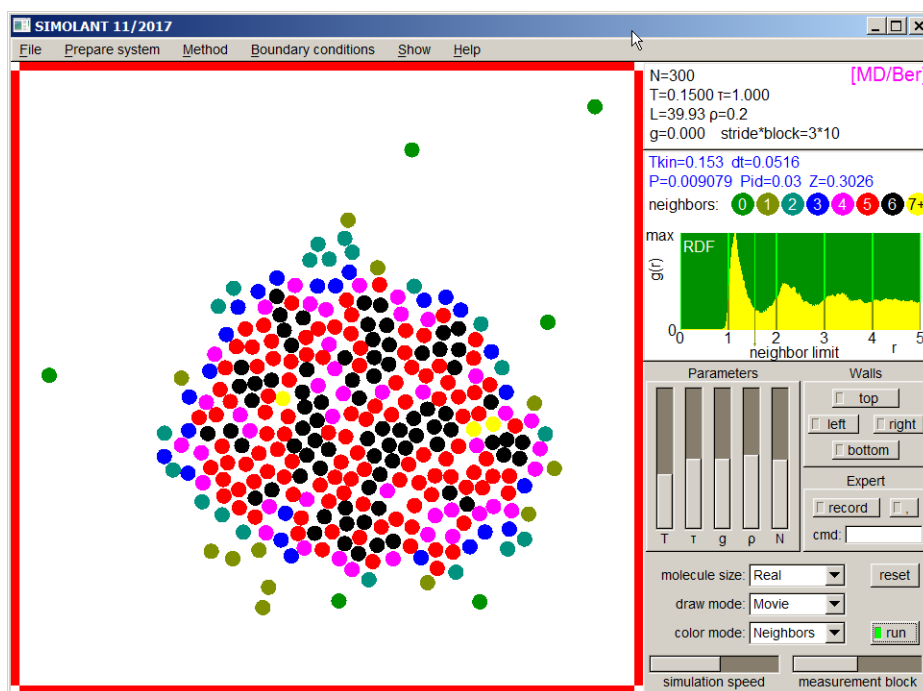# Teaching Physical Chemistry/Molecular Simulations?

SIMOLANT

For free. No ads.

SIMOLANT in teaching physics and chemistry:
A number of phenomena are shown using a two-dimensional molecular model of matter.

- Condensation of gas and crystallization of liquid on cooling
- Melting and evaporation on heating
- Mixing of fluids and gases
- Capillary action
- Crystal defects in motion
- Gas in a gravitational field
- Impact of a solid body (crystal) to a wall
- Nucleation, Ostwald ripening

SIMOLANT in a university course of molecular simulations:
Basic concepts of statistical thermodynamics and molecular simulations can be elucidated.

- Determinism, chaos, ergodicity
- Molecular dynamics at constant energy and temperature (several thermostats)
- Metropolis and Creutz Monte Carlo
- Online converge profile of total energy, timestep dependence
- Online radial distribution function, coordination numbers, density profiles
- Walls or periodic boundary conditions
- Flying icecube problem
- Exercise: simulation verification of the Clausius–Clapeyron equation

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Download: www.vscht.cz/fch/software/simolant

- Windows, MacOS, and Linux executables
- Sources (C++, FLTK)