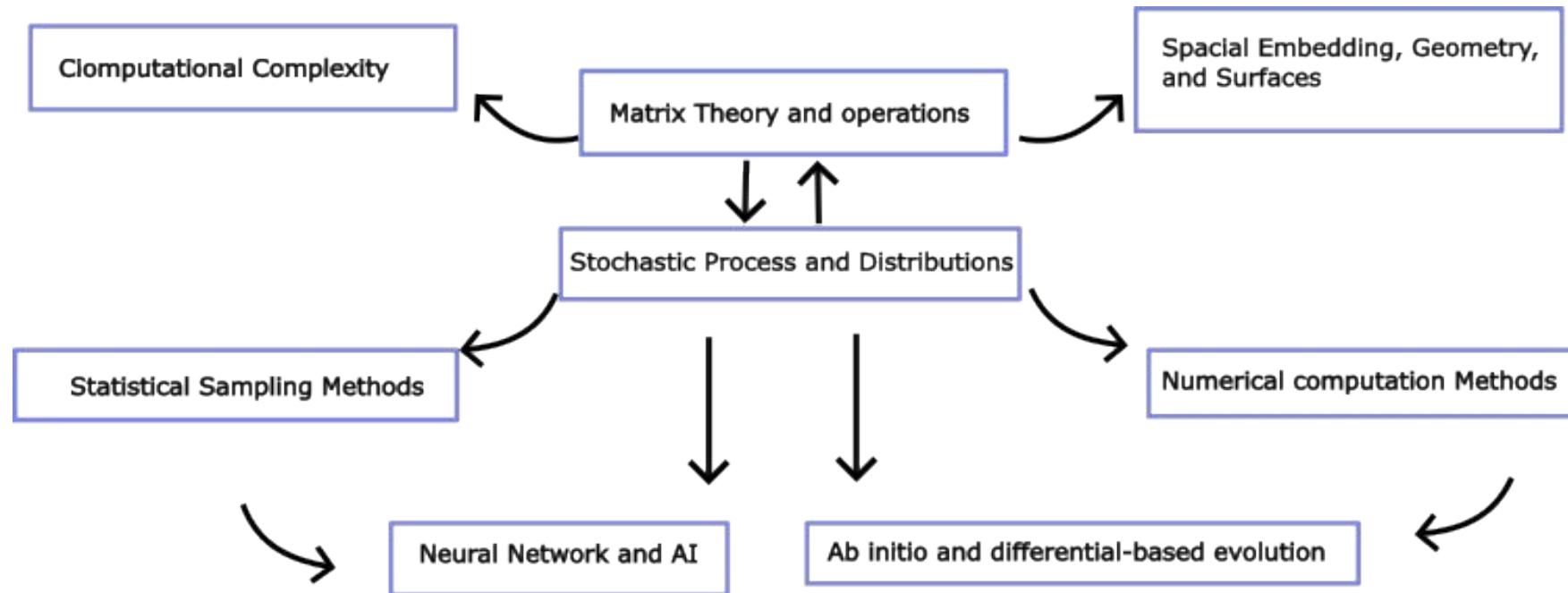


Introduction to Computational Physics

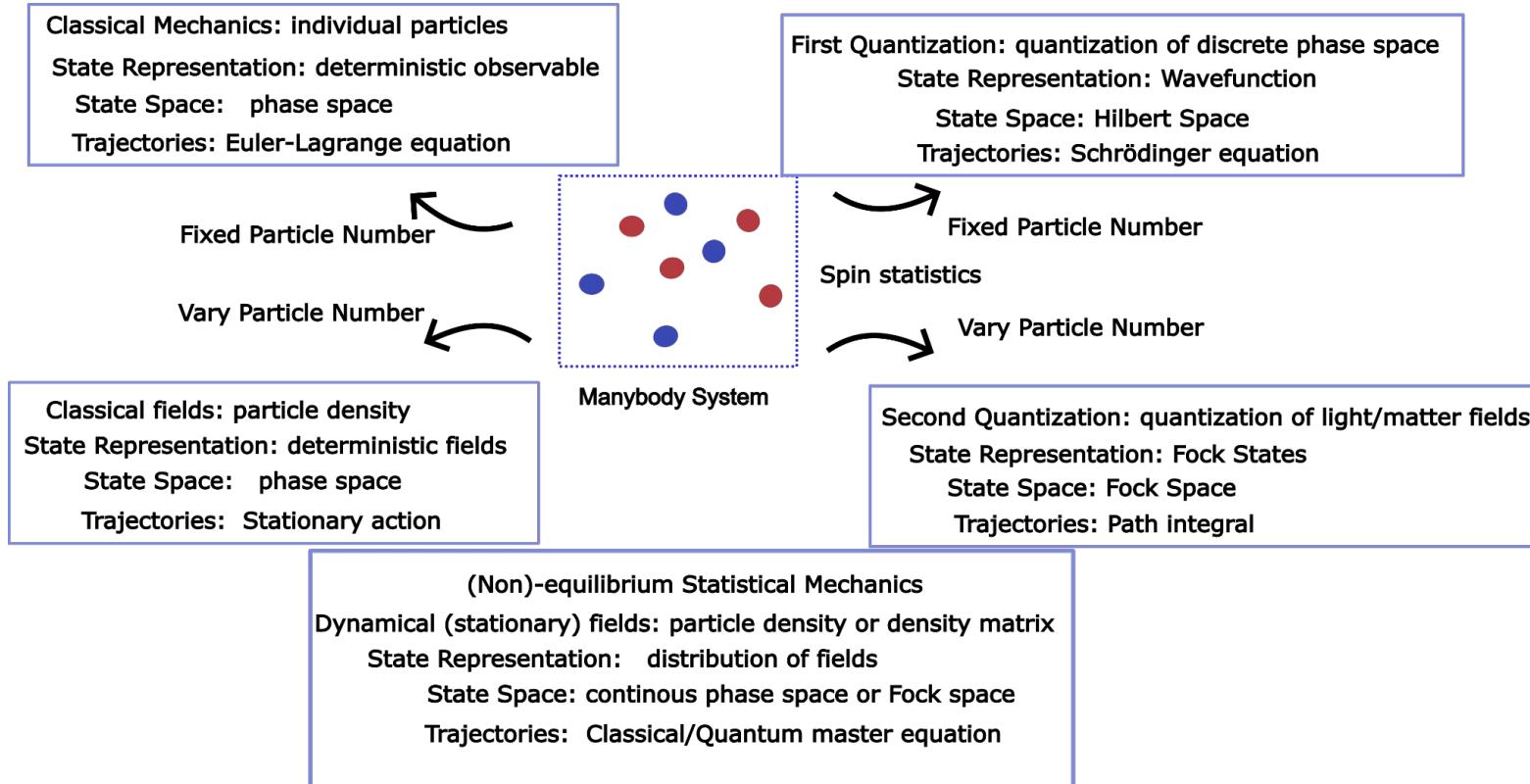
Physics 129AL

Zihang Wang
01/07/2025

Overview



Scope in Physics

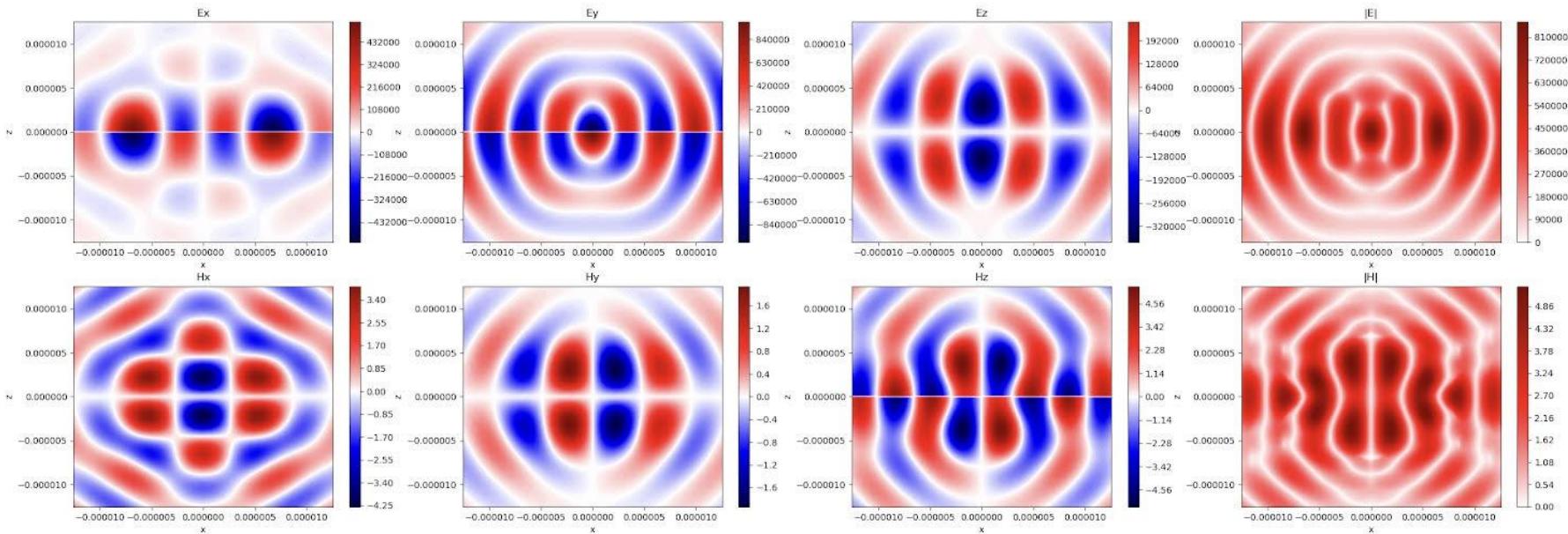
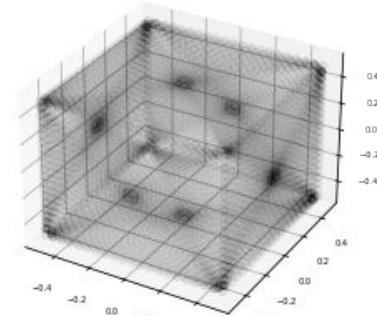


Syllabus

- **Basics in Differential Geometry** matrix, tensors, metric, dual space, generalized coordinate transformation, vector, covector, covariant derivative, parallel transport, geodesic, surface derivatives, first/second fundamental forms, intrinsic/extrinsic curvatures.
- **Basics in Matrix Theory** Gaussian and Gauss-Jacobi elimination, backsubstitution, pivoting, LU decomposition, Cholesky decomposition, QR decomposition, sparse matrix linear algebra, QR decomposition and tridiagonal forms, diagonalization of a symmetric and non-symmetric matrix, principal axes and covariance matrix, singular value decomposition (SVD), normal equations, principal component analysis (PCA) and dimensionality reduction, independent component analysis (ICA)
- **Computational complexity**, decision problem, counting problem, search problem, optimization problem, traveling salesman problem.

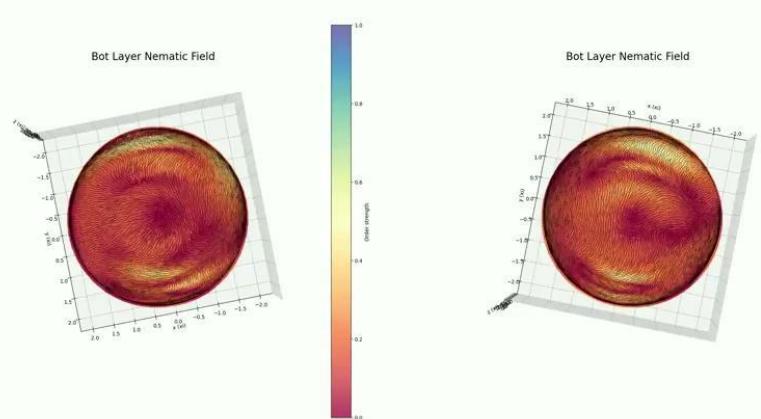
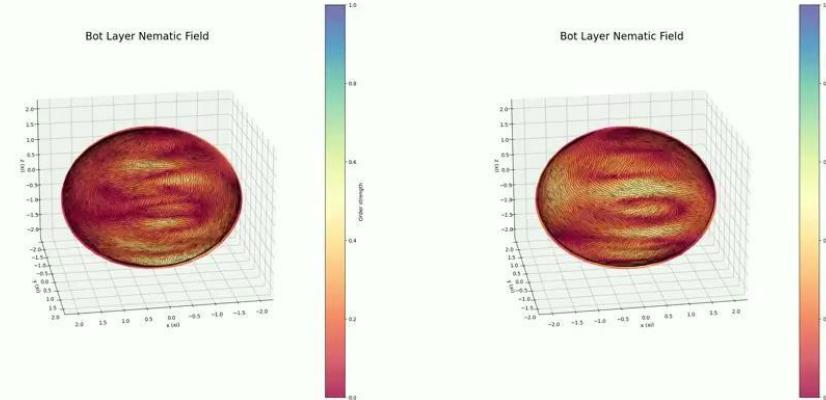
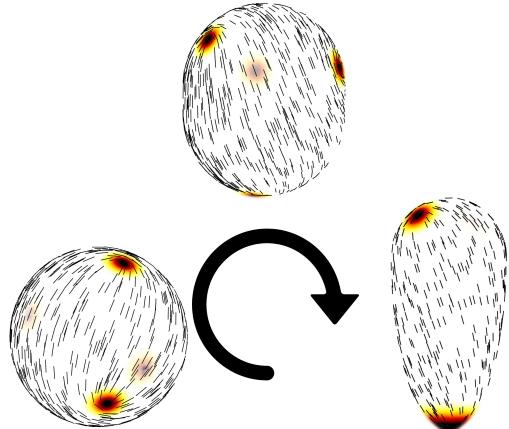
Syllabus

Electric/Magnetic Field Strength, scattering
amplitude on 3D mesh



Syllabus

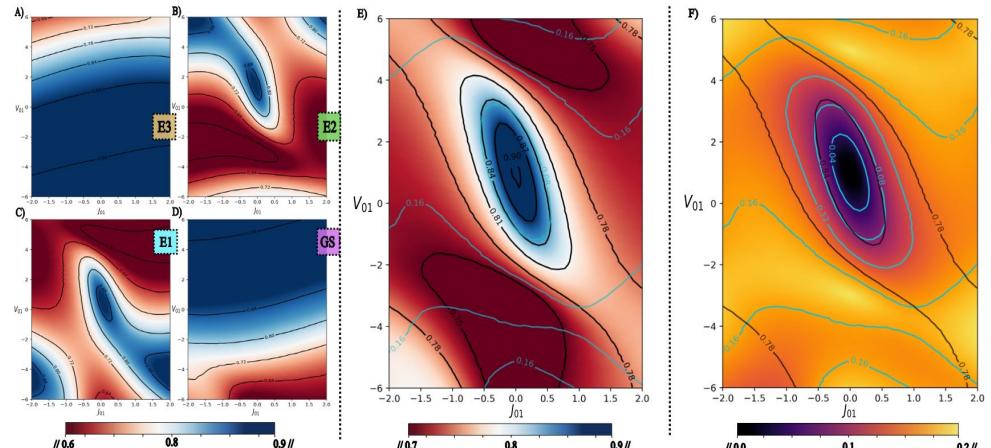
Conserved topological defects on a sphere,
generated via nematic
liquid crystal



Syllabus

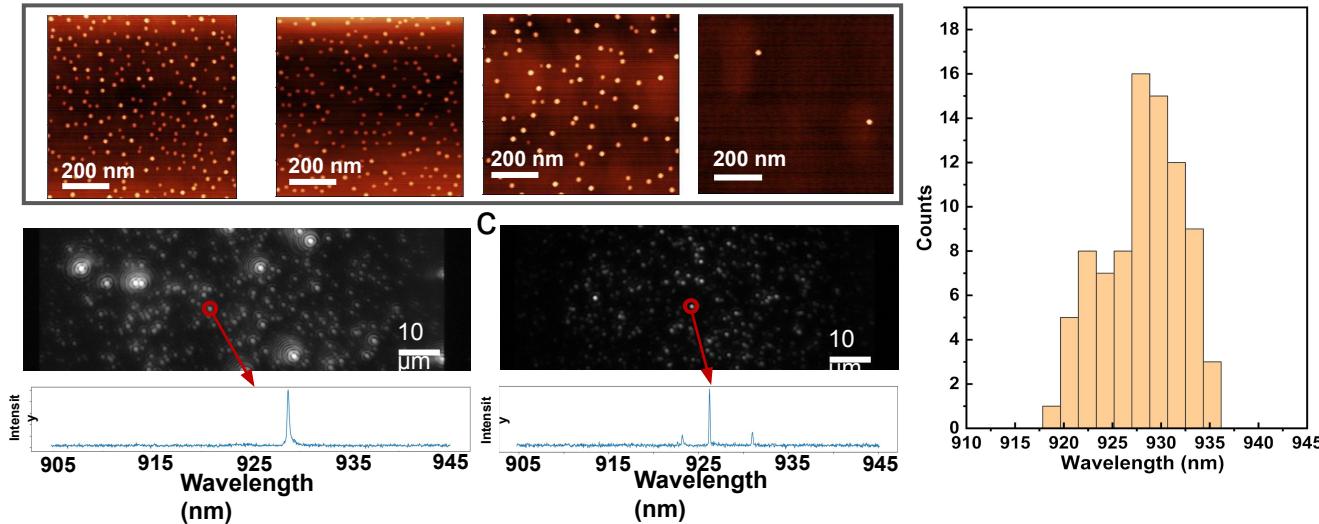
- **Common stochastic processes and statistical distributions in physics**, Concepts in probability and distributions, Bayesian inference and Frequentist statistics. random walk, Markov chain, geometric distribution, central limit theorem, Bernoulli process, binomial process, Poisson process, Lorentz (Cauchy) distribution. Bose–Einstein statistics (Bose-Einstein Condensation), Fermi–Dirac statistics, Maxwell–Boltzmann statistics.

Lower-bound of the entanglement entropy, a Hubbard model with exchange interactions



Syllabus

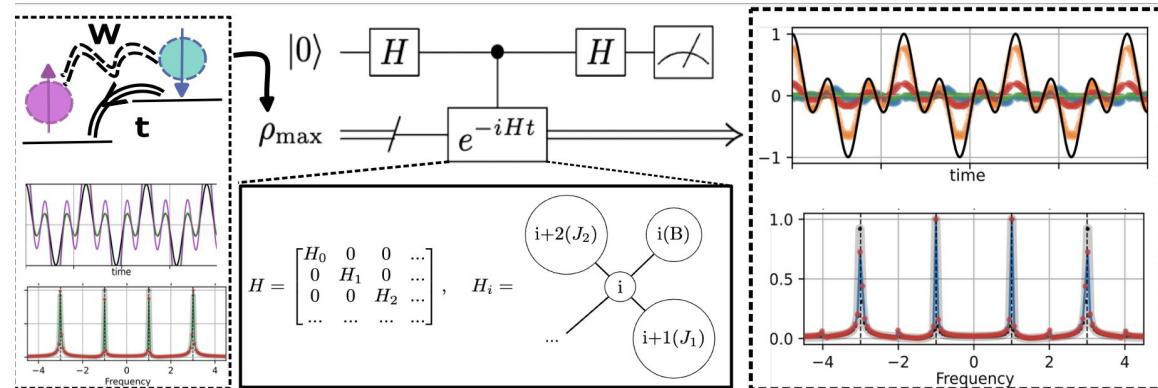
Quantum dot density generated via molecular beam epitaxy



Syllabus

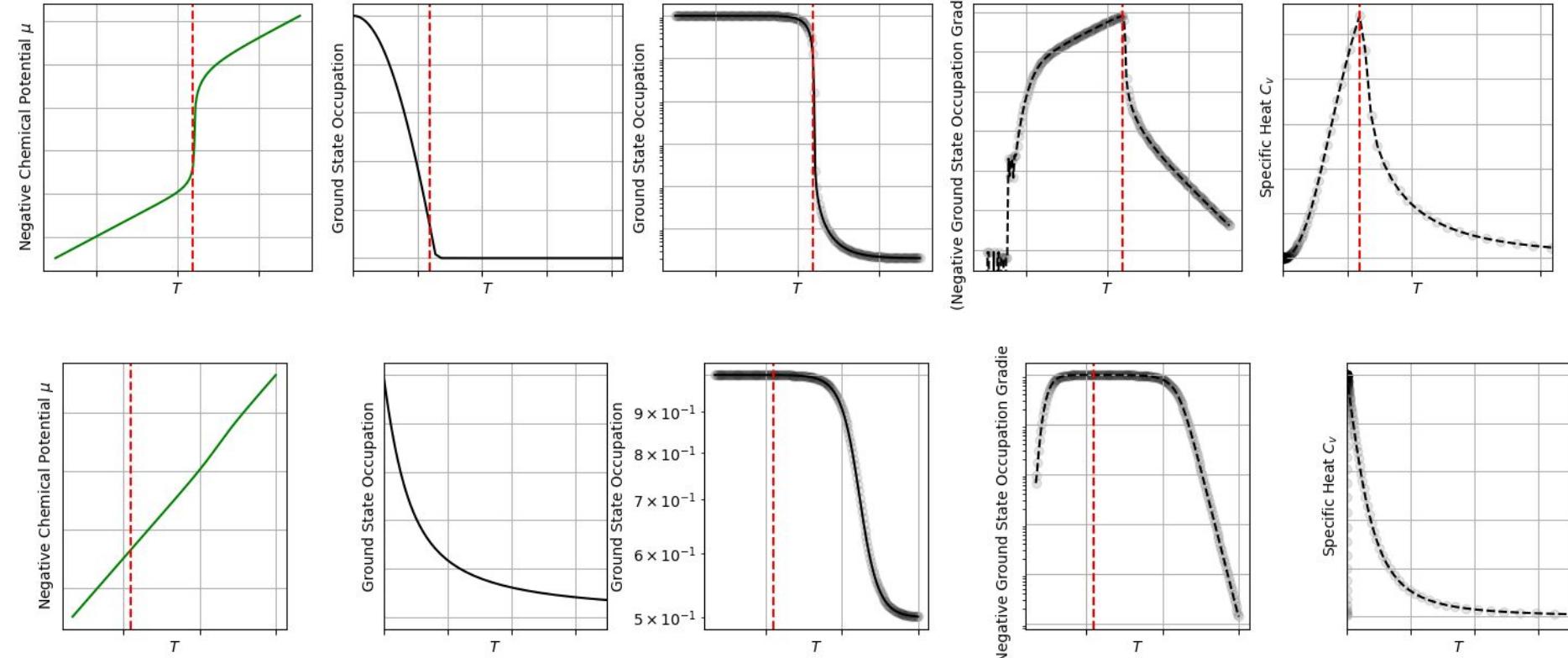
- **Common distribution sampling techniques in physics**, Monte Carlo methods, stochastic sampling, inverse transform sampling, rejection sampling, gibbs sampling, Metropolis–Hastings algorithm, simulated annealing, legendre transform.
- **Common computation techniques in physics**, discrete Fourier transform, numerical integration and differentiation, Gaussian quadrature, orthogonal (Legendre) polynomials, implicit and explicit iterative methods for differential equations, Runge–Kutta methods, Leapfrog, symplectic integrator, (stochastic) gradient descent, explicit/implicit regularization.

State evolution on a quantum computer



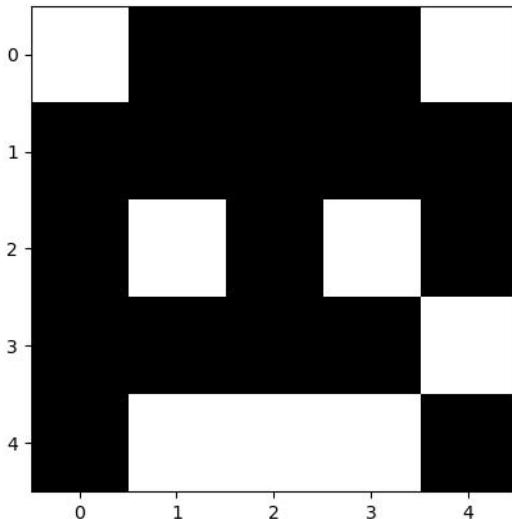
Syllabus

Quantum Phase transitions (bose einstein condensate)



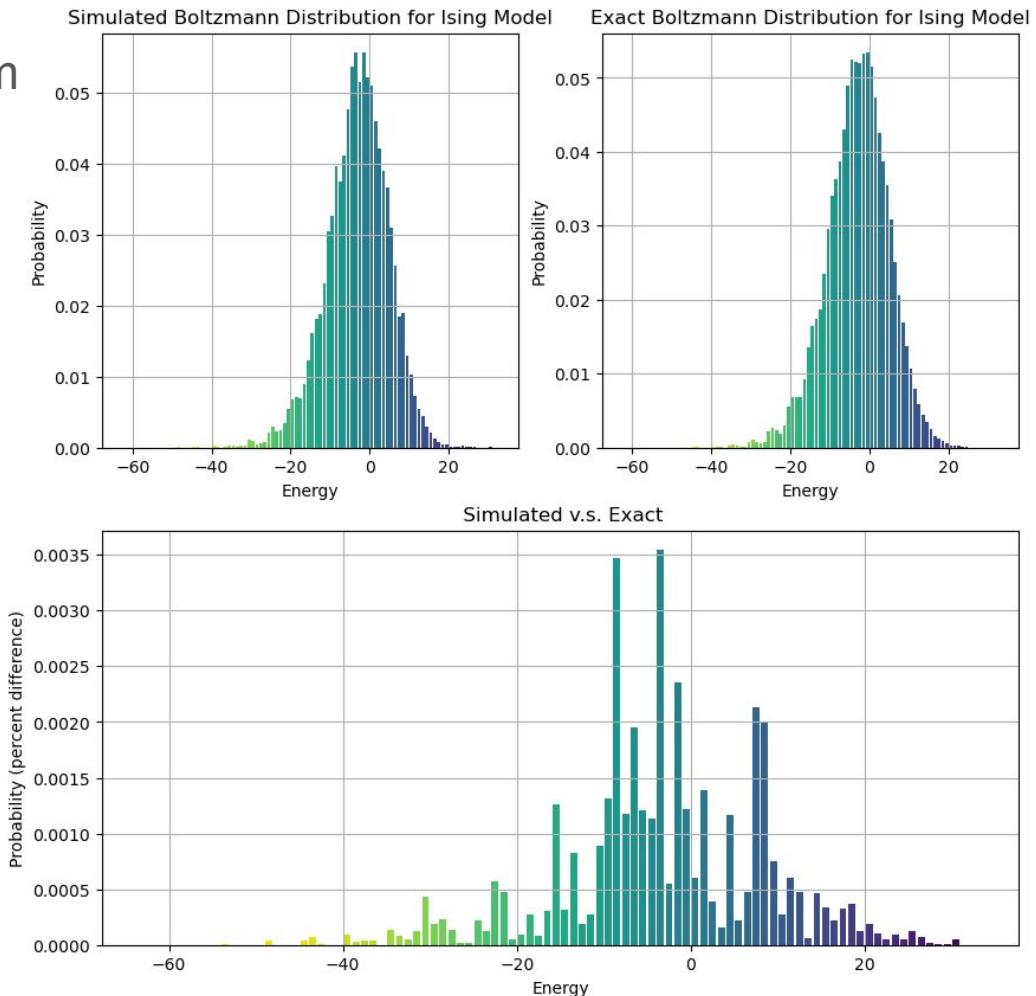
Syllabus

Classical/Quantum
Phase transitions
(Ising model with
transverse field)



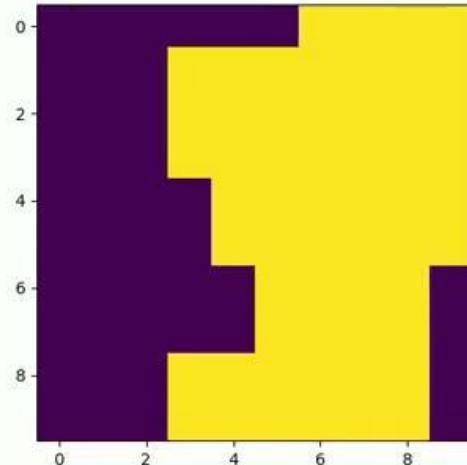
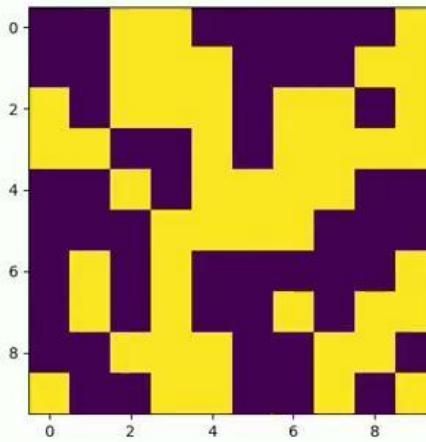
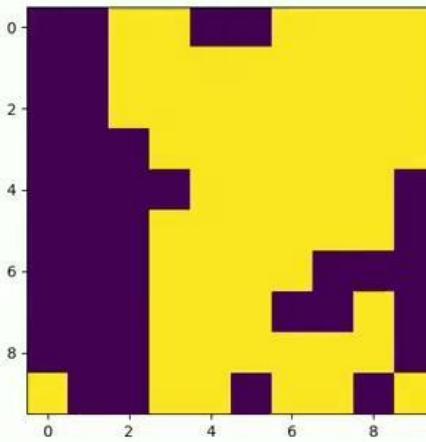
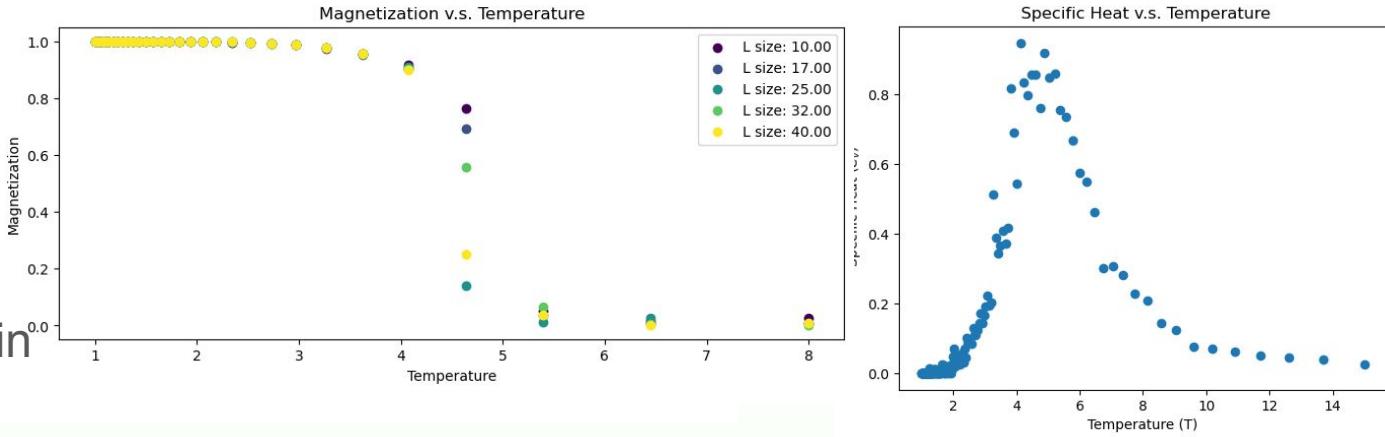
Exact Elapsed Time: 1260.5645 seconds

MC Elapsed Time: 4.4076 seconds

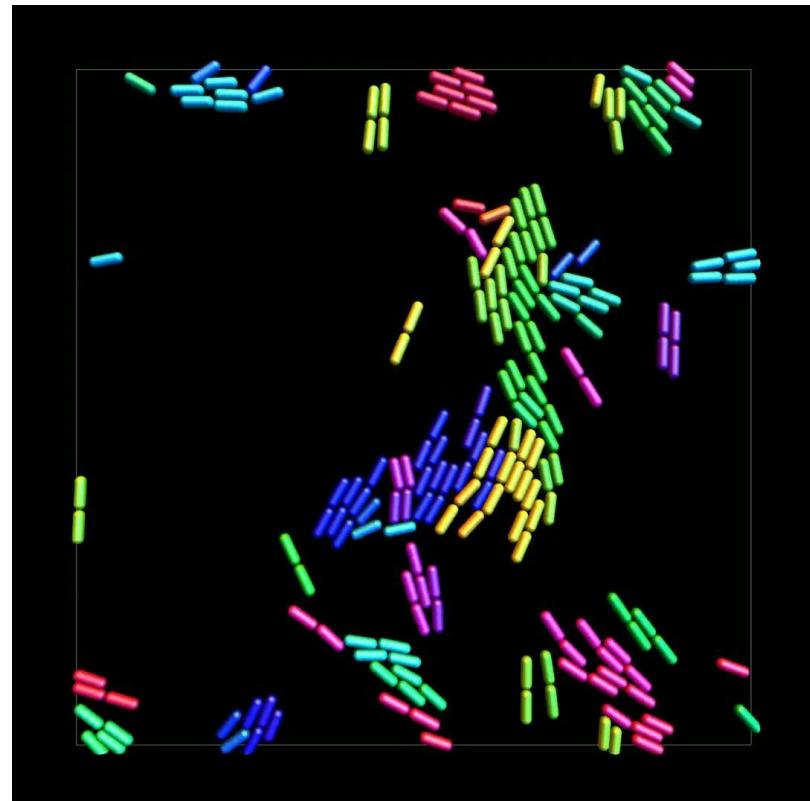
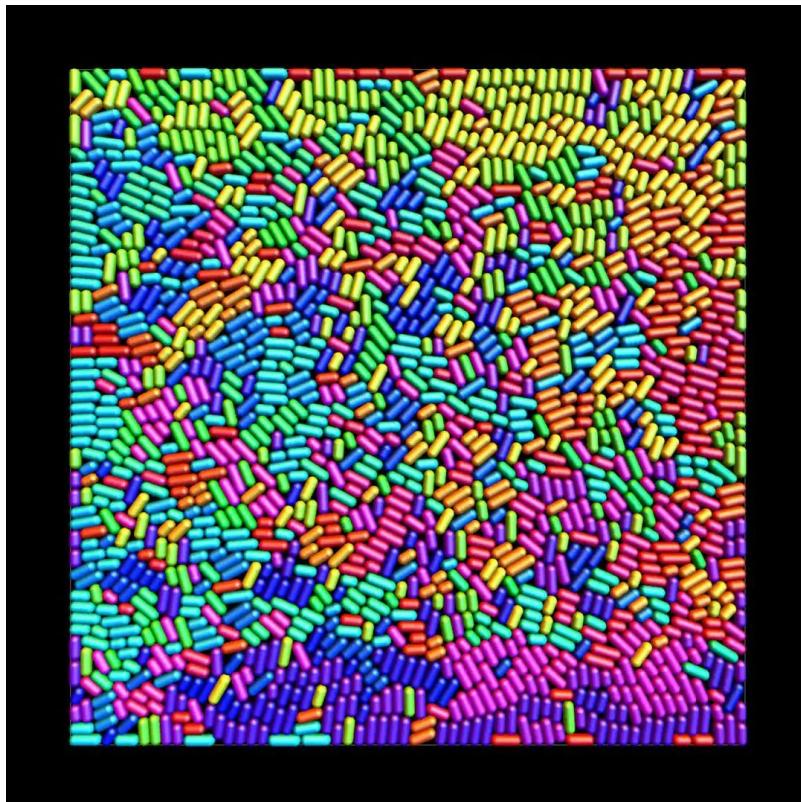


Syllabus

Order parameter in
Phase transitions



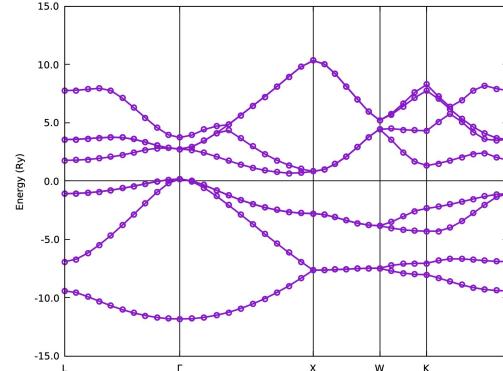
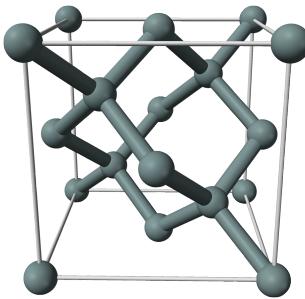
Syllabus Molecular Dynamics that generates Glassy phase transitions in bacteria



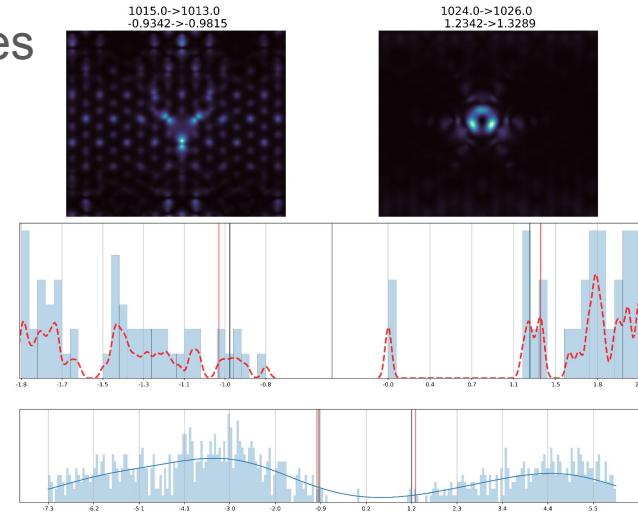
Syllabus

- **Applications in physics**, Electrostatics, Diffusion, Brownian motion, driven system, hydrodynamics, phase transitions, molecular dynamics, *ab initio* approaches to electronic structure, quantum state (density matrix) evolution, surface code, quantum master equation, numerical renormalization group.
- **Software in Modern Computational Physics**, Quantum Espresso and LAMMPS

Self consistent field
calculation for silicon



Localized electronic states



Syllabus

- **Foundations in neural network and artificial intelligence (AI)**, Pytorch, backpropagation, activation, feed-forward neural network, convolutional neural network, recurrent neural networks, generative adversarial network, Transformer, Autoencoder neural networks.

2017

Attention Is All You Need

Ashish Vaswani*
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illia.polosukhin@gmail.com



GPT (Generative Pre-trained
Transformer)

2021

High-Resolution Image Synthesis with Latent Diffusion Models

Robin Rombach¹ * Andreas Blattmann¹ * Dominik Lorenz¹ Patrick Esser^{†§} Björn Ommer¹

¹Ludwig Maximilian University of Munich & IWR, Heidelberg University, Germany [†]Runway ML

<https://github.com/CompVis/latent-diffusion>

Stable Diffusion



Syllabus

- **Foundations in neural network and artificial intelligence (AI)**, Pytorch, backpropagation, activation, feed-forward neural network, convolutional neural network, recurrent neural networks, generative adversarial network, Transformer, Autoencoder neural networks.

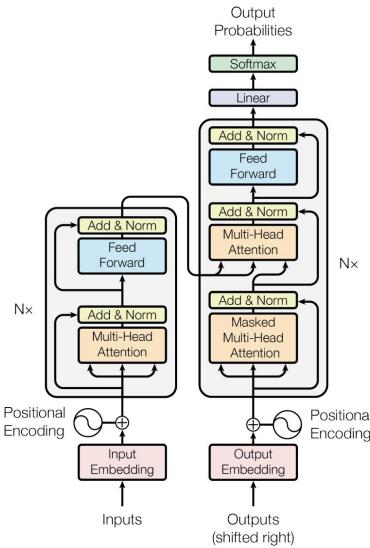


Figure 1: The Transformer - model architecture.

2020

Denoising Diffusion Probabilistic Models

Jonathan Ho
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jonathanho@berkeley.edu

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UC Berkeley
ajayj@berkeley.edu

Pieter Abbeel
UC Berkeley
pabbeel@cs.berkeley.edu

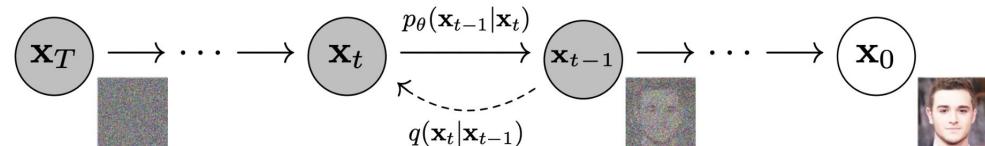


Figure 2: The directed graphical model considered in this work.

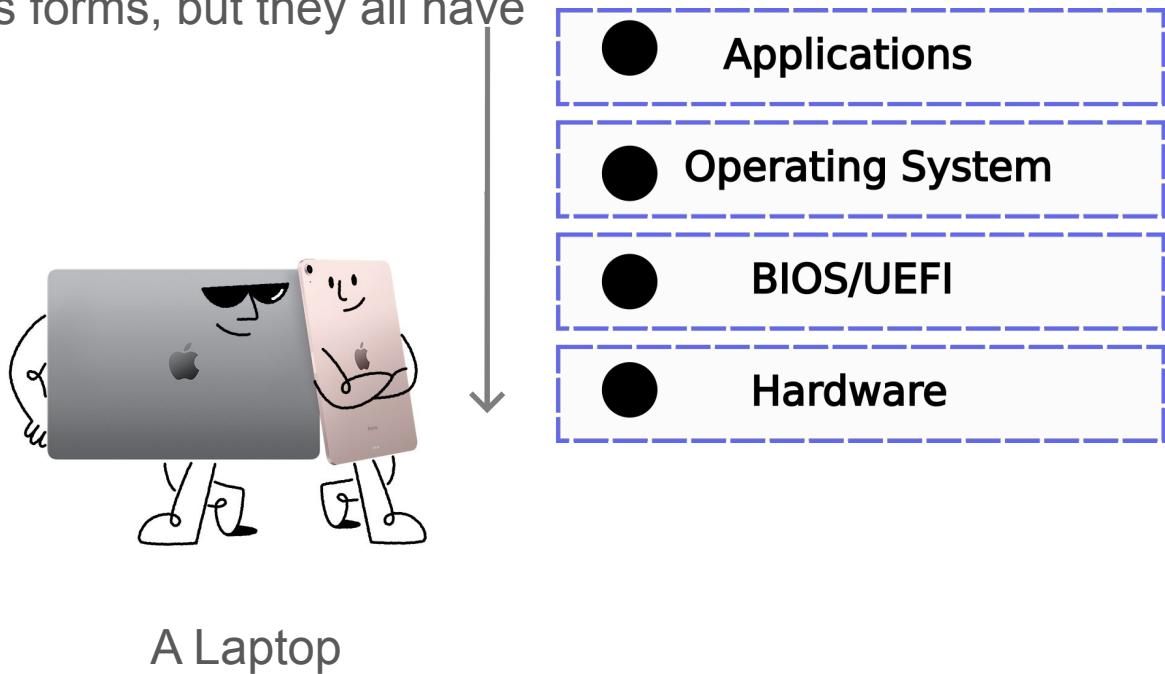
What is happening in a modern computer?

Modern computers have various forms, but they all have similar architectures.



A Supercomputer (HEP)

<https://cs.lbl.gov/news-media/news/2021/berkeley-lab-deploys-next-generation-supercomputer-perlmutter-bolstering-u-s-scientific-research/>



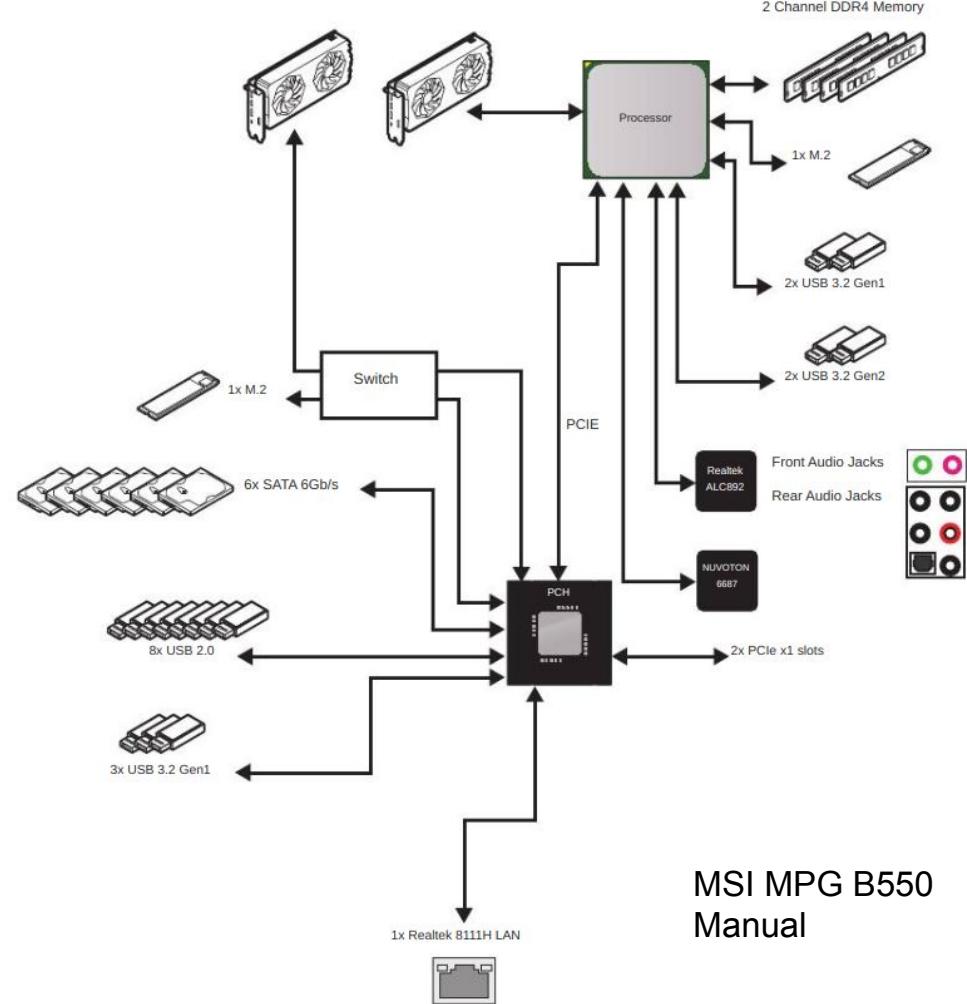
A Laptop

<https://www.apple.com/us-edu/shop/back-to-school>

Hardware

A modern computer requires few essential components: CPU, Memory, Storage, (GPU), and a Motherboard.

As an example, let's look at a typical gaming computer assembly.



BIOS/UEFI

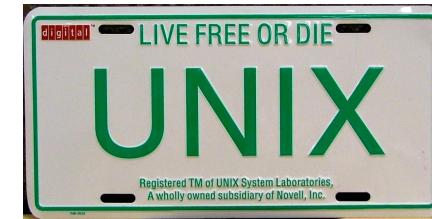
Basic Input/Output System (BIOS) or Unified Extensible Firmware Interface (UEFI) is one example of a firmware that perform low-level control of a hardware, such as booting and interacting with operating system.

The firmware is read-only memory (ROM) and usually stored in a motherboard. For example, the MSI BIOS interface.

MSI MPG B550
Manual



Operating system, UNIX



UNIX was developed in Bell labs (AT&T) in 1969, it is the first attempt for creating a platform for researchers to develop then use on other systems, referring as the Unix philosophy, e.g. make it easy to read and write, make programs work together, choose portability over efficiency. Various OS systems are developed based on the UNIX,

GNU



1983, Richard Stallman

Linux

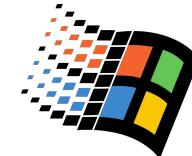


1991, Linus Torvalds

OSX

MacOS
2001

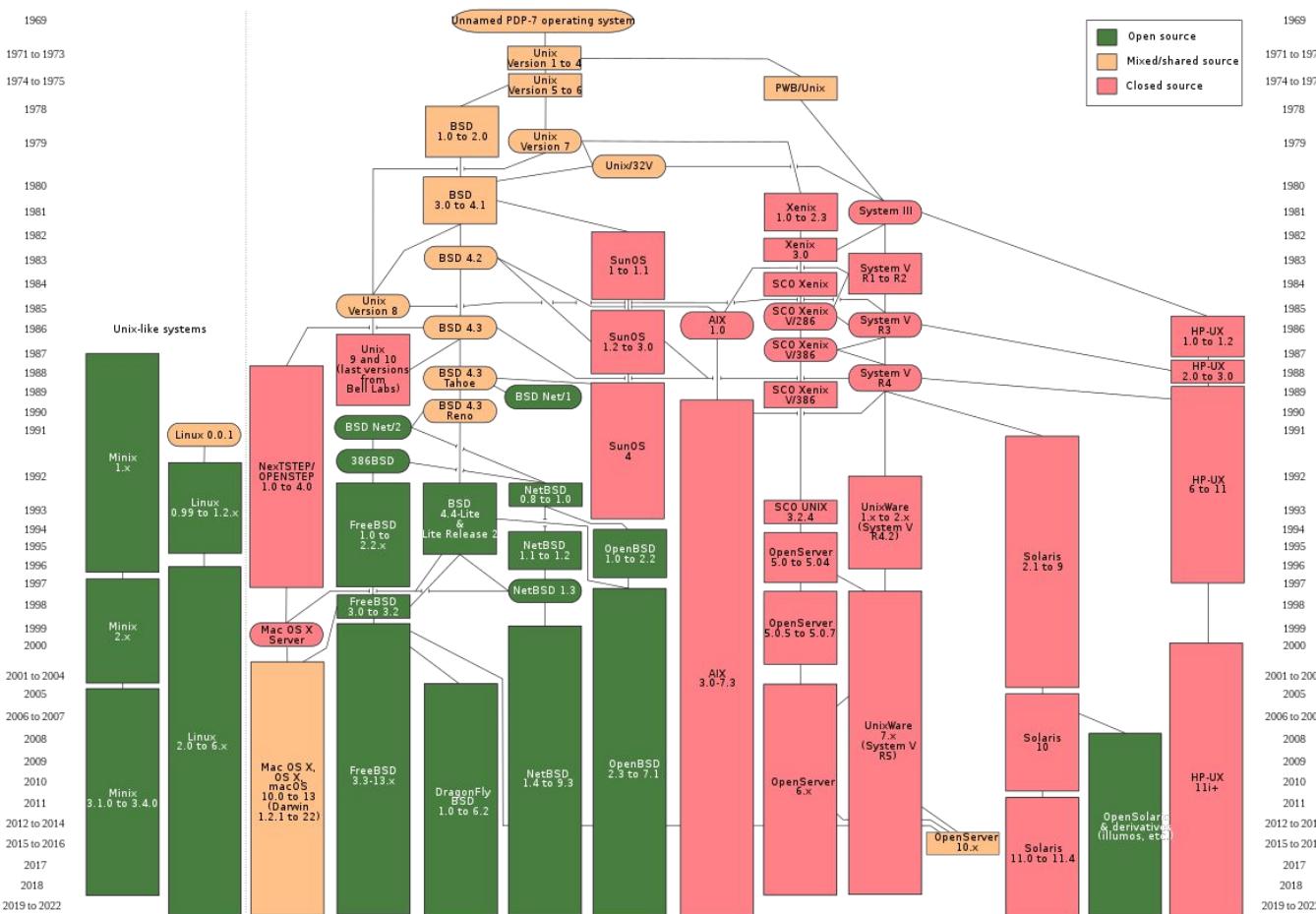
Not this one. At least not directly.



Microsoft Windows

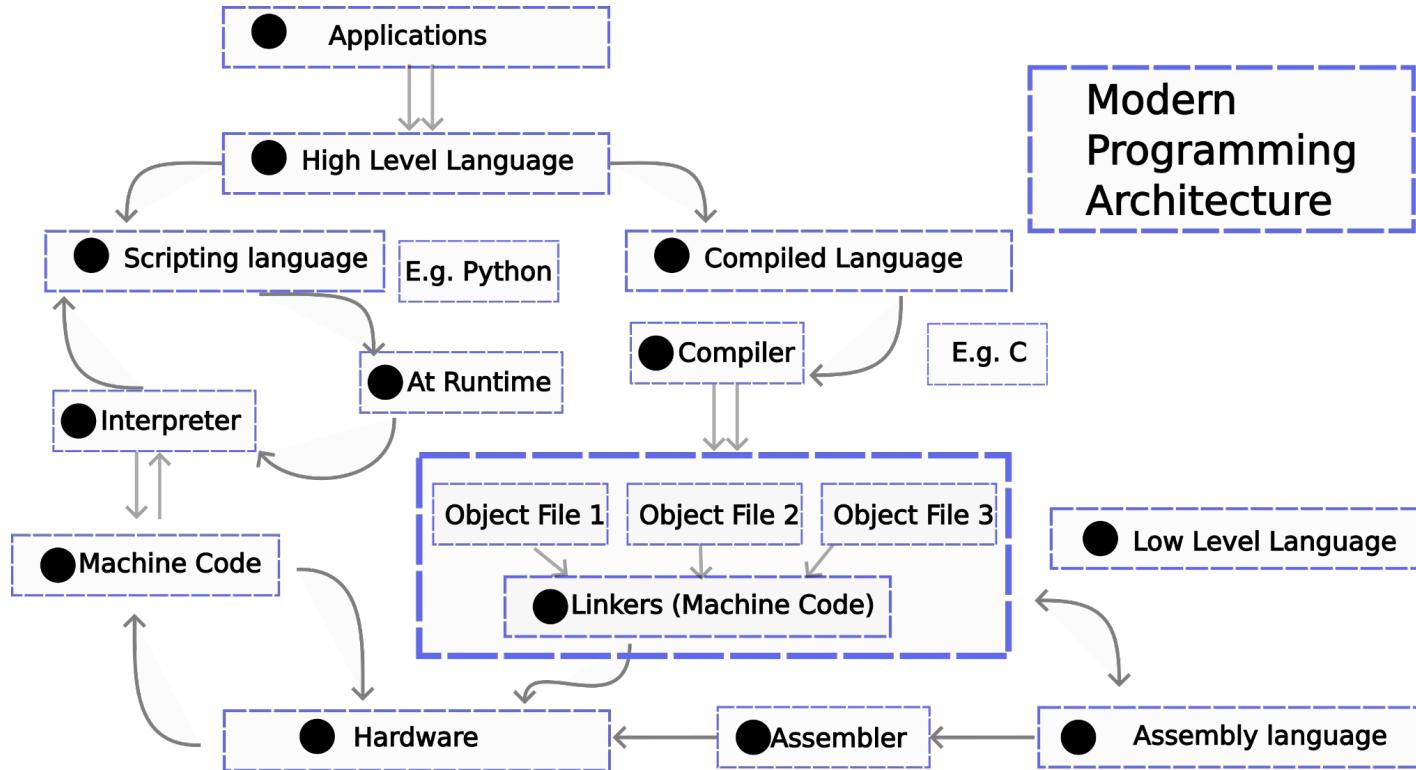
History of UNIX

Over the time, people realize the power of open-source systems...



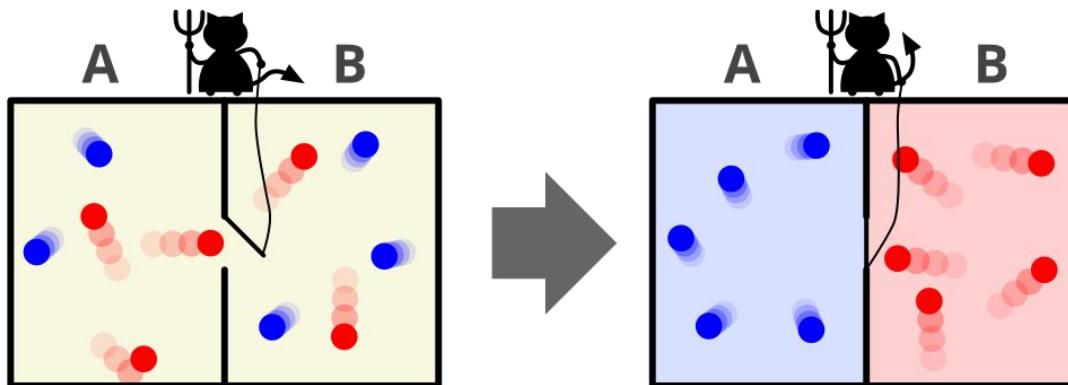
Programming

A program translates the objective of an application to machine-readable language.



Daemons

In Unix-like systems, background processes are called daemons. It was first used in a MIT project (1960s), inspired by "Maxwell's demon," an imaginary agent from physics that tirelessly performs tasks in the background.



information processing has physical consequences.
acquiring, storing, or erasing information generates entropy

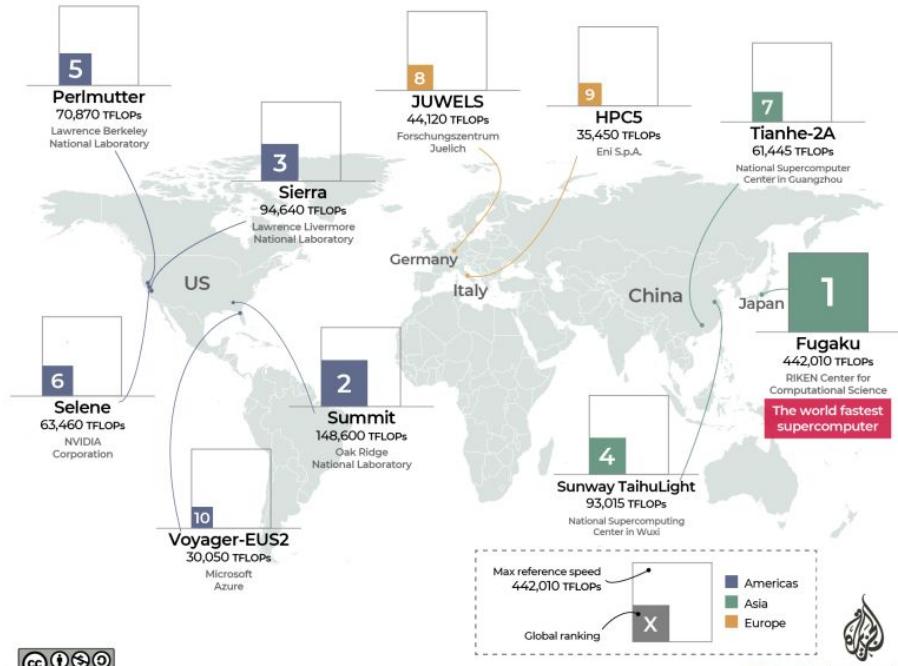
Applications in Science

Computation is an extremely powerful tool in processing practical models where the solution cannot be accessed with any analytical tools. In particular, computation is used to discover new physics phenomena and make predictions, e.g. exotic phase transitions, non-equilibrium models, material properties, biophysical processes, nuclear reactions, particle collision, galactic dynamics, etc...

SUPERCOMPUTERS

The top 10 most powerful supercomputers

Among the ten fastest supercomputers in the world, five are located in the US, two in China and one each in Japan, Germany and Italy.



Source: Top500 | November, 2021

@AJLabs



ALJAZEERA

Git

Git designed to track changes in files (by Linus Torvalds in 2005).

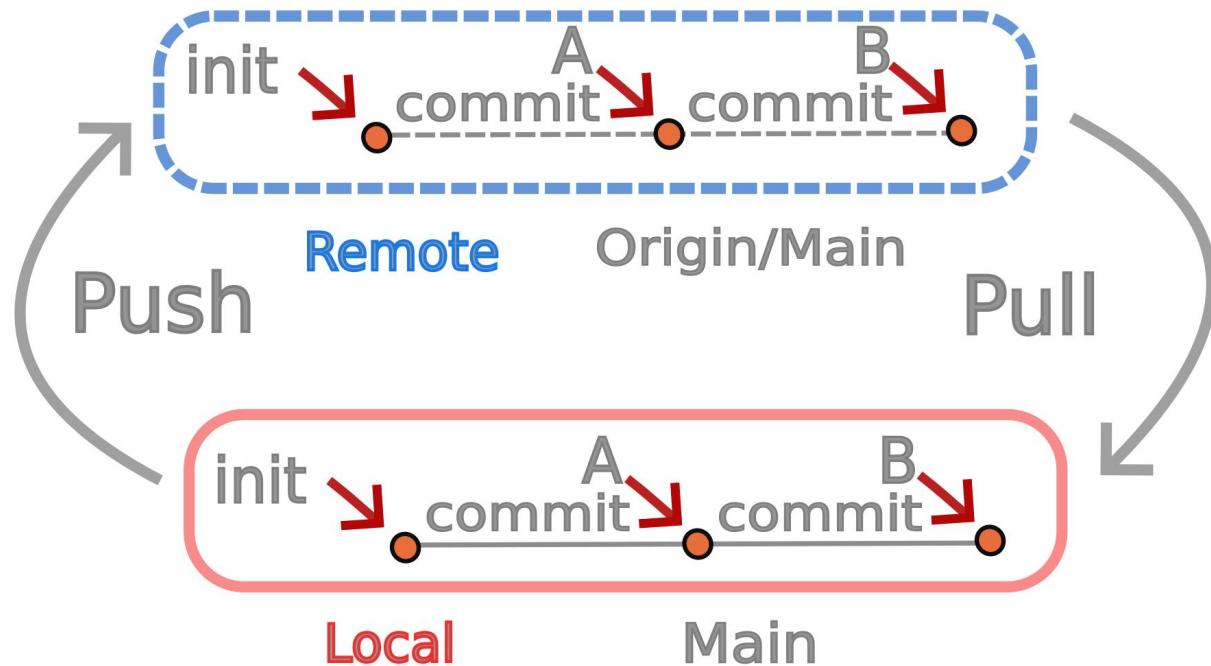


Distributed: every developer has a complete copy of the repository, including its history, on their local machine. This ensures that work can continue without relying on a central server.

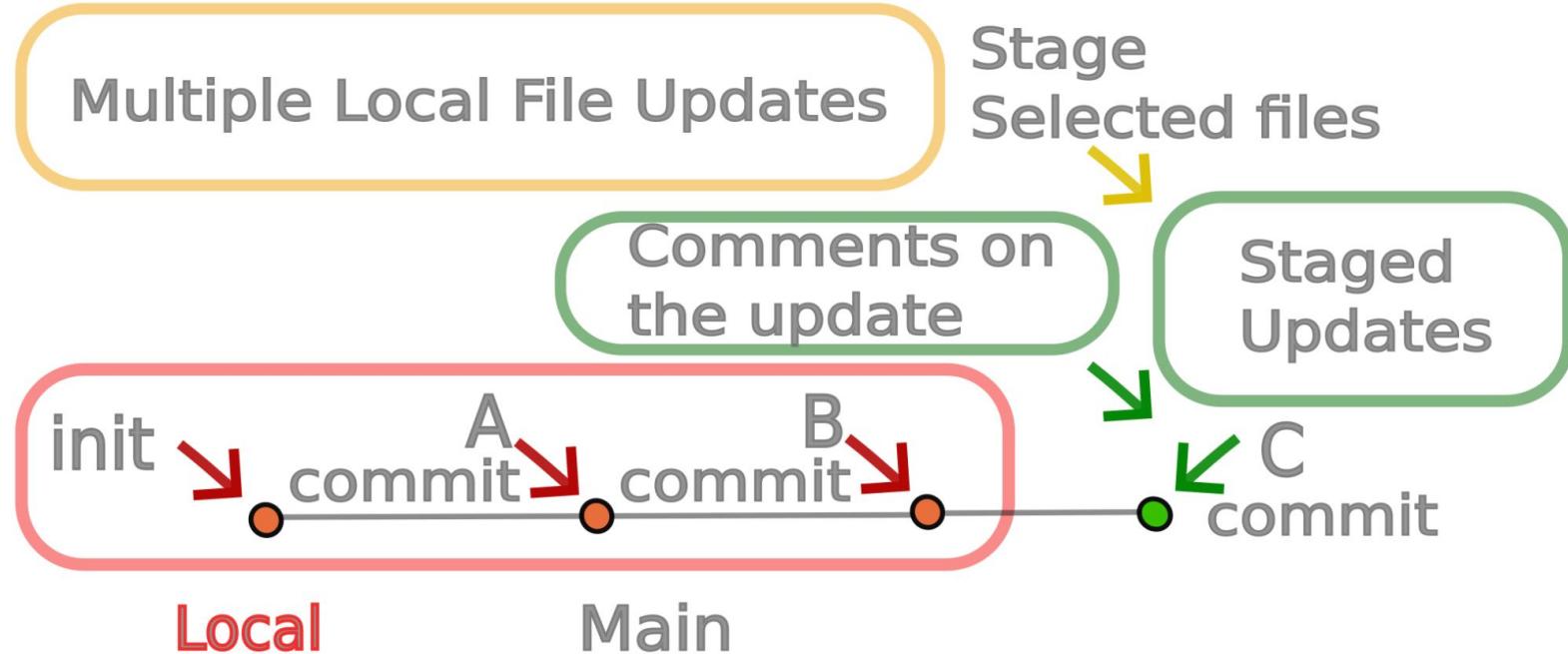
Version Tracking: tracks changes to files and allows developers to view the history of modifications, revert to previous versions, or compare differences between versions.

Non-linear workflows: developers can create branches (**fork**) for new features or experiments without altering the existing mainstream.

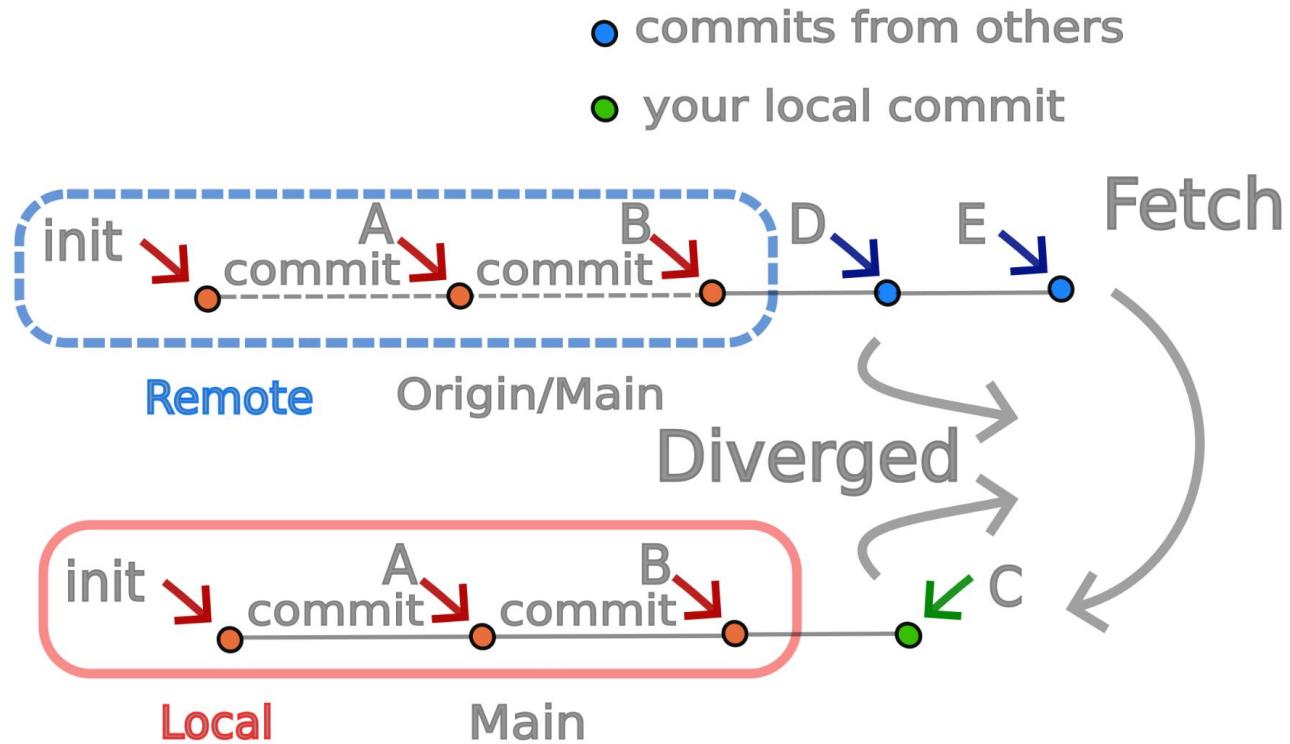
Git: Push and Pull



Git: Commit

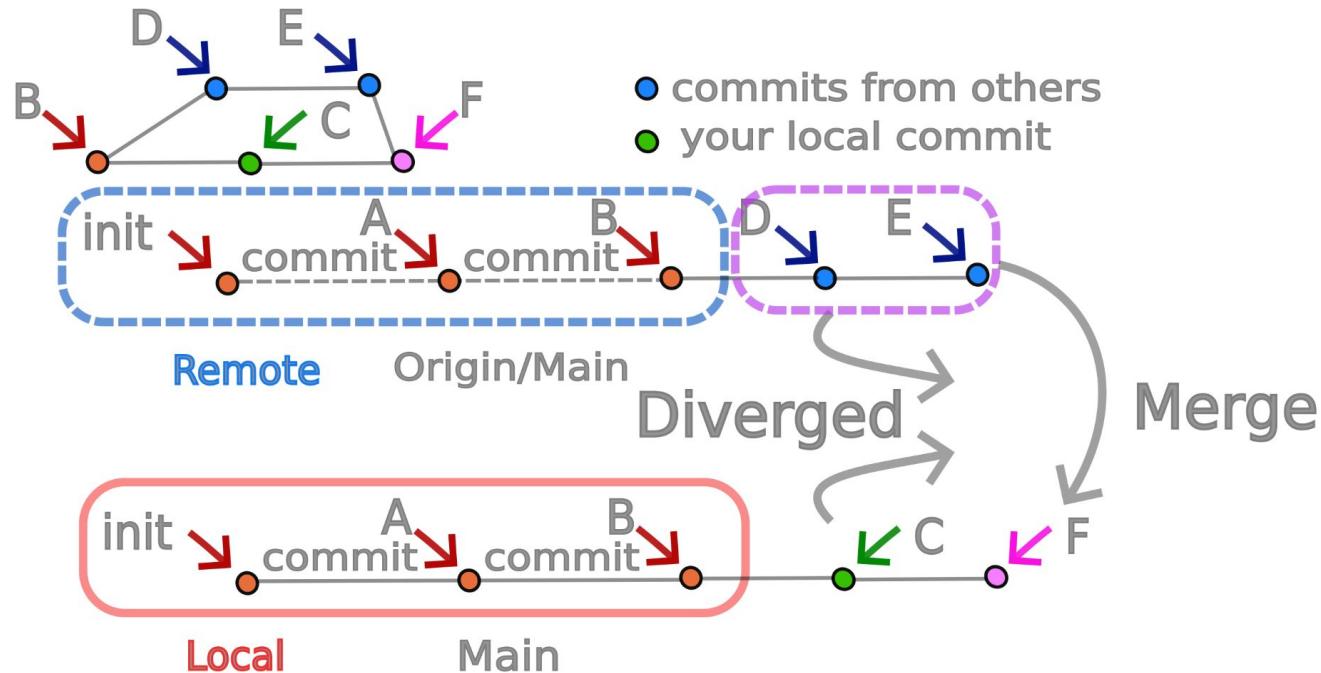


Git: Fetch



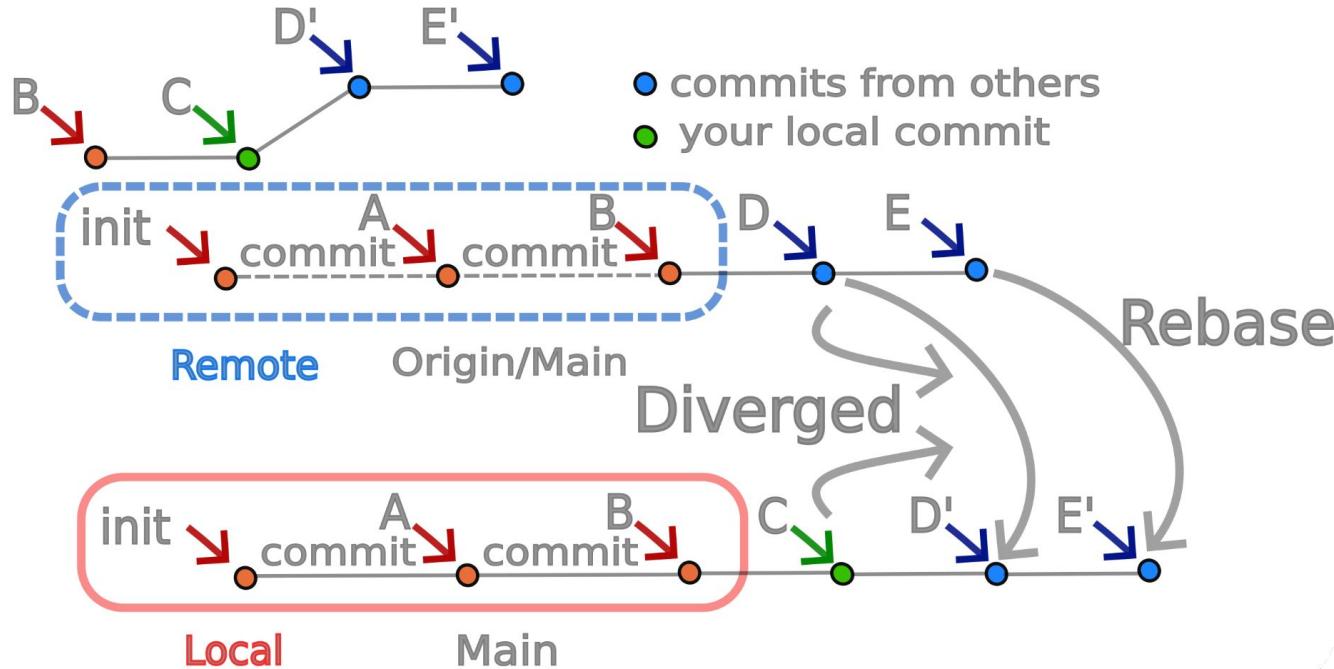
Git: Merge

- A merge commit preserves the branching and merging history, e.g. D,E.



Git: Rebase

A rebase destroy the branching history, assign the D, E commits to a different name D',E'.



Github



Github is a remote repository destination (2007) for git

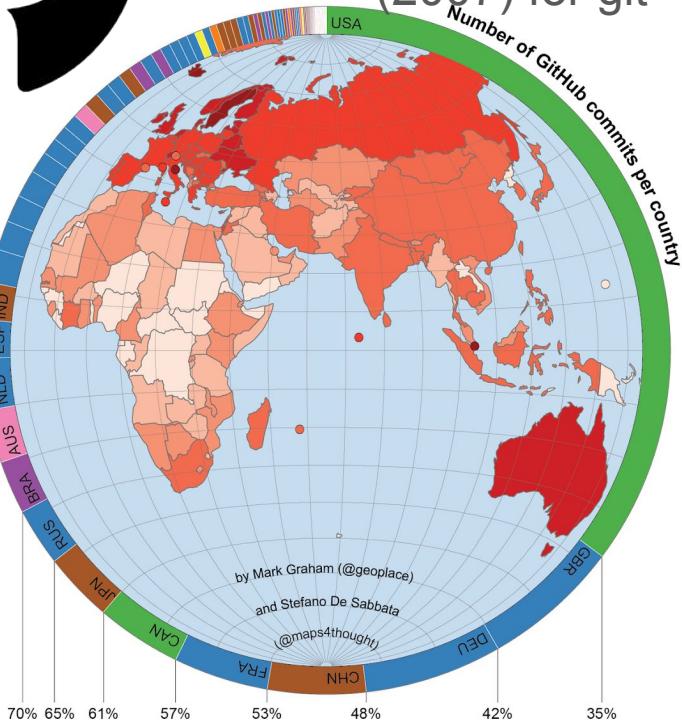
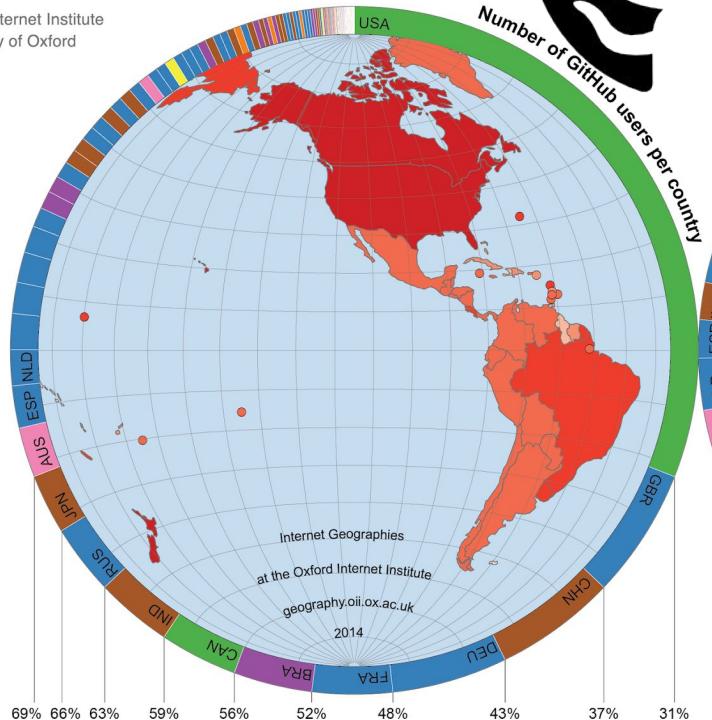
oiioiioi
oiioioioi
oiioioioi
Oxford Internet Institute
University of Oxford

GitHub users per 100,000 Internet users

- > 50
- 25 - 50
- 10 - 25
- 2.5 - 10
- 1 - 2.5
- 0.25 - 1
- < 0.25

- North America
- Latin America & Caribbean
- Sub-Saharan Africa
- Middle East & North Africa
- Europe
- Asia
- Oceania

data sources:
GitHub.com
World Bank
data.worldbank.org



Docker



Containerization (Created in 2013).

Individual Environment on Demand: Lightweight, portable, and isolated environments

Multitasking: Share the host OS kernel instead of requiring a full OS

Reproducibility: consistent behavior across development, testing, and production environments.

Docker Images and Containers



Images are composed of layers. And each of these layers, once created, are immutable.

Container is a specific instance of an **image** that can be created or destroyed on demand.

