

# SF2568: Parallel Computations for Large-Scale Problems

*Lecture 1: Introduction*

January 16, 2024

## Acknowledgements

These slides are an extension of slides by Michael Hanke and Niclas Jansson.

## What is Parallel Computing?

The traditional and basic way software has been written is for *serial* computation

- To be run on a single computer having a single Central Processing Unit (CPU)
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In the most basic form, *parallel computing* is the simultaneous use of multiple compute resources to solve a computational problem

- To be run on multiple CPU cores
- A problem is broken into discrete parts that can be solved concurrently
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The compute resources can include

- A single computer with multiple processors
- An arbitrary number of computers connected by a network
- A combination of both

The computational problem usually demonstrates characteristics such as the ability to

- Be broken apart into discrete pieces of work that can be solved simultaneously
- Execute multiple program instructions at any moment in time
- Be solved in less time with multiple compute resources than with a single compute resource

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## Why Parallel Computations?

The primary reasons for using parallel computing

- Save time - wall clock time
- Solve larger problems

Other reasons might include

- Taking advantage of non-local resources
- Overcoming memory constraints
- Cost saving

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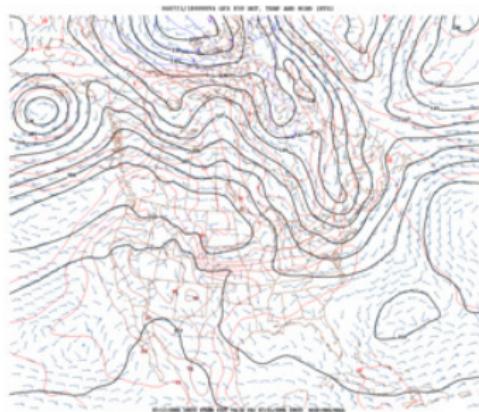
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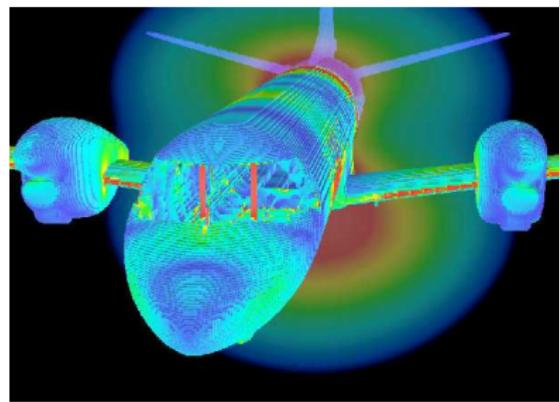
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# Weather Prediction

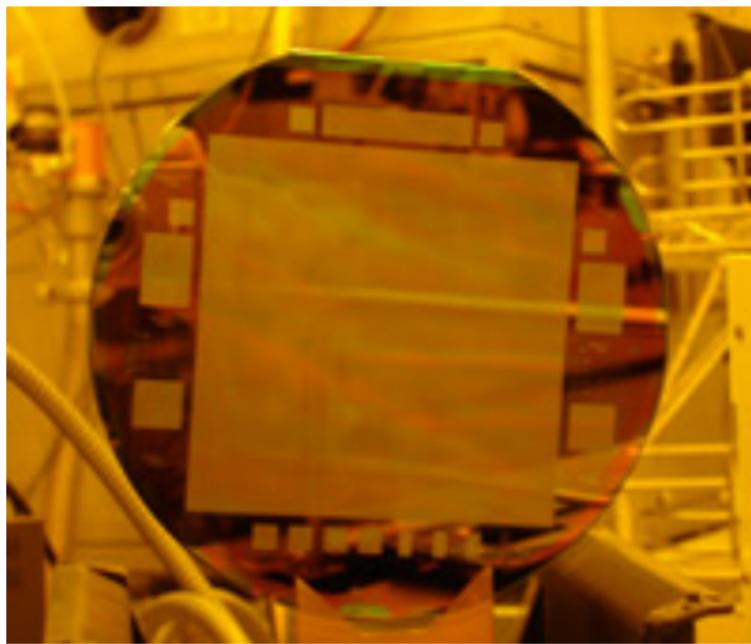


# Computational Electromagnetics

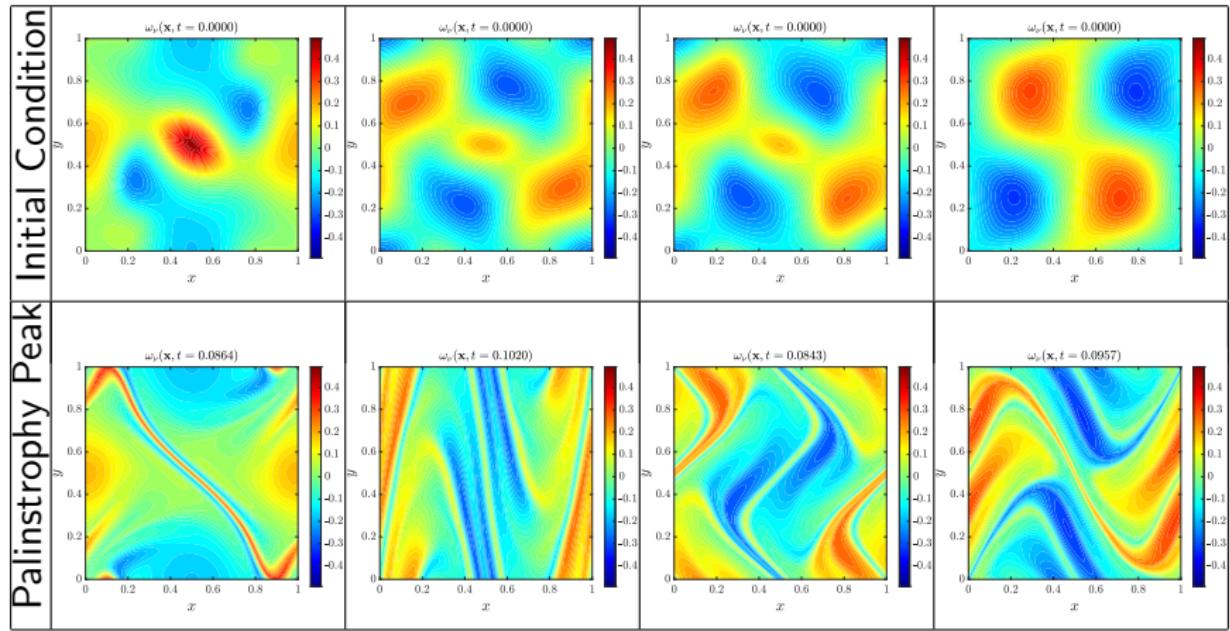


# Real-Time Image Processing

Digital Video Broadcasting (HD-TV)



# Analytic Mathematical Problems



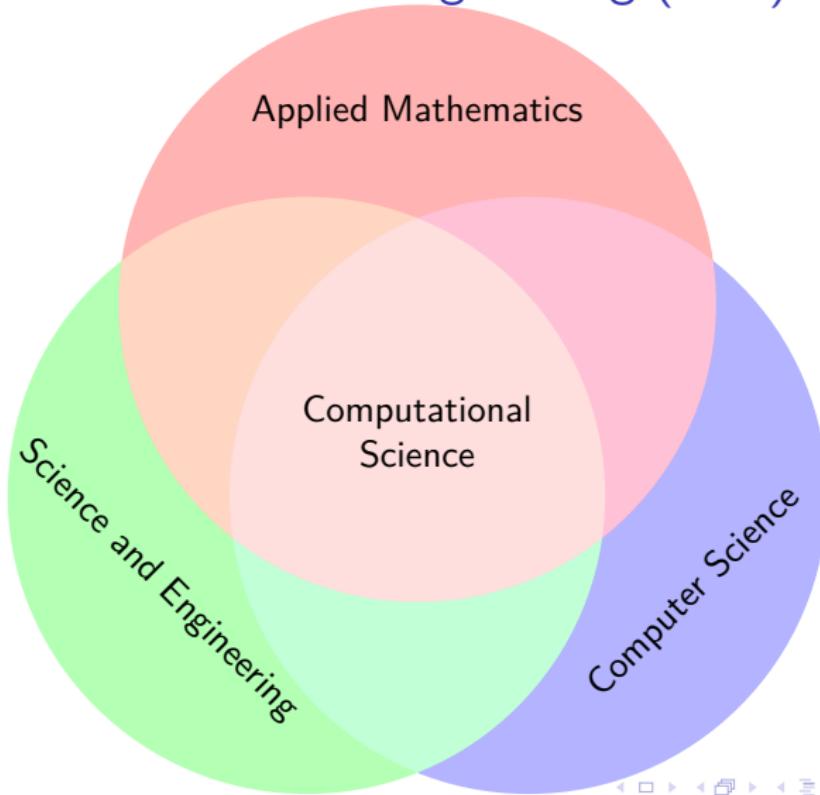
# Computational Science and Engineering (CSE)

- Examples from life sciences (molecular biology), material science (phase transition in welding), fluid dynamics (turbulence)
- The era of petascale computing has been a breakthrough for CSE, with more than 1,000,000,000,000 floating point operations (FLOPs) per second

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# Computational Science and Engineering (CSE)



## Why is Parallelism Necessary

There are limits to serial computing - both physical and practical reasons pose significant constraints to simply building faster serial computers. Parallel computing

- Increases computational power since FLOP rates are limited by the speed of light (30 cm/nanosecond) and molecule sizes, and the transmission limit of copper wire (9cm/nanosecond)
- Increases memory/disk speed, as processor speed on the chip outperform memory/disk subsystem by far
- Avoids communication of distributed data

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## Why is Parallelism Programming Interesting

A well behaved single processor algorithm may behave poorly on a parallel computer, and may need to be *reformulated numerically*

*There is no magic compiler that can turn a serial program into an efficient program all the time and on all machines*

- Performance programming involving low-level details: heavily application dependent
- Irregularity in the computation and its data structures forces us to think even harder. Parallel programs are not naturally deterministic
- Users don't start from scratch — they reuse old code. *Code lives longer than you expect!*

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## Aim of the course

### From the students' handbook

*The goal of the course is to provide a basic understanding of how to develop algorithms and how to implement them in distributed memory computers using the message-passing paradigm*

## Aim of the course

This understanding means that after the course you are able to

- explain *parallelization strategies*
- select and/or develop an algorithm for solving a given problem which has the potential for an efficient parallelization
- select and/or develop data structures for implementing parallel computations
- theoretically analyze a given parallel algorithm with respect to efficiency
- implement a given algorithm on a distributed-memory computer using the message passing library *MPI*
- understand the message flow and avoid unwanted situations (e.g. deadlock, synchronization delays)
- modify and adapt a set of basic routines to special situations
- experimentally evaluate the performance of a parallel program
- explain differences between the theoretically expected performance and the practically observed performance
- understand the challenges of *Green Computing*

## (Preliminary!) Overview of the Course

- Basic ideas of parallel computations
- An Introduction To MPI
- Image Reconstruction And Poisson's Equation
- Matrix-Vector Multiplication And Collective Communication
- Linear Systems of Equations
- Parallel Sorting
- Algorithms On Graphs
- Advanced Topics

# Practical Details

- Prerequisites
  - Basic course in numerical analysis and programming (C, C++ or Fortran). A short introduction to Fortran (or C) will be provided
- Grading
  - Homework assignments (3 assignments, in a group of at most 2 students)
  - A midterm quiz
  - Larger project, topic chosen yourself
- Computer assignments on Dardel at PDC
  - Fastest supercomputer in Sweden
  - Apply for a PDC account [here](#)
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# Examination

The course consists of two components, HEMA and PROA:

- Assignment evaluation and mid-term quiz (HEMA, 4.5 credits):  
There will be 3 assignments and 1 quiz, consisting of Assignment 1 (15 pts), Assignment 2 (12 pts), Assignment 3 (12 pts), the Quiz (17 pts). Maximum number of points is 56 pts for this portion of the course. In order to pass (grade E), *at least one point from each component is required*
- Project report with an oral defense/ presentation (PROA, 3 credits). Projects will be graded based on: Correctness of algorithm, theoretical analysis, implementation, experimental analysis, and the quality of the report.  
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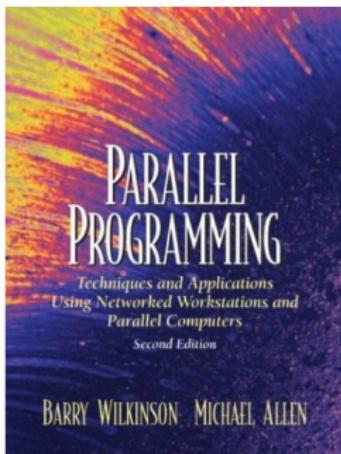
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## Literature

- Course book: Barry Wilkinson, Michael Allan: *Parallel Programming, 2nd edition*
- **Lecture Notes**



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  - Researcher in numerical analysis, studying problems in fluids and approximation functions!
  - Office: Room 3603, Lindstedtsvägen 25
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## The Situation

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# New Challenges: Green Computing and HPC

System	Rmax [TFlops/s]	Power [kW]	[GFlops/W]	[Ext (MW)]
Sweden's 2nd fastest (#110) Berzelius (LiU)	2253	???		
Sweden's fastest (#68) Dardel (KTH) (#5 Green500)	8260	146	57	18
Sweden's fastest (2018) Beskow (KTH)	1802	842	2	500
#2 Top500 Fugaku (JP)	442,010	29,899	15	67
#1 Green500 (#405 Top500) Henri (US)	2,040	31	66	15

Note: Note. The column "Ext" is the virtual power consumption if a computer using the given technology would provide 1 EFlop/s

## New Challenges: Green Computing and HPC

Average power consumption of a city with 100,000 inhabitants  
(2013)

Country	Average power consumption [MW]
US	920
Sweden	683
Germany	515
Japan	475
China	296
India	81

## A Pilot Project at KTH

- Most of the consumed energy is converted to heat
- It is expensive to get rid of the waste heat (cooling)

What if one could reuse this waste heat?

- Problem: The heat appears as warm air and has, therefore, low energy content
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- Basic design:
  - Memory is used to store both program and data instructions
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- A central processing unit (CPU) gets instructions and/or data from memory, decodes the instructions and then **sequentially** performs them

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## Flynn's Classical Taxonomy

- There are different ways to classify parallel computers. One of the more widely used classifications, in use since 1966, is called Flynn's Taxonomy
- Flynn's taxonomy distinguishes multi-processor computer architectures according to how they can be classified along the two independent dimensions of **Instruction** and **Data**. Each of these dimensions can have only one of two possible states: **Single** or **Multiple**

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There are 4 possible classifications according to Flynn

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- SIMD: Single Instruction, Multiple Data
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## Single Instruction, Single Data

- A serial (non-parallel) computer
- Single instruction: only one instruction stream is being acted on by the CPU during any one clock cycle
- Single data: only one data stream is being used as input during any one clock cycle
- Deterministic execution
- This is the oldest and until recently, the most prevalent form of computer

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## Single Instruction, Multiple Data

- A type of parallel computer
- Single instruction: All processing units execute the same instruction at any given clock cycle
- Multiple data: Each processing unit can operate on a different data element
- This type of machine typically has an instruction dispatcher, a very high-bandwidth internal network, and a very large array of very small-capacity instruction units
- Best suited for specialized problems characterized by a high degree of regularity, such as image processing
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## Single Instruction, Multiple Data

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## A First Example: Rank Sort

### Problem

Given  $n$  (pairwise distinct) numbers. Sort the numbers in increasing order.

### Solution

- Let the **rank**  $r_i$  of an element  $a_i$  of the set  $M$  of numbers be the number of elements being less than that element,

$$r_i = \# \{a_j \in M \mid a_j < a_i\}$$

- In a fully sorted list, the position of element  $i$  is just its rank  $r_i$ .

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