Instructor Guide

Basic definitions as shown in the slides:

Diffraction Limit of Light Microscopy: In 1873, the German physicist Ernst Abbe realized that the resolution of optical imaging instruments, including telescopes and microscopes, is fundamentally limited by the diffraction of light. His finding indicated that ultimately the resolution of an imaging instrument is not constrained by the quality of the instrument, but by the wavelength of light used and the aperture of its optics. Specifically, that a microscope cannot resolve objects that are of comparable size to, or smaller than, the wavelength of light that is being used to image it.

"An introduction to super-resolution microscopy of living cells"
https://www.youtube.com/watch?v=E-goSpv7gj8

Density Functional Theory: Electronic scale simulation that performs computational quantum mechanical modelling (i.e., solves the Schrödinger equation) in physics, chemistry and materials science to investigate the electronic structure (or nuclear structure) (principally the ground state) of many-body systems, in particular atoms, molecules, and the condensed phases.

"Basics of DFT in 10 minutes"
https://www.youtube.com/watch?v=UEOrDnwtq6s

Molecular Dynamics (MD): Atomistic scale simulation method that uses Newton's equations of motion to computationally simulate the time evolution of a set of interacting atoms. Such techniques are dependent on a description of how the molecules will interact – a force field (which is typically assumed to be represented via an explicit algebraic equation, such as the Lennard Jones potential) – and are popular in materials chemistry, biochemistry and biophysics.

"Molecular Dynamics in 5 Minutes"
https://www.youtube.com/watch?v=veBZYlD6AF4&t=137s

Metropolis Monte Carlo (MC): Atomistic scale simulation technique to sample the infinite number of available configurations of a material by introducing random motions to the atoms and then either accepting or rejecting them according to the Boltzmann distribution.

Coarse Grained MD/MC: Mesoscopic simulation technique for modeling the behaviour of complex systems using their simplified (e.g.., a pseudo "atom" representing a group of atoms) representation.

Lattice Boltzmann Method/Lattice Gas Automata: Lattice Gas Automata are a type of cellular automaton used to simulate fluid flows, which were the precursor to the Lattice Boltzmann methods. Lattice Boltzmann methods is a very popular CFD method that treats the fluid as "particle densities", whose motion is constrained to a lattice. Fluid properties are accounted for via the "collisions" of these particle densities. It is a very scalable method that can handle large systems with complex boundary conditions very easily.

"Of Foxes, Attackers, ... and the Lattice Boltzmann Method"
https://www.youtube.com/watch?v=8qorVDJS1QA

Continuum Mechanics: Simulation methods that solve conservation equations (e.g.., force, mass, energy balance) in order to model transport phenomena. These methods assume that matter is continuous (i.e., there are no atoms or electrons). Whether or not this is a good assumption is typically quantified using the Knudsen number. Essentially, the average travel distance that particles travel prior to experiencing collisions must be much smaller than the characteristic size of the geometry confining them, in order for the assumption to apply.

Top-Down Machine Learning: Pattern search methods that work by establishing associations in large sets of data. For example, neural networks are patterned after how a human brain learns. These methods do not necessarily have any knowledge of the physics occurring in the system in order to make predictions about it.