

Introduction to Scientific Computing and Data Science

Scientific Computing

Stefan Abi-Karam

Summer 2023

Table of Contents

1. Course Overview
2. About Your Teacher
3. Scientific Computing Overview
4. Closing Advice

Course Goals

- ▶ Overview of topics in **scientific computing, data science, and machine learning**
- ▶ Apply these topics to your own research
- ▶ Familiarize yourself with the tools and software

Course Survey

Topics

- ▶ Programming Foundations
- ▶ Computer Science and Math Foundations
- ▶ Overview of Scientific Computing
- ▶ Exploratory Data Science and Visualization
- ▶ Machine Learning
- ▶ Deep Learning

Tools

- ▶ Python
- ▶ NumPy, SciPy, Pandas
- ▶ Matplotlib, Seaborn
- ▶ Scikit-Learn, Scikit-Image
- ▶ PyTorch

Course Logistics

Refer to the current year's course syllabus for more details.

We will typically split the class into the following components:

- ▶ Lectures: Twice a week
- ▶ Homework: Once a week
- ▶ Office Hours: Typically once a week with demand

Grading is typically split as follows:

- ▶ Homework: 80%
- ▶ Participation + Other: 20%

Communication

- ▶ Email: stefan.abi-karam@ahschool.com
 - ▶ Absence, Personal Concerns, Project Questions and Feedback
 - ▶ Please use your Heritage email address as well
- ▶ Google Classroom
 - ▶ **Homework Assignments**
 - ▶ Class meeting link
 - ▶ Class announcements and changes
- ▶ Campuswire
 - ▶ **Questions about Homework**
- ▶ Office Hours
 - ▶ **Questions about Homework**
 - ▶ **Questions about Projects**
- ▶ Slack
 - ▶ Project Questions and Feedback, Quick Updates, Meeting Links and Reminders

Table of Contents

1. Course Overview
2. About Your Teacher
3. Scientific Computing Overview
4. Closing Advice

About Your Teacher

- ▶ Graduated from American Heritage in 2018
- ▶ B.S. in Electrical Engineering in 2021
- ▶ M.S. in Electrical Engineering in 2022
- ▶ Ph.D. + Research Faculty 2023 and beyond

Research: My research is focused on hardware acceleration of machine learning algorithms and applied machine learning for hardware design tools and emerging technologies.



About Your Teacher

More Details

- ▶ SHARC Lab, ECE, Georgia Tech
- ▶ CIPHER Lab, Georgia Tech Research Institute
- ▶ Georgia Tech Undergraduate Admissions

Hobbies

- ▶ Meteorology
- ▶ Music Production and Analog Music Synthesis
- ▶ Sailing
- ▶ Hobby Electronics and Programming
- ▶ Reading

About Your Teacher



Table of Contents

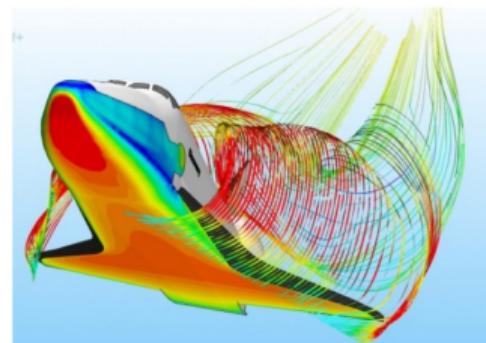
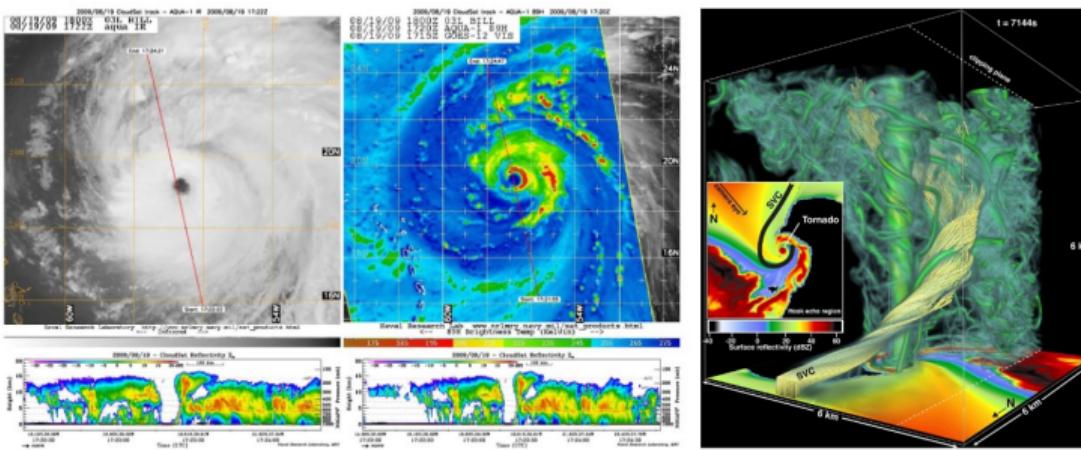
1. Course Overview
2. About Your Teacher
3. Scientific Computing Overview
4. Closing Advice

What is Computing?

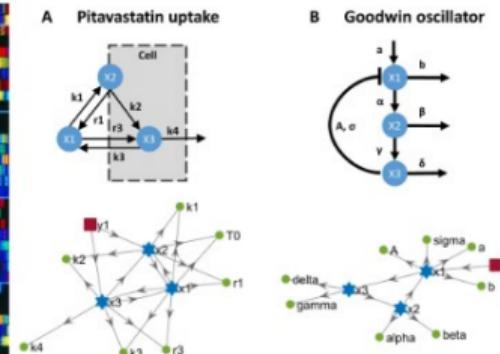
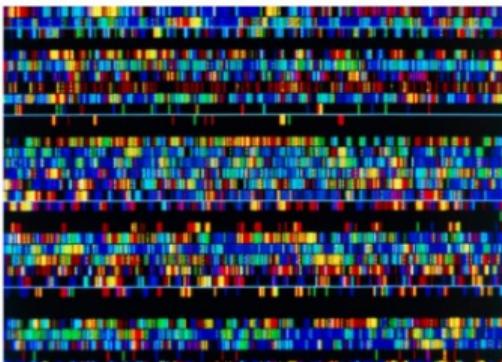
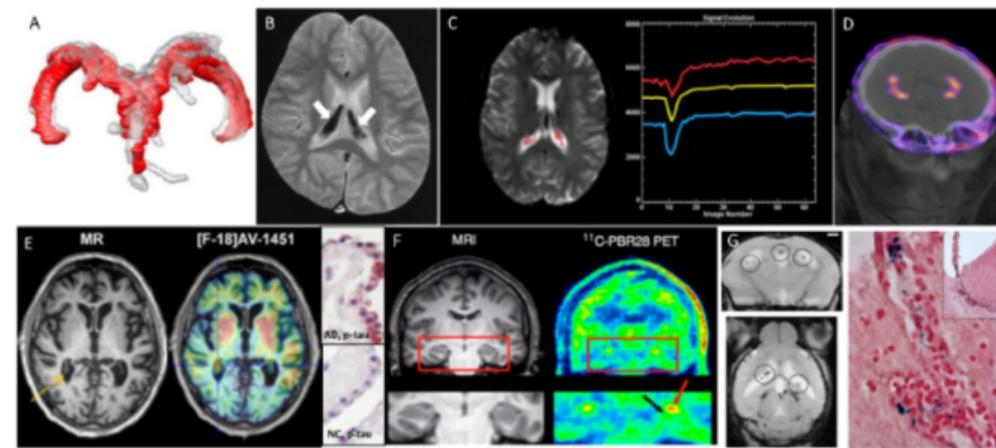
Computer Science is no more about computers than astronomy is about telescopes.

—Edsger W. Dijkstra

Scientific Computing - Earth Science and Engineering



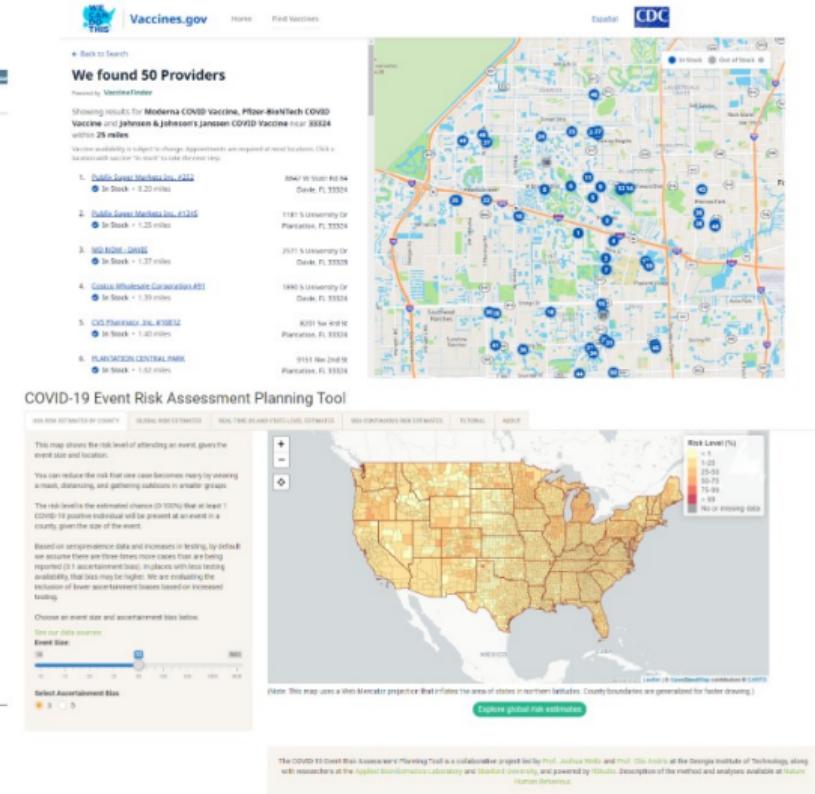
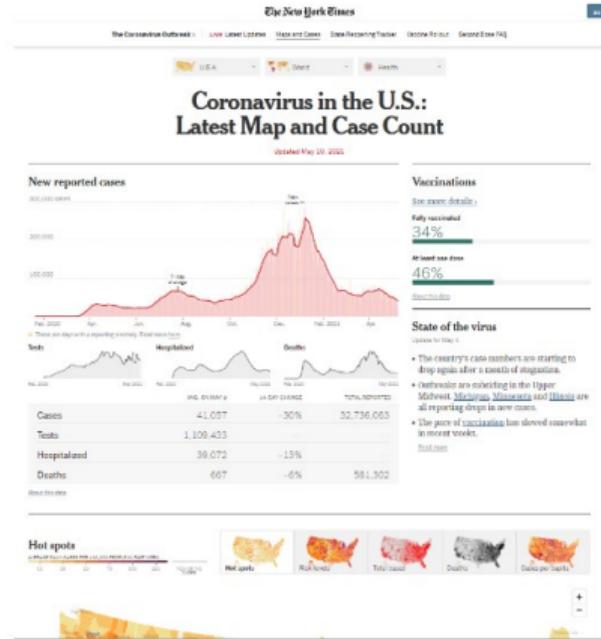
Scientific Computing - Biology and Medicine



What is Data Science?

Data is the new oil.

Data Science - COVID-19



Data Science - General Applications



Loan Default Prediction
Beginners data set for financial analytics
Kamal Das • updated a month ago (Version 2)

Data Tasks (1) Code (6) Discussion (1) Activity Download (269 KB) New Notebook

Usability 10.0 License Data files © Original Authors Tags business, finance, tabular data, banking, beginner



Covid-19 period air-traffic dataset
air traffic data from The OpenSky Network 2020
IshaDS • updated 4 days ago (Version 2)

Data Tasks (1) Code (1) Discussion Activity Download (3 GB) New Notebook

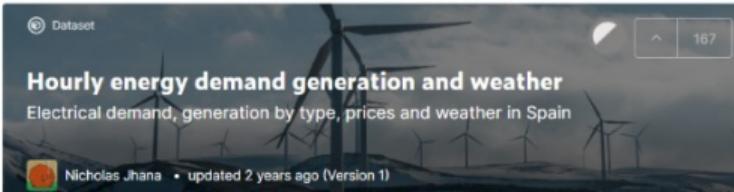
Usability 8.8 License Attribution 4.0 International (CC BY 4.0) Tags transportation, covid19, intermediate, aviation



Heart Attack Analysis & Prediction Dataset
A dataset for heart attack classification
Rashik Rahman • updated 2 months ago (Version 2)

Data Tasks (1) Code (203) Discussion (12) Activity Download (32 KB) New Notebook

Usability 10.0 License CC0: Public Domain Tags health, health conditions, classification, heart conditions, binary classification



Hourly energy demand generation and weather
Electrical demand, generation by type, prices and weather in Spain
Nicholas Jhana • updated 2 years ago (Version 1)

Data Tasks (1) Code (12) Discussion (2) Activity Download (25 MB) New Notebook

Usability 10.0 License CC0: Public Domain Tags business, news, energy, weather and climate, renewable energy

What is Machine Learning?

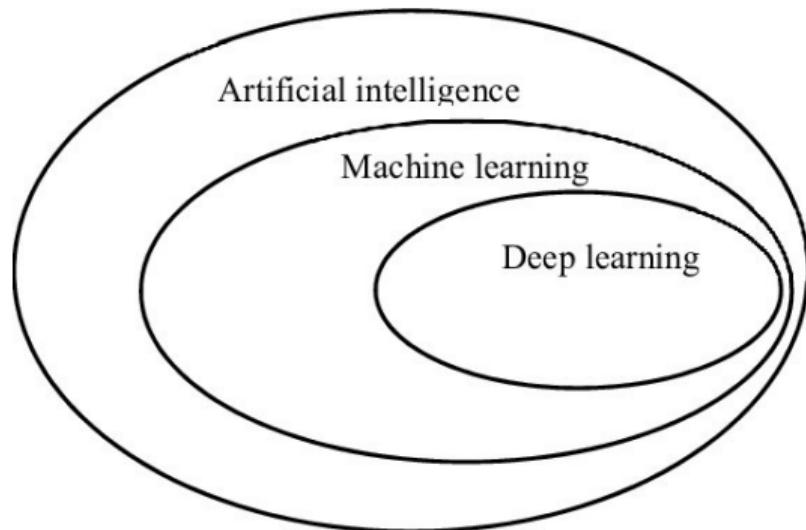
AI is the new electricity.

—Andrew Ng

In the same way that electricity transformed our world, AI will transform our world and will be incorporated into every aspect of our lives.

AI vs. Machine Learning vs. Deep Learning

- ▶ **AI:** The study of how to make computers intelligent.
- ▶ **Machine Learning:** A subfield of computer science that gives computers the ability to learn without being explicitly programmed.
- ▶ **Deep Learning:** A subfield of machine learning that uses neural-network-like structures and large amounts of data to learn.



Machine Learning - Self-Driving Cars



Machine Learning - Generative Models



DreamStudio
beta

MENU

- Dream
- History
- Prompt Guide
- Social
- FAQ
- Support

DreamStudio Lite



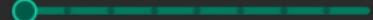
Painting of a cat playing the banjo, abstracted observed, minimal indication, thick outlines, contented peaceful, medium saturation with trichromatic similar hues

Dream



1.0 credits / image

The width of the generated image.



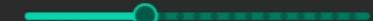
Height

The height of the generated image.



Cfg Scale

Cfg scale adjusts how much the image will be like your prompt. Higher values keep your image closer to your prompt.



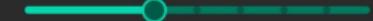
Steps

How many steps to spend generating (diffusing) your image.



Number of Images

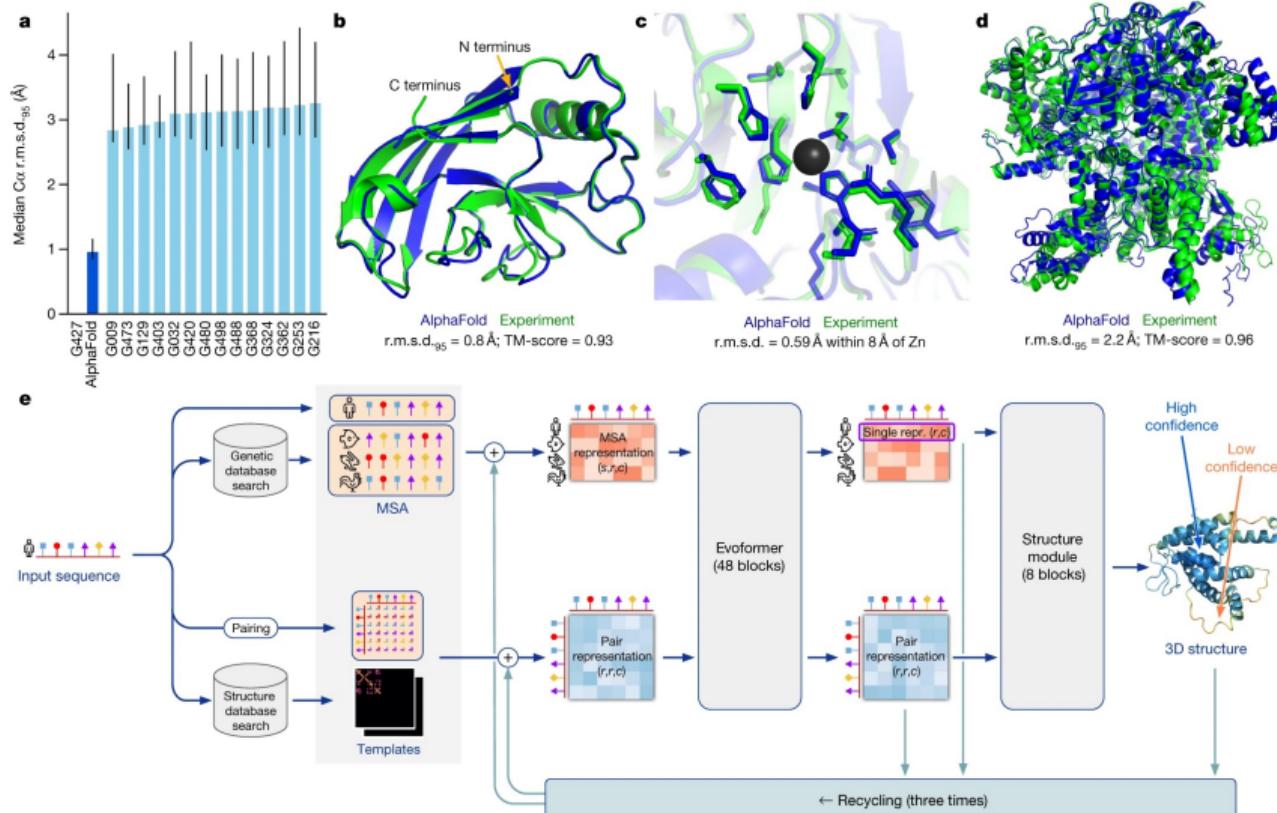
To generate multiple images from one prompt.



Sampler

The diffusion sampling method. Cannot be modified if CLIP Guidance is enabled.

Machine Learning - Protein Folding



Machine Learning - Protein Folding

The screenshot shows the homepage of the AlphaFold Protein Structure Database. At the top, there is a green header bar with the text "Highly accurate protein structure prediction with AlphaFold" and a "PubPeer" link. Below this is a dark blue navigation bar with links for EMBL-EBI, Services, Research, Training, About us, and a logo for EMBL-EBI. The main title "AlphaFold Protein Structure Database" is displayed prominently in white text against a blue background featuring a faint protein structure graphic. Below the title, it says "Developed by DeepMind and EMBL-EBI". A search bar at the bottom left allows users to search for proteins, genes, UniProt accessions, or organisms, with a "BETA" button next to it. Examples of search terms are provided: Free fatty acid receptor 2, At1g58602, Q5VSL9, E. coli, and Help: AlphaFold DB search help. A feedback link "Feedback on structure: Contact DeepMind" is also present.

"Highly accurate protein structure prediction with AlphaFold" has comments on PubPeer

EMBL-EBI Services Research Training About us EMBL-EBI

AlphaFold Protein Structure Database

Home About FAQs Downloads

AlphaFold Protein Structure Database

Developed by DeepMind and EMBL-EBI

Search for protein, gene, UniProt accession or organism

BETA

Search

Examples: Free fatty acid receptor 2 At1g58602 Q5VSL9 E. coli Help: AlphaFold DB search help

Feedback on structure: Contact DeepMind

Table of Contents

1. Course Overview
2. About Your Teacher
3. Scientific Computing Overview
4. Closing Advice

Closing Advice

- ▶ Find connections between your interest and what we will cover and explore those connections; always keep that in the back of your mind.
- ▶ There is no such thing as a dumb question; if you have a question or a gap in your understanding, ask about it as soon as possible.
- ▶ I am flexible about a lot of things if you come to me early and talk to me directly.
- ▶ I have a good sense of humor, so any class or research memes are encouraged.