Why computational physics?

• Why/when computers instead of analytical (exact) approach?

Answer: When it is impractical or impossible to find an analytical solution! (Not when it’s just hard to do!)

• When an precise theory exists (e.g. Newton’s laws, Schrodinger Eq., statistical mechanics, electrodynamics), typically the “exactly solvable” applications are very few.

• To find solutions that can be tested against experiments, numerical methods become an important (or even essential) approach.
Important problems/applications

• Large systems of coupled differential equations
  
  Examples: Schrodinger’s equation, trajectories of many interacting particles/masses

• Large systems of linear equations (linear algebra/matrices)
  
  Examples: Normal modes, solutions to differential equations in a basis, eigenvalues/eigenvectors

• Nonlinear differential equations
  
  Examples: Fluid dynamics, plasma physics, chaos

• Analysis of large amounts of data
  
  Examples: Spectral methods, fitting data to functions
What tools are commonly used/available?

• Ordinary desktop/laptop
  Convenient, cheap, limited in power, serial

• Supercomputer facility
  Extremely powerful, usually parallel machines, run by experts, funded by govt. agencies, competitive grants. National Center for Supercomputer App. (NCSA), NERSC, etc.

• Beowulf computer
  Large parallel machine built from desktops, “do-it-yourself”, relatively cheap, widely used
What other tools might one use?

• Software tools/numerical libraries
  
  Tools for common numerical tasks, e.g. manipulation of large matrices in linear algebra

• Software for specific applications
  
  Fluid dynamics, electronic structure of molecules and crystals, modeling thermodynamics of alloys, etc.

• As computational methods continue to become more widespread, strong chance of “reinventing the wheel”.