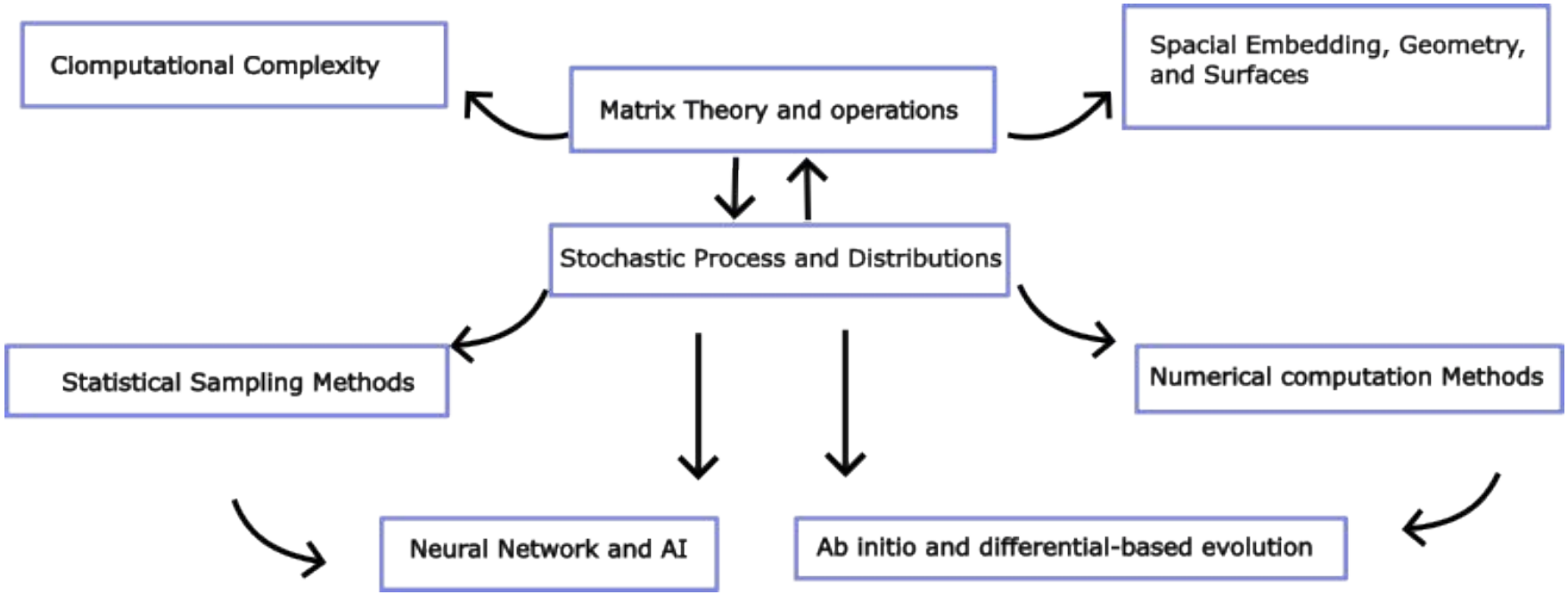
Introduction to Computational Physics

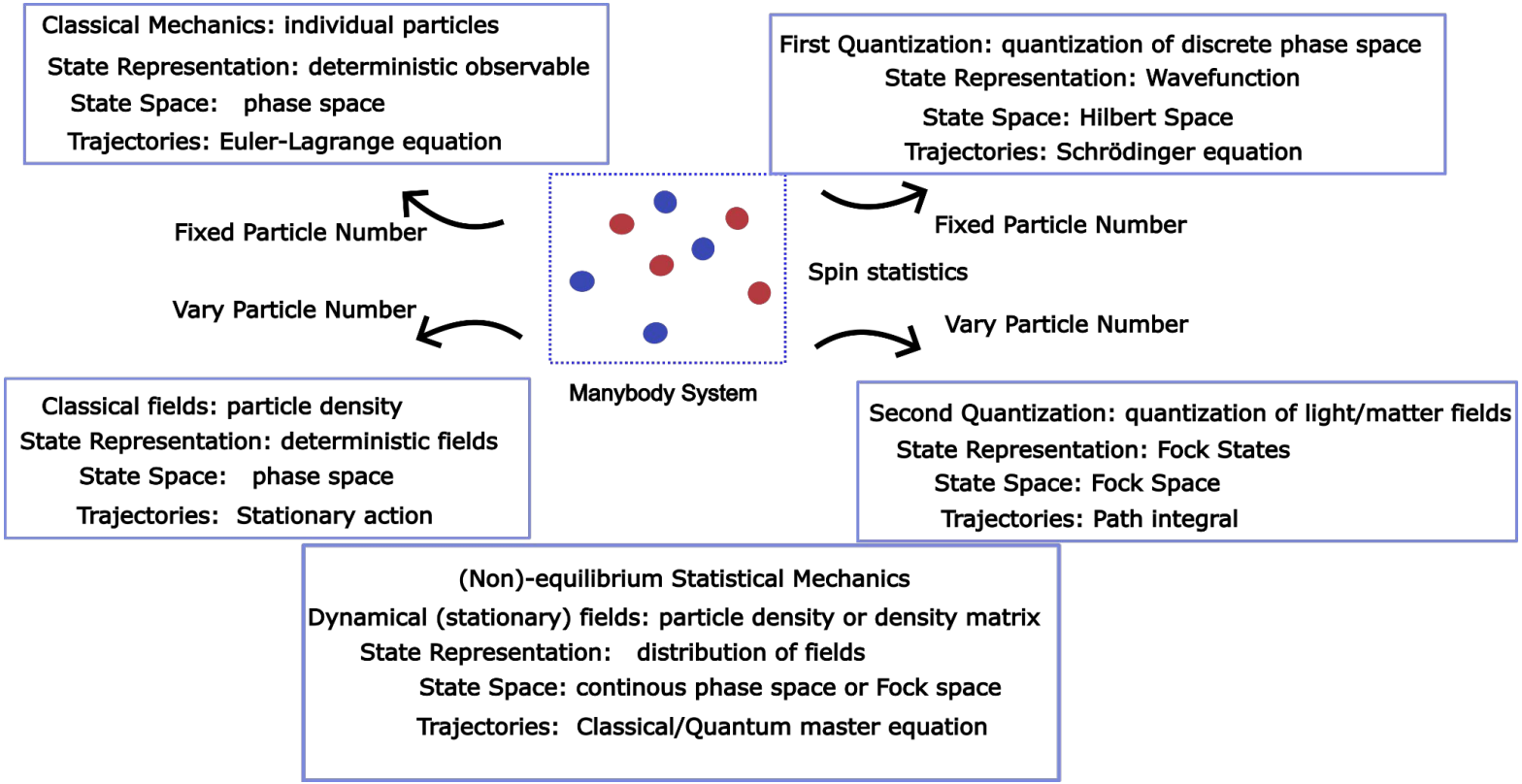
Physics 129AL

Zihang Wang
01/07/2025

Overview


Clomputational Complexity
Matrix Theory and operations
Spacial Embedding, Geometry, and Surfaces
Stochastic Process and Distributions
Statistical Sampling Methods
Numerical computation Methods
Neural Network and AI
Ab initio and differential-based evolution

Scope in Physics



Syllabus

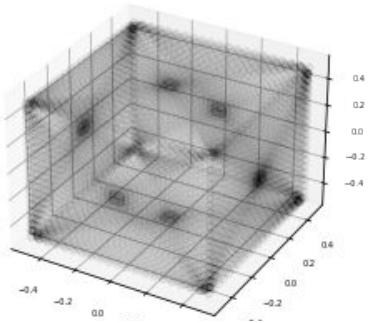
- **Basics in Differential Geometry** matrix, tensors, metric, dual space, generalized coordinate transformation, vector, covector, covariant derivative, parallel transport, geodesic, surface derivatives, first/second fundamental forms, intrinsic/extrinsic curvatures.

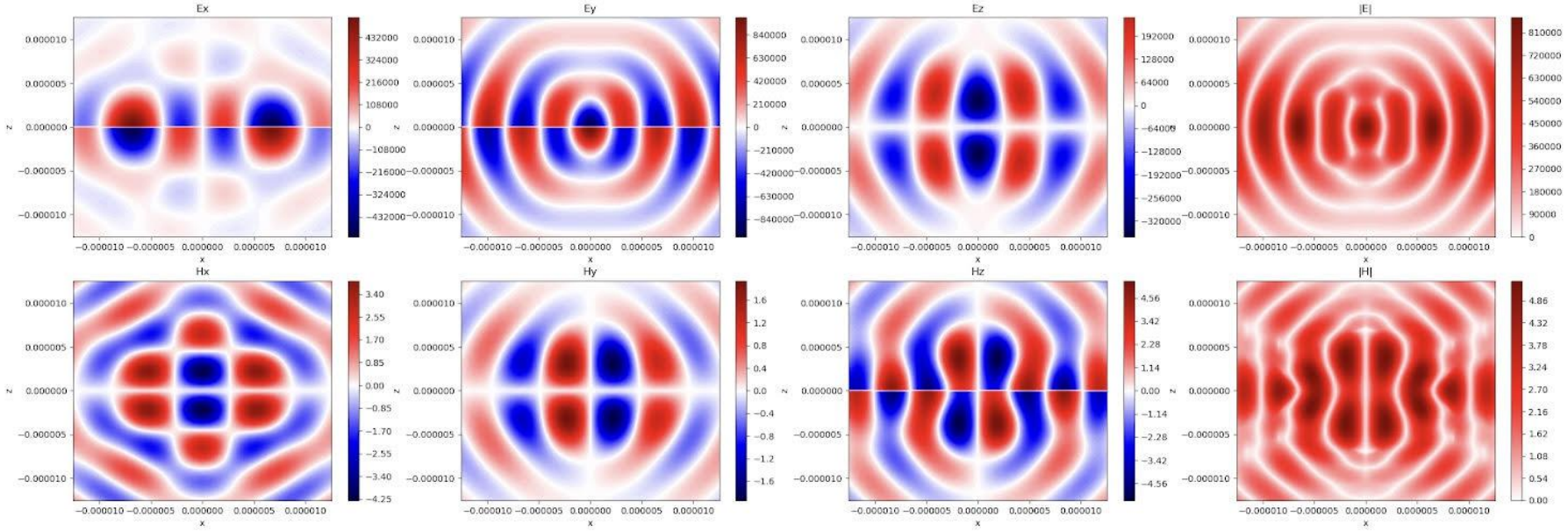
- **Basics in Matrix Theory** Gaussian and Gauss-Jacobi elimination, backsubstitution, pivoting, LU decomposition, Cholesky decomposition, QR decomposition, sparse matrix linear algebra, QR decomposition and tridiagonal forms, diagonalization of a symmetric and non-symmetric matrix, principal axes and 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

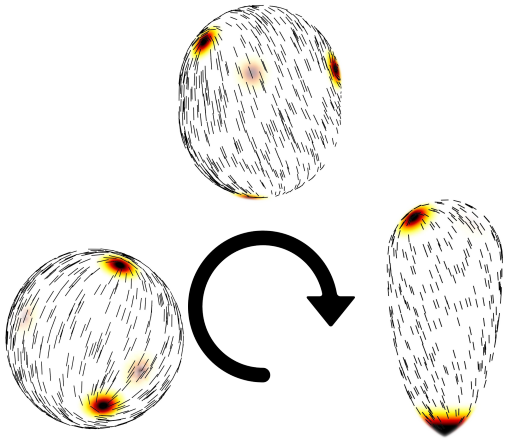
Electric/Magnetic Field Strength, scattering amplitude on 3D mesh

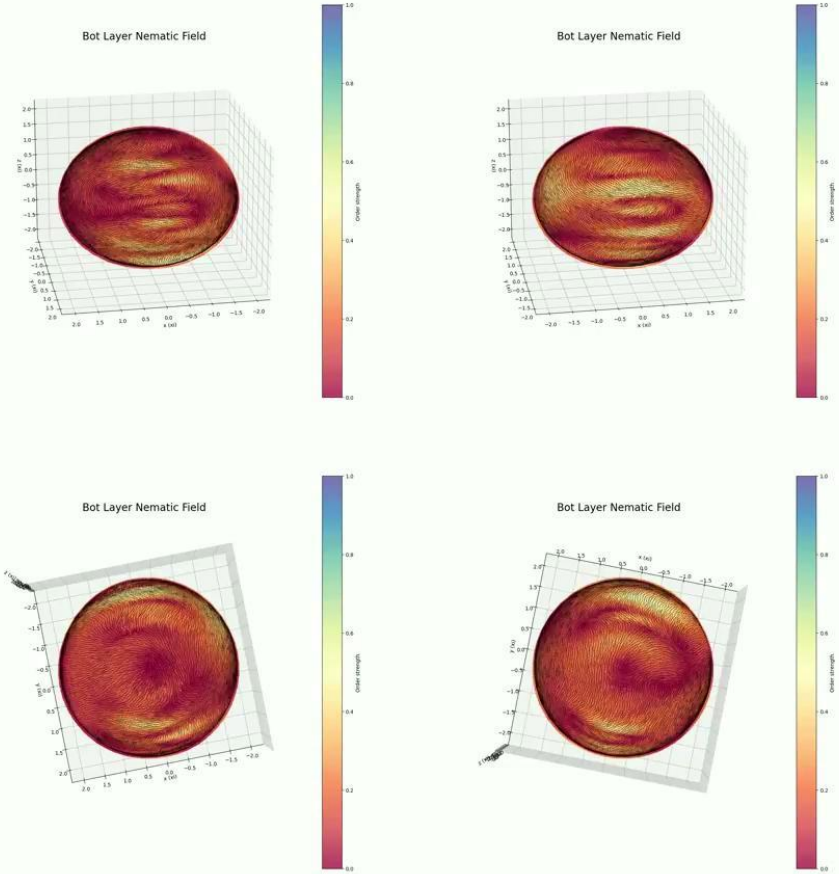




Syllabus

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

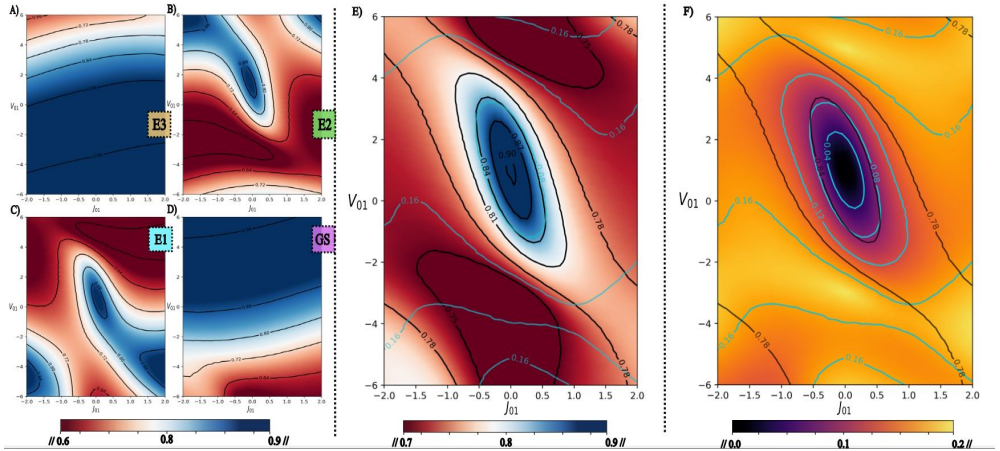




Syllabus

- **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



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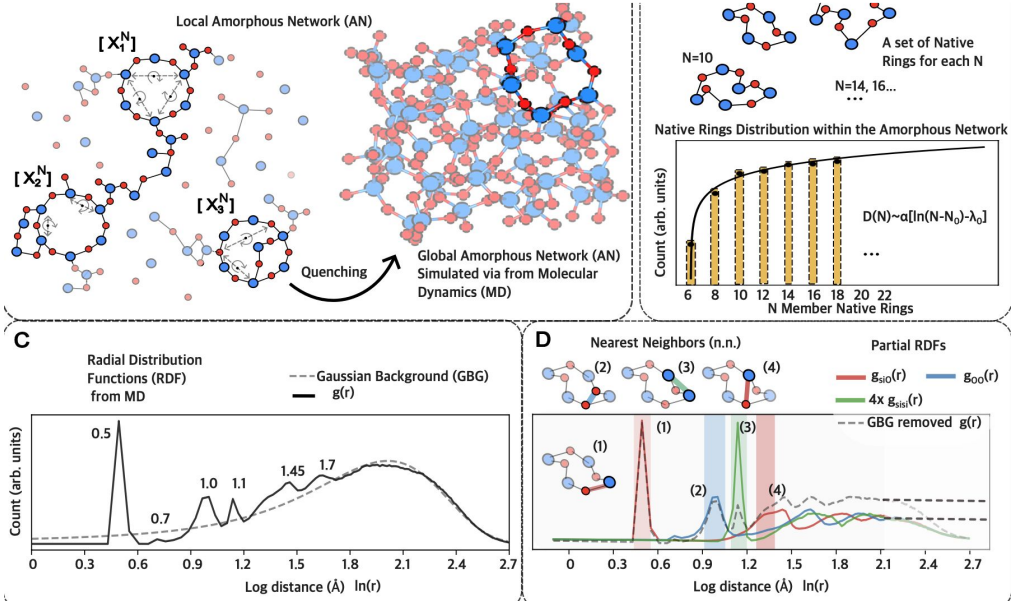
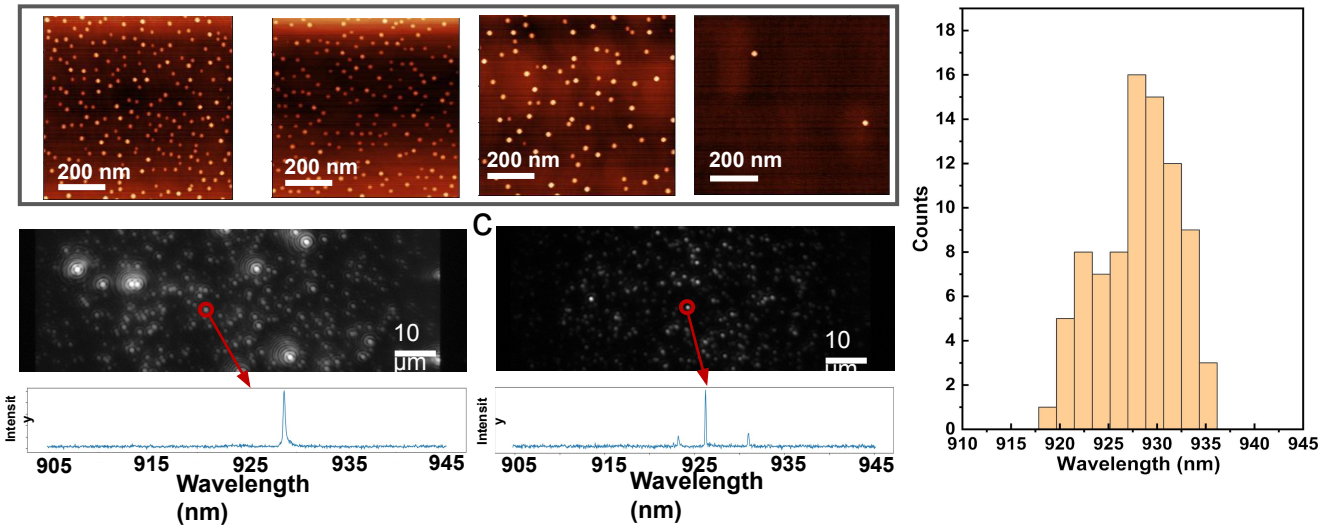
Amorphous network generation and anisotropy statistics



Syllabus

Quantum dot density generated via molecular beam epitaxy

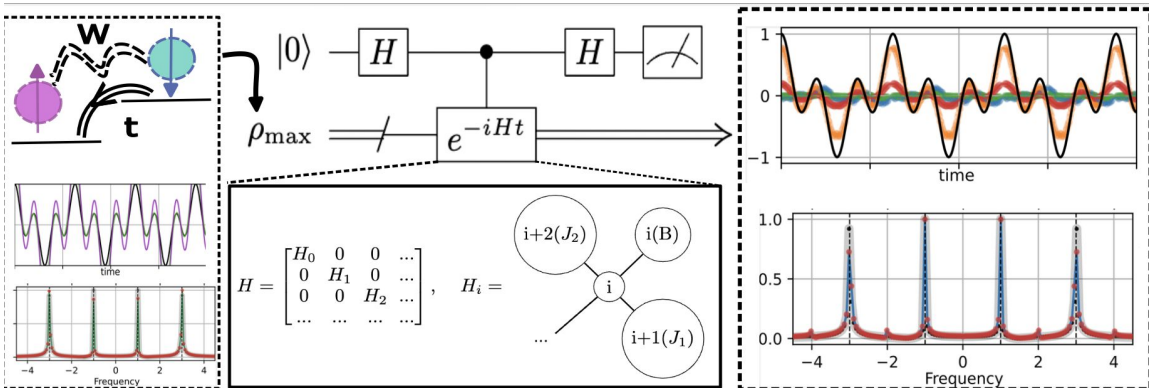


Syllabus

- **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.

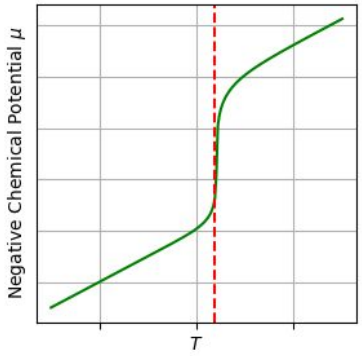
- **Common computation techniques in physics**, discrete Fourier transform, numerical integration and differentiation, Gaussian quadrature, orthogonal (Legendre) polynomials, implicit and explicit iterative methods for differential equations, Runge–Kutta methods, Leapfrog, symplectic integrator, (stochastic) gradient descent, explicit/implicit regularization.

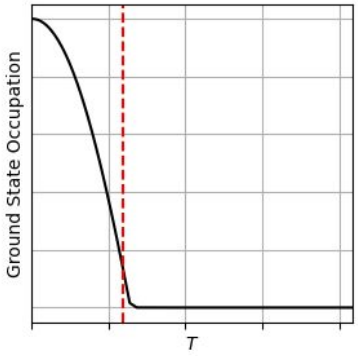
State evolution on a quantum computer

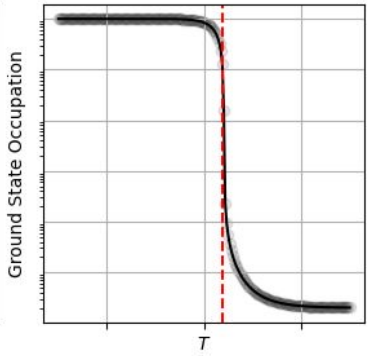


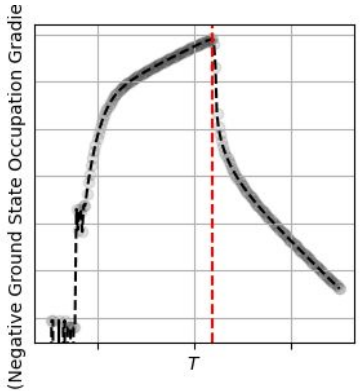
Syllabus

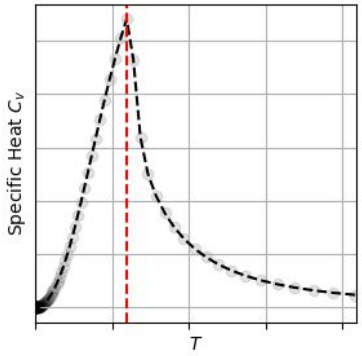
Quantum Phase transitions (bose einstein condensate)

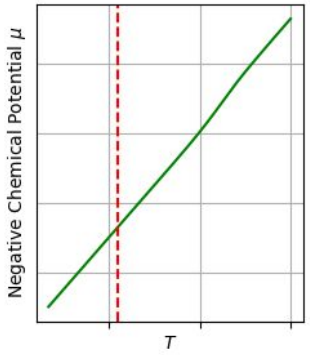


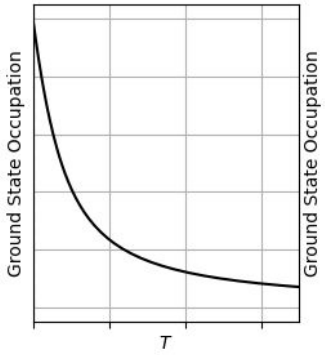


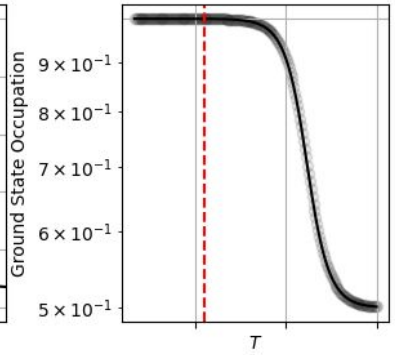


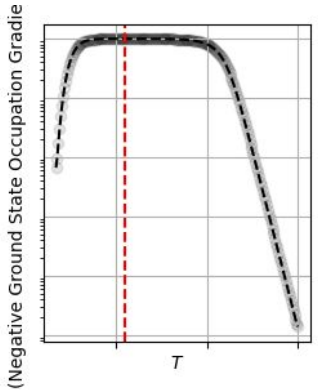


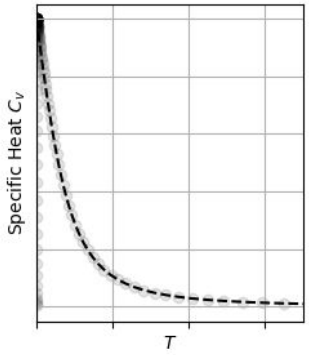






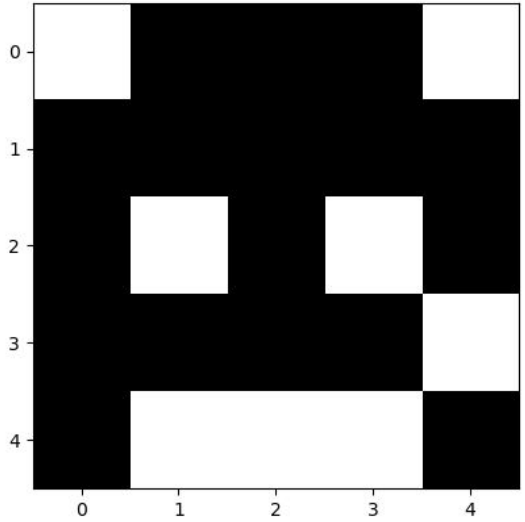






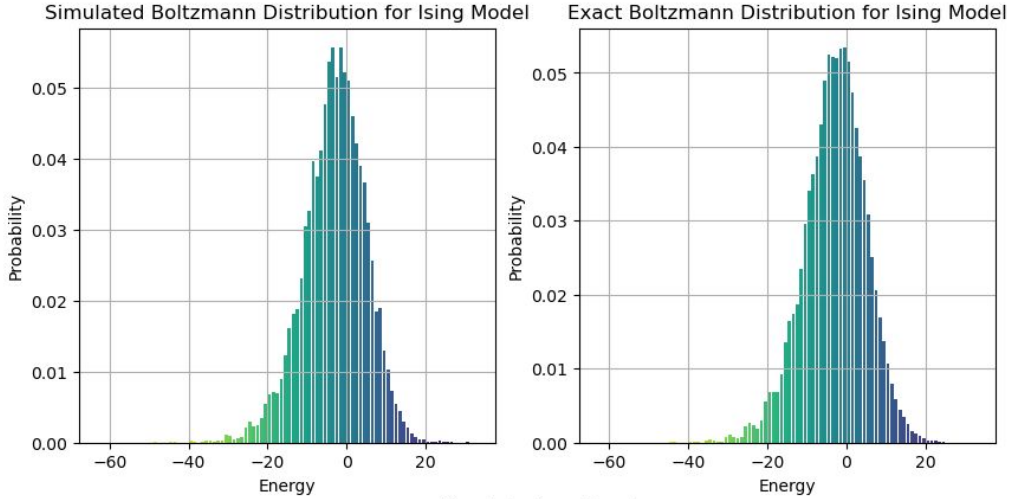
Syllabus

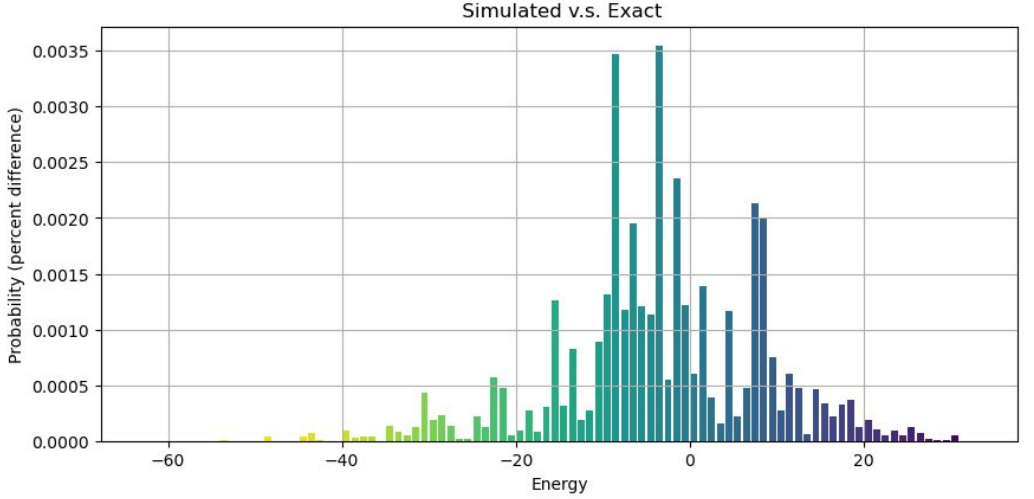
Classical/Quantum Phase transitions (Ising model with transverse field)



Exact Elapsed Time: 1260.5645 seconds

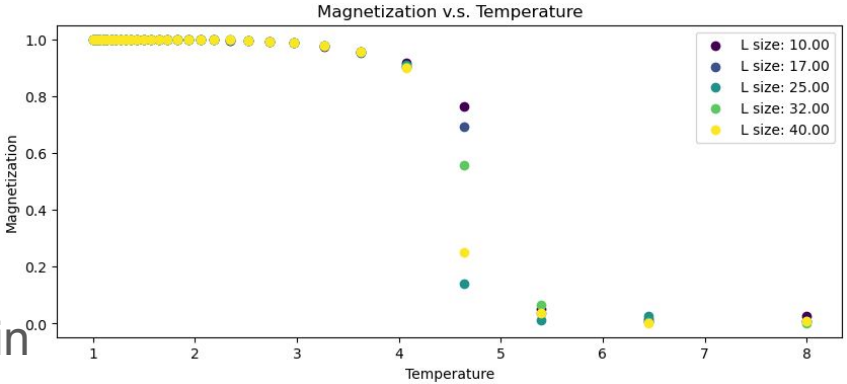
MC Elapsed Time: 4.4076 seconds

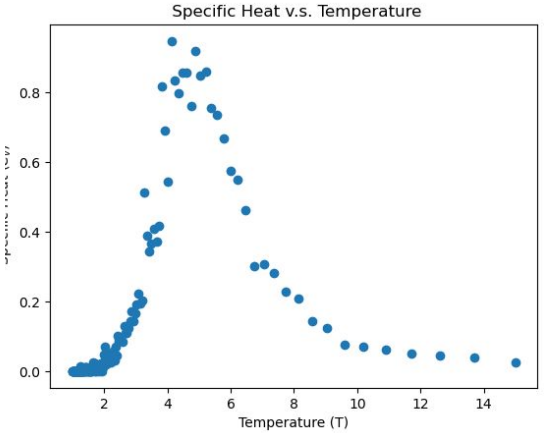


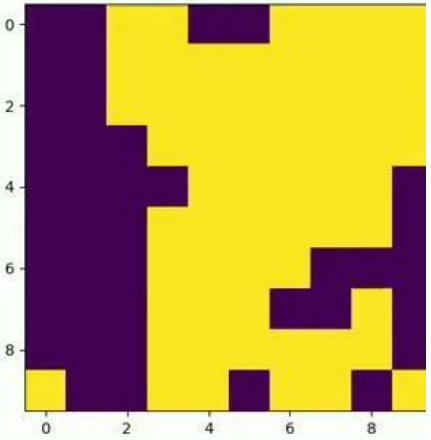


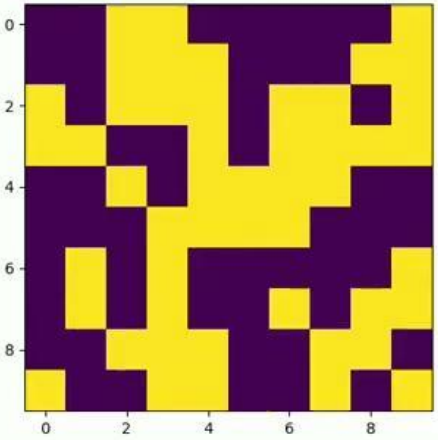
Syllabus

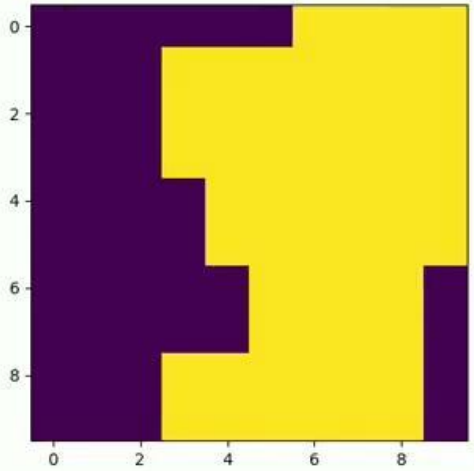
Order parameter in Phase transitions



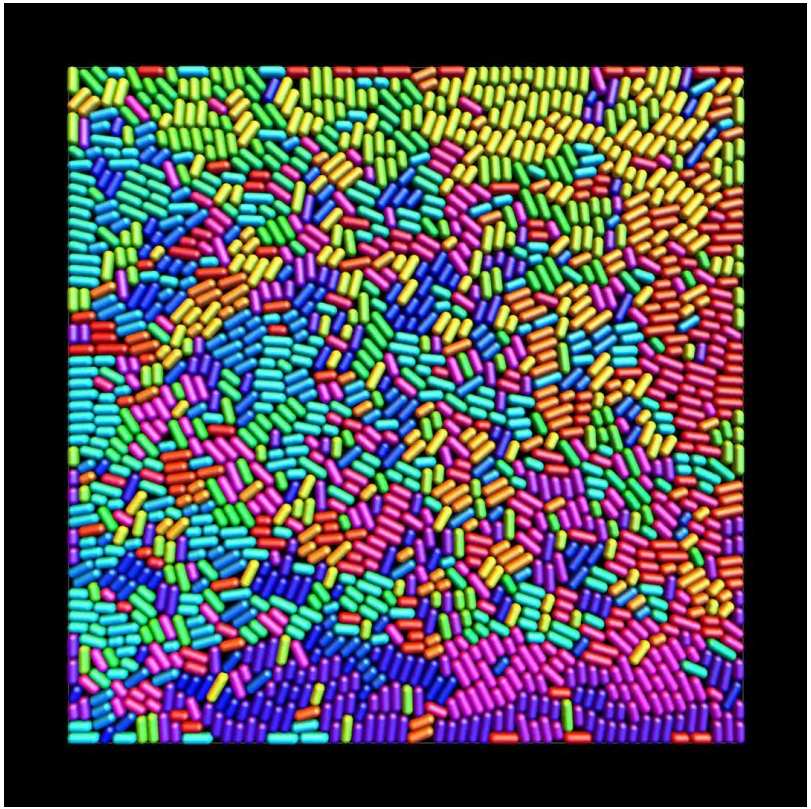


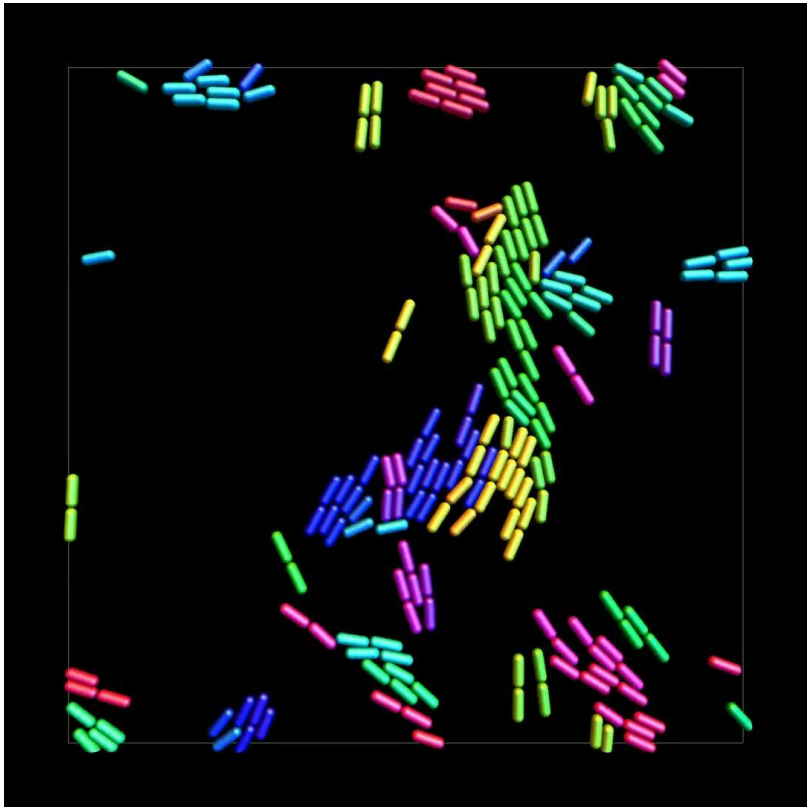






Syllabus Molecular Dynamics that generates Glassy phase transitions in bacteria

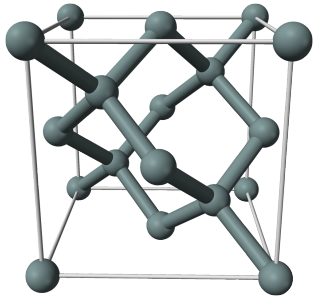


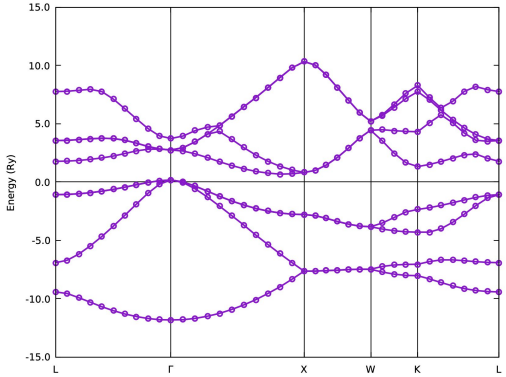


Syllabus

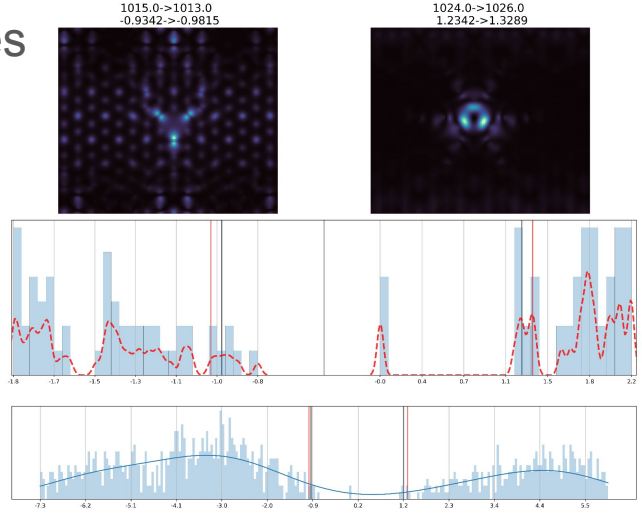
- **Applications in physics**, Electrostatics, Diffusion, Brownian motion, driven system, hydrodynamics, phase transitions, molecular dynamics, *ab initio* approaches to electronic structure, quantum state (density matrix) evolution, surface code, quantum master equation, numerical renormalization group.
- **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* Google Brain avaswani@google.com

Noam Shazeer* Google Brain noam@google.com

Niki Parmar* Google Research nikip@google.com

Jakob Uszkoreit* Google Research usz@google.com

Llion Jones* Google Research llion@google.com

Aidan N. Gomez* † University of Toronto aidan@cs.toronto.edu

Łukasz Kaiser* Google Brain lukaszkaiser@google.com

Illia Polosukhin* ‡ illia.polosukhin@gmail.com

GPT (Generative Pre-trained Transformer)

2021

High-Resolution Image Synthesis with Latent Diffusion Models

Robin Rombach[1] * Andreas Blattmann[1] * Dominik Lorenz[1] Patrick Esser[R] Björn Ommer[1]

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

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

Stable Diffusion

Syllabus

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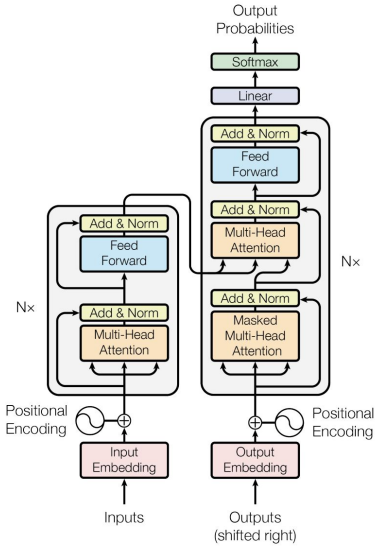


Figure 1: The Transformer - model architecture.

2020 **Denoising Diffusion Probabilistic Models**

Jonathan Ho
UC Berkeley
jonathanho@berkeley.edu

Ajay Jain
UC Berkeley
ajayj@berkeley.edu

Pieter Abbeel
UC Berkeley
pabbeel@cs.berkeley.edu

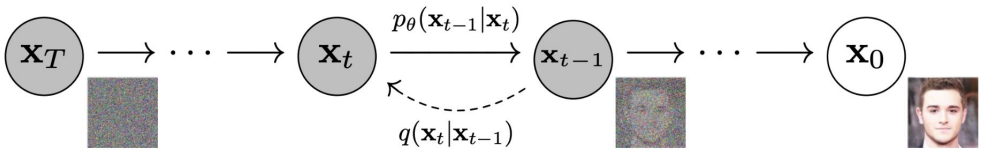


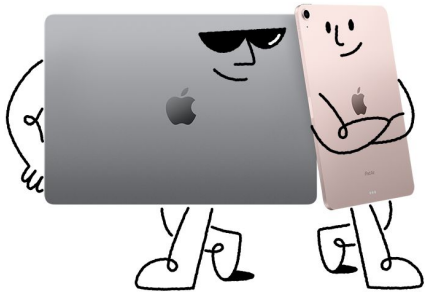
Figure 2: The directed graphical model considered in this work.

What is happening in a modern computer?

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

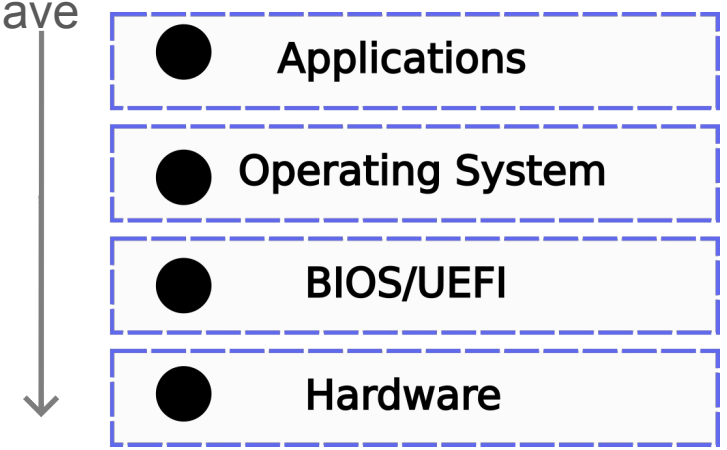
A Supercomputer (HEP)

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



A Laptop

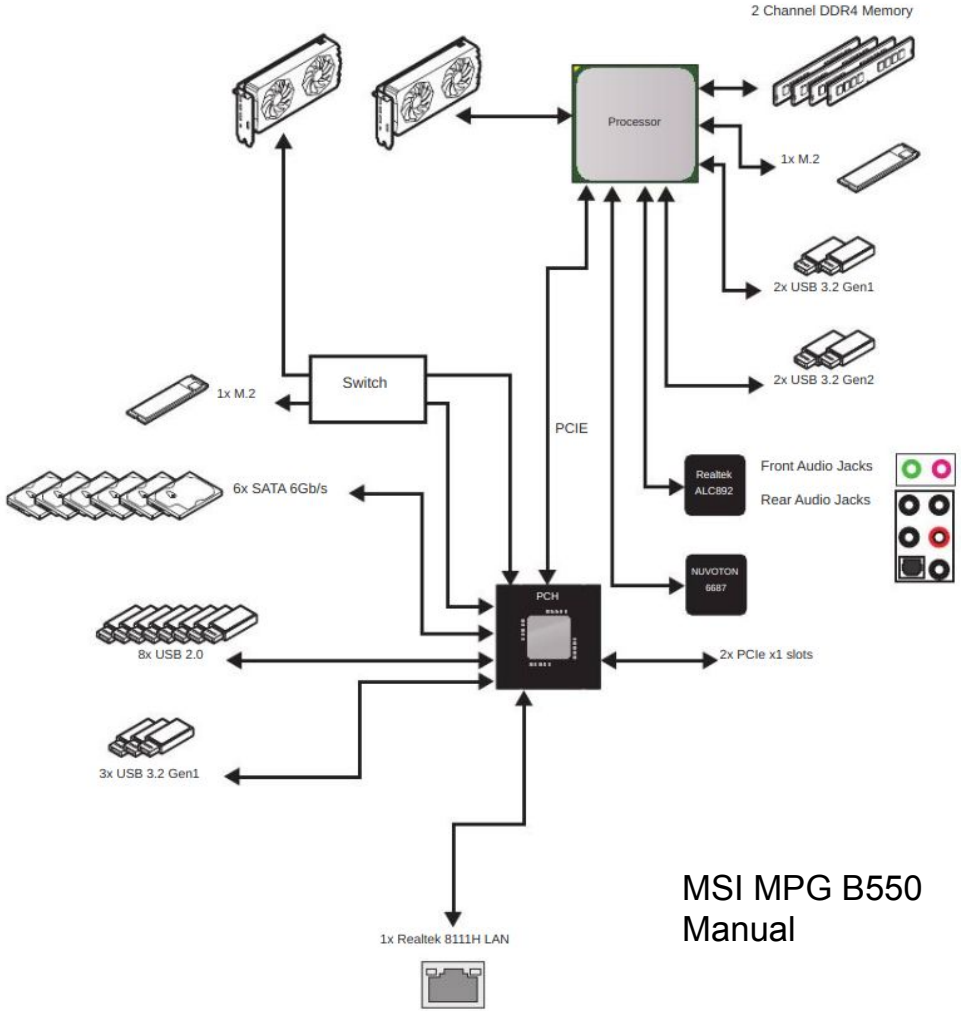
https://www.apple.com/us-edu/shop/back-to-school



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.

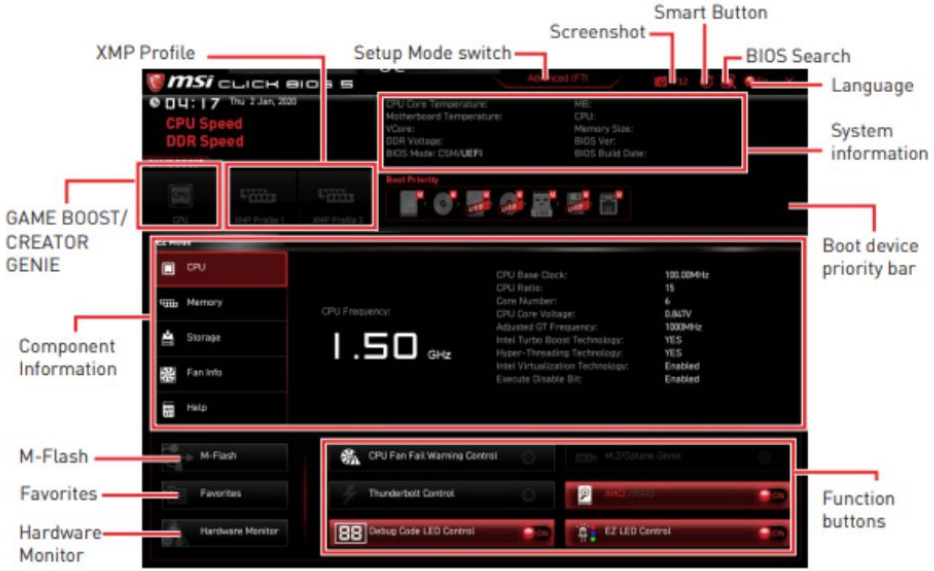


MSI MPG B550 Manual

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

OS X

MacOS

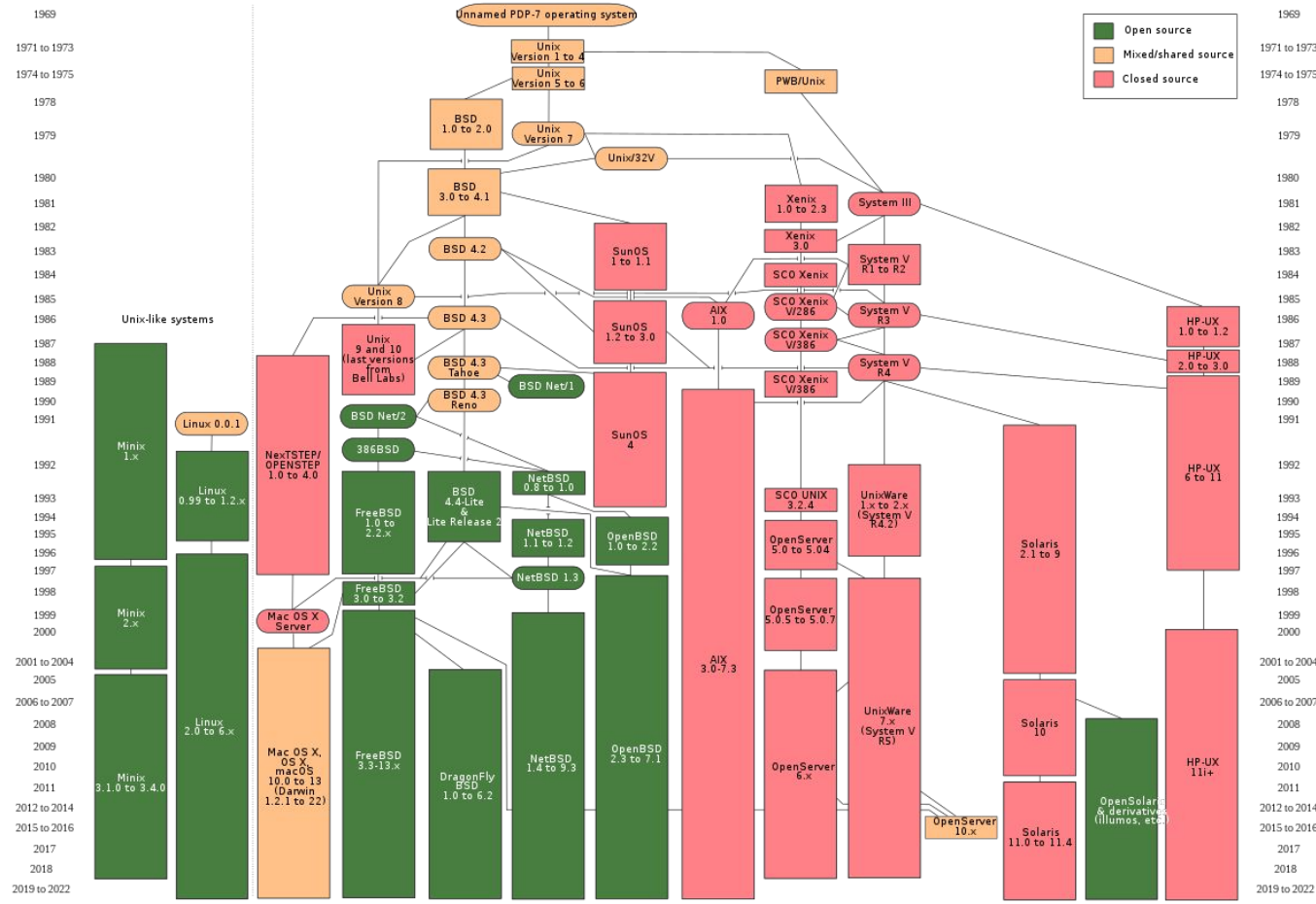
2001

Not this one. At least not directly.

Microsoft Windows

History of UNIX

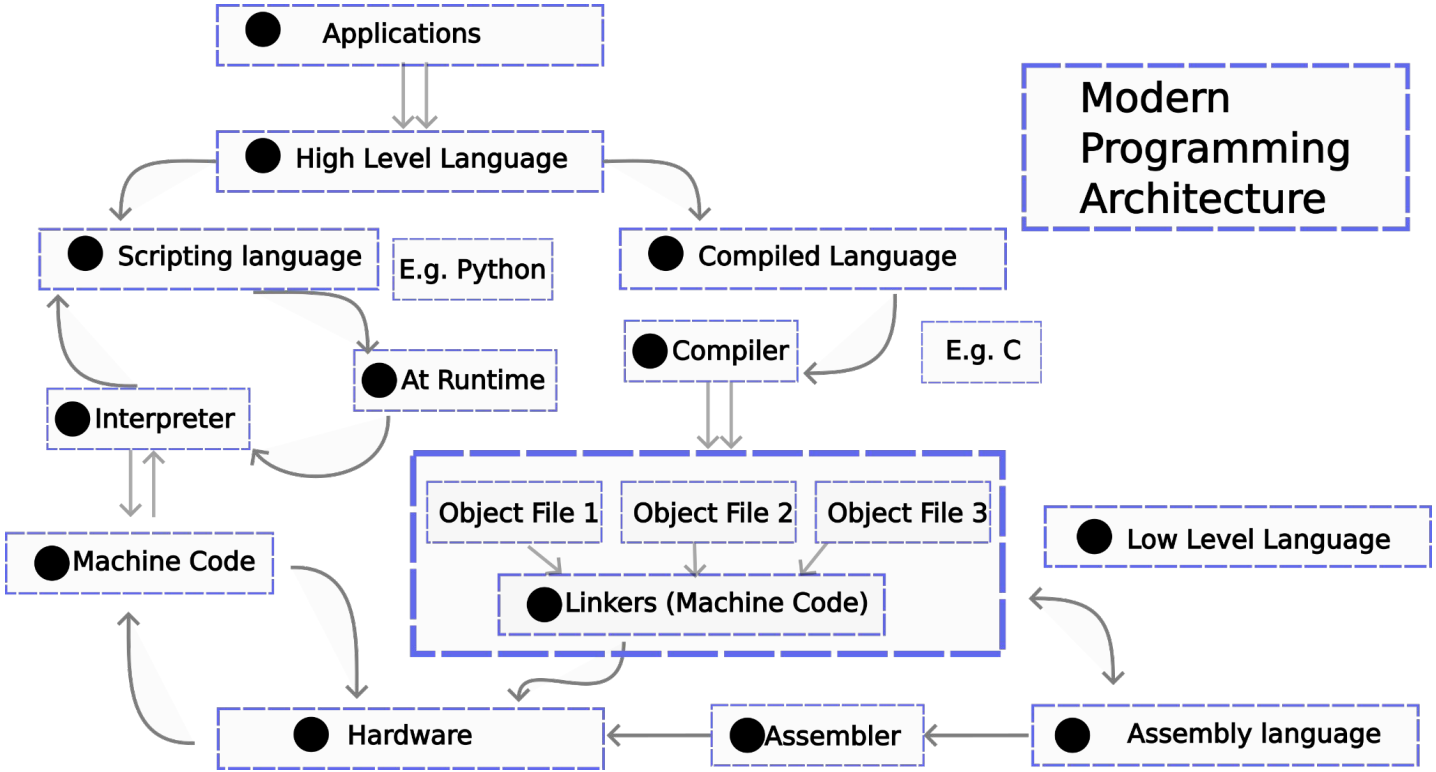
Over the time, people realize the power of open-source systems…



https://en.wikipedia.org/wiki/Unix-like

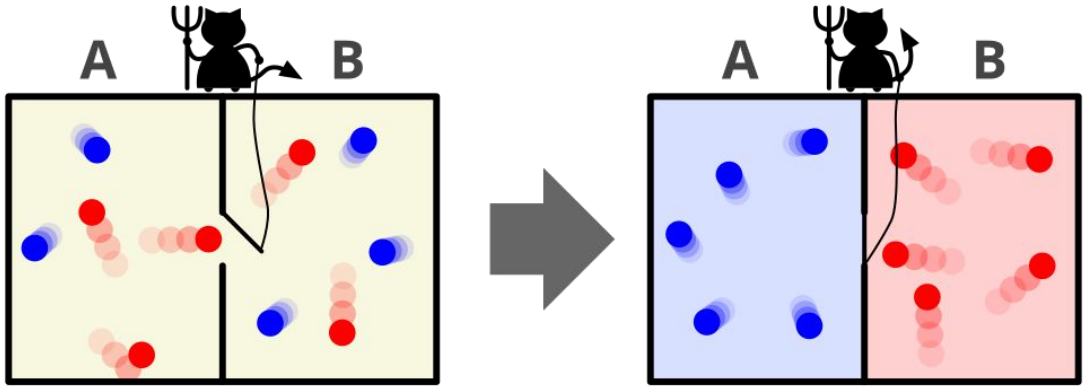
Programming

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.

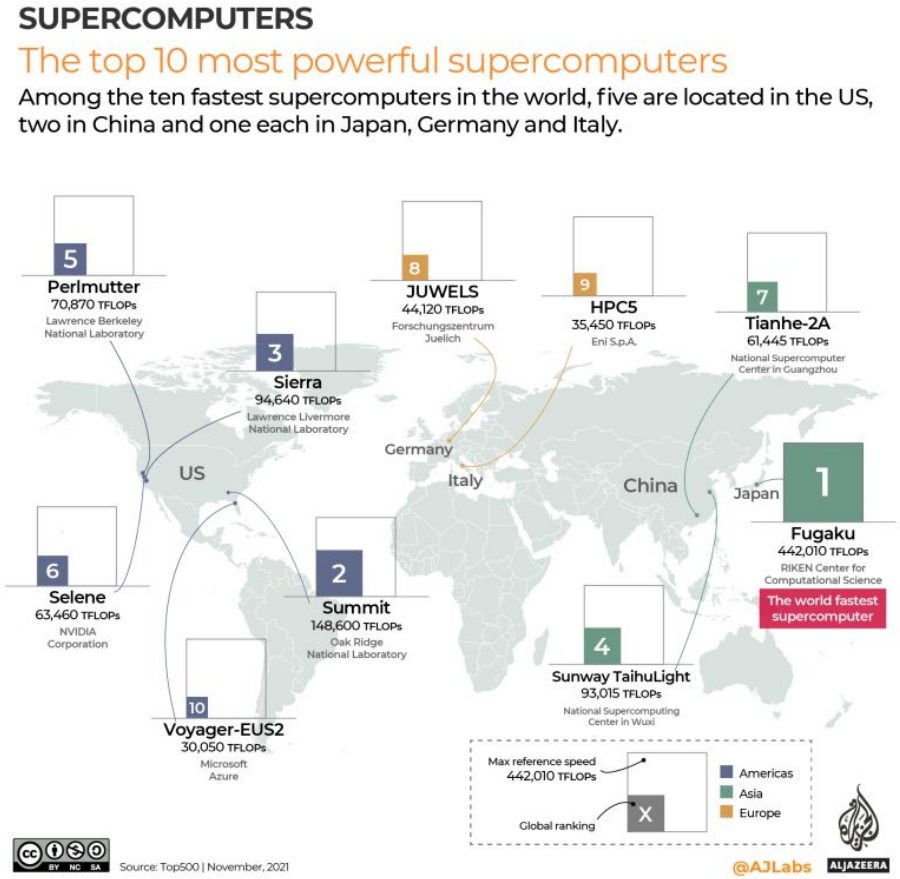


https://en.wikipedia.org/wiki/Maxwell's_demon

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…



https://www.aljazeera.com/news/2022/1/14/infographic-visualising-race-build-world-fastest-supercomputers-interactive

Git

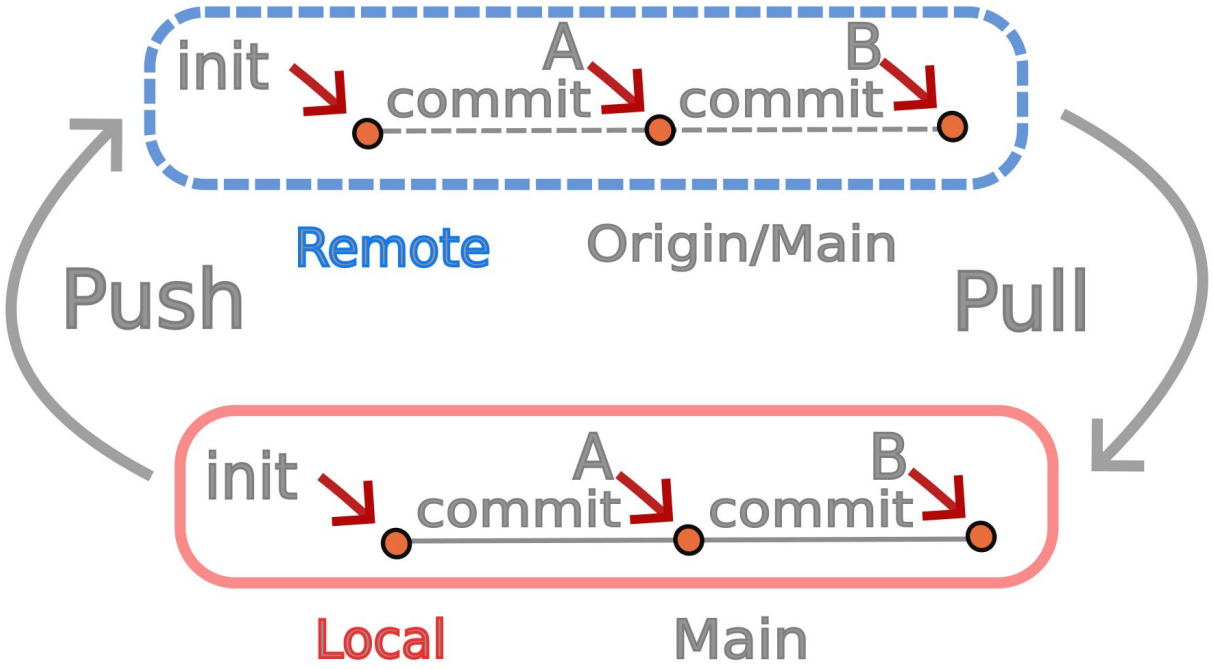
Git designed to track changes in files (by Linus Torvalds in 2005).

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.

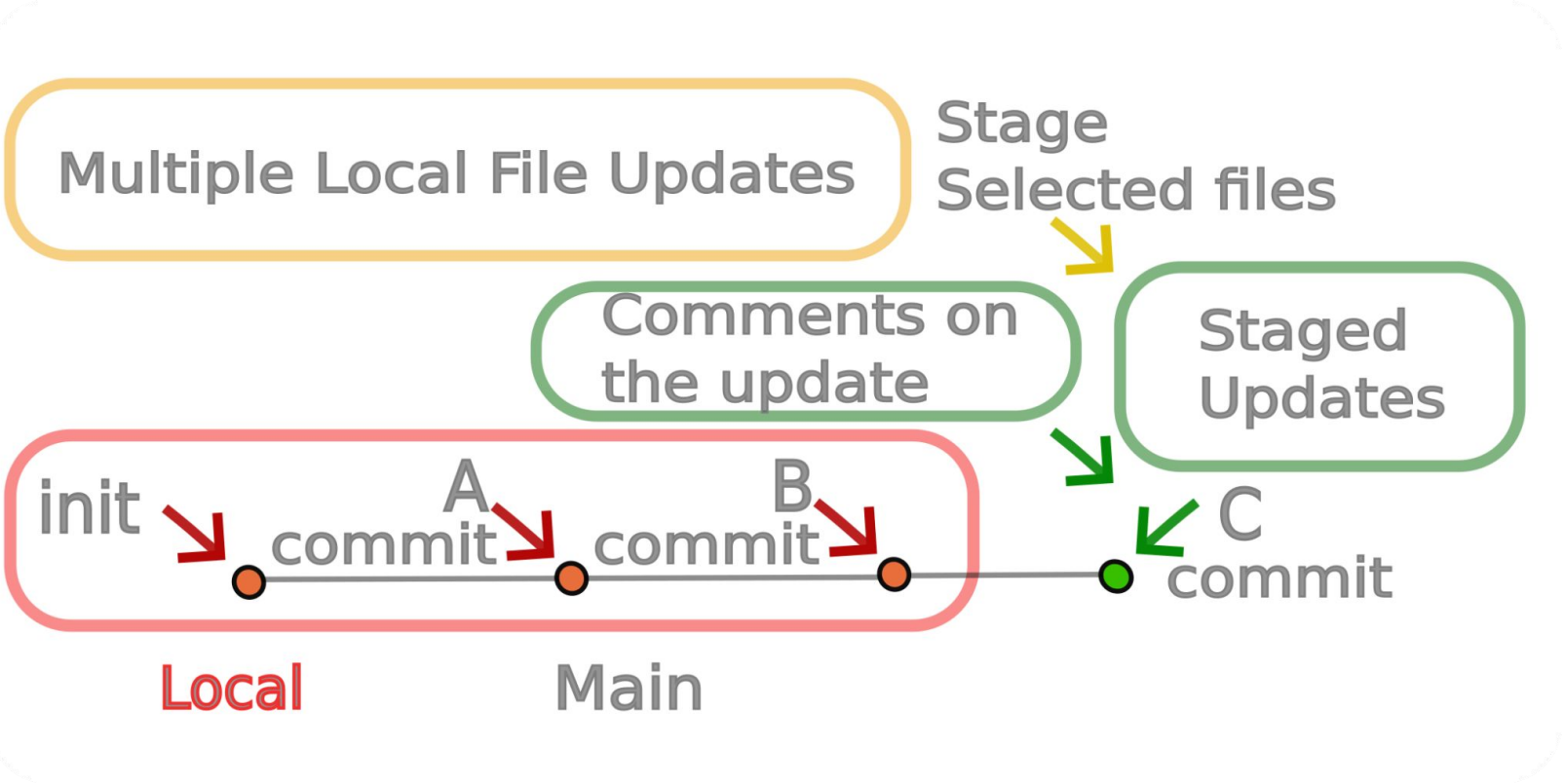
Version Tracking: tracks changes to files and allows developers to view the history of modifications, revert to previous versions, or compare differences between versions.

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

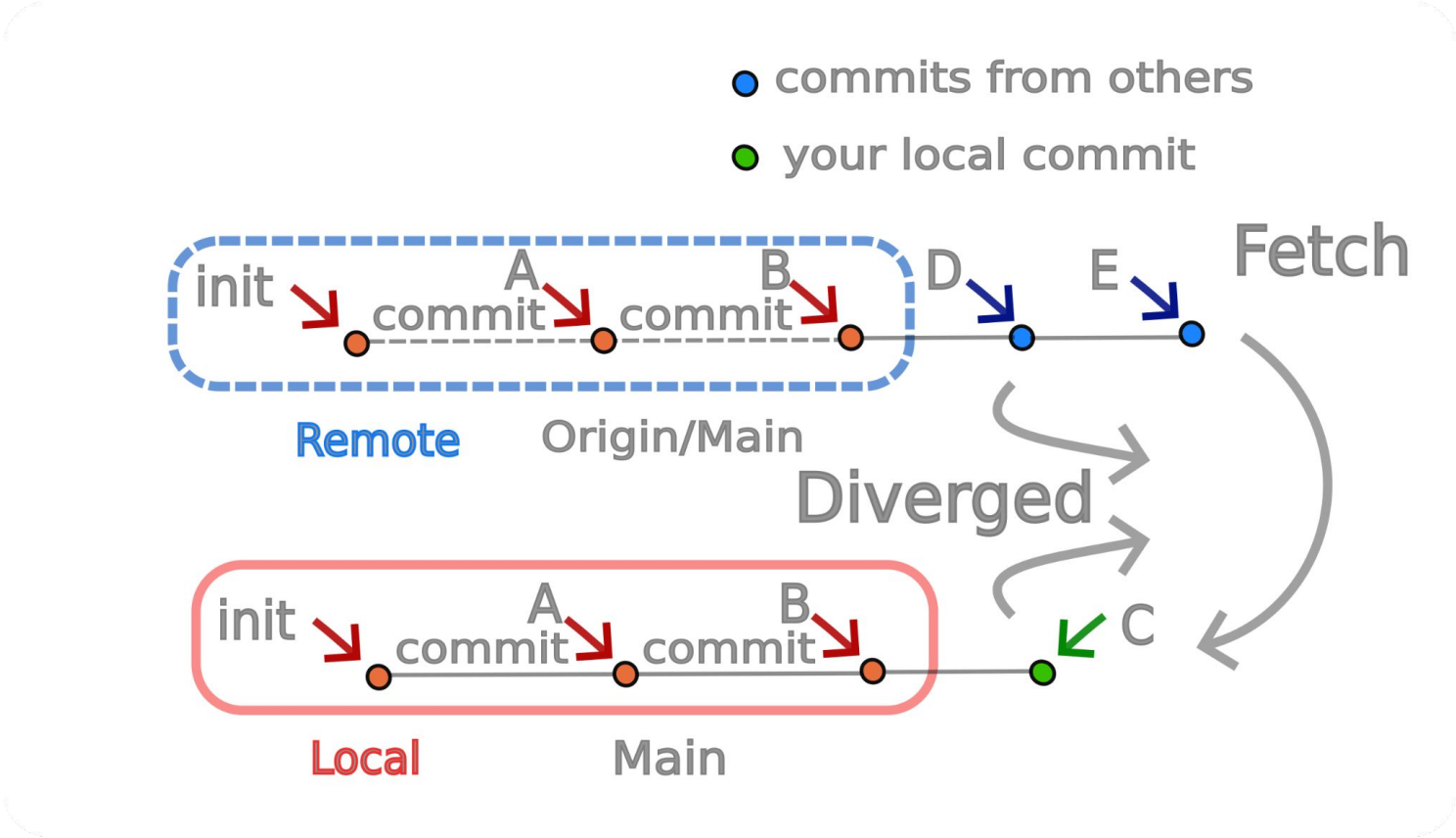
Git: Push and Pull



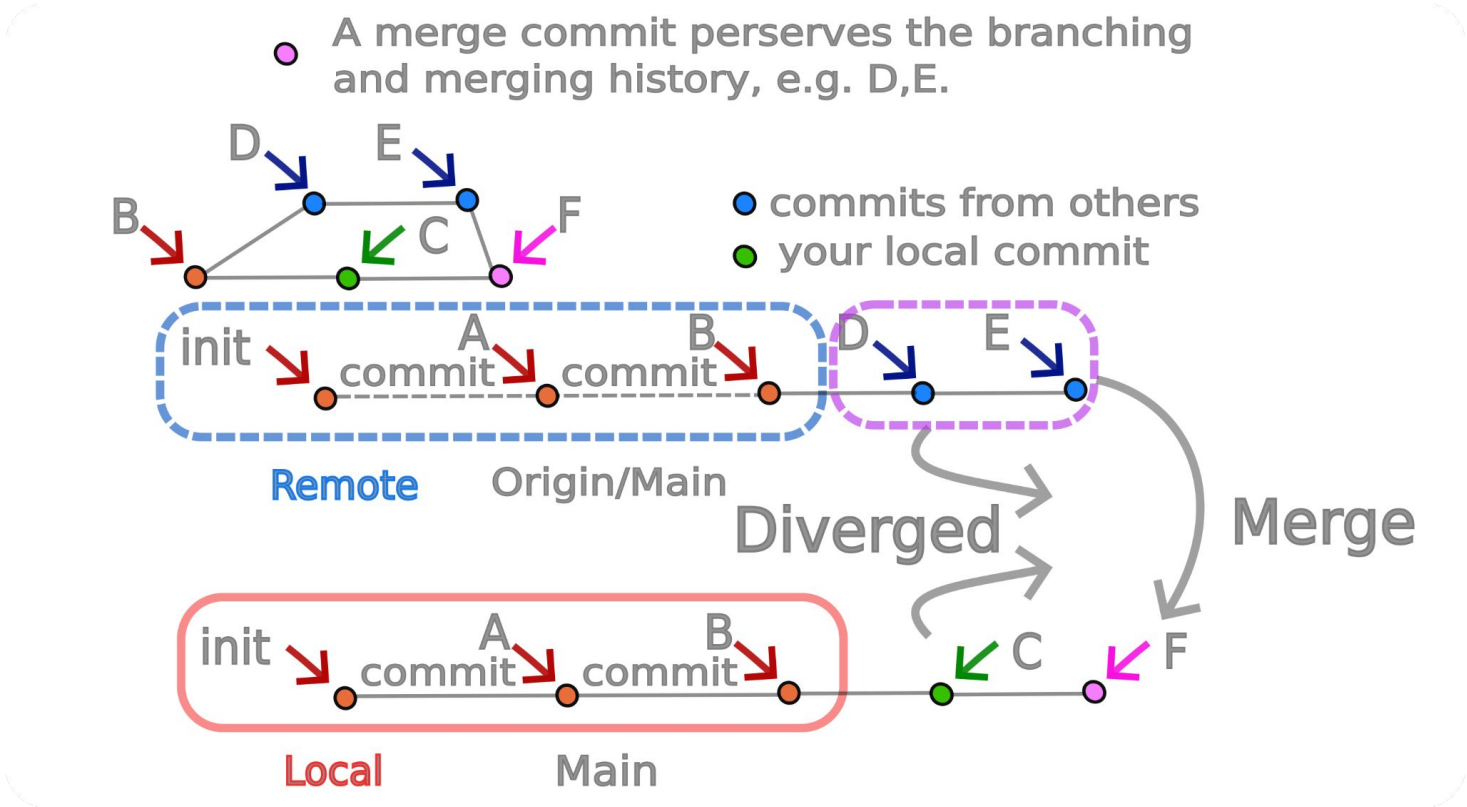
Git: Commit


Multiple Local File Updates
Stage
Selected files
Comments on
the update
Staged
Updates
init
A
commit
B
commit
C
commit
Local
Main

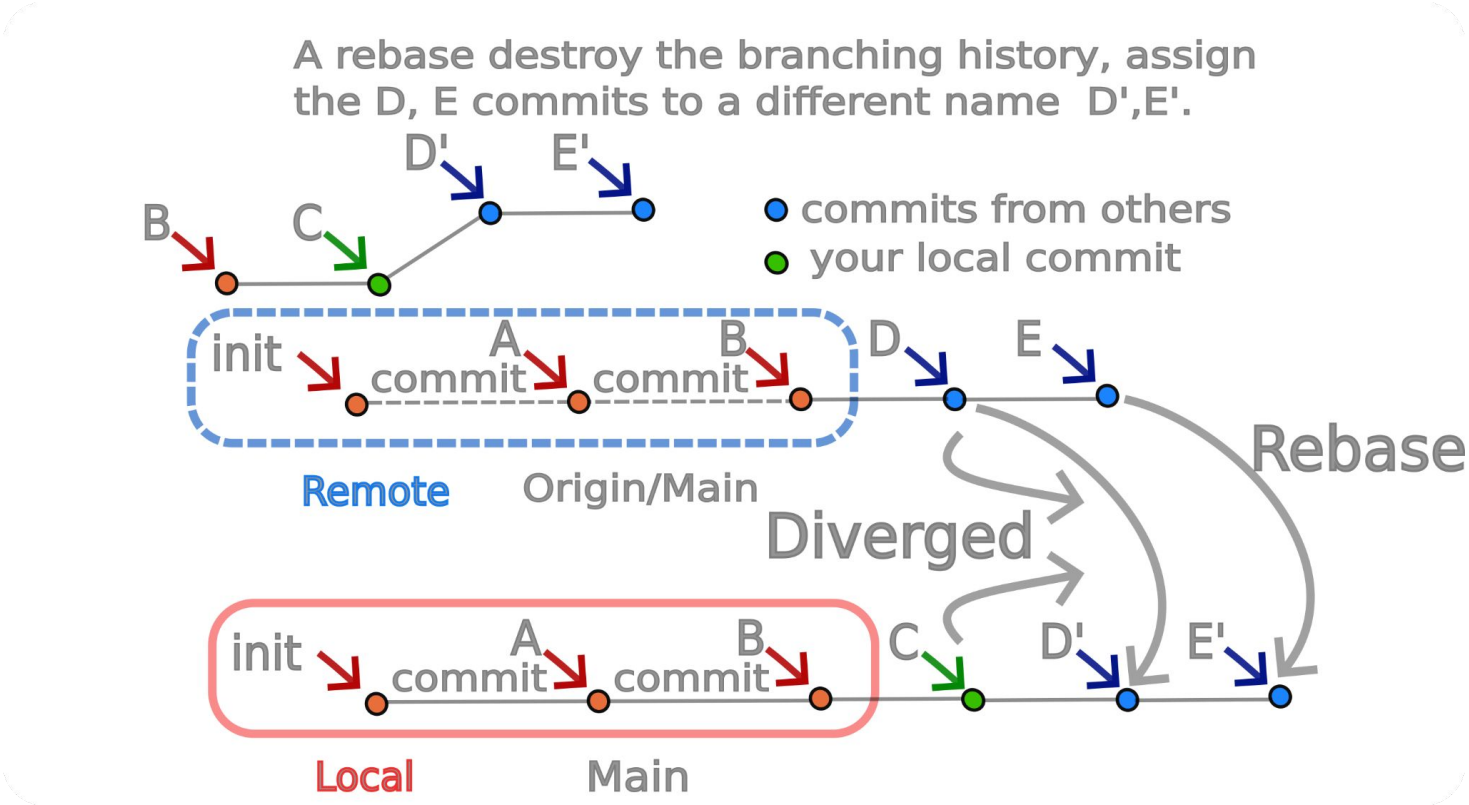
Git: Fetch


commits from others
your local commit
init
A
commit
B
commit
D
E
Fetch
Remote
Origin/Main
Diverged
init
A
commit
B
commit
C
Local
Main

Git: Merge

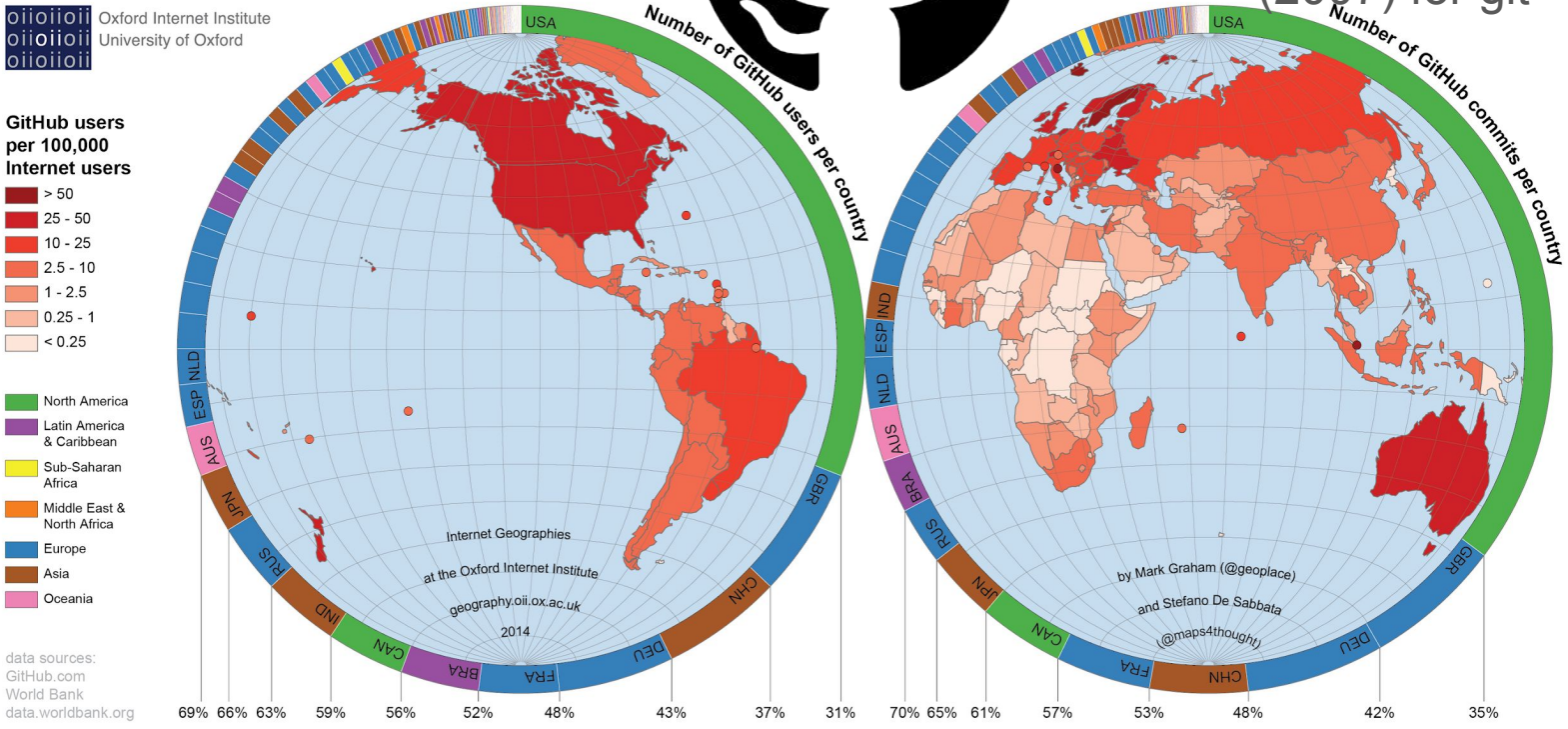

A merge commit perserves the branching and merging history, e.g. D,E.
D
E
B
C
F
commits from others
your local commit
init
A
commit
B
commit
D
E
Remote
Origin/Main
Diverged
Merge
init
A
commit
B
commit
C
F
Local
Main

Git: Rebase


A rebase destroy the branching history, assign the D, E commits to a different name D',E'.
D'
E'
B
C
commits from others
your local commit
init
A
commit
B
commit
D
E
Rebase
Remote
Origin/Main
Diverged
init
A
commit
B
commit
C
D'
E'
Local
Main

Github

Github is a remote repository destination (2007) for git



GitHub | Mapping collaborative software

Docker

Containerization (Created in 2013).

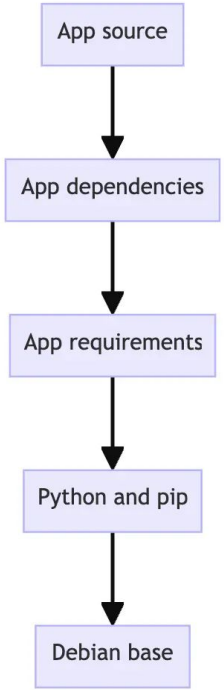
Individual Environment on Demand: Lightweight, portable, and isolated environments

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.