Specialized Numerical Methods for Transport Phenomena

Introduction and course plan

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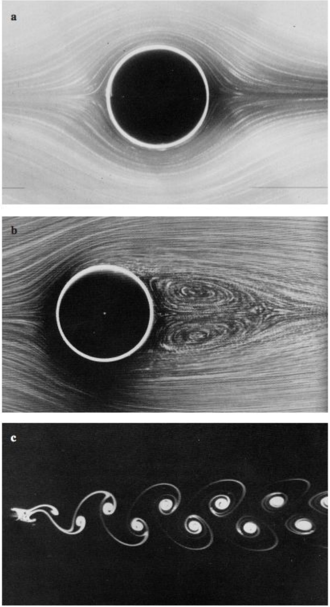

FIG. 8. – Photographs of streamlines (a, b) or streaklines (c) for steady flow past a circular cylinder at different values of the Reynolds number (M.Van Dyke, 1982): (a) $Re \ll 1$, (b) $Re = 26$, (c) $Re = 105$.

Outline

Why numerical modeling?

Getting to know each other

Course plan

The phenomena we will simulate

What are computers?

The steps in numerical modeling?

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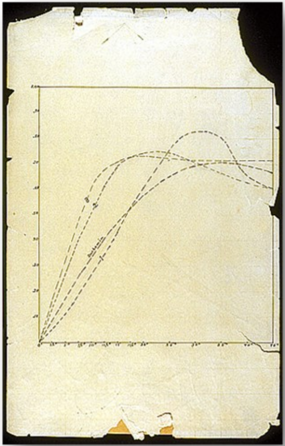
Classical Paradigm

Theory (Physics and Mathematics) is combined with experience (and chance) to predict nature, design objects and processes

- The Wright brothers' first plane
- Penicillin by Fleming
- Haber-Borsch process



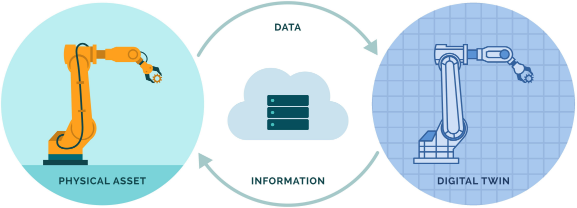
Modern Paradigm

Modern objects and processes are much more complex than before. An Airbus 380 contains 4 million components. Modern refineries contain dozens of distillation columns, thousands of pipes.

In the modern paradigm, theory (physics and mathematics) is solved by **numerical modeling** and is combined with experience to predict nature and design processes and objects.

Digital twins

A **digital twin** is a dynamic virtual copy of a physical asset, process, system or environment that looks like and behaves identically to its real-world counterpart. With a digital twin, you can predict possible performance outcomes and issues that the real-world product might undergo.

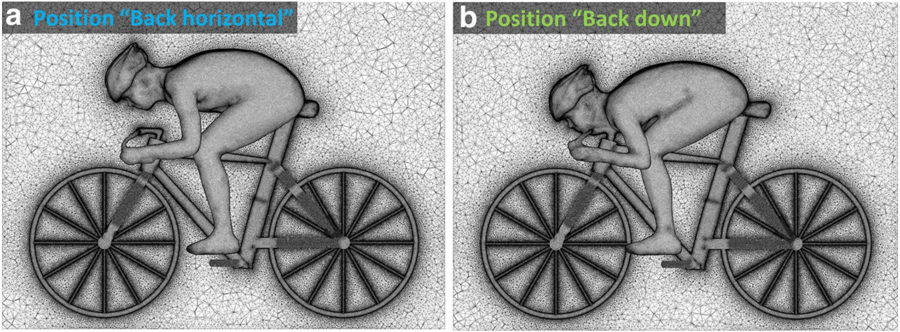


Wind turbine

Chemical reactor - Velocity profile

Chemical reactor - Residence time

Cyclist posture



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Getting to know you

- Which program are you in?
- What level?
- What do you wish to acquire from this class?
- What is your experience in numerical modeling?
  - Internship?
  - Previous classes?
- What are your biggest fears or concerns?

About us: Bruno Blais

- B. Eng. in Chemical Engineering
- D. Ing. in Mechanical Engineering
- Master in Physics
- Ph.D. in Chemical Engineering
- 3 years industrial experience as a researcher for the National Research Council Canada
- Assistant professor (2018-2022) and Associate professor (2022-) at Polytechnique Montréal

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About us: Laura Prieto Saavedra

- B. Sc. in Chemical Engineering
- M. Sc. in Computational Science and Engineering
- Ph.D. candidate in Chemical Engineering
  $\rightarrow$ working on the implementation of efficient numerical methods to simulate turbulent flows

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Goal of this class

Numerical simulations software/methods have evolved

Simulation-based engineering is in constant evolution. New paradigms have arisen in the last two decades:

- High-performance computing (HPC)
- Highly performant open-source implementation of classical methods
- Novel numerical methods

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Difficult to access

These methods and software platform require specialized knowledge:

- Working in a Linux environment (terminal)
- Learning how to compile and modify specialized software
- Understanding the underlying numerics and methods

The goal of this class is to acquire this knowledge for both a classical method (the Finite Element Method) and novel numerical methods.

The Finite Element Method (FEM)

A common method in simulation-based engineering. Used for solid mechanics, heat transfer, electrodynamics and fluid dynamics.
The method is challenging:

- Mathematically involved
- Difficult to program

In the 6 weeks we dedicate to it, we will use the deal.II library to minimize the amount of core software development. By the mid-semester, we will have developed our own CFD solver using FEM.

Specialized methods

Lattice Boltzmann Method (LBM)

Based on the Boltzmann equation, LBM allows us to rapidly and efficiently write a solver for the Navier-Stokes equations.

Discrete Element Method (DEM)

The Discrete Element Method simulates the flow of spherical (or even non-spherical) granular material.

Objectives

- Choose the most appropriate numerical method (classical or specialized) for the solution of a given transport phenomena
- Describe the main mathematical foundations of standard/specialized numerical methods in order to understand their limitations
- Evaluate and critique the performance and accuracy of various specialized/standard numerical methods for scientific computing
- Evaluate and control errors in the numerical solution of scientific problems by understanding their significance
- Apply finite element, lattice Boltzmann and discrete element methods to the simulation of the simulation of exchange phenomena
- Evaluate the quality of the numerical model used in the context of the application studied

Evaluations

Nature	Amount	(Individual/Team)	Weight
Homework	7	Team of two	70%
Final exam	1	Individual	30%

Important: All homework must be handed in before the specified date on the Moodle website. Delays will be penalized by 10% for each day.

Plagiarism will be punished.

Programming

Programming is a key element of this course. We will program every numerical method we use in C++.

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Why?

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- Allows us to identify the limitations of the method.
- Will enable you to tackle any equation you face in your own research/work.

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Homeworks will require a **lot** of programming. Reports will be simple. Templates will be given with every assignment to simplify the process.

Outline

Diffusion

The Poisson equation describes diffusion processes (heat transfer, mass transfer). An example we will often use is the heat transfer equation.

Steady-state heat transfer equation

$$-\alpha \nabla^2 T = Q \tag{1}$$

Where $\alpha = \frac{k}{\rho C_p}$. is the thermal diffusivity and Q is a heat source. This assumes constant physical properties.

Transient heat transfer equation

$$\frac{\partial \rho C_p T}{\partial t} = \alpha \nabla^2 T + Q \tag{2}$$

Advection-diffusion

This equation allows us to calculate the steady-state temperature profile in a liquid moving with a velocity $\boldsymbol{u}$. By a balance we can establish the advection-diffusion equation. The balance includes a diffusion component and a transport component.

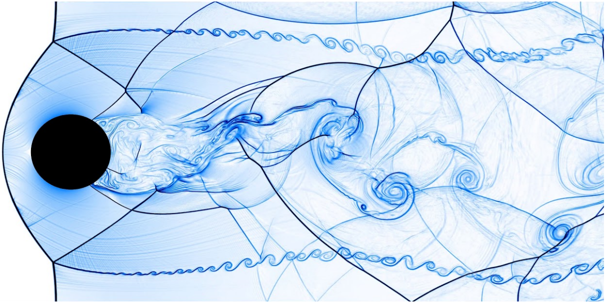
$$\underbrace{\rho C_p \boldsymbol{u} \cdot \nabla T}_{Advection} = \underbrace{k \nabla^2 T}_{Diffusion}$$

Incompressible fluid dynamics

The Navier-Stokes equations describe the behavior of fluids (gas or liquid) in flow around obstacles, inside processes, and are also the basis of meteorological predictions. In this course, we will solve them in their incompressible form:

$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{\nabla} \cdot \boldsymbol{u} \otimes \boldsymbol{u} = -\frac{1}{\rho} \boldsymbol{\nabla} \boldsymbol{p} + \boldsymbol{\nabla} \cdot \bar{\bar{\tau}} + \boldsymbol{g}$$



Granular flows

A large part of the industrial and chemical process involve material in granular form.

Although particles (e.g. sand) flow, they can also form clumps at rest.

Advanced techniques based on force balances and ordinary differential equations based on Newton's second law allow to simulate their behavior. This will be the Discrete Element Method.

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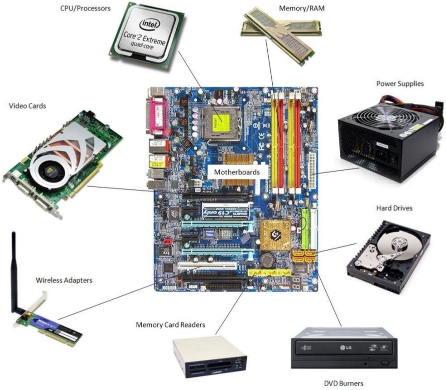
The modern computer

What constitutes a modern computer?

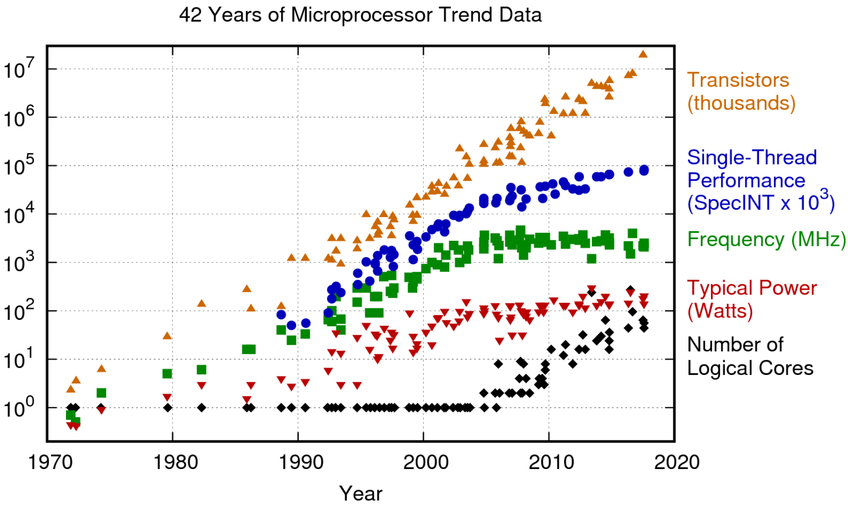
The modern computer

What is the modern computer made of?

- A motherboard
- One or more processors (1 to 4) which contain multiple cores(1 to 64+)
- Evanescent memory (RAM)
- Storage
- A GPU
- Power supply
- Network connection



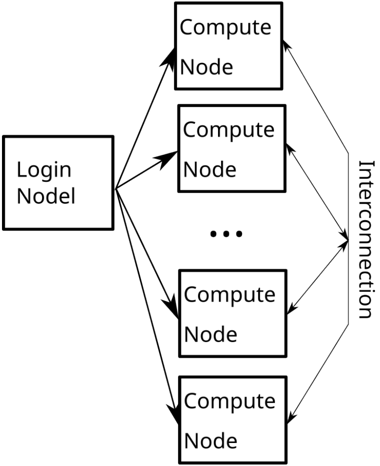
Moore's law



Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten
New plot and data collected for 2010-2017 by K. Rupp

High-performance computing

A high-performance computer uses a different strategy.
It connects several nodes (computers) by an extremely fast interconnection.
A simulation will run on several computers at the same time. This requires a particular programming paradigm (MPI).



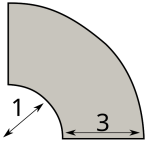
Example of a computer cluster

Narval

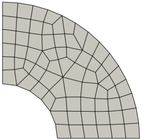
- 78000 cores on 1200 nodes
- $>$ 300 TB of ram
- $>$ 20PB of storage

Outline

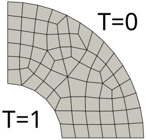
1. Preprocessing



Constructing a model of the geometry

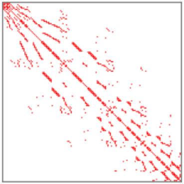


Meshing the geometry



Establishing boundary conditions

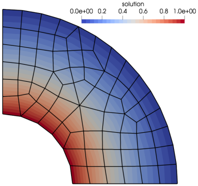
2. Solution



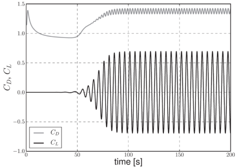
$A\mathbf{x}=\mathbf{b}$

or recurrence

3. Postprocessing



Visualisation of the results

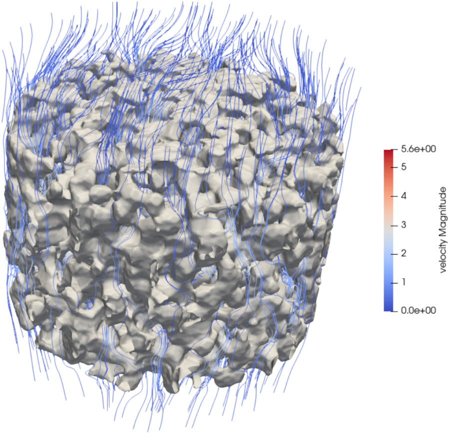


Extraction of the quantity of interest

Preprocessing

Preparing a digital representation of a geometry can be trivial or very difficult. This requires CAD software.

Making a mesh (discretization) of the geometry is a second step. It affects the underlying accuracy of the method.



Postprocessing

Visualisation

Visualisation of the result requires dedicated software. In this course we will use Paraview, but there are other alternatives.

More than just images

Simulation for engineering purposes generally require you to go beyond producing nice images. Postprocessing also entails calculating quantities such as:

- Drag coefficients
- Lift coefficients
- Heat fluxes
- Residence time
- Mixing time
- ...

What's next?

Rest of the week

- Hackathon to install deal.II and paraview on your machines.
- Refresher on tensor notation and tensor calculus.
- Basics of C++ and Linux.
- Begin Homework 1

Please ensure that everything is installed before the next class.

Next week

- Advanced C++ programming