Module 1

Introduction

1.1 Computing vs scientific computing?

1.2 Pre-requisites

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MATH, IIT KANPUR

Module 1

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Introduction: Computing vs scientific computing

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What is scientific computing?

Introduction: Computing vs scientific computing

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What is scientific computing?

Scientific method

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What is scientific computing?

Scientific method

Experiment

Observations

Theory

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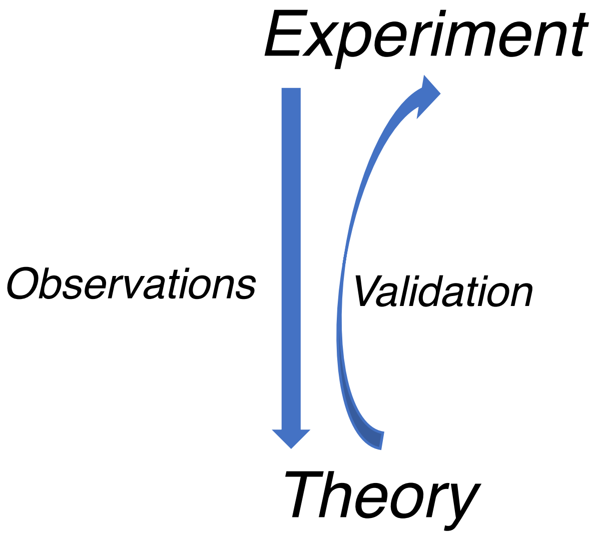
What is scientific computing?

Scientific method



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What is scientific computing?

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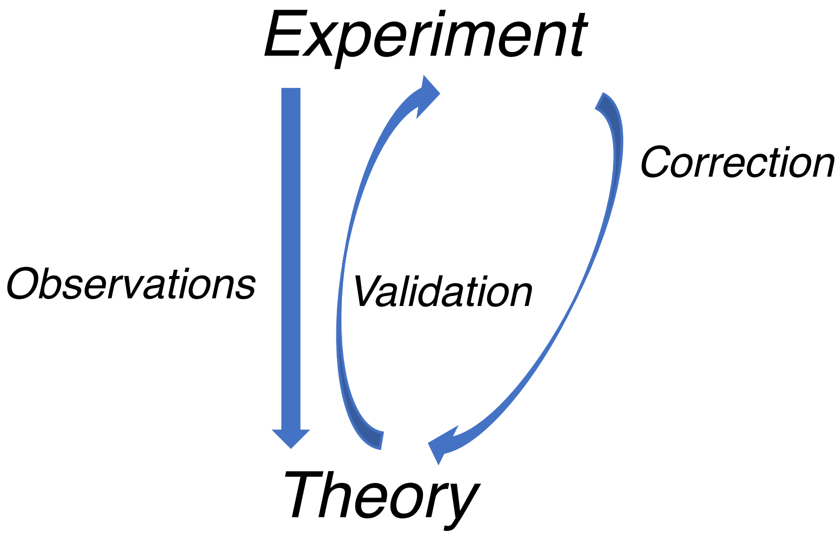

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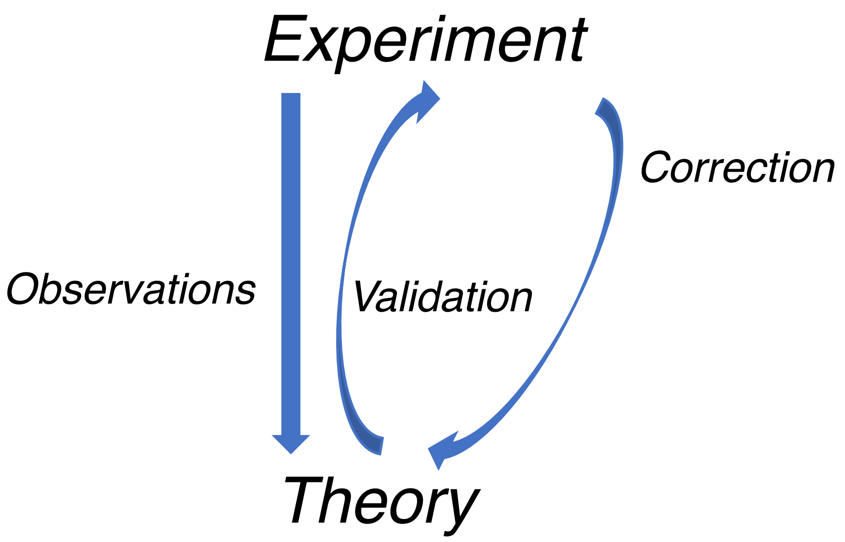

Computation

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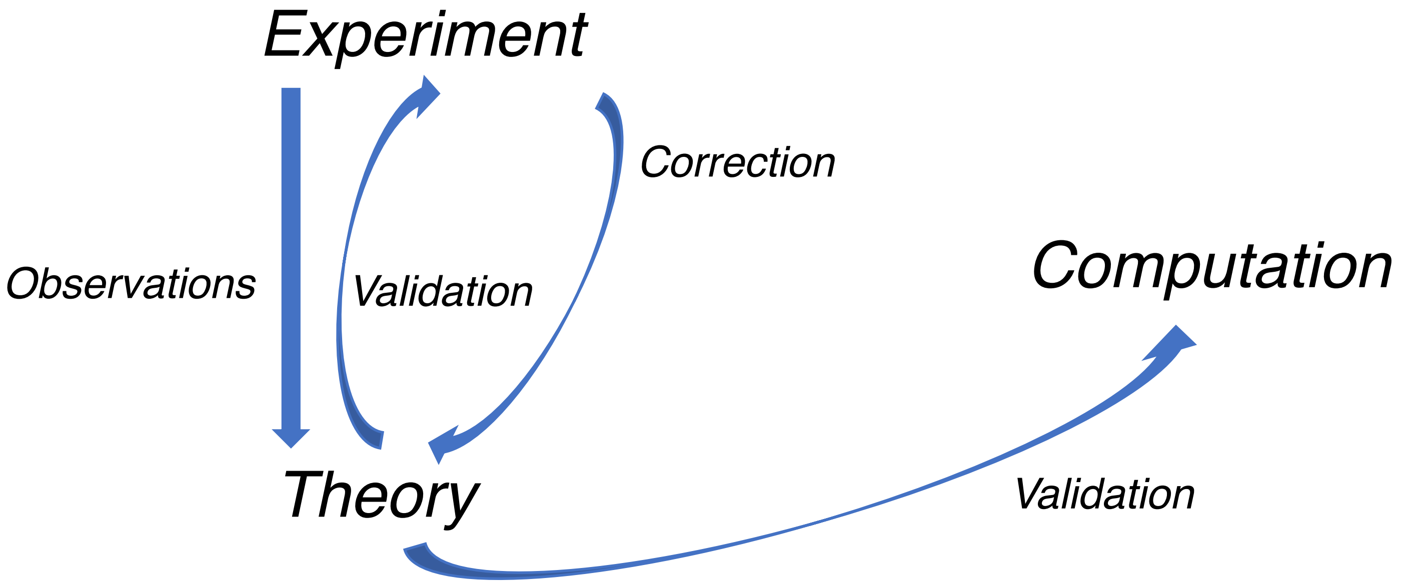
What is scientific computing?

Scientific method



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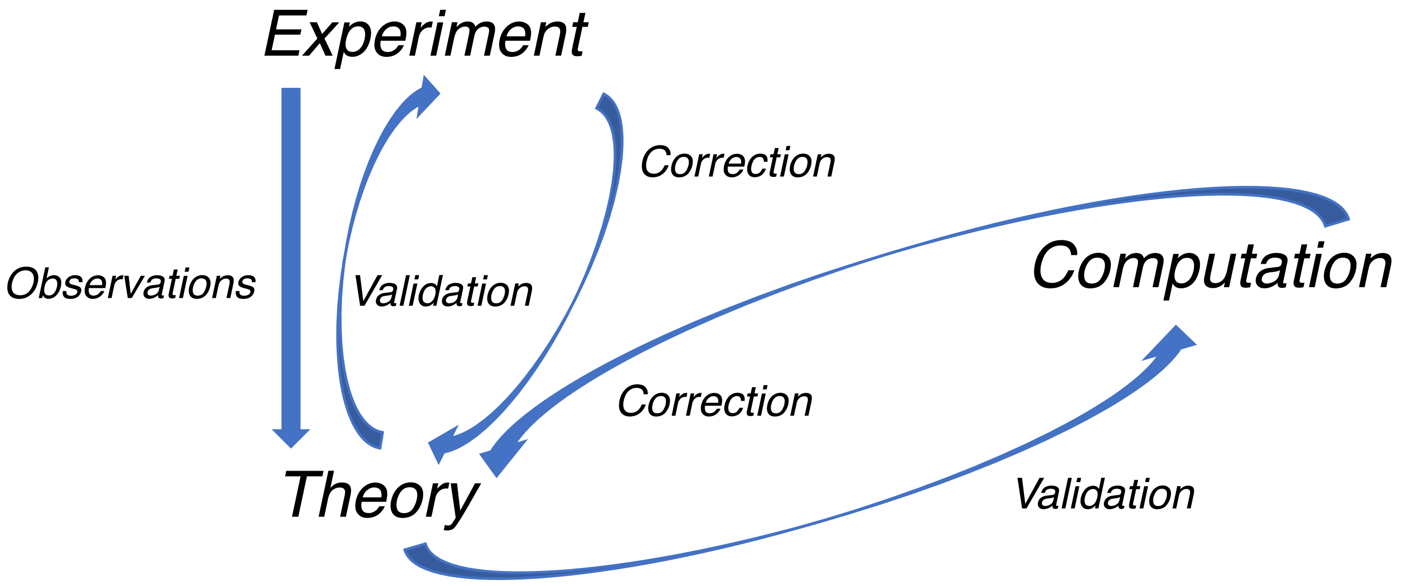

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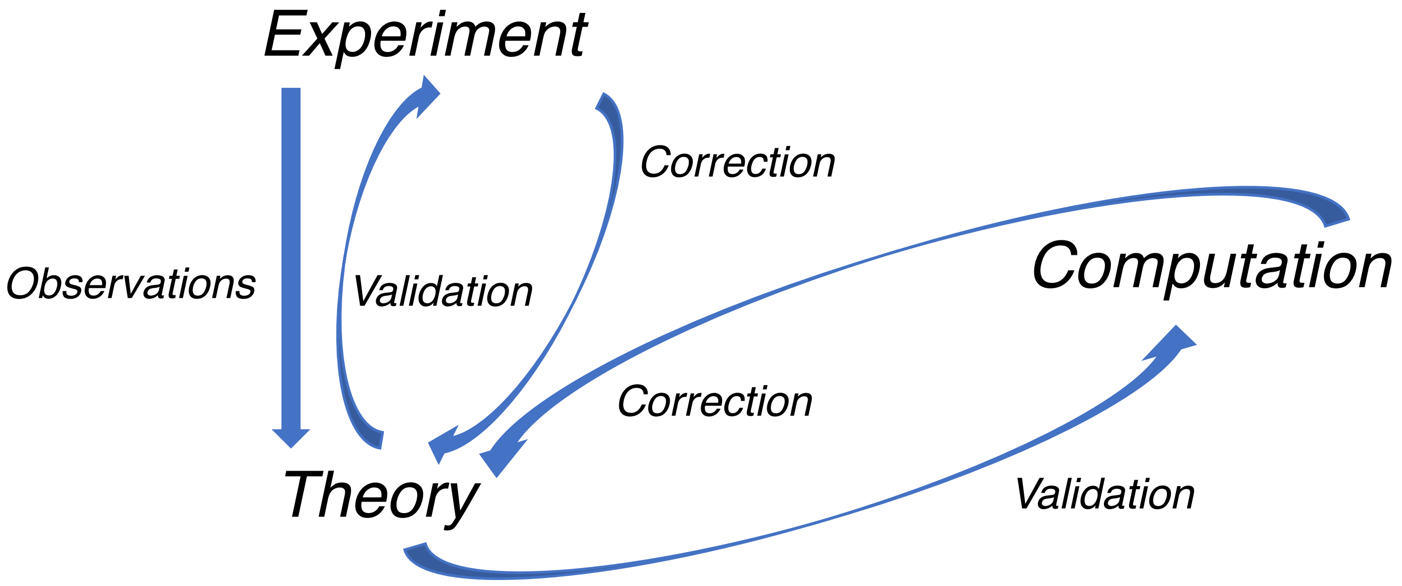
What is scientific computing?

Scientific method

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



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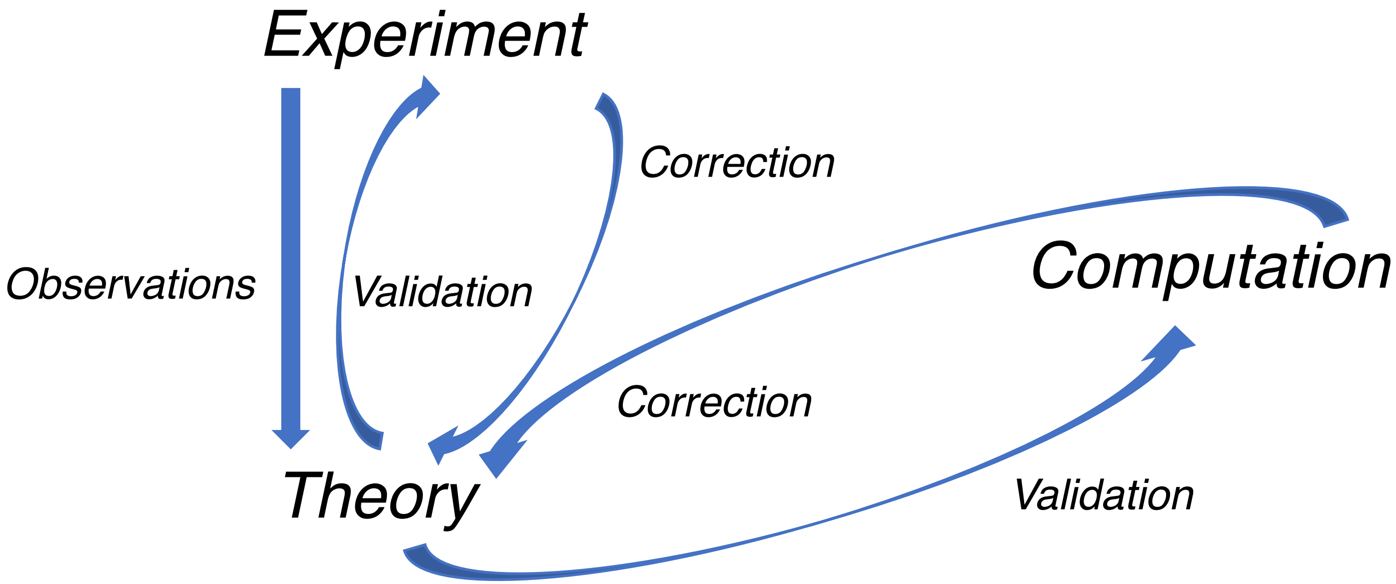

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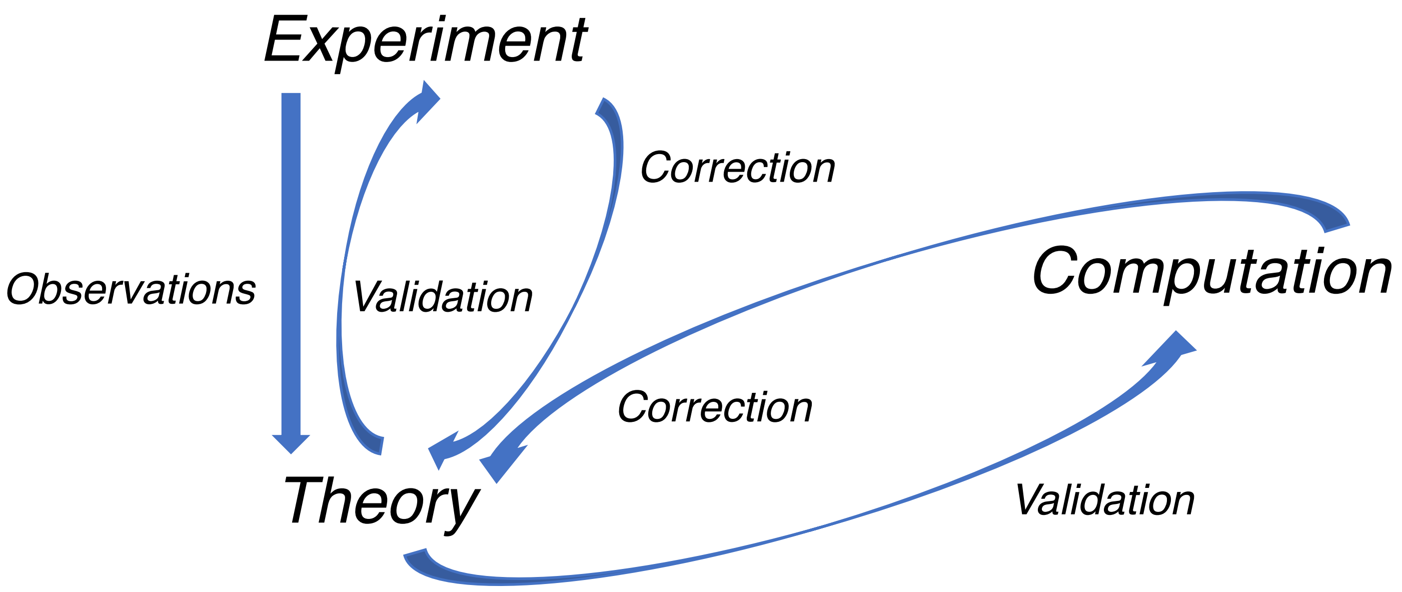

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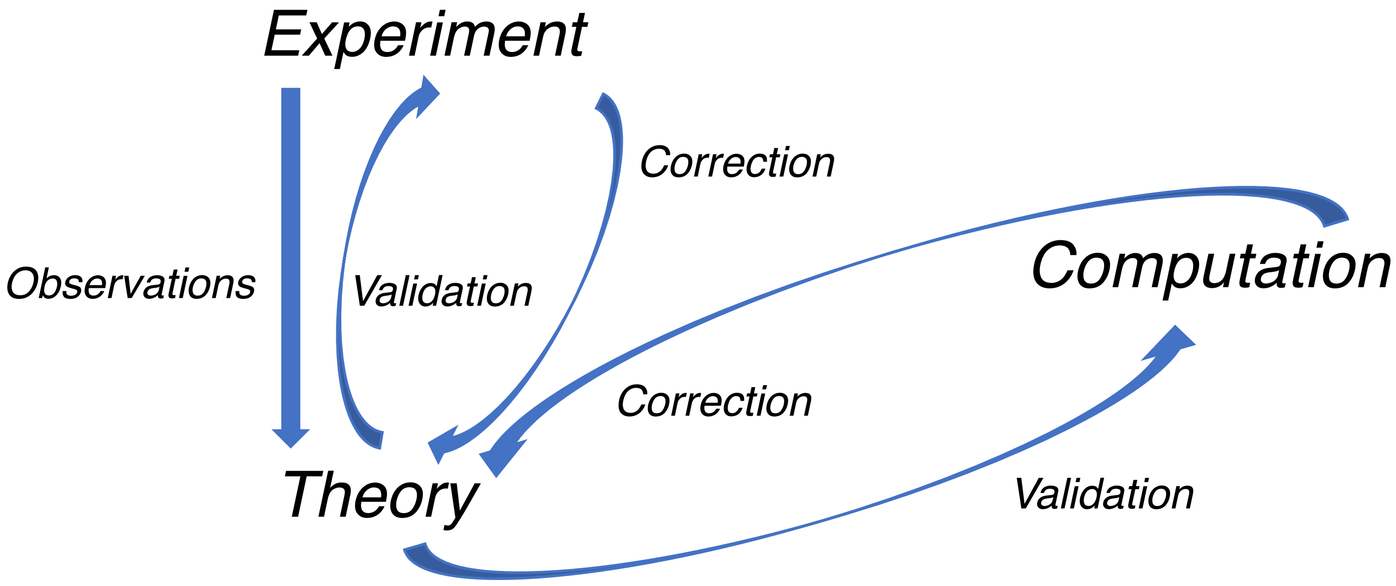

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... cost advantage

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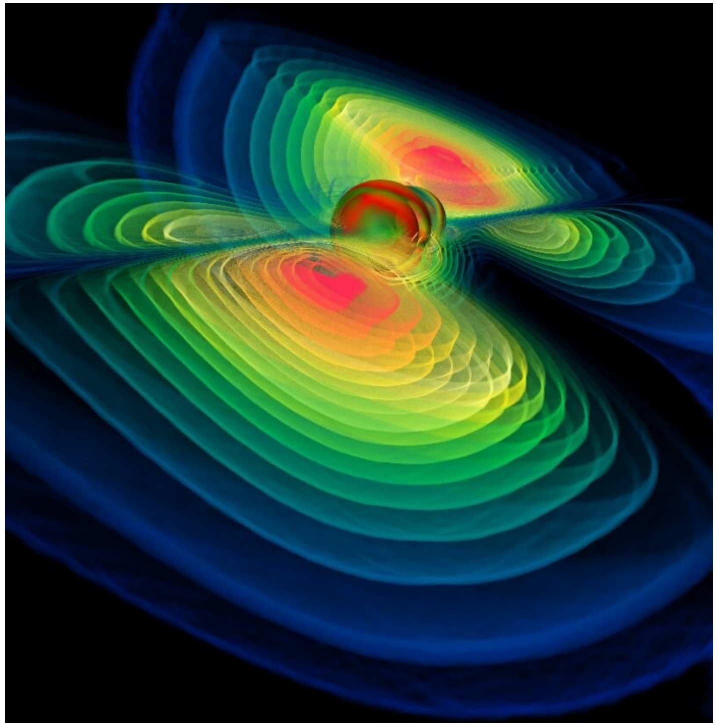
What is scientific computing?

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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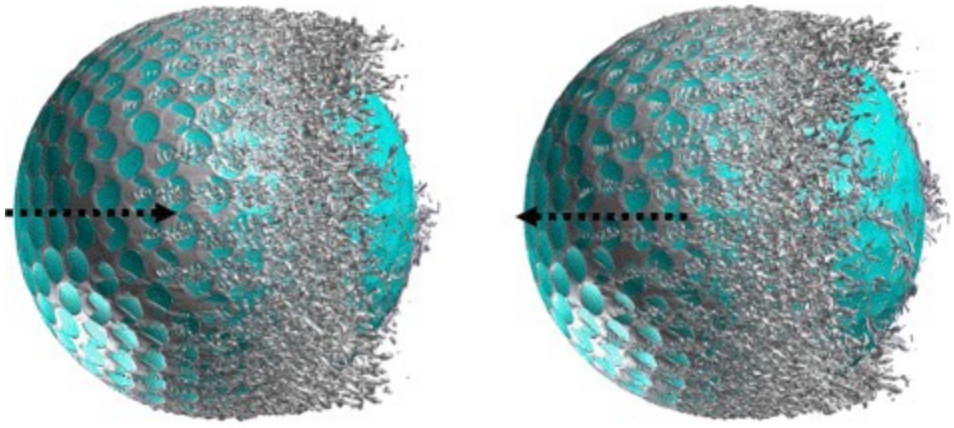
What is scientific computing?

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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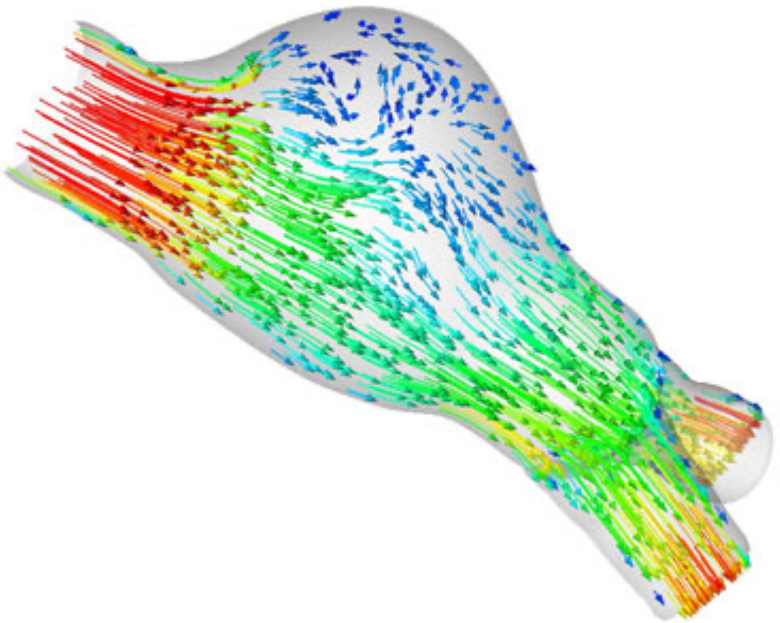
What is scientific computing?

Example

Abdominal aortic aneurysm



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

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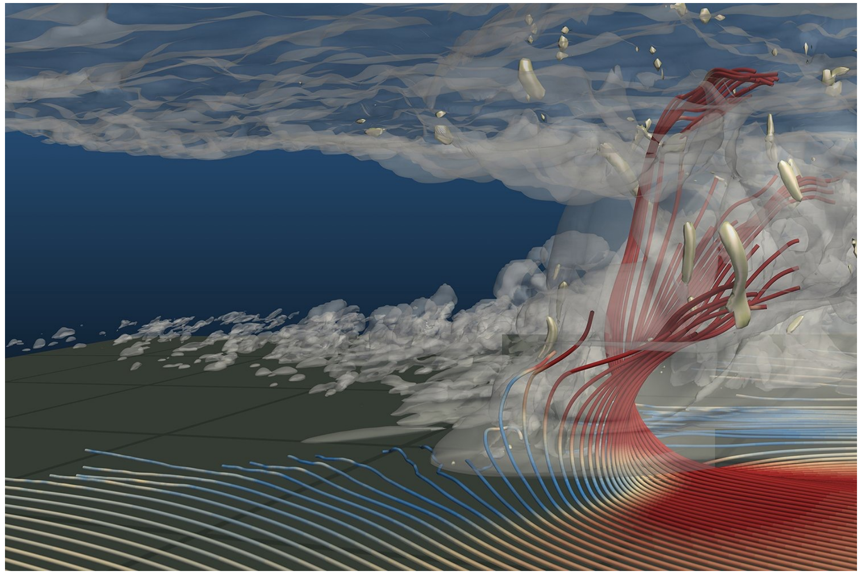
What is scientific computing?

Example

Updraft in a hypothetical supercell simulation



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

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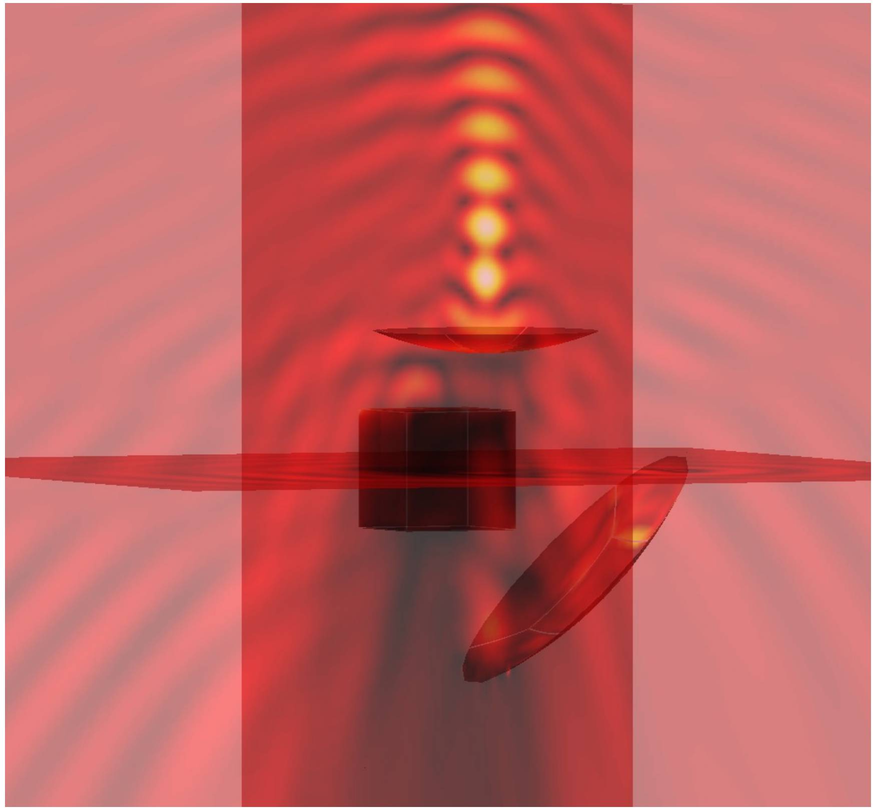
What is scientific computing?

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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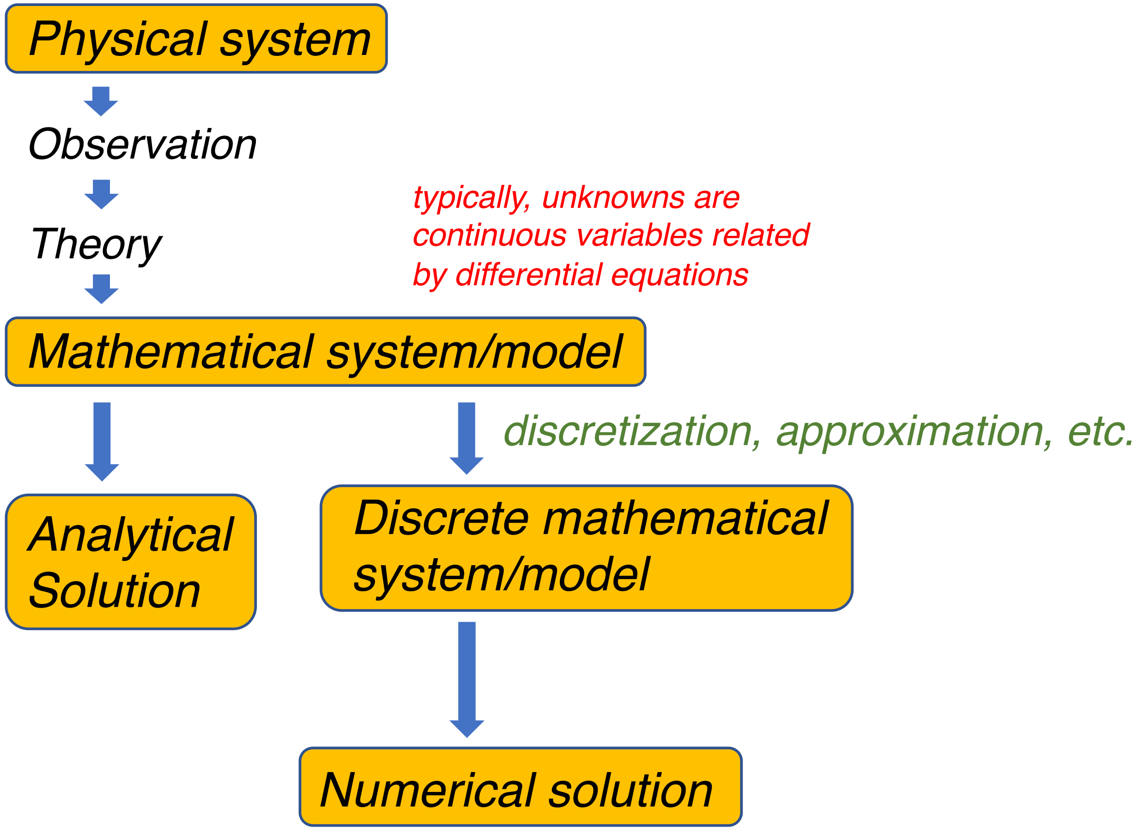

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typically, unknowns are continuous variables related by differential equations

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

Numerical solution

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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

↓ 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

→ 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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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

A robotic vehicle departs at 30 km/h, but, due to battery drain, its speed decreases by 1/10 km/h for each kilometer travels.

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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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A simple example

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Discrete system

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Using 10 intervals of 1 hour gives *195.39647 km*

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Using 10 intervals of 1 hour gives	*195.39647 km*
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

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

- *Approximation of*
  - *functions,*
  - *derivatives,*
  - *integrals.*

- *Solution of (system of)*
  - *linear equations and*
  - *non-linear equations.*

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,*
  - *integrals.*

- *Solution of (system of)*
  - *linear equations and*
  - *non-linear equations.*

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.

Module 2

Initial Value Problems

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Initial Value Problems

2.0 First-order system of ODE

2.1 Well-posedness

2.2 Stability

2.3 Euler's method

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Initial Value Problems: First order system of ODE

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Recall that a kth order ODE is said to be explicit if it can be written in the form

$$u^{(k)} = f\left(t, u, u', u'', \ldots, u^{(k-1)}\right)$$

where $f : \mathbb{R}^{kn+1} \to \mathbb{R}^n.$

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Introduce new variables

$$y_1(t) = u(t), y_2(t) = u'(t), \ldots, y_k(t) = u^{(k-1)}(t)$$

so that the original kth order system becomes a system of kn first order equations

$$y' = \begin{bmatrix} y_1' \\ \vdots \\ y_{k-1}' \\ y_k' \end{bmatrix} = \begin{bmatrix} y_2 \\ \vdots \\ y_k \\ f\left(t, y_1, y_2, \cdots, y_k\right) \end{bmatrix}$$

Module 2

Initial Value Problems

Initial Value Problems: Well-posedness

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We want to study the methods for numerical solution of a first order system of ordinary differential equations with initial conditions,

$$y' = f(t, y), \qquad y(t_0) = y_0,$$

where $y\colon [a, b] \to \mathbb{R}^n$ *and* $f\colon \mathbb{R}^{n+1} \to \mathbb{R}^n$.

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Before we study the numerical solution, we need to investigate the well-posedness of the problem, that is, we study if the problem has following three properties:

*(i) existence of a solution (**existence**),*

*(ii) uniqueness of the solution (**uniqueness**), and*

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This investigation, however, is the main subject matter of the course on Ordinary Differential Equations (ODE) and we, in this course, will only recall the relevant discussions.

Initial Value Problems: Well-posedness

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Let $D = [a, b] \times \Omega \subseteq \mathbb{R}^{n+1}$ *be a closed and bounded set.*

Suppose that $f: \mathbb{R}^{n+1} \to \mathbb{R}^n$ *is a Lipschitz continuous function in* y *on* D*, that is, there is a constant* L *such that for any* $t \in [a, b]$ *and for any* y *and* $\hat{y} \in \Omega$*,*

$$\|f(t, \hat{y}) - f(t, y)\| \le L\, \|\hat{y} - y\|.$$

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Recall, from your ODE course, that for such functions, the following Initial Value Problem (IVP)

$$y' = f(t, y), \qquad y(t_0) = y_0,$$

has a unique solution in a subinterval of $[a, b]$ *containg* y_0*.*

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Example: If f is differentiable, then f is Lipschitz continuous with

$$L = \max_{(t,y)\in D} \|f'(t, y)\|,$$

where f' is the $n{\times}n$ Jacobian matrix of f with respect to y, $[f'(t, y)]_{ij} = \frac{\partial f_i(t,y)}{\partial y_j}$.

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If the function is also perturbed so that we have $\hat{y}' = \hat{f}(t, \hat{y})$, then for $t \geq t_0$,

$$\|\hat{y}(t) - y(t)\| \leq e^{L(t-t_0)}\, \|\hat{y}_0 - y_0\| + \frac{e^{L(t-t_0)} - 1}{L}\, \|\hat{f} - f\|,$$

where

$$\|\hat{f} - f\| = \max_{(t,y)\in D} \|\hat{f}(t, y) - f(t, y)\|.$$

These perturbation bounds show that the unique solution to the IVP is a continuous function of the problem data, and hence the problem is well-posed.

Module 2

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Initial Value Problems: Stability

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We will see that the stability of the solution plays a significant role in the propagation of error, introduced by a numerical method, over time; they can either get amplified or diminished depending on the stability.

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Also recall that a solution of the ODE $y' = f(t, y)$ *is said to be stable if for every* $\epsilon > 0$, *there exists a* $\delta > 0$ *such that if* $\hat{y}(t)$ *satisfied the ODE and* $\|\hat{y}(t_0) - y(t_0)\| \leq \delta$, *then* $\|\hat{y}(t) - y(t)\| \leq \epsilon$ *for all* $t \geq t_0$.

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Thus, for a stable solution, if the initial value is perturbed, then the perturbed solution remains close to the original solution, which rules out the exponential divergence of perturbed solution allowed by the perturbation bound

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$$\|\hat{y}(t) - y(t)\| \le e^{L(t-t_0)} \|\hat{y}_0 - y_0\|.$$

A stable solution is said to be asymptotically stable if $\|\hat{y}(t) - y(t)\| \to 0$ *as* $t \to \infty$. *This stronger form means that the original and perturbed solution not only remain close to each other, but they converge toward each other over time.*

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Examples:

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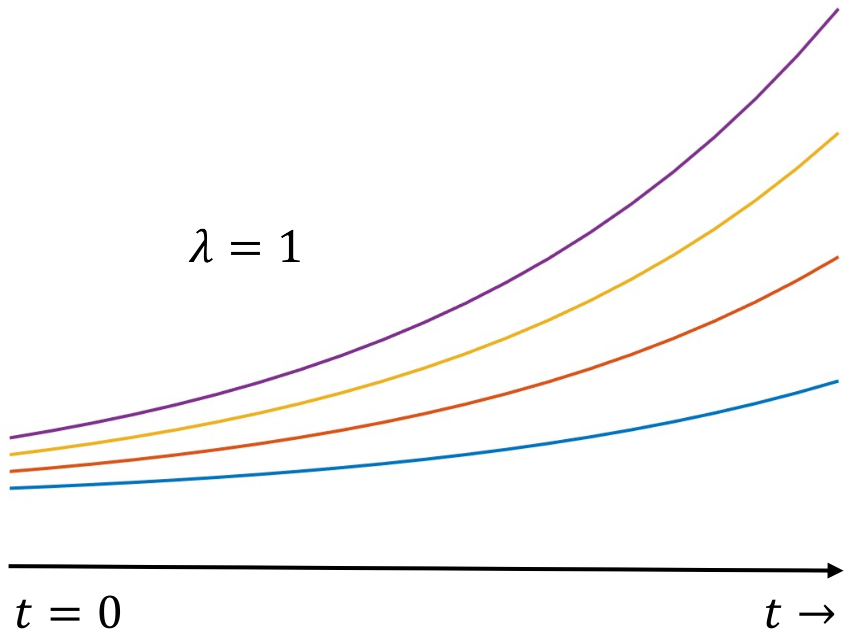

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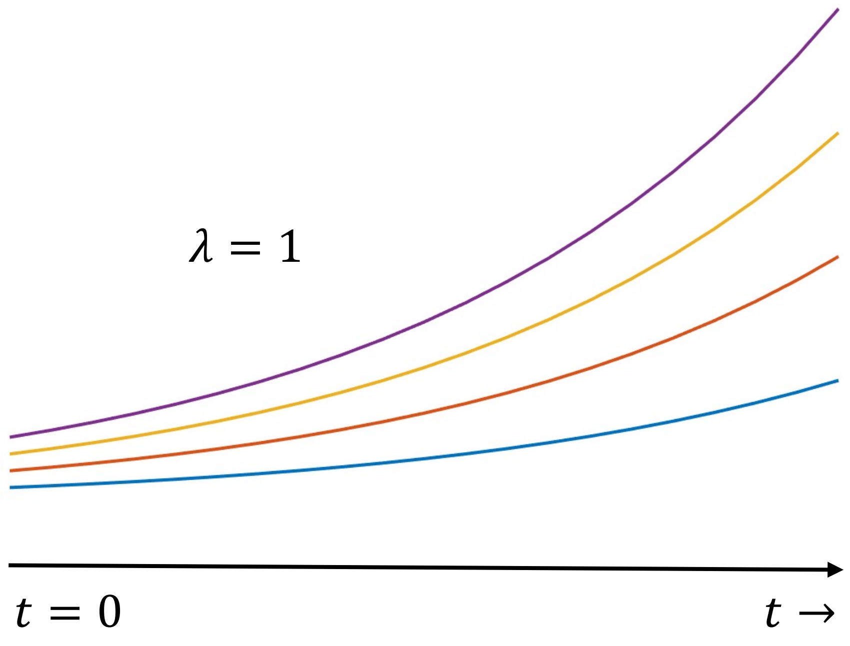

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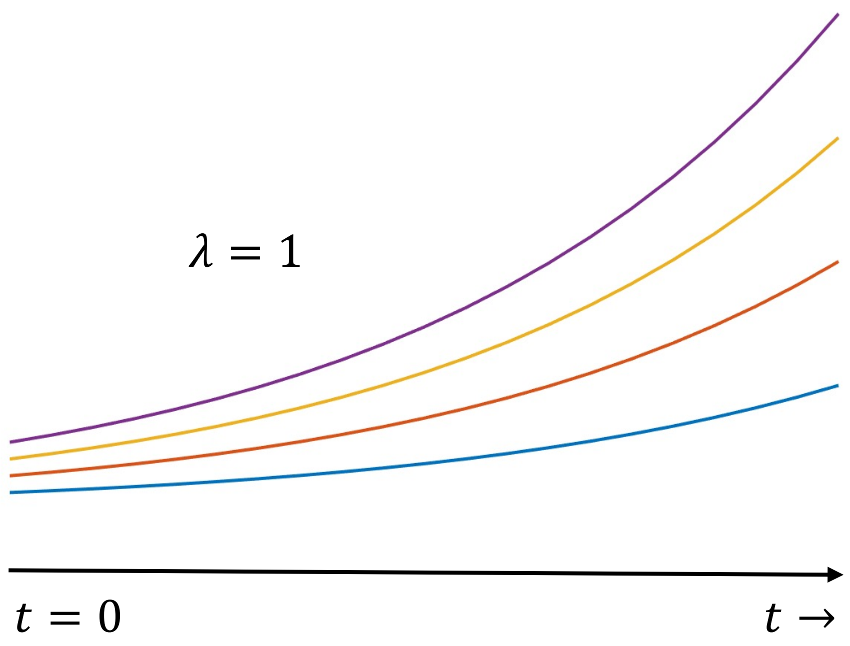

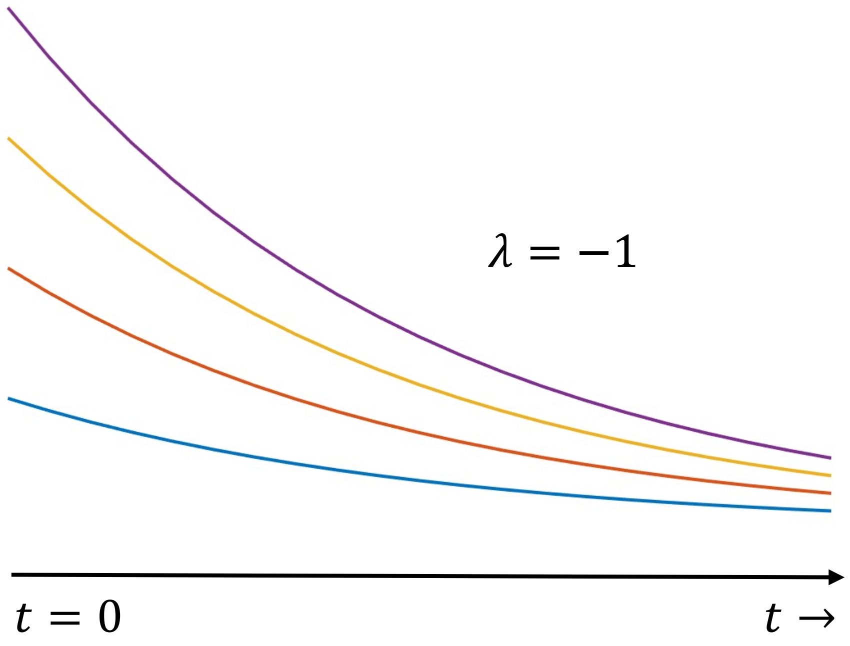

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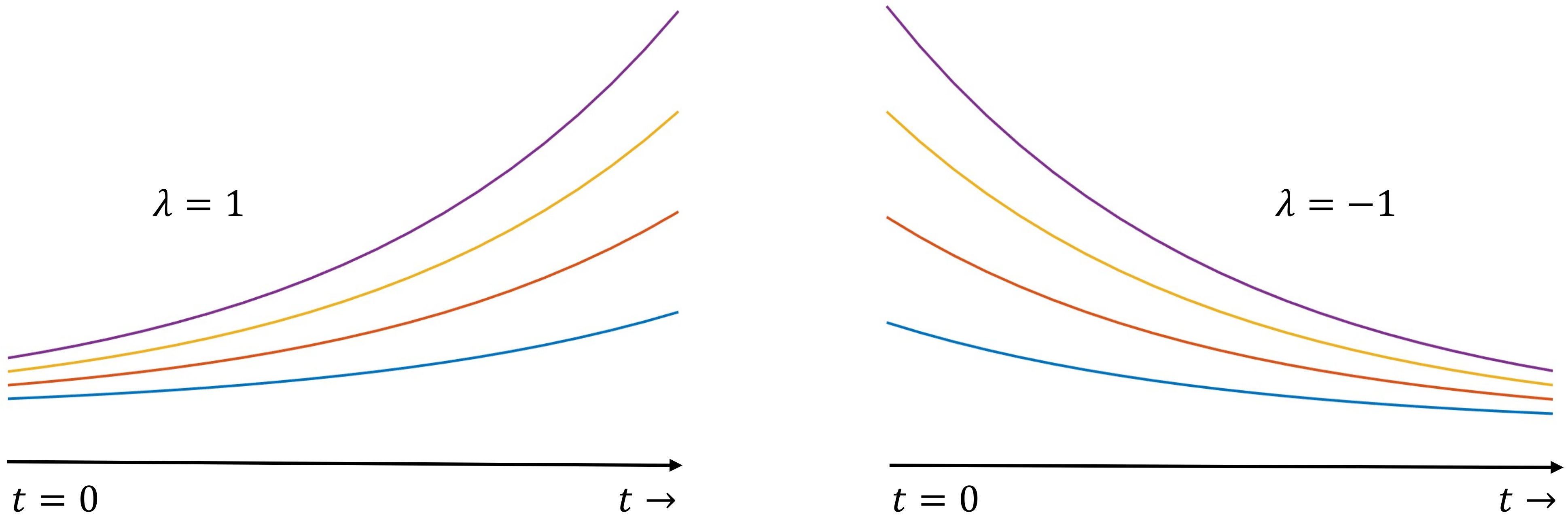

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(iii) A linear homogeneous system of ODEs with constant coefficients has the form

$$y' = Ay,$$

where A is an $n \times n$ matrix. Suppose we have the initial condition $y(0) = y_0$. Discuss the stability of the solutions if

(a) A is diagonalizable, and
(b) A is not diagonalizable.

*(**Exercise**)*

Module 2

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Starting at time t_0 with the given initial value y_0, we would like to track the solution tragectory governed by the ODE

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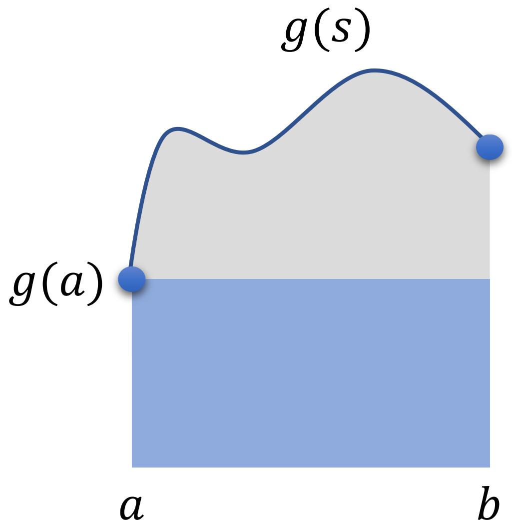

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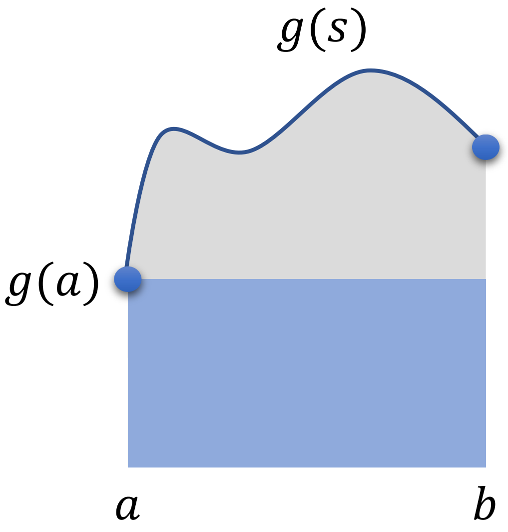

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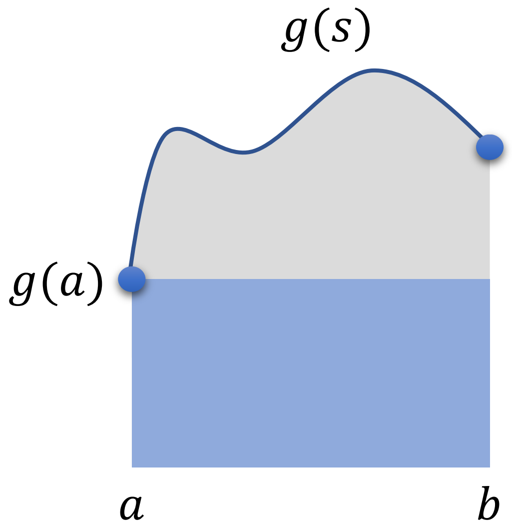

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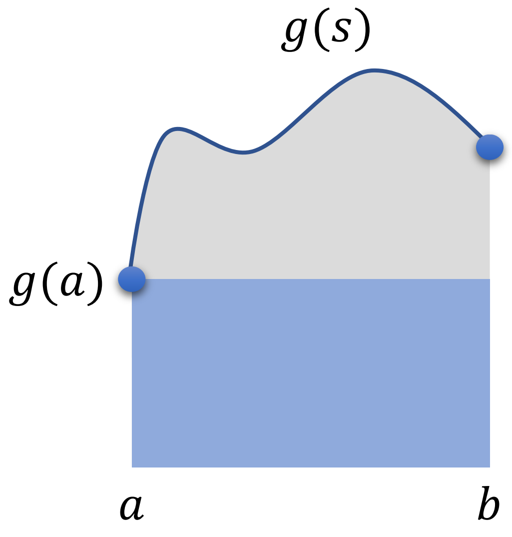

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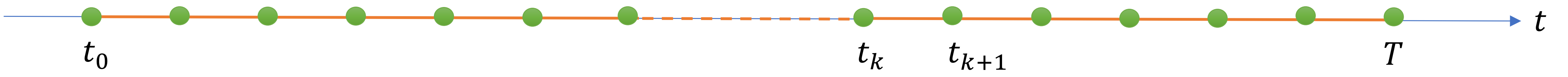

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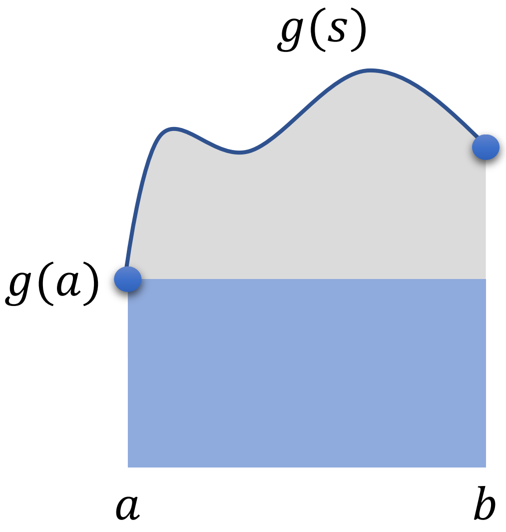

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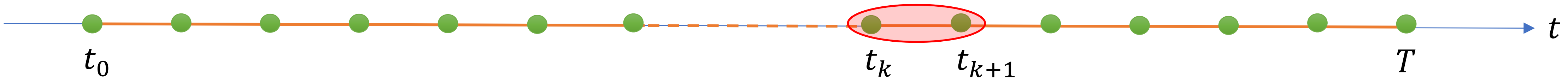

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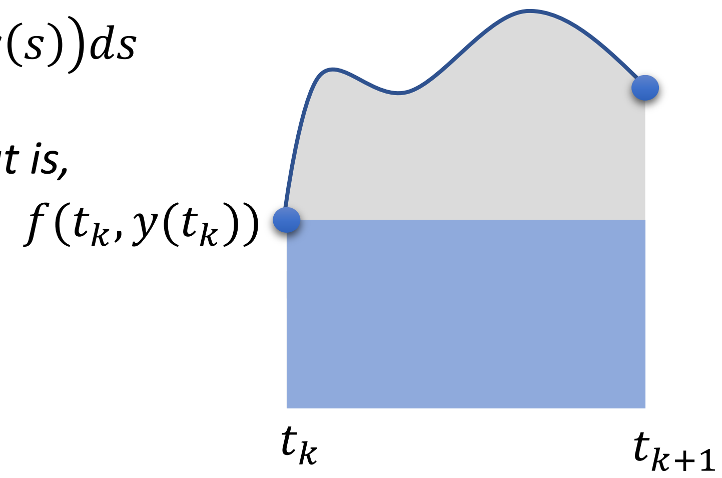

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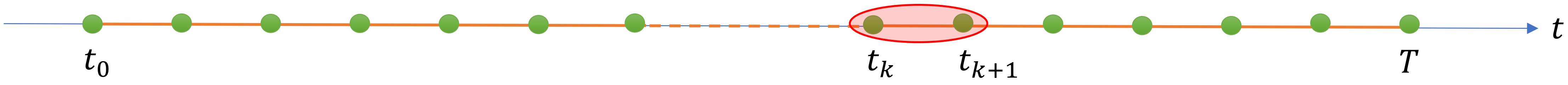


Initial Value Problems: Euler's method

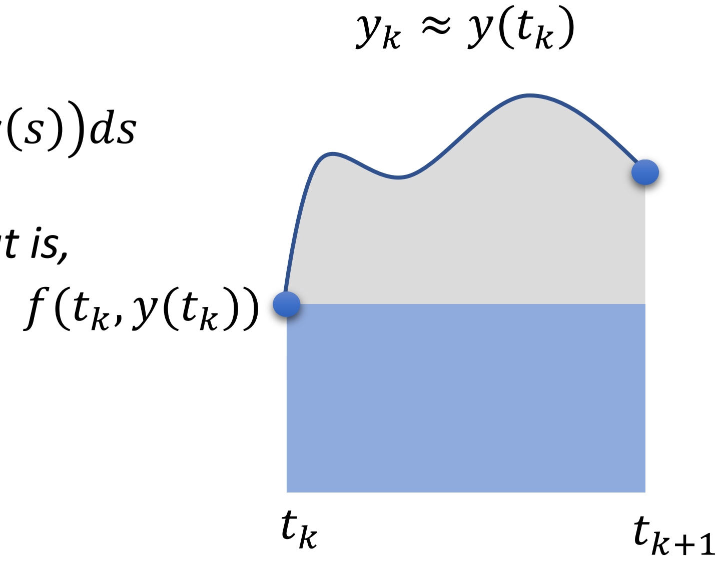
Akash Anand
MATH, IIT KANPUR

Starting at time t_0 with the given initial value y_0, we would like to track the solution tragectory governed by the ODE

$$y' = f(t, y)$$

The fundamental theorem of calculus tells us that

$$y(t_{k+1}) = y(t_k) + \int_{t_k}^{t_{k+1}} y'(s)ds = y(t_k) + \int_{t_k}^{t_{k+1}} f\big(s, y(s)\big)ds$$



The simplest approximation for the integral is by using the left end-point rule, that is,

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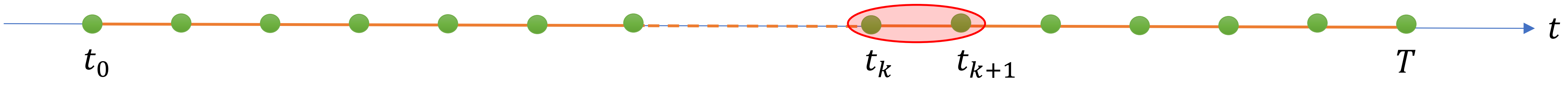

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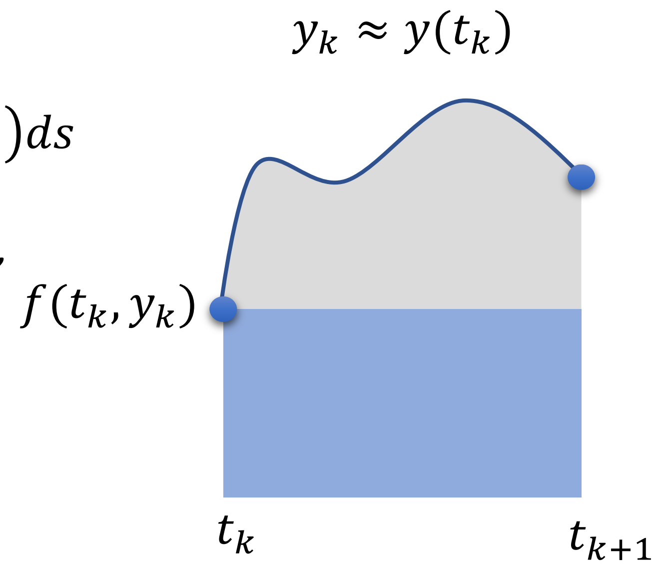

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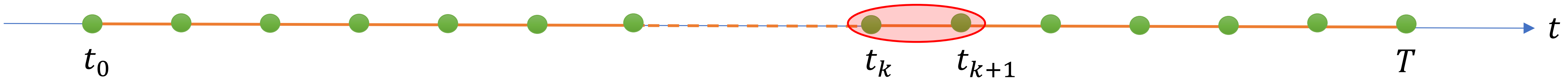

Initial Value Problems: Euler's method

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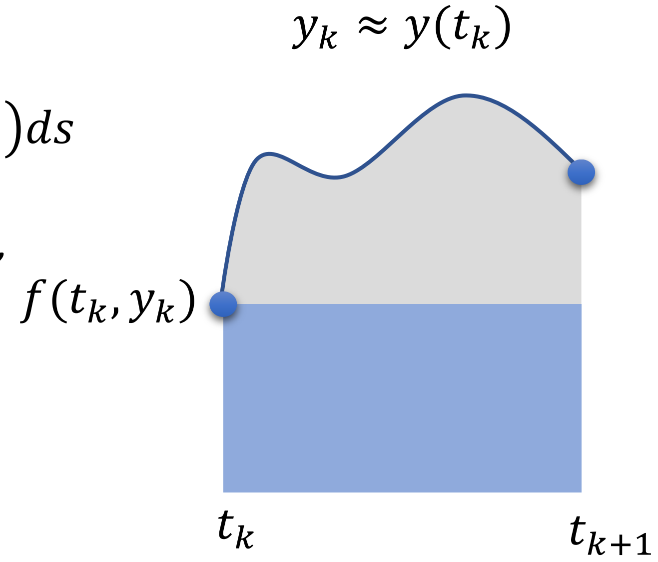

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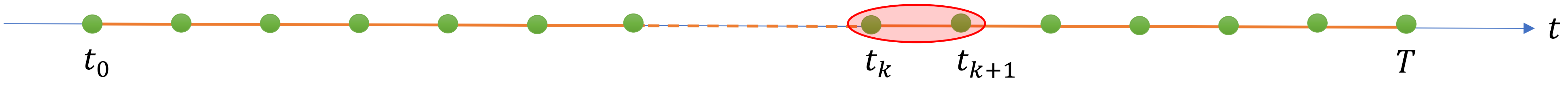

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Initial Value Problems: Euler's method

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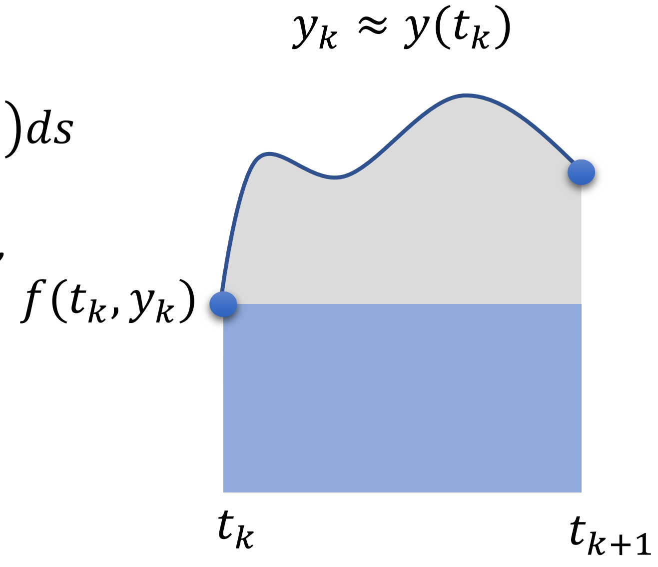

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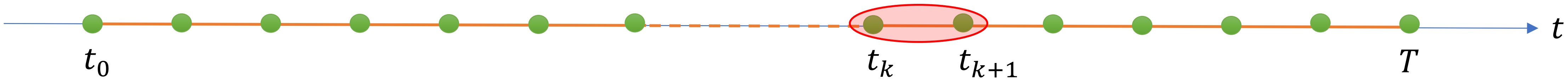

Euler's method

$$\boxed{y_{k+1} = y_k + (t_{k+1} - t_k)f(t_k, y_k)}$$

Module 2

Initial Value Problems

2.1 Well-posedness

2.2 Stability

2.3 Euler's method

- Derivations

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Derivation using Taylor series

Initial Value Problems: Euler's method

Derivation using Taylor series

Consider the Taylor series

$$y(t_{k+1}) = y(t_k) + (t_{k+1} - t_k)y'(t_k) + \frac{(t_{k+1} - t_k)^2}{2} y''(t_k) + \cdots$$

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The Euler's method results from taking $y_k = y(t_k)$, $y'(t_k) = f(t_k, y_k)$ *and dropping terms of second and higher orders!*

Initial Value Problems: Euler's method

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Derivation using finite difference approximation

Initial Value Problems: Euler's method

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Derivation using finite difference approximation

Replacing the $y'(t)$ in the ODE $y' = f(t, y)$ by a first order forward difference approximation, we obtain an algebraic equation

$$\frac{y_{k+1} - y_k}{t_{k+1} - t_k} = f(t_k, y_k)$$

that yields the Euler's method.

Initial Value Problems: Euler's method

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Derivation using polynomial interpolation

Initial Value Problems: Euler's method

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Derivation using polynomial interpolation

One point Hermite polynomial $p(t)$ *that matches the function and derivative data at* $t = t_k$*, that is,*

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Initial Value Problems: Euler's method

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Initial Value Problems: Euler's method

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Derivation using the method of undetermined coefficients

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Derivation using the method of undetermined coefficients

At $t = t_k$, *we know the values* y_k *and* y_k', *and based on these values we want to predict the value* y_{k+1}.

Initial Value Problems: Euler's method

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Derivation using the method of undetermined coefficients

At $t = t_k$, we know the values y_k and y_k', and based on these values we want to predict the value y_{k+1}. A predictor based on their linear combination has the form

$$y_{k+1} = \alpha y_k + \beta y_k'$$

where α and β are coefficients to be determined.

Initial Value Problems: Euler's method

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Initial Value Problems: Euler's method

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Initial Value Problems: Euler's method

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implying $\alpha = 1$ *and* $\beta = t_{k+1} - t_k$ *resulting in the Euler's method.*

Module 2

Initial Value Problems

2.1 Well-posedness

2.2 Stability

2.3 Euler's method

- Errors and error propagation

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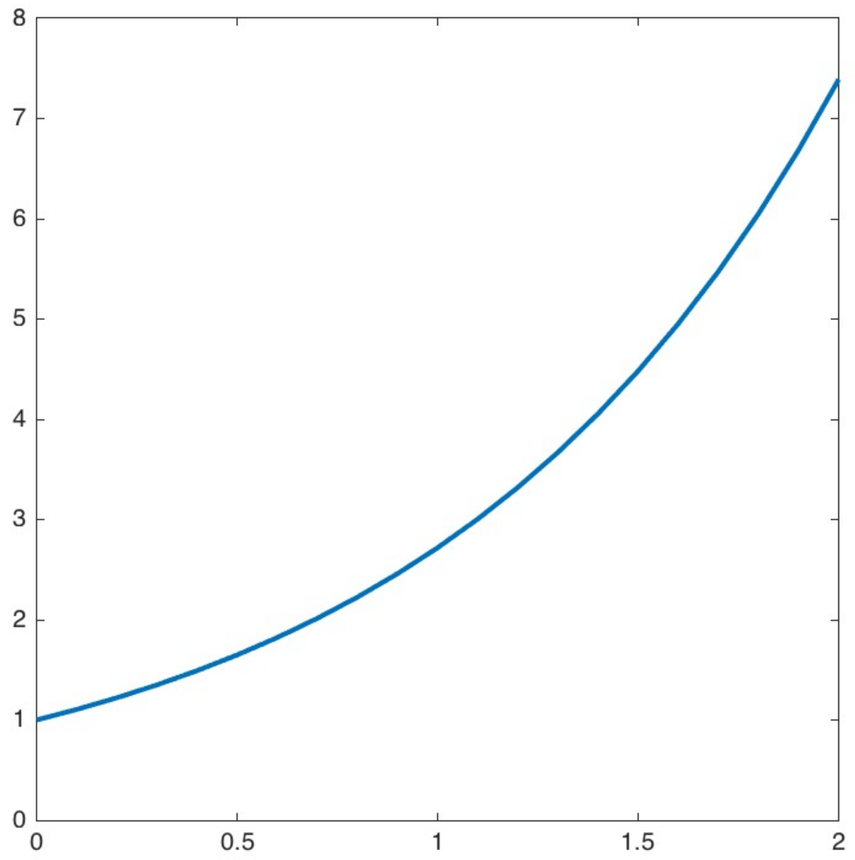
MATH, IIT KANPUR

Initial Value Problems: Euler's method

Example

Let us solve $y' = y,\; y(0) = 1$ *using the Euler's method taking the uniform step size* $h = h_k = t_{k+1} - t_k = 0.5$.

$$y_1 = 1 + h,\quad y_2 = y_1 + hy_1 = (1+h)^2,\quad y_3 = y_2 + hy_2 = (1+h)^3, \ldots,\quad y_k = (1+h)^k, \ldots$$



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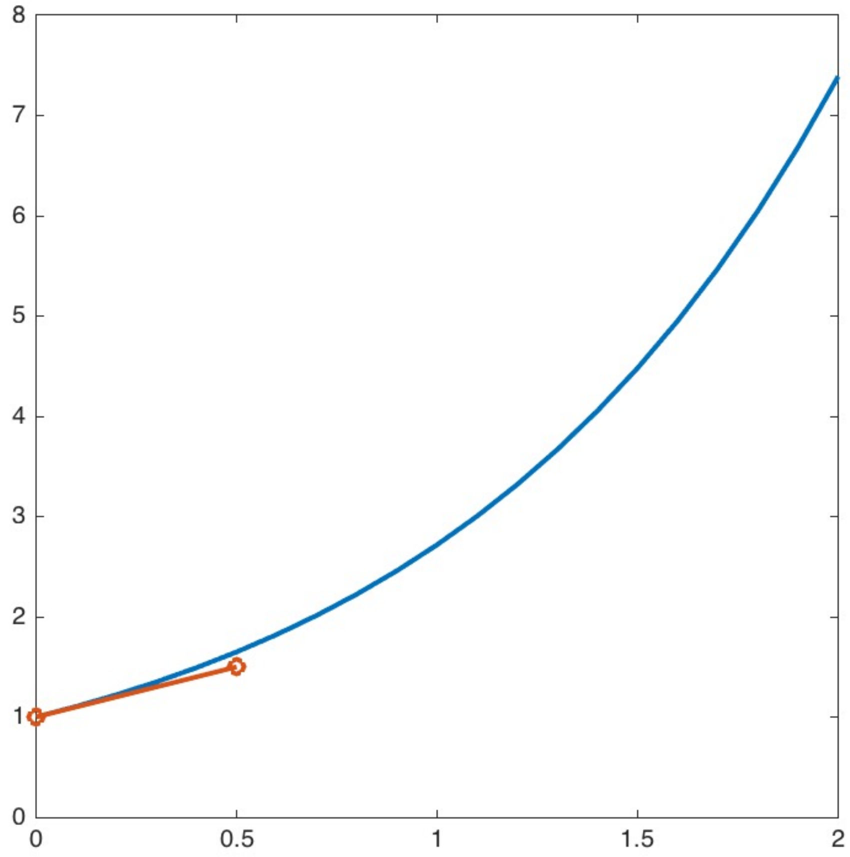

Initial Value Problems: Euler's method

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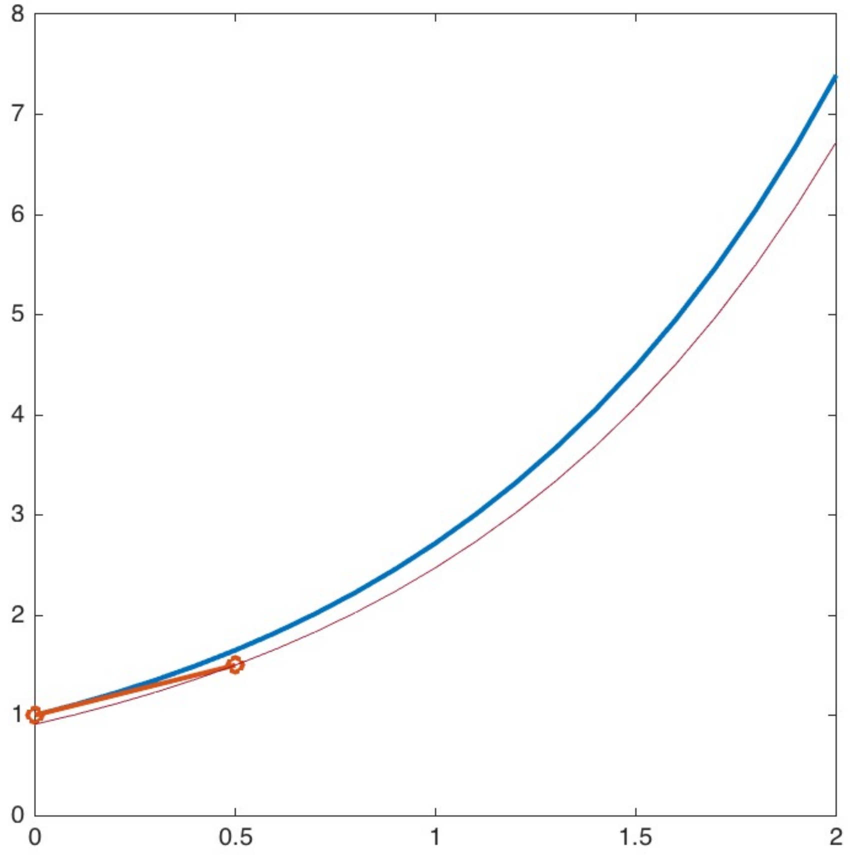

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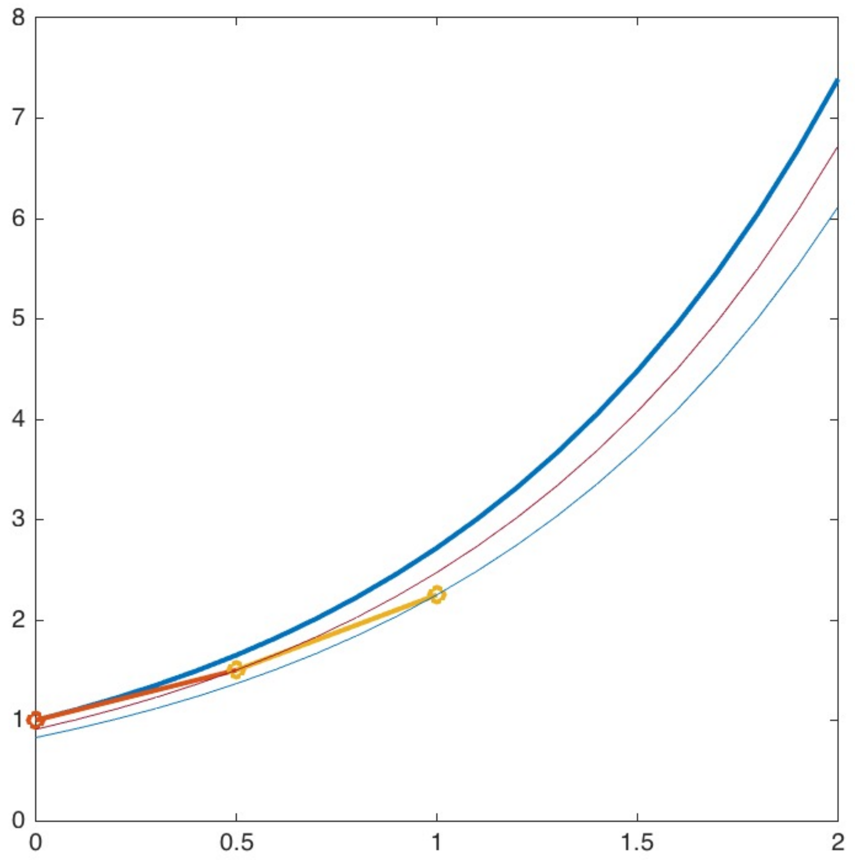

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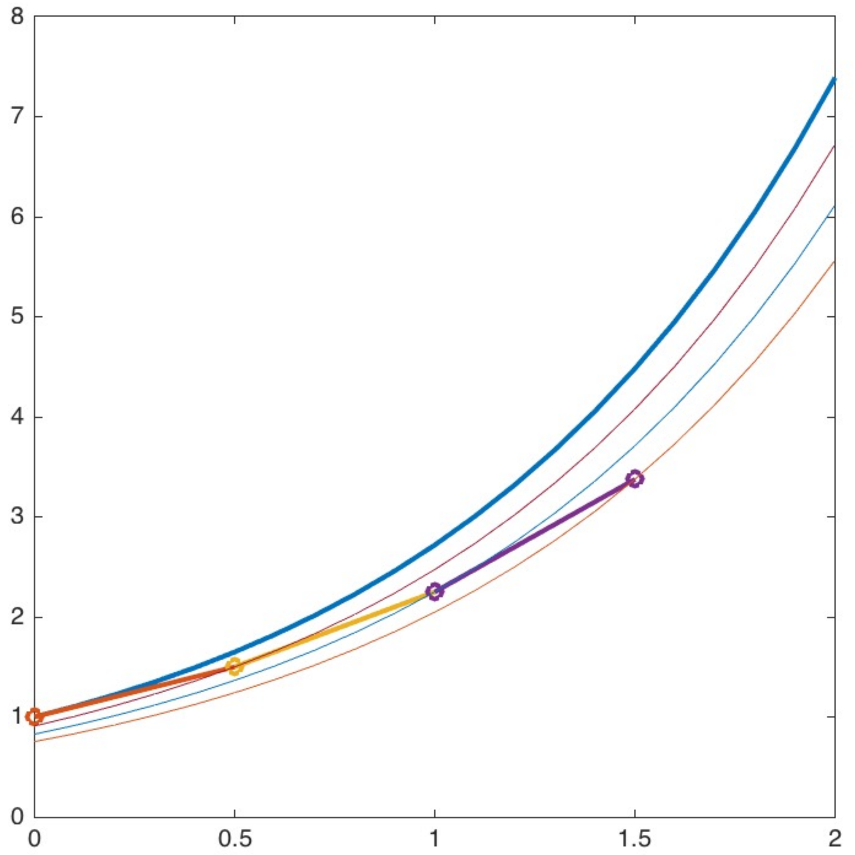

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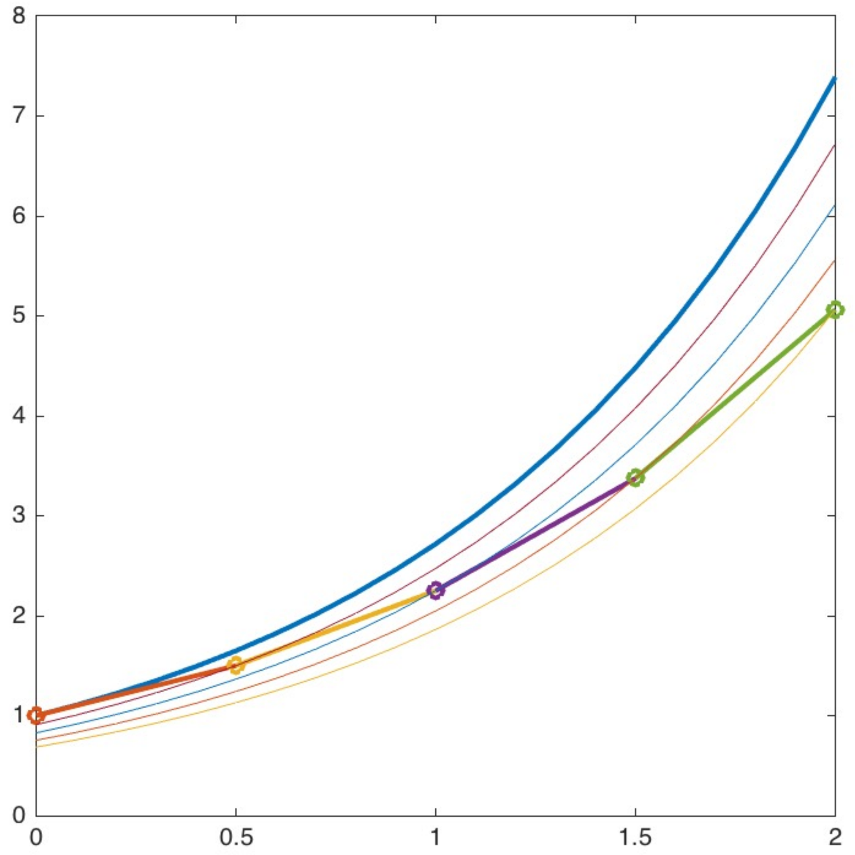

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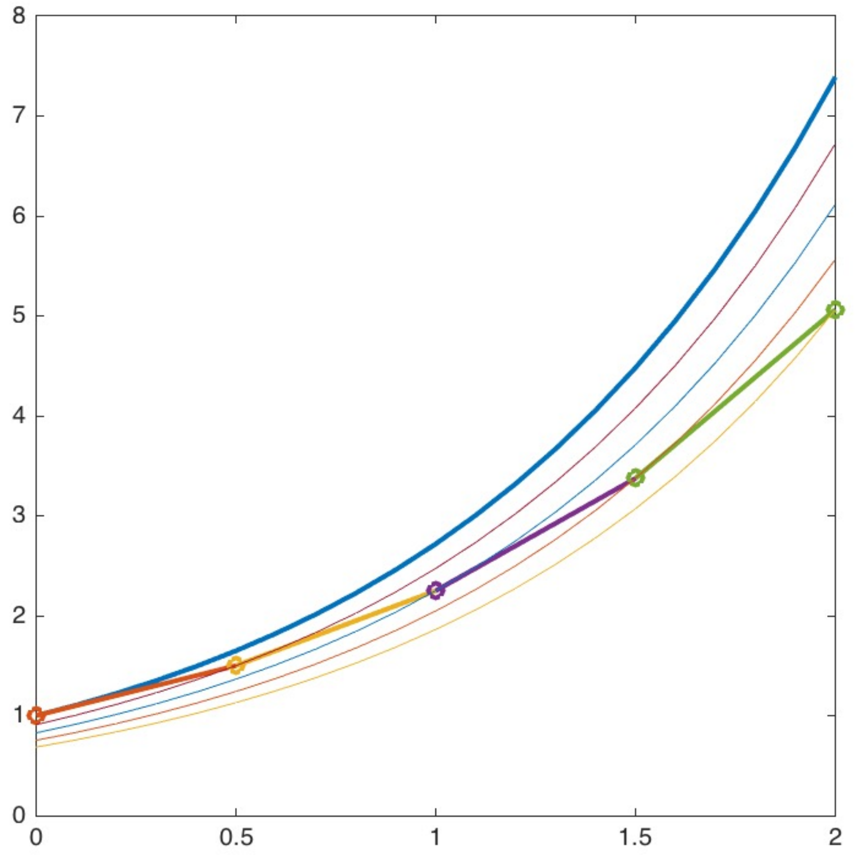

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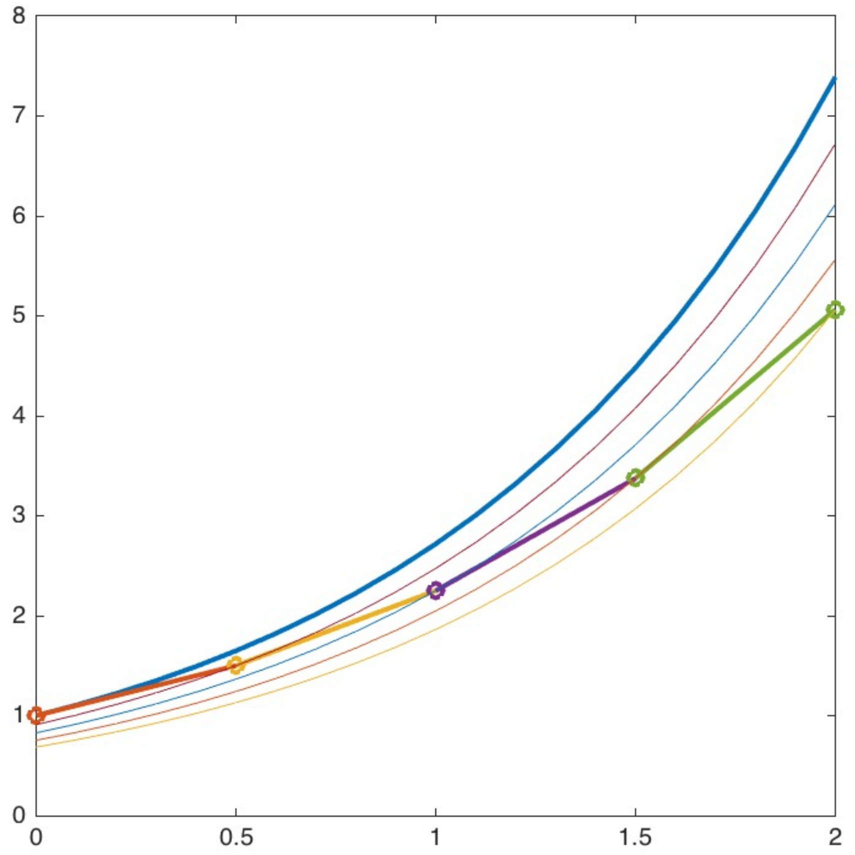

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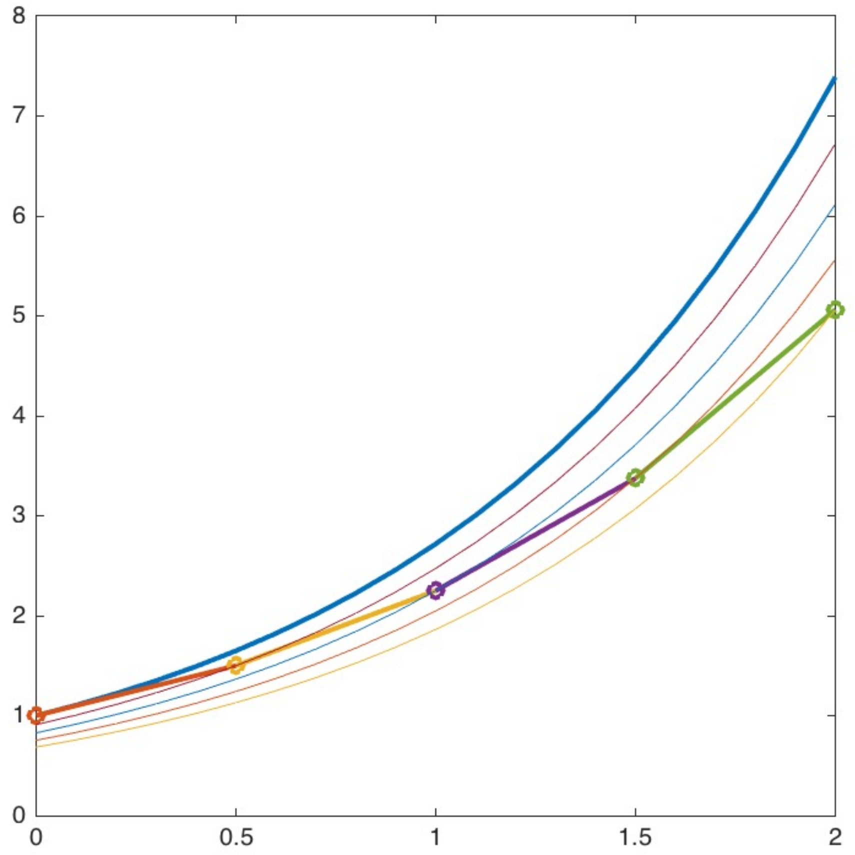

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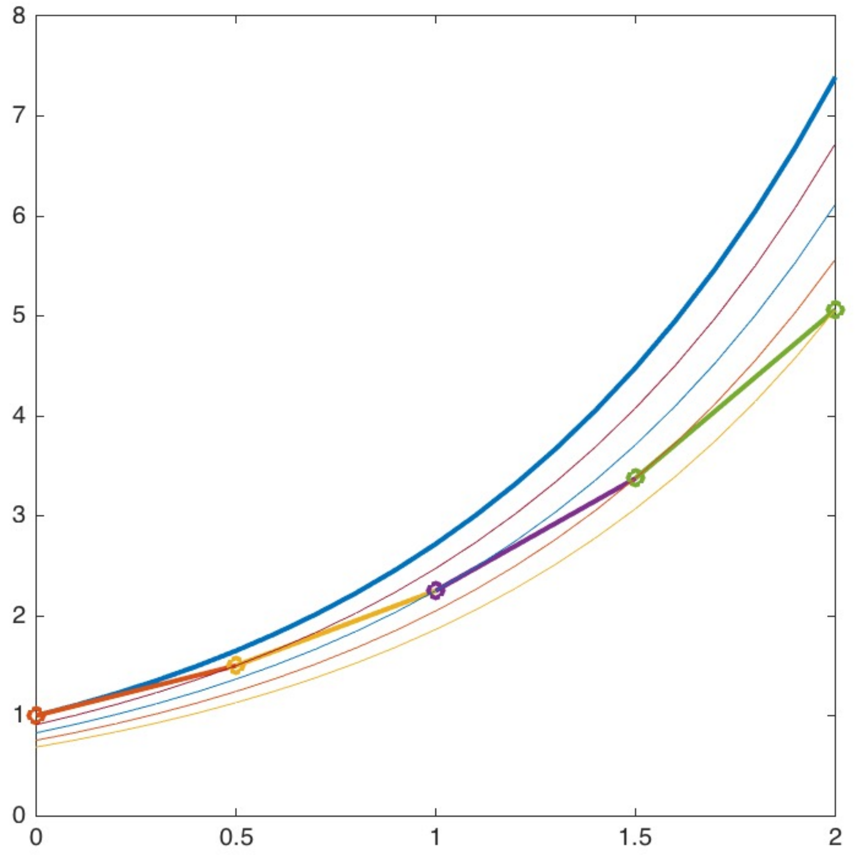

With each step, we hop from one solution of the ODE to another.

Initial Value Problems: Euler's method

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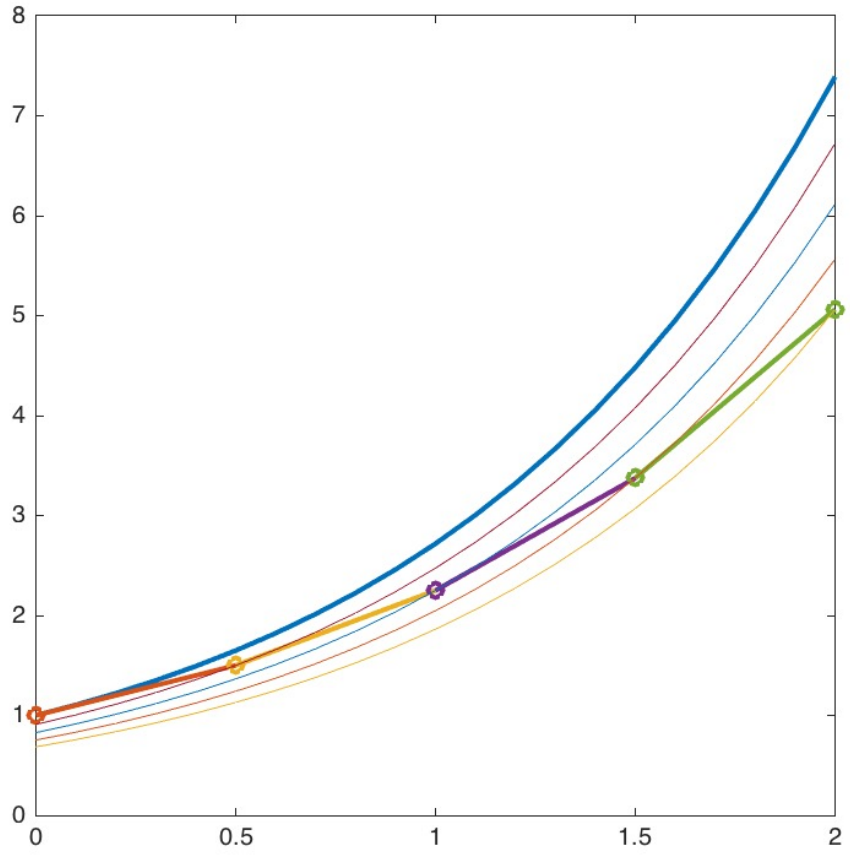

With each step, we hop from one solution of the ODE to another.

Local errors get amplified if the solutions to the ODE are unstable.

Initial Value Problems: Euler's method

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Example

Let us solve $y' = y,\ \ y(0) = 1$ *using the Euler's method taking the uniform step size* $h = h_k = t_{k+1} - t_k = 0.5.$

$$y_1 = 1 + h,\ \ y_2 = y_1 + hy_1 = (1+h)^2,\ \ y_3 = y_2 + hy_2 = (1+h)^3, \ldots,\ \ y_k = (1+h)^k, \ldots$$

With each step, we hop from one solution of the ODE to another.

Local errors get amplified if the solutions to the ODE are unstable.

Source: https://youtu.be/714HgSO0h7g

Example

Let us solve $y' = -y,\ y(0) = 1$ *using the Euler's method taking the uniform step size* $h = 0.5$.

Example

Let us solve $y' = -y,\ y(0) = 1$ *using the Euler's method taking the uniform step size* $h = 0.5$.

$$y_1 = 1 - h,\quad y_2 = y_1 - hy_1 = (1-h)^2,\quad y_3 = y_2 - hy_2 = (1-h)^3, \dots,\quad y_k = (1-h)^k, \dots$$

Initial Value Problems: Euler's method

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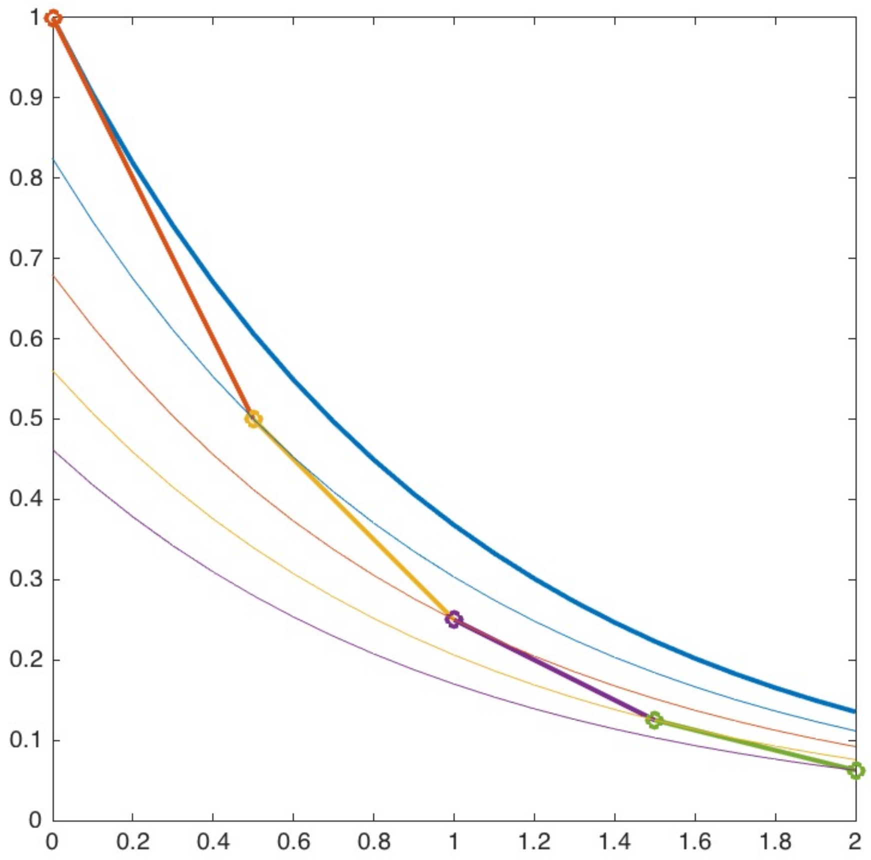
Example

Let us solve $y' = -y,\ y(0) = 1$ *using the Euler's method taking the uniform step size* $h = 0.5$.

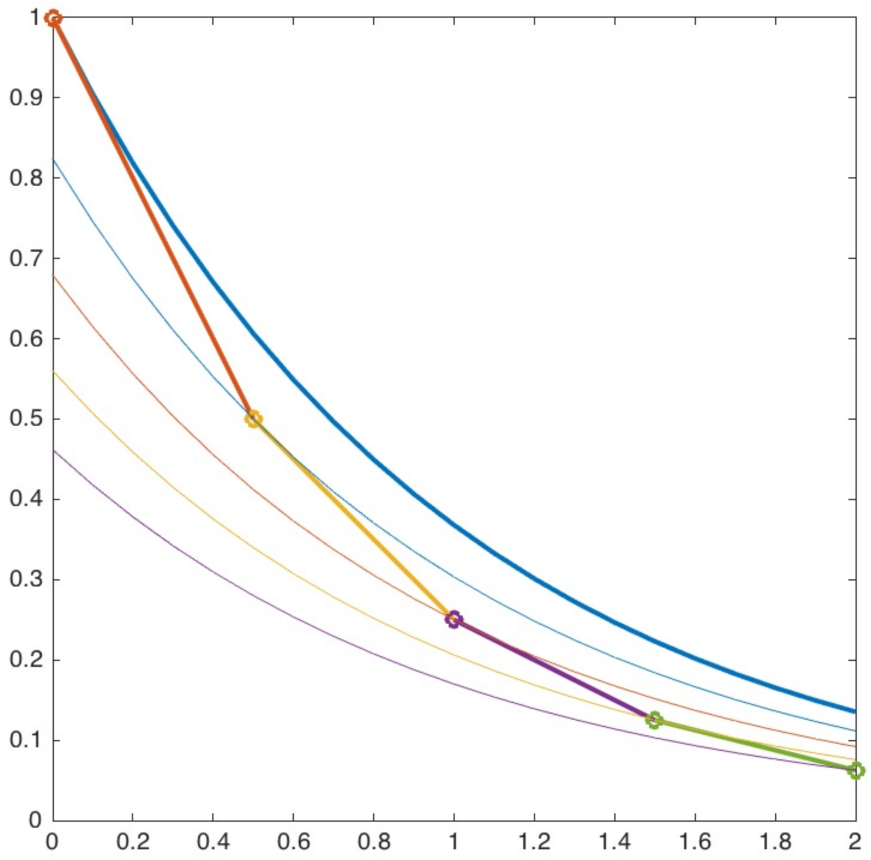
$$y_1 = 1 - h,\ \ y_2 = y_1 - hy_1 = (1-h)^2,\ \ y_3 = y_2 - hy_2 = (1-h)^3, \ldots,\ \ y_k = (1-h)^k, \ldots$$



Example

Let us solve $y' = -y,\ y(0) = 1$ *using the Euler's method taking the uniform step size* $h = 0.5$.

$$y_1 = 1 - h,\ \ y_2 = y_1 - hy_1 = (1-h)^2,\ \ y_3 = y_2 - hy_2 = (1-h)^3, \dots,\ \ y_k = (1-h)^k, \dots$$



For an equation with stable solutions, the errors in the numerical solution do not grow, and for equations with asymptotically stable solutions, the errors diminish with time.