

Introduction to Computational Methods

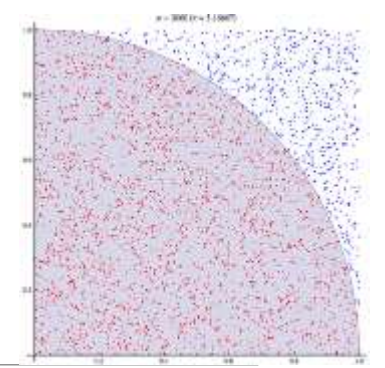
LECTURE 1

What is Computational Science?



- Computational Science is the “science” of representing a physical system in a computer to aid in understanding, designing or optimization of real systems.
- One way to understand nature (besides experimental or deductive/theoretical approach).
- Involves application of simulations or algorithms to replicate and better understand nature or real phenomena.
- Could also be concerned with development of algorithms that draw inspiration from systems/phenomena that occur in the real world (e.g. Ant foraging algorithms)

What is Scientific Computing?



- Development of algorithms for computer solution of large-scale problems in mathematics.” CSE Paper
- Comprises numerical algorithms for
 - Differential equations, *optimization algorithms*, discrete event simulations, or *Monte Carlo algorithms*.
- Scientific computing is part of computational science, but not the whole.
- https://kids.kiddle.co/Monte_Carlo_algorithm

Modeling and Simulation



- Modeling and Simulation important to computational science
- Modeling
 - Involves communication, experience, science philosophy
 - Many application sciences courses “teach” modeling as it applies to their domain (and use tools, such as GUIs)
 - But general problem of model building is not covered
- Types of Models
 - Evolutionary, Optimization, Statistical, Simulation, Grammatical, etc.

Modeling and Simulation

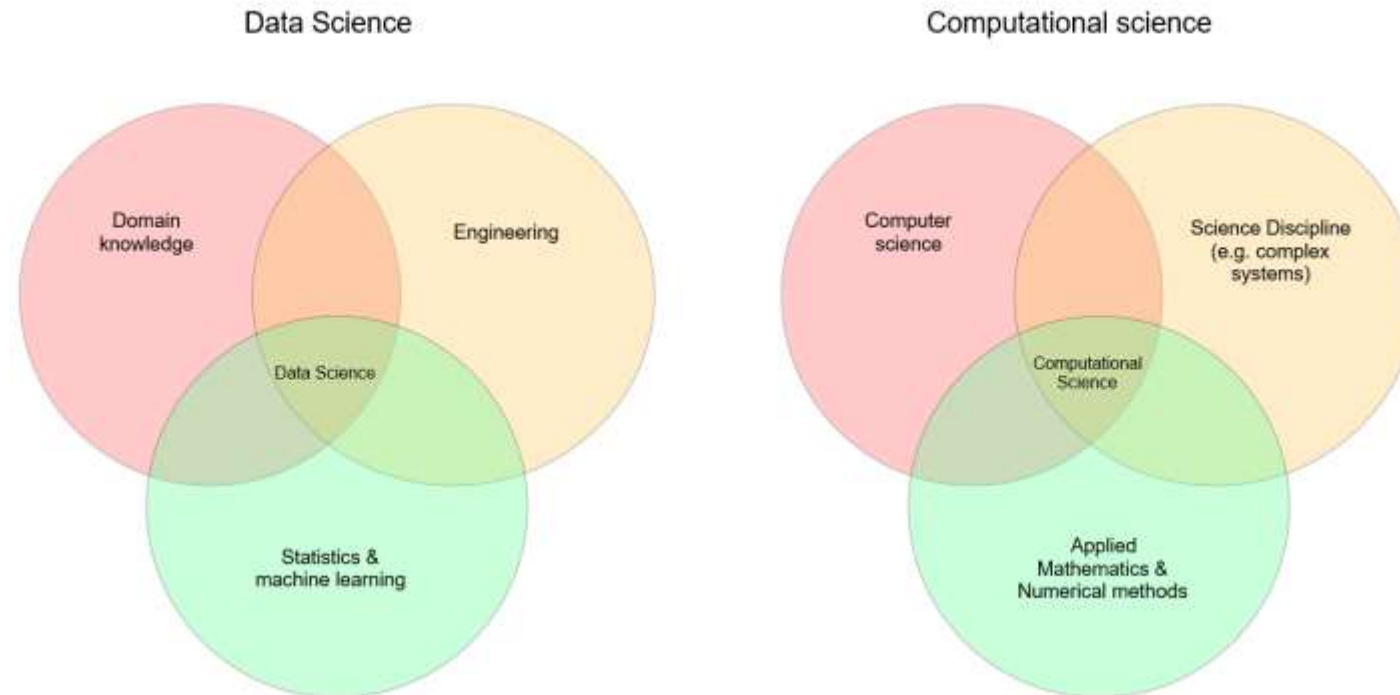
- Simulation
 - “Imitation of the operation of a real-world process or system over time. Simulations require the use of models; the model represents the key characteristics or behaviors of the selected system or process, whereas the simulation represents the evolution of the model over time.” [Wikipedia](#)



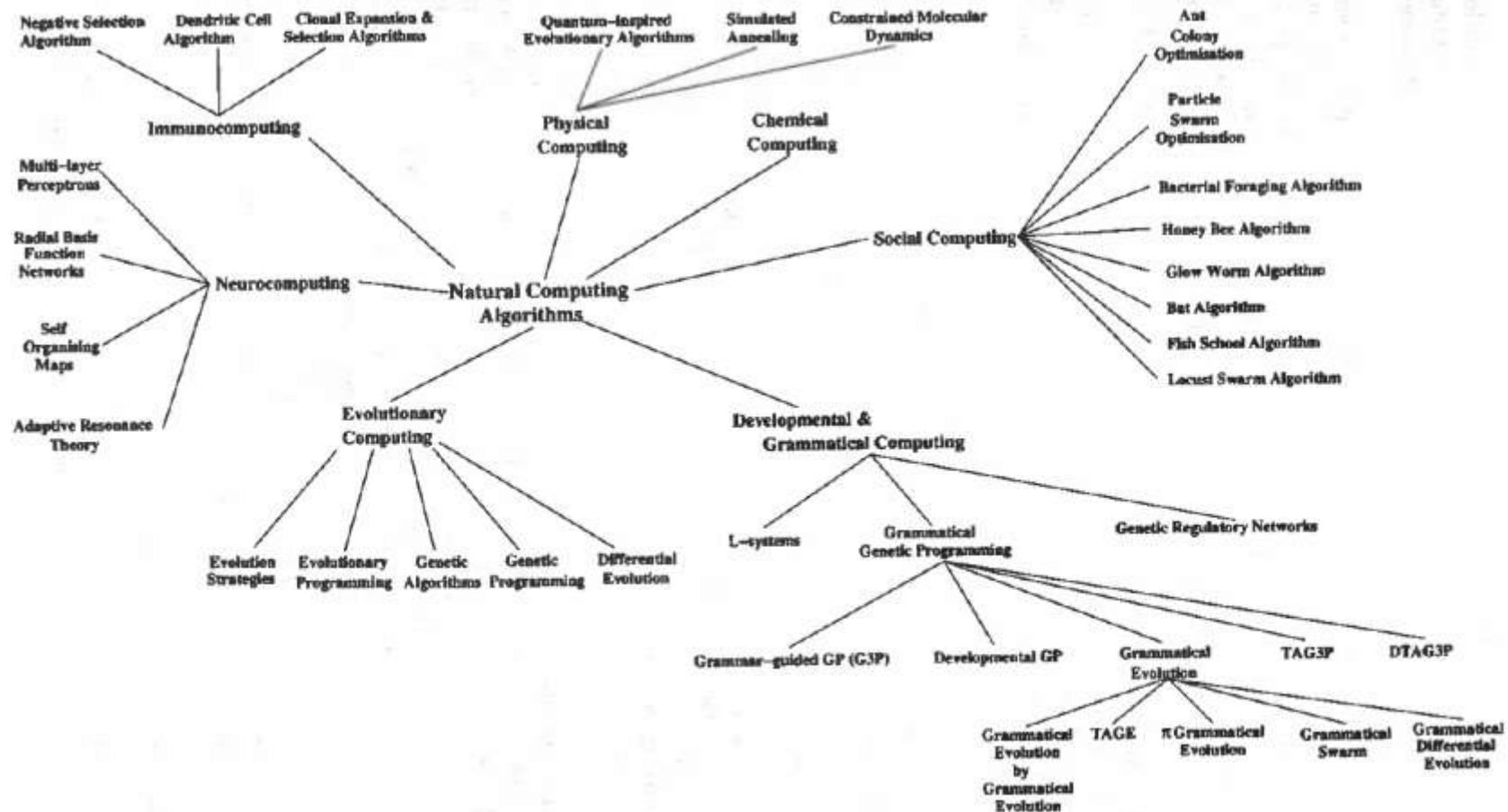
What is Data Science?

- Data science is an *interdisciplinary* field that uses scientific methods, processes, algorithms and systems to extract knowledge and insights from structured and unstructured data, and apply knowledge and actionable insights from data across a broad range of application domains. [Wikipedia](#)
- Relies on computer science (data structures, algorithms, visualization, big data support and general programming), statistics, and domain knowledge.

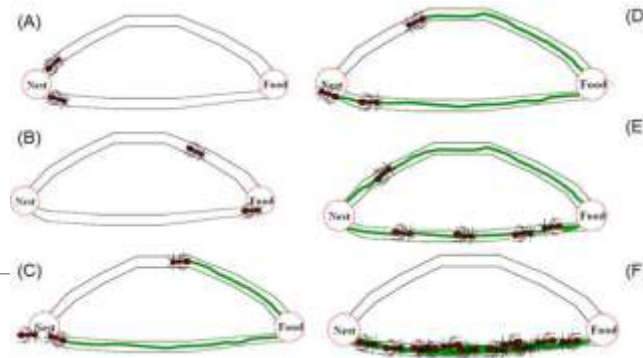
Computational Science: Multidisciplinary



Taxonomy of Nature Inspired Algorithms



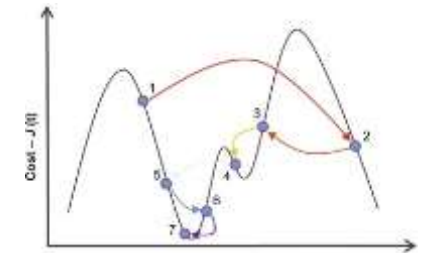
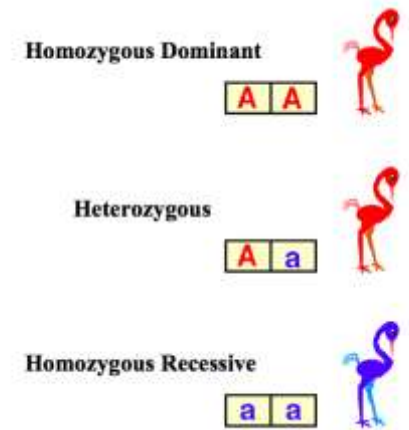
Examples

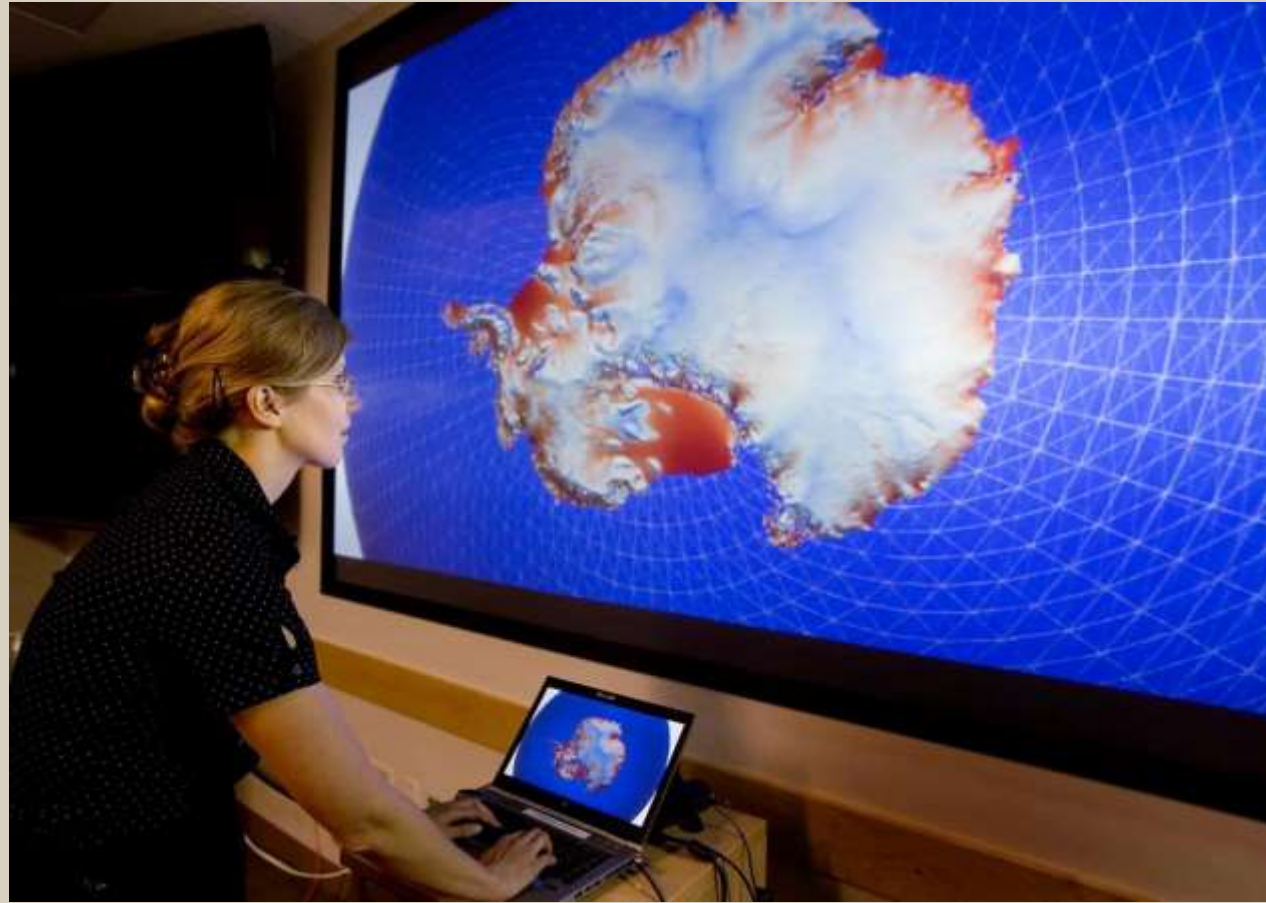


- Evolutionary
 - Genetic Algorithms – “DNA”, Selection (Survival of fittest), Mutations
 - Constrained Optimizations – Population Density
- Social Computing
 - Particle Swarm Optimization (PSO) – Fish, Bats, Birds, Locusts
 - Foraging algorithms, Ant, Honey Bee, Bacteria
- Neurocomputing – Model of the brain, predictions, classifications..
- Immunocomputing – Natural, Innate, Adaptive Immune Systems, useful for optimization and classification algorithms

Examples

- Developmental and Grammatical Computing
 - Genotype and Phenotype Mapping
 - Genome encoding
 - Image compression
- Physically Inspired Computed
 - Simulated Annealing – interactions of physical bodies (atomic, quantum level)
- Plant Inspired Algorithms
 - Root Foraging
 - Adaptive algorithms (Sunflowers)
- Chemically Inspired Algorithms – emerging area (Chemical reactions)





Irina Tezaur (8700), a 2019 recipient of the Presidential Early Career Award for Scientists and Engineers, examines the computer modeling of land ice evolution in Antarctica, a model for which she was a lead developer. (Photo by Dino Vournas)