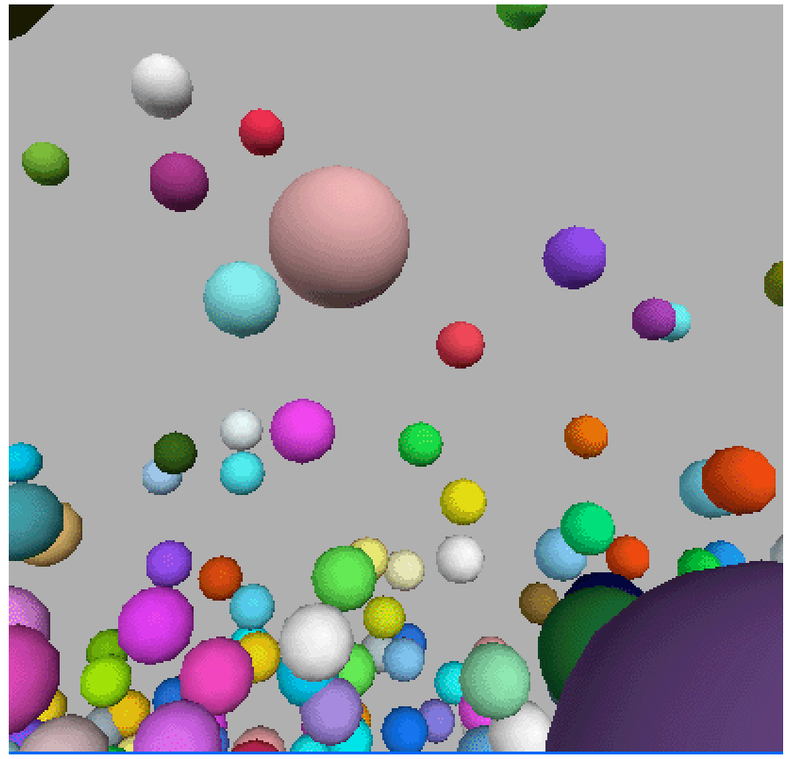
Molecular Dynamics, Digital Material, and Design Patterns

Physics 7682 / CIS 6229: Computational Methods for Nonlinear Systems

- Molecular dynamics
  - Integration of Newton's 2nd law for a large collection of particles

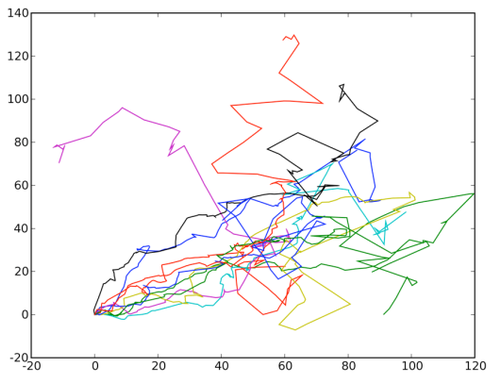
$$\vec{F} = m\vec{a}$$



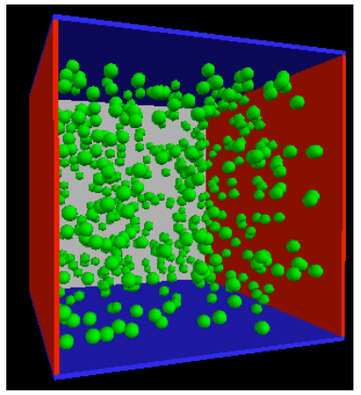
- physics
  - thermodynamics of (non)interacting gases
  - structure, energetics, and dynamics of liquids, crystalline solids and defects (e.g., dislocations, cracks), disordered systems (e.g., glasses)
  - interatomic potentials, increasingly derived from quantum mechanical calculations
- biology
  - structure, energetics, and dynamics of macromolecules (e.g., proteins)
  - details of protein conformations, protein-ligand binding
  - interatomic potentials typically empirically derived (AMBER, CHARMM, etc.)

Molecular Dynamics module

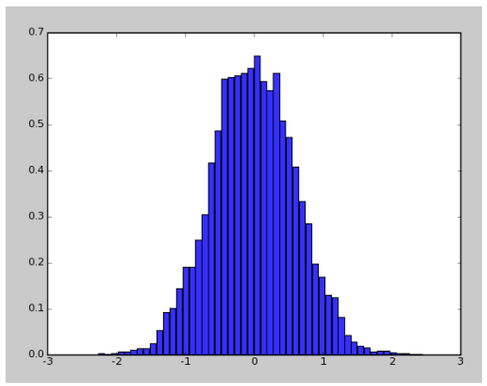
- Not usual hints+fill-in-the-missing code structure
  - focused more on use of existing package (Digital Material) and analysis of simulation data
  - uses VPython (visual) for animated graphics
- Exercises
  - Perfume Walk: random walk due to collisions
  - Pressure: emergence of pressure from collisions
  - Equilibration: convergence to equilibrium from nonequilibrium state
  - Exponential Atmosphere: thinning of atmosphere under gravity
  - Pair Distribution Function: positional correlations in gas, liquid, solid



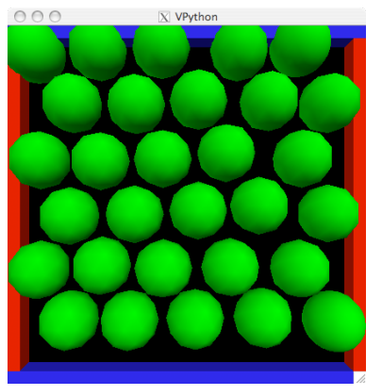
Perfume Walk



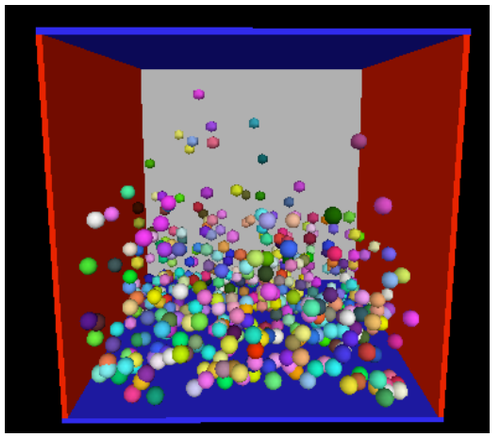
Pressure

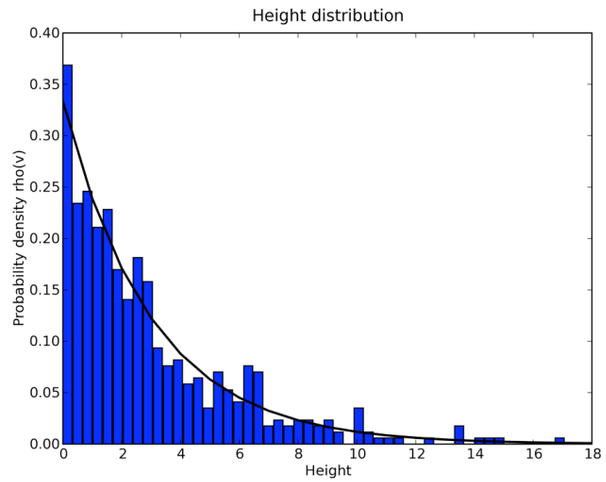


Equilibration



Pair Distribution

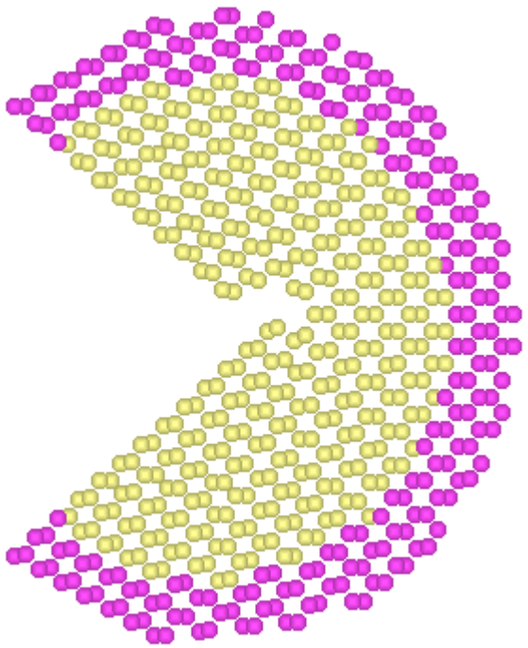


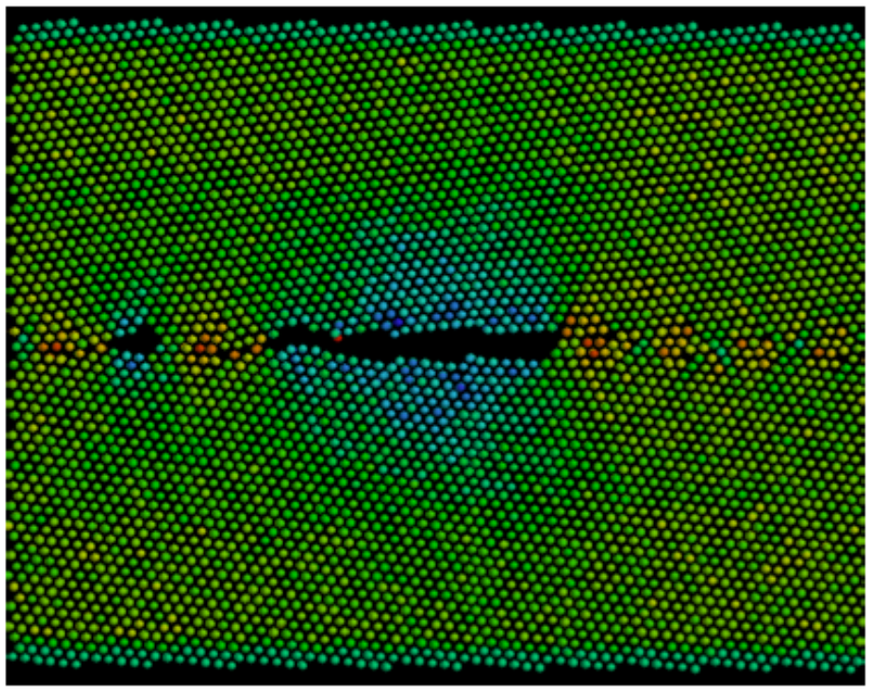


Exponential Atmosphere

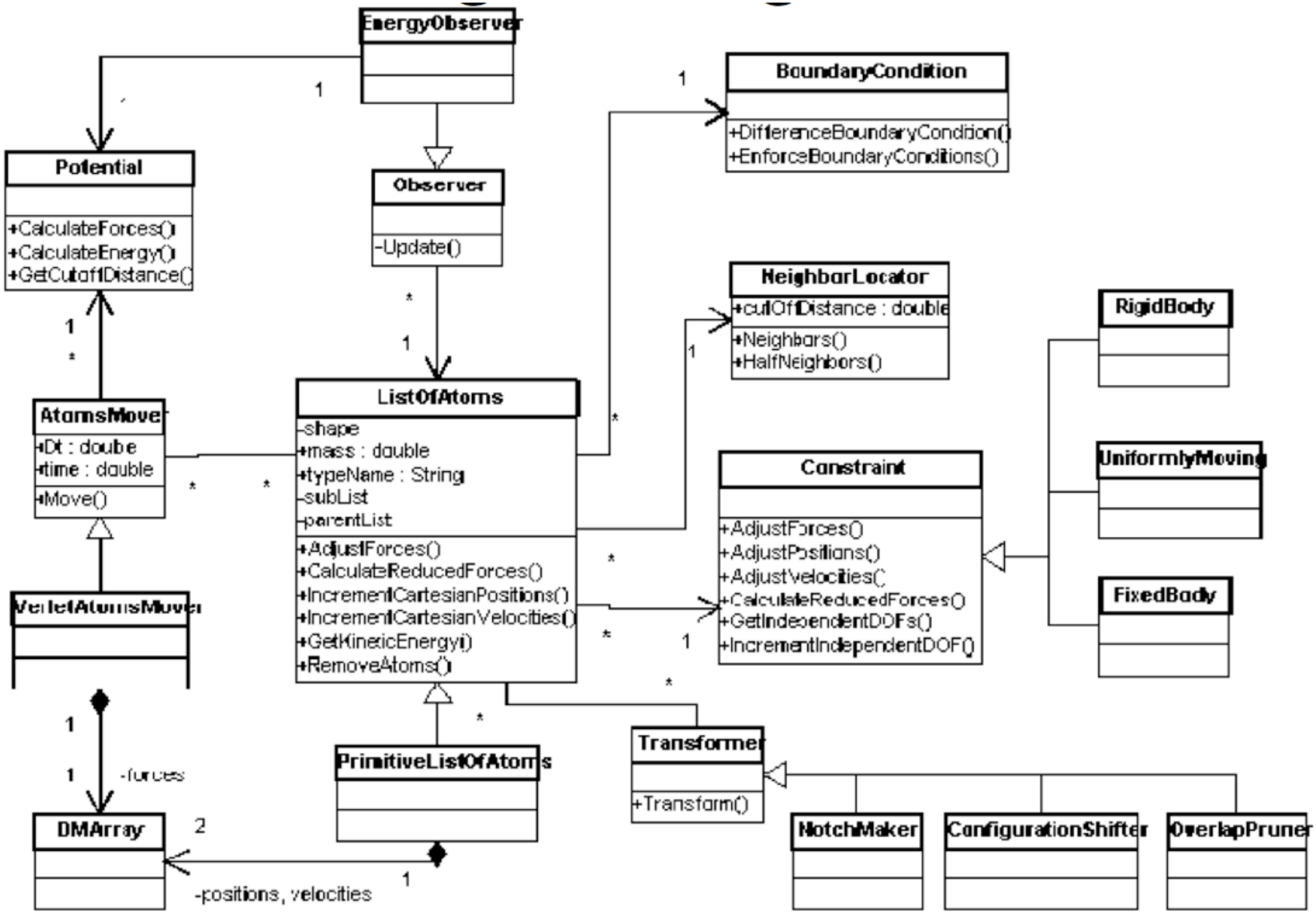
Digital Material package

- Grew out of a multiscale materials modeling effort (Sethna, Myers, et al. 1998-2002)
  - emphasis on investigating the structure and dynamics of defects in crystalline and polycrystalline materials relevant for deformation and failure
    - ➡ dislocations, dislocation tangles, grain boundaries, cracks
  - emphasis on construction and manipulation on nontrivial, heterogeneous defect geometries and coupling to coarse-grained models (e.g., finite-element analysis)
  - original code in C++ with minimal Python wrapper; ported to Python for Phys 682 / CIS 629 by Sethna

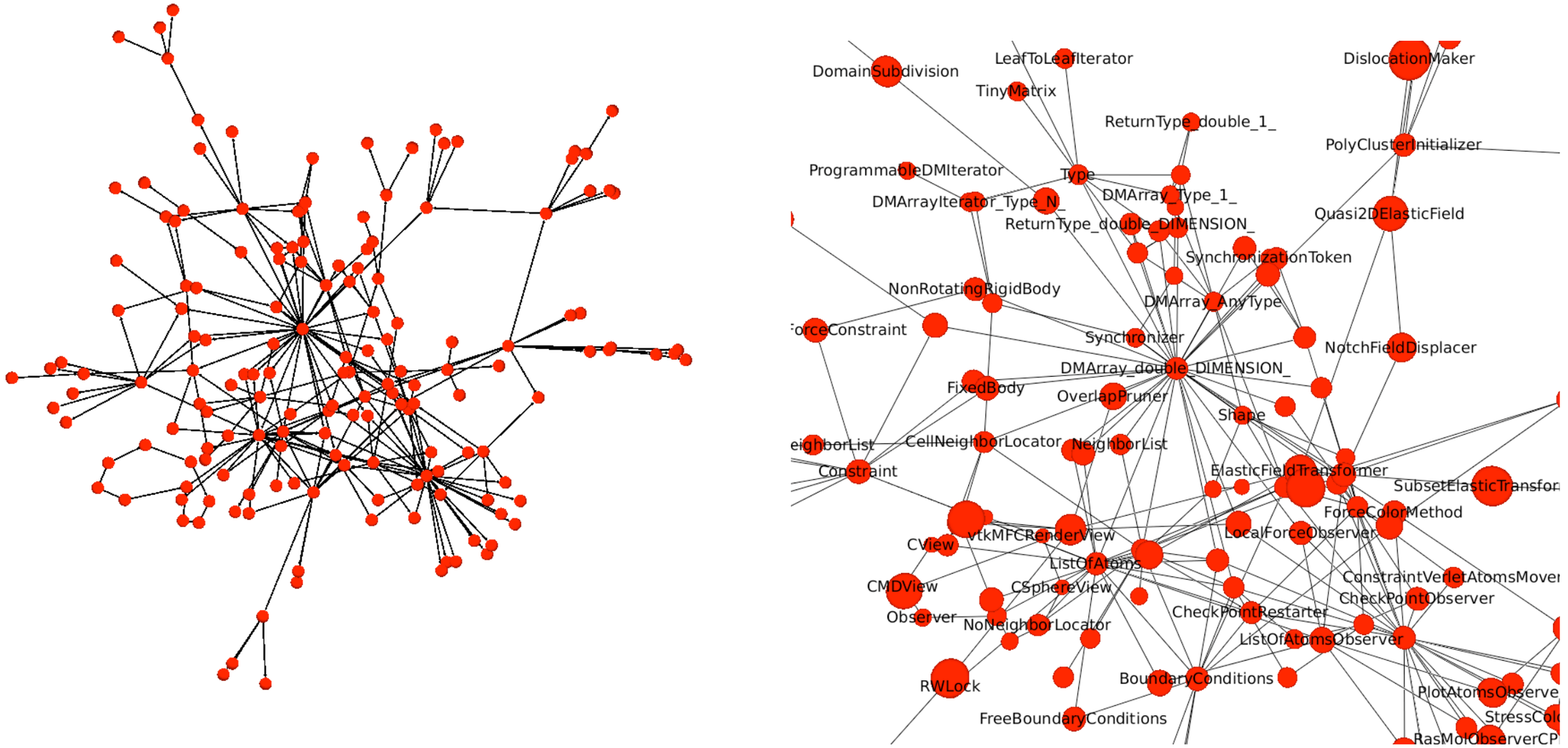




Class Diagram: interactions among classes in OO code



Class Diagram: interactions among classes in OO code



CRM, "Software systems as complex networks...", Phys. Rev. E (2003)

Design patterns

- Object-oriented design methodology for building code that can easily incorporate changes
  - collaborations among sets of classes/objects to encapsulate highly variable pieces
  - different patterns encapsulate different types of variability, e.g.,
    - factories address variability in the construction of objects
    - observers address variability in views/analyses of a central data repository
    - strategies address variability in algorithms
    - adapters address variability in class/object interfaces
  - emphasis on having many smaller objects working together (more reconfigurable), rather than more specialized and monolithic pieces that are harder to change
  - initially catalogued in the well-known book by Gamma et al. ("Gang of Four", of GoF)

- Design patterns in Digital Material
  - ListOfAtoms: efficient collections of atoms
  - Initializers and transformers: decoupled algorithms for manipulating structure
  - Movers: decoupling structure from dynamics (use different algorithms)
  - Observers: decoupling analysis from dynamics (generic Update() interface)
  - Boundary conditions: decoupling enforcement of boundary conditions from dynamics
  - NeighborLocators: decoupling structure from force computation

Gravity cluster

```
gravityPotential = GravityPotential(g=g)
LennardJonesPotential = LennardJonesCutPotential()
potential = CompositePotential([gravityPotential,
                                LennardJonesPotential])
boundaryConditions = ReflectiveBoundaryConditions(L)
neighborLocator = SimpleNeighborLocator(LennardJonesPotential.cutoff,
                                        boundaryConditions)
atoms = TriangularSphericalClusterListOfAtoms(
                R=R, center=[L/2., L/2.], temperature=T,
                radius=LennardJonesPotential.latticeSpacing/2.0)
displayObserver = VisualDisplayAtomsObserver(atoms,L)
energyObserver = EnergyObserver(potential, neighborLocator,
                                boundaryConditions)
observers = [displayObserver, energyObserver]
mover = RunVelocityVerlet;
sys = MDSystem(L, atoms, observers, neighborLocator,
               boundaryConditions, potential, mover)
```