



MATHEMATICAL, NUMERICAL, BAYESIAN, AND CAUSAL PROBLEM SOLVING

MSE 420/MSE510

Instructor: Sergei V. Kalinin

Co-instructor: Richard Liu

Times and locations: 9:10-10:00

MWF, Ferris Hall 502

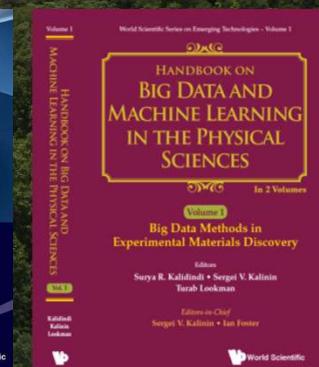
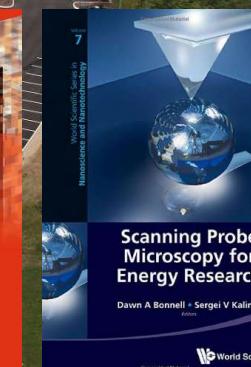
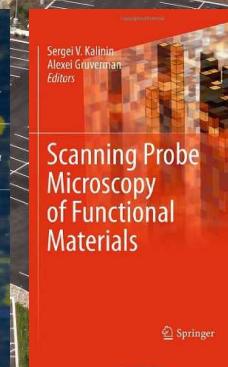
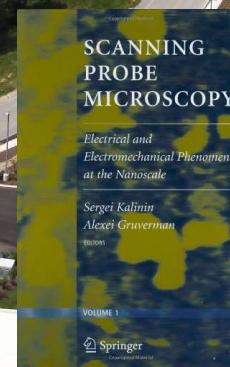
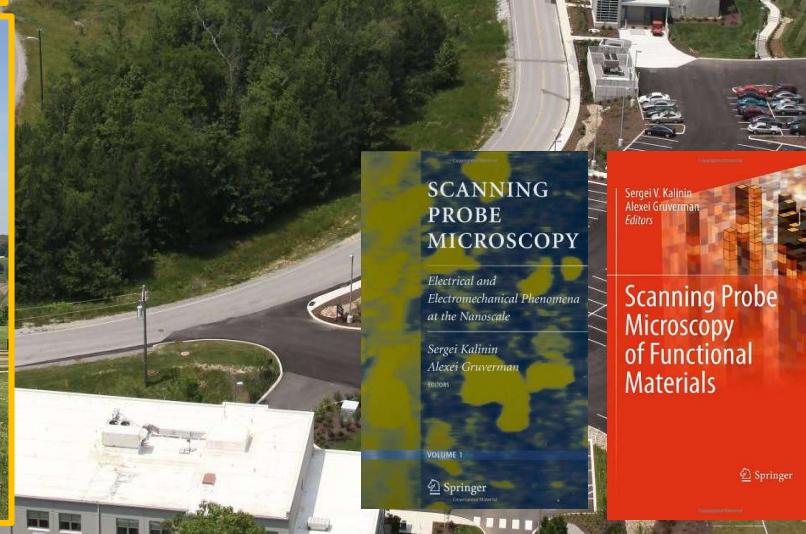
2002 - 2022

Since ~2010



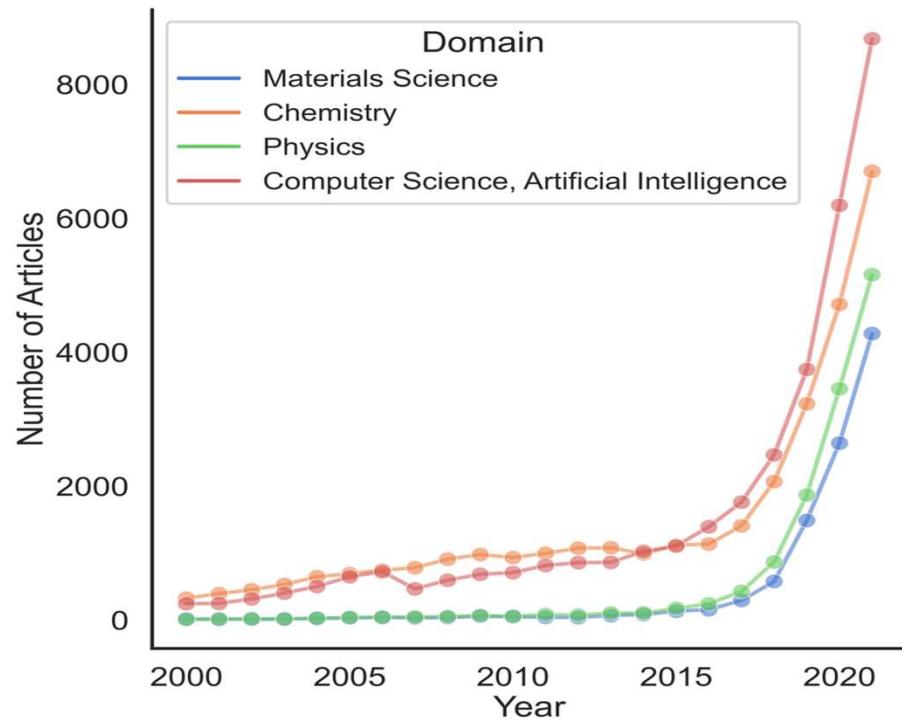
2022 -2023

amazon

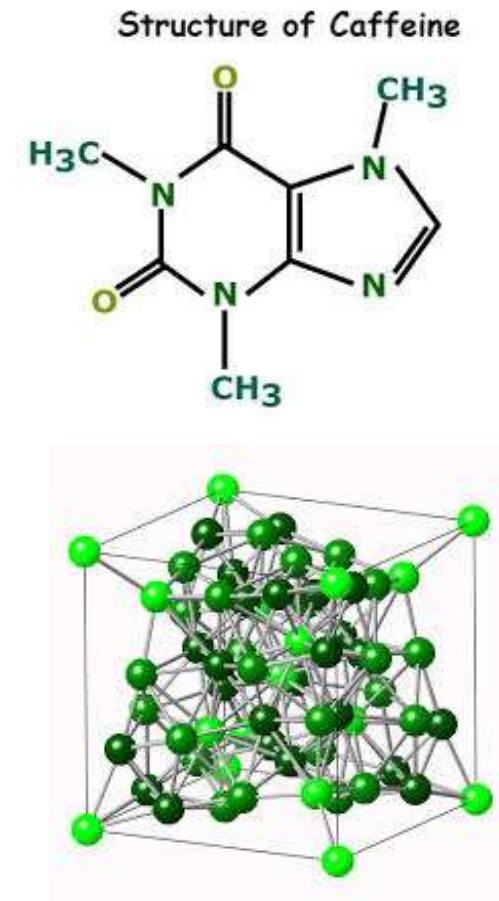


There is no computation
without representation

ML in Domain Sciences



Analysis by B. Blaiszik, Argonne



- The rapid adoption of ML in domain sciences and industrial R&D is a very recent trend
- Technologies and workforce emerge from academia into industry
- We can estimate potential growth rates comparing to cloud computing 15 - 20 years ago

What are our objects?



Quantitative Variables:

- 3 apples, 2 oranges

Categorical Variables:

- Apple and Orange

Schemas:

- "Fruit," "Type," and "Quantity"

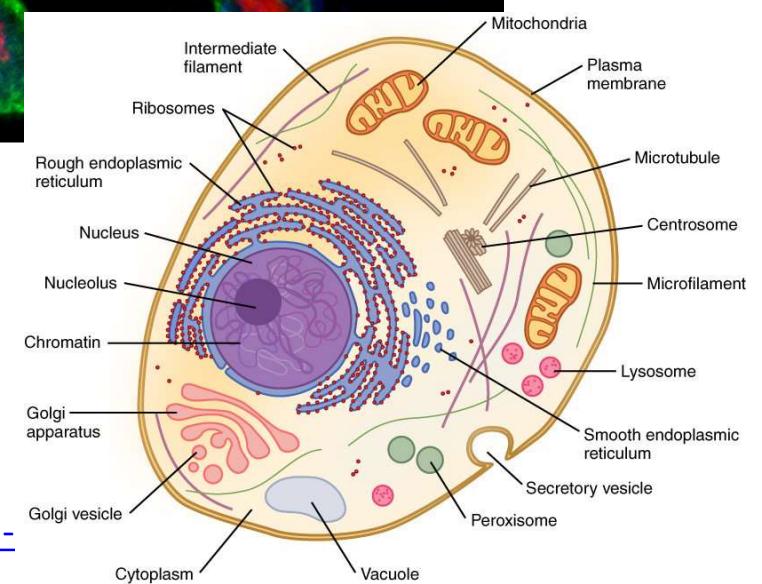
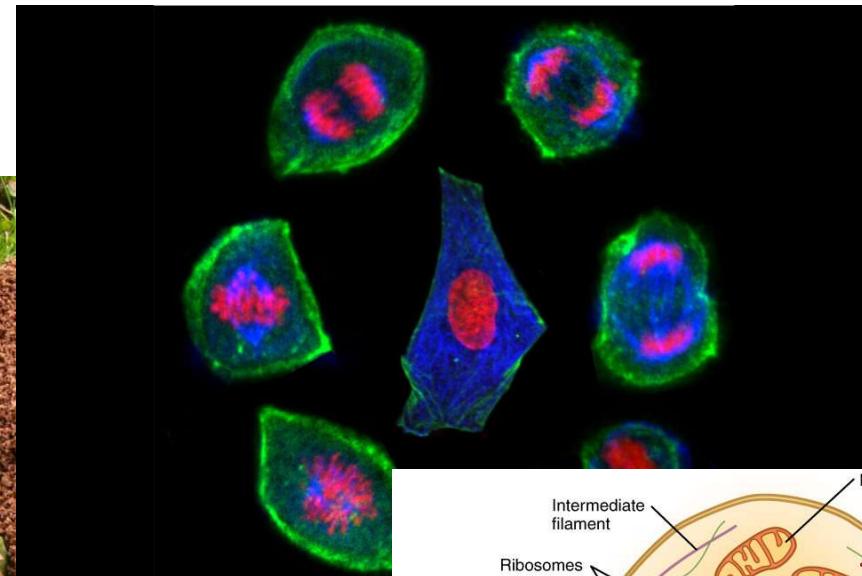
Ontologies:

- "Apple is a type of Fruit"

Knowledge Graphs:

- Connection between "Apple," "Fruit," "Vitamin C content," and "Growth Regions."

No equations (or ML) without representation!



<https://phys.org/news/2021-10-cell-life-optical-tweezers.html>

<https://doi.org/10.1080/00150193.2020.1722012>

<https://www.pointepestcontrol.net/inside-the-ant-hill/>

https://www.researchgate.net/figure/Schematic-representation-of-a-cell-20-with-organelles-delimited-or-made-of-lipid_fig5_350133282

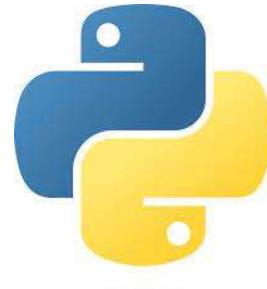
Symbols, numbers, data

- Numbers
- Patterns
- Magnitude
- Shapes and forms

- Symbols
- Algorithms
- Logic

- Correlations

- Prior Knowledge
- Causality
- Workflows



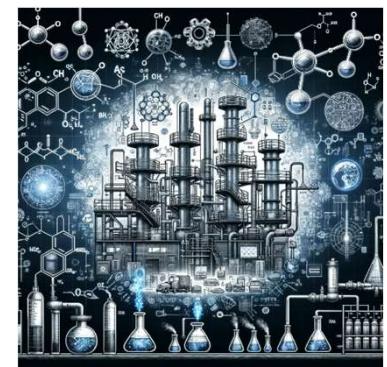
Materials science



Physics



Chemical engineering



Chemistry



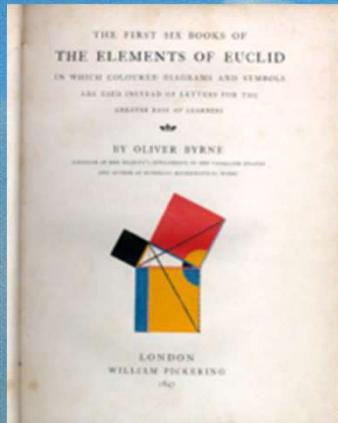
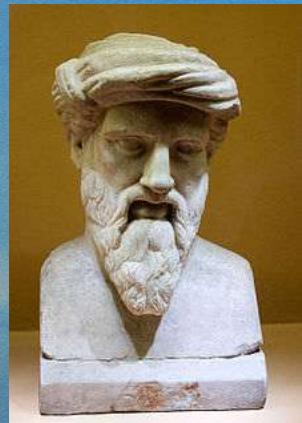
- 
- Taxes:
 - Grain allotments
 - Workers
 - Weights of silver
 - Geometry
 - Pythagoras theorem
 - Linear, quadratic, and cubic equations
 - Hexadecimal system

<https://www.independent.co.uk/news/science/babylonians-trigonometry-develop-more-advanced-modern-mathematics-3700-years-ago-ancient-civilisation-a7910936.html>

- Composite and prime numbers
- Arithmetic, geometric and harmonic means
- Simple number theory
- Power of correlations

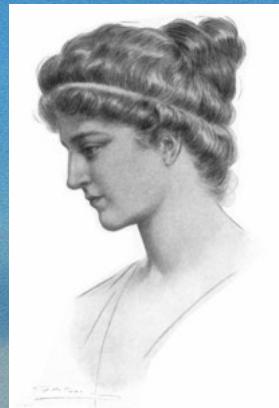


<https://www.pyramid-of-giza.com/plan-your-visit-pyramids-of-giza/>



Pythagoras

Euclides



Fictional portrait
of Hypatia of
Alexandria by
Jules Maurice
Gaspard



https://assets.editorial.aetnd.com/uploads/2010/03/ancient_greece_gettyimages-475594807.jpg

India and China



The Tsinghua Bamboo Slips, containing the world's earliest decimal multiplication table, 305 BC during the Warring States period



The Nine Chapters on the Mathematical Art, one of the earliest surviving mathematical texts from China (2nd century AD)

**TABLE SHOWING THE PROGRESS OF NUMBER FORMS
IN INDIA**

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



- Algebra
- Algorithms
- Early calculus
- Trigonometry
- Cryptography
- Frequency analysis

<https://www.newscientist.com/people/muhammad-ibn-musa-al-khwarizmi/>

Medieval Europe

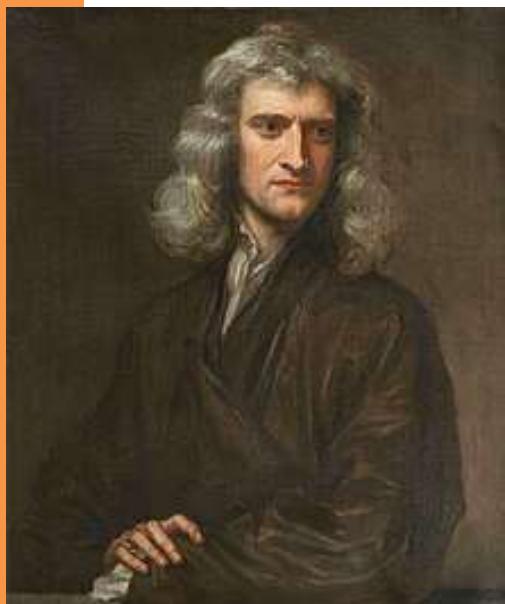
Primary drivers:

- Manufacturing
- Taxes
- Philosophy
- Theology

<https://www.discovermiddleages.co.uk/medieval-life/medieval-life-and-times>



Renaissance



Isaac Newton
(1642 – 1726)



Leonhard Euler
(1707 – 1783)



Friedrich Gauss
(1777 – 1855)



Joseph Fourier
(1768 – 1830)

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

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

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

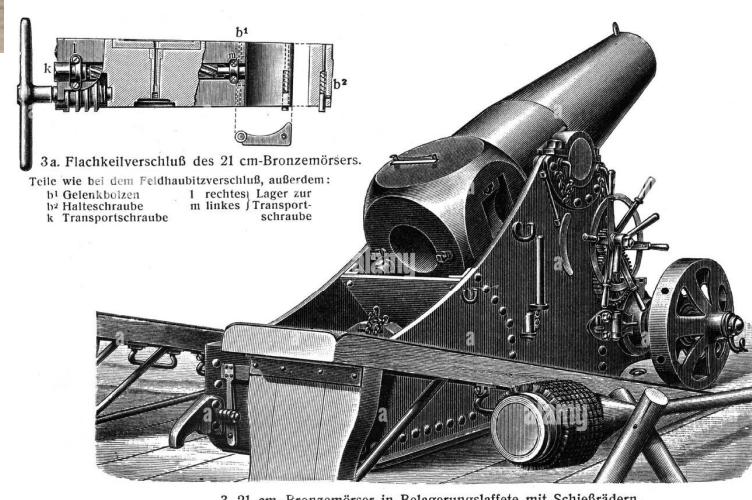
https://en.wikipedia.org/wiki/Joseph_Fourier

- Mechanics
- Electromagnetism
- Heat conduction

From Renaissance to XX Century



https://en.wikipedia.org/wiki/Reffye_85_mm_cannon



alamy



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

<https://www.alamy.com/stock-photo-military-artillery-guns-german-21-cm-mortar-wood-engraving-late-19th-28829542.html>

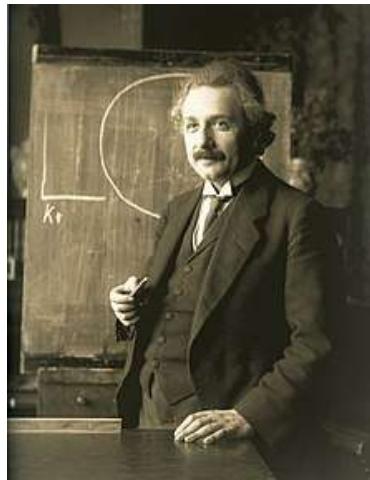
Gödel proved that the world of pure mathematics is inexhaustible; no finite set of axioms and rules of inference can ever encompass the whole of mathematics; given any finite set of axioms, we can find meaningful mathematical questions which the axioms leave unanswered. I hope that an analogous Situation exists in the physical world. If my view of the future is correct, it means that the world of physics and astronomy is also inexhaustible; no matter how far we go into the future, there will always be new things happening, new information coming in, new worlds to explore, a constantly expanding domain of life, consciousness, and memory.

— Freeman Dyson

From Lecture 1, 'Philosophy', in a series of four James Arthur Lectures, 'Lectures on Time and its Mysteries' at New York University (Autumn 1978).

Printed in 'Time Without End: Physics and Biology in an Open Universe', *Reviews of Modern Physics* (Jul 1979), **51**, 449.

The Quantum Era



Einstein



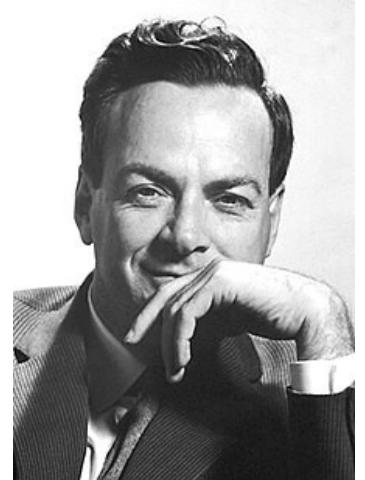
Bohr



Noether



Schwinger



Feynman

- Quantum mechanics
- Relativity
- Quantum electrodynamics
- Discovery of spin
- ... and so on

For a physicist mathematics is not just a tool by means of which phenomena can be calculated, it is the main source of concepts and principles by means of which new theories can be created.

— Freeman Dyson

In 'Mathematics in the Physical Sciences', *Scientific American* (Sep 1964), **211**, No. 3, 129.

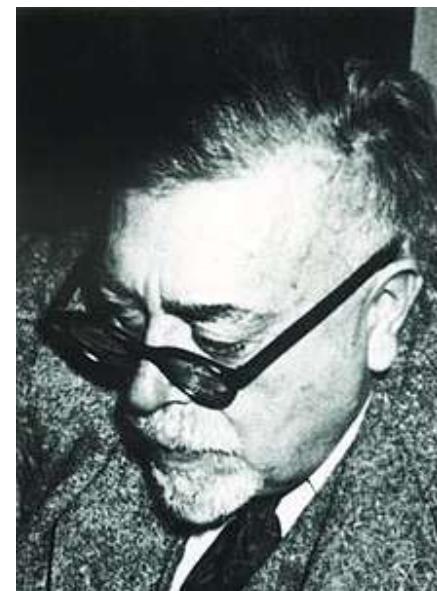
Science and Engineering of Big Numbers



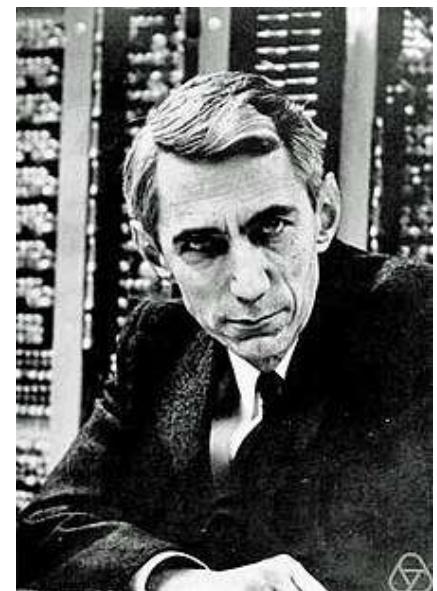
John von Neumann
(1903 – 1957)



Eugene Wigner
(1902 – 1995)



Norbert Wiener
(1894 – 1964)



Claude Shannon
(1916 – 2001)

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

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

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

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

Science and Engineering of Big Numbers



Grace Hopper
(1906 –1992)



Margaret Hamilton
(1936 -)



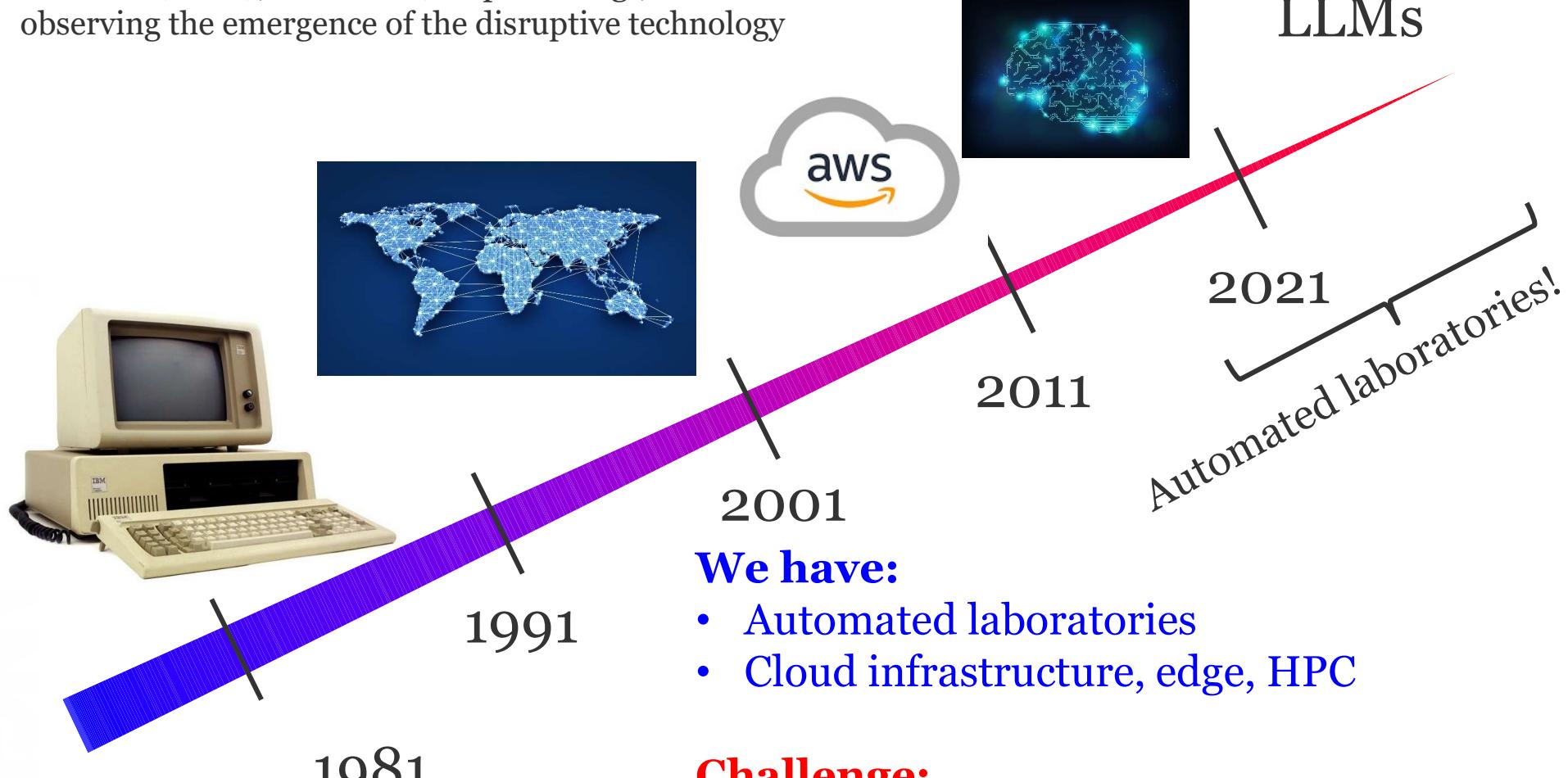
Katherine Johnson
(1918 –2020)

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

[https://en.wikipedia.org/wiki/Margaret_Hamilton_\(software_engineer\)](https://en.wikipedia.org/wiki/Margaret_Hamilton_(software_engineer))

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

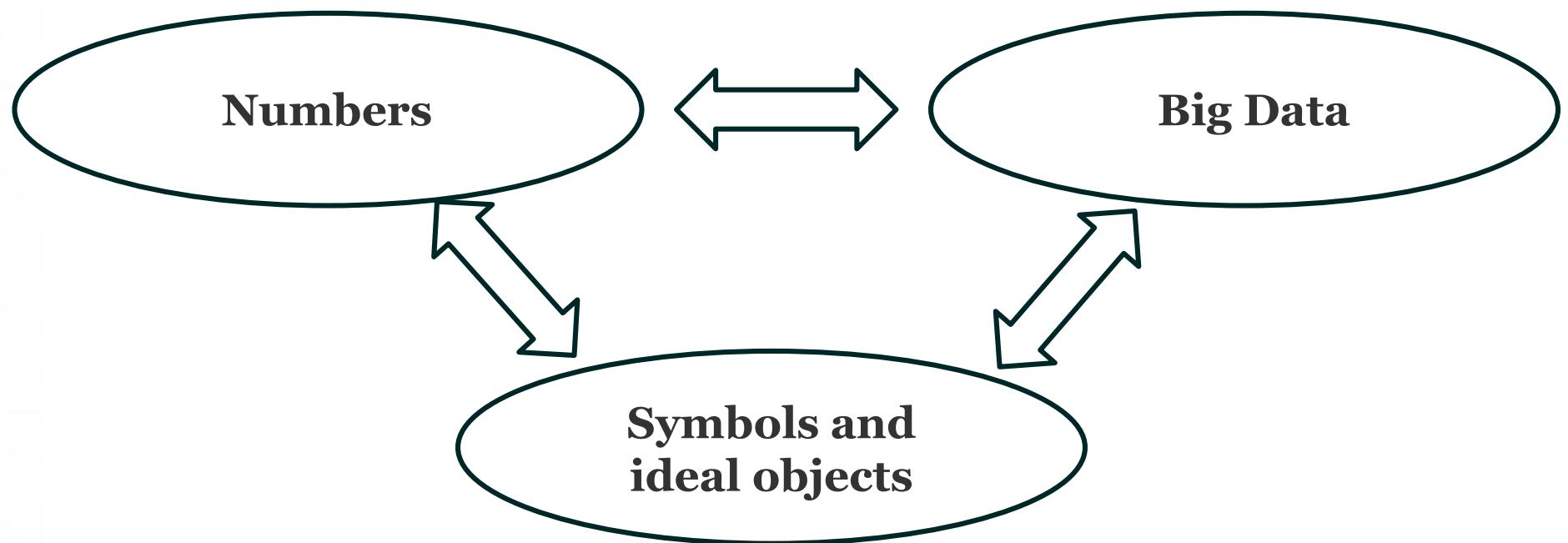
Much like in early 80ies (PCs), mid-90ies (Internet), mid-2000 (cloud), and 2012 (Deep learning), we are now observing the emergence of the disruptive technology



<https://www.computerhistory.org/timeline/1981/>

New addition: big data

We are now entering the new era of science when in addition to classical mathematics and physics tools we have new intuition and methods of big data



Course Information

Faculty Contact Information:

Instructor: Prof. Sergei V. Kalinin,
Office: 314 IAMM
E-mail: sergei2@utk.edu
Teaching Assistant: TBD

Instructor Availability:

Please don't hesitate to email me with updates, questions, or concerns. I will typically respond within 24 hours during the week and 48 hours on the weekend. I will notify you if I will be out of town and if connection issues may delay a response.

Meeting Time: 9:10-10:00 MWF, Ferris Hall 502

The lectures and materials will be posted on Canvas and at GitHub:

https://github.com/SergeiVKalinin/MSE_Spring2026

Office Hours:

Friday 1:30 - 3:00 PM are open for 1:1 meetings to discuss any course related item. Please set time by e-mail.

Course Outline

1. Mathematical Methods in Physical Science
2. Introduction to Python and the SciPy Ecosystem
3. Classical Numerical Methods with Python
4. Regression Methods
5. Mathematical Representation of the Real World
6. Differentiable Modeling and Physics-Informed Neural Networks
7. Bayesian Data Analysis
8. Causal Methods
9. Gaussian Processes, Bayesian Optimization, and Active Learning
10. Gaussian Processes Meet Physics
11. Decision Loops, Model-Based Control, and State Estimation
12. Use of LLMs for Decision-Making Workflows

Value Proposition

1. Achieve proficiency in scientific Python, tapping into its diverse mathematical applications.
2. Gain the ability to solve both foundational and advanced equations with confidence.
3. Deep dive into data analysis, mastering tools that empower data-driven decisions.
4. Grasp the nuances of Bayesian methods, learning how to weave together data with prior knowledge.
5. Explore the intricate landscape of causal analysis within the ML spectrum.
6. Develop a solid understanding of probabilistic techniques for decision-making in uncertain scenarios.

Prerequisites

To be successful in this course you will need a general background in materials science. Python or similar programming experience, while not essential, will be extremely useful. Students without any prior programming experience should expect to spend extra time outside of class learning basic skills.

Outcomes

1. This course aims to provide students with the skills needed to link physics, numerical methods, and big data
2. Students should learn how to combine intuition from mathematics, physics, and machine learning methods
3. The course is designed to provide students with basic knowledge of numerical methods, causal analysis, and Bayesian methods
4. Preparedness for the Future of Science and Industry: With insights into automated labs, large language models in scientific workflows, and federated tools and workflows, students will be prepared for the future of industry. These skills are increasingly important as companies automate processes and incorporate AI into their workflows. This knowledge can help students stand out in the job market and be prepared for the careers of the future.

This and that

Learning Environment:

The class will be delivered as in-person lectures. The Jupyter notebooks, code libraries, and videos provided. Weekly programming exercises will be assigned via Google Colabs and those students wishing to interact with the instructor in person should attend office hours.

Use of ChatGPT:

Strongly encouraged both for programming and written assignments. However, the students have to be aware of the limitations of the generative models.

Grading & Policies:

- | | |
|-----------------|-----|
| • Midterms (2) | 30% |
| • Homeworks | 40% |
| • Final Project | 30% |

Reference Materials

I will provide copies of lecture notes, presentations, and Colabs on GitHub and Canvas. There is no specific textbook for the course, and we will take material from a variety of sources including:

- Andrew Bird et al, Python Workshop, <https://www.packtpub.com/product/the-python-workshop/9781839218859>
- Oswaldo Martin, Bayesian Analysis with Python - Second Edition, <https://subscription.packtpub.com/book/data/9781789341652/>
- Alexander Molak, Causal Inference and Discovery in Python, <https://subscription.packtpub.com/book/data/9781804612989/>

Homework 1:

- Create new Colab, <https://colab.google/>
- Chapter 1-4 and 10, Python Workshop.

Homework, midterm, and finals format

- All homeworks, midterms, and finals will be in the Google Colab format
- Use the code for programming exercises and markdown fields for text responses
- Share in the “comment” or “editor” modes
- The Colabs should save all graph outputs
- The Colabs should be able to run from the beginning to end (e.g. if I restart the runtime and run all)
- Submit to sergei2vk@gmail.com

Homework 1:

- Create new Colab, <https://colab.google/>
- Chapter 1-4 and 10, Python Workshop.