POTSDAM INSTITUTE FOR CLIMATE IMPACT RESEARCH

Technische Universität München

Machine Learning of Dynamical Systems

Workshop Critical Earth Winter School at TU Munich IAS

Maximilian Gelbrecht and Alistair White, 20th/21st February 2023

Who Are We?

A little introduction

- Alistair White, alistair.white@tum.de
- Maximilian Gelbrecht, maximilian.gelbrecht@tum.de
- Future Lab Artificial Intelligence in the Anthropocene at the Potsdam Institute for Climate Impact Research
- Earth System Modelling Group at TUM

- Our research deals with combining dynamical systems with machine learning for climate modelling, you'll see a lot of example during the next two days!

Schedule

	Monday	Tuesday
9:00 - 10:45	**Introduction** **ML for Dynamical Systems: Overview and Project Topics**	**Project Q&A**
11:15 - 13:00	**Solving Dynamical Systems in Julia**	**Project Work**
14:00 - 15:45	**Project Introductions and Q&A**	**from 15:00 Project Presentations**
16:15 - 18:00	**Project Work**	

Projects

- Work in groups of ~4 people
- We'll introduce three main topics, and a few project ideas for each of them
- We prepared a lot of Jupyter notebooks with plenty of code to get you started

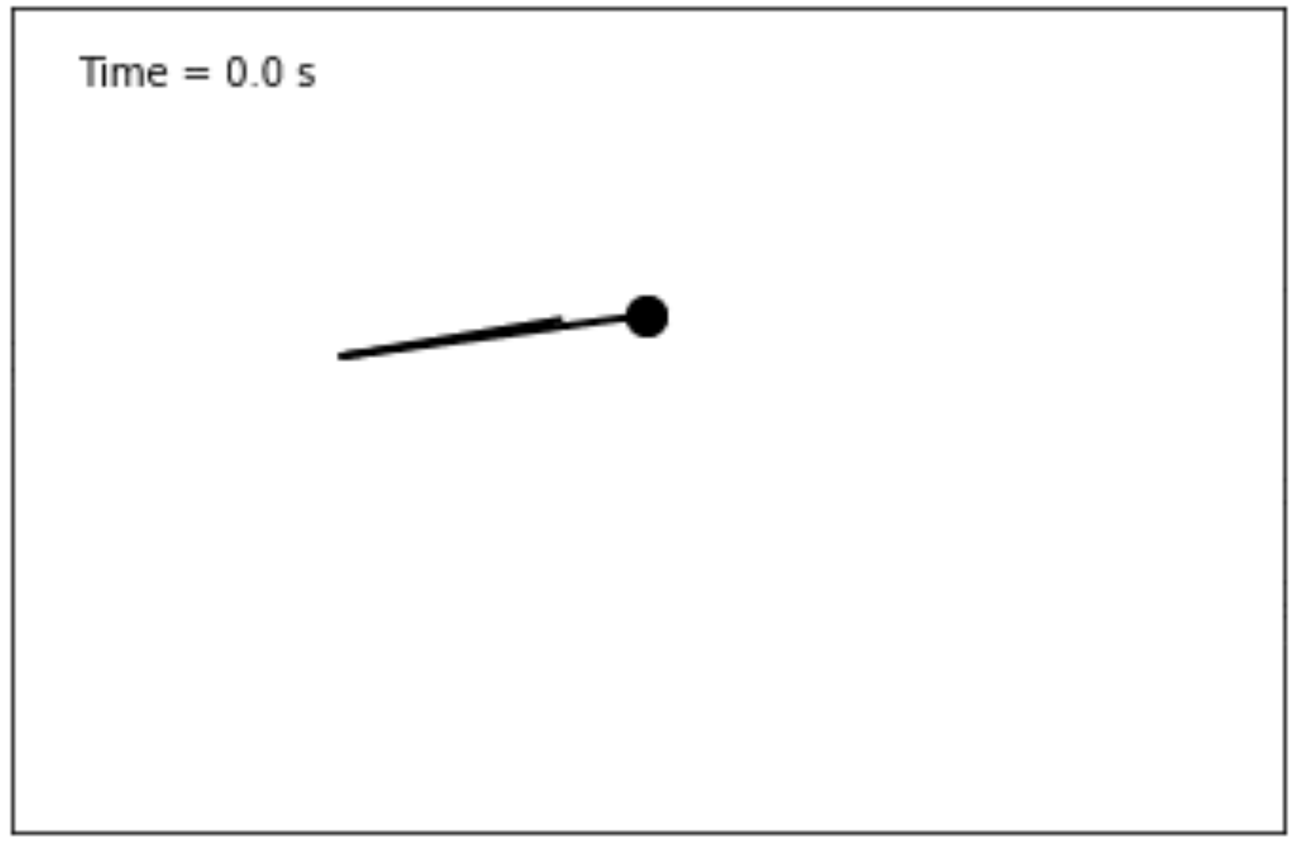
Resources

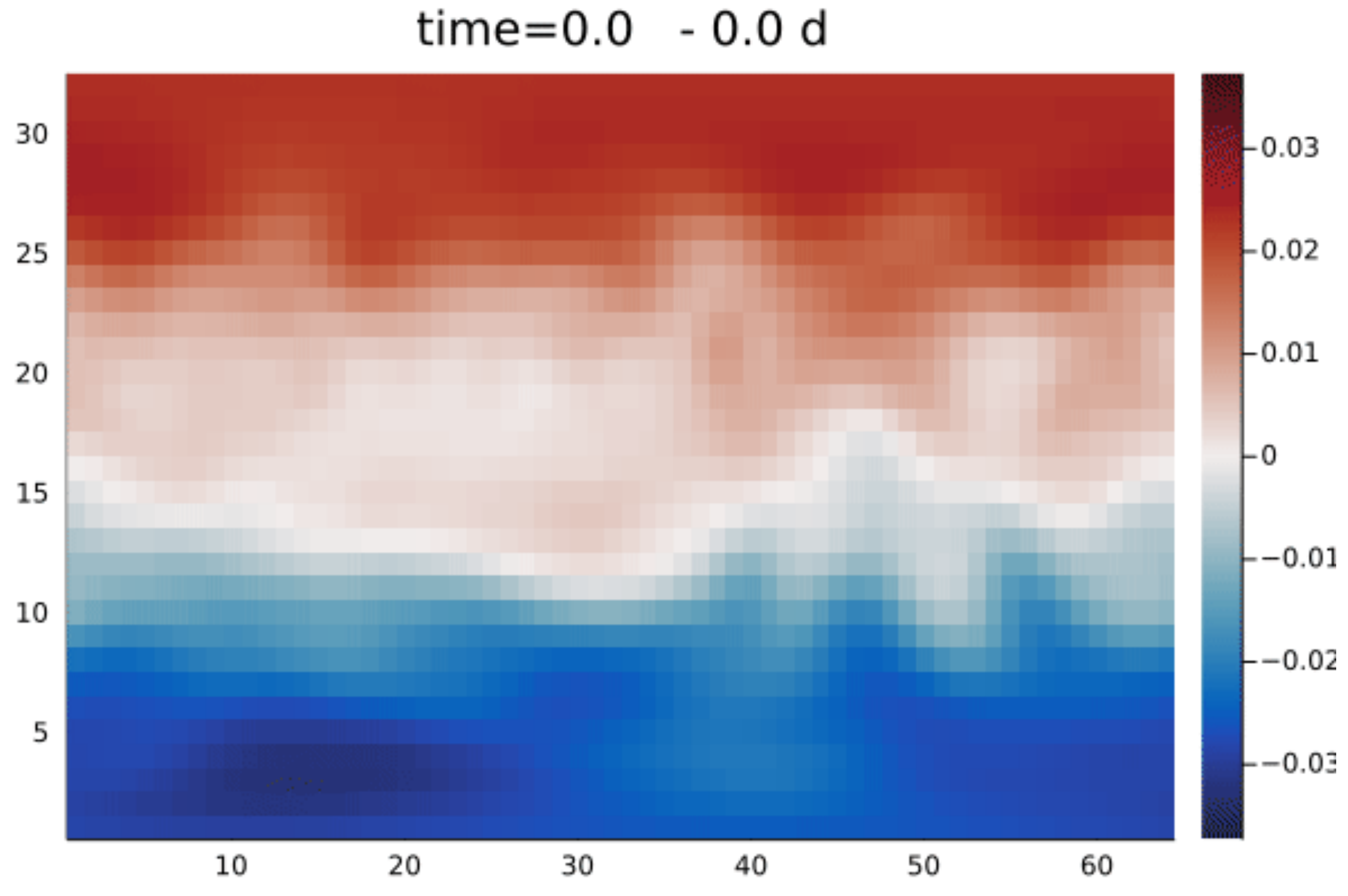
We prepared a lot of additional material for you!

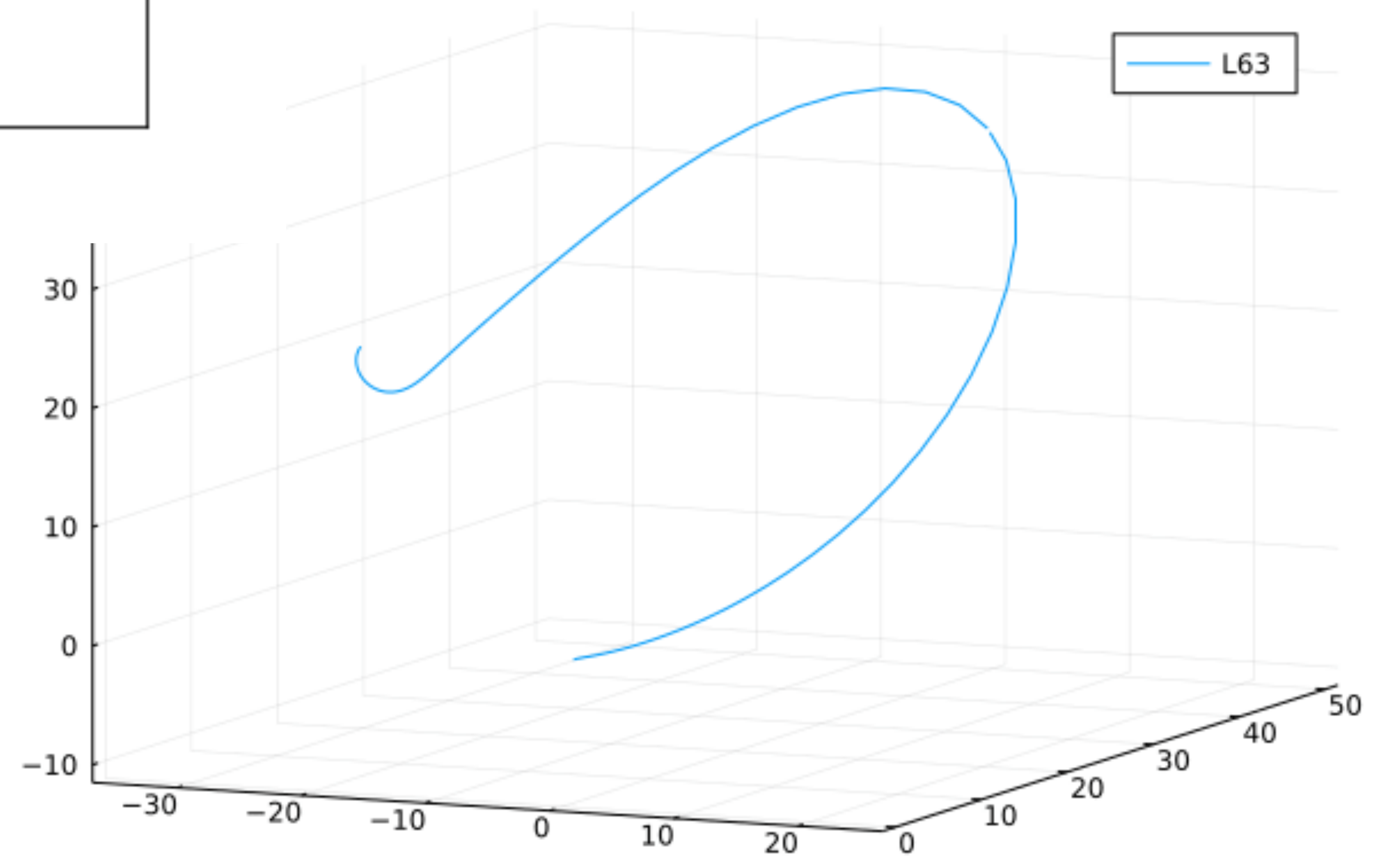
- All workshop material is available at https://github.com/TUM-PIK-ESM/ML-DS-Workshop-23
- All lectures
- Project descriptions and Jupyter notebooks to get you started
- Programming Cheat Sheet

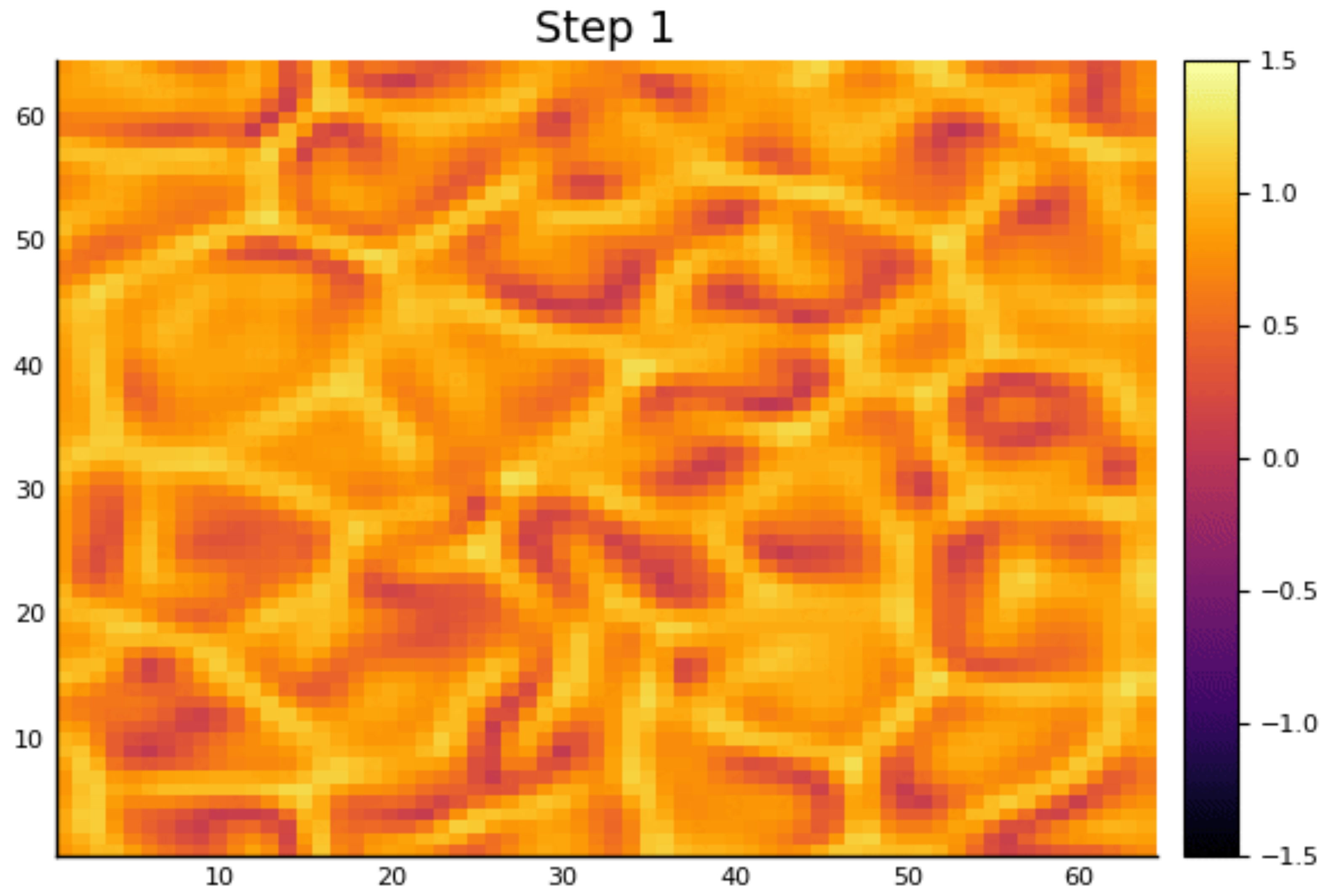
Machine Learning ~~of~~ and Dynamical Systems

Dynamical Systems









Dynamical Systems

A few definitions

- In this workshop we will mostly consider ordinary differential equations (ODEs)

$$\frac{d\mathbf{x}(t)}{dt} = f(\mathbf{x}(t), t; \boxed{\theta})$$

Right-hand side (rhs)

→ Parameters

with $x \in \mathbb{R}^n, f : \mathbb{R}^n \rightarrow \mathbb{R}^n$

- Most of the methods and approaches however do generalise to other kinds of dynamical systems like PDEs, SDEs, etc
- Ask us about it, if you want to work with those systems in your projects!

Dynamical Systems

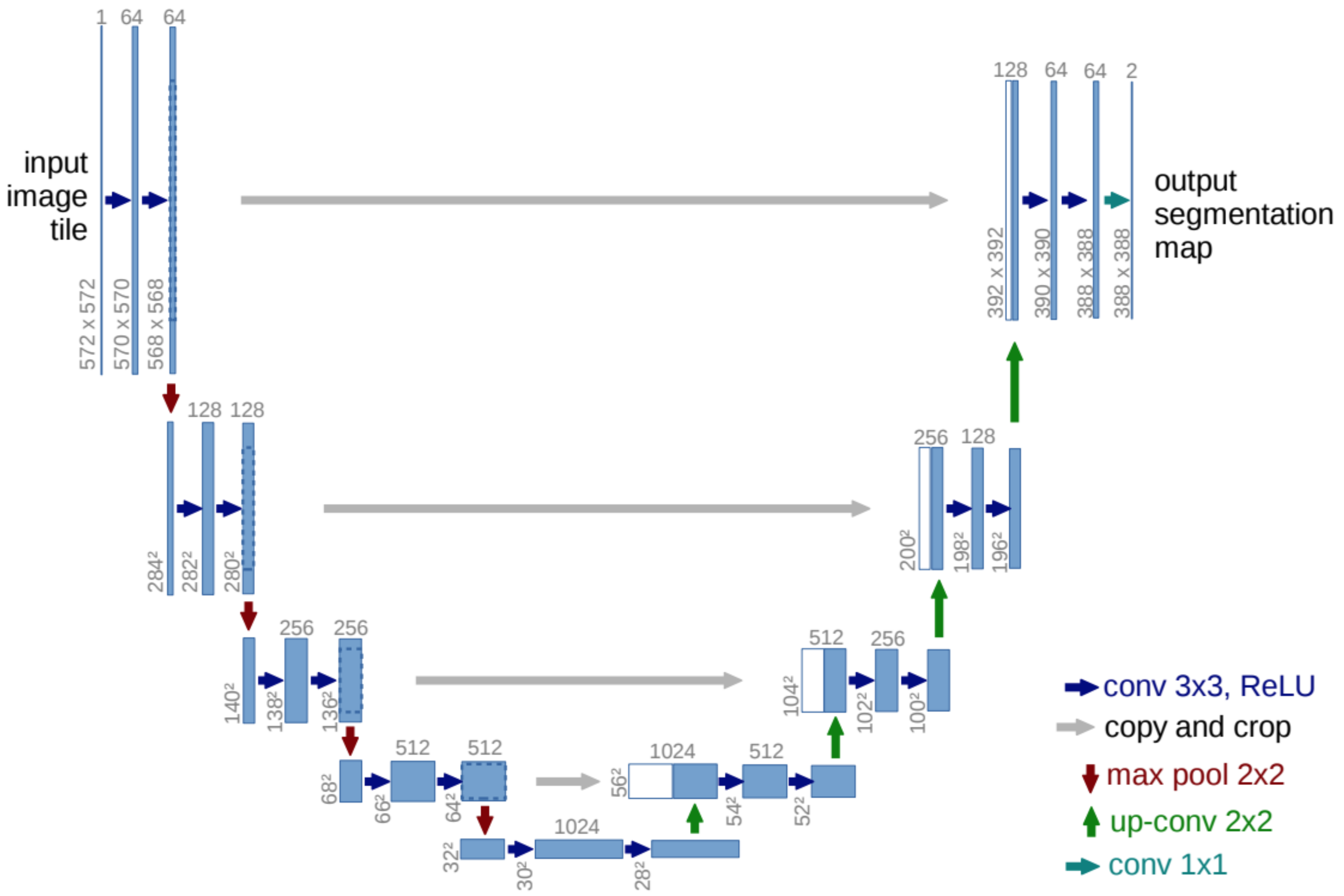
A few definitions

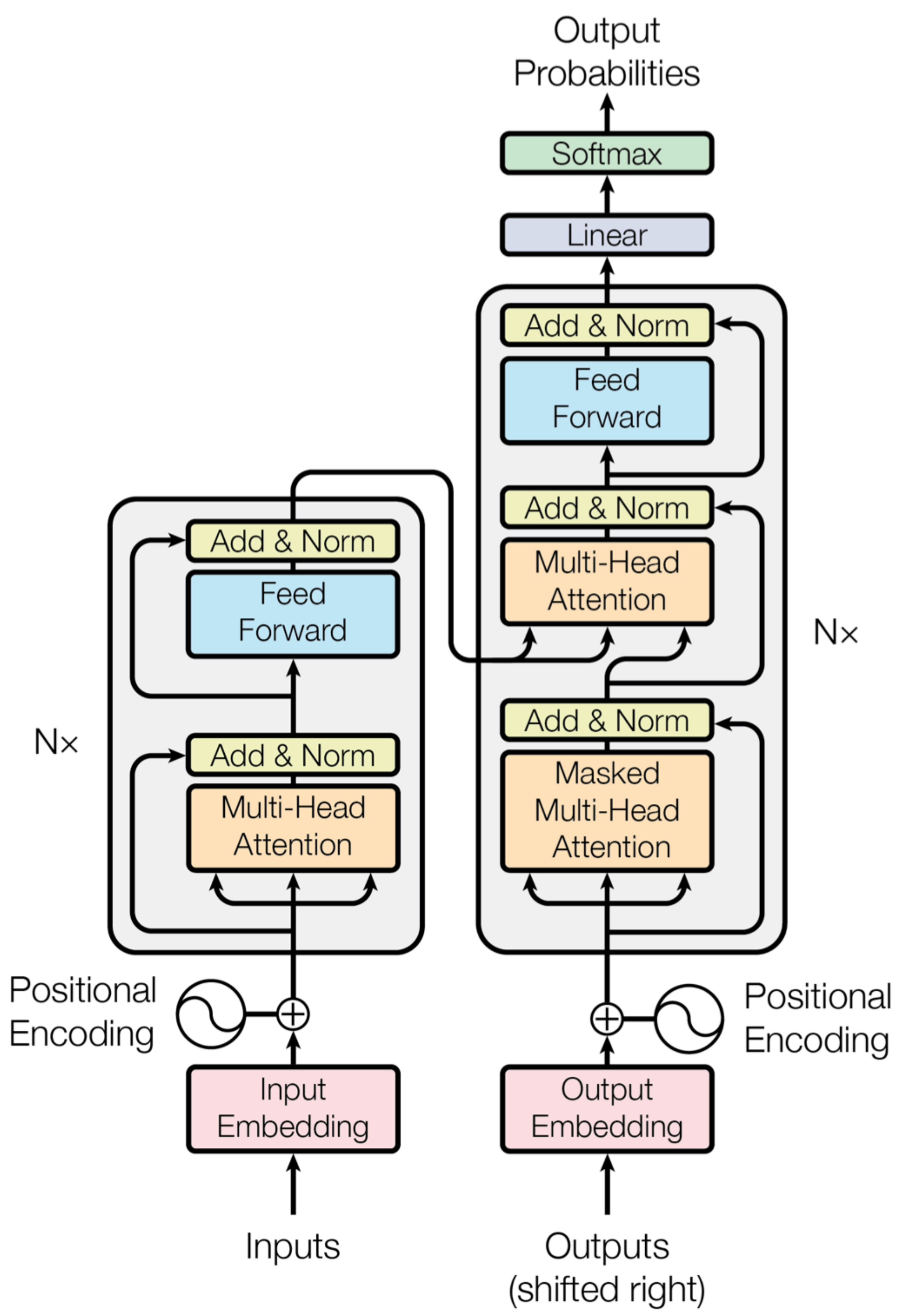
- We will be mostly concerned with numerically solving nonlinear, chaotic ODEs starting from an initial condition $\mathbf{x}_0 = \mathbf{x}(0)$, therefore we have an initial value problem (IVP) that is solved by a ODE solver

- In the second part of this initial lecture we will go into a lot more detail on this process

Machine Learning

A Zoo of Architectures





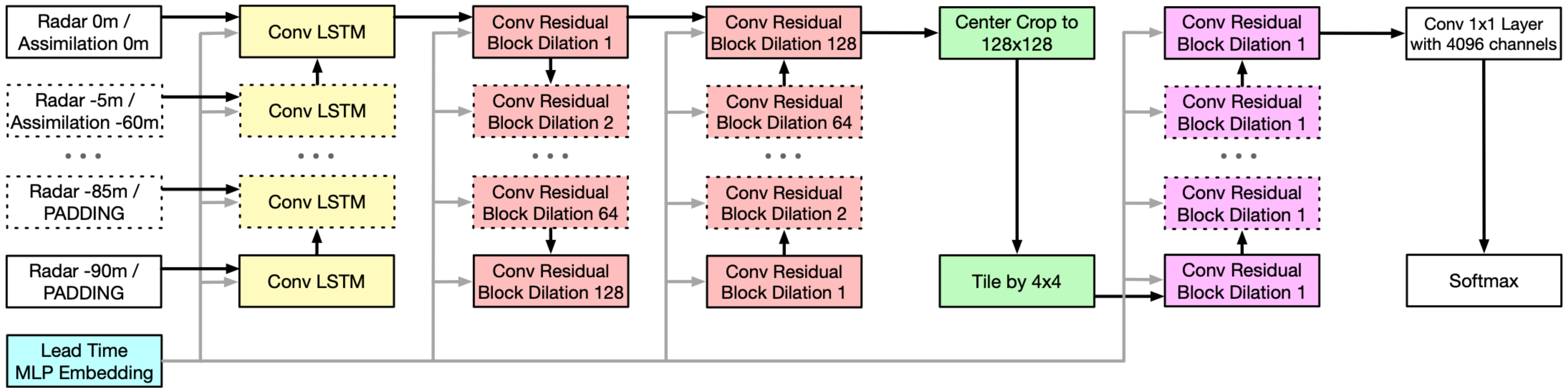


Image sources: https://towardsdatascience.com/paper-summary-u-net-convolutional-networks-for-biomedical-image-segmentation-13f4851ccc5e
Espeholt et al 2021, Vasvami et al 2017

Machine Learning

A few further definitions

- Methods that build parametrised models that can approximate functions from data
- In this workshop, we will be mostly concerned with **supervised machine learning**
- We have pairs of observations $(\mathbf{x}_i, \mathbf{y}_i), \mathbf{x}_i \in \mathbb{R}^n, \mathbf{y} \in \mathbb{R}^m$ of an unknown function $f : \mathbb{R}^n \to \mathbb{R}^m$
- And want to approximate this function with a parametrised model $g(\mathbf{x}_i; \theta)$ by using the observations $(\mathbf{x}_i, \mathbf{y}_i)$, usually by optimising an objective function minimising the difference between $g(\mathbf{x_i}; \theta)$ and $\mathbf{y}_i$, so that g approximates f

Machine Learning

A few further definitions

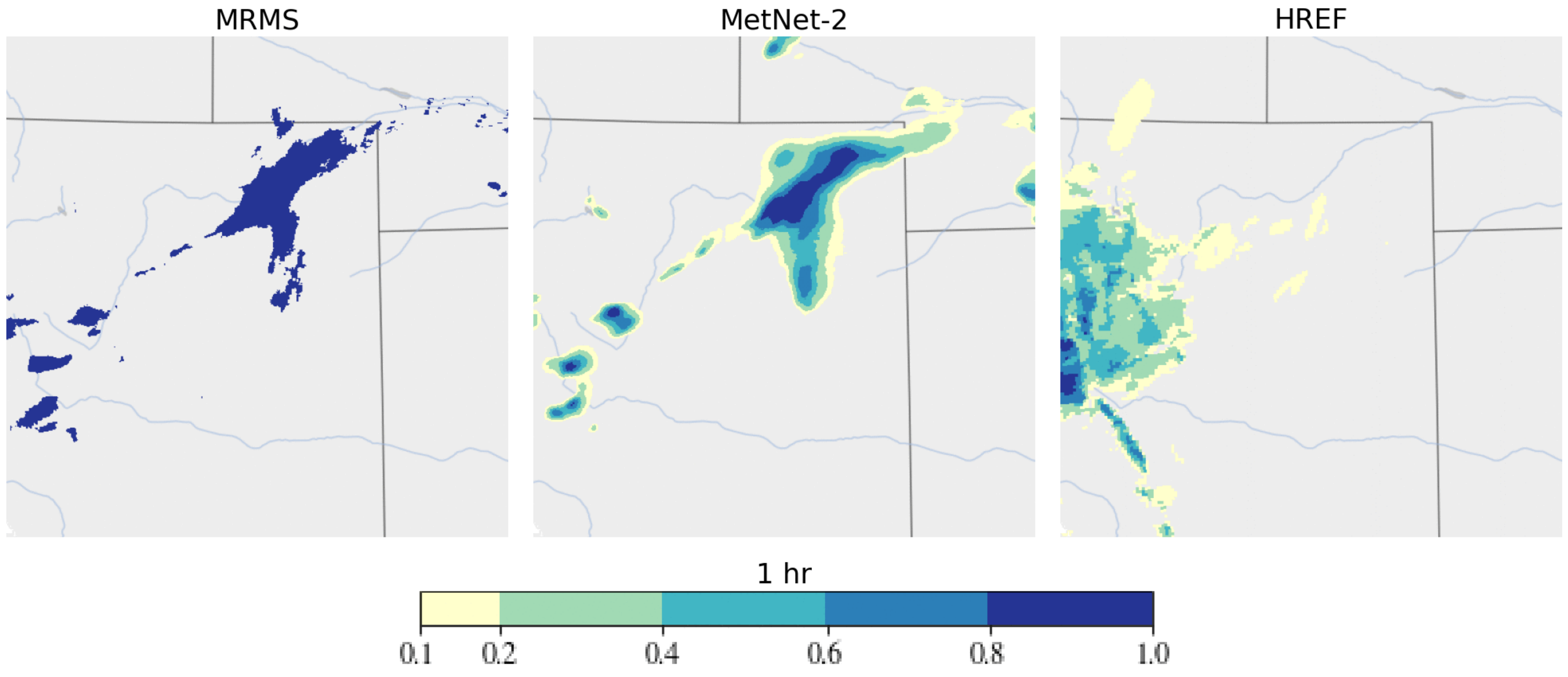
- In this workshop, we will mostly work with **artificial neural networks** as our choice of parametrised models
- We will also mostly restrict ourselves to multilayer perceptrons (more on that a bit later)

How do we apply this to climate science and in particular Earth system modelling?

How to Combine DS and ML?

And why?

- We can have a data from an unknown DS and want to you make predictions of it: ENSO forecast, Weather Forecast, etc…..



Source: MetNet2, L Espeholt et al, 2021

How to Combine DS and ML?

And why?

- We have an imperfect model and we have data
  - Can we improve the model with the data?
  - Can we use model and the data to get better predictions of our system than with each individually?
  - Does the ML component still fulfil physical constraints?
- **Physics-informed machine learning** or **scientific machine learning**

How to Combine DS and ML?

And why?

- Advantages will differ for the actual, concrete implementation, but they can be:
    - Ability to train with less data
    - Improved accuracy (esp. for extrapolation)
    - Improved interpretability

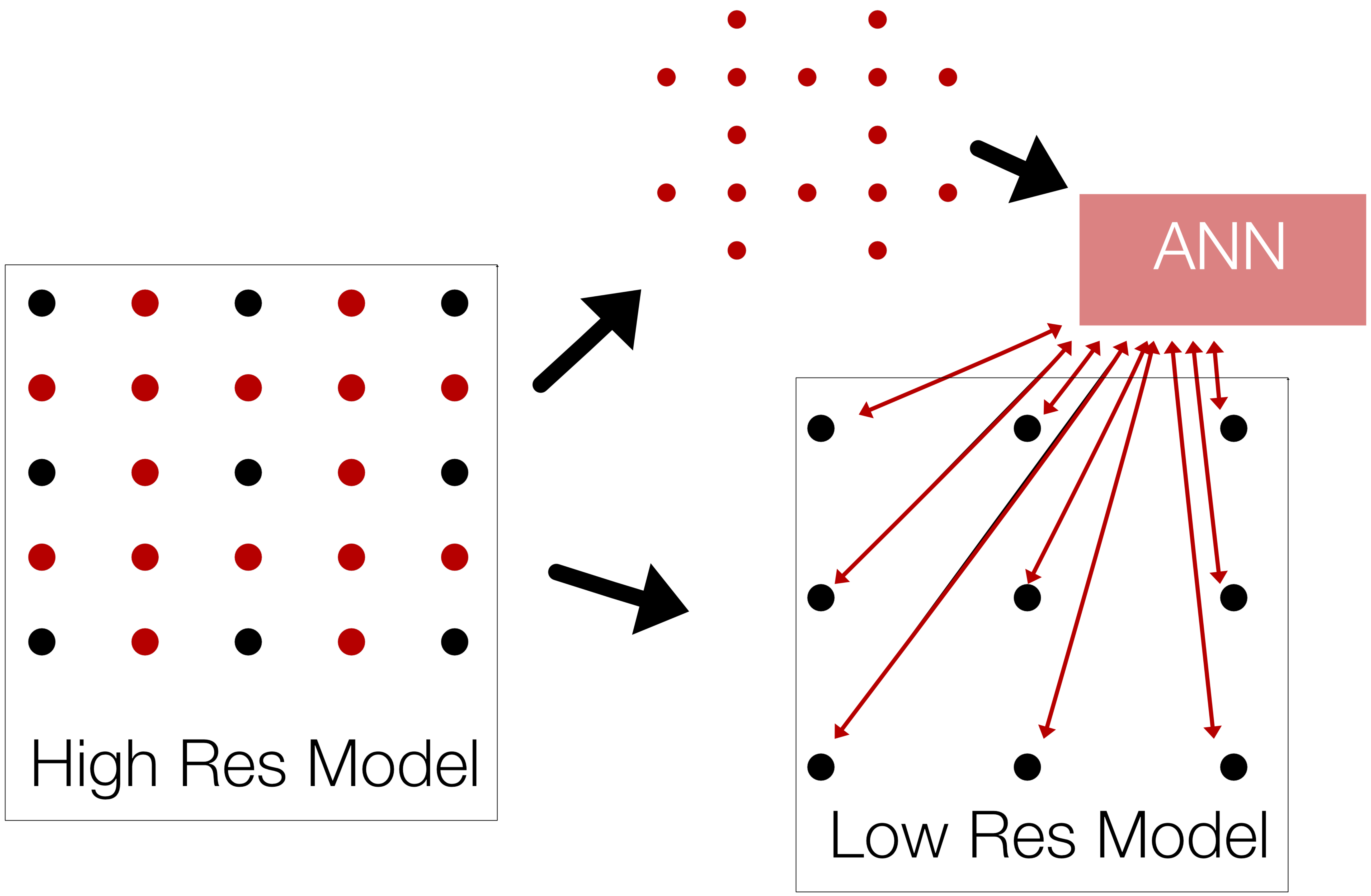
- In Earth System science we have great comprehensive models, but also a lot of data, it’s a great area to explore these methods

Subgrid Parametrizations with ANNs

One type of hybrid model

- Parametrization of processes
  that need a finer resolution with ANNs

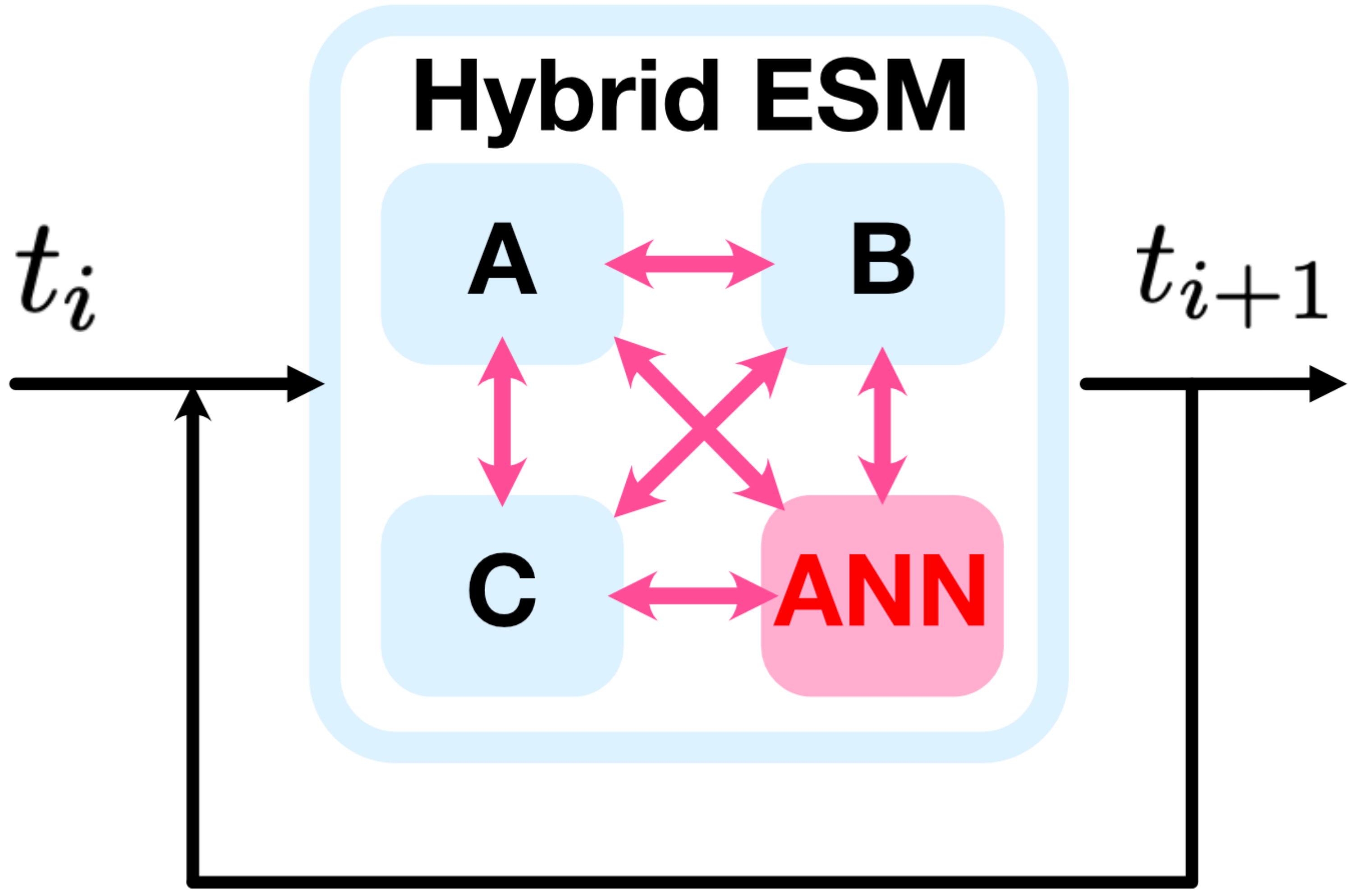
- E.g. (Yuval et al 2021) for atmospheric processes or (Um et al 2020) for a more general CFD scenario

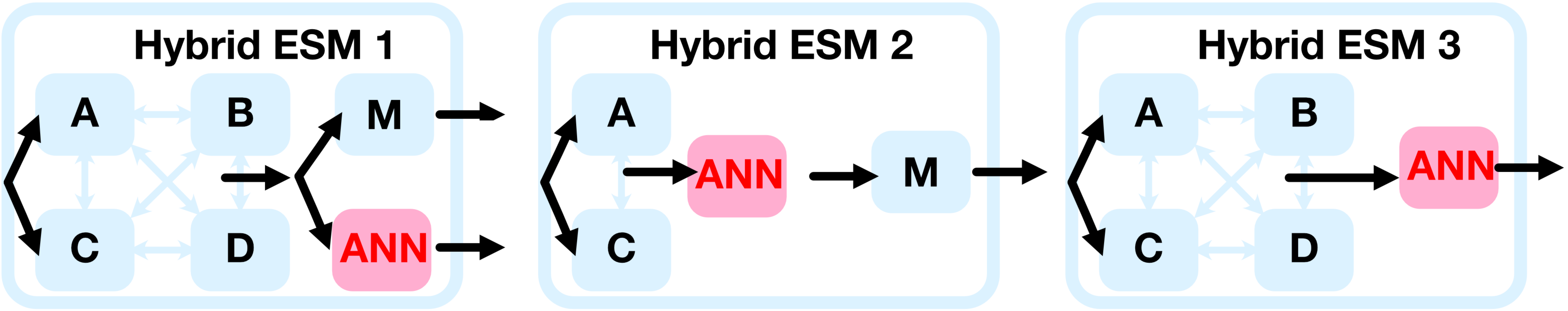


Hybrid Earth System Models

A small pitch

- E.g. (de Bezenac et al, 2019) for SST prediction, or (Kraft et al 2021) for a hybrid hydrology model





Challenges

So why don't we already have some with hybrid ESMs?

- Integrating the old (Fortran) code base into these approaches is not easy
- Differentiable models are needed (e.g. using Python JAX or Julia Enzyme/Zygote)
- The behaviour of the models themselves is also quite complex!
- So, in our workshop we start with prototypical dynamical systems that are
  - Easier to understand
  - Easier to implement in just a few lines of code

Plan for the Workshop

What are you doing these two days?

- We want you to apply one of three ML techniques to a dynamical systems problem (and maybe climate data)
- First, we'll speak about some basics of numerically solving differential equation problems in the Julia language
- Then, we'll present the three ML techniques
- You form groups and pick one and we provide with you material, code and tips & tricks to get started quickly
- Tomorrow afternoon you present what you were able to do

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