Physics-informed machine learning for glacier modelling

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Facundo Sapienza

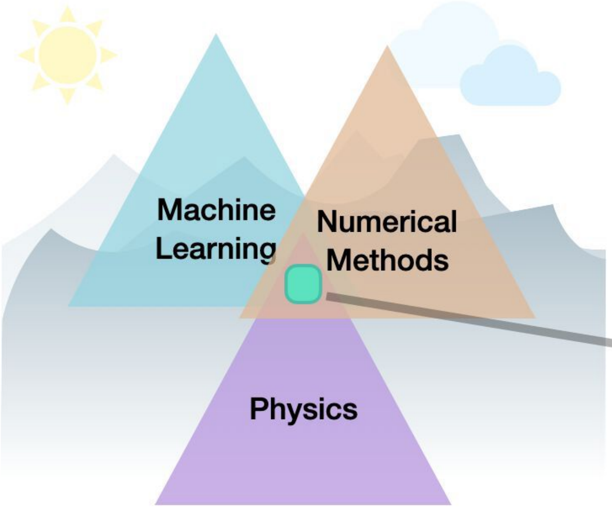
Introduction

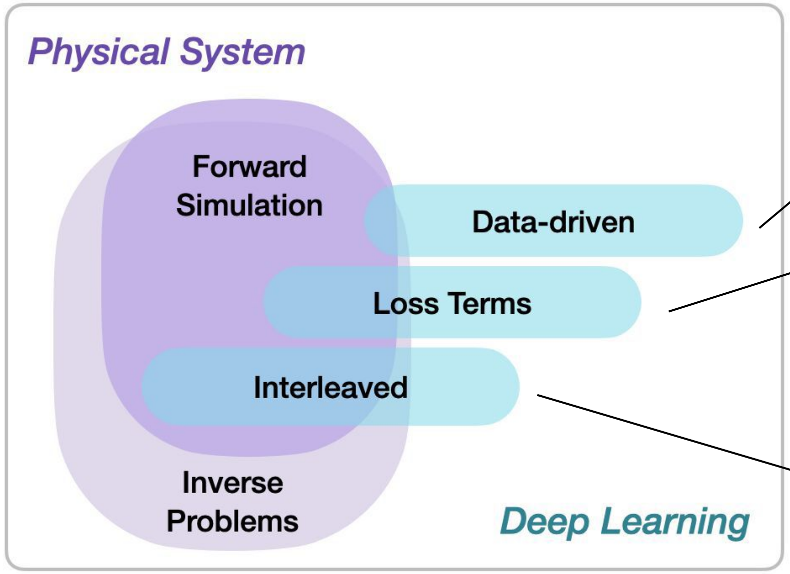
Prediction/inference is complicated with a purely data-driven approach

- “Blackbox” model
- Difficult to extrapolate beyond observations
- Difficult to gain knowledge about the underlying physical processes

New research opportunities to overcome these limitations

Physics-informed machine learning





Physics-Based Deep Learning,
Thuerey et al. (2021)

3 main categories:

a. **Data-driven**: classic ML

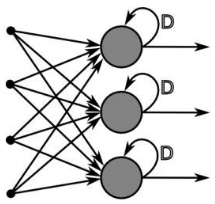
b. **Soft constraints**: Physics-informed Neural Networks (PINNs)

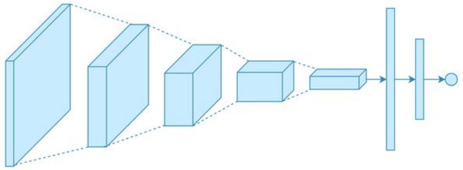
c. **Hard constraints**: differentiable programming + solvers + neural networks

a) **Data-driven machine learning**

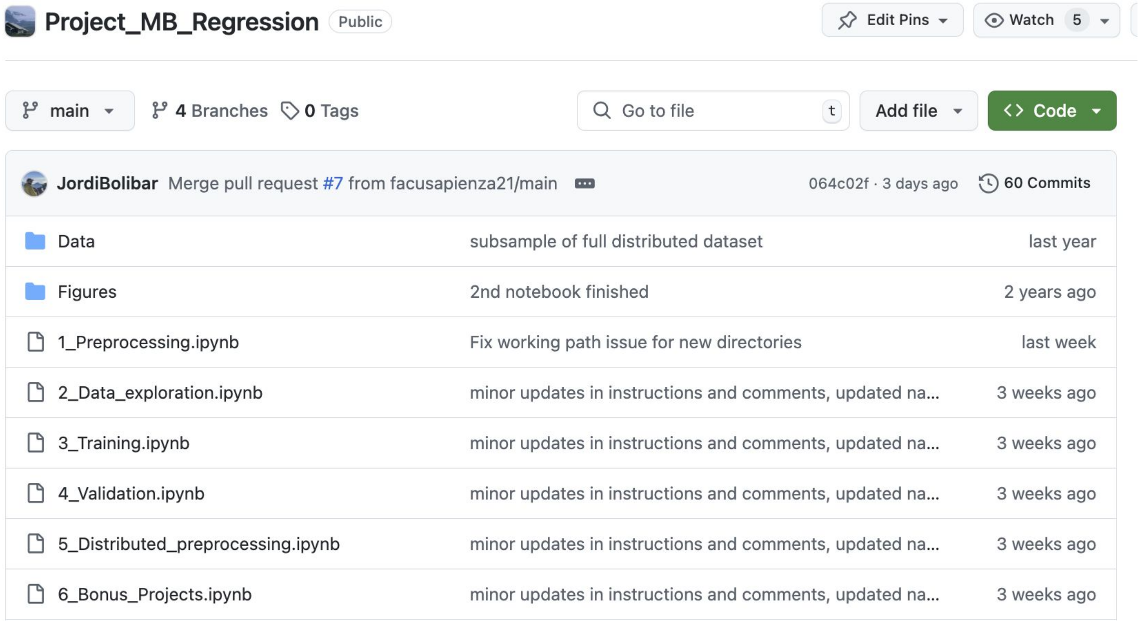
- Output: constrain within physically plausible values
- Loss function: choose one that suits the target data

- For neural networks: choose an architecture that matches the nature of the dataset
  - Recurrent NNs for time dependencies
  - Convolutional NNs for spatial dependencies

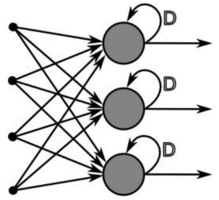


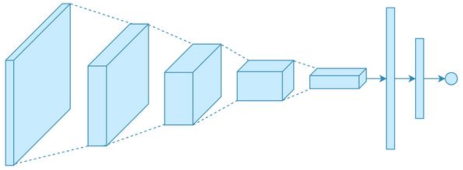


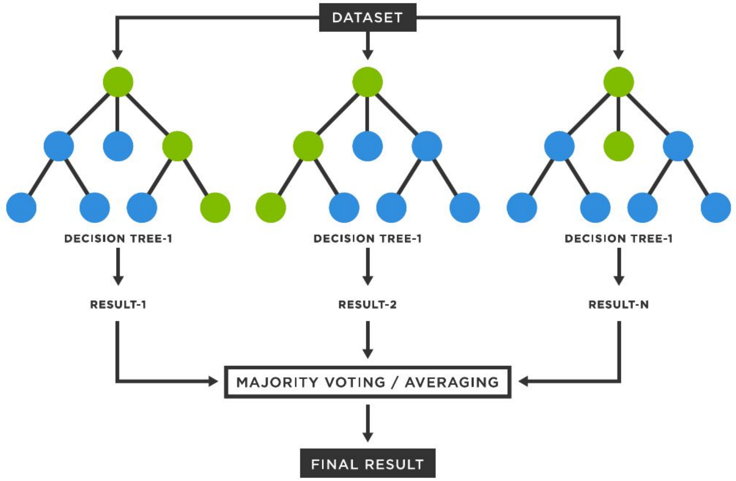
a) Data-driven machine learning



MassBalanceMachine







a) Data-driven machine learning

Advantages:

- Straightforward model design
- Flexibility: great for physical processes for which we don’t have much previous knowledge
- Data exploration: great way to explore a novel dataset to obtain a first model to learn from the data

Disadvantages:

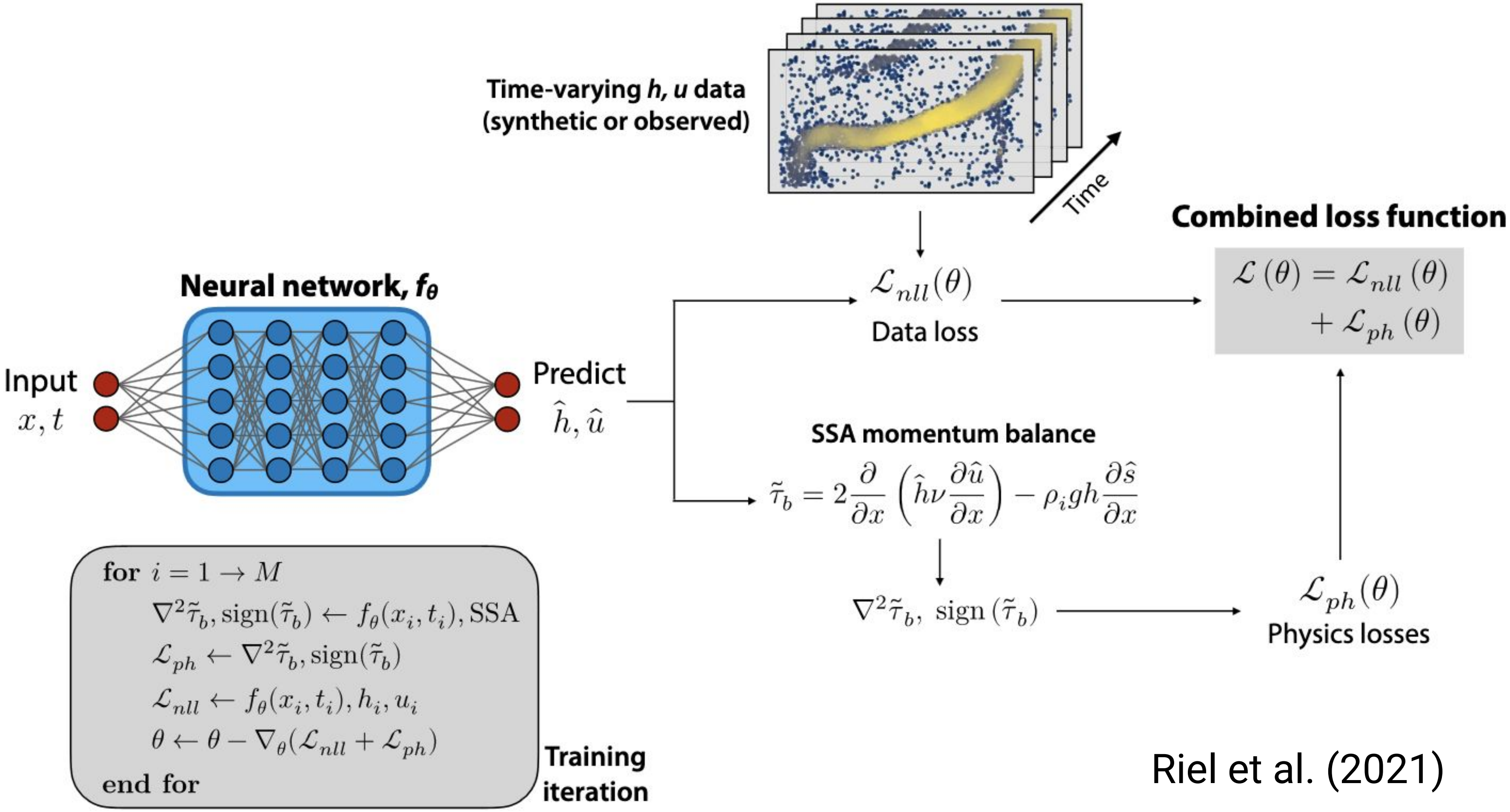
- Requires more validation to make sure physical properties are respected
- General lack of interpretability

b) Soft constraints

- Physical (soft) constraints are added in the NNs loss function
  - E.g. Physics-Informed Neural Networks (PINNs)
  - Based on regularization
  - NN learns the (numerical) **solution** of the differential equation
  - It can be used also to learn unknown parts of the equation

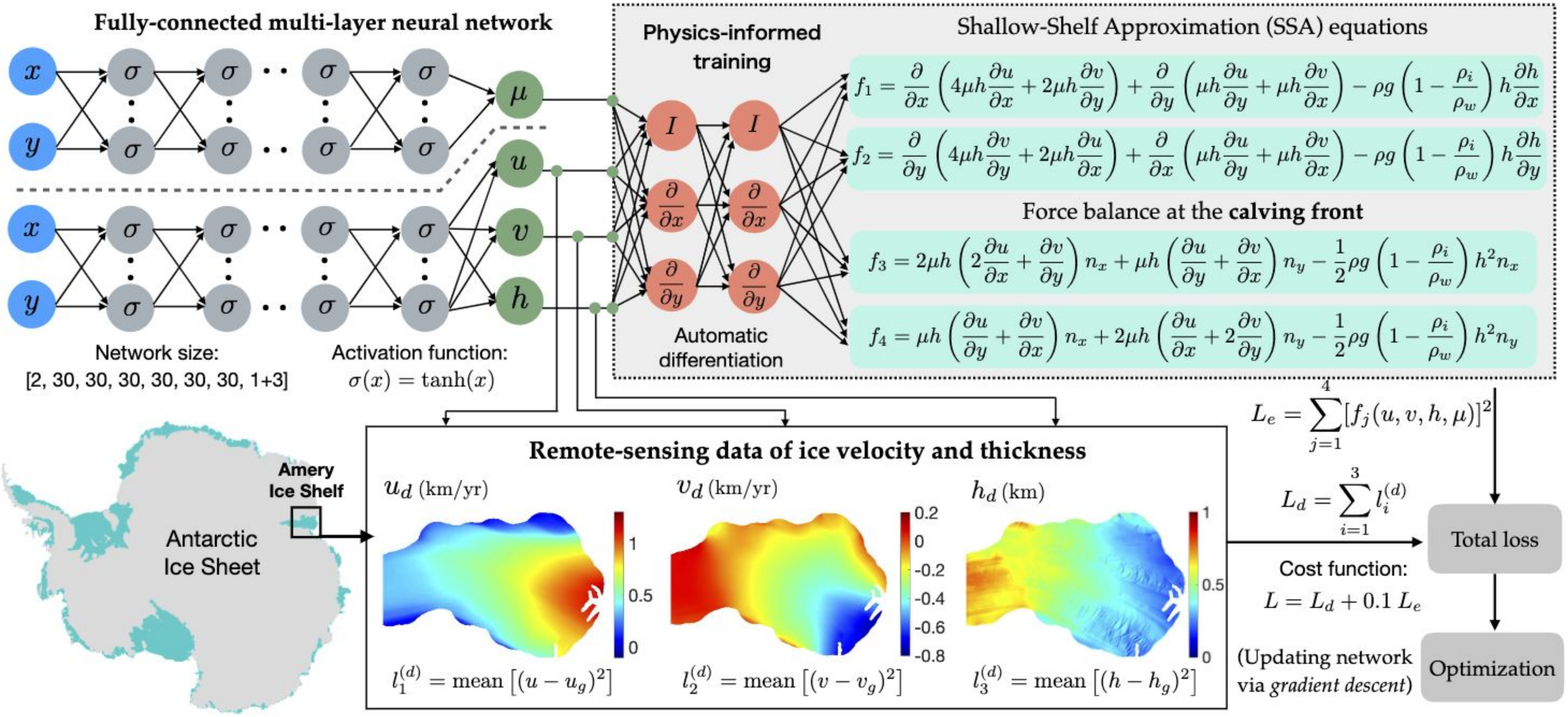
$$\boxed{\mathcal{L} = \mathcal{L}_{data-driven} + \mathcal{L}_{physics}}$$

b) Soft constraints: PINNs



Riel et al. (2021)

b) Soft constraints: PINNs



Wang et al. (2022)

b) Soft constraints

Advantages:

- Physical constraints: the model can reliably respect the imposed physical conditions
- Very fast to execute once trained

Disadvantages:

- Very hard to train
- High computational cost for training: needs to learn the numerical solver and/or the "classic" regression
- Difficult to work with high-order derivatives

c) Hard constraints

- Combine numerical solvers with neural networks (hard constraints)
- E.g. Universal Differential Equations or Neural Differential Equations
- Requires a good automatic differentiation (AD) framework:

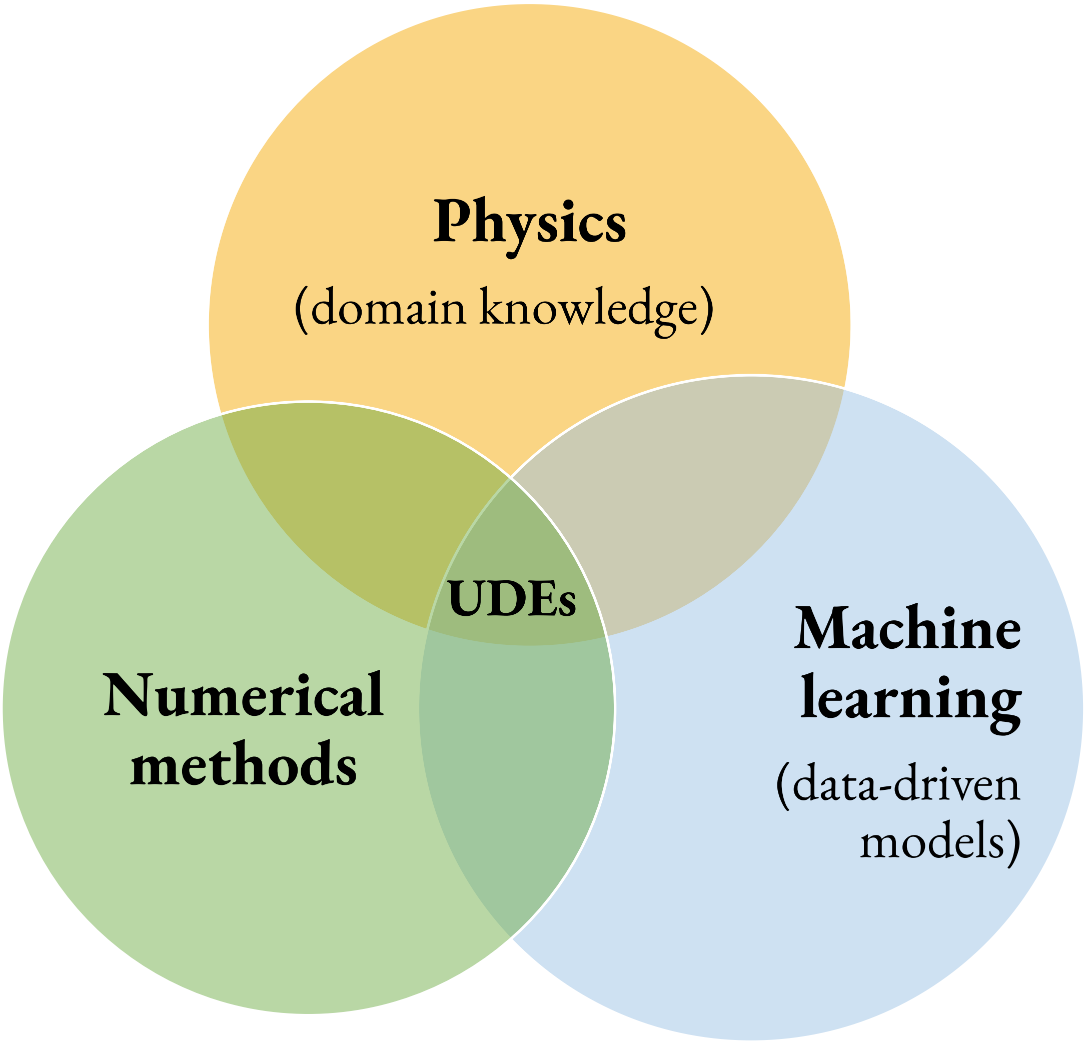
  The model needs to be fully differentiable!

  PyTorch TensorFlow JAX julia

- They can tackle more complex inverse problems:

  New opportunities for **identifying** physical laws/parameterizations

Hard constraints: Universal Differential Equations

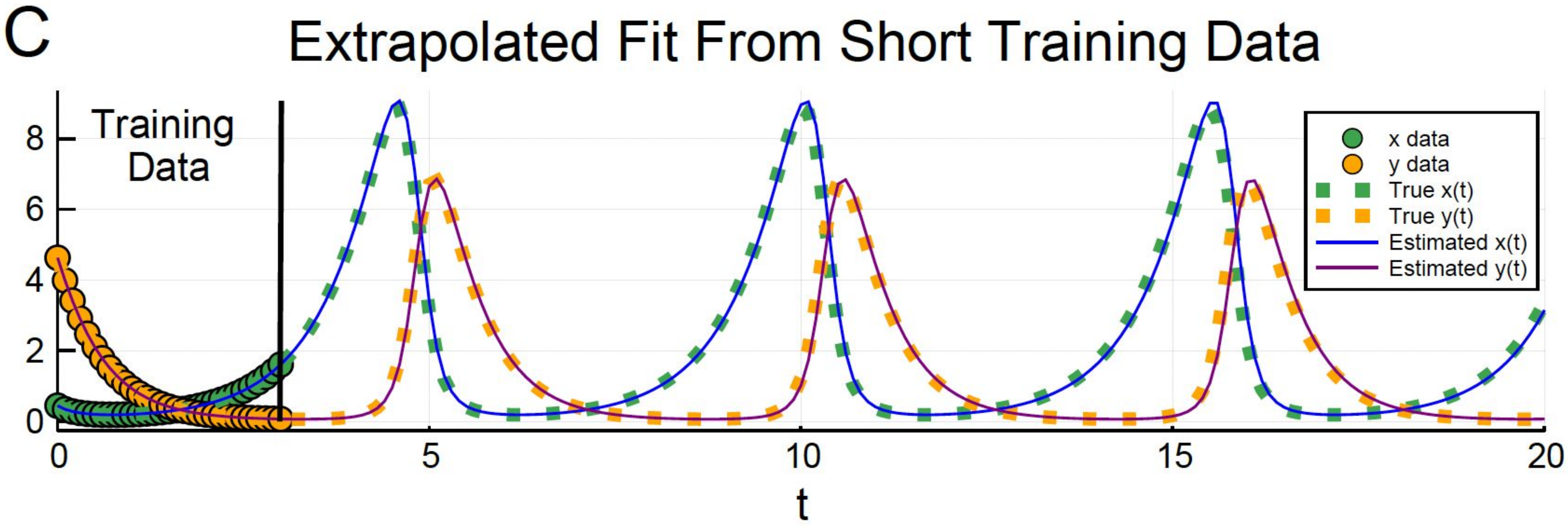


$$\boxed{\frac{\partial H}{\partial t} = \boxed{\dot{b}} + \nabla(\boxed{D}\nabla S)}$$

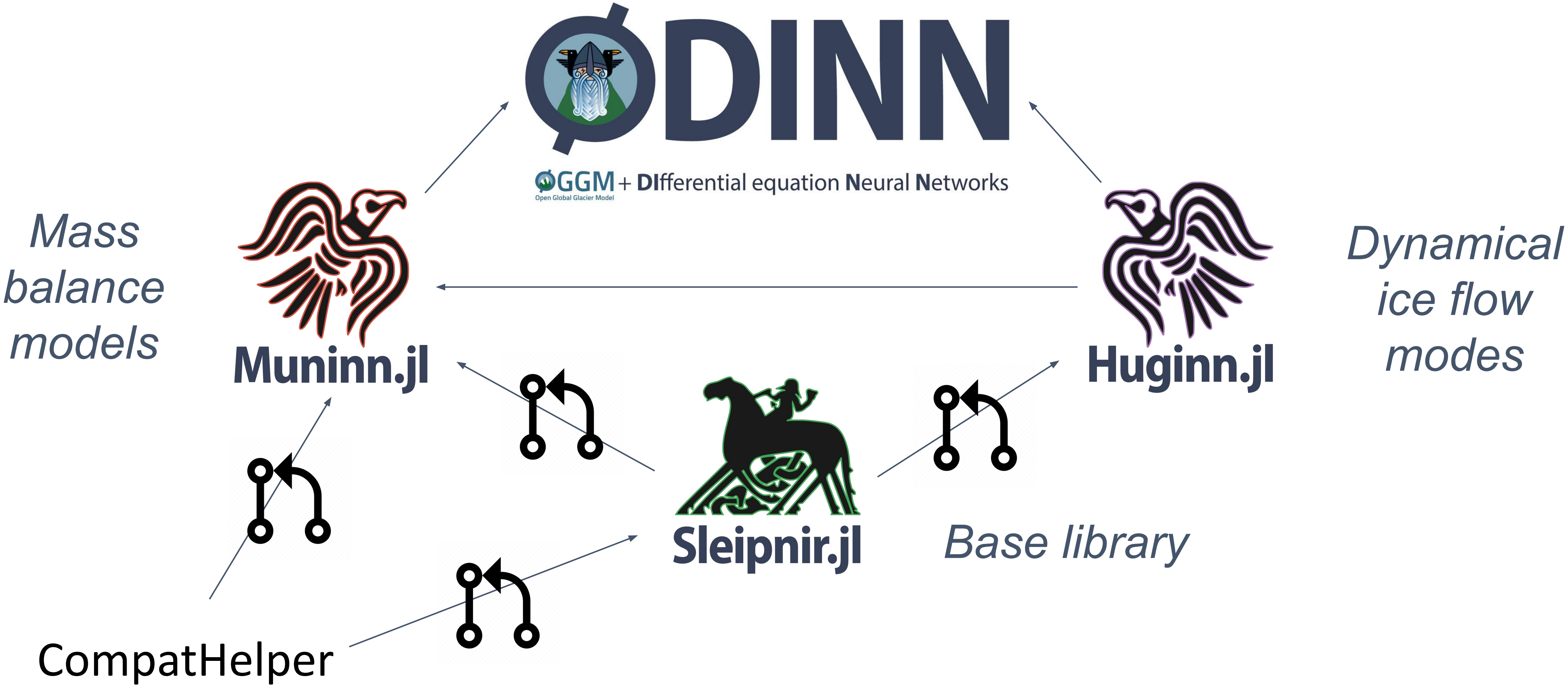
New modelling philosophy

1. Make use of as much existing knowledge as possible
2. ONLY use regressors (e.g. machine learning) for what you DON'T know

Hard constraints: Universal Differential Equations



c) An example of UDEs: ODINN



c) An example of UDEs: ODINN

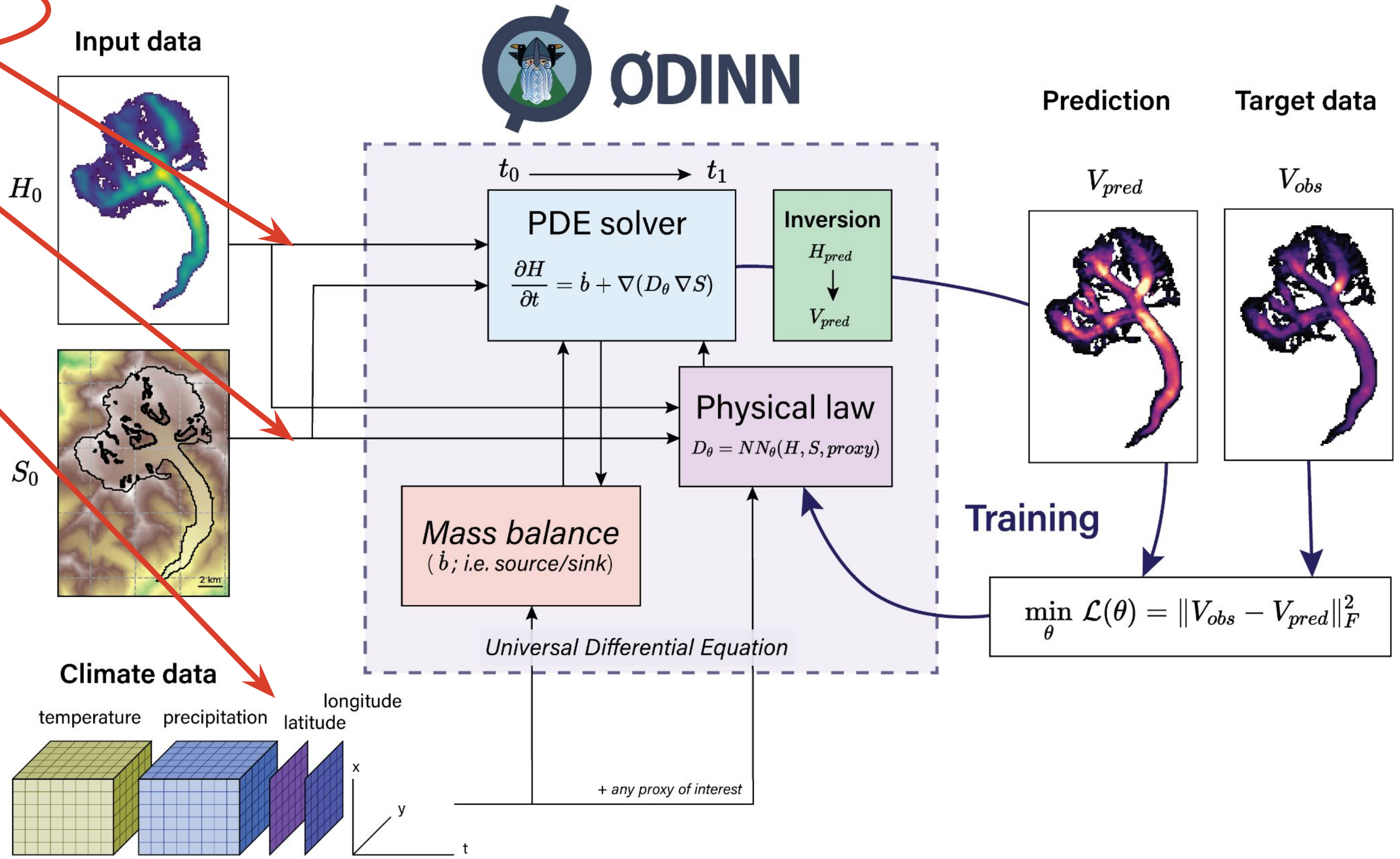
Data gathering and preprocessing

Functional inverse modelling

Forward modelling / predictions

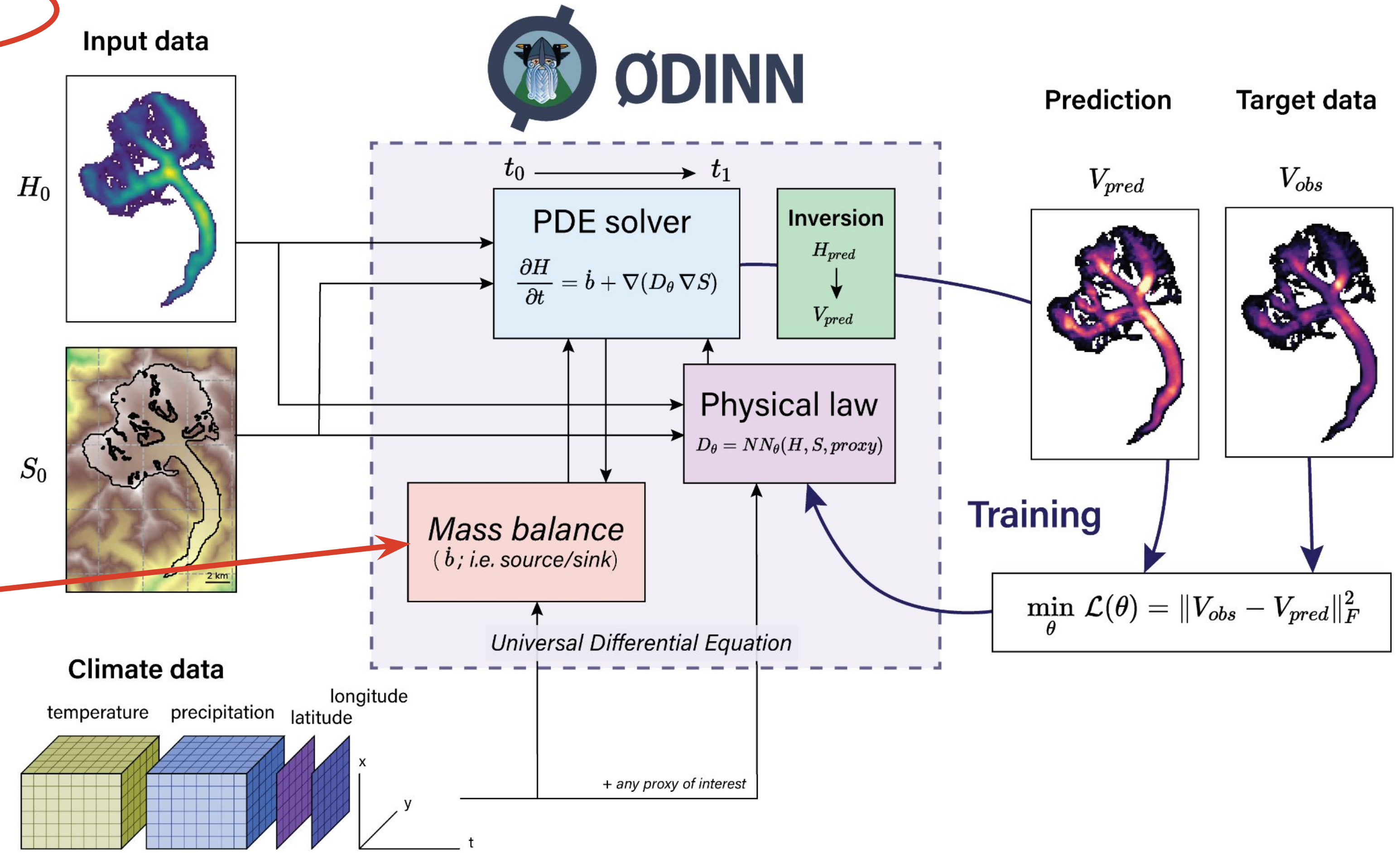
Dataset production and output features

Preprocessing



Bolibar, Sapienza et al., GMOD 2023, *Universal Differential Equations for glacier ice flow modelling*

Preprocessing



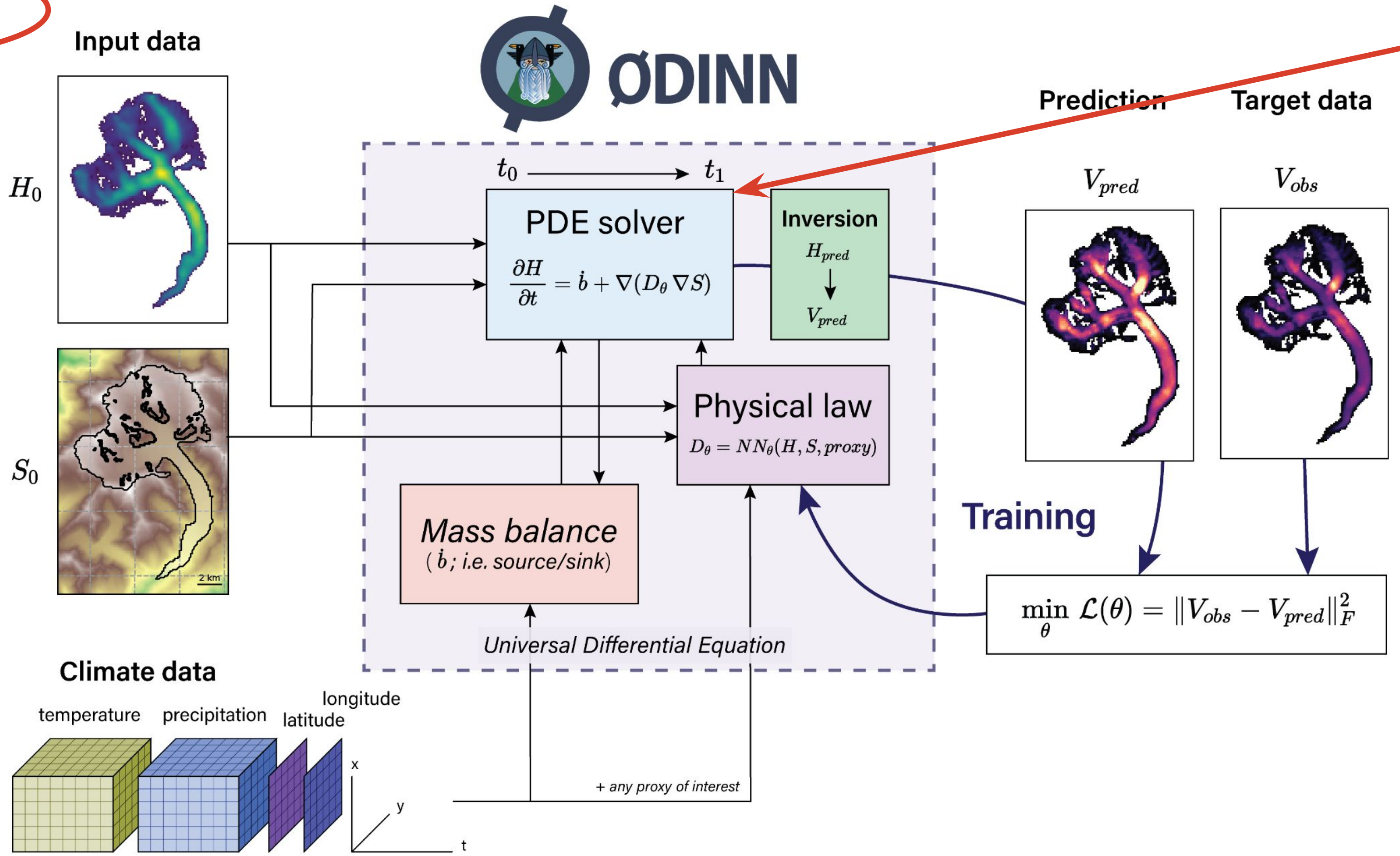
Mass balance model

Bolibar, Sapienza et al., GMOD 2023, *Universal Differential Equations for glacier ice flow modelling*

Preprocessing

Numerical solution of SIA equation

Mass balance model



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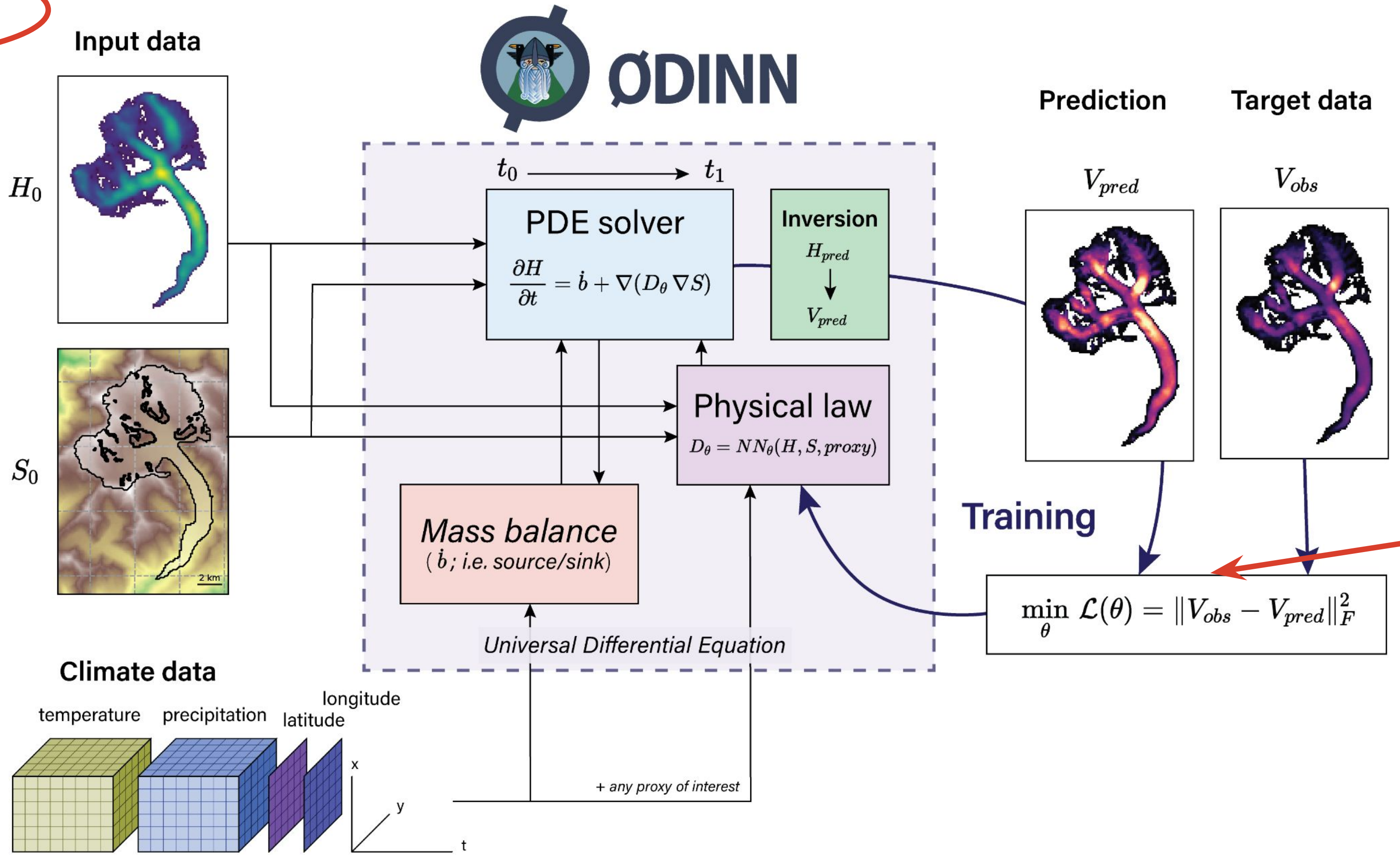
Preprocessing

Mass balance model



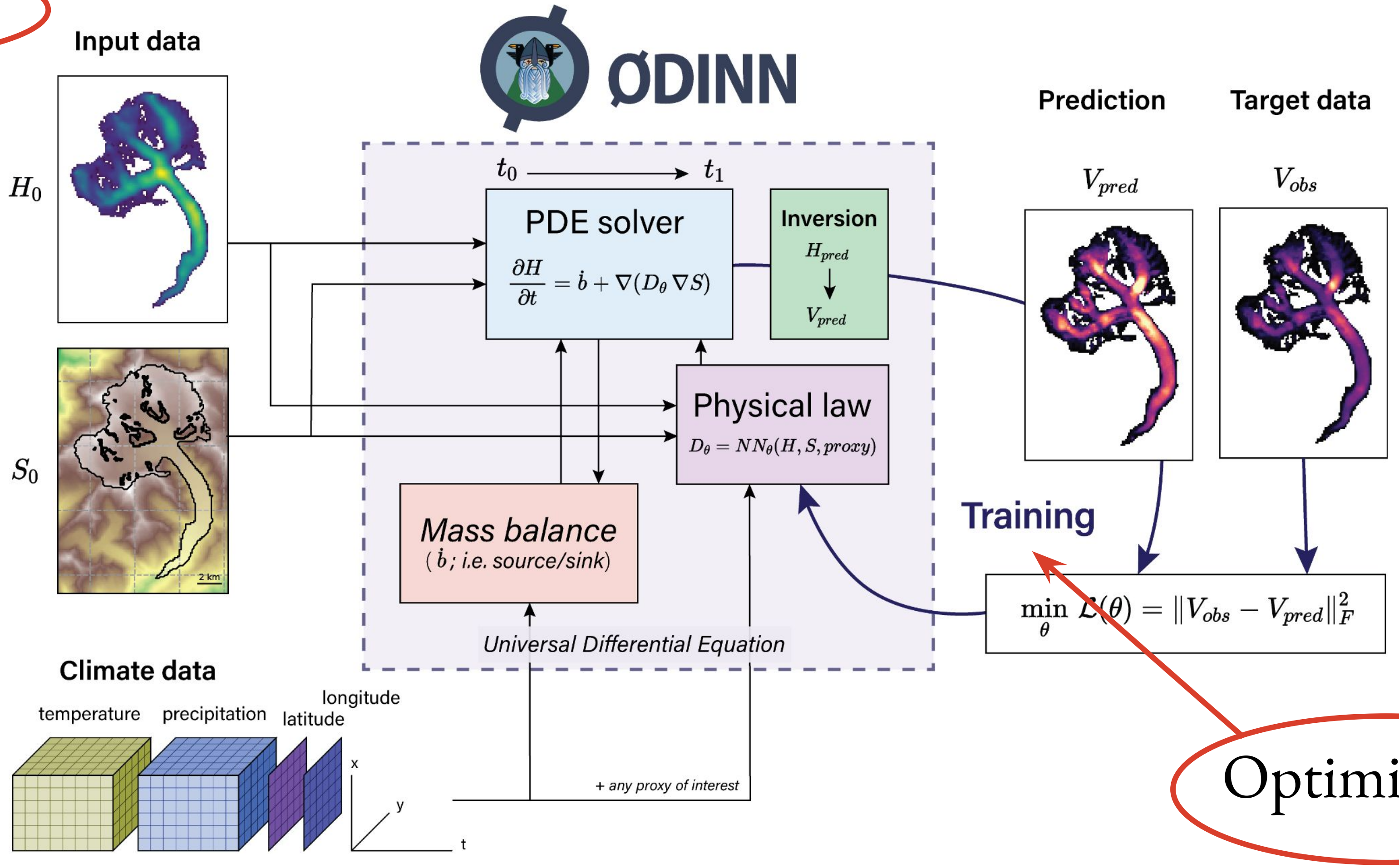
Numerical solution of SIA equation

Computation of gradients

Bolibar, Sapienza et al., GMOD 2023, *Universal Differential Equations for glacier ice flow modelling*

Preprocessing

Numerical solution of SIA equation



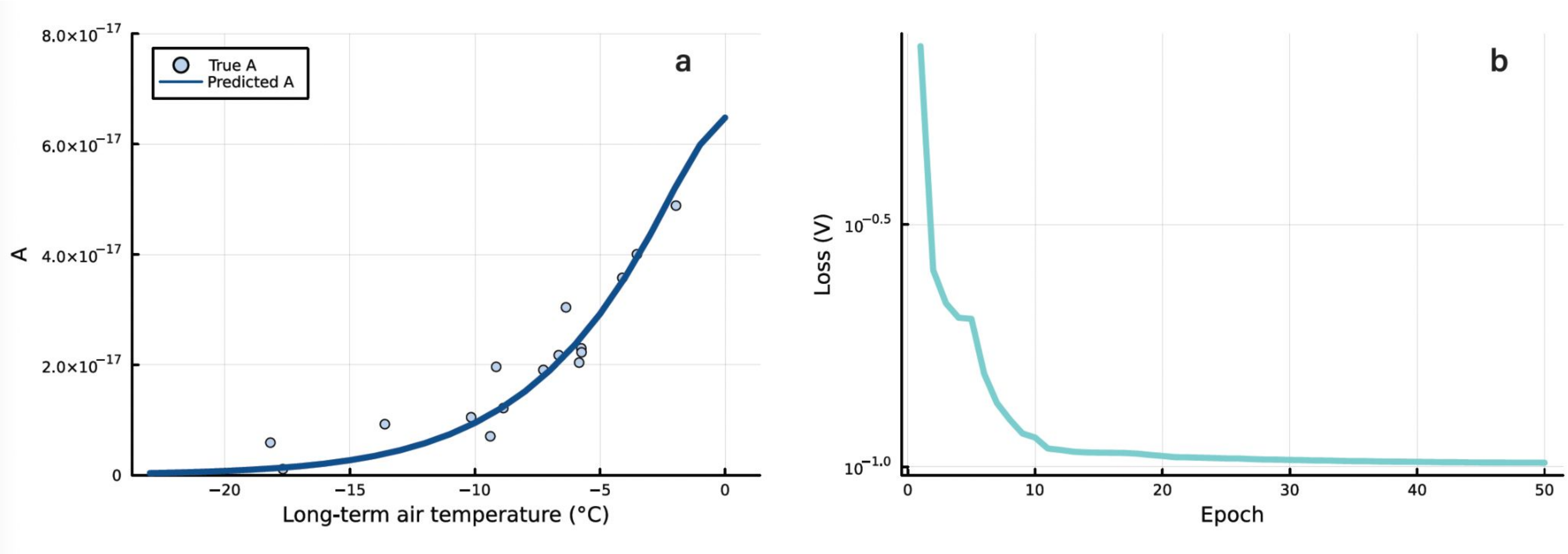
Mass balance model

Computation of gradients

Optimization

Bolibar, Sapienza et al., GMOD 2023, *Universal Differential Equations for glacier ice flow modelling*

c) Training of Universal Differential Equations



c) Hard constraints

Advantages:

- Targeted ML approach, compatible with small data
- Faster and easier to train than PINNs
- Functional inversions: new tool to discover physical/empirical laws

Disadvantages:

- More technically complex to implement: requires a good AD framework
- Generally slower to execute than PINNs and data-driven ML models

These methods are based on **differentiable programming**

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Programming paradigm to compute gradients/sensitivities of a computer program

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Required for training/calibration of complex models with many parameters

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Programming paradigm to compute gradients/sensitivities of a computer program

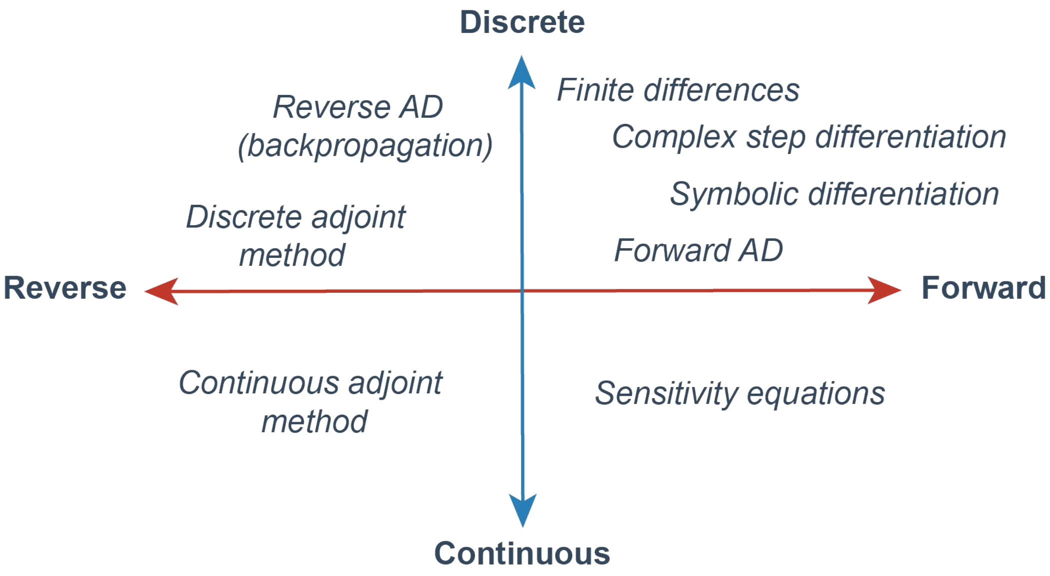
Required for training/calibration of complex models with many parameters

In geophysical modelling based on differential equations, we need to differentiate through the numerical solver!

Sapienza et al., *A review on sensitivity methods for differential equations (In Preparation)*

Differentiable programming for differential equations

Different methods to evaluate the gradient of systems based on solutions of differential equations:



Differentiable Programming for Differential Equations: A Review

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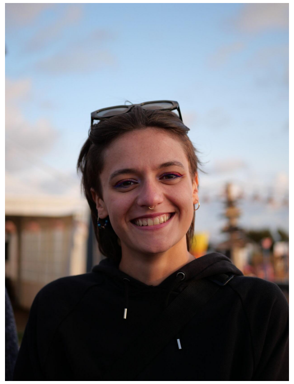

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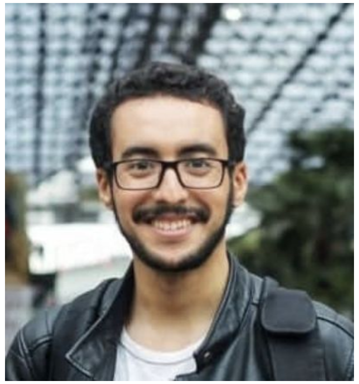

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