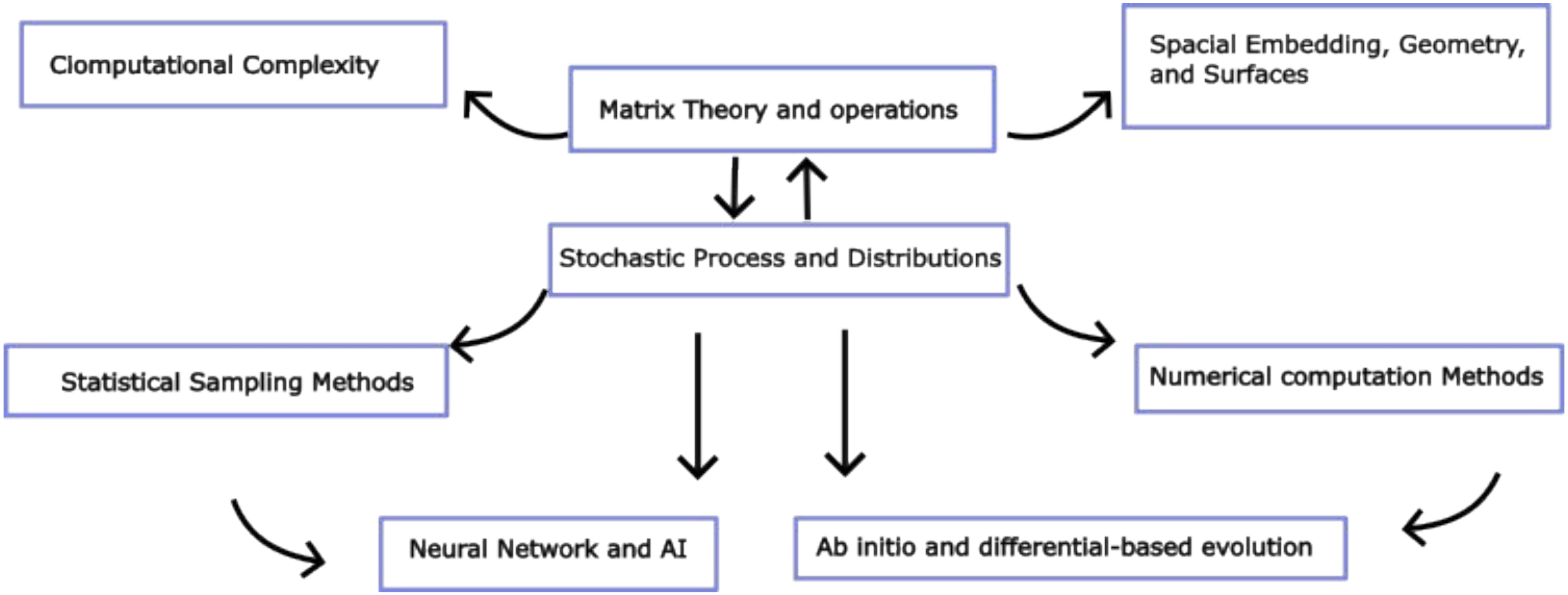
Introduction to Computational Physics

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

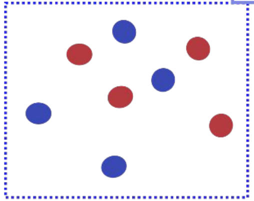
Scope in Physics

Classical Mechanics: individual particles
State Representation: deterministic observable
State Space: phase space
Trajectories: Euler-Lagrange equation

First Quantization: quantization of discrete phase space
State Representation: Wavefunction
State Space: Hilbert Space
Trajectories: Schrödinger equation

Fixed Particle Number

Vary Particle Number



Manybody System

Fixed Particle Number

Spin statistics

Vary Particle Number

Classical fields: particle density
State Representation: deterministic fields
State Space: phase space
Trajectories: Stationary action

Second Quantization: quantization of light/matter fields
State Representation: Fock States
State Space: Fock Space
Trajectories: Path integral

(Non)-equilibrium Statistical Mechanics
Dynamical (stationary) fields: particle density or density matrix
State Representation: distribution of fields
State Space: continous phase space or Fock space
Trajectories: Classical/Quantum master equation

Syllabus

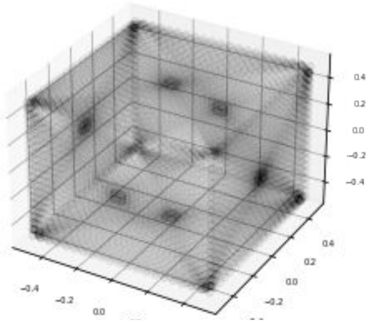
- **Basics in Differential Geometry** matrix, tensors, metric, dual space, generalized coordinate transformation, vector, covector, covariant derivative, parallel transport, geodesic, surface derivatives, first/second fundamental forms, intrinsic/extrinsic curvatures.

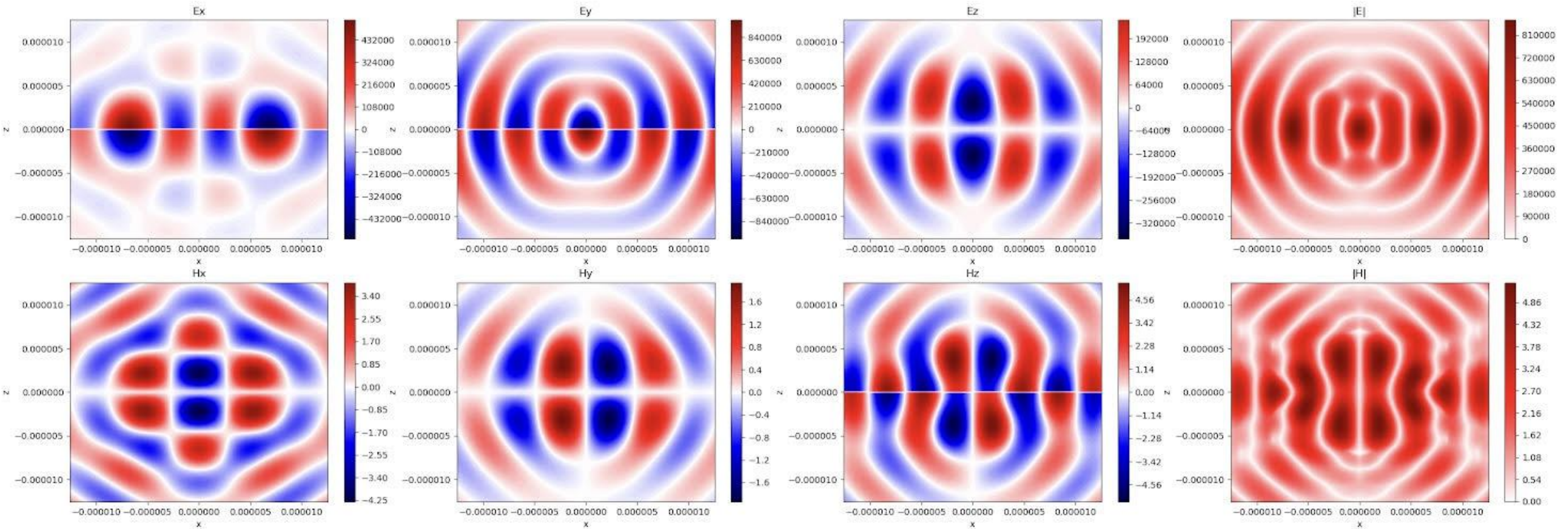
- **Basics in Matrix Theory** Gaussian and Gauss-Jacobi elimination, backsubstitution, pivoting, LU decomposition, Cholesky decomposition, QR decomposition, sparse matrix linear algebra, QR decomposition and tridiagonal forms, diagonalization of a symmetric and non-symmetric matrix, principal axes and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

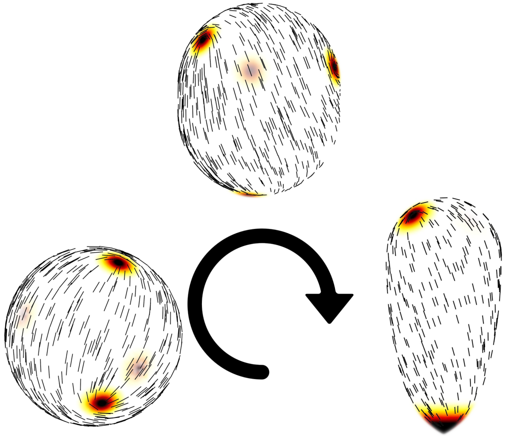
Electric/Magnetic Field Strength, scattering amplitude on 3D mesh

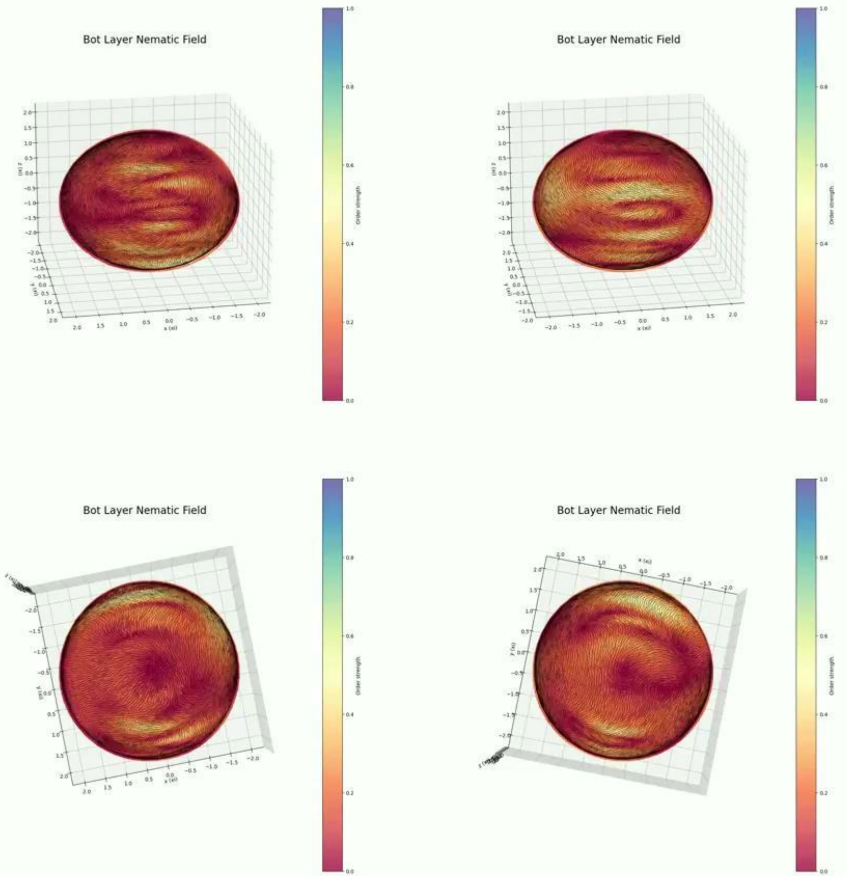




Syllabus

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

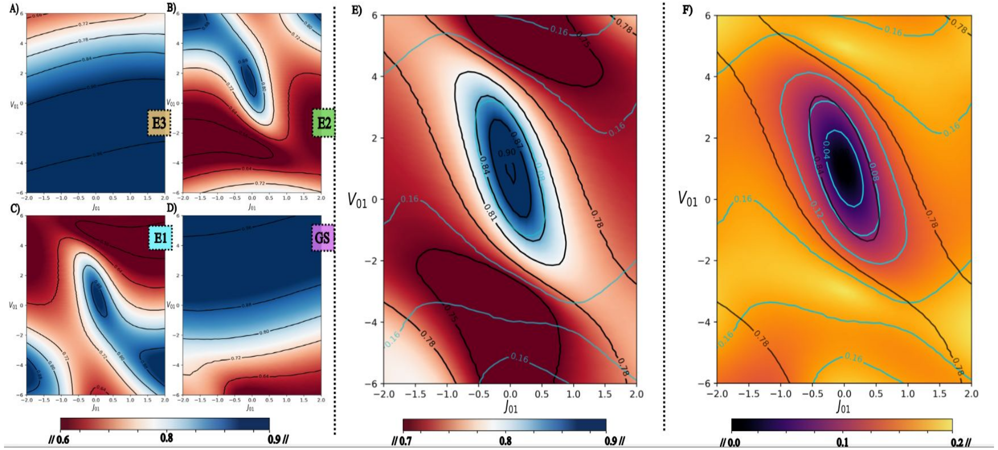




Syllabus

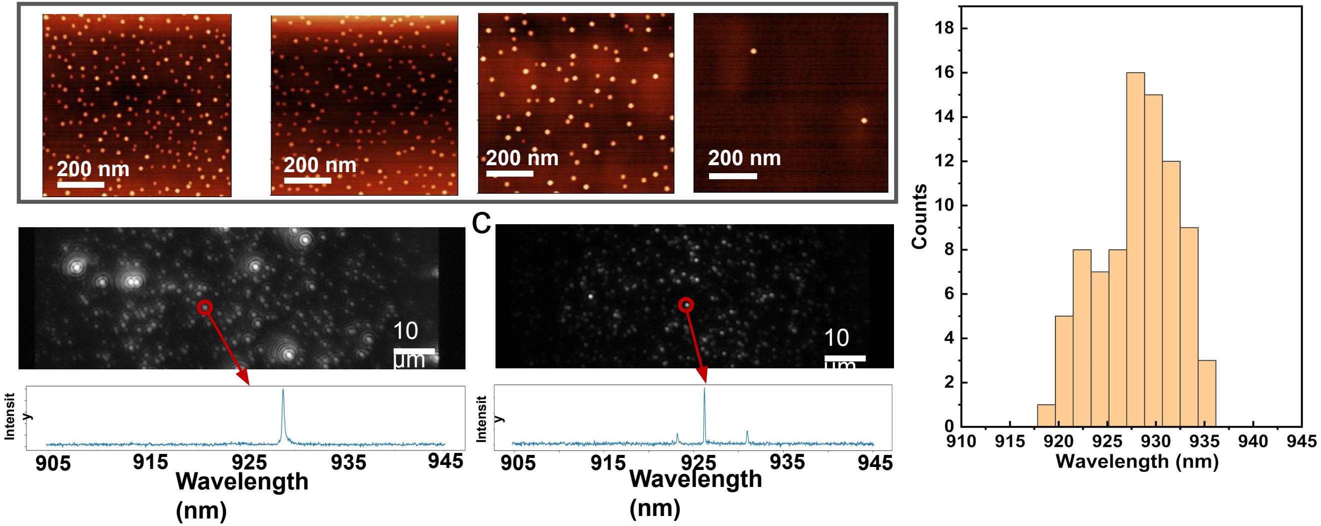
- **Common stochastic processes and statistical distributions in physics**, Concepts in probability and distributions, Bayesian inference and Frequentist statistics. random walk, Markov chain, geometric distribution, central limit theorem, Bernoulli process, binomial process, Poisson process, Lorentz (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

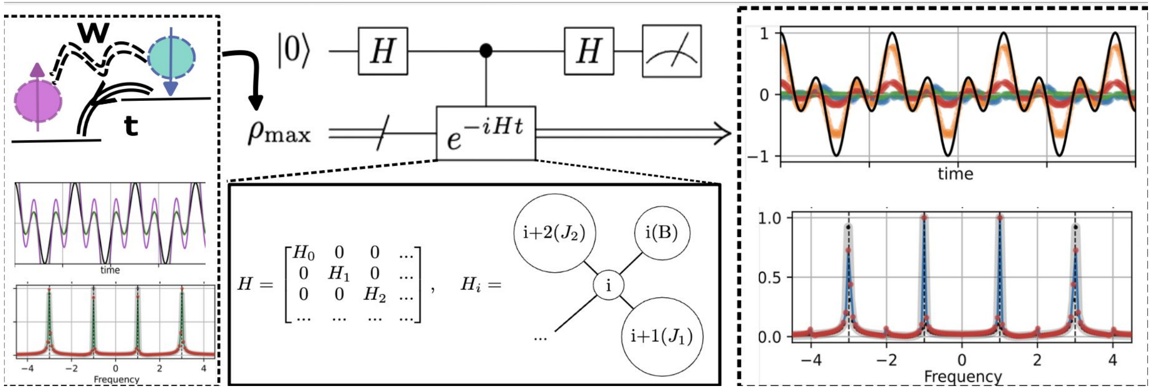


Syllabus

- **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.

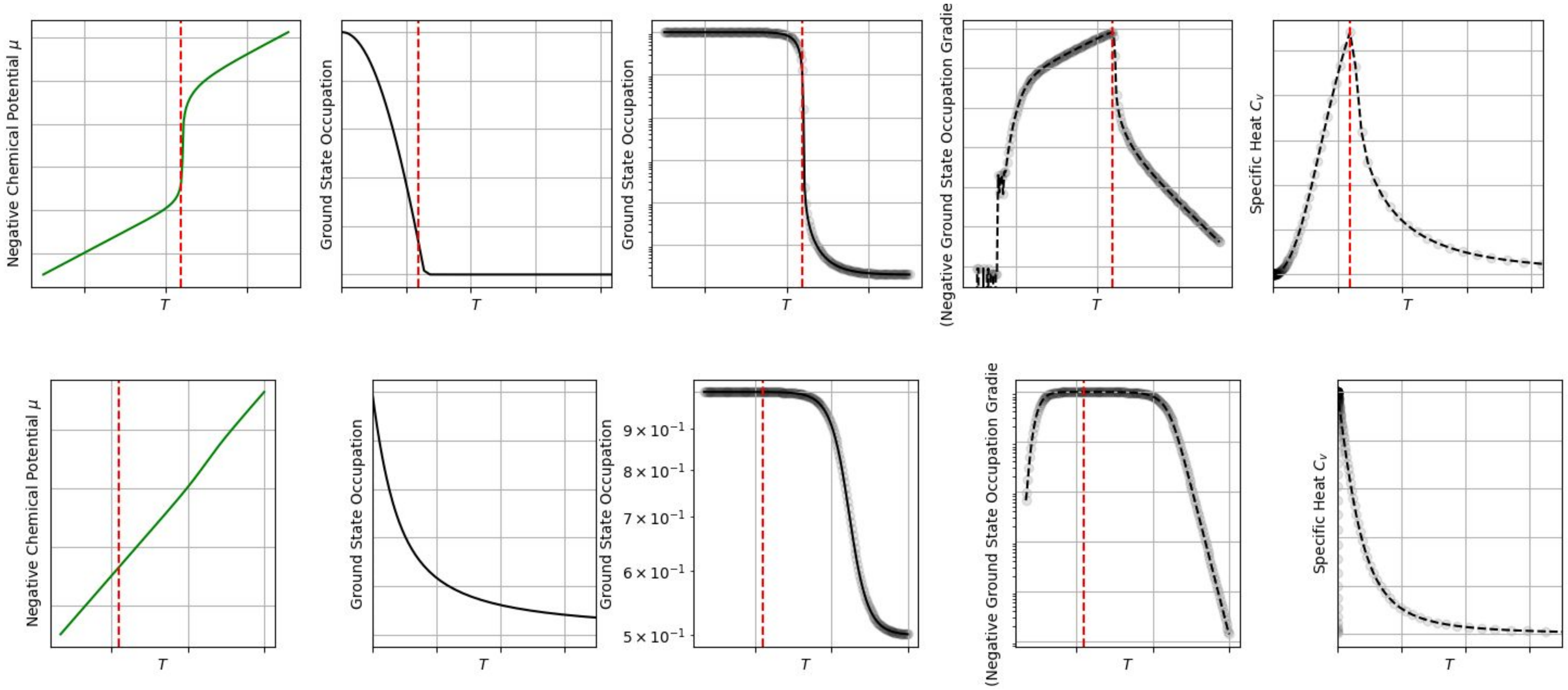
- **Common computation techniques in physics**, discrete Fourier transform, numerical integration and differentiation, Gaussian quadrature, orthogonal (Legendre) polynomials, implicit and explicit iterative methods for differential equations, Runge–Kutta methods, Leapfrog, symplectic integrator, (stochastic)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

State evolution on a quantum computer



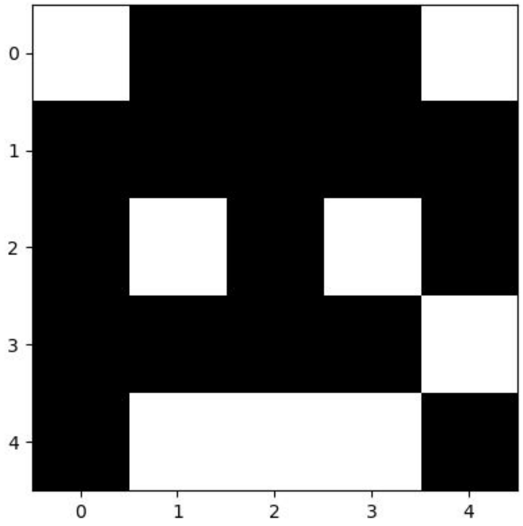
Syllabus

Quantum Phase transitions (bose einstein condensate)



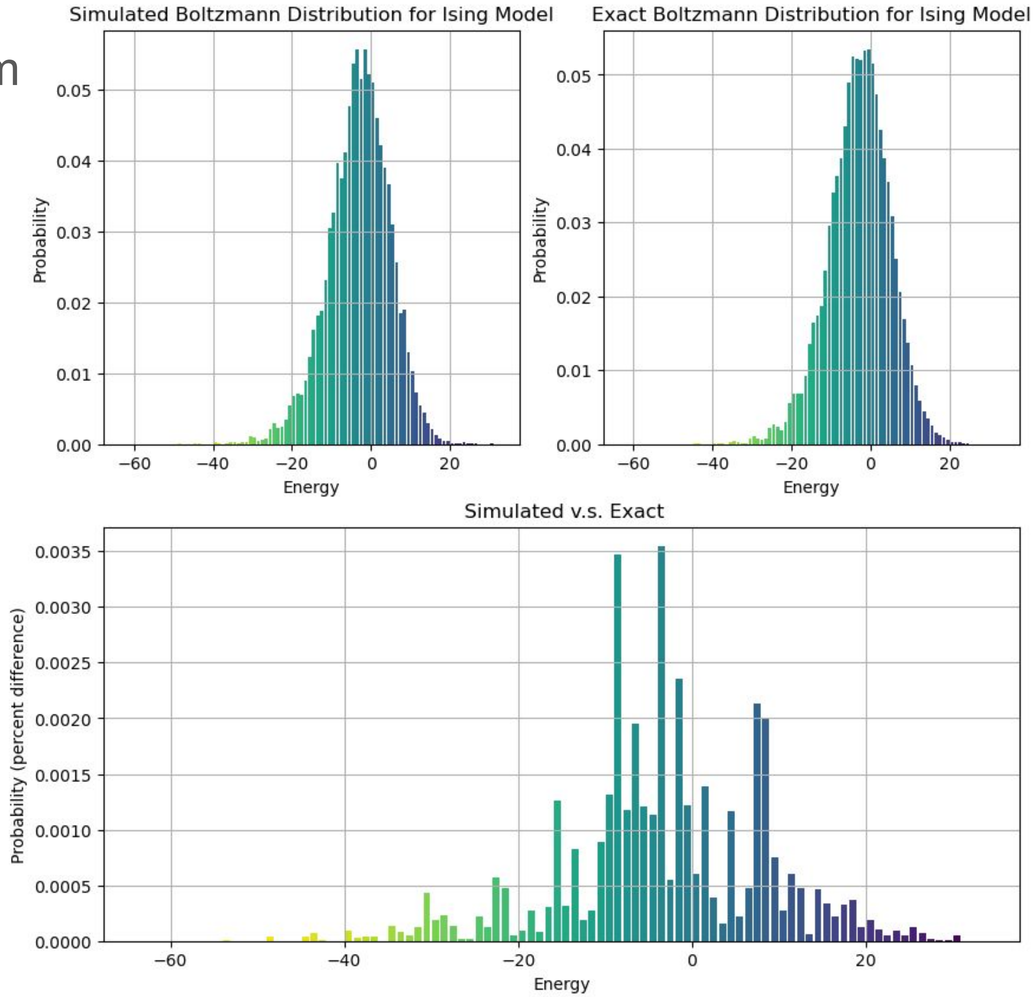
Syllabus

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



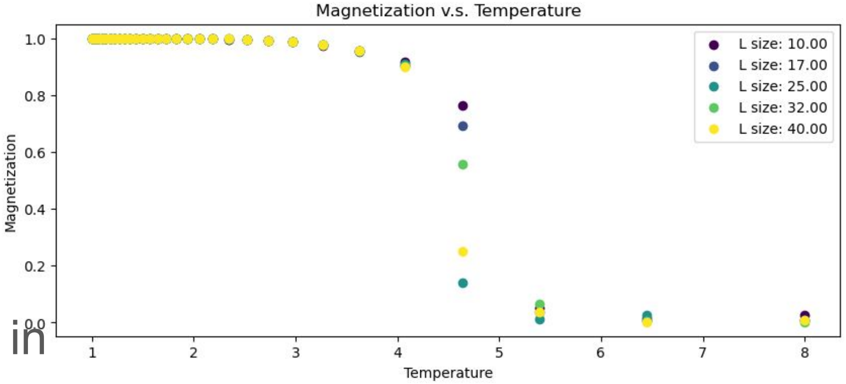
Exact Elapsed Time: 1260.5645 seconds

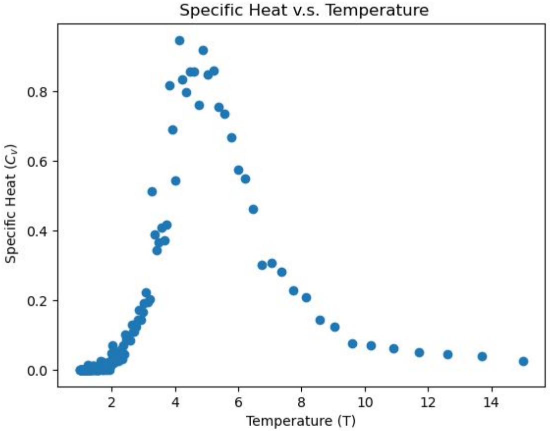
MC Elapsed Time: 4.4076 seconds

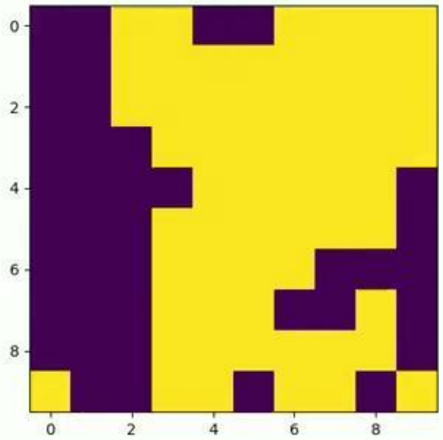


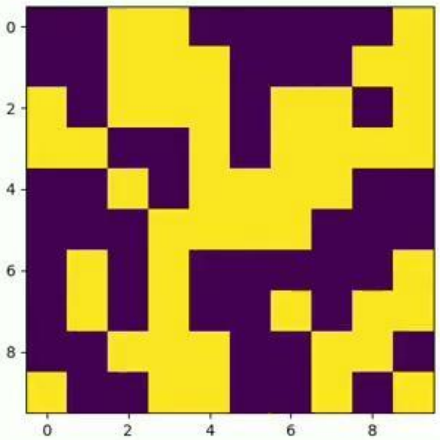
Syllabus

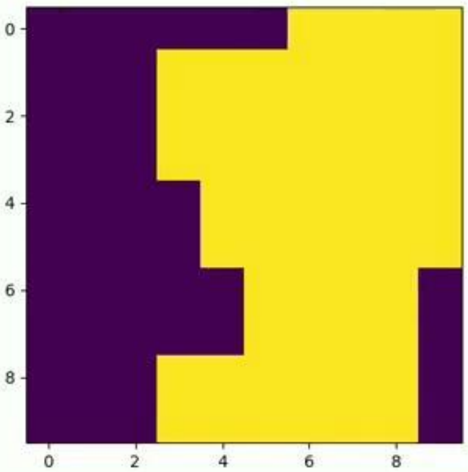
Order parameter in Phase transitions



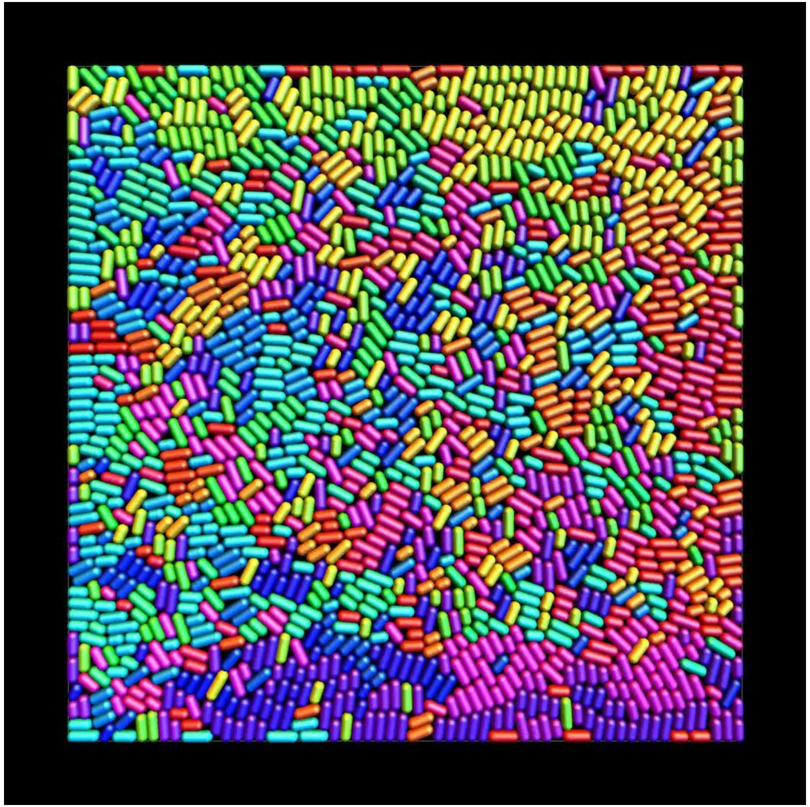


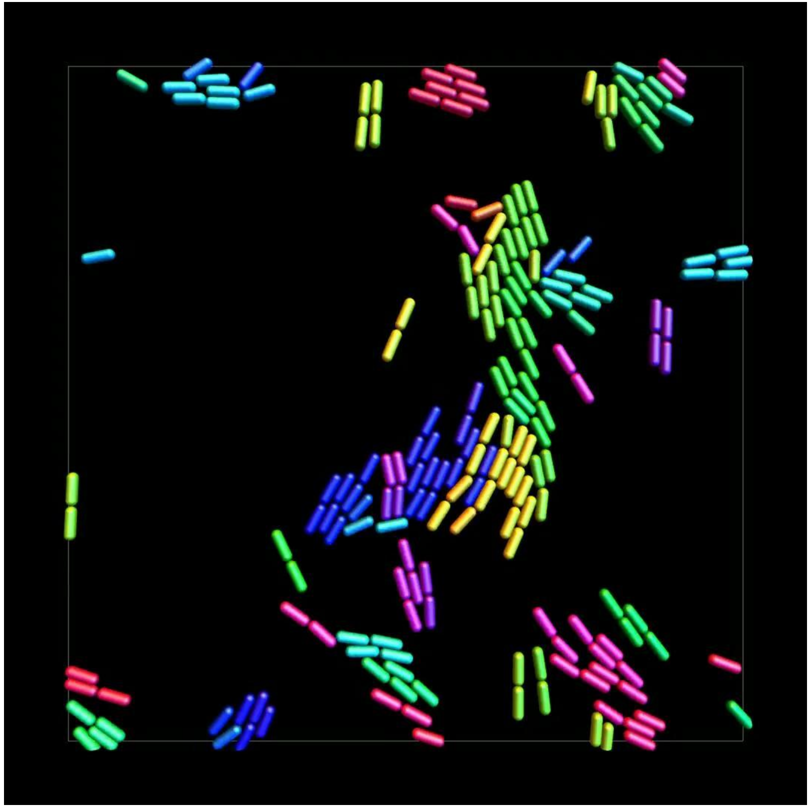






Syllabus Molecular Dynamics that generates Glassy phase transitions in bacteria

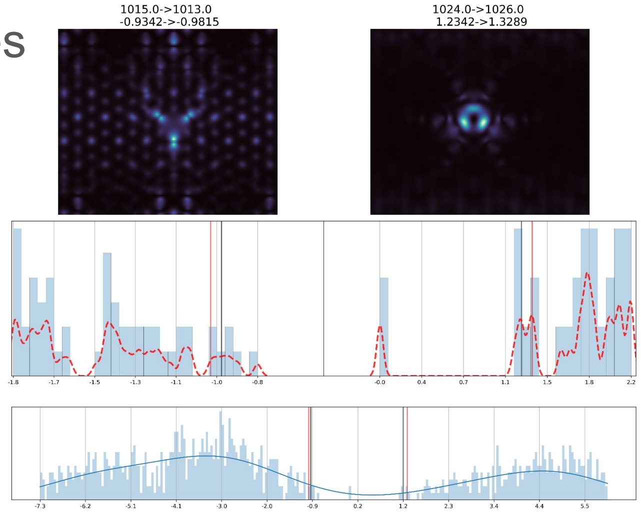




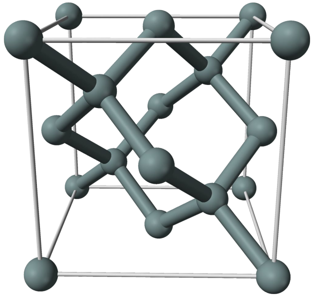
Syllabus

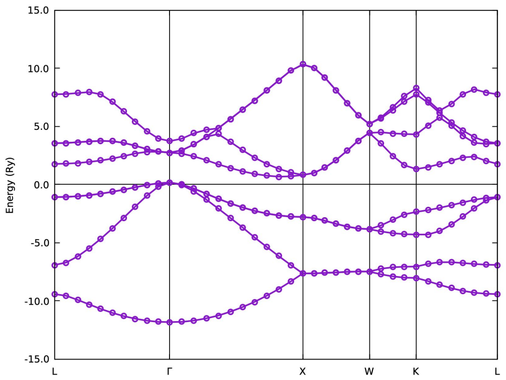
- **Applications in physics**, Electrostatics, Diffusion, Brownian motion, driven system, hydrodynamics, phase transitions, molecular dynamics, *ab initio* approaches to electronic structure, quantum state (density matrix) evolution, surface code, quantum master equation, numerical renormalization group.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

Localized electronic states



Self consistent field calculation for silicon





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)

GPT-4o

2021

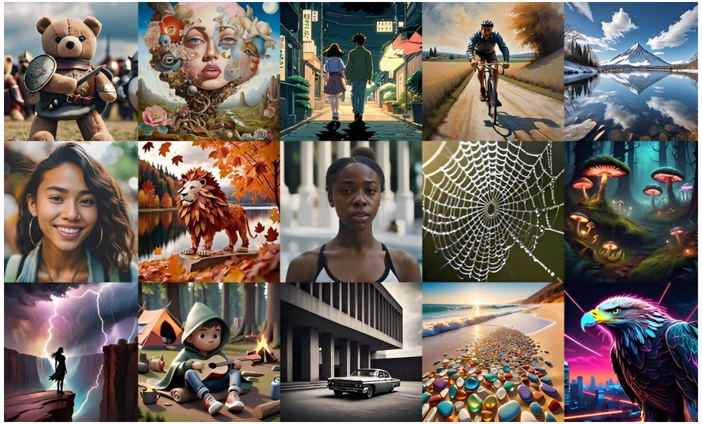
High-Resolution Image Synthesis with Latent Diffusion Models

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

- **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.

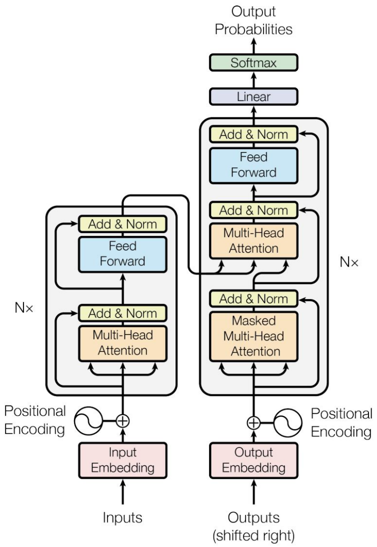


Figure 1: The Transformer - model architecture.

2020

Denoising Diffusion Probabilistic Models

Jonathan Ho
UC Berkeley
jonathanho@berkeley.edu

Ajay Jain
UC Berkeley
ajayj@berkeley.edu

Pieter Abbeel
UC Berkeley
pabbeel@cs.berkeley.edu

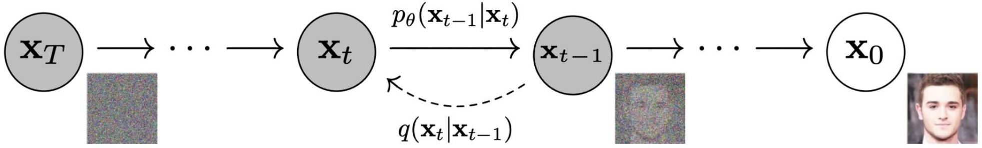


Figure 2: The directed graphical model considered in this work.

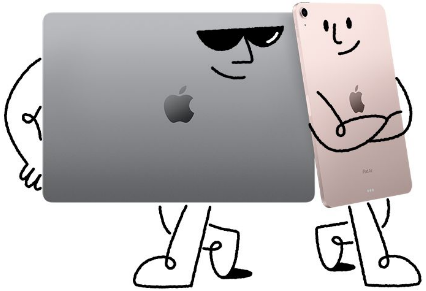
What is happening in a modern computer?

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

- Applications
- Operating System
- BIOS/UEFI
- Hardware

A Supercomputer (HEP)

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



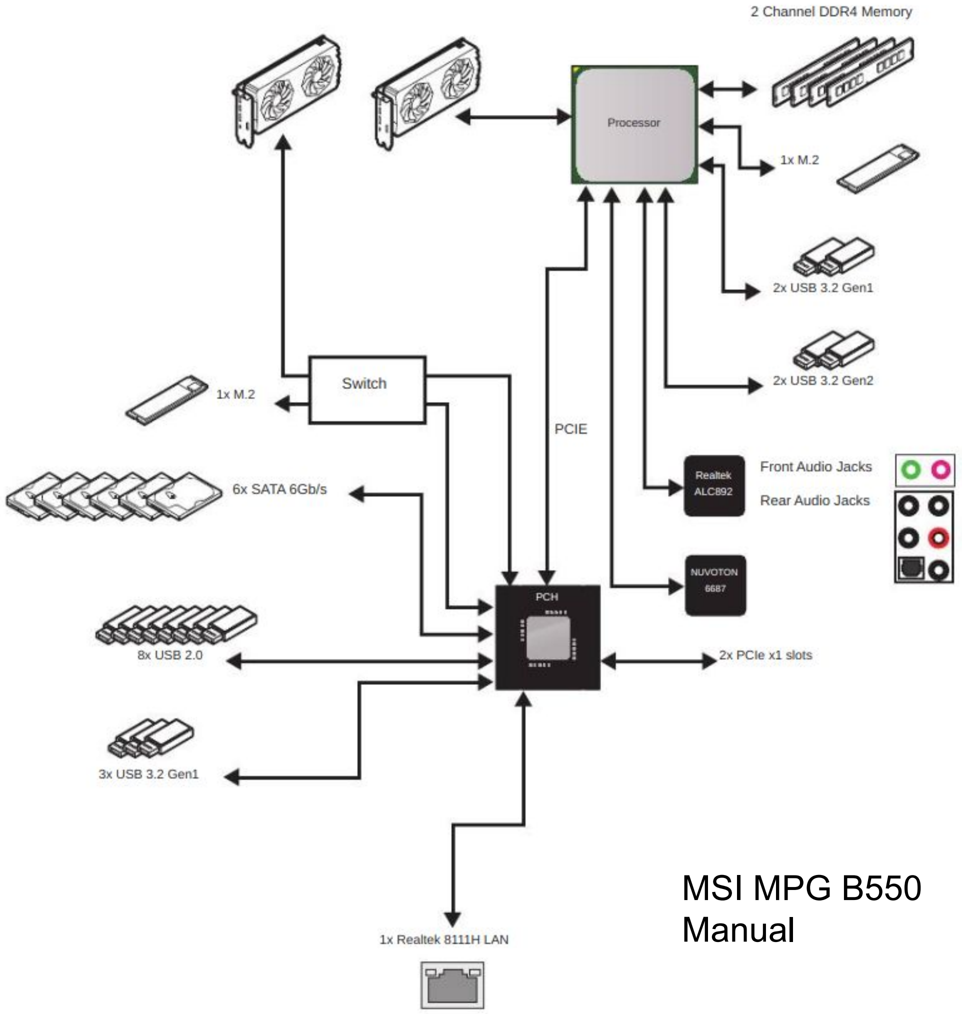
A Laptop

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.

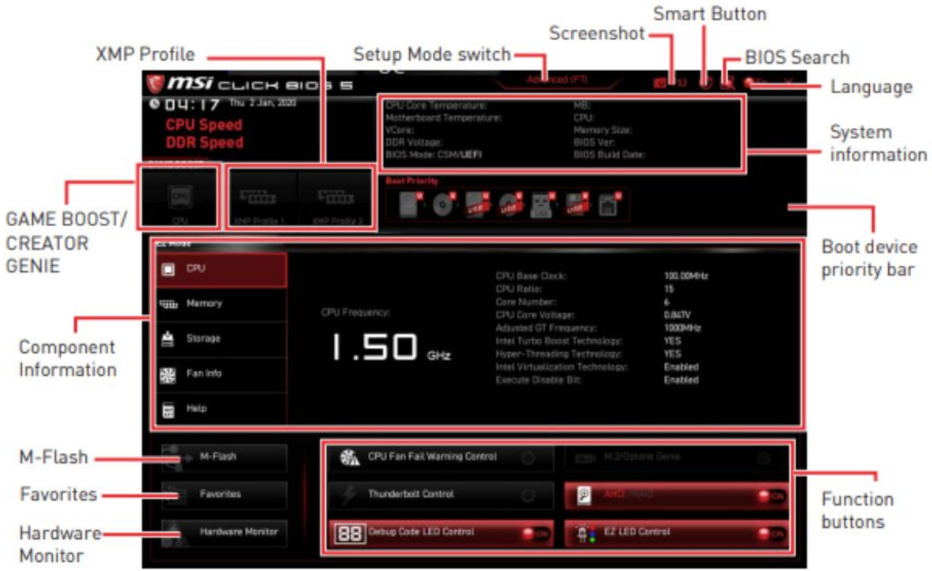


MSI MPG B550 Manual

BIOS/UEFI

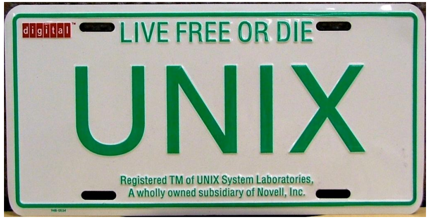
Basic Input/Output System (BIOS) or Unified Extensible Firmware Interface (UEFI) is one example of a firmware that perform low-level control of a hardware, such as booting and interacting with operating system.

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

OSX

MacOS

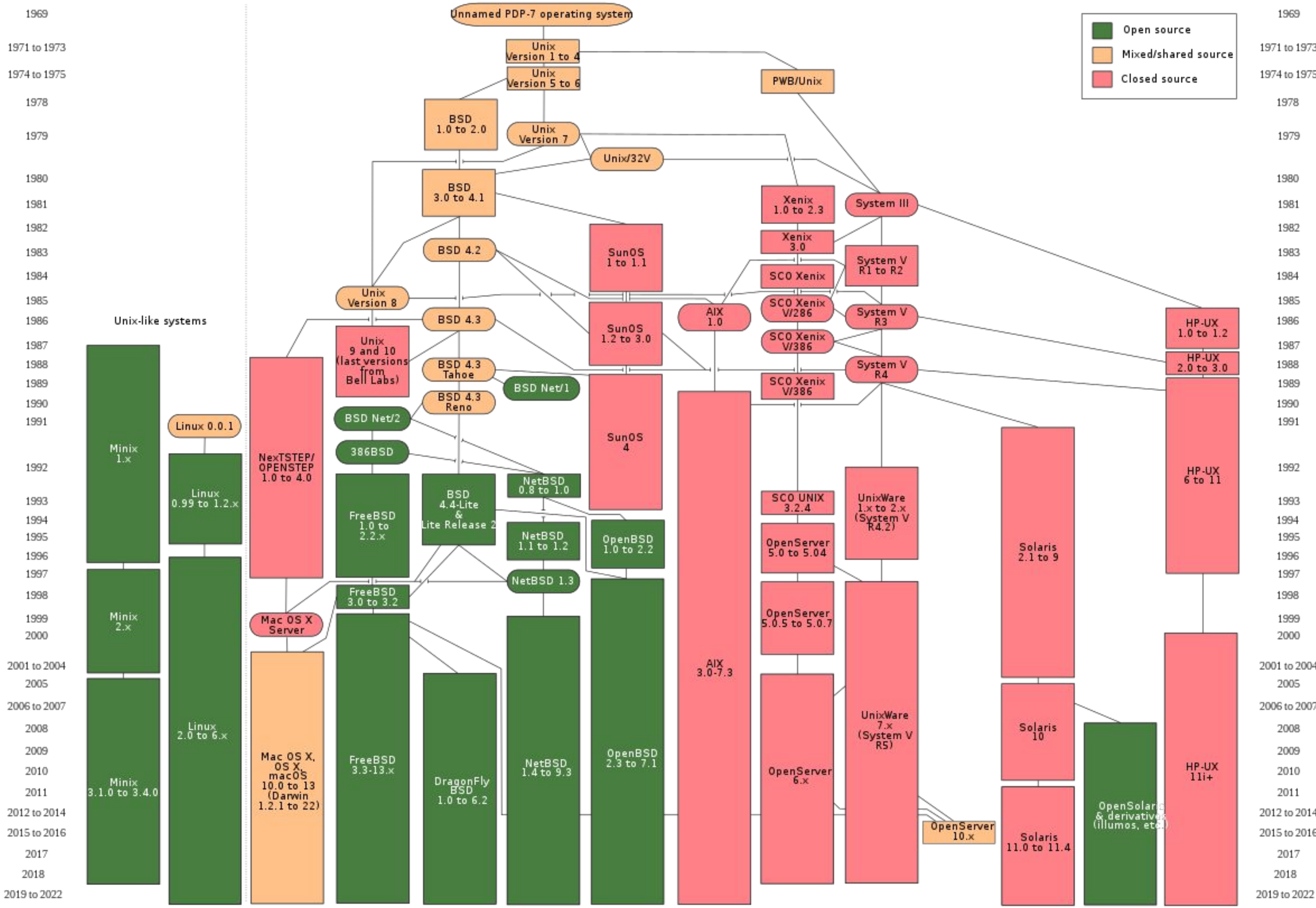
2001

Not this one. At least not directly.

Microsoft Windows

History of UNIX

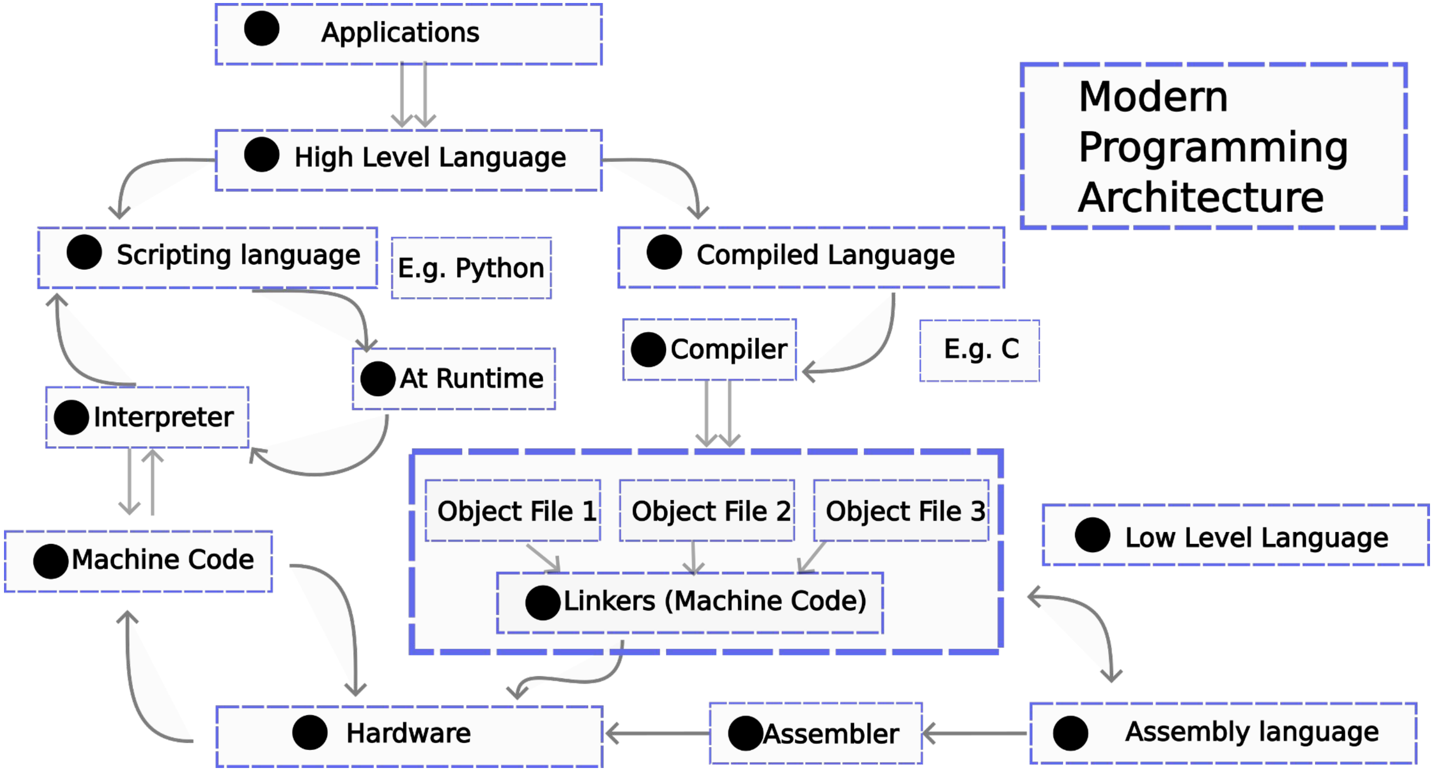
Over the time, people realize the power of open-source systems…



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

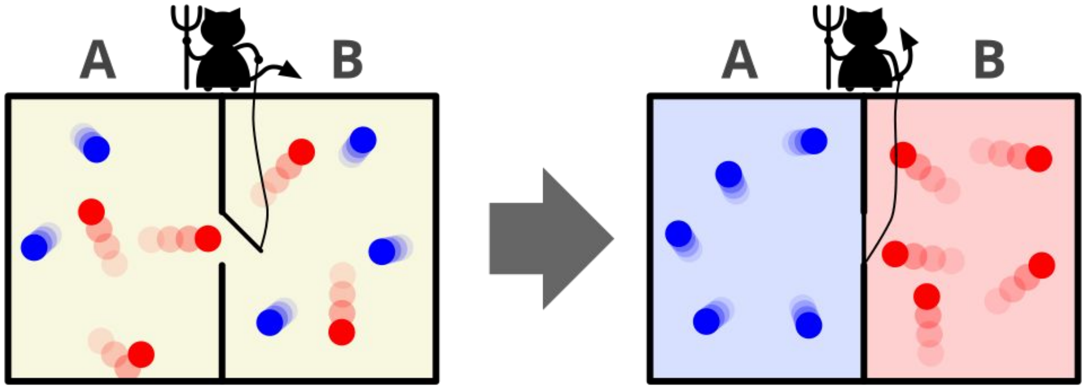
Programming

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.

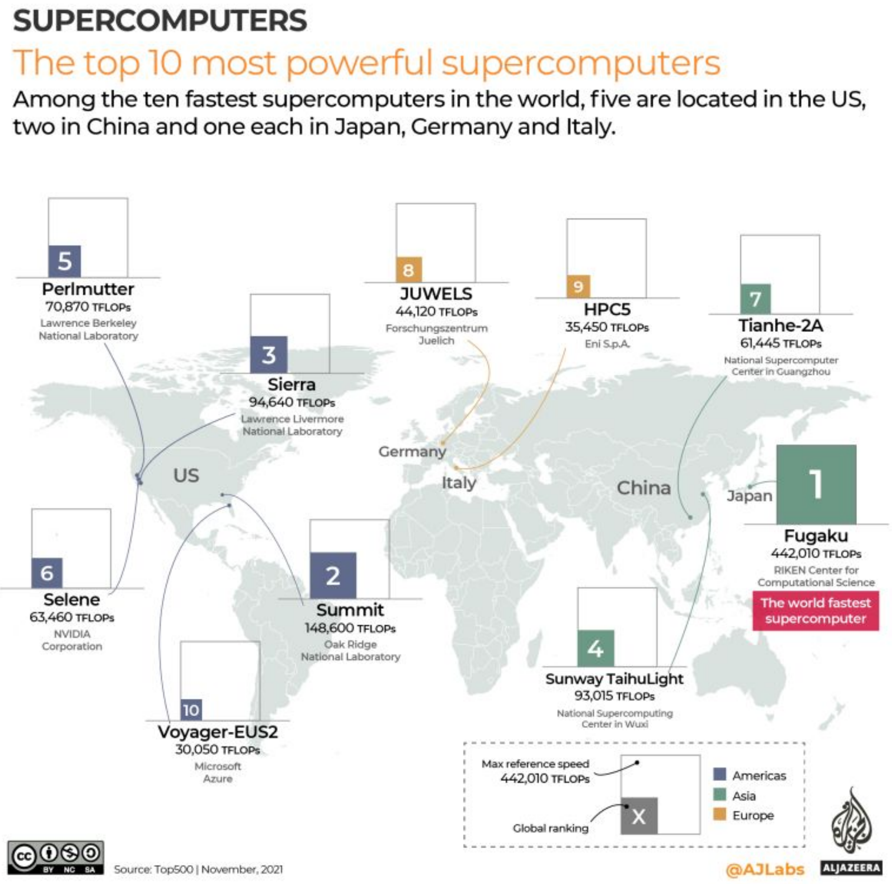


information processing has physical consequences. acquiring, storing, or erasing information generates entropy

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

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

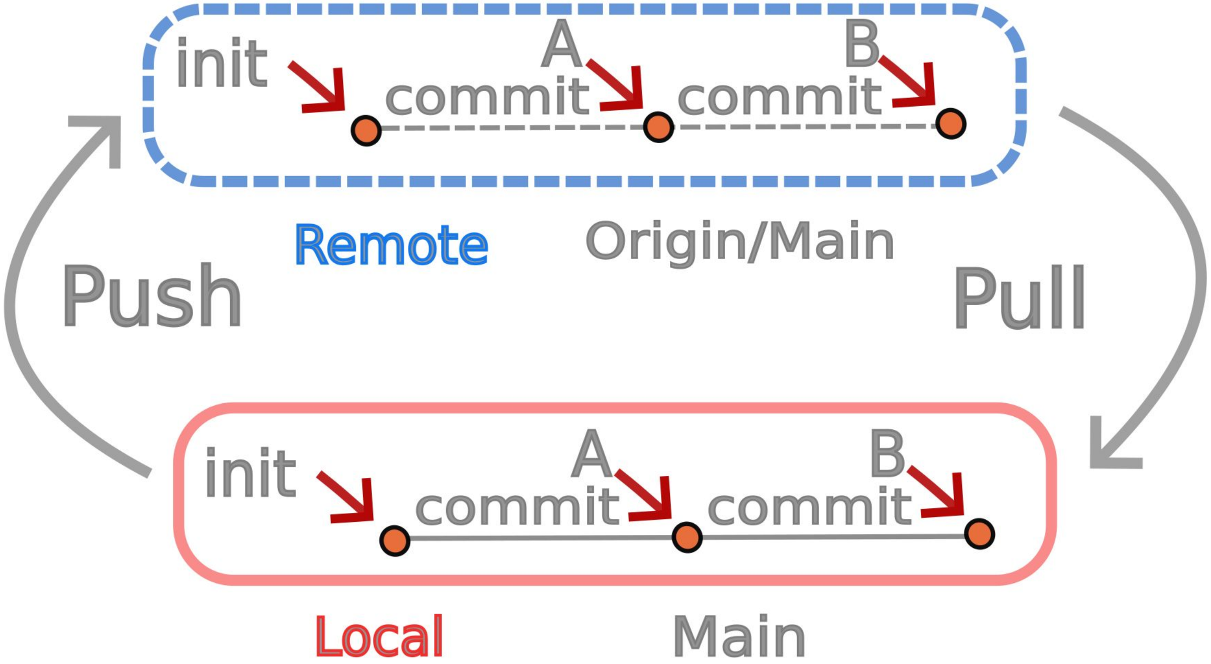
Git designed to track changes in files (by Linus Torvalds in 2005).

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.

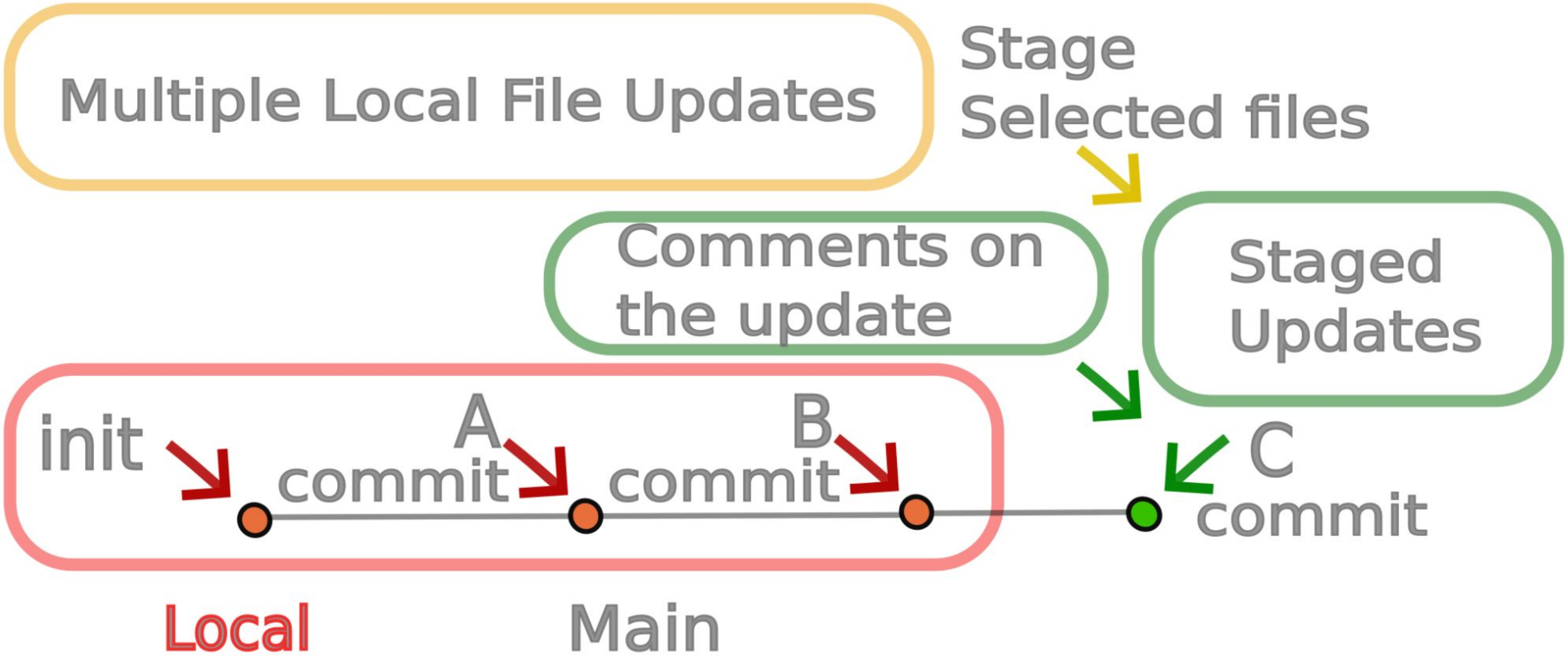
Version Tracking: tracks changes to files and allows developers to view the history of modifications, revert to previous versions, or compare differences between versions.

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

Git: Push and Pull

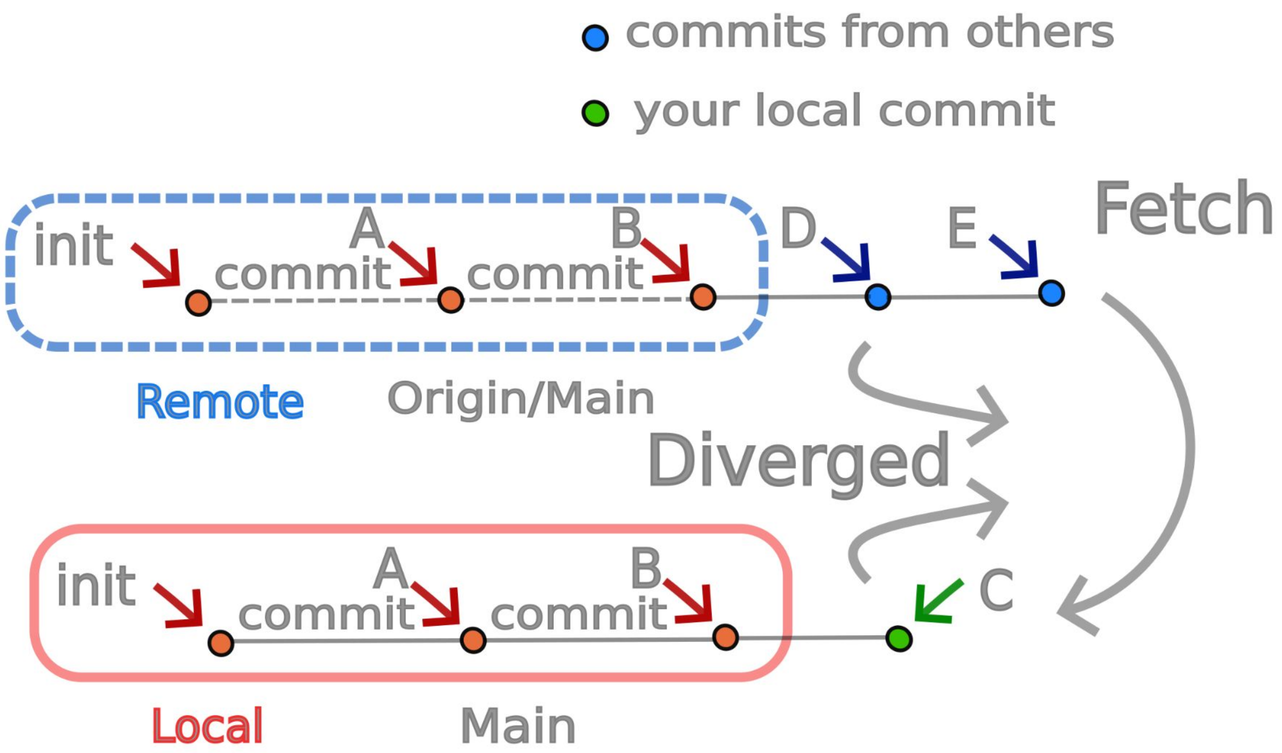


Git: Commit

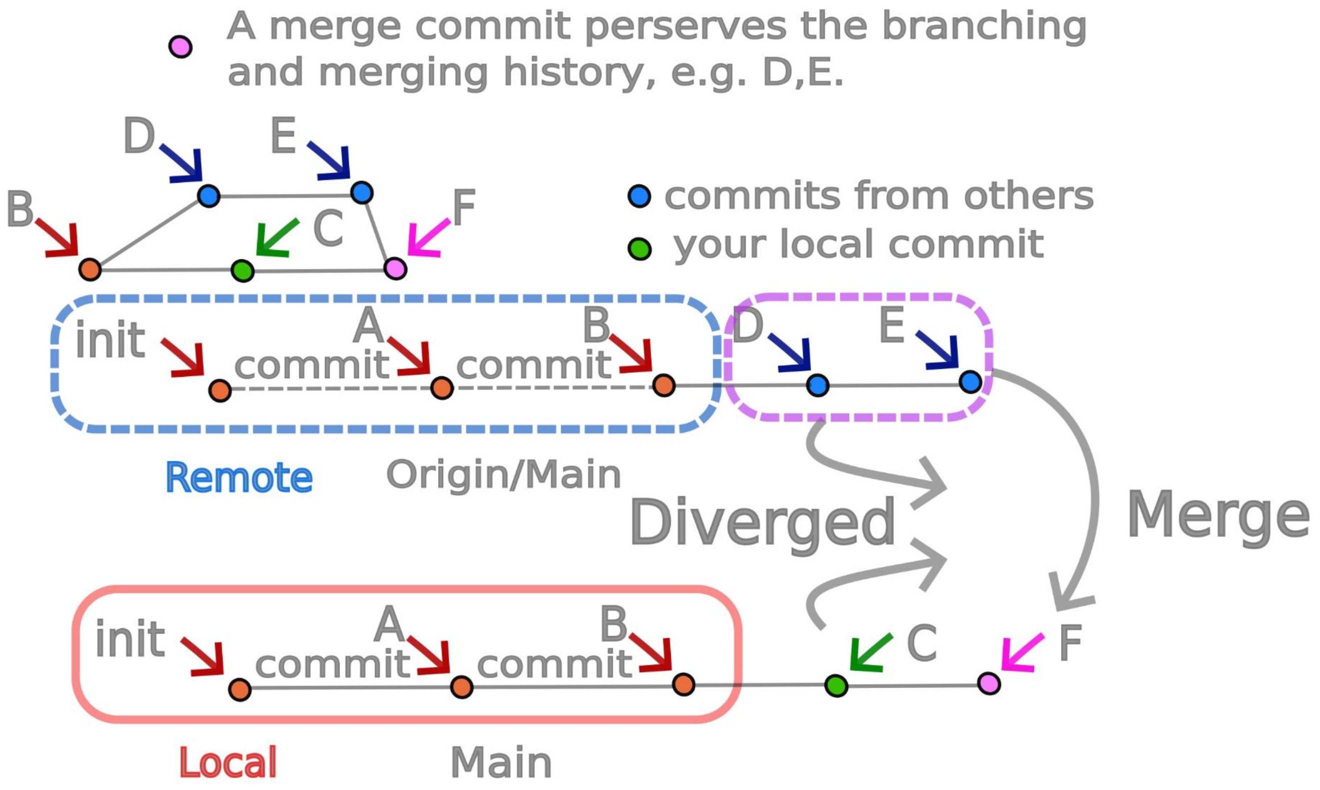


Multiple Local File Updates
Stage
Selected files
Comments on
the update
Staged
Updates
init
A
commit
B
commit
C
commit
Local
Main

Git: Fetch

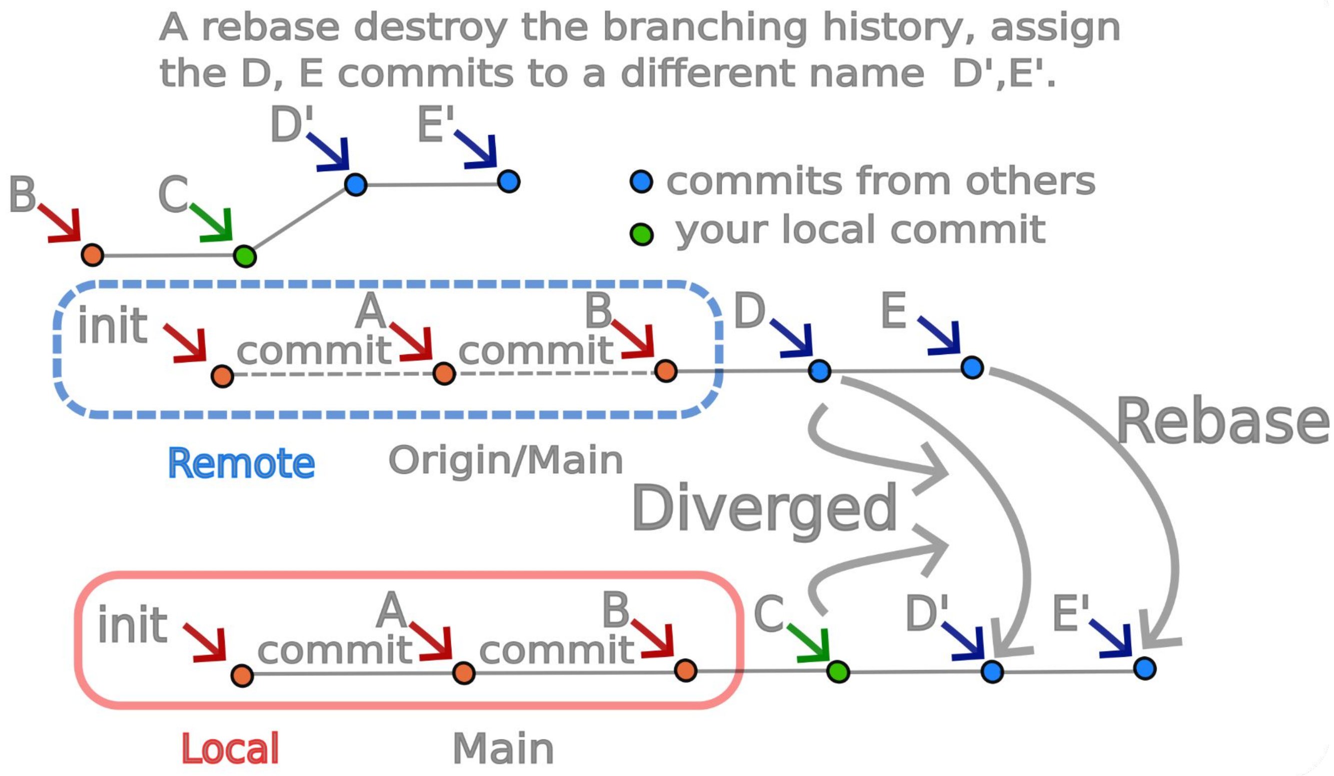

commits from others
your local commit
init
A
commit
B
commit
D
E
Fetch
Remote
Origin/Main
Diverged
init
A
commit
B
commit
C
Local
Main

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

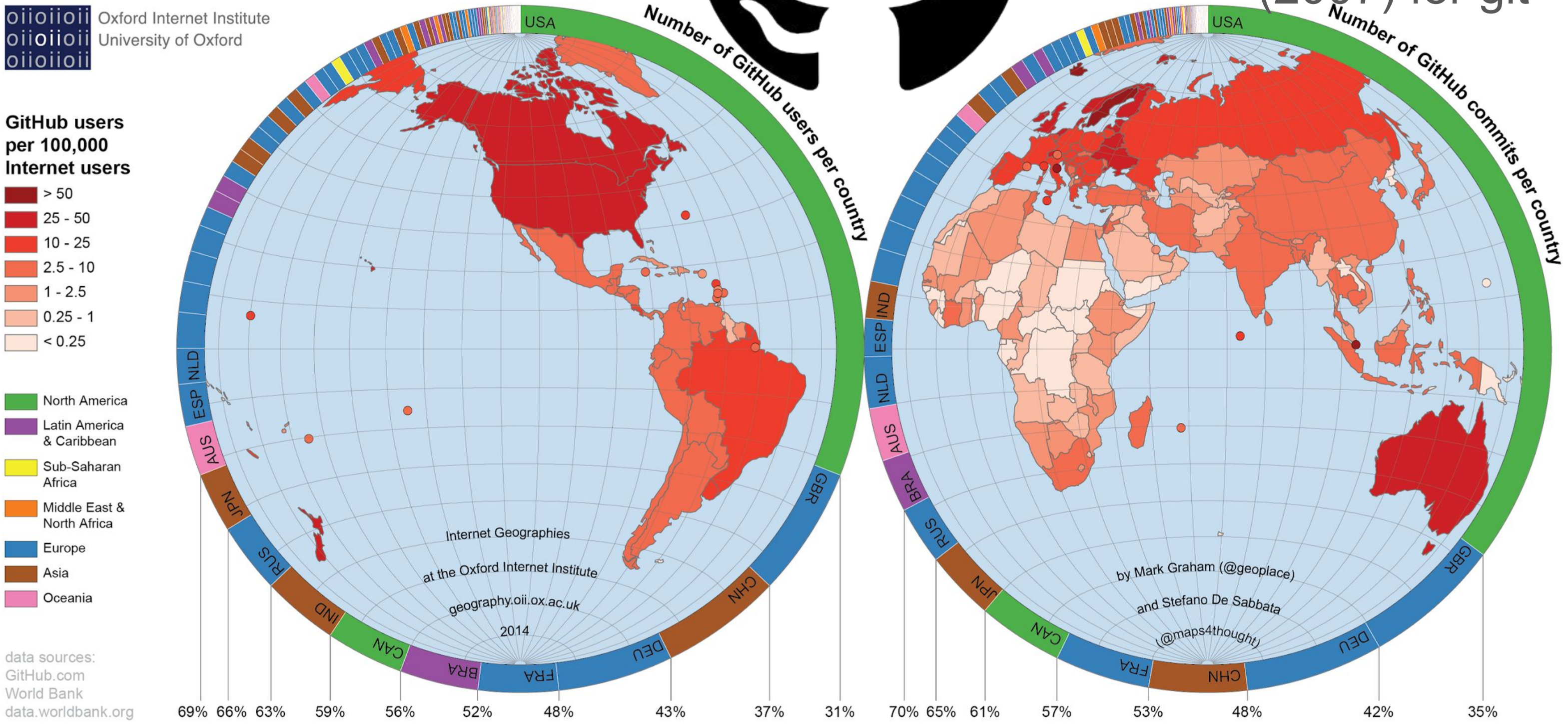
Git: Rebase



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

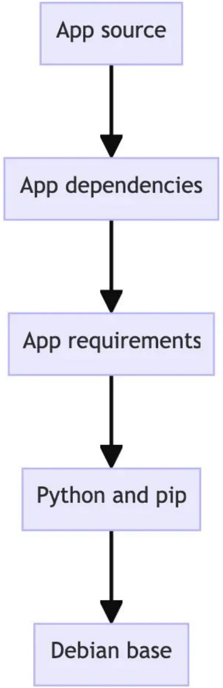
Multitasking: Share the host OS kernel instead of requiring a full OS

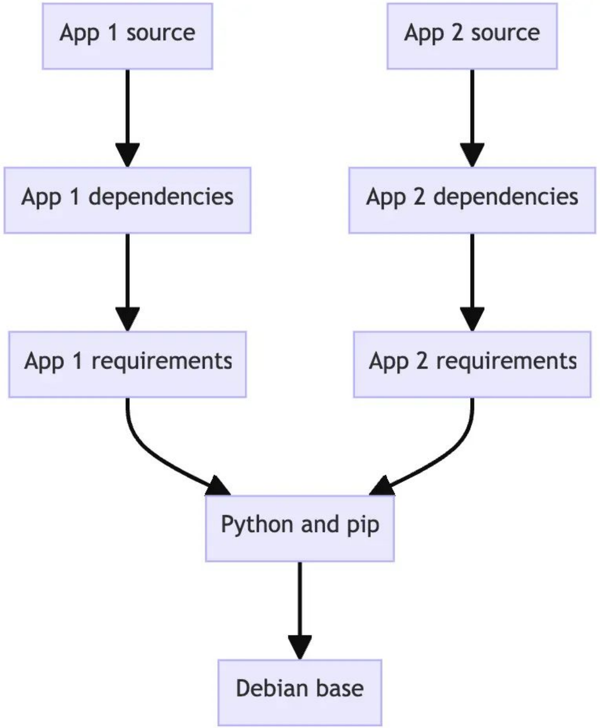
Reproducibility: consistent behavior across development, testing, and production environments.

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.





Network types

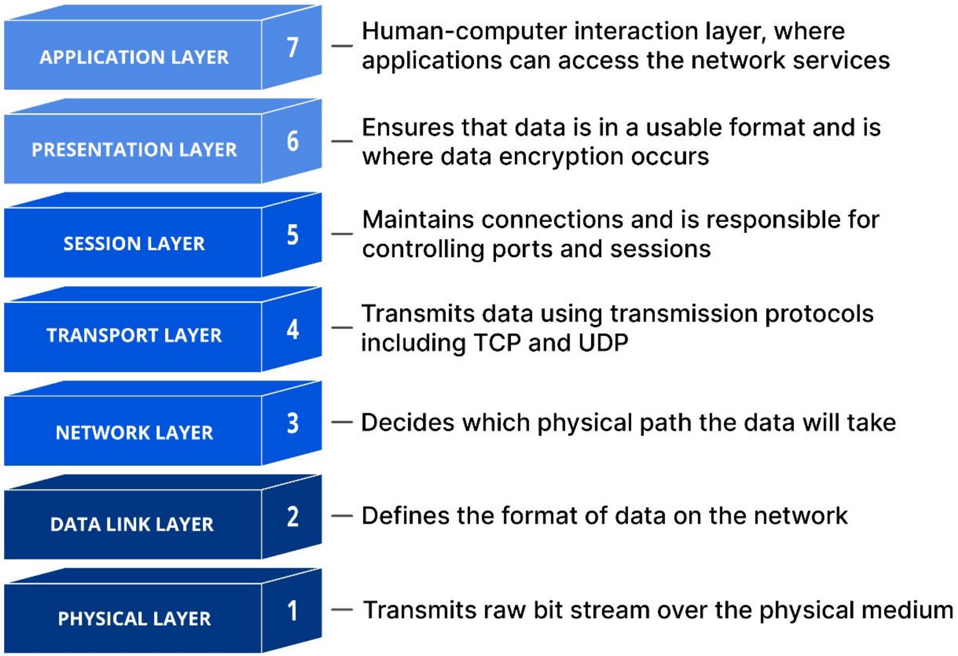
Computer networks can be classified into various types based on their scale, purpose, and geographic coverage.

Local Area Network (**LAN**): small-scale networks within a local area.

Wide Area Network (**WAN**): large-scale networks (for example, internet).

Network Protocols

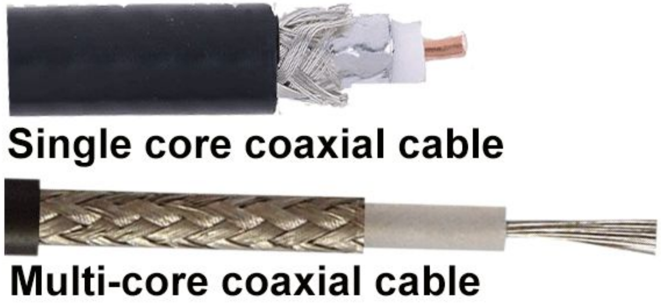
Open systems interconnection (OSI) model contains network protocols that govern the communication and data exchange between devices and systems over a network.



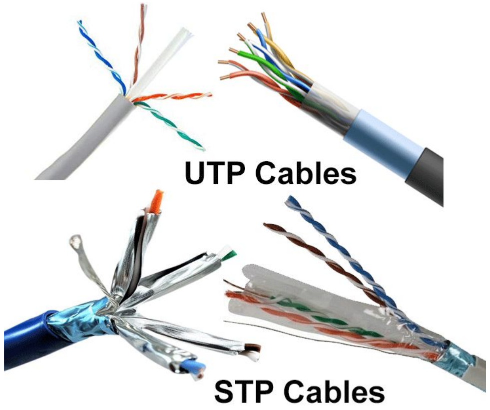
https://www.cloudflare.com/learning/ddos/glossary/open-systems-interconnection-model-osi/

Layer 1: Physical Layer

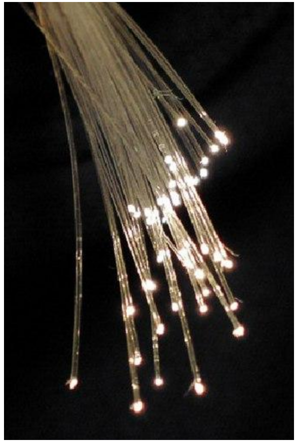
Physical layer is the foundation of network communication, responsible for managing the physical infrastructure and transmission of raw binary data over the network medium.



Coaxial Cable (retired)



Ethernet cable

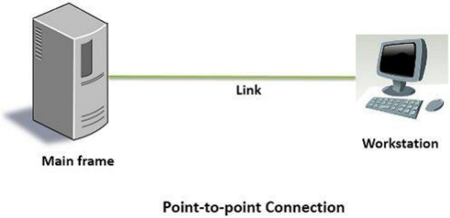


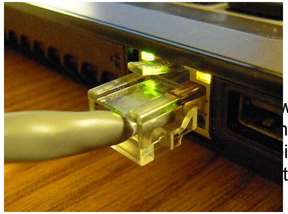
Optical Fibers

https://www.computernetworkingnotes.com/networking-tutorials/network-cable-types-and-specifications.html

https://en.wikipedia.org/wiki/Optical_fiber

Layer 2: Data Link Layer





wikipedia.org/wiki/Ethernet
ndifferences.com/difference-b
int-to-point-and-multipoint-co
tml

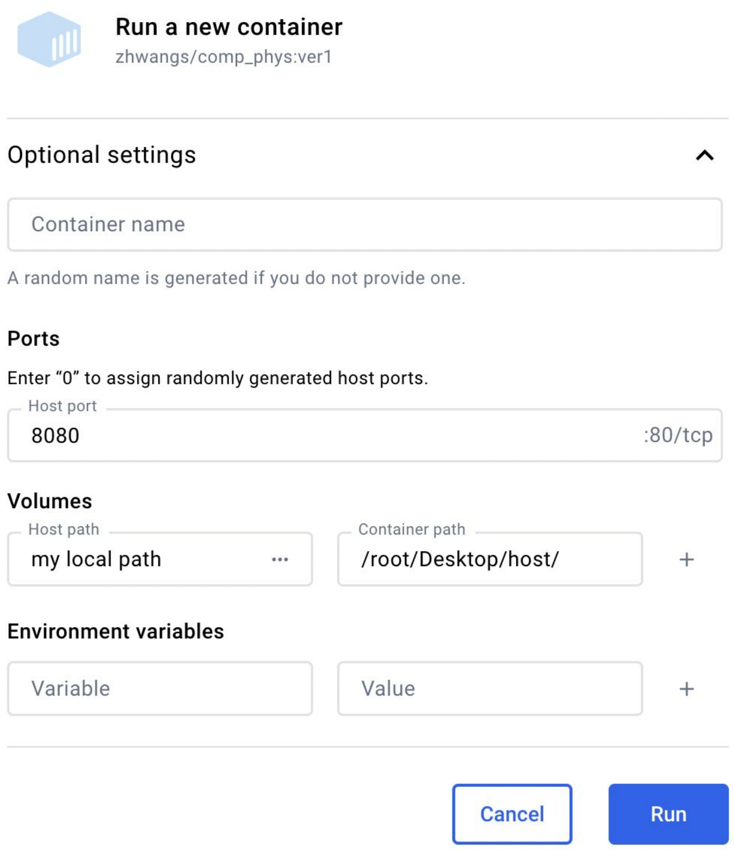
The data link layer provides for the transfer of data frames (packages) between devices connected to the physical link. This layer is communication between devices on the same local network (LAN) segment, e.g. via Ethernet protocol, Wi-Fi 802.11 (802.11a/b: Operates in the 5/2.4 GHz frequency)**.The protocol is limited by device-device communication.**

Physical Addressing: Media Access Control (MAC) address

Flow Control and Error Detection and Correction

Layer 3: Network layer

The network layer is responsible for routing data packets between devices in different networks or local subnets.The protocol is determining the best path for data packets to travel from the source to the destination across a network (Including Firewalls and Tunnelling). Internet Protocol (IP): Devices in a network are assigned unique logical addresses.



Check Network Configuration

We can check network configuration using the command, **ifconfig**

```
eno2: flags=4163<UP,BROADCAST,RUNNING,MULTICAST>  mtu 1500
        inet 192.168.0.85  netmask 255.255.255.0  broadcast 192.168.0.255
        inet6 fe80::5e3d:5eae:2785:656b  prefixlen 64  scopeid 0x20<link>
        ether 00:d8:61:34:de:5f  txqueuelen 1000  (Ethernet)
        RX packets 390992  bytes 327740646 (327.7 MB)
        RX errors 0  dropped 0  overruns 0  frame 0
        TX packets 237951  bytes 75474925 (75.4 MB)
        TX errors 0  dropped 0 overruns 0  carrier 0  collisions 0
        device interrupt 16  memory 0xa4300000-a4320000
```

```
lo: flags=73<UP,LOOPBACK,RUNNING>  mtu 65536
        inet 127.0.0.1  netmask 255.0.0.0
        inet6 ::1  prefixlen 128  scopeid 0x10<host>
        loop  txqueuelen 1000  (Local Loopback)
        RX packets 57626  bytes 3703927 (3.7 MB)
        RX errors 0  dropped 0  overruns 0  frame 0
        TX packets 57626  bytes 3703927 (3.7 MB)
        TX errors 0  dropped 0 overruns 0  carrier 0  collisions 0
```

```
tun0: flags=4305<UP,POINTOPOINT,RUNNING,NOARP,MULTICAST>  mtu 1400
        inet 128.111.237.46  netmask 255.255.255.255  destination 128.111.237.4
6
        inet6 fe80::6686:1568:18c2:35f2  prefixlen 64  scopeid 0x20<link>
        unspec 00-00-00-00-00-00-00-00-00-00-00-00-00-00-00-00  txqueuelen 500
 (UNSPEC)
        RX packets 67829  bytes 53849086 (53.8 MB)
        RX errors 0  dropped 0  overruns 0  frame 0
        TX packets 51273  bytes 17367846 (17.3 MB)
        TX errors 0  dropped 0 overruns 0  carrier 0  collisions 0
```

```
wlo1: flags=4099<UP,BROADCAST,MULTICAST>  mtu 1500
        ether f4:d1:08:a7:9c:89  txqueuelen 1000  (Ethernet)
        RX packets 0  bytes 0 (0.0 B)
        RX errors 0  dropped 0  overruns 0  frame 0
        TX packets 0  bytes 0 (0.0 B)
        TX errors 0  dropped 0 overruns 0  carrier 0  collisions 0
```

eno2, physical Ethernet network interface: main internet access from the service provider.

lo, loopback interface: It is used for communication within the local device itself, and any data sent to this interface is looped back and delivered internally.

tun0, tunneling interface: it allows network traffic to be encrypted and routed through a remote VPN server.

wlo1, wireless network interface: it allows the computer to connect to and communicate with wireless networks, such as Wi-Fi networks.

Local: Layer 1-3

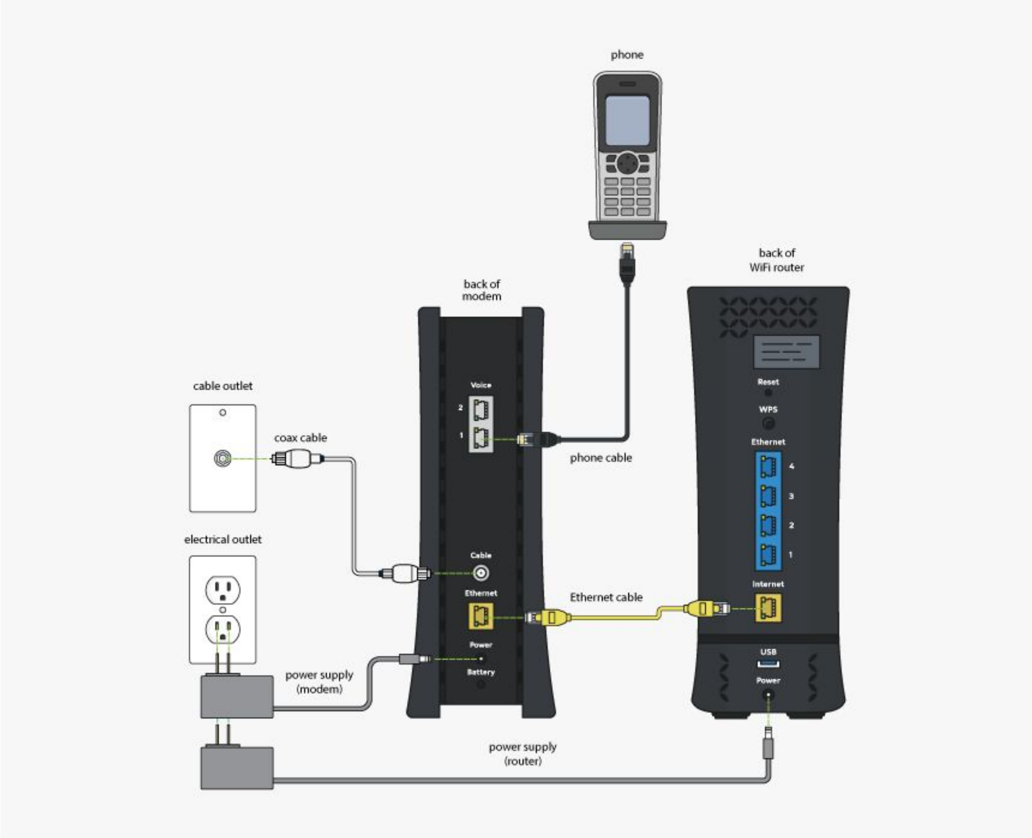
Modem and router are two distinct devices that play essential roles in networking.

Modem (Modulator-Demodulator)

(Layer 1-2) A device that modulates and demodulates digital data into analog signals for transmission over a specific medium and then converts incoming analog signals back into digital data.

Router:

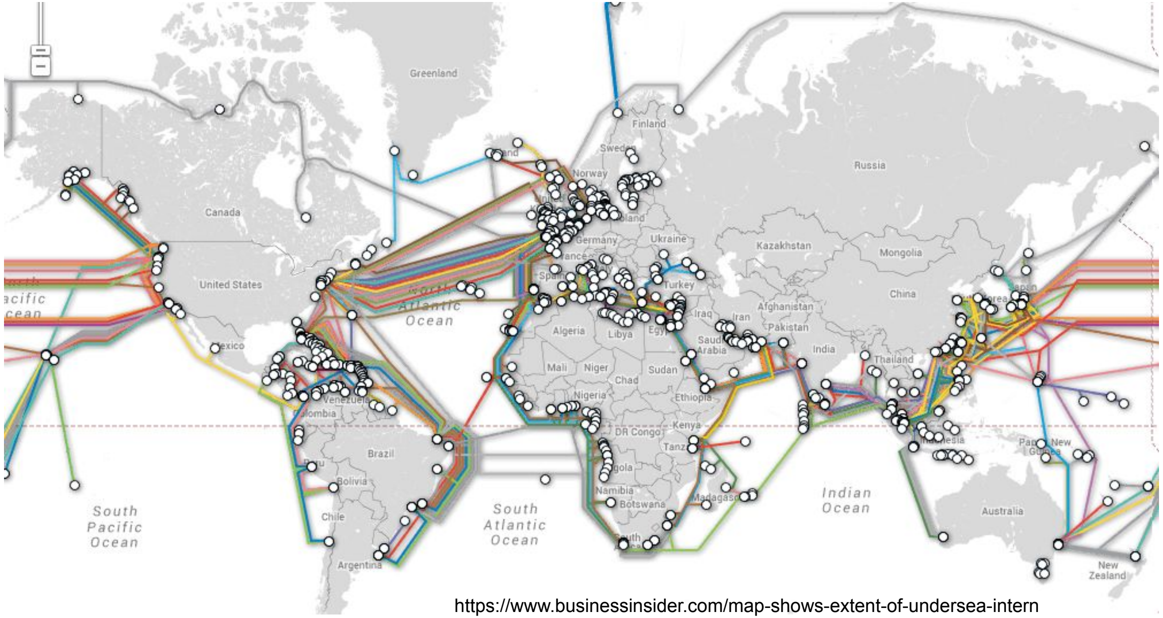
(Layer 2-3) A router is a networking device that connects multiple devices within your local network and routes data packets between them.



https://www.pngitem.com/middle/xbwwoR_setting-up-spectrum-wifi-spectrum-modem-and-router/

Global: Layer 1-3

Network nodes (e.g. data centers) are critical for global data and communication connectivity, allowing data to travel between continents and regions through the extensive undersea cable network.



https://www.businessinsider.com/map-shows-extent-of-undersea-internet-cables-that-russians-could-cut-2017-12

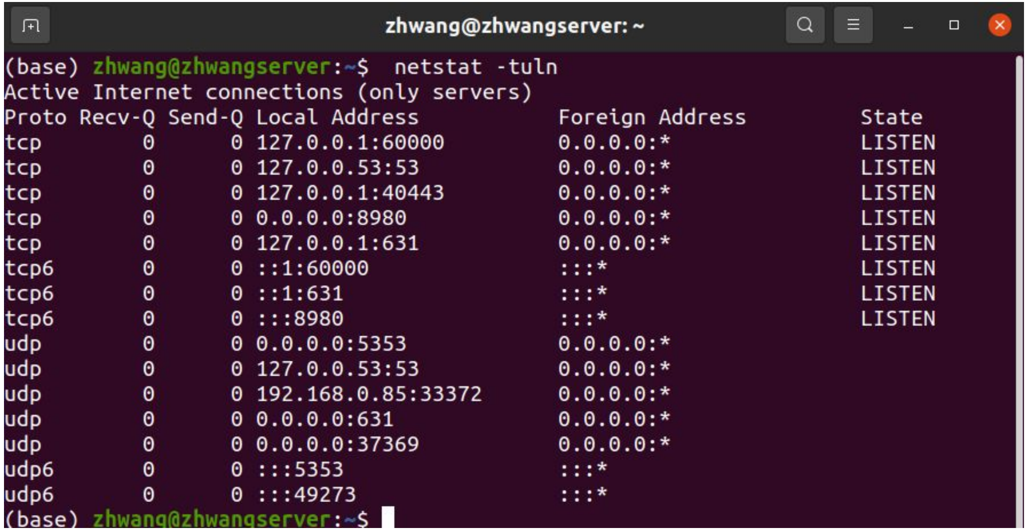
https://www.windsystemsmag.com/the-latest-advancements-in-submarine-cables-protection/

Layer 4: Transport Layer

The transport layer is responsible for ensuring end-to-end communication between devices across a network, namely the **sockets**.Two common protocols are TCP (Transmission Control Protocol) and UDP (User Datagram Protocol).

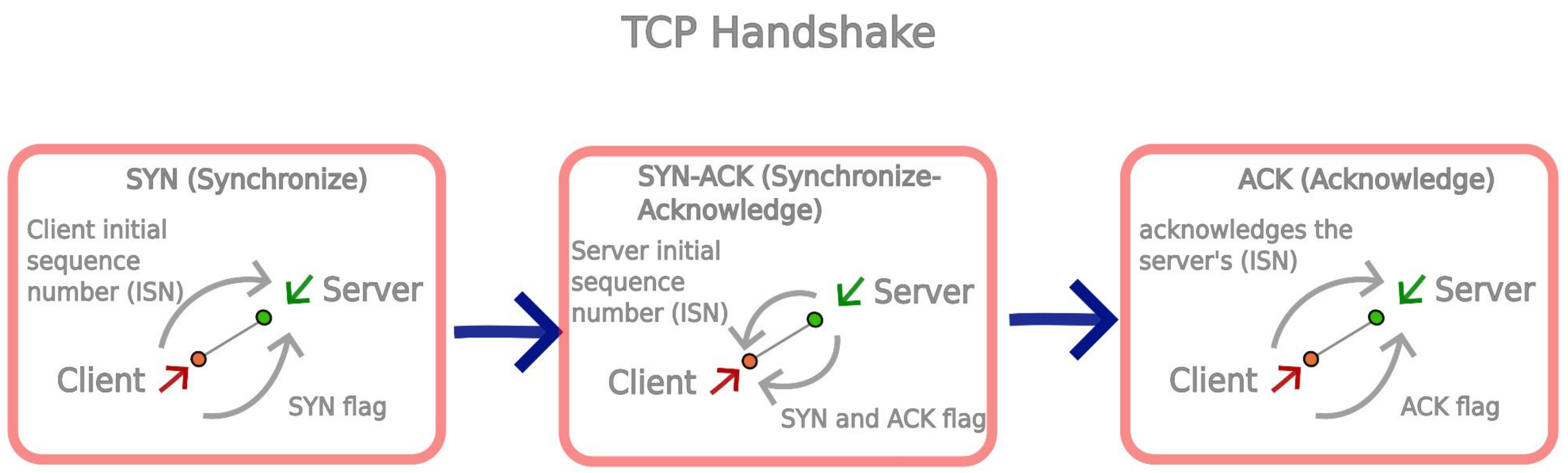
TCP:preserve data integrity, connection-oriented communication.

UDP: prioritize speed over data integrity, connectionless communication.



TCP Handshake

TCP handshake is designed to ensure that both devices agree to establish a reliable communication channel before exchanging data.



Port binding and Reserved IP Address

When a device wants to provide a service over TCP, it binds to a specific port number and listens for incoming connections on that port. Some ports are reserved for specific purposes, such as HTTP (port 80), HTTPS (443), and SSH (22).

Private IP Address

Private IP addresses are used within local networks, such as home or corporate networks, to allow multiple devices to communicate with each other.

10.0.0.0 to 10.255.255.255

172.16.0.0 to 172.31.255.255

192.168.0.0 to 192.168.255.255

Loopback IP Address

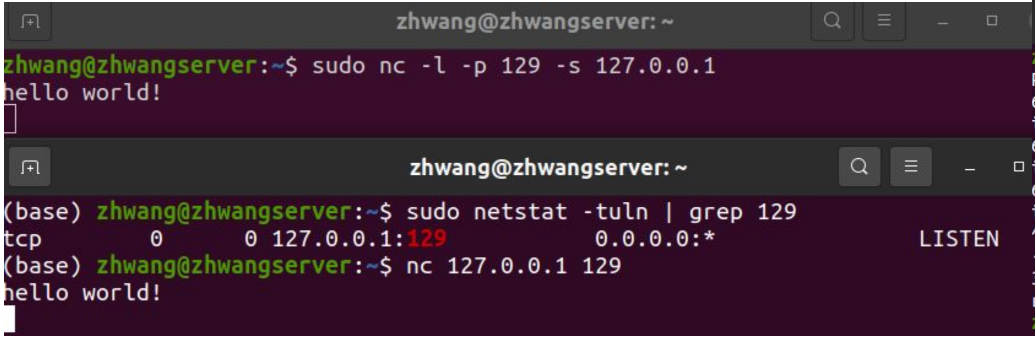
It is used for local network communication within a device itself, and it always refers to the local host,

127.0.0.0 to 127.255.255.255

TCP Sessions and Ping

We can create TCP sessions with **netcat** in a local network. The option -s gives local address.

TCP sessions on a local network



Ping an IP address