K20 and K40 GPUs

Intel Xeon Phi support officially launched with latest update to PMEMD (AMBER 14)

Preinstalled Amber Certified GPU Workstations and Clusters now available with GTX-980, GTX-Titan-Black, K20, K40 and K80

Quick links

Amber force fields

Assisted Model Building with Energy Refinement

Search

"Amber" refers to two things: a set of molecular mechanical *force fields* for the simulation of biomolecules (which are in the public domain, and are used in a variety of simulation programs); and a *package of molecular simulation programs* which includes source code and demos.

Amber is distributed in two parts: *AmberTools15* and *Amber14*. You can use AmberTools15 without Amber14, but not *vice versa*. See *below* for information on how to obtain Amber14.

When citing Amber14 or AmberTools15 please use the following:

D.A. Case, J.T. Berryman, R.M. Betz, D.S. Cerutti, T.E. Cheatham, III, T.A. Darden, R.E. Duke, T.J. Giese, H. Gohlke, A.W. Goetz, N. Homeyer, S. Izadi, P. Janowski, J. Kaus, A. Kovalenko, T.S. Lee, S. LeGrand, P. Li, T. Luchko, R. Luo, B. Madej, K.M. Merz, G. Monard, P. Needham, H. Nguyen, H.T. Nguyen, I. Omelyan, A. Onufriev, D.R. Roe, A. Roitberg, R. Salomon-Ferrer, C.L. Simmerling, W. Smith, J. Swails, R.C. Walker, J. Wang, R.M. Wolf, X. Wu, D.M. York and P.A. Kollman (2015), AMBER 2015, University of California, San Francisco.

A good general overview of the Amber codes can be found in:

R. Salomon-Ferrer, D.A. Case, R.C. Walker. An overview of the Amber biomolecular simulation package. *WIREs Comput. Mol. Sci.* **3**, 198-210 (2013). (*PDF*)

CHARMM

Program

Development

Documentation

To get CHARMM

CHARMM

CHARMM News (Nov. 10, 2014):

Michael Crowley and Antti-Pekka Hynninen will be giving a webinar on November 11 regarding the new GPU- capable DOMDEC functionality. Additional information may be found at the main page for the webinar. An early version of the DOMDEC GPU code is available in CHARMM version c39b1. A more robust implementation will be available in c40b1, expected for release in August, 2015.

CHARMM News (Oct. 22, 2012):

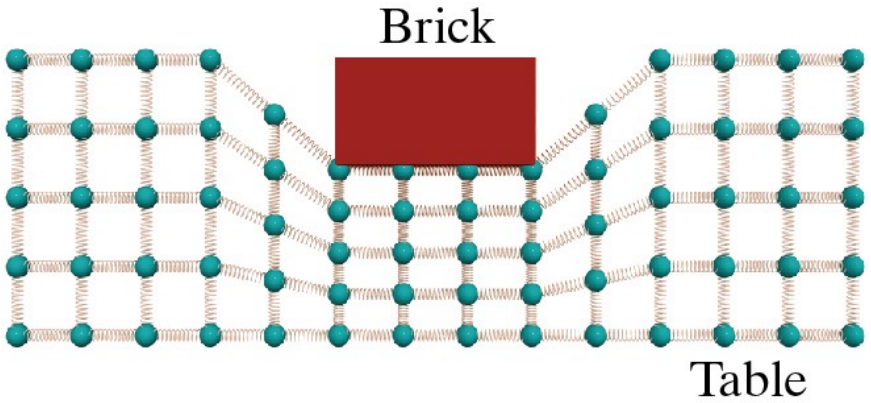
The most recent release of CHARMM makes available to users significant performance enhancements for conventional molecular dynamics calculations, e.g., MD with explicit solvent and periodic boundary conditions using PME. This enhanced performance comes from the development and introduction of the DOMDEC module, by Antti-Pekka Hynninen and Michael Crowley, for simulations on parallel architectures, and for GPU accelerated molecular dynamics from the CHARMM/OpenMM interface, developed by Michael Garrahan and Charles Brooks, which leverages the relatively mature OpenMM API developed by Vijay Pande and coworkers at Stanford. For more information, please see this page.

CHARMM (Chemistry at HARvard Macromolecular Mechanics):

- is a versatile and widely used molecular simulation program with broad application to many-particle systems
- has been developed with a primary focus on the study of molecules of biological interest, including peptides, proteins, prosthetic groups, small molecule ligands, nucleic acids, lipids, and carbohydrates, as they occur in solution, crystals, and membrane environments

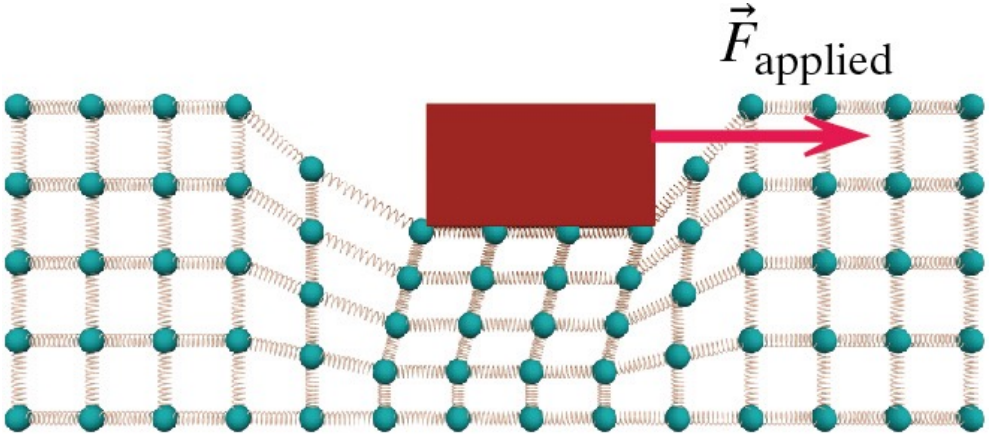
The Normal Force

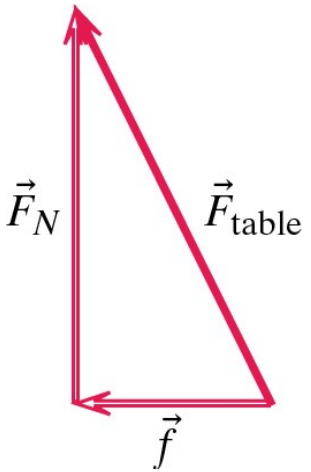
- Bond between atoms in the table are stretched and compressed
- The bonds (modeled as springs) apply forces to restore bond lengths to equilibrium
- Vector summing forces due to all bonds near the “brick” gives a net upward force



The Friction Force

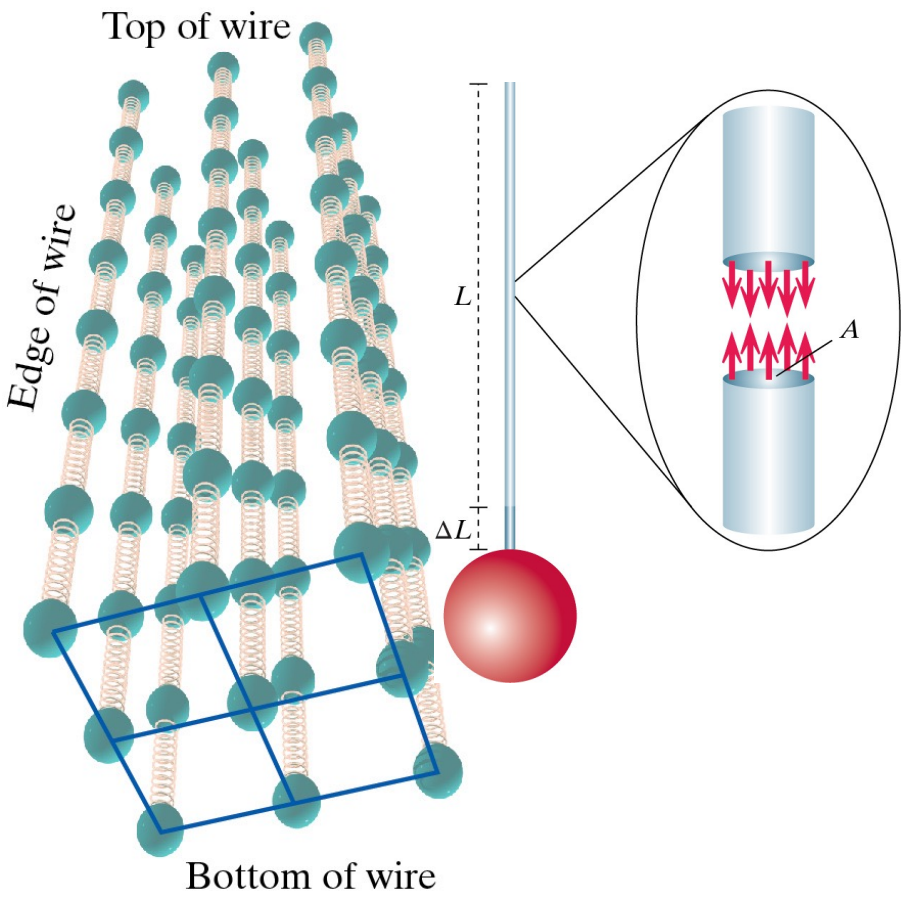
- Bond between atoms in the surface are stretched and compressed
- The bond forces “oppose” the motion of the object
- Vector summing forces due to all bond pulled to the right give a net force to the left
- Also (to be discussed in Chap. 9), there are weak bonds between the object and surface atoms





The Tension Force

- Ropes, wires, string, … can be models as packets of stiff springs connected in series
- Applying a force to one end, the bonds stretch
- By Newton's 3rd law, the bonds apply a force to return to equilibrium
- "Applied" force is propagated from one end of wire to the other



General Solution for SHM

- Systems which display simple harmonic motion (often called harmonic or oscillatory) can have various initial conditions
- Introduce a phase ϕ (or phase factor or phase shift)
- Three independent, constant properties of the system A, ω, and ϕ