CS-E4002 - Special Course in Computer Science D: Large-scale Computing and Data Analysis

2 – Presentation of topics

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23.4.2021

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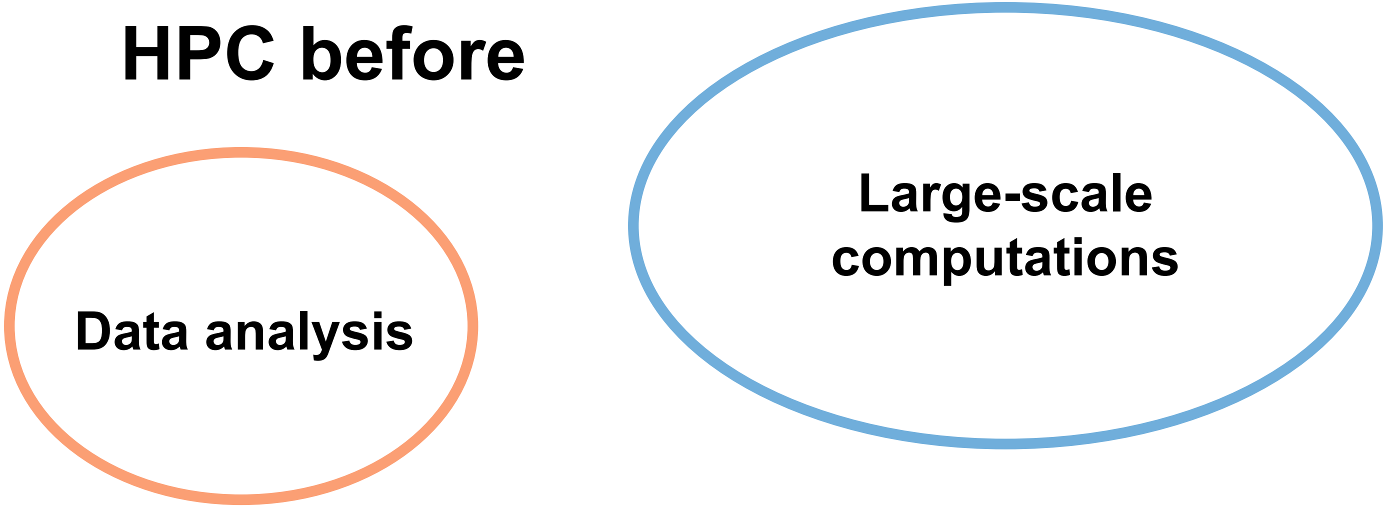
Context

HPC before

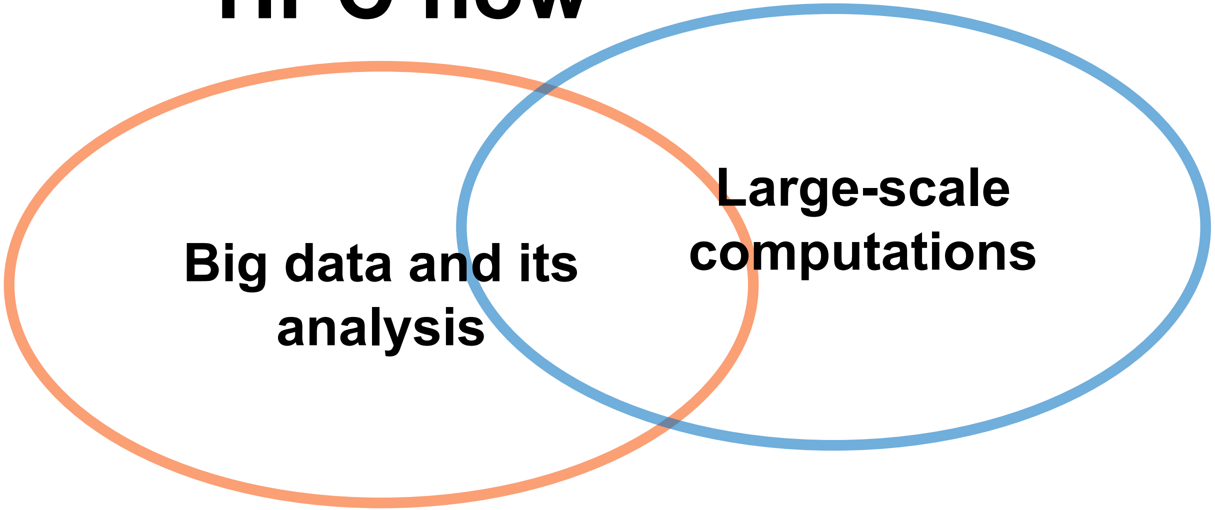


Data analysis

Large-scale computations

Context

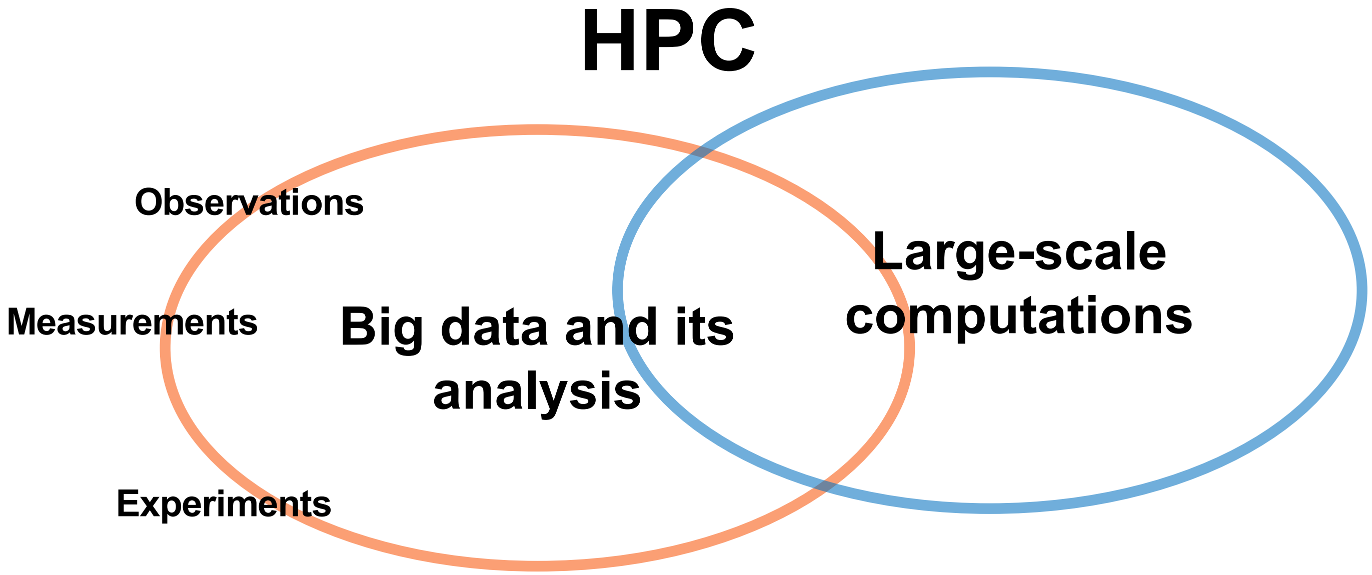
HPC now



Big data and its analysis

Large-scale computations

Sources



HPC

Observations

Measurements

Experiments

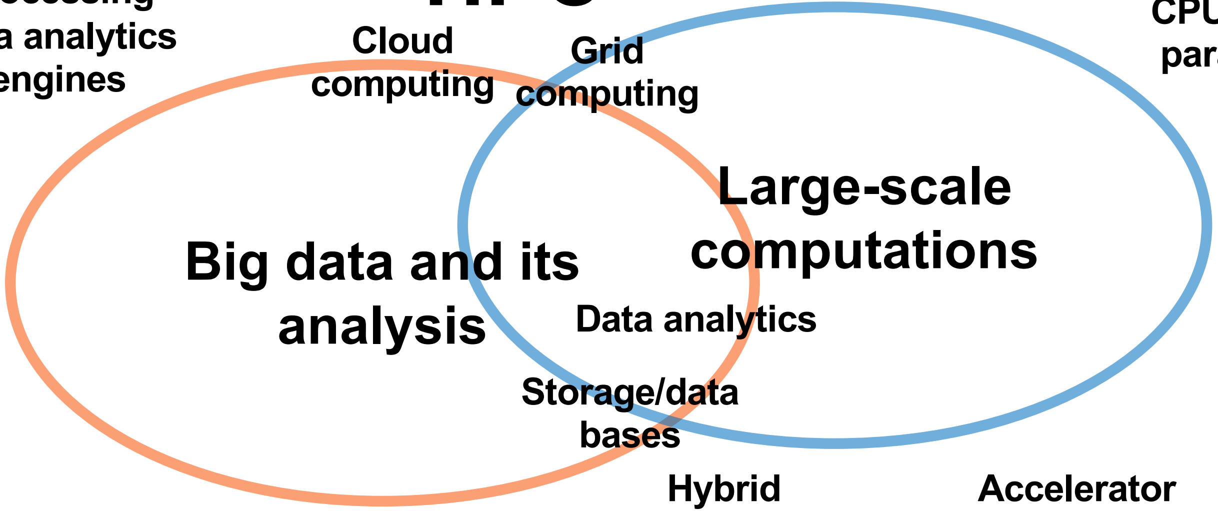
Big data and its analysis

Large-scale computations

Simulations of complex systems:

- physics
- chemistry
- Engineering
- …

Concepts



HPC

Stream processing data analytics engines

Cloud computing

Grid computing

CPU + MPI paradigm

Big data platforms

Big data and its analysis

Large-scale computations

Data analytics

Storage/data bases

Ingest systems

Hybrid architectures

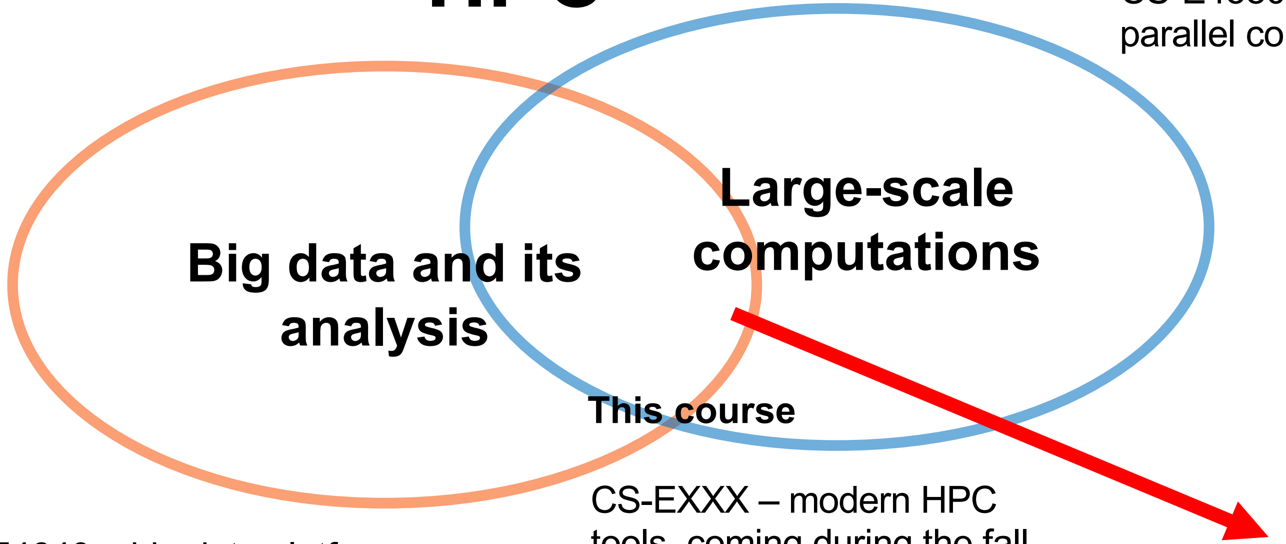
Accelerator paradigms

Batch processing data analytics engines

Course coverage at CS

HPC

CS-E4580 – programming parallel computers



Big data and its analysis

Large-scale computations

This course

CS-E4640 – big data platforms

CS-EXXX – modern HPC tools, coming during the fall 2021

The following two topics

Acute issues I, LS computing

- **Arithmetic performance** is currently increasing faster than the **memory and network bandwidth**: **communication** has become the bottleneck of HPC computing at large scale
- Optimizing for data movements has become a key issue in designing and implementing solvers for complex systems.
- Data analysis on-the-fly will/must be sacrificed from efficiency point-of-view
- Currently, in a communication-bound applications you end up **”dumping” mammoth-sized system states to be analyzed in post-processing**

Data analysis pipeline for LS computing application

- How do we perform the data analysis?
- Can modern data analytics engines (such as Hadoop/Spark,…) provide us with efficient solutions?

Possible project: Develop a data analysis pipeline, where a typical system state (as a binary blob), from a complex system simulation, is ingested to (e.g.) Apache Spark, and perform some typical wanna-make reductions (e.g. compute averages, probability distribution functions) on it, and assess the performance. One type of mystery data set will be provided, containing a feature that you should extract, or you can produce/bring in your own data set.

Acute issues II, LS computing

- The situation is made even worse by the **emergence of accelerator platforms, such as graphical processing units (GPUs).**
- Even more arithmetic power, the communication bound limit is reached even earlier.
- Design and implementation of algorithms needs to be done keeping the hardware in mind at all times; from safe, sound, and easy to uncharted, ever changing, and complicated
- Learning this paradigm **is a must if you desire to do the biggest and coolest simulations existing**.

Learn to use a multi-node GPU solver

- Some solutions exist already, and have been designed in a way that generic computations of certain types are easy
    - Stencil operations
    - E.g., domain specific language (DSL)

Possible project: Learn to use the MPI-aware Cuda library Astaroth to perform stencil operations. Choose a problem from your own field of study, implement it with the DSL, and assess what you can achieve with it. Or, use an existing setup for magnetised fluids, and study the problematics of communication bound systems.

Topic: funcX for large-scale computing

- **How does HPC/large-scale data analytics benefit from the emerging function-a-a-service (serverless) computing model?**
- **funcX is an attempt to enable function-as-a-service for HPC**
  - Very recent development
- **Our goal is to evaluate funcX**
  - We need to evaluate it to support domain scientists and further development function-a-a-service features for HPC

Topic: human-in-the-loop for ML/data analytics workflows

- **Human-in-the-loop is critical for steering and tuning the analytics**
  - large-scale analytics is very expensive (resources and energy)
  - Can human interactions prevent the analytics leads to useless results or the analytics failure in the middle of analytics
- **How do we support human-in-the-loop with current known ML/analytics tools/workflows?**
  - which kind of human tasks and how to integrate humans into the workflows?

Topic: GPU and containers

- **Virtualization of GPUs for HPC with containers: a way to achieve portable HPC application deployment for HPC workload with GPU?**
  - Ease the management of Deep learning/ML deployment in GPU-enabled HPC systems
- **What kind of supports and how to manage an ensemble of containerized GPU nodes for the user?**
  - HPC systems have many different rigorous ways to acquire resources → sometimes it is not easy for the user to manage an ensemble for application-specific workload

Topic: data locality optimization patterns for modern data analysis

- **Modern ML/data analysis**
  - Involve data sources and data movement between cloud storage, HPC shared file systems and specific cluster node local file systems
  - Different types of workload might require different ways of handling data locality and movement
- **What would be suitable design patterns, best practices?**
  - Which data movement and buffering strategies are useful for which situations?