Piotr Luszczek

Introduction

to

Numerical Libraries for Linear Algebra

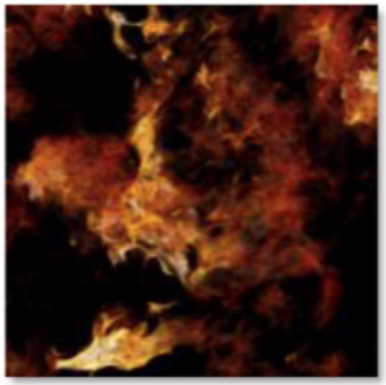
January 10, 2017

Topics and Schedule

- General topics
  - Tuesday Jan 10 Hardware for numerical software
    - Lab: download, install, test
  - Wednesday Jan 11 CUDA: beyond basics. Libraries' basics
    - Lab: nvprof, nvvp, measure performance, locate bottlenecks
  - Thursday Jan 12 Numerical libraries: dense, batch
    - Lab: profiling libraries
  - Friday Jan 13 Numerical libraries: batch (cont.), sparse
    - Lab: profiling libraries
- Schedule
  - 9:30-11:00 Lecture
  - Break
  - 11:30-13:00 Lecture
  - Lunch break
  - 14:00-17:00 Lab

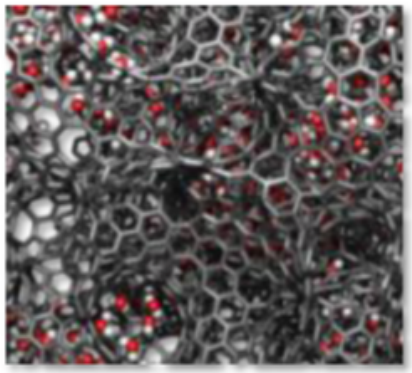
Computational Science

Applications to Energy



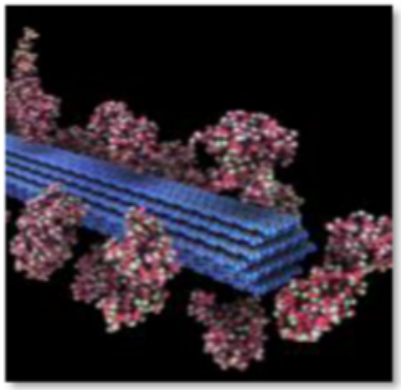
Turbulence

Understanding the statistical geometry of turbulent dispersion of pollutants in the environment.



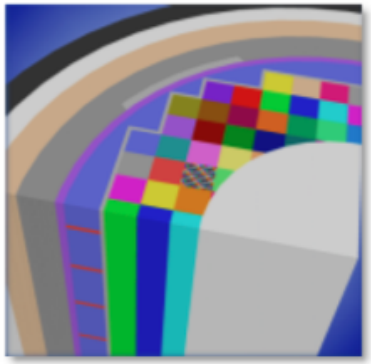
Energy Storage

Understanding the storage and flow of energy in next-generation nanostructured carbon tube supercapacitors



Biofuels

A comprehensive simulation model of lignocellulosic biomass to understand the bottleneck to sustainable and economical ethanol production.

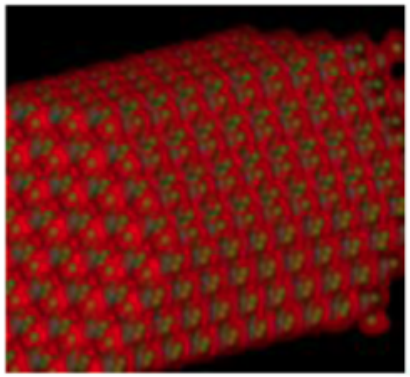


Nuclear Energy

High-fidelity predictive simulation tools for the design of next-generation nuclear reactors to safely increase operating margins.

Smart Truck

Aerodynamic forces account for ~53% of long haul truck fuel use. ORNL's Jaguar predicted 12% drag reduction and yielded EPA-certified 6.9% increase in fuel efficiency.



Nano Science

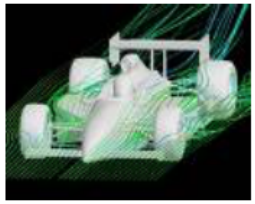
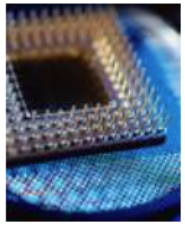
Understanding the atomic and electronic properties of nanostructures in next-generation photovoltaic solar cell materials.

Source: Steven E. Koonin, DOE

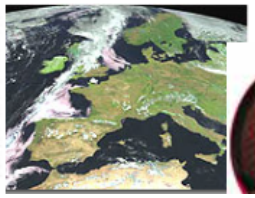
Industrial Use of Supercomputers

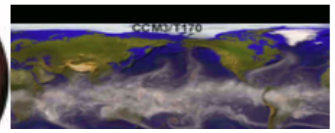
50% of the 500 fastest supercomputers worldwide are used by industry





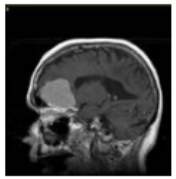





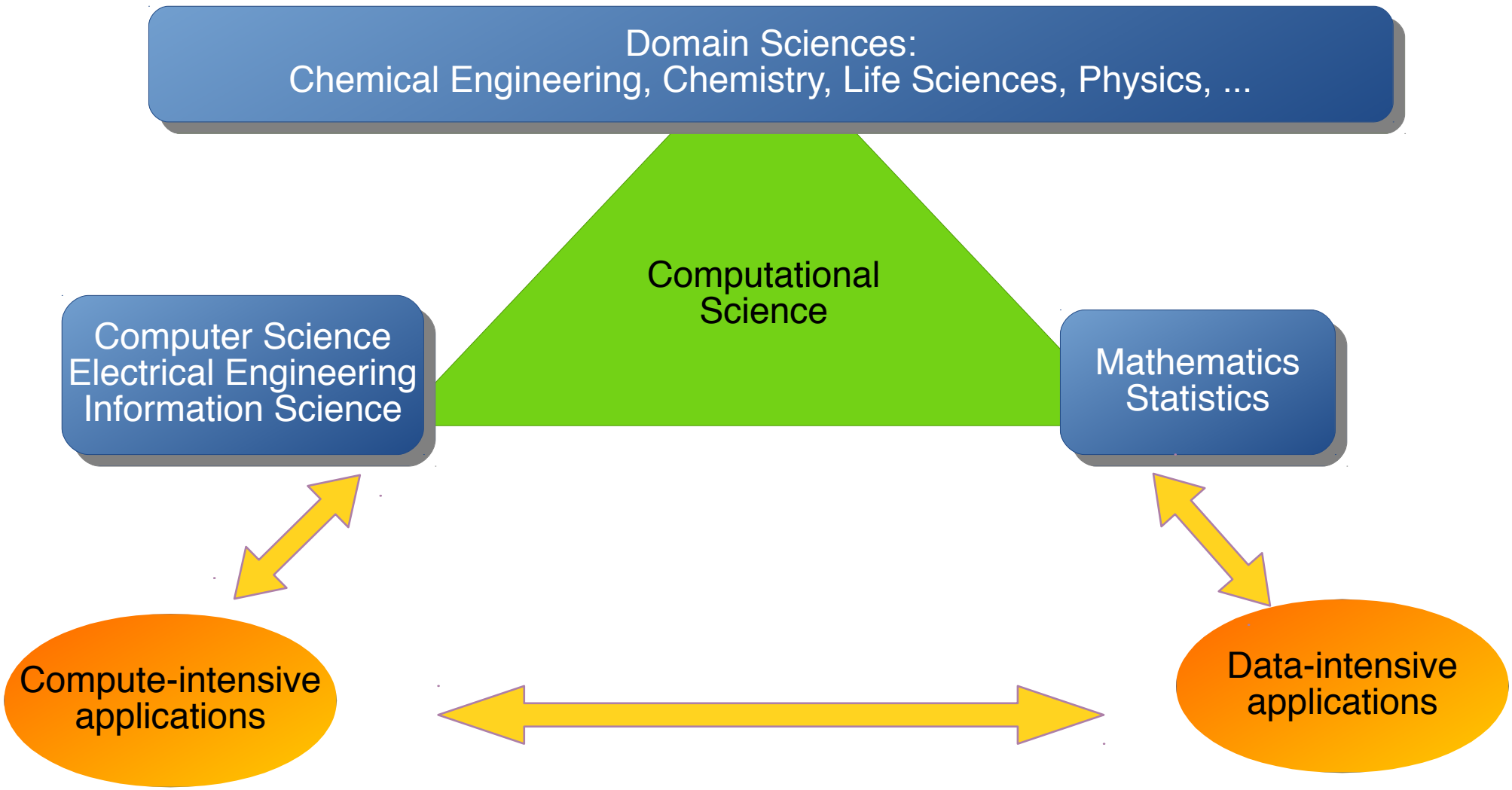

- Aerospace
- Automotive
- Biology
- CFD
- Database
- Defense
- Digital Content Creation
- Digital Media
- Electronics
- Energy
- Environment
- Finance
- Gaming
- Geophysics
- Image Proc./Rendering
- Information Processing Service
- Information Service
- Life Science
- Media
- Medicine
- Pharmaceutics
- Research
- Retail
- Semiconductor
- Telecomm
- Weather and Climate Research
- Weather Forecasting






Computational Science Fuses 3 Elements



Units of Measure

- High Performance Computing (HPC) units are:
  - flop: floating point operation, usually double precision unless noted
  - flop/s: floating point operations per second
  - bytes: size of data (a double precision floating point number is 8)
  - Note: computer scientists like to abbreviate byte(s) as B forgetting about units of loudness (Bells): dB.
- Typical sizes are millions, billions, trillions…

Mega	Mflop/s = 10^6 flop/s	MiB = 2^{20} = 1048576 ~ 10^6 bytes
Giga	Gflop/s = 10^9 flop/s	GiB = 2^{30} ~ 10^9 bytes
Tera	Tflop/s = 10^{12} flop/s	TiB = 2^{40} ~ 10^{12} bytes
Peta	Pflop/s = 10^{15} flop/s	PiB = 2^{50} ~ 10^{15} bytes
Exa	Eflop/s = 10^{18} flop/s	EiB = 2^{60} ~ 10^{18} bytes
Zetta	Zflop/s = 10^{21} flop/s	
Yotta	Yflop/s = 10^{24} flop/s	

- Currently fastest (public) machine ~ 90 Pflop/s (www.top500.org)

More Units: Power and Energy

- Power
  - Watt
    - Single server chip: 100, 200, 300 W
  - MW
    - Supercomputer: 10 MW
    - Data center: 50 MW
- Energy
  - Joule
    - Single register instruction: 1 pJ
  - kWh
    - Electricity cost: 10 cents per kWh

Looking at the Gordon Bell Prize

- Founding principles and goals
  Recognize outstanding achievement in high-performance computing applications and encourage development of parallel processing
- 1988 1 Gflop/s Cray Y-MP 8 Processors
  - Static finite element analysis
- 1998 1 Tflop/s Cray T3E 1024 Processors
  - Modeling of metallic magnet atoms, using a variation of the locally self-consistent multiple scattering method
- 2008 1 Pflop/s Cray XT5 $1.5*10^5$ Processors
  - Superconductive materials
- 2018(?) 1 Eflop/s ??? 10^7 Processors (10^9 threads)
  - Machine learning? Artificial Intelligence?