ME 471/571

Parallel Scientific Computing

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COVID SAFETY RULES

- We need to wear mask on our nose and mouth at all times inside University buildings
- When you have symptoms or feel under the weather, attend the class on Zoom, or review the recording later
- No food or drink in class

TELL ME ABOUT YOURSELF

- Why did you take this course?
- What do you expect to learn?

slido.com

Join at

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#342 454

WARSAW UNIVERSITY OF TECHNOLOGY

- Aeronautical Engineering
- Computational Fluid Dynamics

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THE UNIVERSITY OF WARWICK

Coventry, UK

- Scientific Computing
- Turbulence Simulations

NAVAL POSTGRADUATE SCHOOL

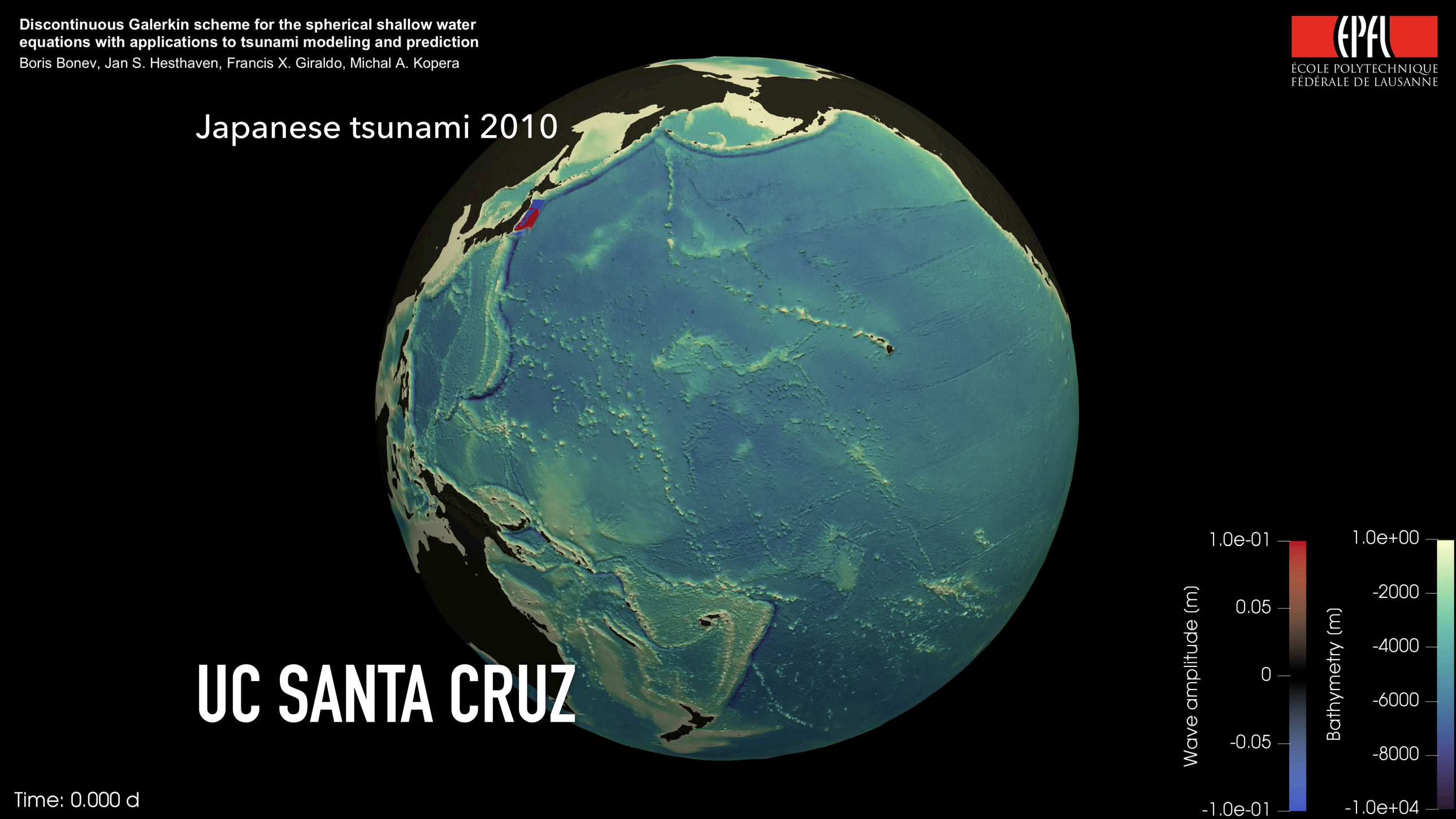
Monterey, CA

- Atmospheric modeling
- High Performance Computing

Discontinuous Galerkin scheme for the spherical shallow water equations with applications to tsunami modeling and prediction

Boris Bonev, Jan S. Hesthaven, Francis X. Giraldo, Michal A. Kopera

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE



- Computational Math
- High performance computing
- Mathematical methods for ocean modeling

BY THE END OF THIS COURSE WE WILL:

- run code on a **supercomputer**
- design **parallel algorithms** which take advantage of multiple processors working together
- measure **efficiency** and **scalability** of programs
- learn how to use a supercomputer to **accelerate your research**

WHAT ARE WE GOING TO LEARN ABOUT?

PARALLEL

SCIENTIFIC

COMPUTING

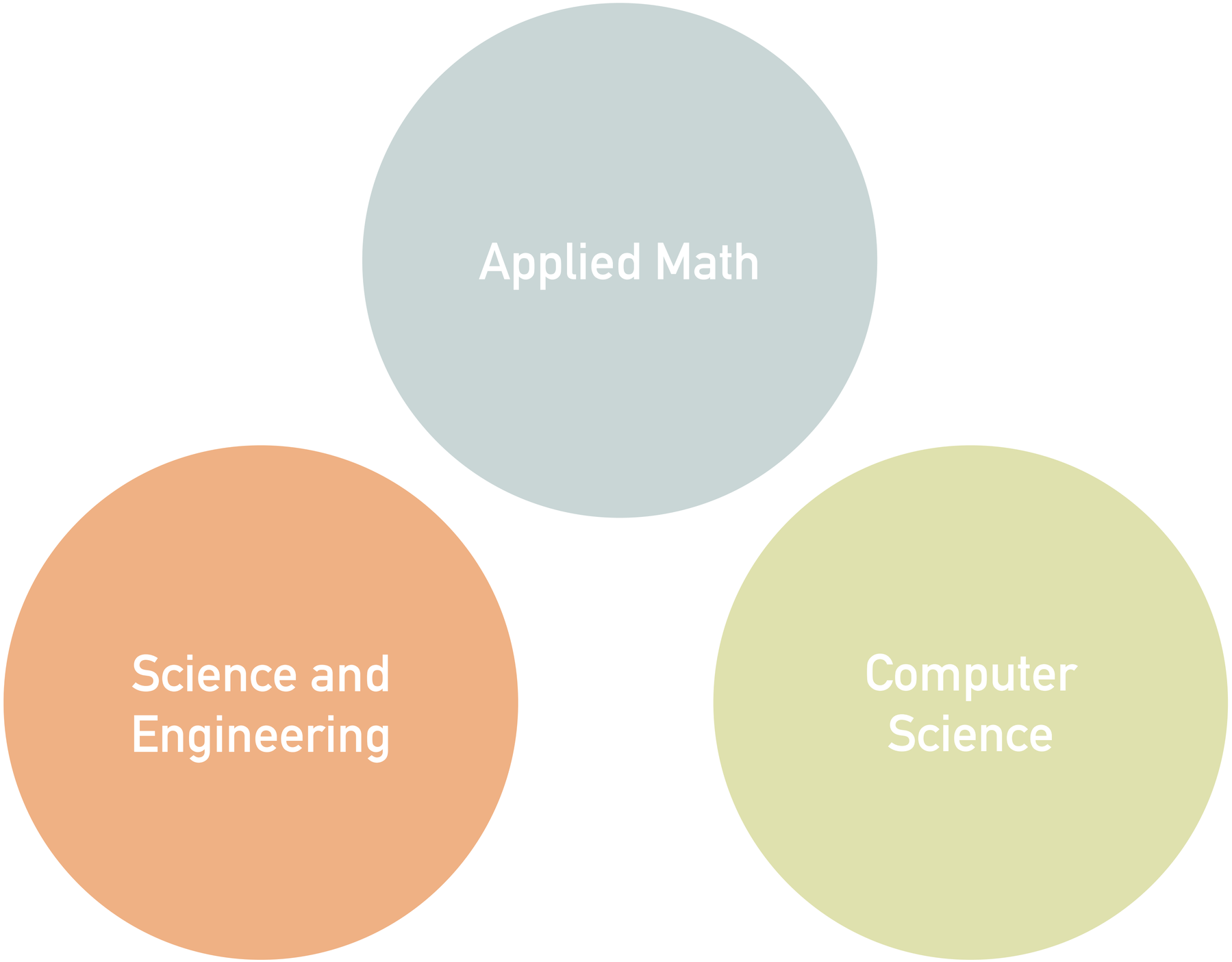
WHAT ARE WE GOING TO LEARN ABOUT?

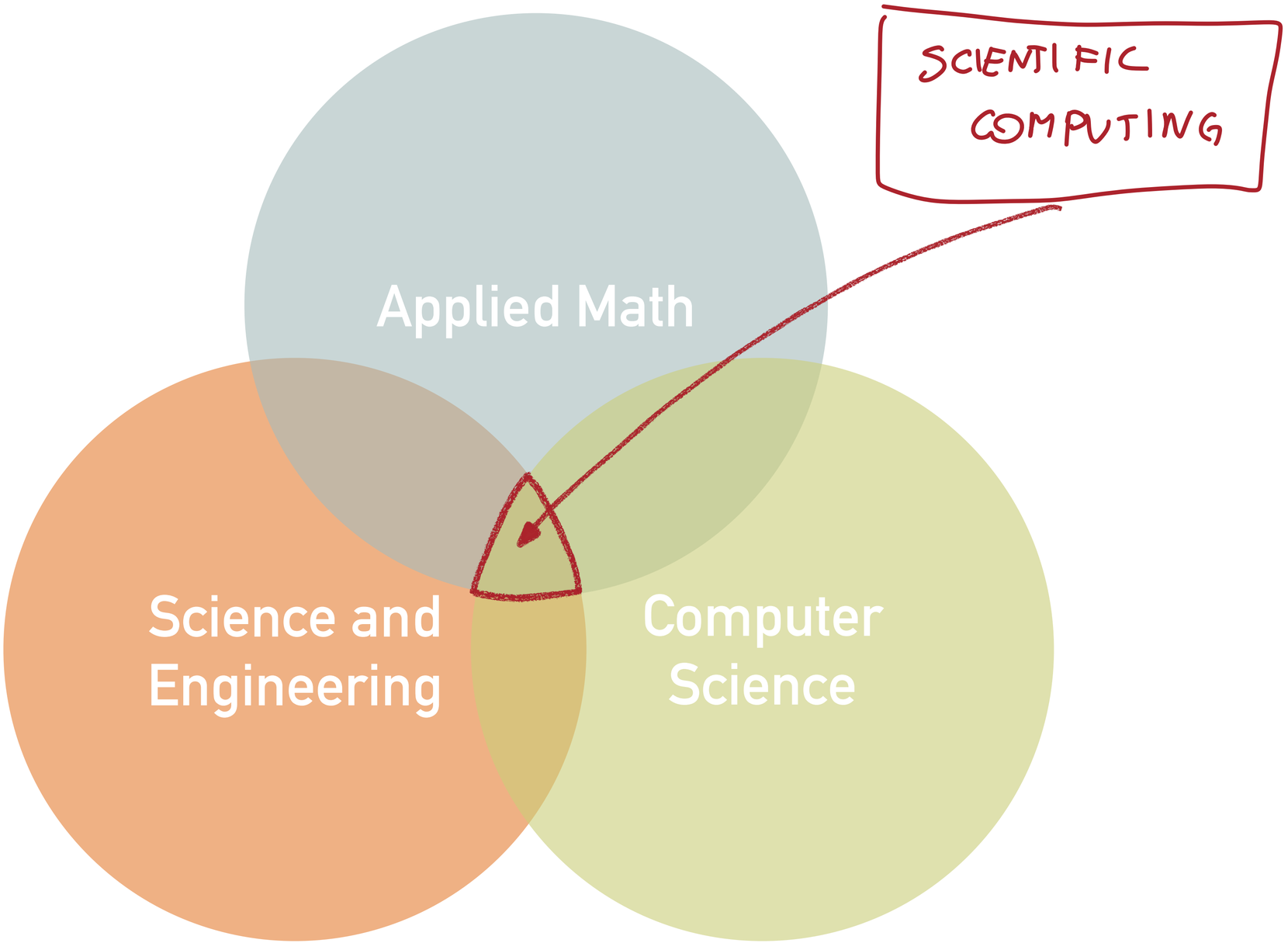
SCIENTIFIC COMPUTING

"Computational science has become the **third pillar of scientific enterprise**, a peer alongside theory and physical experiment"

"… is a rapidly growing **multidisciplinary** field that uses **advanced computing capabilities** to understand and solve **complex problems.**"

President's Information Technology Advisory Committee,
Report to the President, June 2005

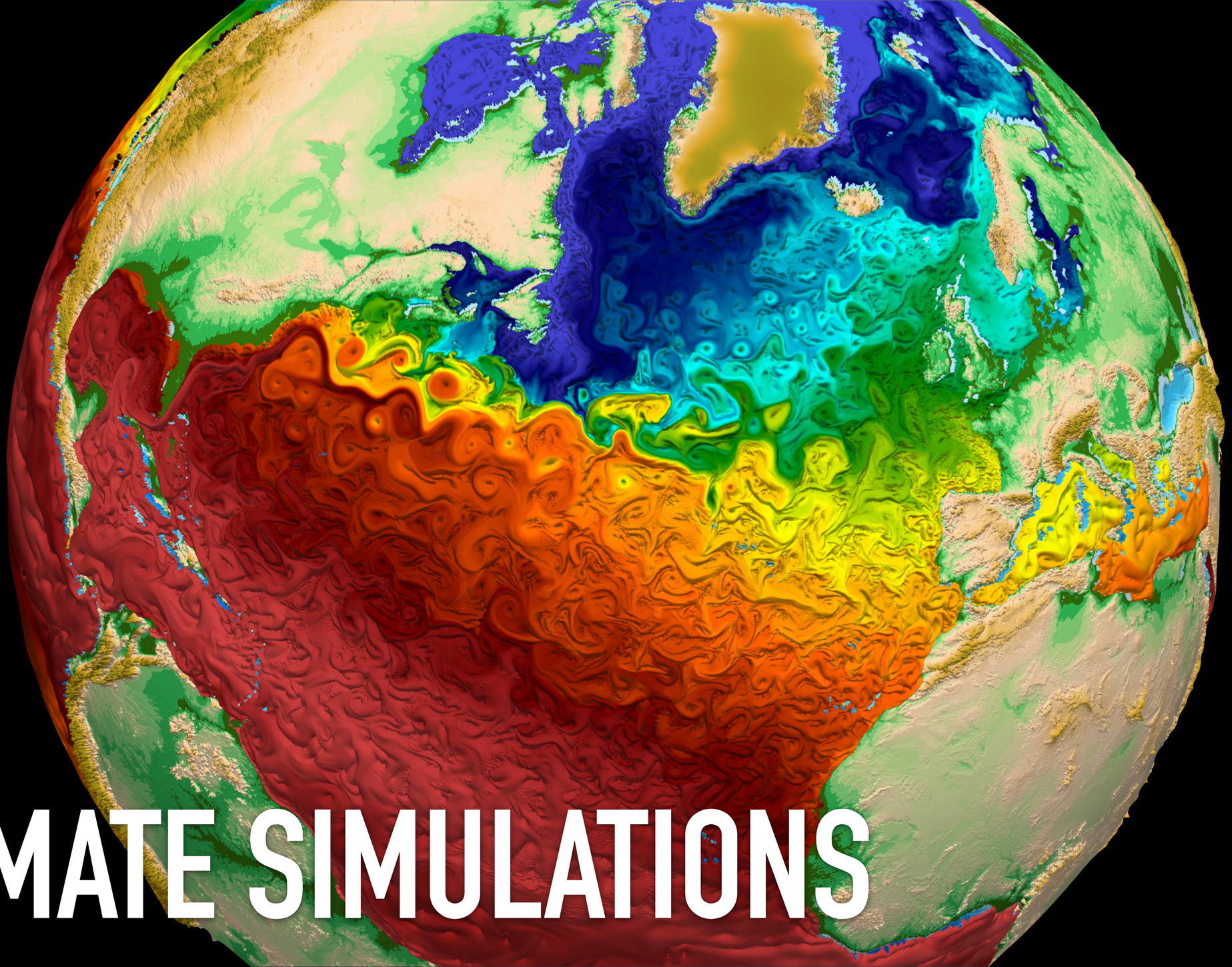

Applied Math
Science and Engineering
Computer Science


Applied Math
Science and Engineering
Computer Science
SCIENTIFIC COMPUTING

DECODING HUMAN GENOME

FORMATION OF STARS AND GALAXIES

(credits: phys.org)



CLIMATE SIMULATIONS

EXAMPLE – WEATHER FORECAST

10 km resolution = 5×10^6 points

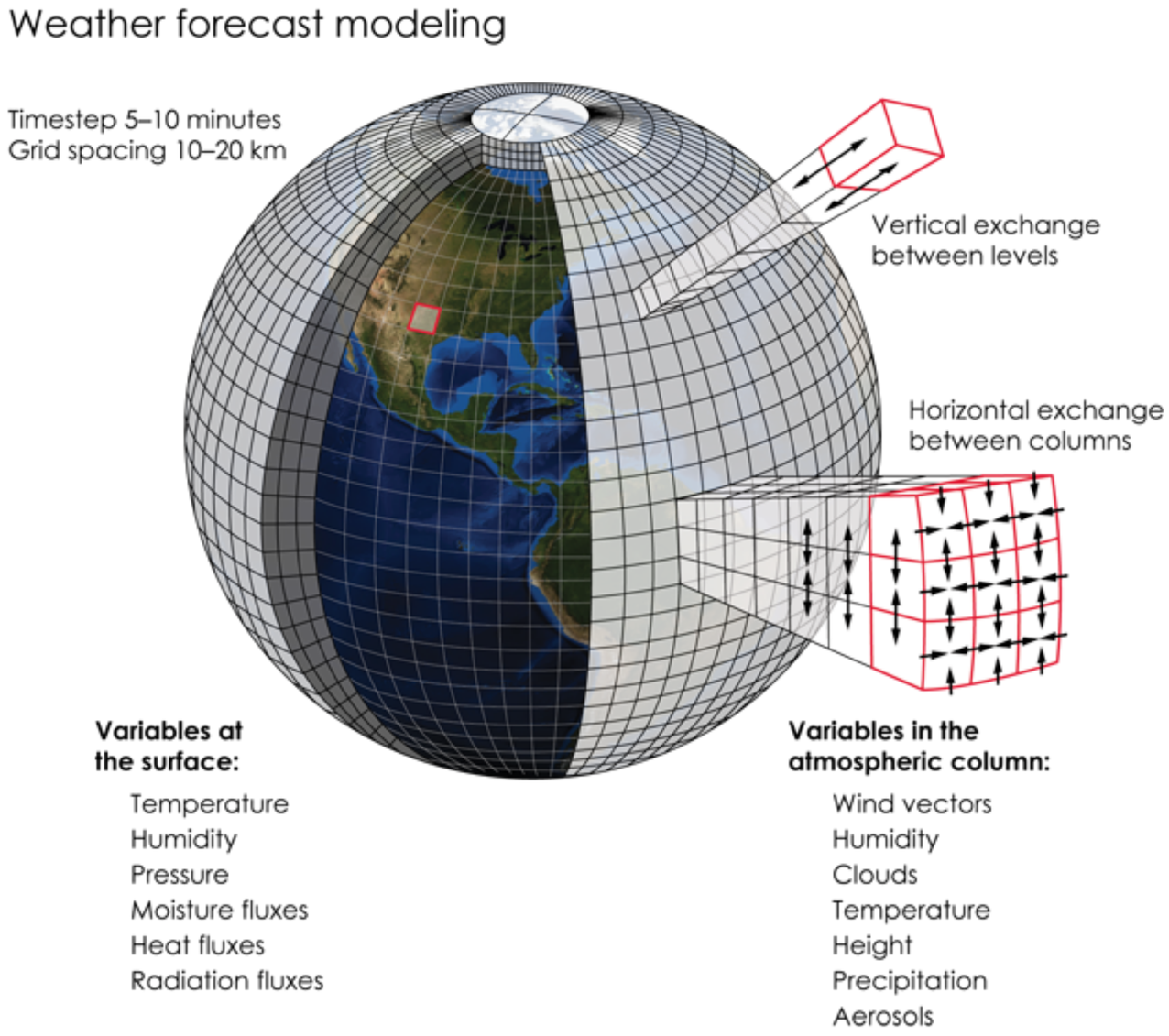
x 100 vertical levels = 5×10^8 points

x 10 variables = **5×10^9 DOF**

per time-step…

dt = 5 min gives ~300 time-steps per day

source: ECMWF



EXAMPLE – WEATHER FORECAST

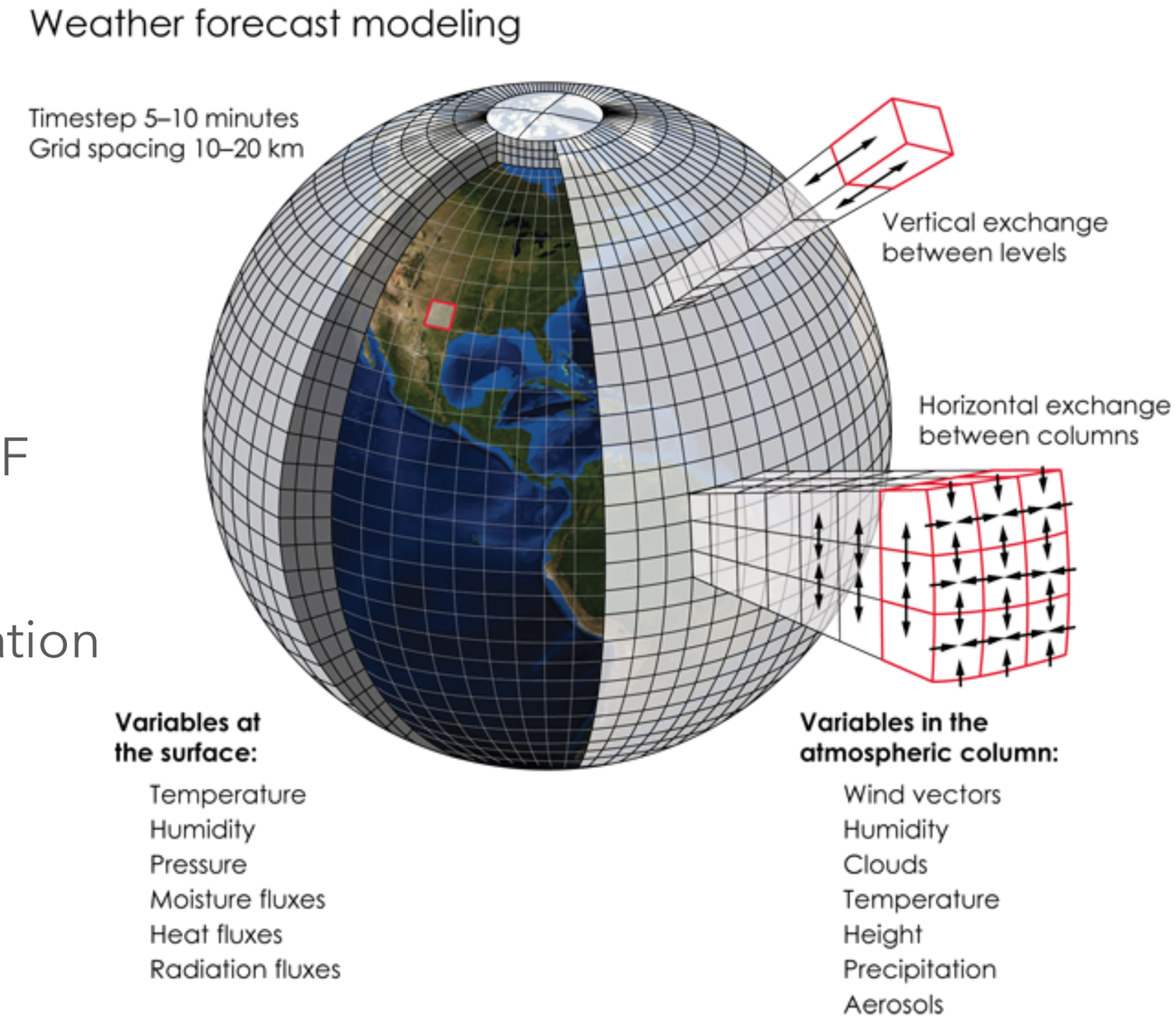
source: ECMWF

x 10 variables = **5 x 10^9 DOF**

dt = 5 min gives ~300 time-steps per day

say 1 time-step requires ~100 flop per DOF

that gives **1.5 x 10^{14} flop** per day of simulation



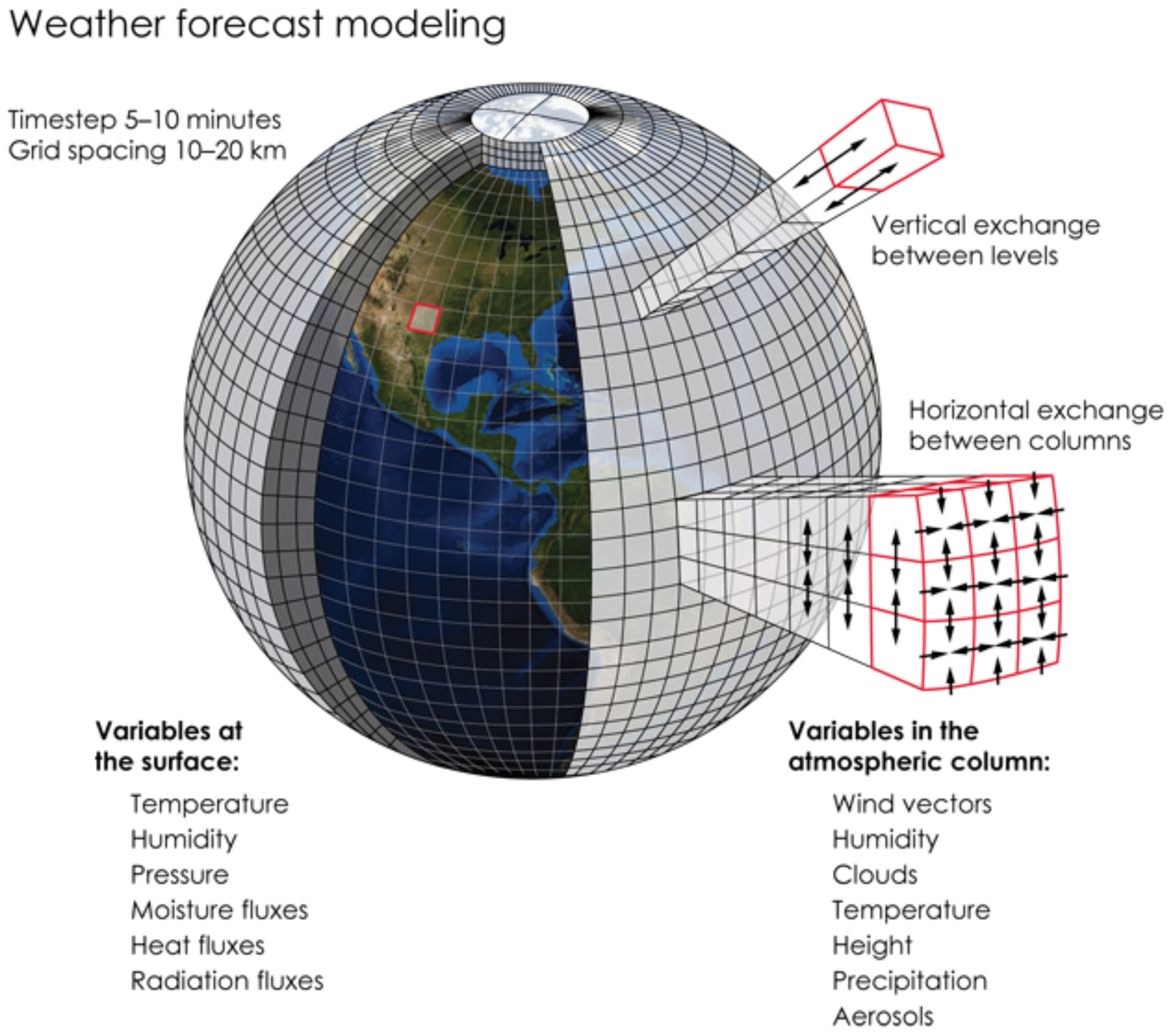
EXAMPLE – WEATHER FORECAST

source: ECMWF

that gives **1.5 x 10^{14} flop** per day of simulation

a laptop can do ~1 x 10^{9} flop/s

… but that is only a theoretical peak performance, excluding accessing memory, not to mention storage required to accommodate 1.5 billion DOFs.



EXAMPLE – WEATHER FORECAST

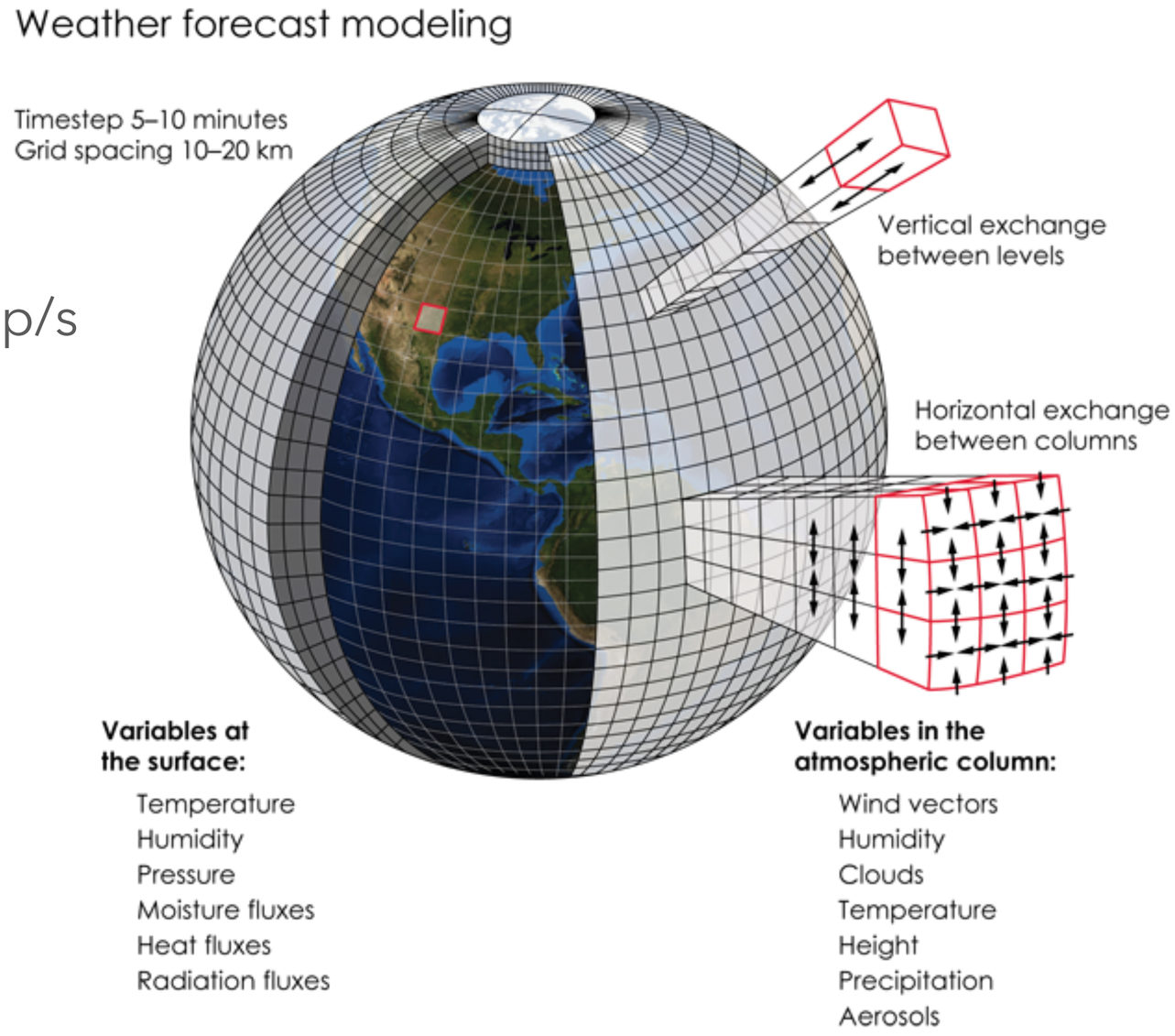
that gives **1.5 x 10^{14} flop** per day of simulation

say a laptop can **realistically** do ~1 x 10^{8} flop/s

then a 1 day weather forecast would take… **~17 days** of laptop's runtime

and that excludes creating initial conditions from satellite data, result post-processing and dissemination.

source: ECMWF

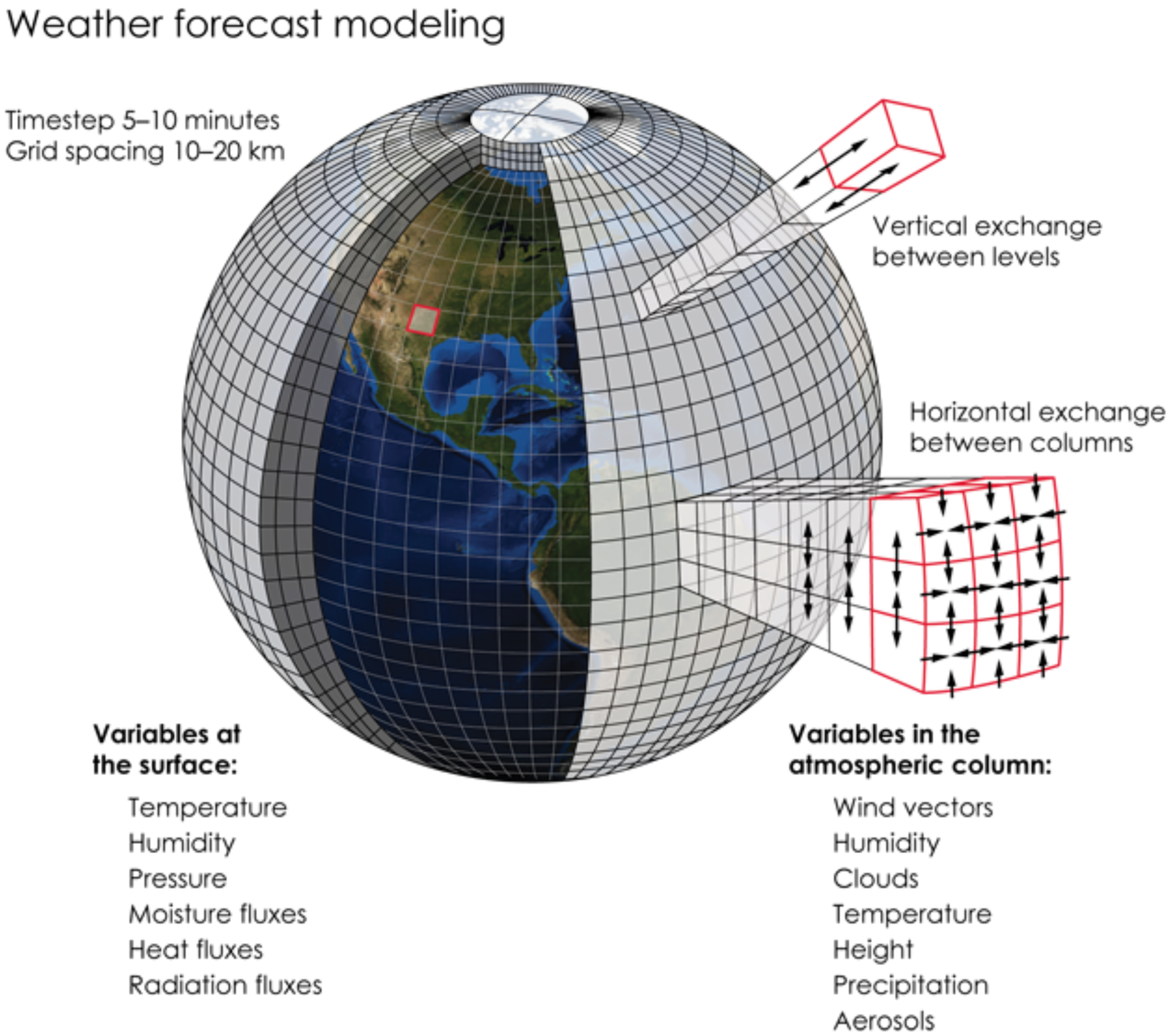


EXAMPLE – WEATHER FORECAST

source: ECMWF

in reality **10 day** forecast takes **1 hour**

using a 10000 processor supercomputer



PARALLEL SCIENTIFIC COMPUTING

creating **scientific software** capable of exploiting **parallel supercomputers**

PARALLEL SOFTWARE

- Parallel software is not easy to write
  - automated serial-to-parallel translation program exist, but rarely give satisfactory results
  - you need to rewrite your serial programs for parallel computers
  - sometimes, the best way is to take a step back and devise a completely new algorithm

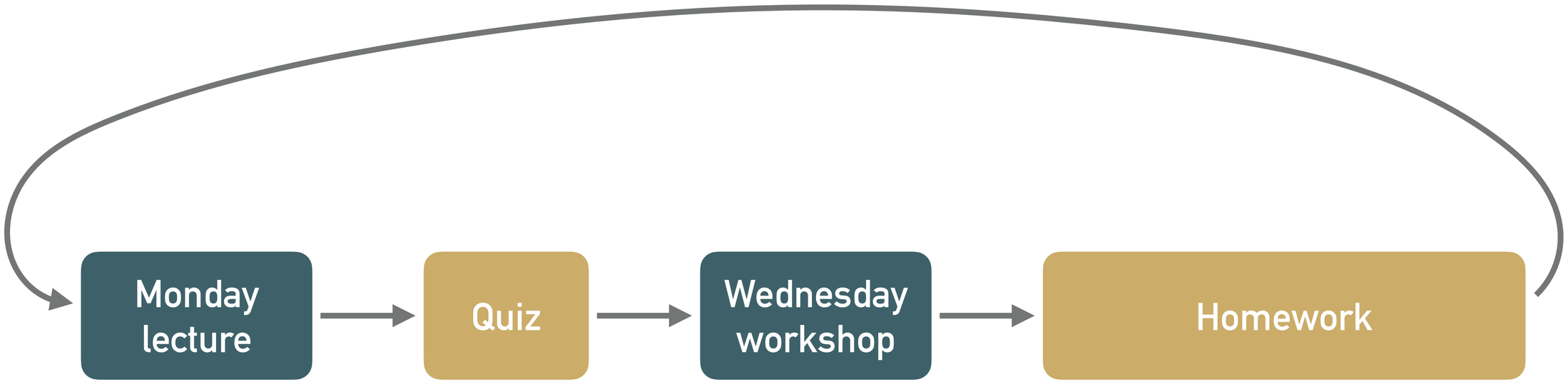
- This is why **we need YOU!**

WHAT DO I NEED TO SUCCEED?

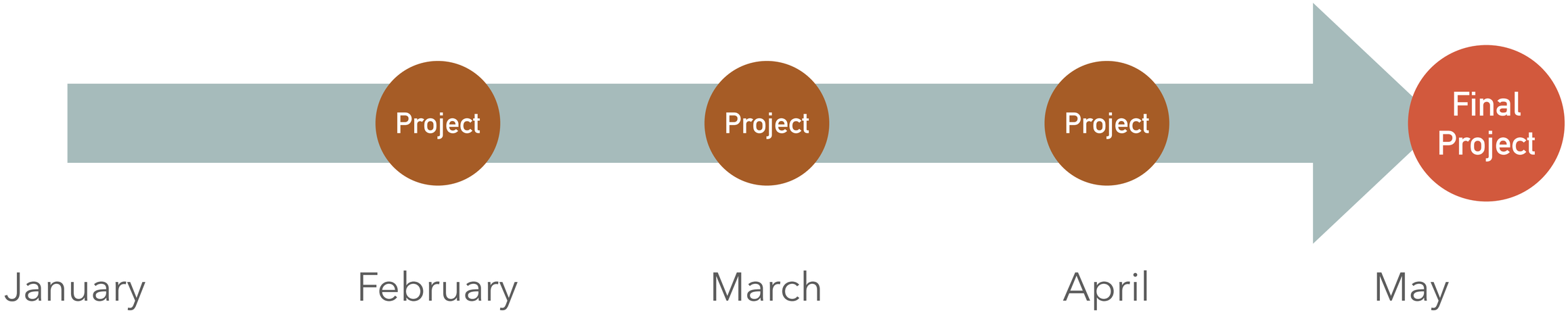
- Access to a computer (preferably UNIX based)
- **Set time** in your calendar to work on the coursework
- Textbooks:
  - Chopp, D. L. (2019). Introduction to High Performance Scientific Computing (Vol. 30). SIAM
  - Eijkhout, V. (2021). Parallel Programming, **online for free**

See the course Canvas website for Syllabus and more info!

WEEKLY CLASS CYCLE



ASSESSMENTS



WHAT I EXPECT OF YOU

- Want to learn and put in the work
- Reach out if you are stuck (Slack)
- Read the Syllabus
- Know basic C programming
- Be able to pick up basic unix, shell script

WHAT CAN YOU EXPECT OF ME

- I will support you to succeed
- I will reply to Slack by the end of the day
- I will give you prompt feedback
- I will listen to your feedback

TO DO THIS WEEK

- Set up Google Drive folder with your name and share it with me
- Join Slack channel
- Make sure you have a terminal app on your computer
- Look out for info from OIT regarding your R2 account