SMCEF 23/24

Review

What did we see

- Quick review of python and introduction to numpy and pyplot
  - Forest fires simulation
- Monte Carlo simulations
  - Random walk, simple, self-avoiding and growing self-avoiding
  - Ising model of Ferromagnetism
- Initial Values Problems numerical methods
  - Euler and Euler-Cromer methods
  - High order methods - Runge-Kuta 2nd and higher order methods
  - Implicit methods

What did we see? 2

- Brief introduction/review of computer architecture
- Brief introduction to complexity theory
- Introduction to multiprocessing within python
  - Conflicts when multiple processes write on the same memory
  - Cache misses take on efficiency
- Tools to measure execution time and most costly code sections
  - timeit
  - prun, profilers

But also...

Any minimally complex code should be approach as an **engineering** project!

Plan before type

Measure before and after any optimization attempt. Have at least an educated guess what would be the improvement expected and compared it with the one obtained!

But also… 2

What are the model parameters

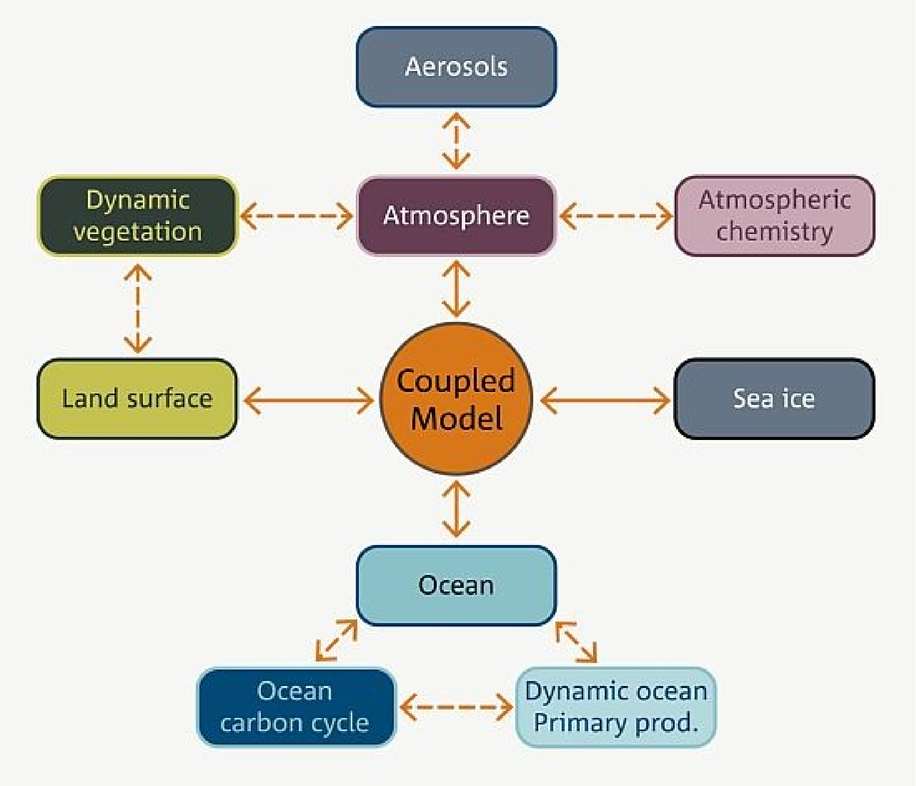
What are the model/method meta-parameters

Are the results obtain a good approximation to the system being modeled/simulated?

What we have not seen

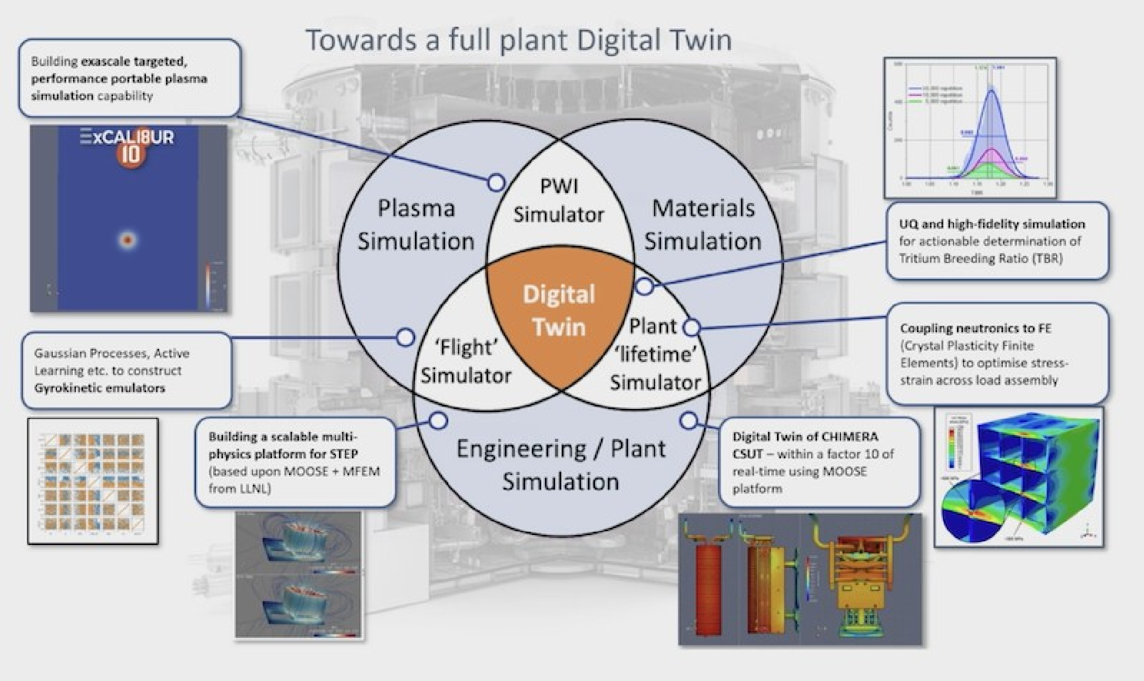
- Fine Element Models
- Optimization methods
- Diffusion, scattering and transport models
- Adaptive time steps methods
- Interaction between several models – having simultaneously different models modeling different aspects of the system and interacting with each other
- And a lot more ...

Climate Models



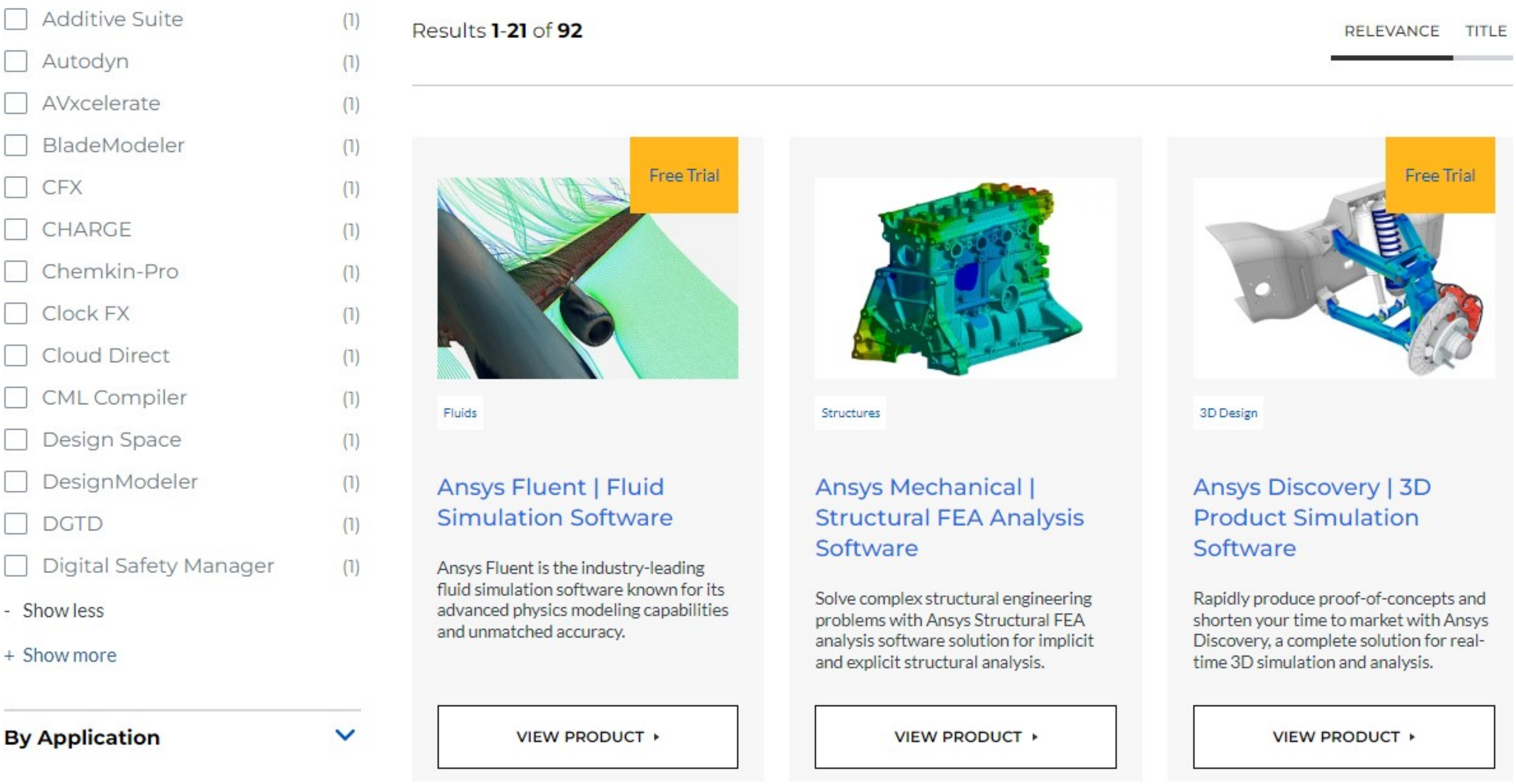
CLIMATE CHANGE IN AUSTRALIA

Fusion plant modeling



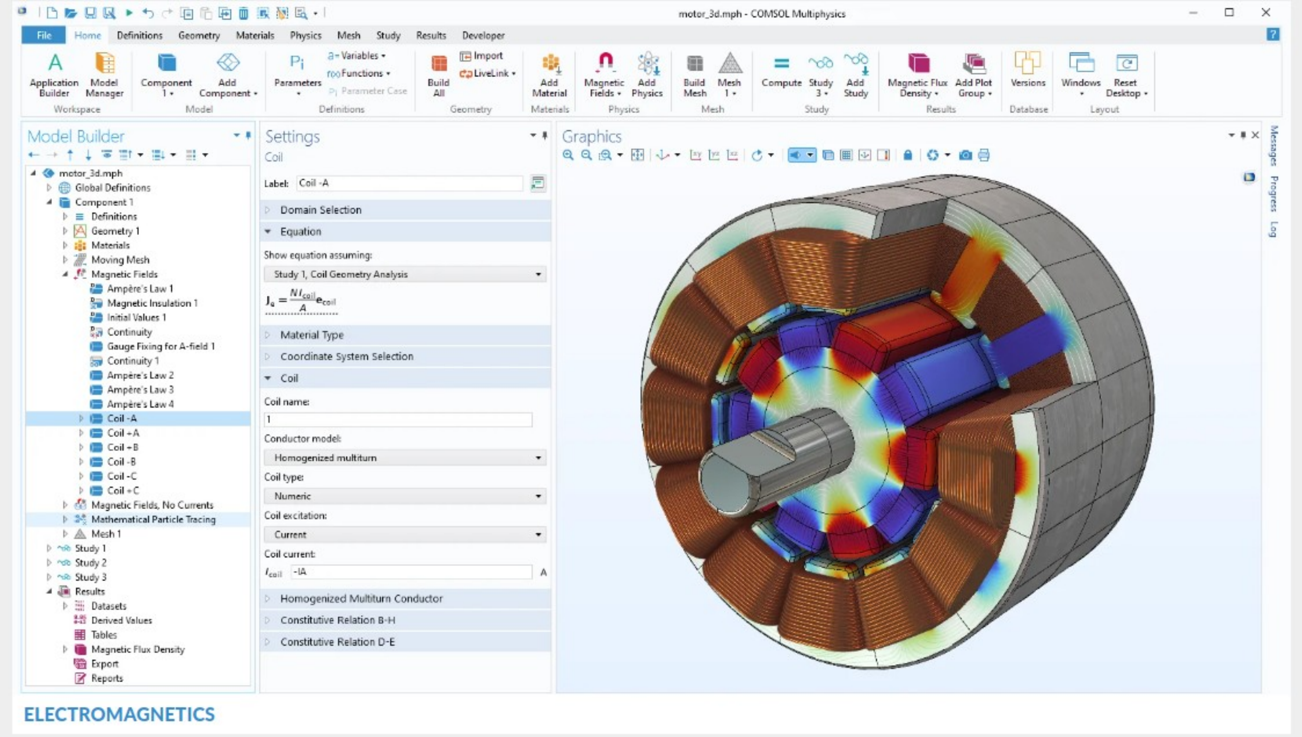
The Grand Challenge of Simulating Nuclear Fusion: An Overview with UKAEA's Rob Akers

Modeling and simulation software



Ansys

Modeling and simulation software

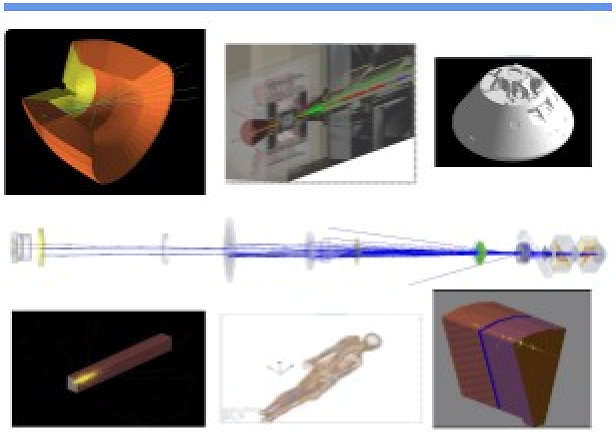


Comsol

Modeling and simulation software

Geant4

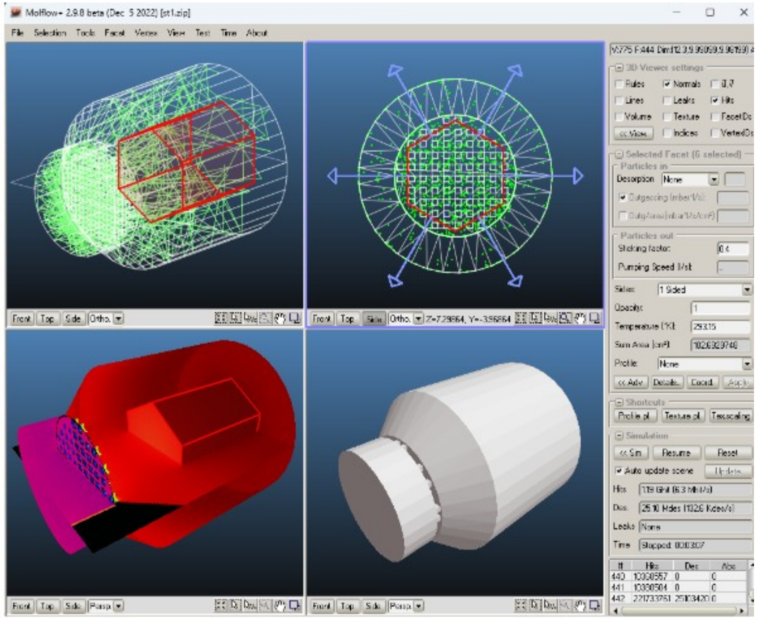
Toolkit for the simulation of the passage of particles through matter. Its areas of application include high energy, nuclear and accelerator physics, as well as studies in medical and space science.

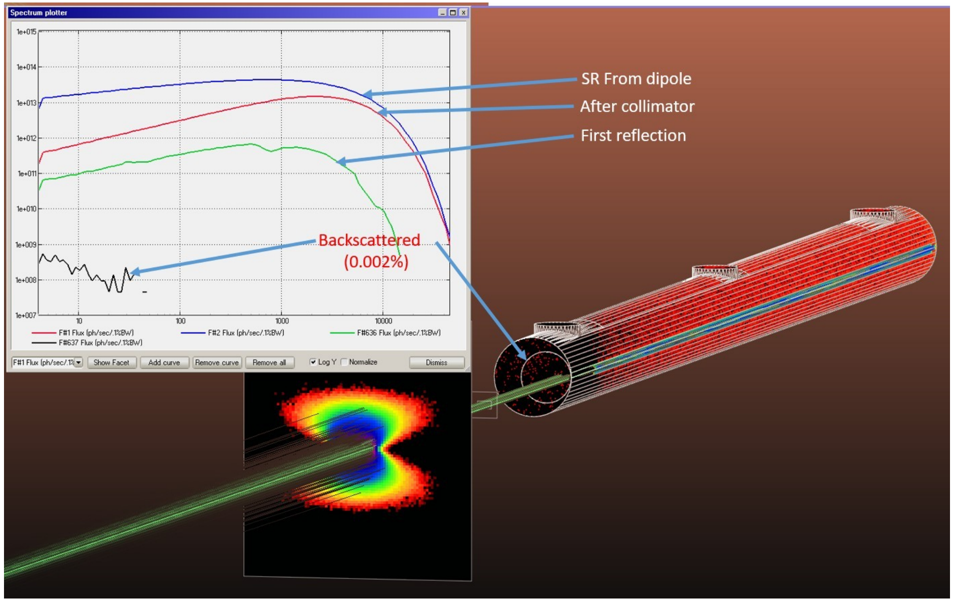


Geant4

Modeling and simulation software

MolFlow+

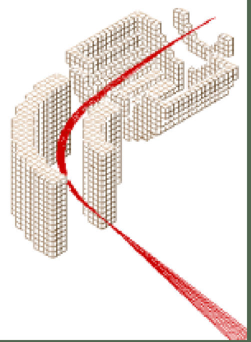




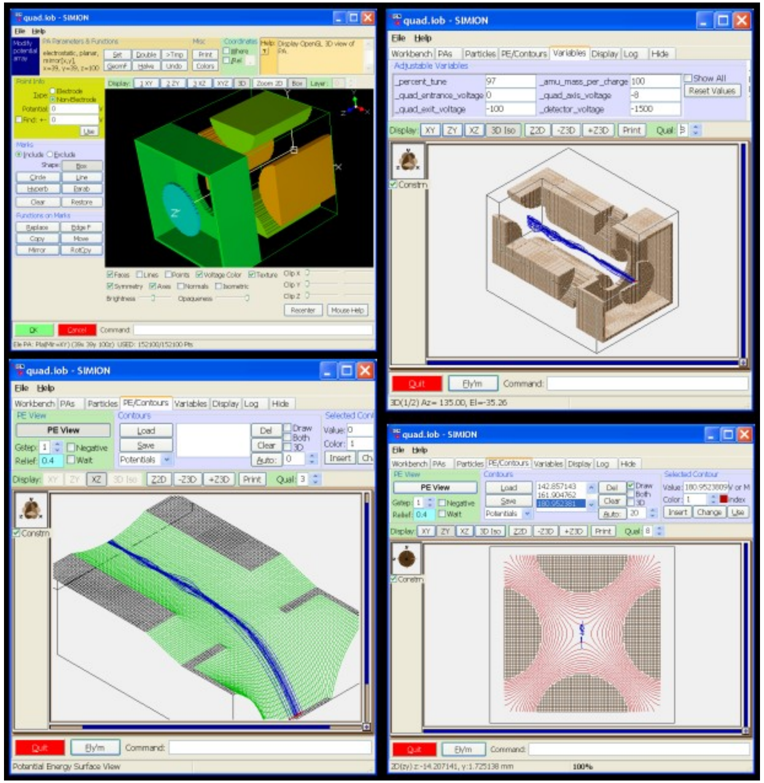
Molflow+/Synrad+

Modeling and simulation software

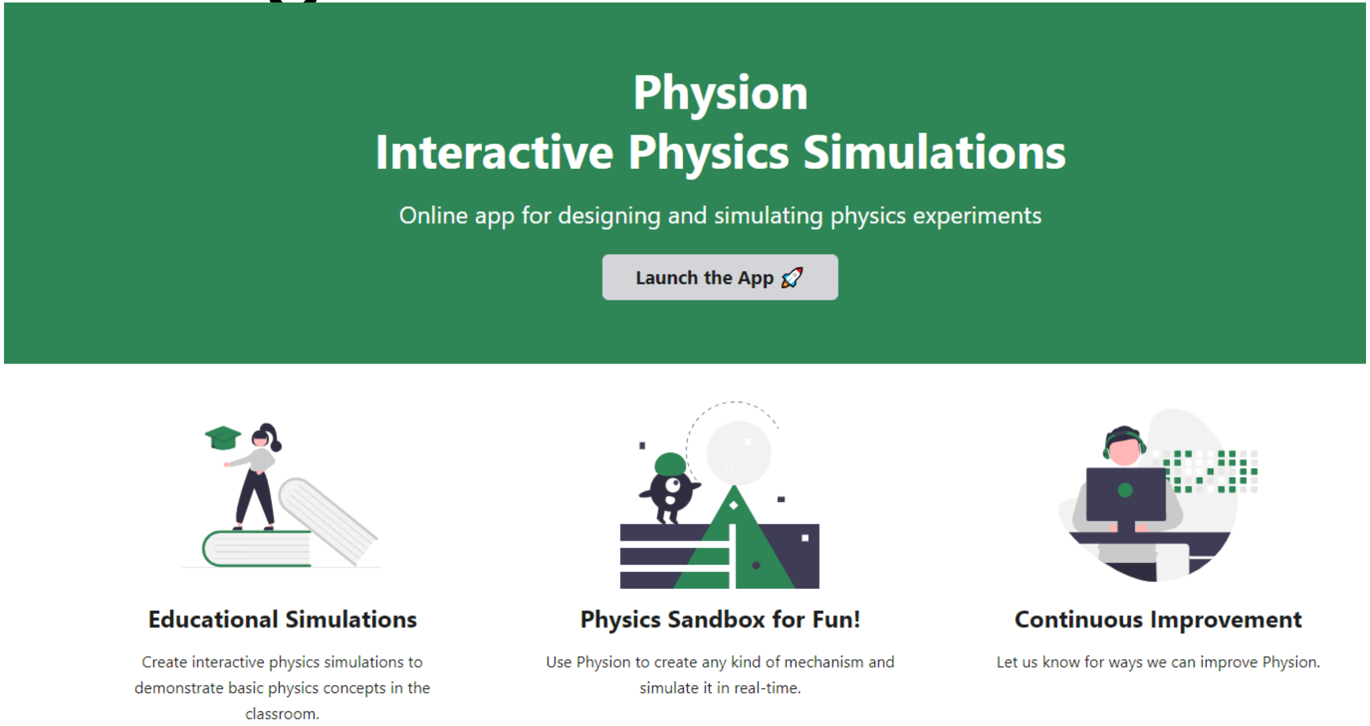
SIMION® Version 2020



Overview: SIMION is a software package primarily used to calculate electric fields and the trajectories of charged particles in those fields when given a configuration of electrodes with voltages and particle initial conditions, including optional RF (quasistatic), magnetic field, and collisional effects. In this, SIMION provides extensive supporting functionality in geometry definition, user programming, data recording, and visualization. It is an affordable but versatile platform, widely used for over 30 years to simulate lens, mass spec, and other types of particle optics systems.



Modeling and simulation software

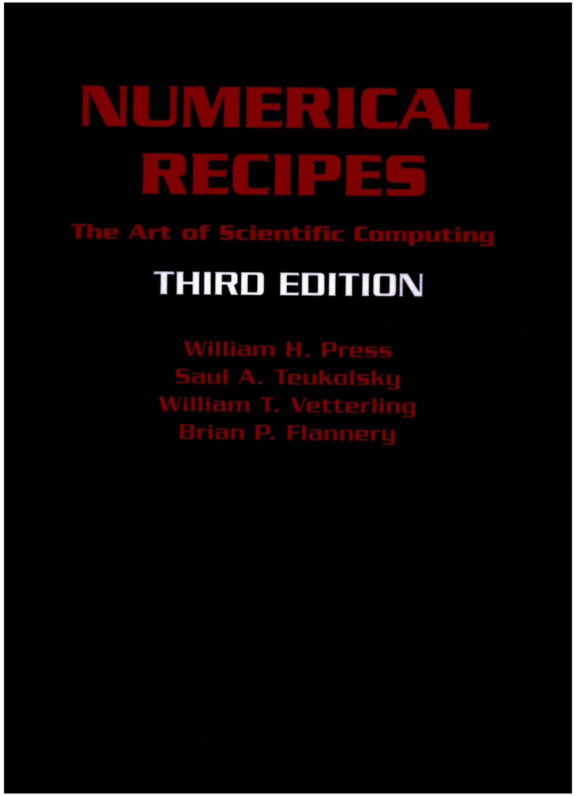


Physion

Sources

- Computer Science course
  - Computer Architecture
  - Operation System Foundations
  - Computer Theory
  - Algorithms and Data Structures
  - Algorithm Analysis and Design
  - Concurrency and Parallelism
  - High Perfomance Computation

Sources



Numerical Recipes:
https://numerical.recipes/

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

https://github.com/geographerwang/Numerical-Recipes

Sources

- MITx • 6.00.1x - Introduction to Computer Science and Programming Using Python
- MITx • 6.00.2x - Introduction to Computational Thinking and Data Science
- MITx • CSE.0002x - Introduction to Computational Science and Engineering
- UChicagoX • PS280x - Modeling Climate Change

Future

- Read the help information of the functions you use, explore the algorithms used
- Parallel computation – Single machine, clusters, supercomputers
- Accelerators:
  - GPU
  - Quantum Computers