# Metodi Numerici dell'Informatica

## Introduzione

Emanuele Rodolà
rodola@di.uniroma1.it

SAPIENZA
Università di Roma

# Logistics

- **Docenti:** Prof. Emanuele Rodolà

- **Assistenti:** Dr. Riccardo Marin e Dr. Emilian Postolache
  Codice, esercitazioni, supporto tecnico

# Logistics

- **Docenti:** Prof. Emanuele Rodolà

- **Assistenti:** Dr. Riccardo Marin e Dr. Emilian Postolache
  Codice, esercitazioni, supporto tecnico

- **Quando:** Mercoledi 10:00–**12:30** e Giovedi 14:00–**15:30**

# Logistics

- **Docenti:** Prof. Emanuele Rodolà

- **Assistenti:** Dr. Riccardo Marin e Dr. Emilian Postolache
  Codice, esercitazioni, supporto tecnico

- **Quando:** Mercoledi 10:00–**12:30** e Giovedi 14:00–**15:30**

- **Dove:**
  In presenza: Aula G50 - Edificio RM115 (complesso Regina Elena,
  Edificio G)
  Aula virtuale: Zoom, Meeting ID: 475 234 9941, Passcode: 3K7xrM

# Logistics

- **Docenti:** Prof. Emanuele Rodolà

- **Assistenti:** Dr. Riccardo Marin e Dr. Emilian Postolache
  Codice, esercitazioni, supporto tecnico

- **Quando:** Mercoledi 10:00–**12:30** e Giovedi 14:00–**15:30**

- **Dove:**
  In presenza: Aula G50 - Edificio RM115 (complesso Regina Elena, Edificio G)
  Aula virtuale: Zoom, Meeting ID: 475 234 9941, Passcode: 3K7xrM

- **Ricevimento:** Inviare una mail al docente o agli assistenti

- **Sito del corso:** https://erodola.github.io/NumMeth-s2-2022/
  Controllare giornalmente per informazioni e materiale

# Repository

The course is hosted on Github at the url:

https://github.com/erodola/NumMeth-s2-2022

# Repository

The course is hosted on Github at the url:

https://github.com/erodola/NumMeth-s2-2022

You can use github to ask questions, in particular:

- Start a discussion to create a new topic / question
  (this replaces the issue system used last year)

- Reply to discussions started by others

- Please use discussions instead of direct emails to the Professor,
  unless you have private reasons.

# Disclaimer

This is a new course.

- All the material is new

# Disclaimer

This is a new course.

- All the material is new

- We will alternate between theoretical and lab classes

# Disclaimer

This is a new course.

- All the material is new

- We will alternate between theoretical and lab classes

- We may change the balance depending on your feedback

Try to enjoy the course!

Take this as an opportunity to learn in depth.

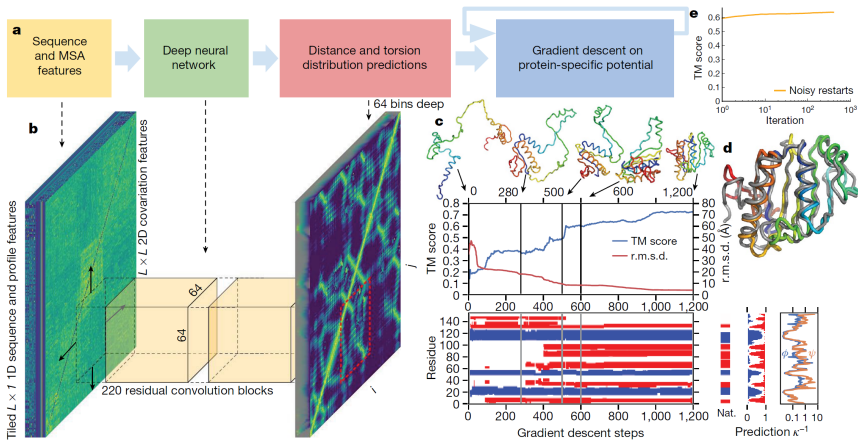Ask questions when in doubt.

# Who am I?

- Had research positions at U Tokyo, TU Munich, U Lugano and visiting positions at Harvard, Stanford, Ecole polytechnique, Technion among others

- Research: digital geometry processing, geometric deep learning

- Team: ~25 members from physics, engineering, computer science **GLADIA** group of Geometry, Learning and AI

- If you have ideas, approach us for projects / theses

# nature methods

**a**

| Sequence and MSA features | → | Deep neural network | → | Distance and torsion distribution predictions | ⇒ | Gradient descent on protein-specific potential |

**b**

Tiled $L \times 1$ 1D sequence and profile features

$L \times L$ 2D covariation features

64

64

64

220 residual convolution blocks

64 bins deep

$i$

$j$

**c**

0    280    500    600    1,200

TM score / r.m.s.d. (Å)

— TM score
— r.m.s.d.

0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1

80
70
60
50
40
30
20
10

0    200    400    600    800    1,000    1,200

Residue

140
120
100
80
60
40
20

0    200    400    600    800    1,000    1,200
Gradient descent steps

Nat.    0    1    0.1  1  10
Prediction $\kappa^{-1}$

**d**

**e**

TM score

0.6
0.4
0.2

$10^0$    $10^1$    $10^3$
Iteration

— Noisy restarts

https://deepmind.com/research/case-studies/alphafold

# Pre-requisites and reading material

"Numerical Algorithms" by Justin Solomon, CRC Press 2015.

Specific references will be given throughout the course in the form of book chapters and scientific articles.

## Pre-requisites and reading material

"Numerical Algorithms" by Justin Solomon, CRC Press 2015.

Specific references will be given throughout the course in the form of book chapters and scientific articles.



Pre-requisites:

- Programming fundamentals. We will use Python

- Welcome (not mandatory): linear algebra, calculus

# Grading

1. Midterm self-evaluation (*not graded*)
   When: first half of April

# Grading

1. Midterm self-evaluation (*not graded*)
   When: first half of April

2. Written exam
   When: June 15th and July 6th

# Grading

1. Midterm self-evaluation (*not graded*)
   When: first half of April

2. Written exam
   When: June 15th and July 6th

3. Optional: oral exam, contributing $\pm 3$ points to the final grade

# Grading

1. Midterm self-evaluation (*not graded*)
   When: first half of April

2. Written exam
   When: June 15th and July 6th

3. Optional: oral exam, contributing $\pm 3$ points to the final grade

In class, be prepared:

- Download/print the slides beforehand
- Take notes: not everything will be on the slides
- Bring your laptop: we'll do live coding sessions

## What will you get out of this course?
(if you study)

- You will acquire solid fundamental skills for understanding, analyzing, and applying numerical methods and algorithms in diverse application scenarios
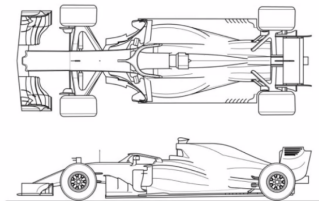
Overall objective

# What will you get out of this course?
### (if you study)

- You will acquire solid fundamental skills for understanding, analyzing, and applying numerical methods and algorithms in diverse application scenarios

- You will be able to grasp and elaborate on more advanced topics in several other applied disciplines and scientific areas
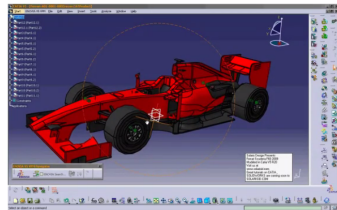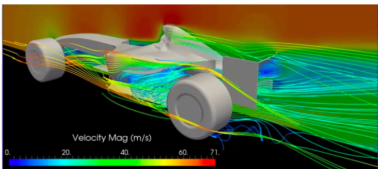
Overall objective

## What will you get out of this course?
### (if you study)

- You will acquire solid fundamental skills for understanding, analyzing, and applying numerical methods and algorithms in diverse application scenarios

- You will be able to grasp and elaborate on more advanced topics in several other applied disciplines and scientific areas

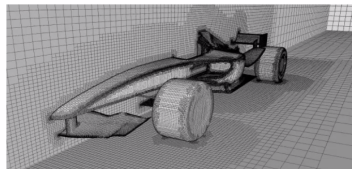- You will get practical development expertise on applied problems

Sketch

3d model

Aerodynamic simulation

Velocity Mag (m/s)
0.      20.      40.      60.      71.

Volumetric mesh

Image: Edoardo Remelli, EPFL