Numerical Analysis & Scientific Computing II

Module 1
Introduction

1.1 Computing vs scientific computing?

1.2 Pre-requisites

Akash Anand
MATH, IIT KANPUR

Module 1

Introduction

1.1 Computing vs scientific computing?

1.2 Pre-requisites

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Introduction: Computing vs scientific computing

What is scientific computing?

Introduction: Computing vs scientific computing

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What is scientific computing?

Scientific method

Introduction: Computing vs scientific computing

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What is scientific computing?

Scientific method

Experiment

$\Big\downarrow$ *Observations*

Theory

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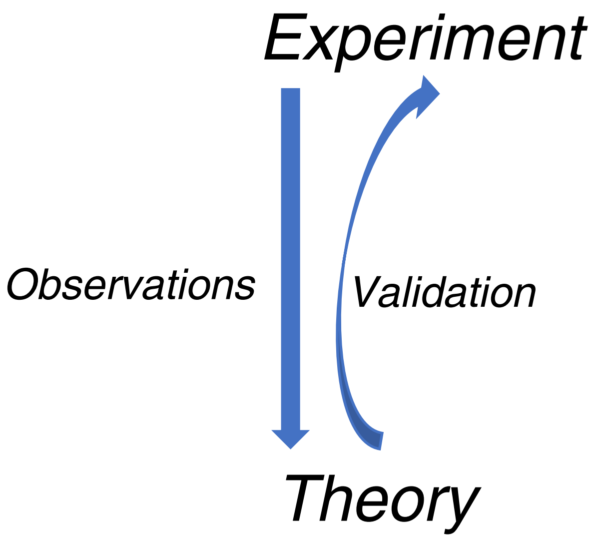
What is scientific computing?

Scientific method



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What is scientific computing?

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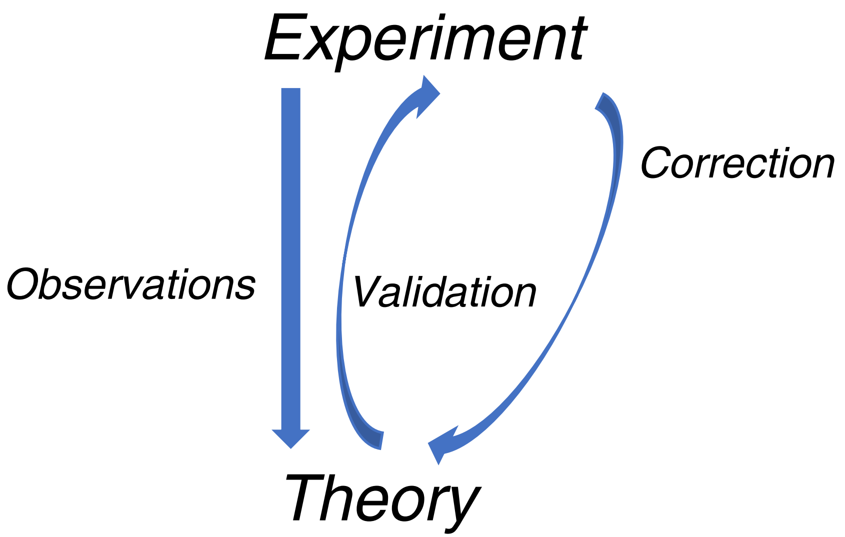

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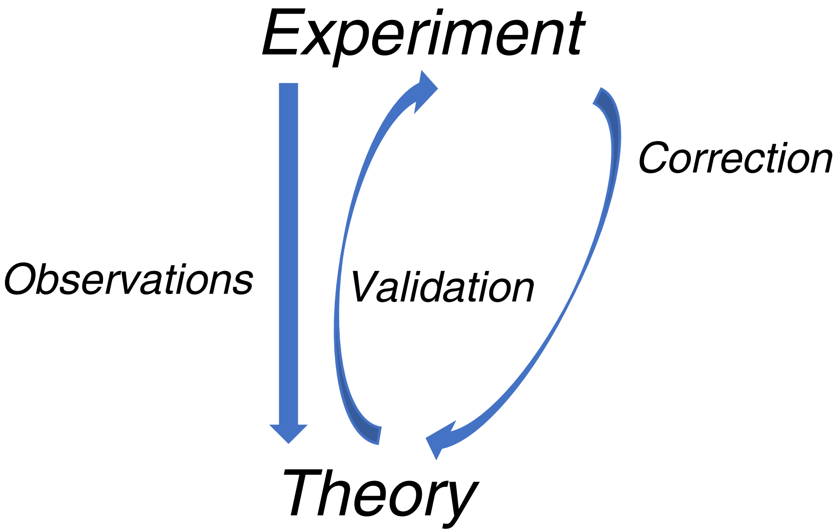

Computation

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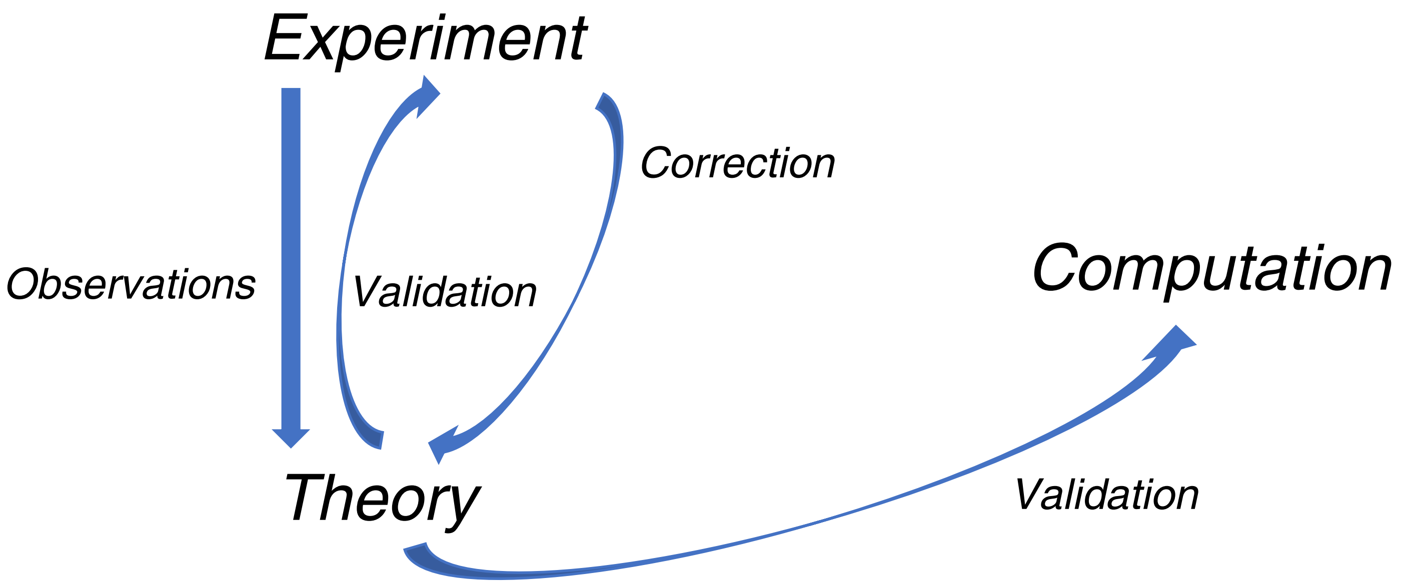
Scientific method



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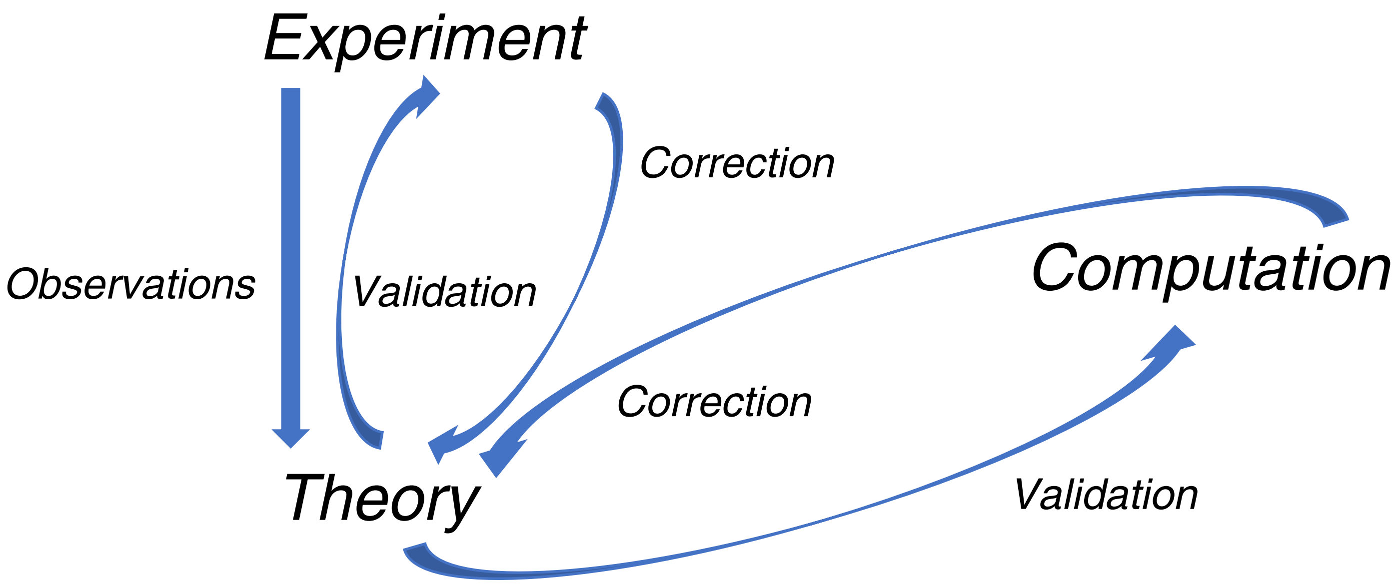

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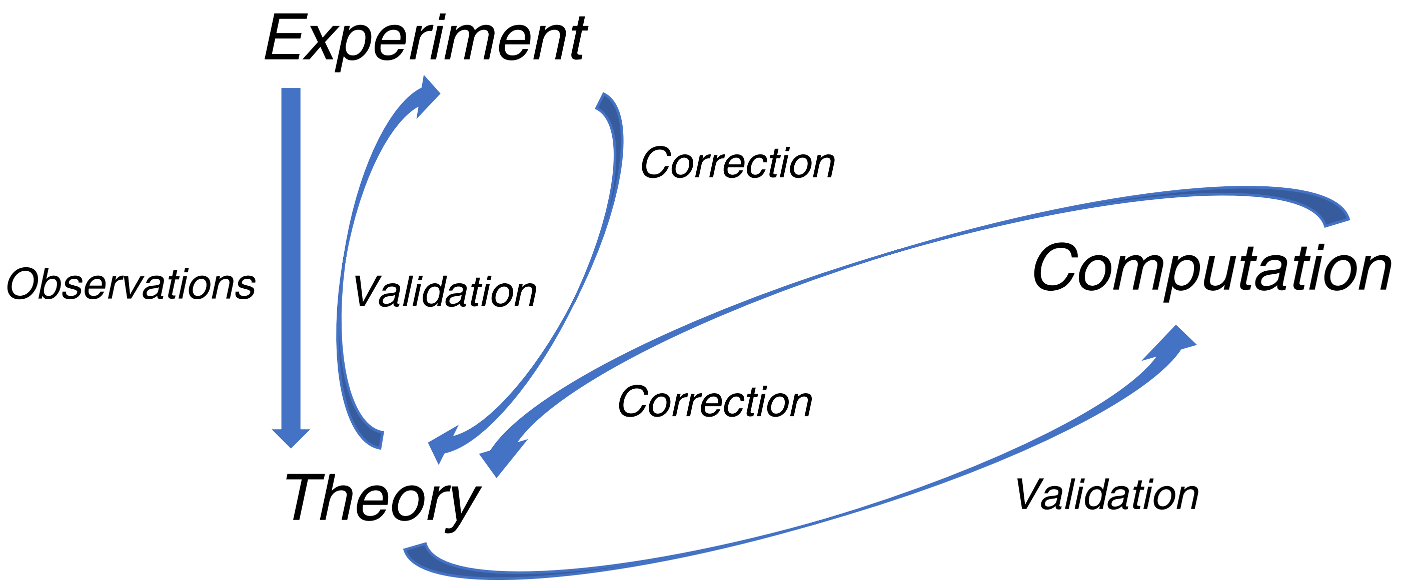
We can to things with computation that we could not do with experiments …



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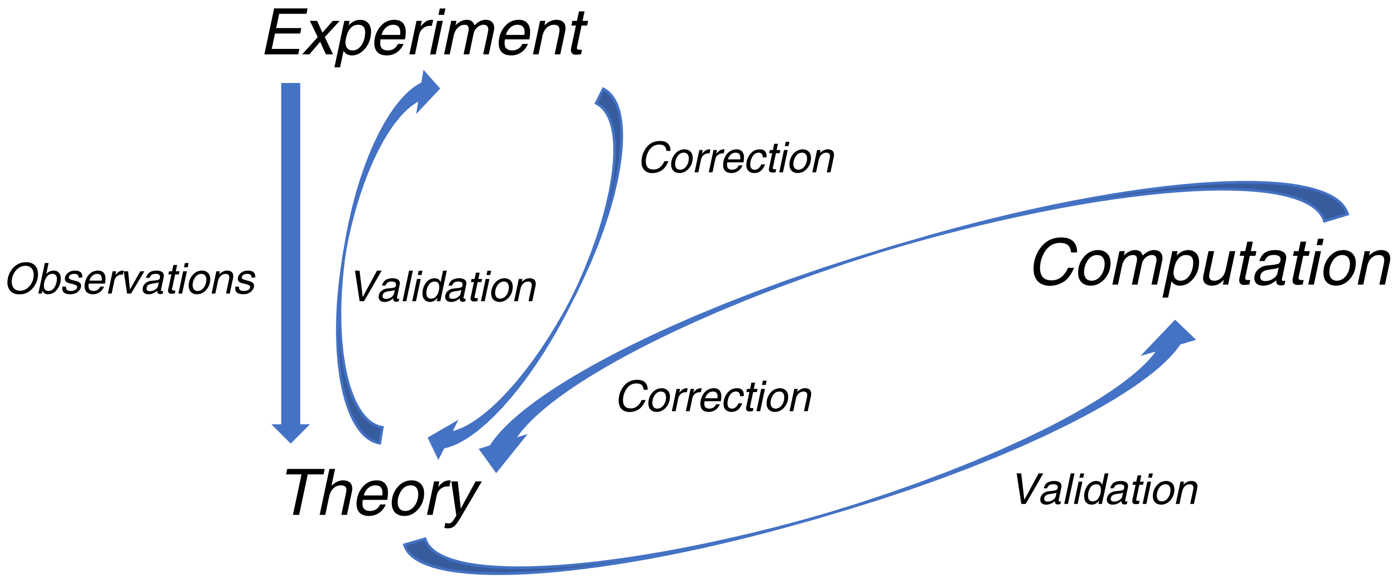

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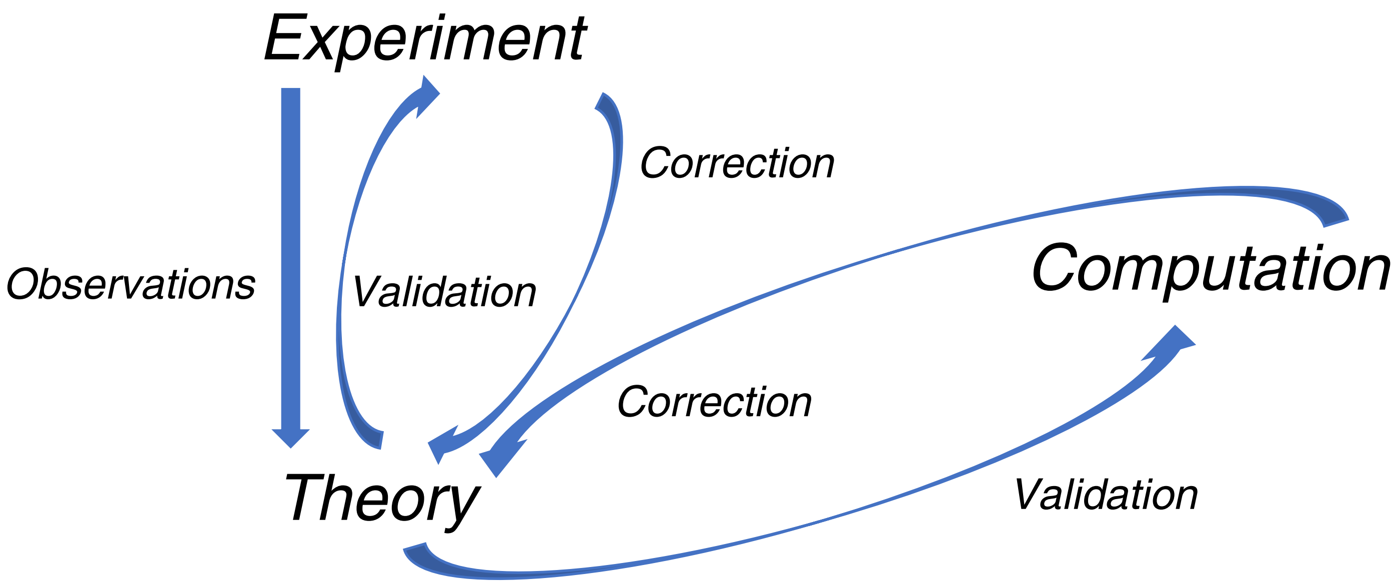

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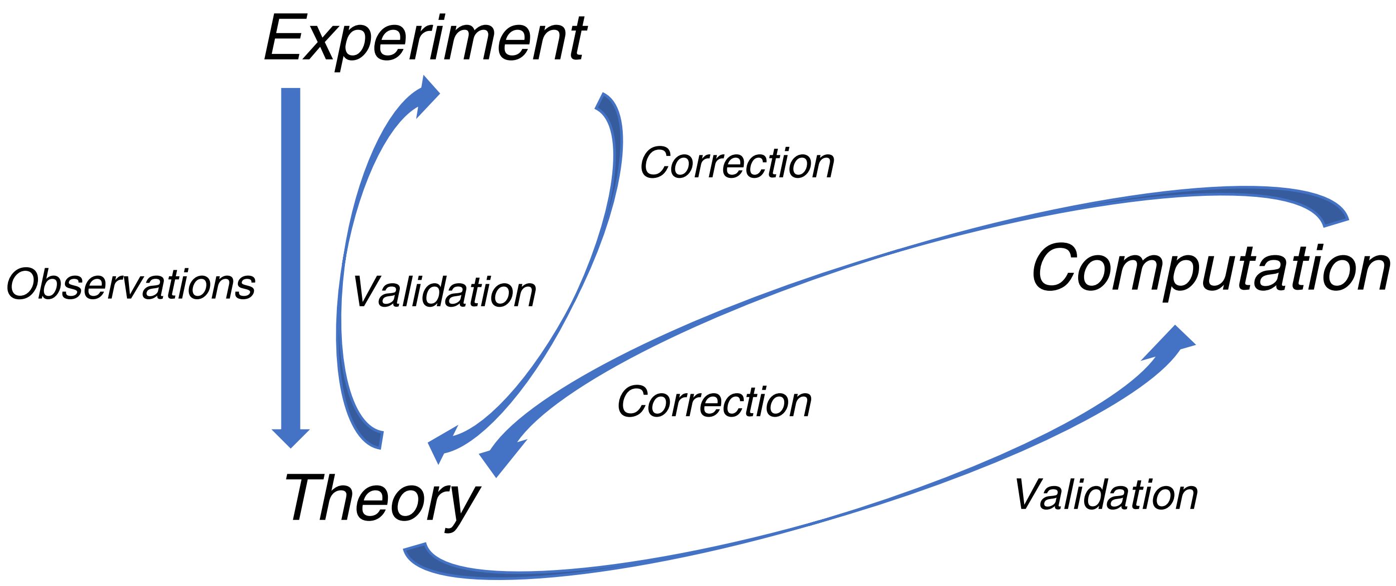

We can to things with computation that we could not do with experiments …

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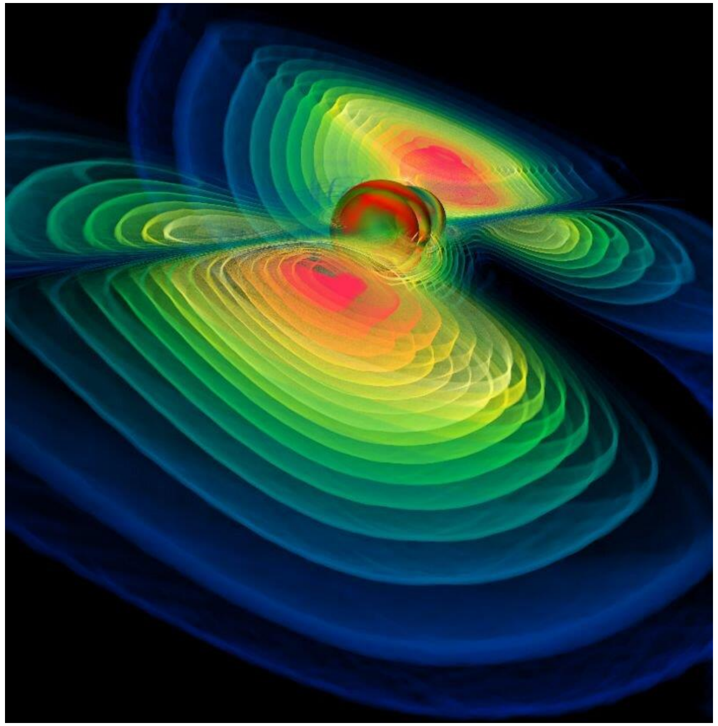
... cost advantage

…

What is scientific computing?

Example

A numerical simulation showing the gravitational radiation emitted by the violent merger of two black holes



Source:
Approaching the Black by Numerical Simulations by Christian Fendt

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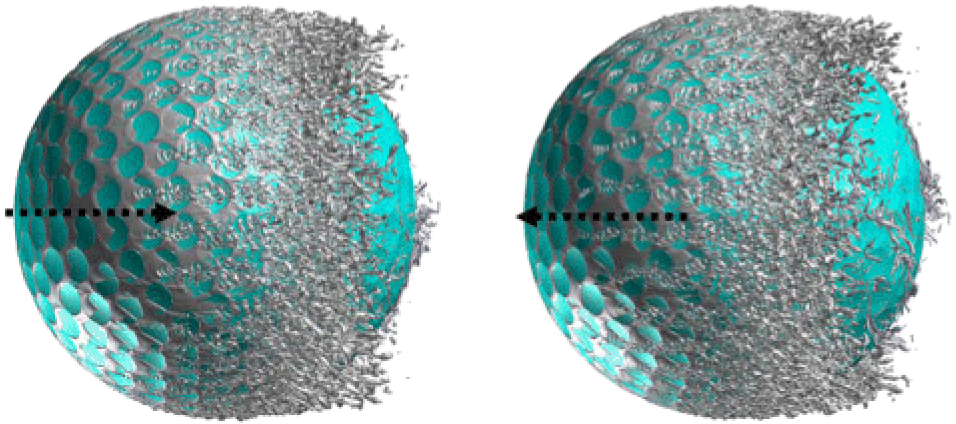
What is scientific computing?

Example

Visualization of the instantaneous vortical structures around the golf ball



Source:
Numerical Investigation of the Flow Past a Rotating Golf Ball and its comparison with a rotating smooth sphere by Jing Li, Makoto Tsubokura, Masaya Tsunoda

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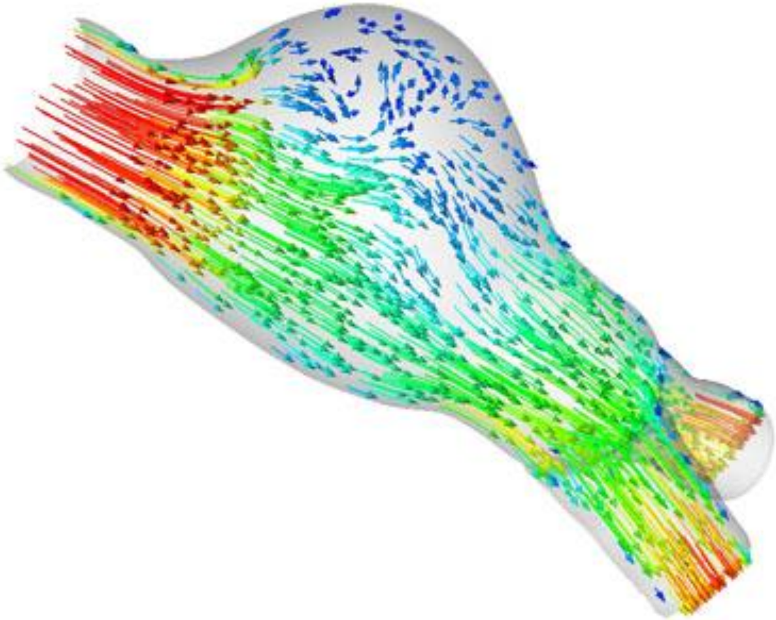
What is scientific computing?

Example

Abdominal aortic aneurysm



Source:
Team for Advanced Flow Simulation and Modeling (https://www.tafsm.org/PROJ/CVFSI/PSCMADBF)

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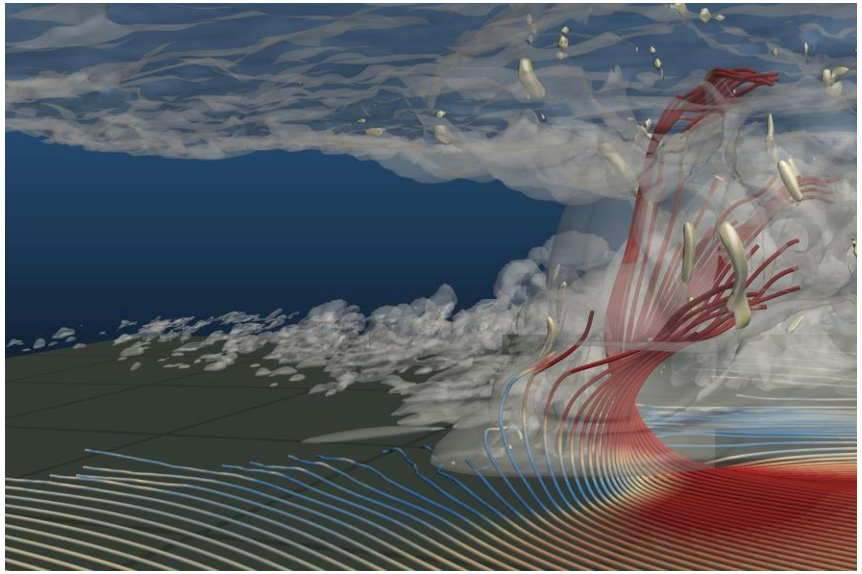
What is scientific computing?

Example

Updraft in a hypothetical supercell simulation



Source:
Texas Advanced Computer Center, University of Texas at Austin

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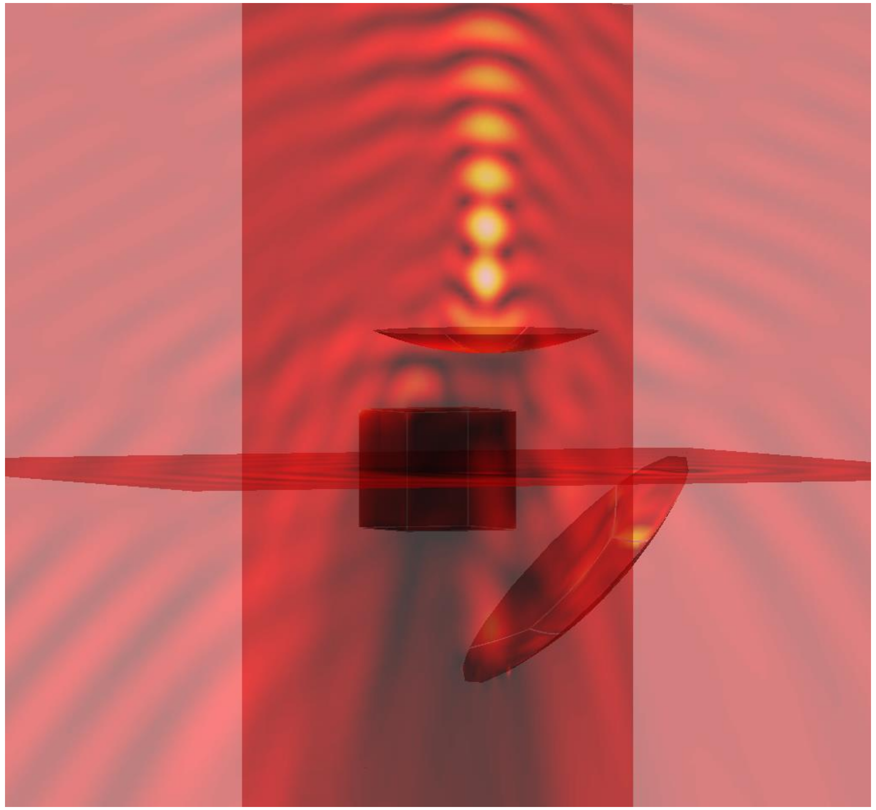
What is scientific computing?

Example

Wave-satellite interaction



Source: Anand et al.

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What is scientific computing?

The basic paradigm

Physical system

↓

Observation

↓

Theory

↓

Mathematical system/model

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Mathematical system/model

typically, unknowns are continuous variables related by differential equations

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Analytical Solution

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typically, unknowns are continuous variables related by differential equations

↓ **Analytical Solution**

↓ **Discrete mathematical system/model** → ↓ **Numerical solution**

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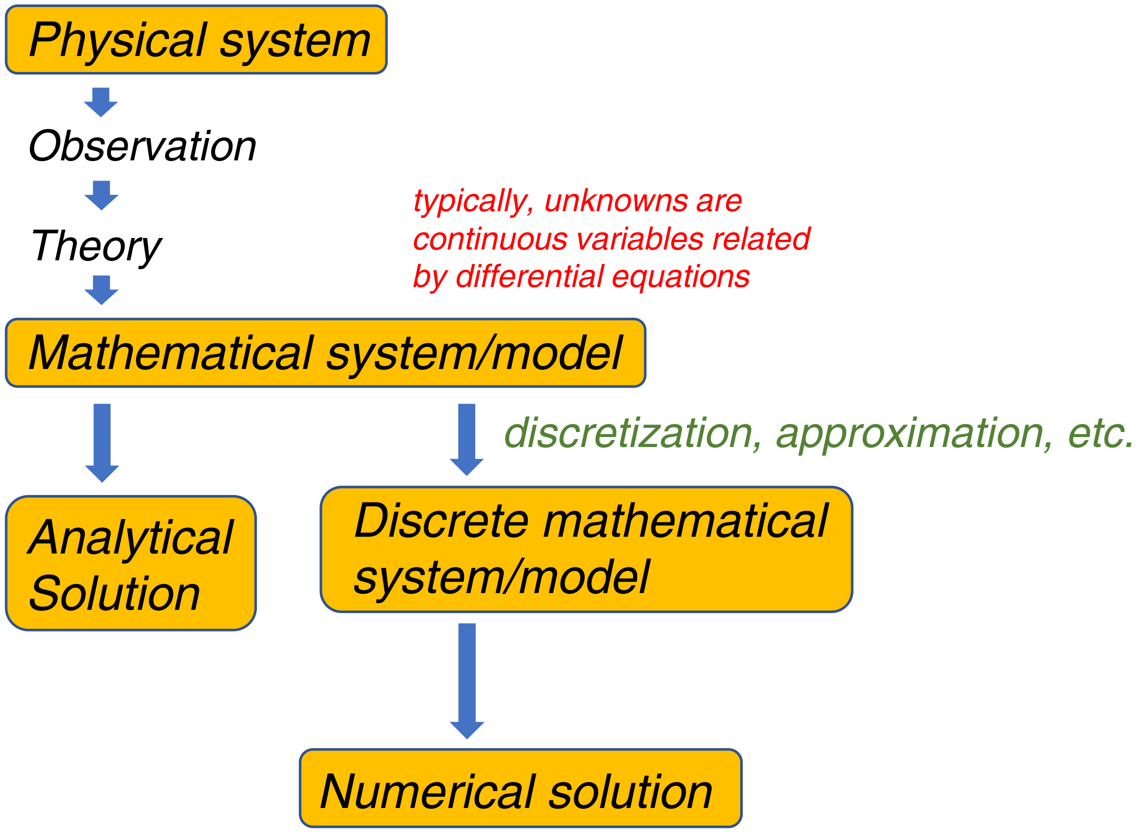

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Mathematical system/model

typically, unknowns are continuous variables related by differential equations

↓ Analytical Solution

↓ *discretization, approximation, etc.*

Discrete mathematical system/model

typically, large number of discrete unknowns, related by a large number of algebraic equations

↓

Numerical solution

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Theory

↓

Mathematical system/model

typically, unknowns are continuous variables related by differential equations

↓ → *Analytical Solution*

↓ *discretization, approximation, etc.* → *Discrete mathematical system/model*

typically, large number of discrete unknowns, related by a large number of algebraic equations

↓ *algorithm, code, computers, etc.*

Numerical solution

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typically, unknowns are continuous variables related by differential equations

Mathematical system/model

discretization, approximation, etc.

Analytical Solution

Discrete mathematical system/model

typically, large number of discrete unknowns, related by a large number of algebraic equations

algorithm, code, computers, etc.

Numerical solution

Need to deal with large number of algebraic equations in a large number of unknowns – need efficient algorithms, codes, and computers.

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What is scientific computing?

The basic paradigm

Physical system

↓

Observation

↓

Theory

↓

Mathematical system/model

typically, unknowns are continuous variables related by differential equations

↓ Analytical Solution

↓ discretization, approximation, etc.

Discrete mathematical system/model

typically, large number of discrete unknowns, related by a large number of algebraic equations

↓ algorithm, code, computers, etc.

Numerical solution

Numerical analysis is the design, analysis, and validation of the discretization.

Validation is a key point as we need provably correct answers!

Need to deal with large number of algebraic equations in a large number of unknowns – need efficient algorithms, codes, and computers.

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A simple example

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$$v(t) = 30 - \frac{1}{10}x(t)$$

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Mathematical system

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Mathematical system

The "first discretization" of differential equations is due to Euler in 1768.

Euler's method partitions the 10 hour time interval into many short intervals and successively computes the distance travelled in each interval using the speed at the start.

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Discrete system

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Using 10 intervals of 1 hour gives 195.39647 km

A simple example

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Recomputing using 600 intervals of 1 minute gives	189.72820 km

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Numerical solution

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Numerical solution

Reliability/accuracy?

Speed of calculation?

Module 1

Introduction

1.1 Computing vs scientific computing?

1.2 Pre-requisites

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Introduction: Pre-requisites

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In the first course on Numerical Analysis & Scientific Computing, you should have seen the following topics:

- *Approximation of*
  - *functions,*
  - *derivatives,*
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- *Solution of (system of)*
  - *linear equations and*
  - *non-linear equations.*

Introduction: Pre-requisites

Akash Anand
MATH, IIT KANPUR

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In addition, it is useful to know the well-posedness of initial and/or boundary value problems for ODEs and PDEs, a subject matter of theoretical courses on ODE/PDE.