Math 381 - Fall 2022

Jay Newby

University of Alberta

Week 1

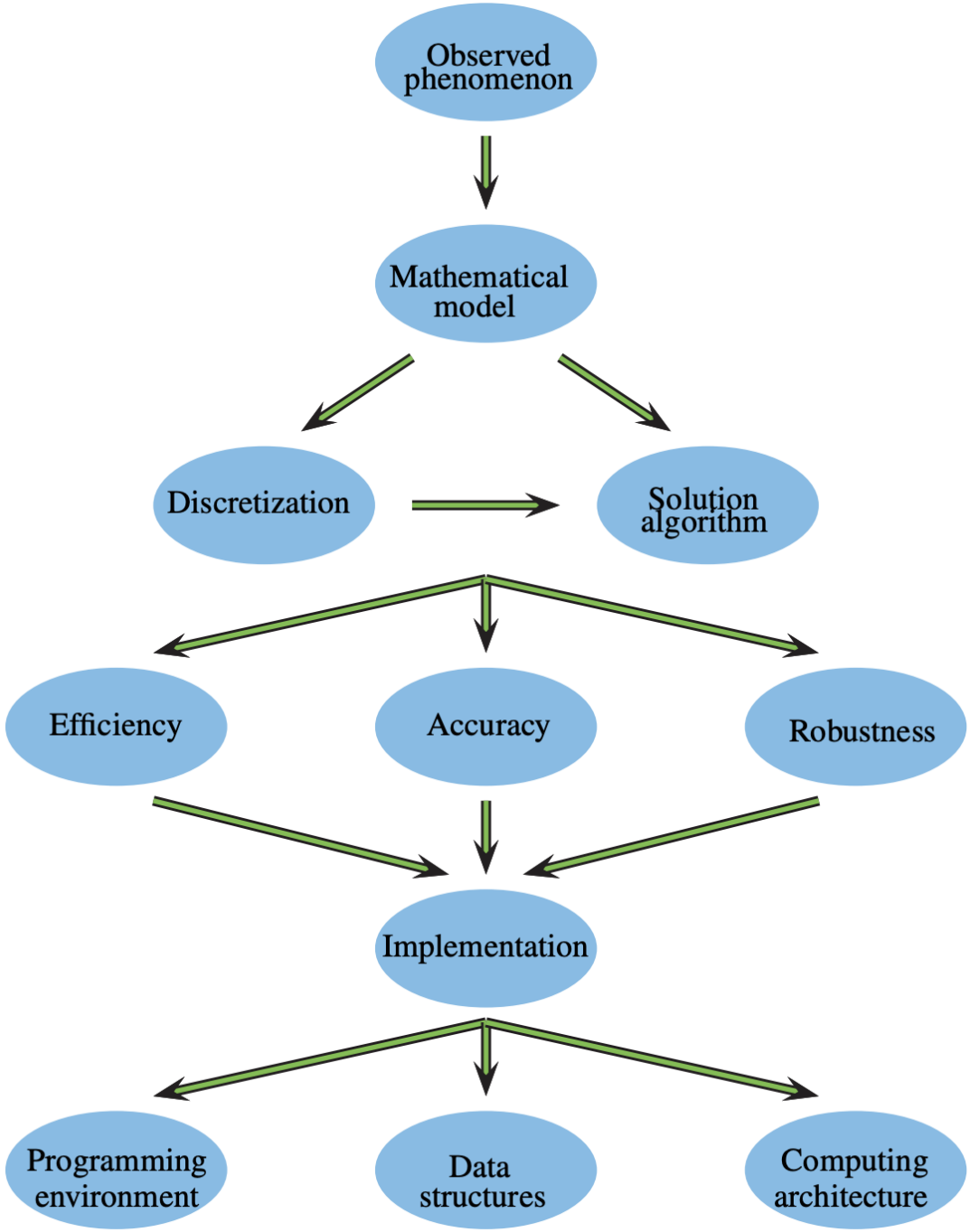
This Week: Introduction to scientific computing

1. Programming
2. Hardware
3. Approximation and Error
4. Algorithm Properties
    - Accuracy
    - Efficiency
    - Robustness

Numerical Analysis

Definition: Numerical analysis [Trefethen and Bau]

Numerical analysis is the study of algorithms for the problems of continuous mathematics


Observed phenomenon
Mathematical model
Discretization
Solution algorithm
Efficiency
Accuracy
Robustness
Implementation
Programming environment
Data structures
Computing architecture

Part 1: Programming

Algorithms

Definition: algorithm

An abstract procedure that can be implemented in code to solve or approximate the solution to a mathematical problem

Compiled languages

- Require extreme precision for greater speed
- Can create applications used by many people
- Make loads of $$

Examples: commonly used for scientific computing

C, C++, Fortran

Scripting languages

- Requires less precision at the cost of slower speed
- Often have an interactive command interface
- Greater portability
- Can serve as an everyday tool for individual use

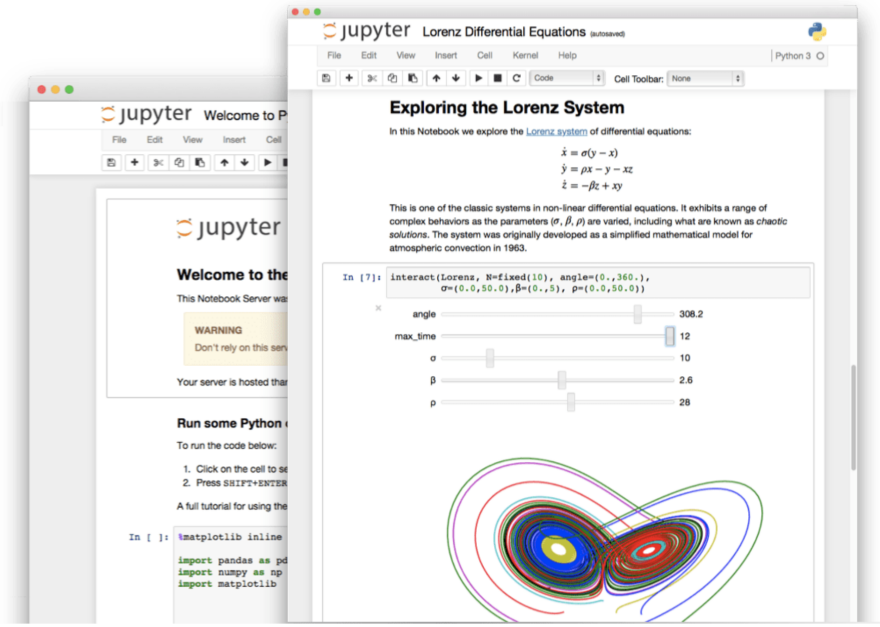
Examples: commonly used for scientific computing

Python, Matlab, Javascript, R, Julia

Additional Examples:

Bash, HTML, LaTeX, Perl, etc

Jupyter

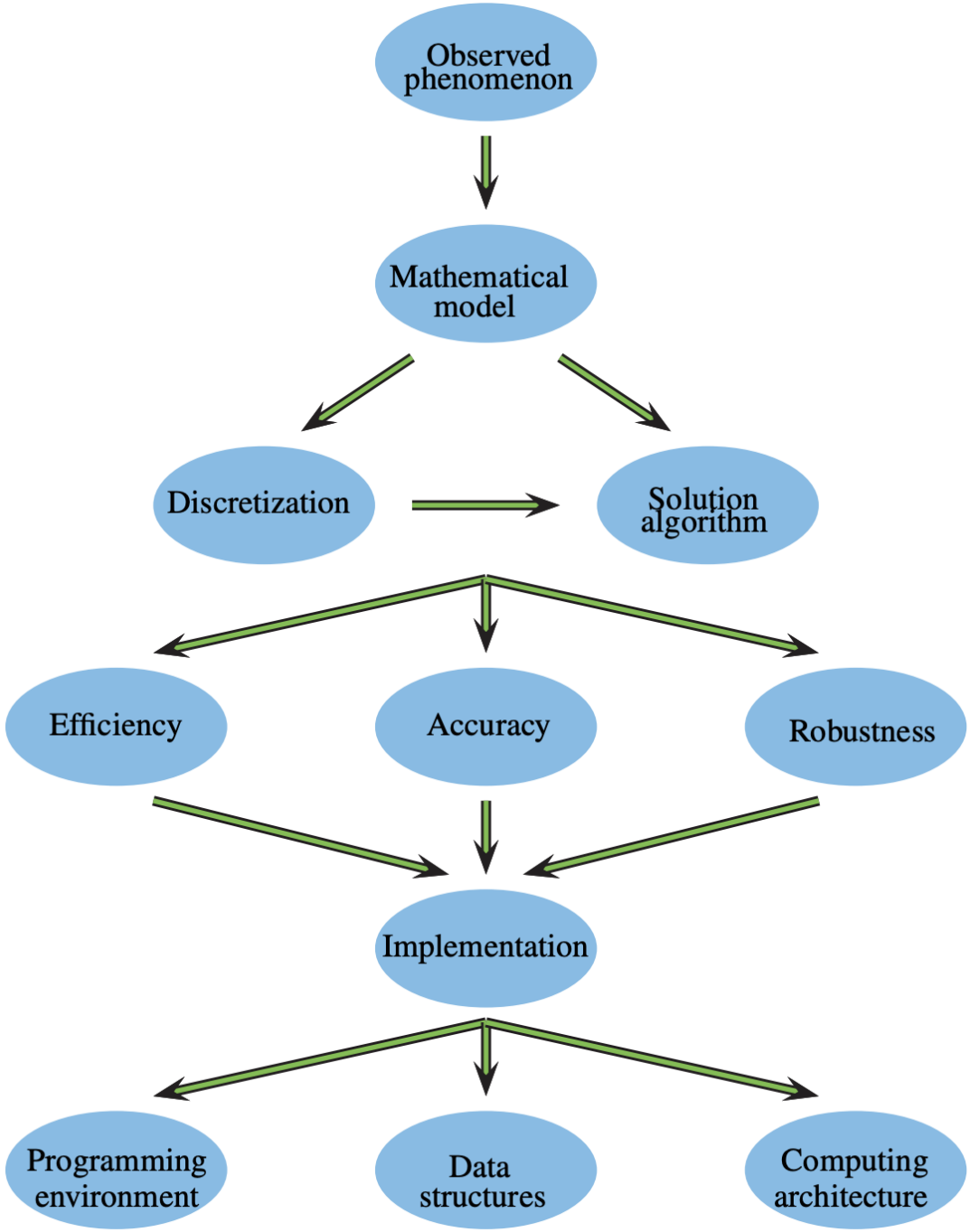


The Jupyter Notebook is an open-source web application that allows you to create and share documents that contain live code, equations, visualizations and narrative text. Uses include: data cleaning and transformation, numerical simulation, statistical modeling, data visualization, machine learning, and much more.

Syzygy

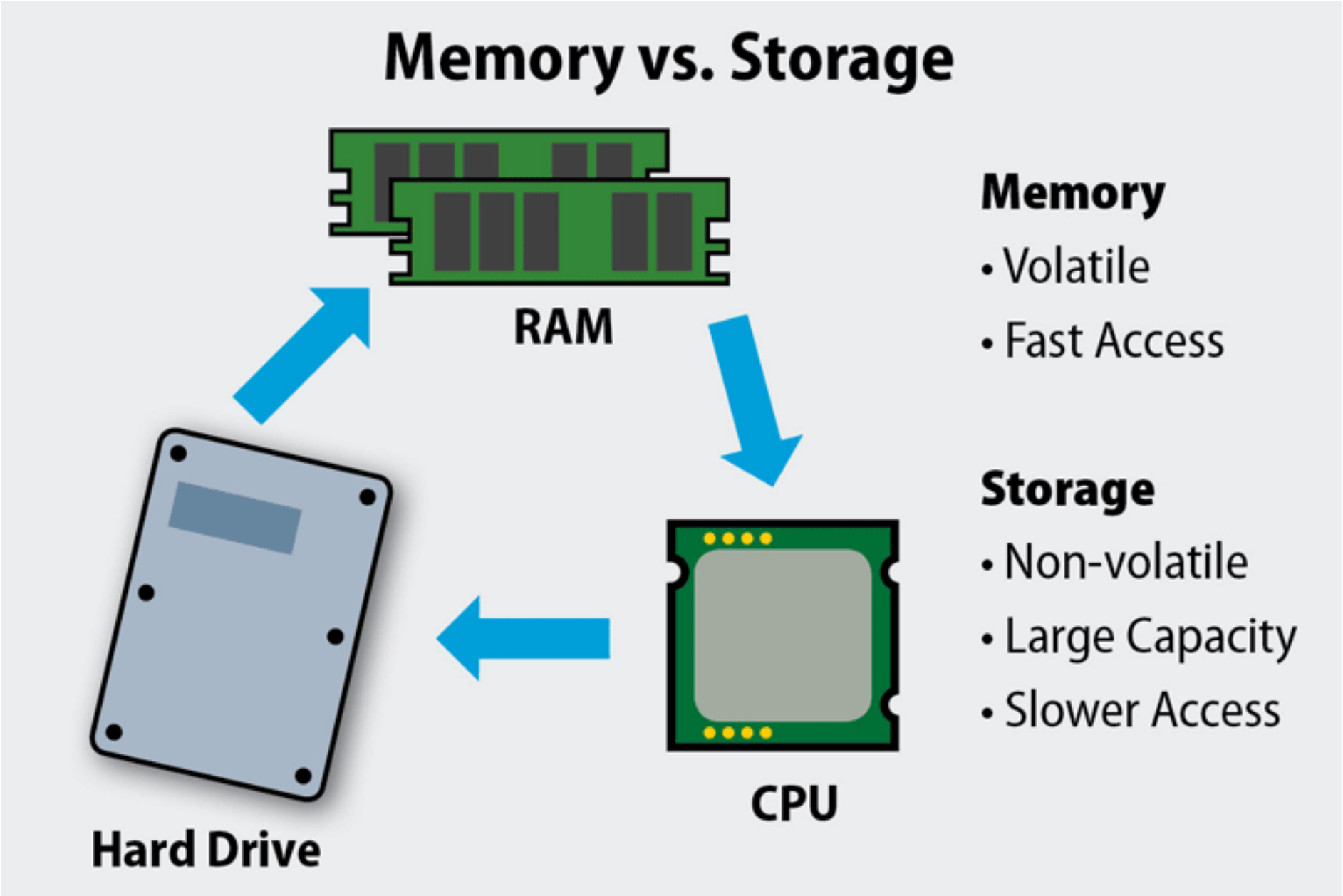
You do not need to install any software to use Jupyter. We will be using the uAlberta Syzygy server. https://ualberta.syzygy.ca

[Show example and take a brief tour]


Observed phenomenon
Mathematical model
Discretization
Solution algorithm
Efficiency
Accuracy
Robustness
Implementation
Programming environment
Data structures
Computing architecture

Part 2: How hardware constrains scientific computing

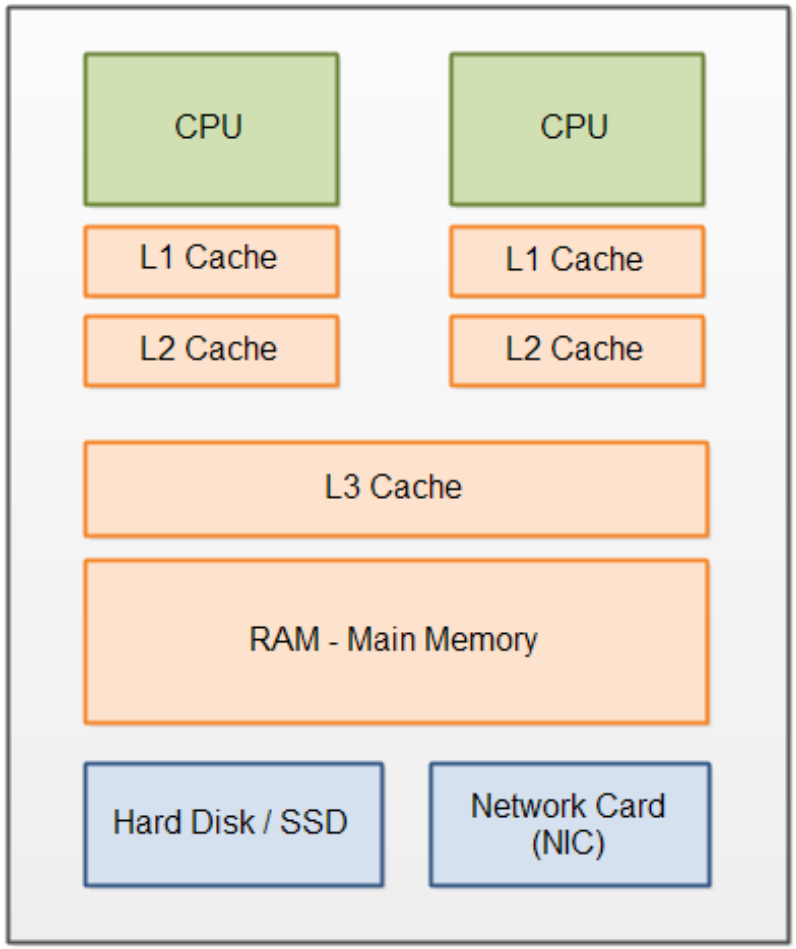
Basic parts


Memory vs. Storage
RAM
Memory
• Volatile
• Fast Access
Storage
• Non-volatile
• Large Capacity
• Slower Access
CPU
Hard Drive

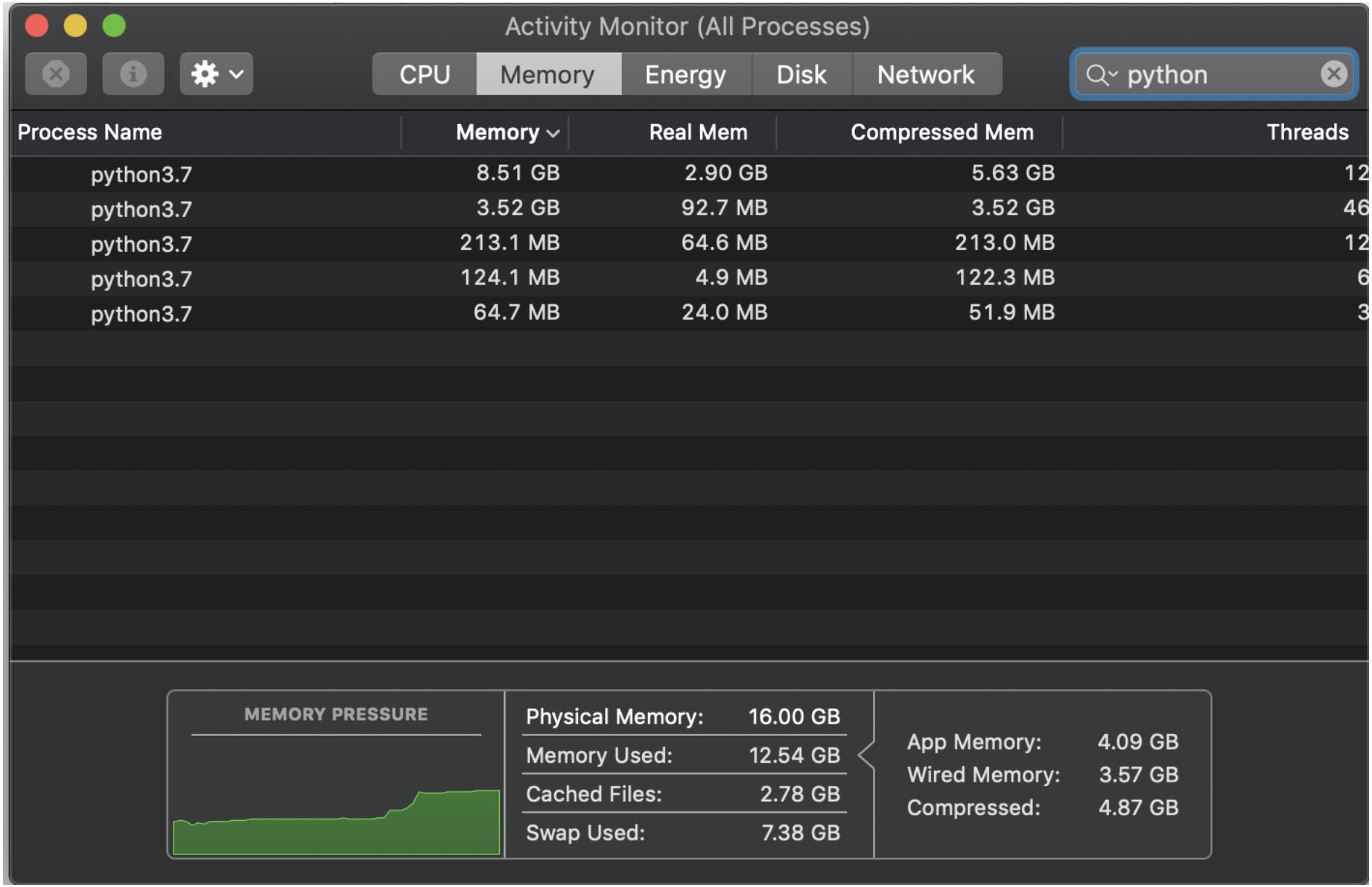
How CPUs can influence algorithms

- Architecture (Cache)
- Parallel processing

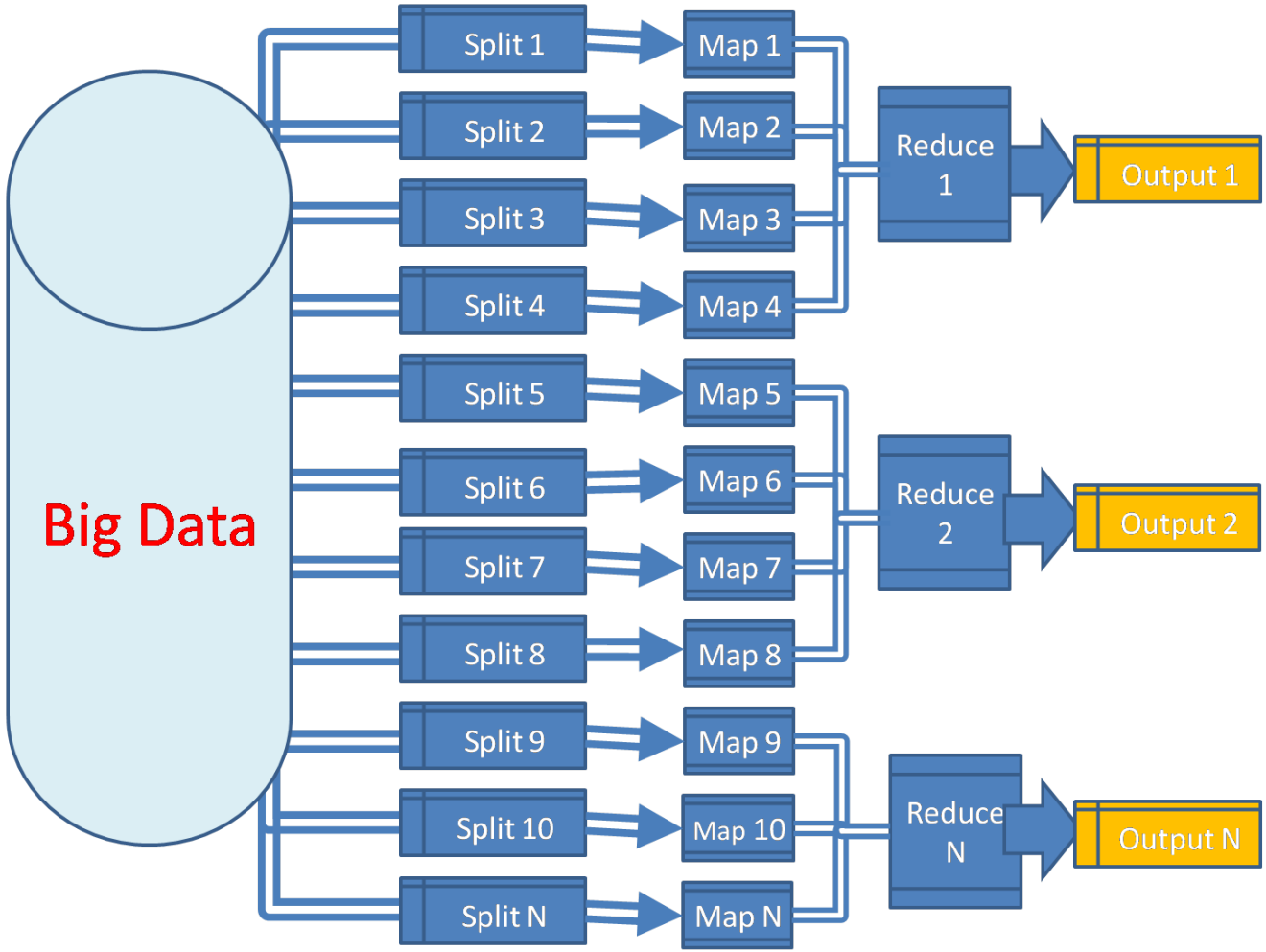
CPU Cache system



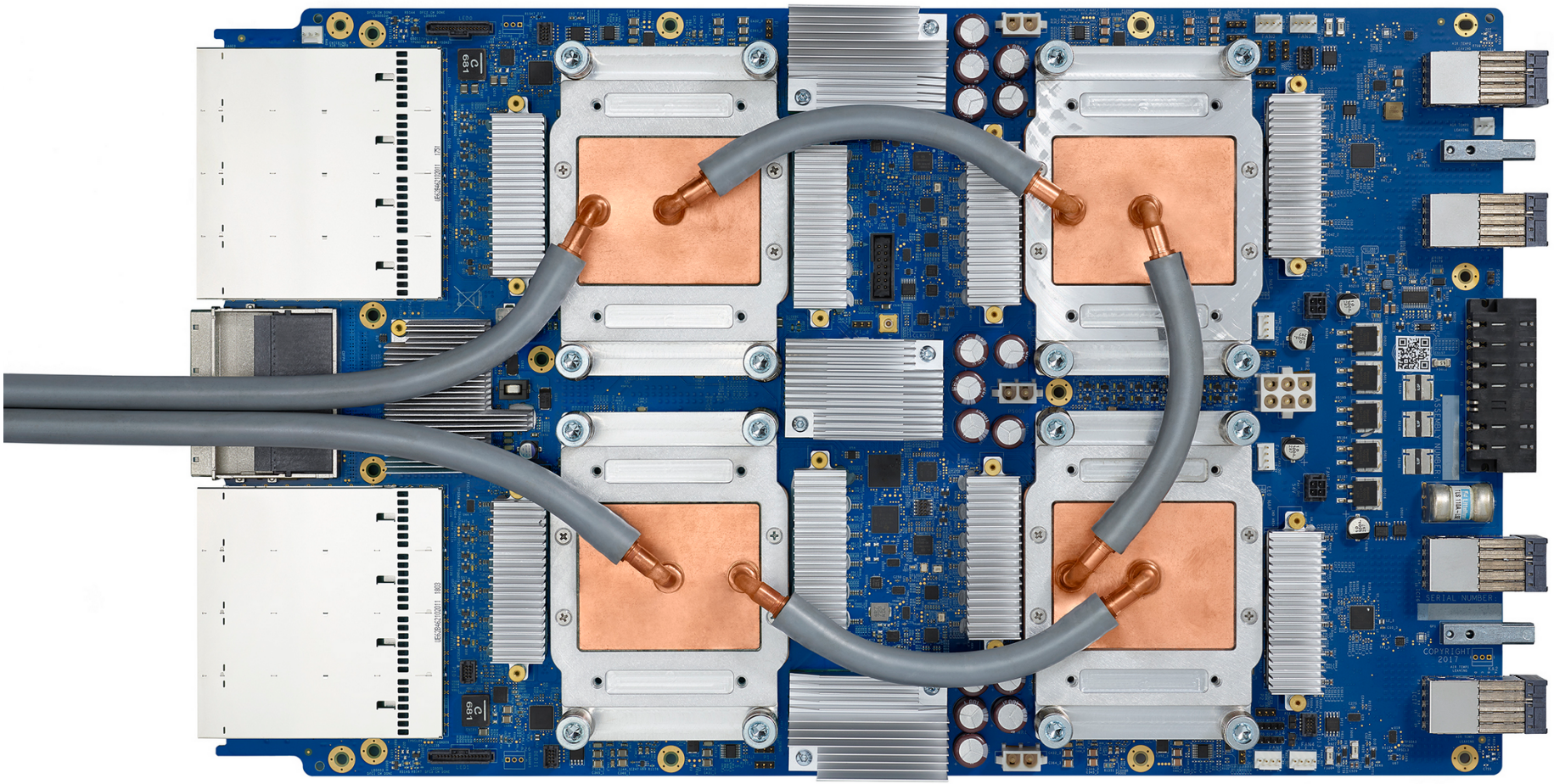
How memory constrains algorithms



How storage constrains algorithms



Graphical Processing Unit (GPUs) and ASIC hardware



Part 3: Numerical Approximation and Error

Origins of Error

- Error between mathematical representations of error and reality
- Error from measurements and collection of empirical data
- Numerical errors
  - Discretization errors
  - Convergence errors
  - Roundoff error

Absolute and Relative Error

Suppose we have the exact solution to a problem $x \neq 0$, and an approximate solution $\hat{x} \in \mathbb{R}$.

Absolute Error:

$$\mathcal{E}_{\text{abs}} = |\hat{x} - x|$$

Relative Error:

$$\mathcal{E}_{\text{rel}} = \frac{|\hat{x} - x|}{|x|}$$