SYMPOSIUM OP'24

Ocean Predict

In partnership with

unesco
Intergovernmental Oceanographic Commission

2021 2030 United Nations Decade of Ocean Science for Sustainable Development

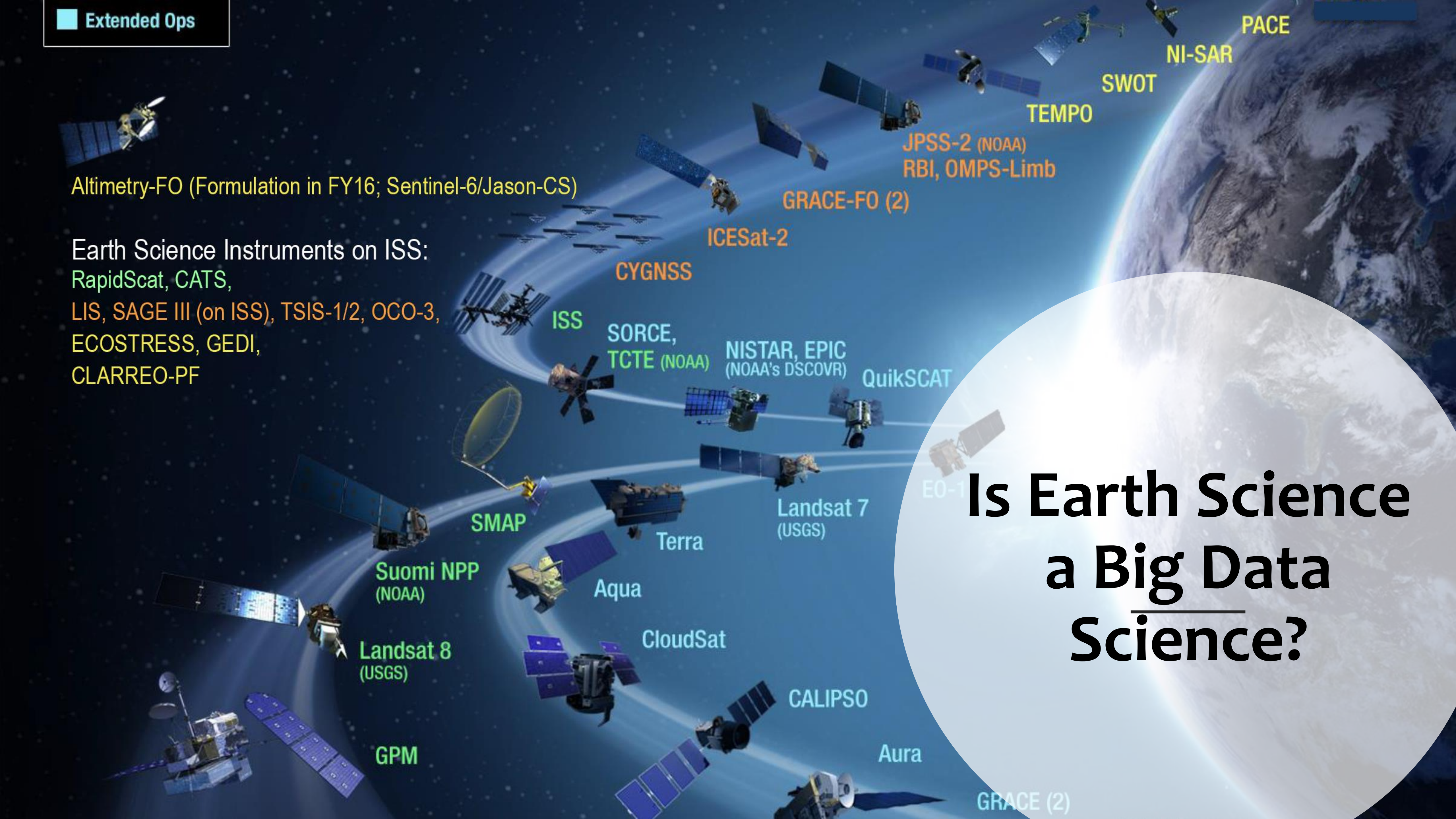
Learning from (sparse) observations through the lens of models

Patrick Heimbach &
The DJ4Earth & ECCO groups

The University of Texas at Austin

ODEN INSTITUTE
FOR COMPUTATIONAL ENGINEERING & SCIENCES

Is Earth Science a Big Data Science?



Is Oceanography a “big data” science?

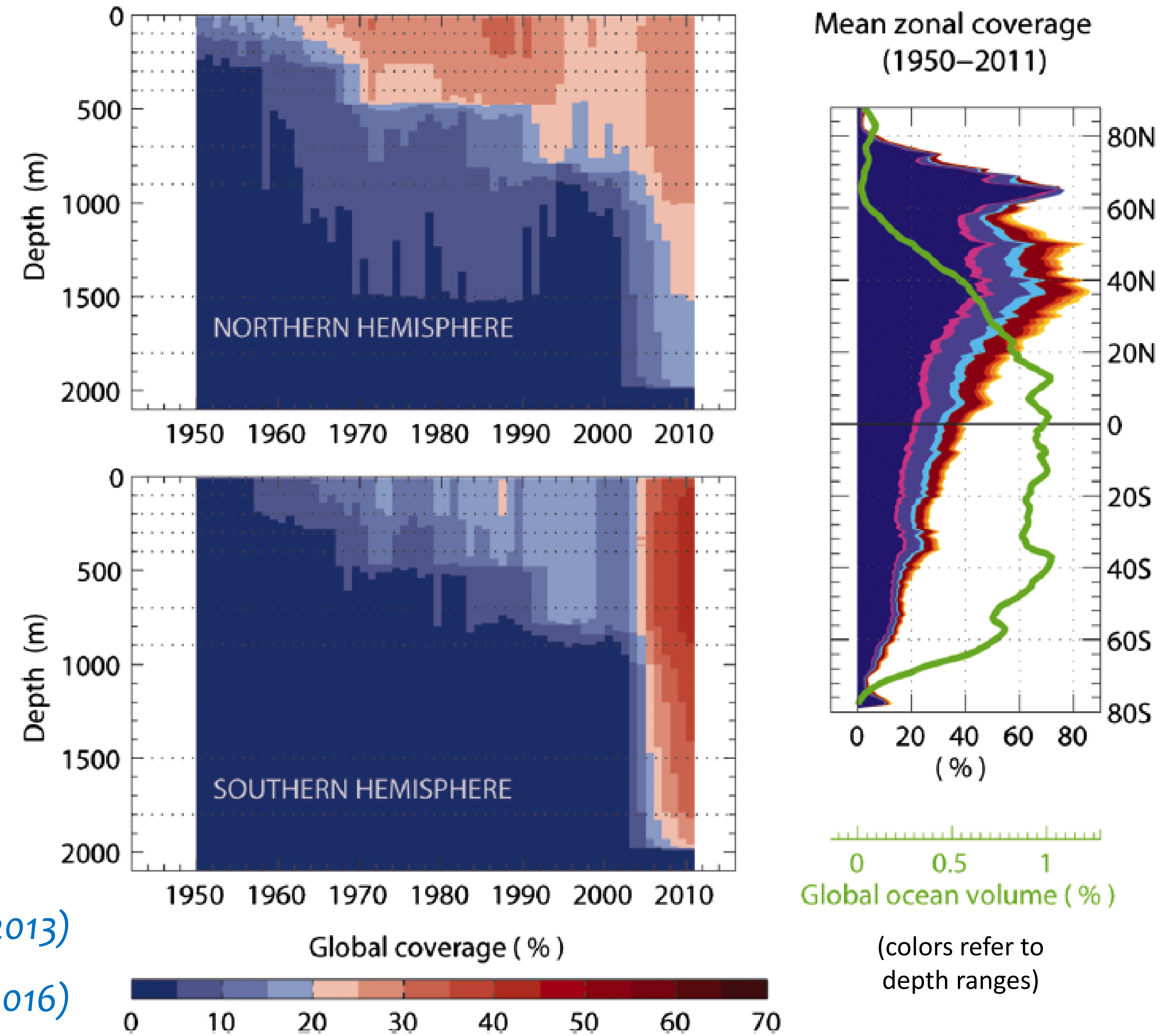
Yes & No …

Oceanography: <u>A *sparse data* problem</u> …

Observational sampling coverage for ocean temperature in the upper 2000 m
1950 – 2010
(mean ocean depth: ~ 3900 m)

Abraham et al., Rev. Geophys. (2013)

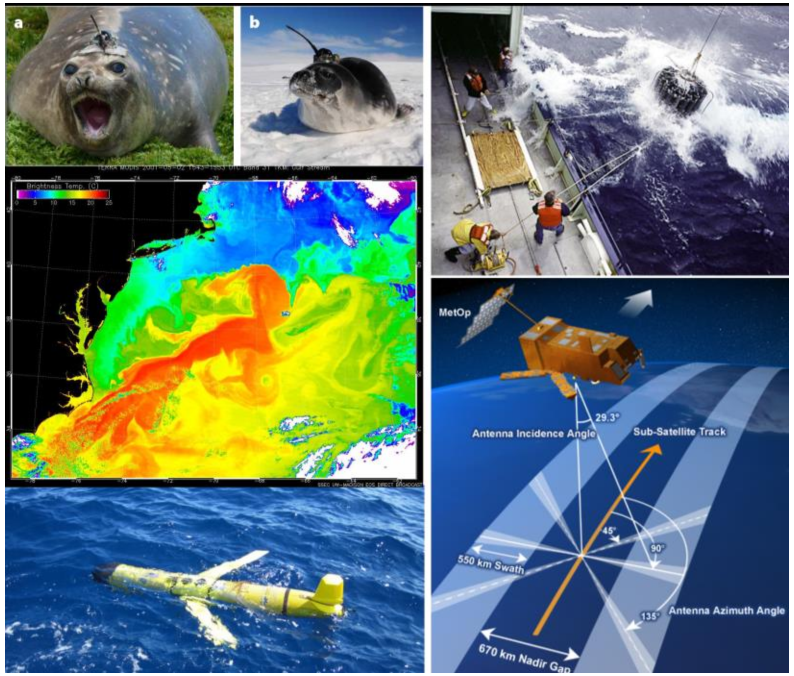
Wunsch, Annual Reviews (2016)



Two incomplete knowledge reservoirs

an eclectic, patchy, heterogeneous

observing system



numerical models

that require

uncertain

inputs

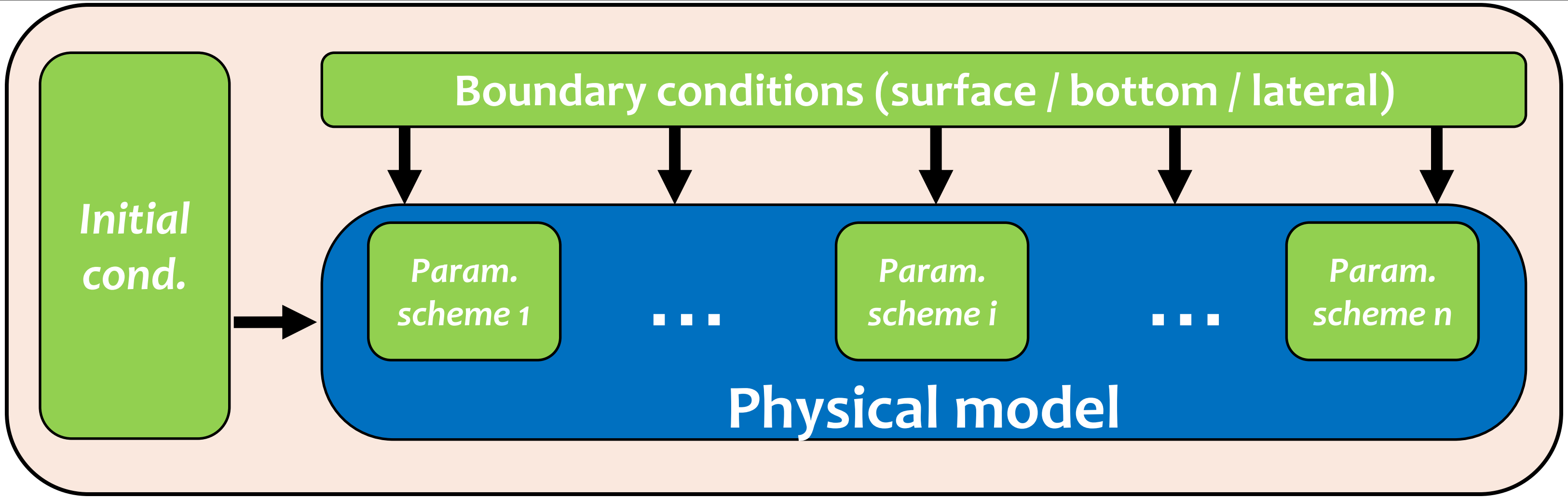
Parameter & state estimation

The data assimilation / inverse method *is learning from* …

- a set of **usually sparse, heterogeneous** observations
- … *AND* known (albeit uncertain) physics/dynamics,
- … by solving a gigantic least-squares model-data misfit minimization

What do we mean by ***"Learning"***?

Learn …

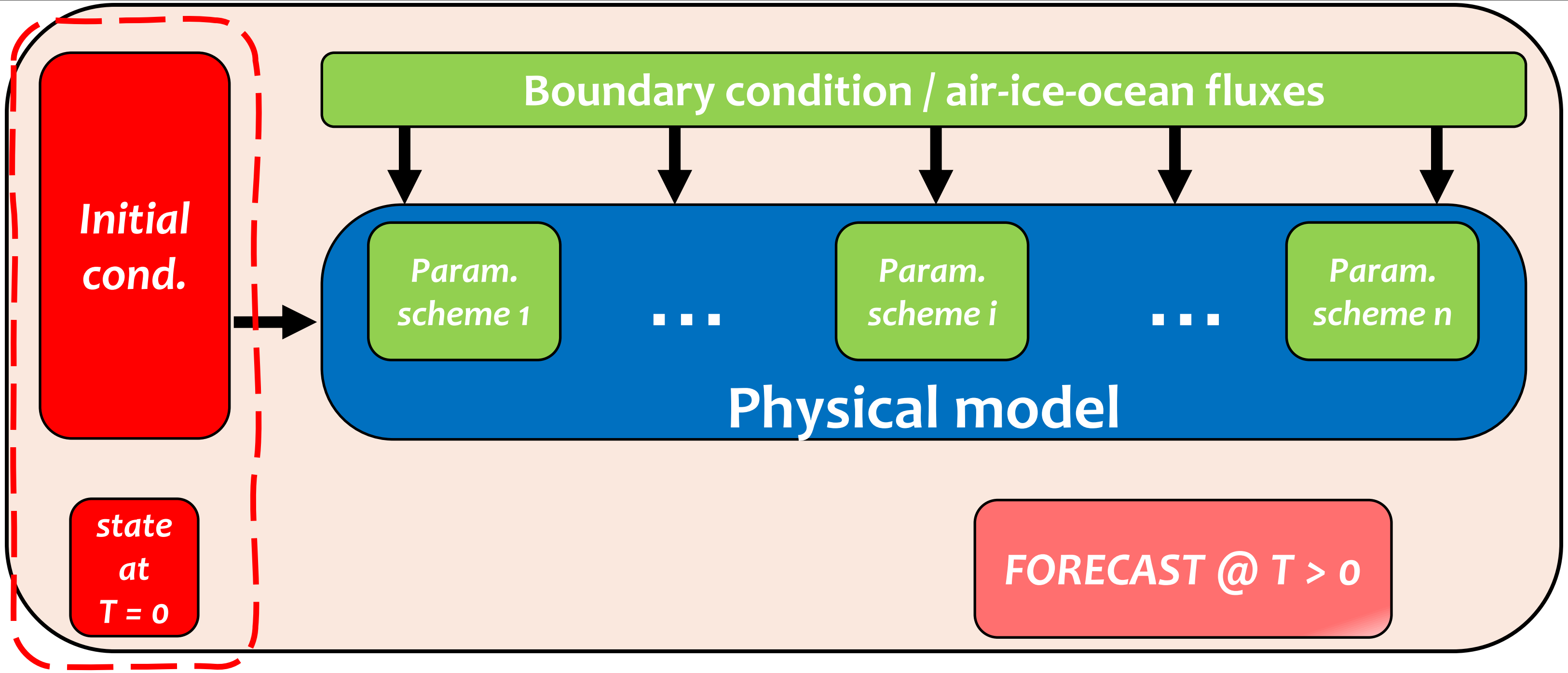


Boundary conditions (surface / bottom / lateral)
Initial cond.
Param. scheme 1
…
Param. scheme i
…
Param. scheme n
Physical model

Learn model *initial conditions*

Find best initial conditions that will produce optimal forecast …

*The **filtering** problem of optimal estimation & control*



Learn model *initial conditions*

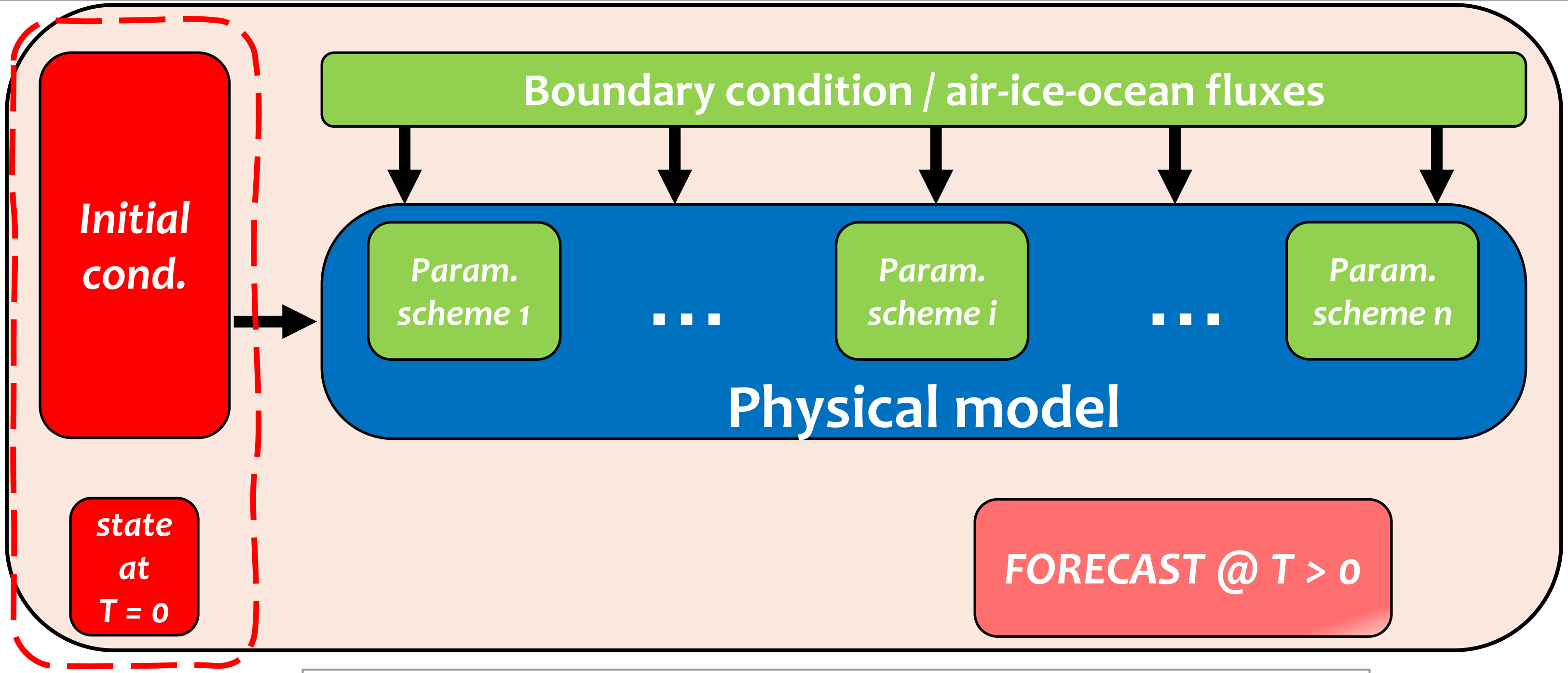
Find best initial conditions that will produce optimal forecast …

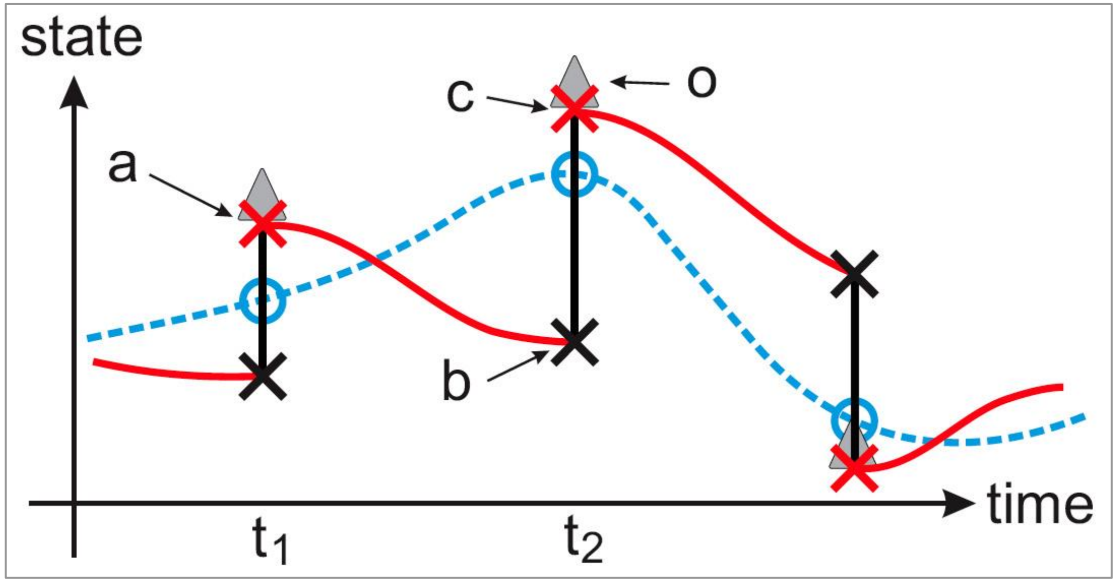
*The **filtering** problem of optimal estimation & control*

Initialization for prediction/extrapolation

as practiced in short-term

weather & ocean prediction





Learn model *initial conditions*

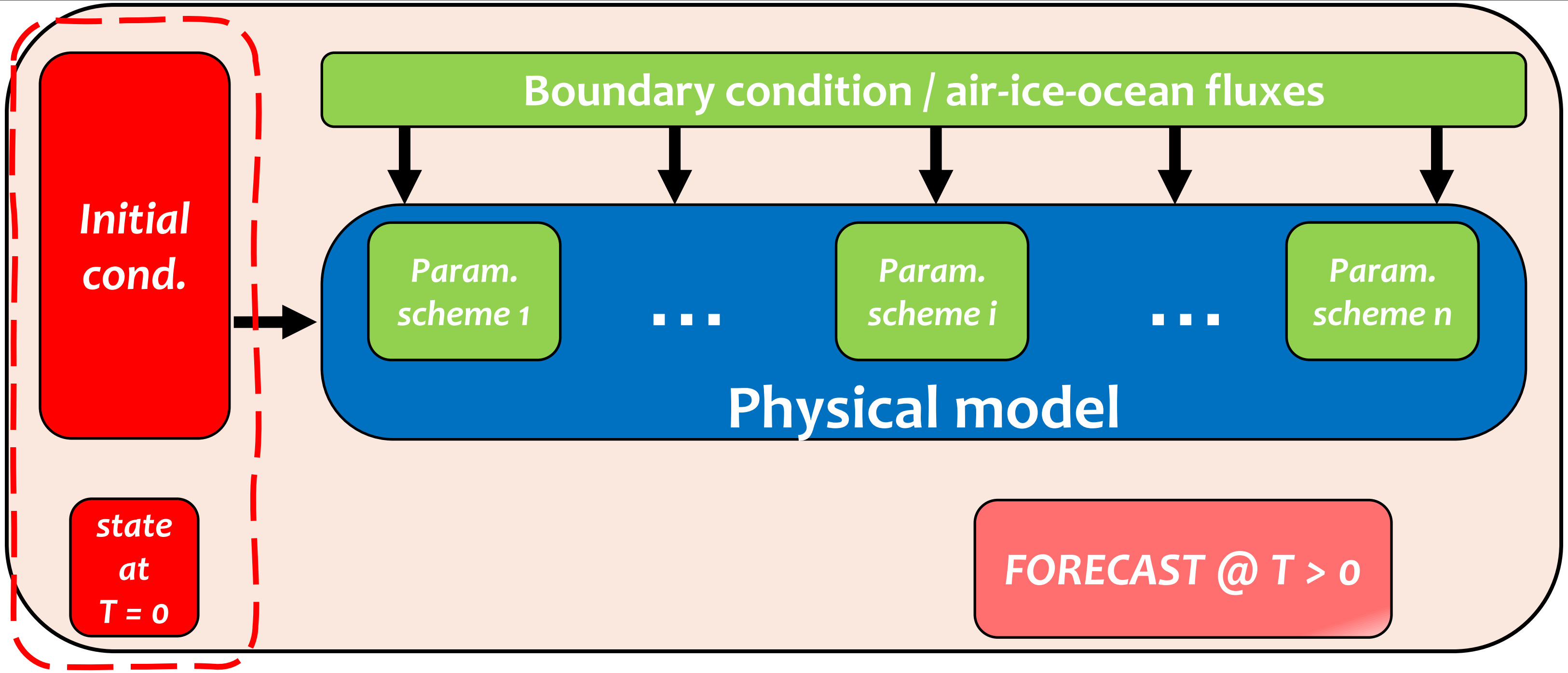
Find best initial conditions that will produce optimal forecast …

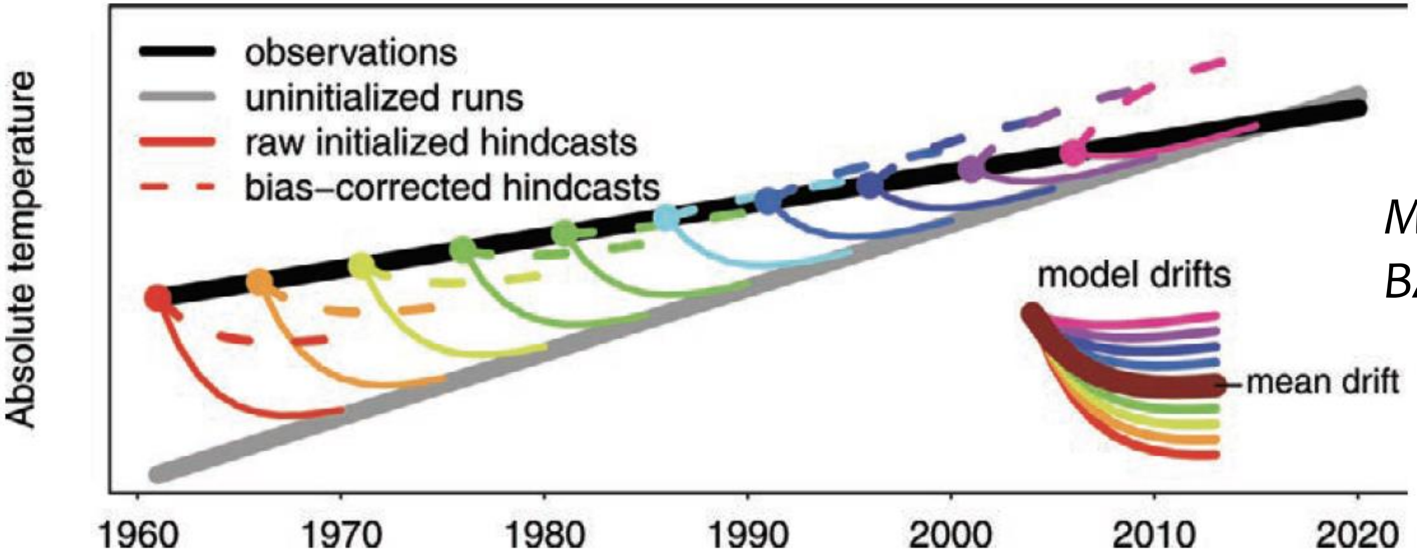
*The **filtering** problem of optimal estimation & control*

Initialization for prediction/extrapolation

as practiced in

interannual to decadal prediction



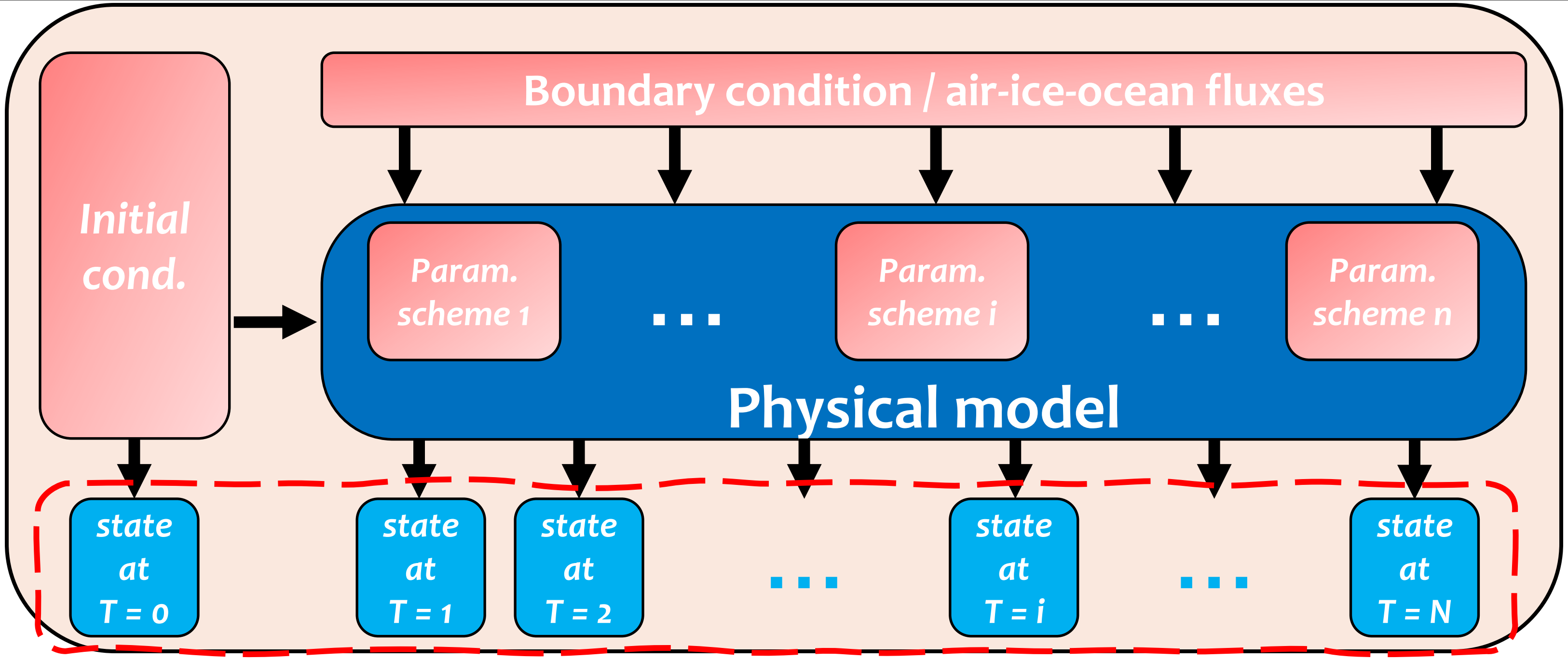


Meehl et al. BAMS (2014)

Learn model *time-evolving state*

Find model inputs (in red) that produce the best dynamically consistent state

*The **smoothing** problem of optimal estimation & control*



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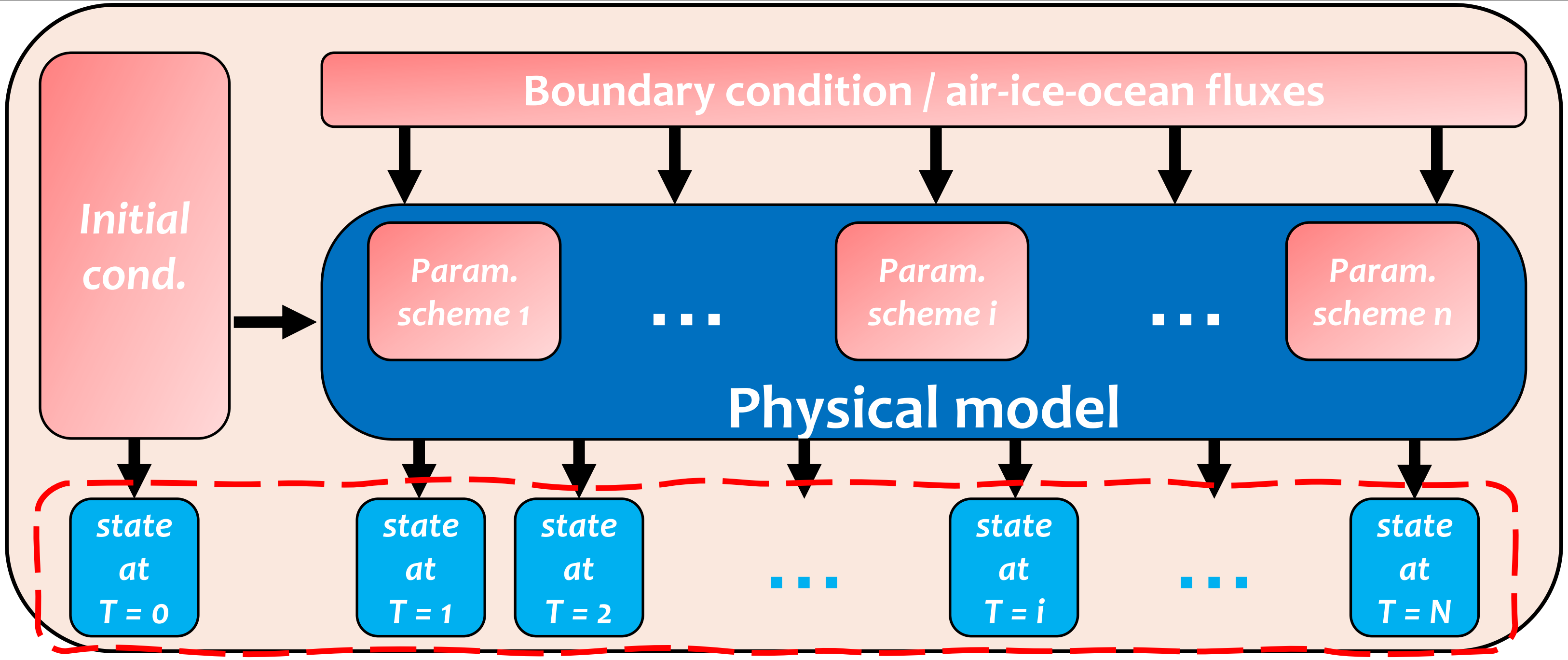
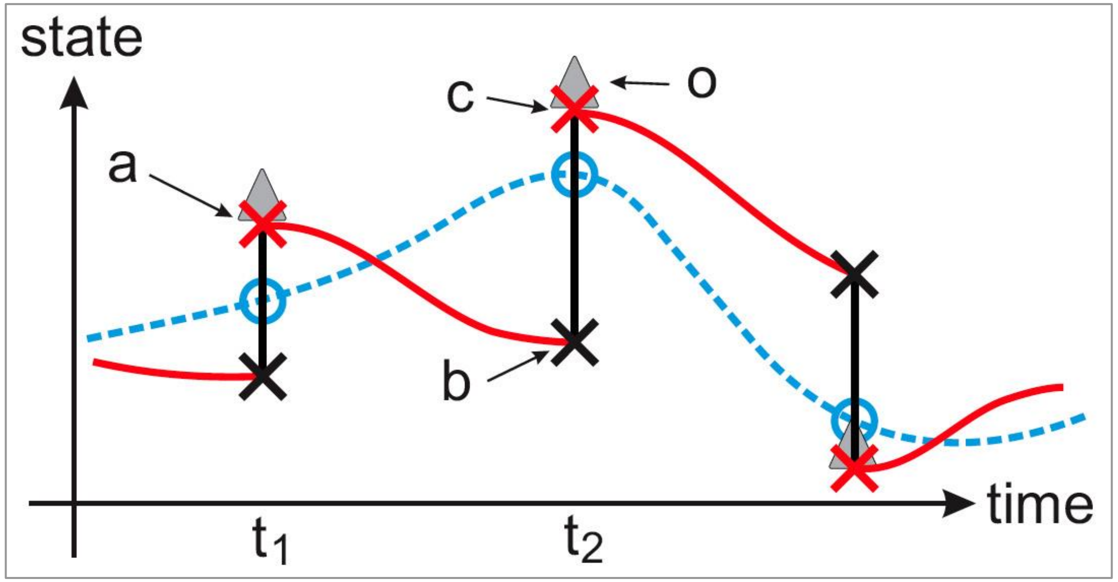


State & parameter estimation for:

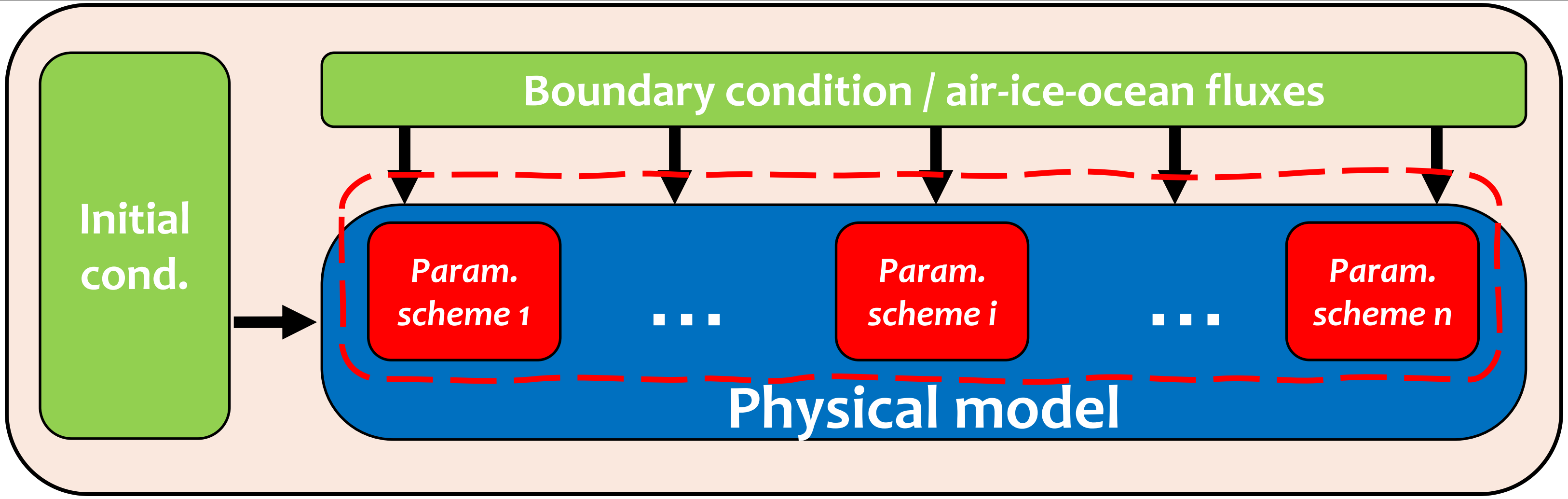
- ***Interpolation/reconstruction***
- ***(transient calibration)***

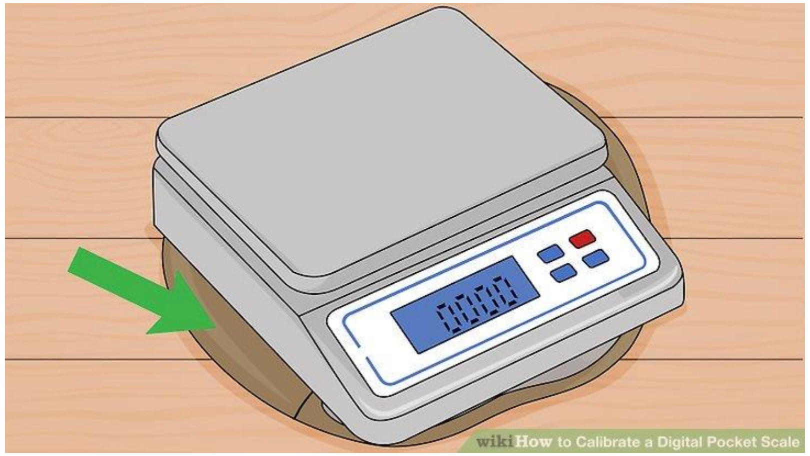


Learn model *parameters*

Physical model has many empirical parameters:

- constitutive laws
- subgrid-scale parameterization schemes





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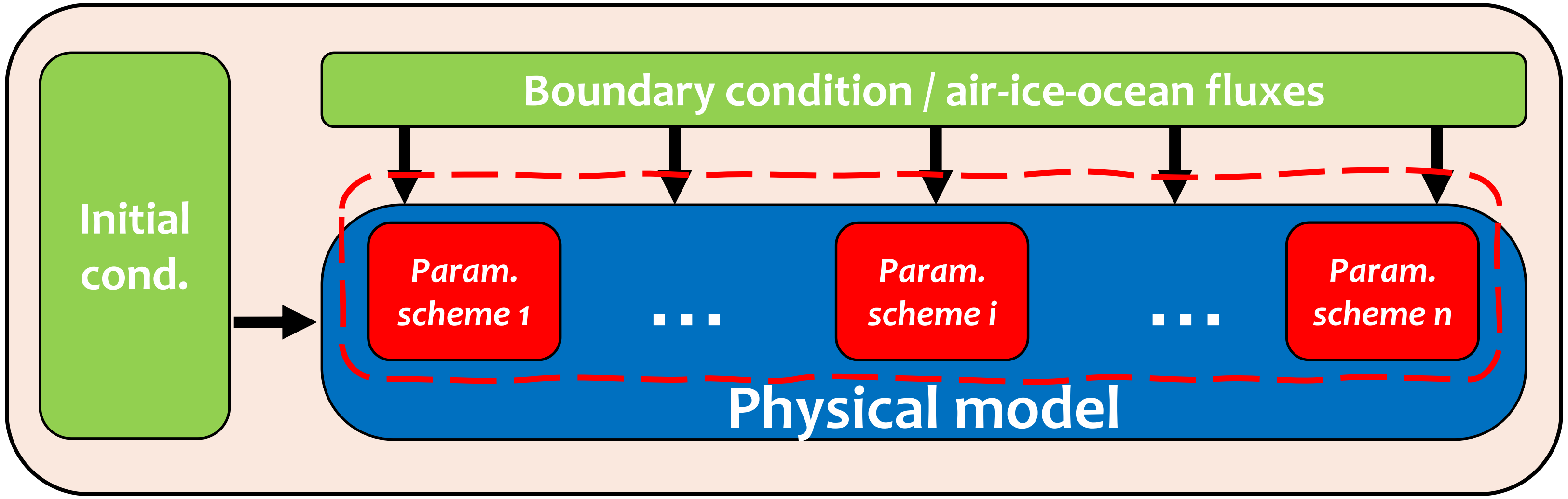
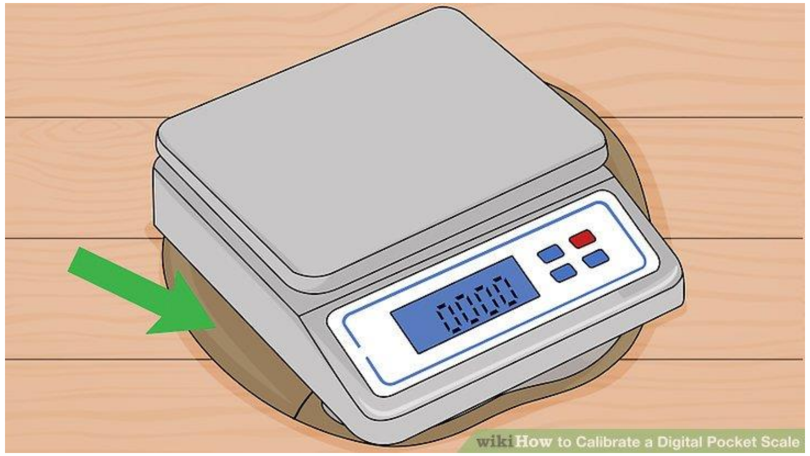


parameter estimation using observations is essential



THE ART AND SCIENCE OF CLIMATE MODEL TUNING

BAMS

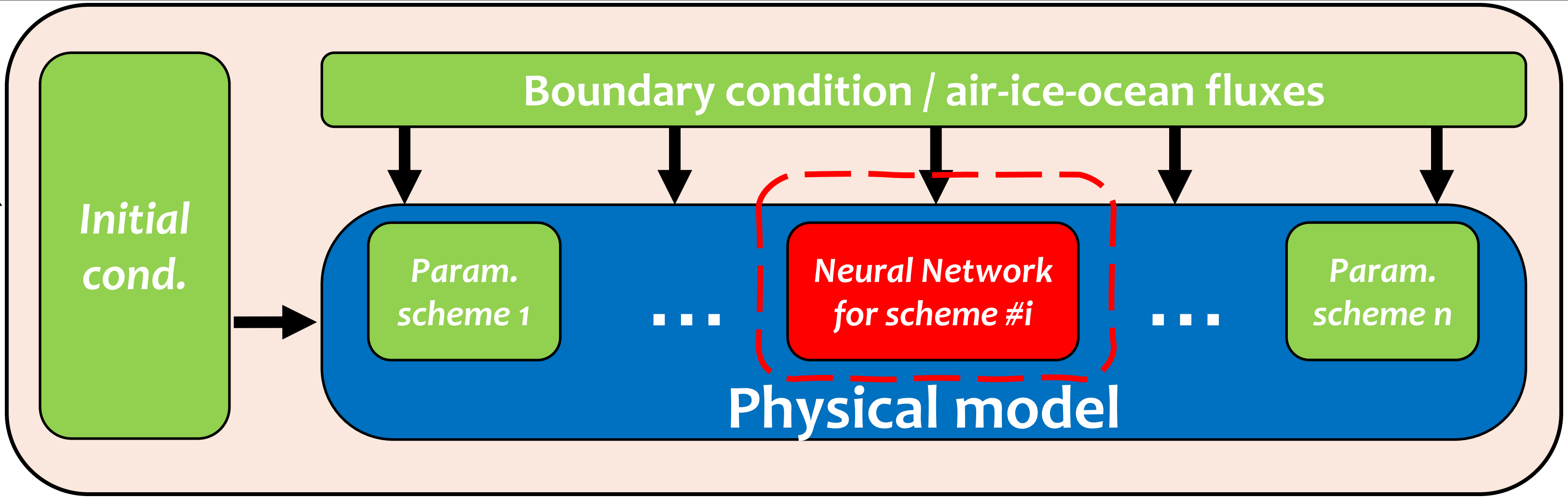
Frédéric Hourdin, Thorsten Mauritsen, Andrew Gettelman, Jean-Christophe Golaz, Venkatramani Balaji, Qingyun Duan, Doris Folini, Duoying Ji, Daniel Klocke, Yun Qian, Florian Rauser, Catherine Rio, Lorenzo Tomassini, Masahiro Watanabe, and Daniel Williamson

We survey the rationale and diversity of approaches for tuning, a fundamental aspect of climate modeling, which should be more systematically documented and taken into account in multimodel analysis.

Learn surrogate (e.g., NN) of *model's parameterization scheme*

Parameterization scheme(s) is replaced by neural network

NN is trained on high-fidelity simulation data which resolve scales to be parameterized



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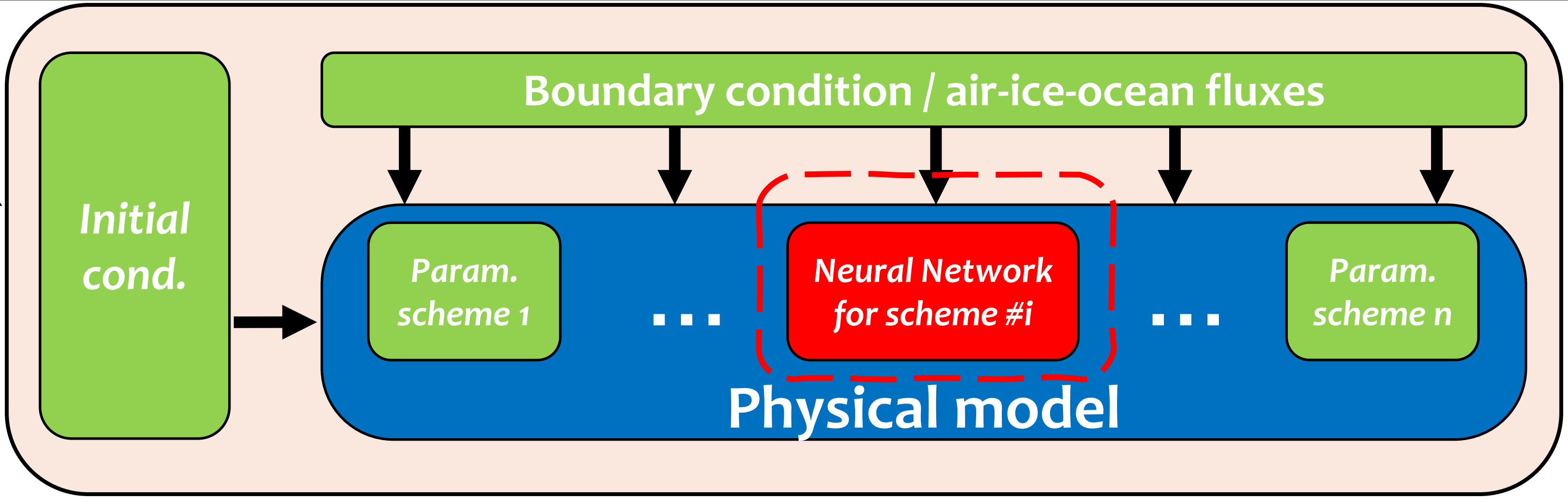

Parameterization scheme(s) is replaced by neural network

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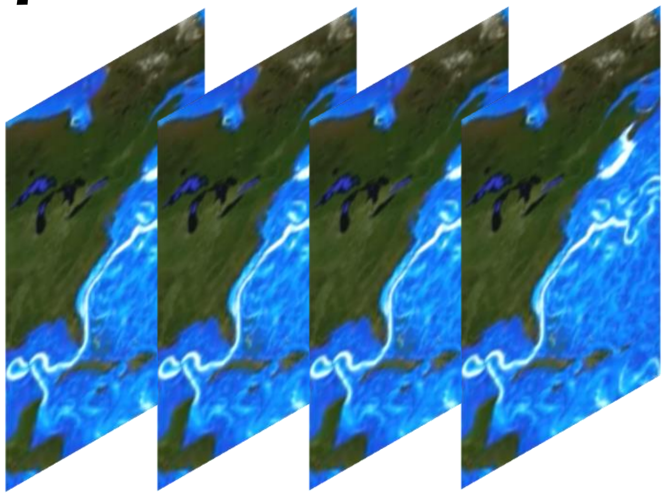
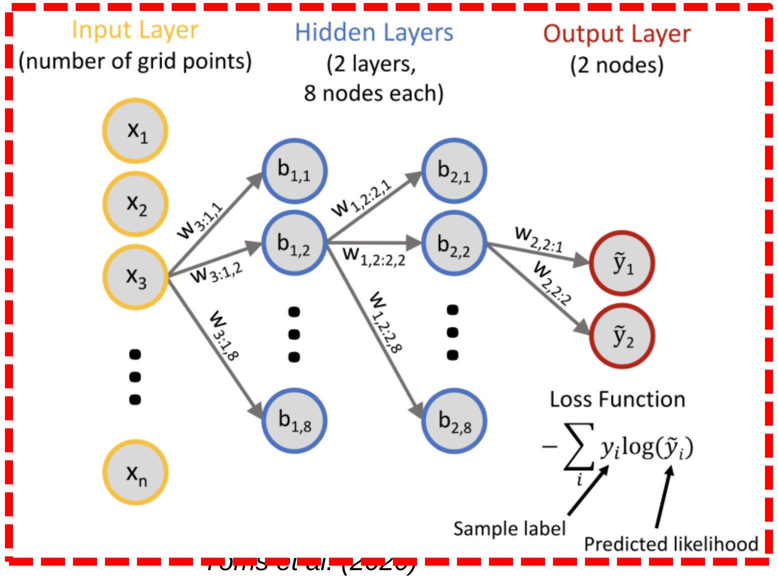
$$\frac{\partial \overline{\Phi}}{\partial t} + (\overline{\mathbf{u}} \cdot \nabla)\, \overline{\Phi} = \nabla \cdot (\kappa \nabla \overline{\Phi}) + \overline{F}_{\Phi} + \nabla \cdot \mathbf{S}$$

$$\nabla \cdot \mathbf{S} = \nabla \cdot \left(\overline{\mathbf{u}\,\Phi} - \overline{\mathbf{u}}\,\overline{\Phi} \right) =$$





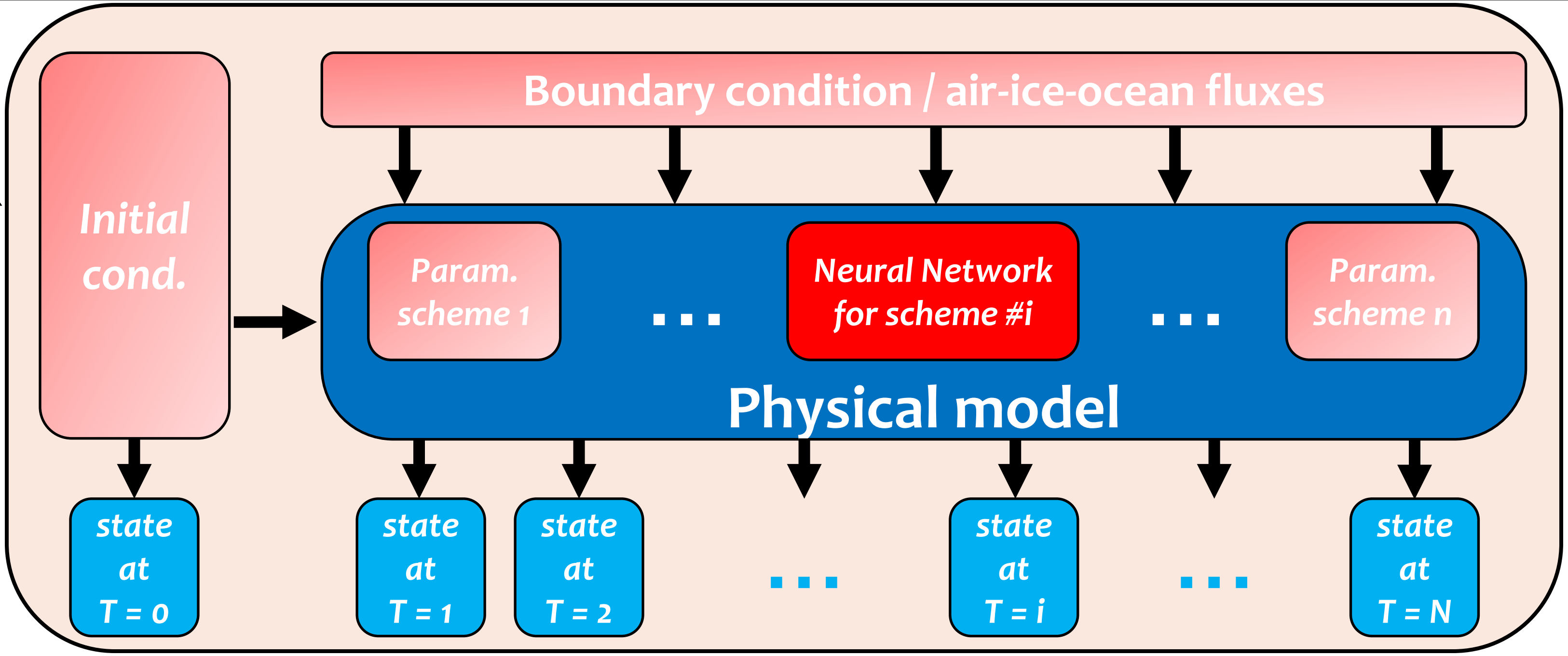
a priori / offline learning

Frezat et al. (2019), Zanna & Bolton (2021)

Learn *hybrid* physical/surrogate (NN) model

Parameterization scheme(s) is replaced by neural network

Training of the NN is part of "training" of the physical model on state variables



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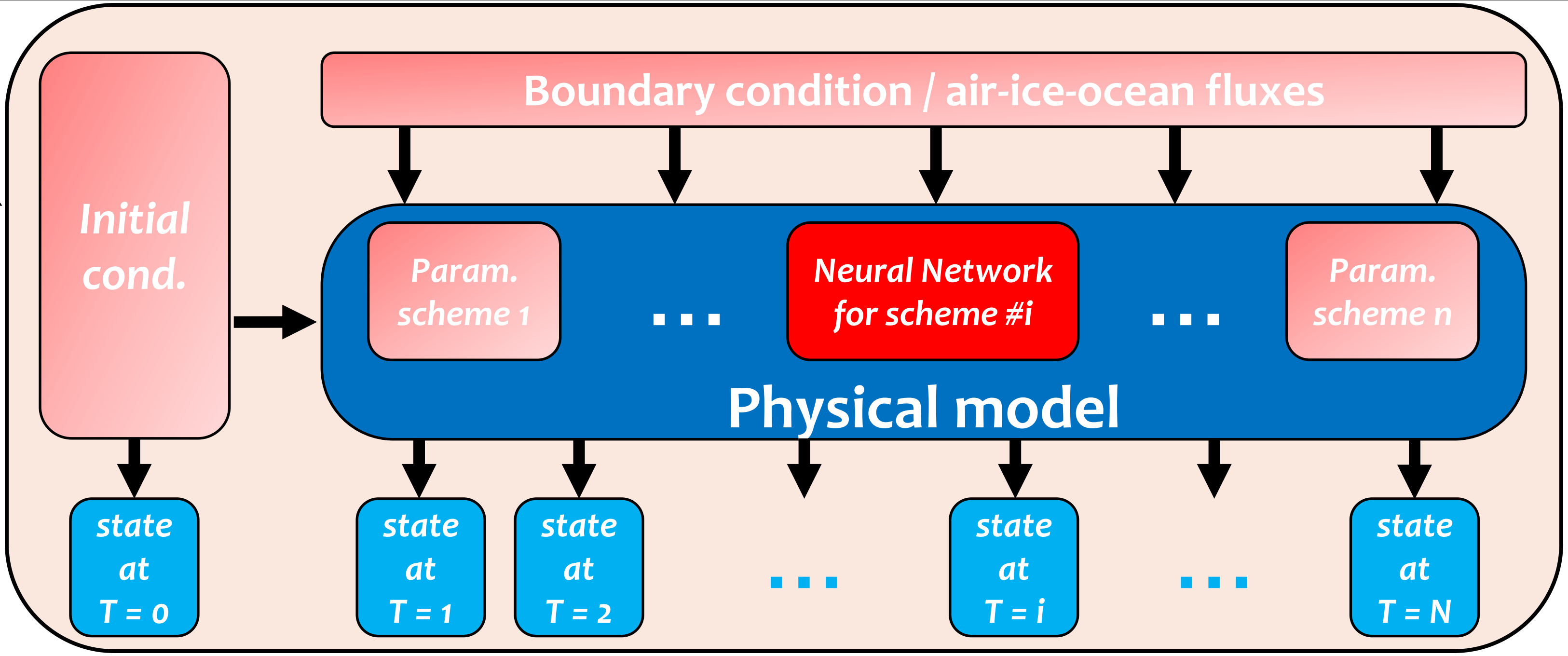
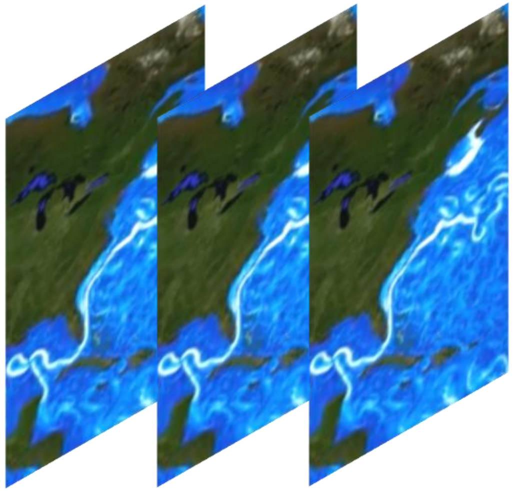


a posteriori / full-model / online / end-to-end learning



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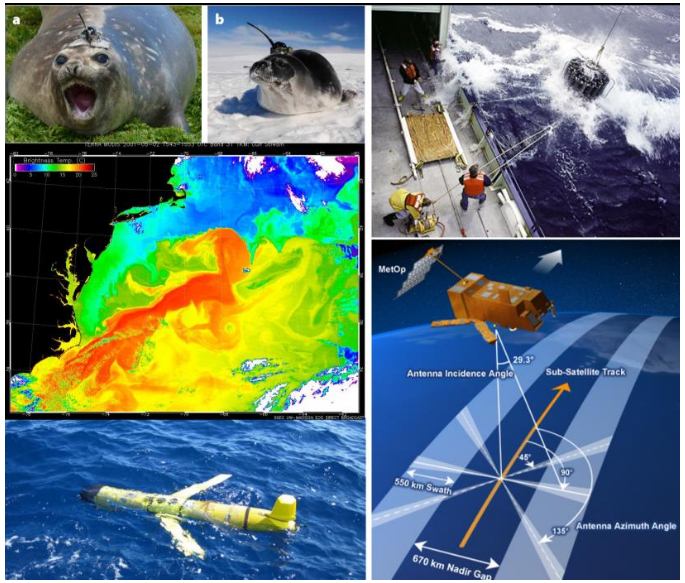
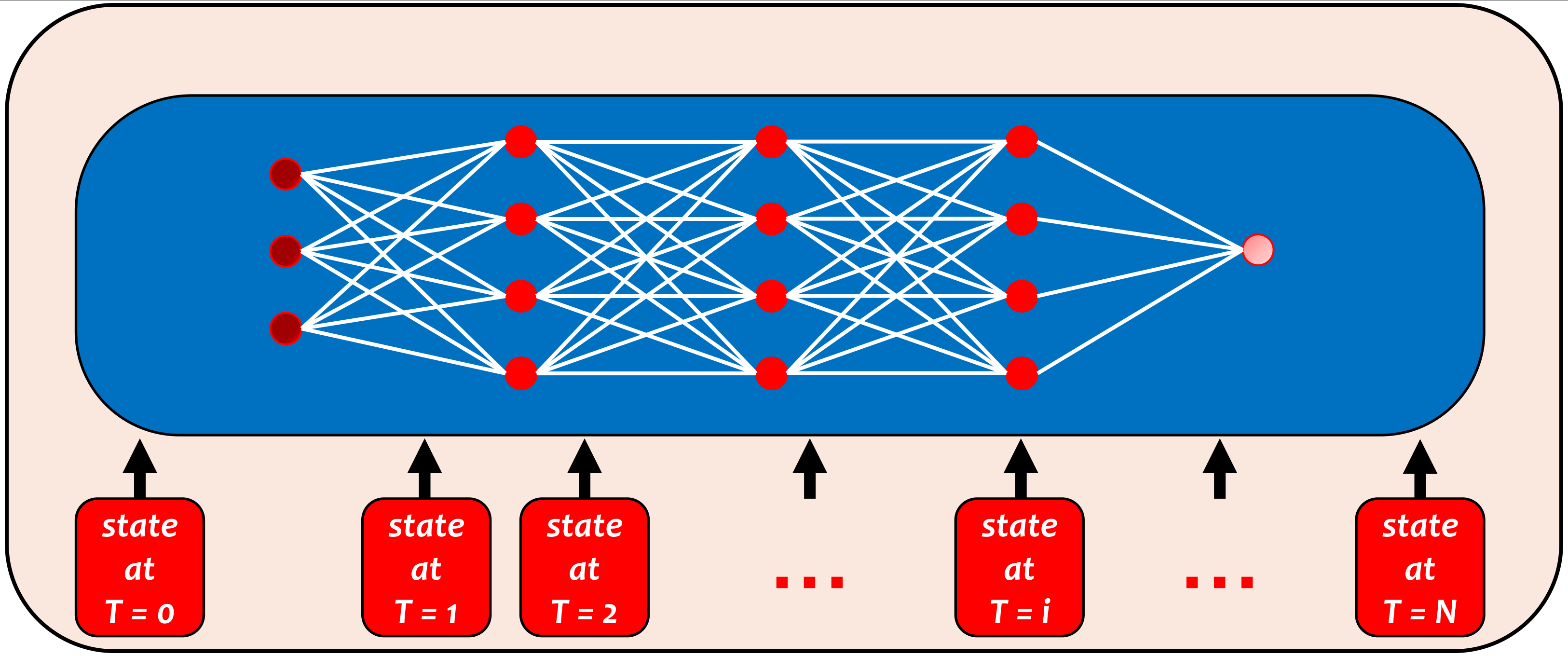


Learn surrogate (e.g., NN) of the *entire* physical model

Physical model is replaced entirely by surrogate model, e.g., neural network (NN):

purely data-driven learning

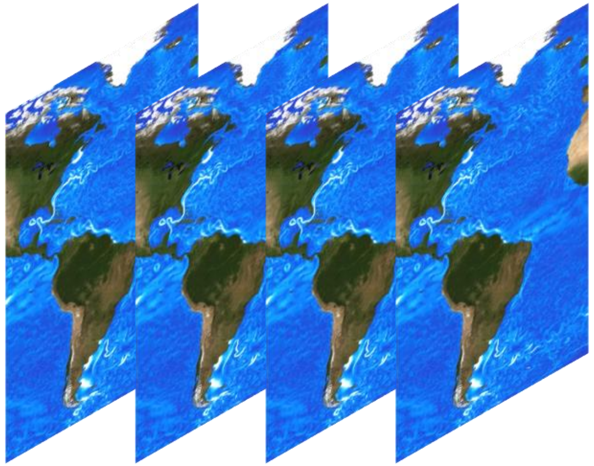


Weights of neural network trained on simulated model states, either

- ***high-fidelity models***

  or

- ***reanalyses***



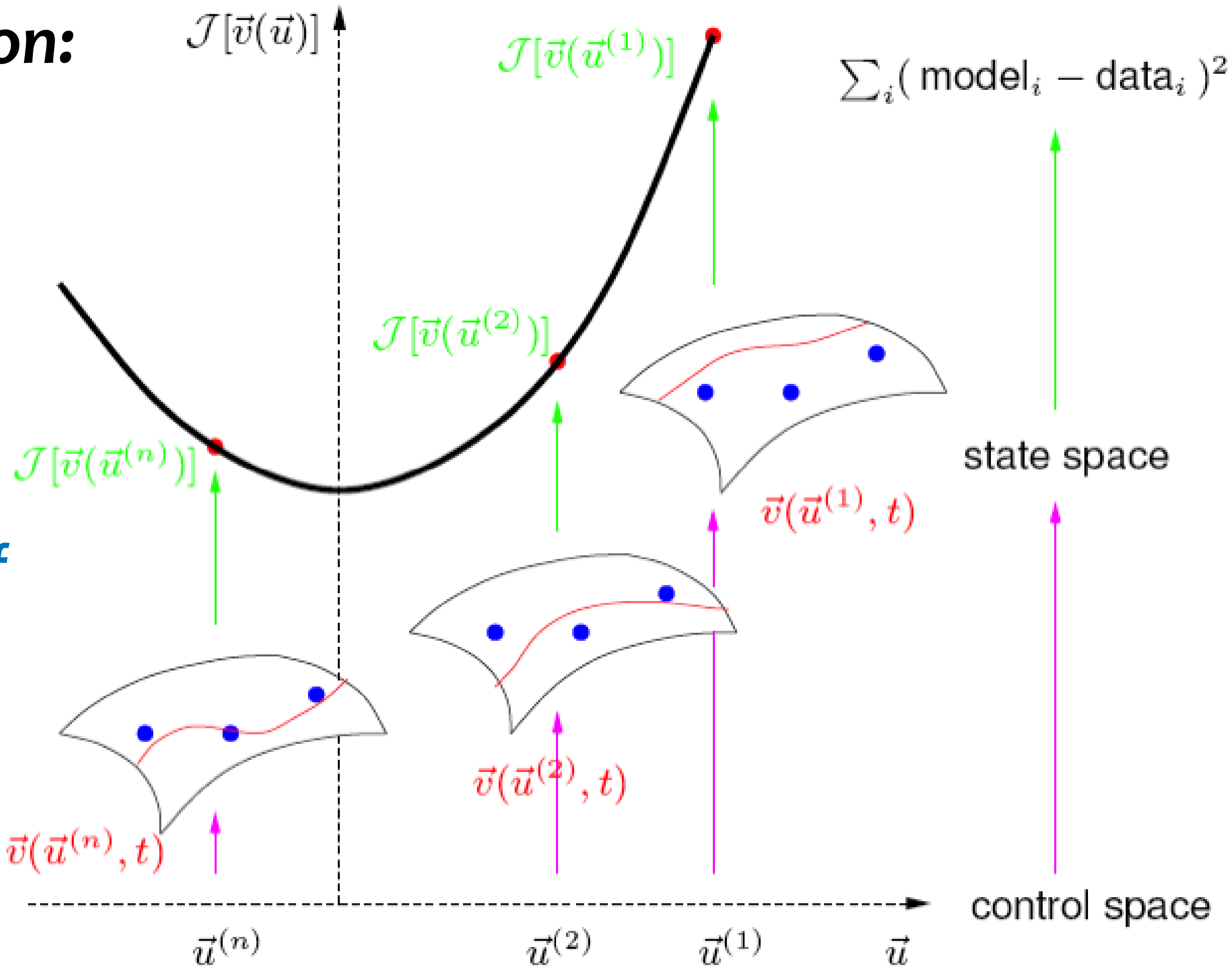
A key unifying computational framework of “*learning from data*”

Gradient-based optimization:

- *inversion* (physical models)
  - ***seek uncertain input / control variables / parameters***
- *training* (neural networks)
  - ***seek uncertain weights of NN representation***

Adjoint / backpropagation

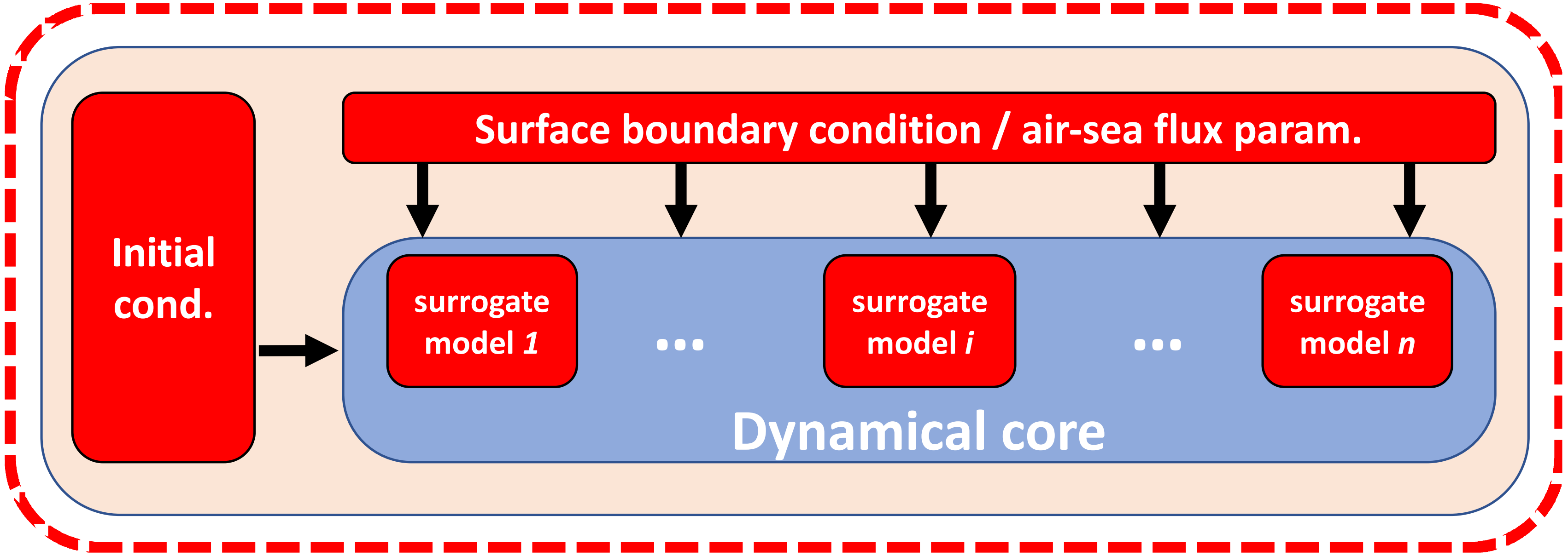
essential tool for computing high-dimensional gradients!



Full-model learning

Can we integrate the surrogate model training within full-model calibration

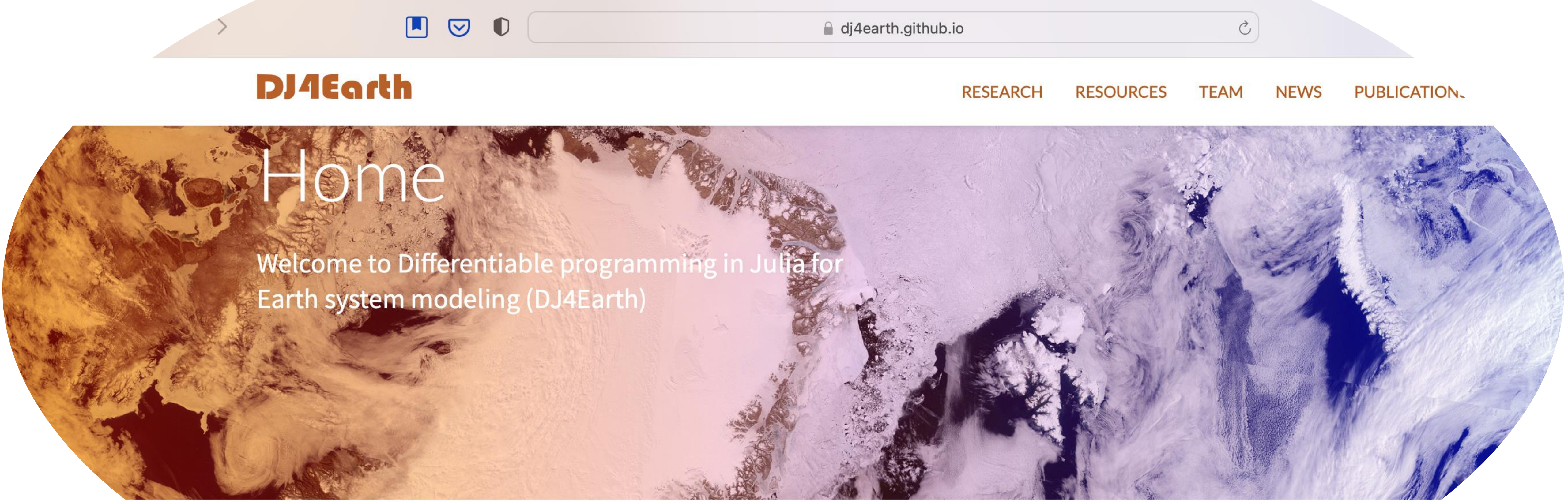
An end-to-end adjoint enables full-model calibration & initialization



Here: use of full-model ***differentiable programming*** to

- replace parts of model by appropriate surrogates
- use all available observations to train/calibrate all uncertain variables
- combines inverse modeling and ML in ***end-to-end learning***

relies on general-purpose automatic differentiation (AD)



Cyberinfrastructure for Sustained Scientific Innovation (CSSI)

https://DJ4Earth.github.io

NSF CSSI: *DJ4Earth*

Convergence of Bayesian inverse methods and scientific machine learning through universal differentiable programming

Since 2023 the idea of differentiable programming has taken off …

Geosci. Model Dev., 16, 3123–3135, 2023
https://doi.org/10.5194/gmd-16-3123-2023

Geoscientific
Model Development
Open Access

Differentiable programming for Earth system modeling

Maximilian Gelbrecht[1,2], Alistair White[1,2], Sebastian Bathiany[1,2], and Niklas Boers[1,2,3]

[1]Earth System Modelling, School of Engineering and Design, Technical University of Munich, Munich, Germany
[2]Potsdam Institute for Climate Impact Research, Potsdam, Germany
[3]Department of Mathematics and Global Systems Institute, University of Exeter, Exeter, UK

Since 2023 the idea of differentiable programming has taken off …

Geosci. Model Dev., 16, 3123–3135, 2023
https://doi.org/10.5194/gmd-16-3123-2023

Geoscientific
Model Development
Open Acces

Differentiable programming

Maximilian Gelbrecht[1,2], **Alistair White**[1,2], **Sebastia**

[1]Earth System Modelling, School of Engineering and De
[2]Potsdam Institute for Climate Impact Research, Potsdam,
[3]Department of Mathematics and Global Systems Institute,

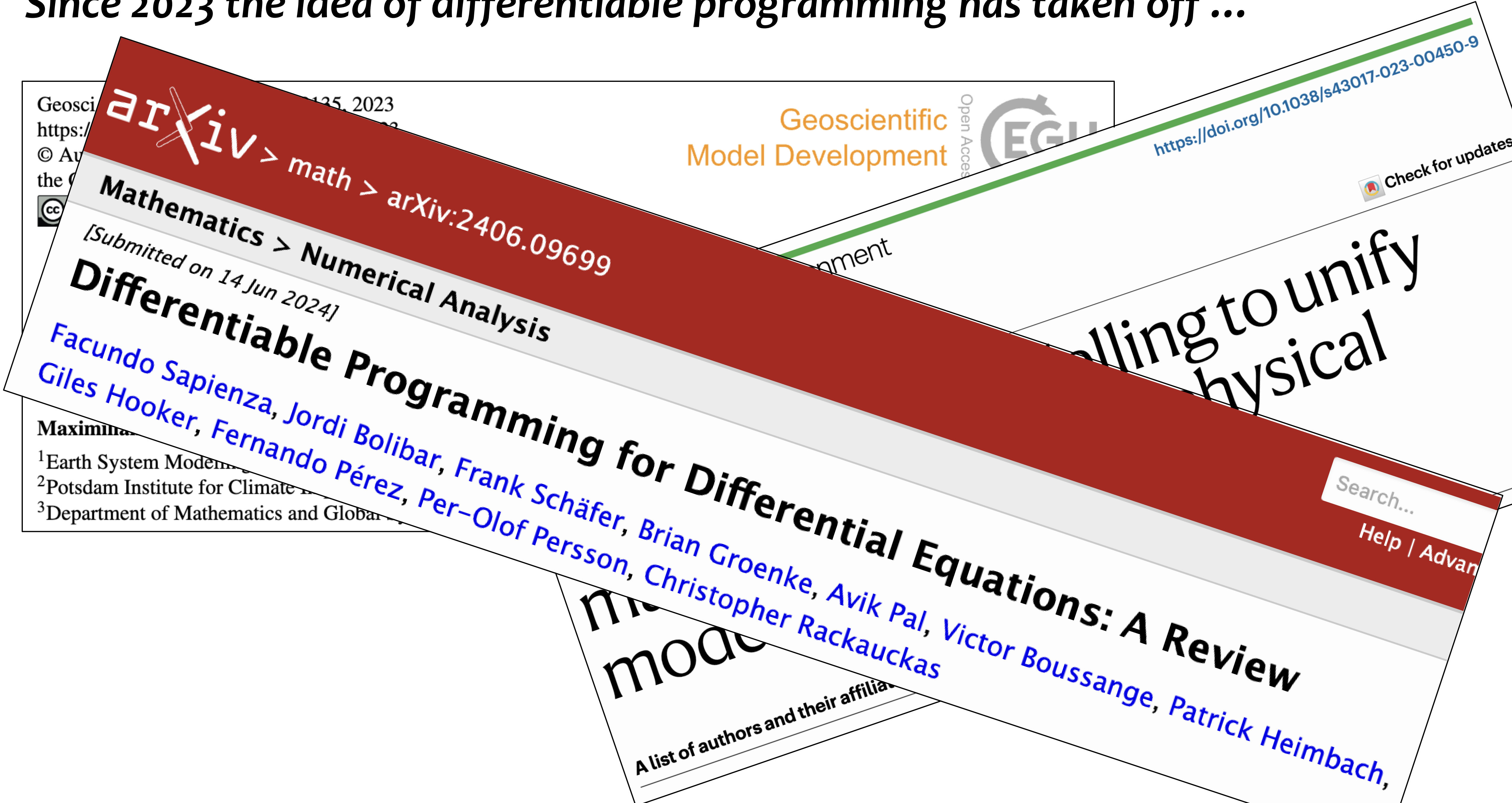
https://doi.org/10.1038/s43017-023-00450-9
Check for updates
nature reviews earth & environment

Perspective

Differentiable modelling to unify machine learning and physical models for geosciences

A list of authors and their affiliations appears at the end of the paper

Since 2023 the idea of differentiable programming has taken off ...



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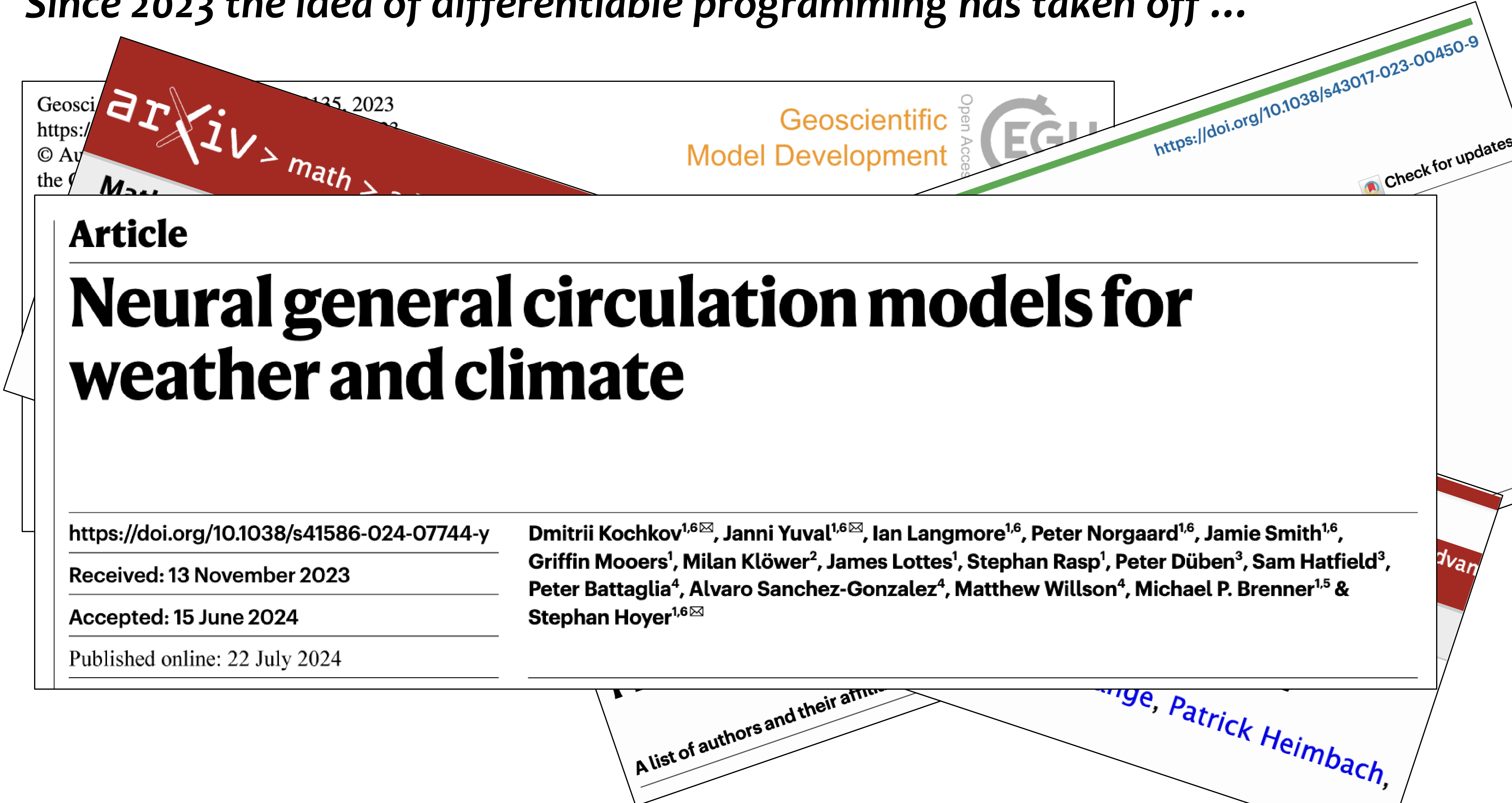


Geoscientific Model Development

https://doi.org/10.1038/s43017-023-00450-9

Check for updates

Article

Neural general circulation models for weather and climate

https://doi.org/10.1038/s41586-024-07744-y

Received: 13 November 2023

Accepted: 15 June 2024

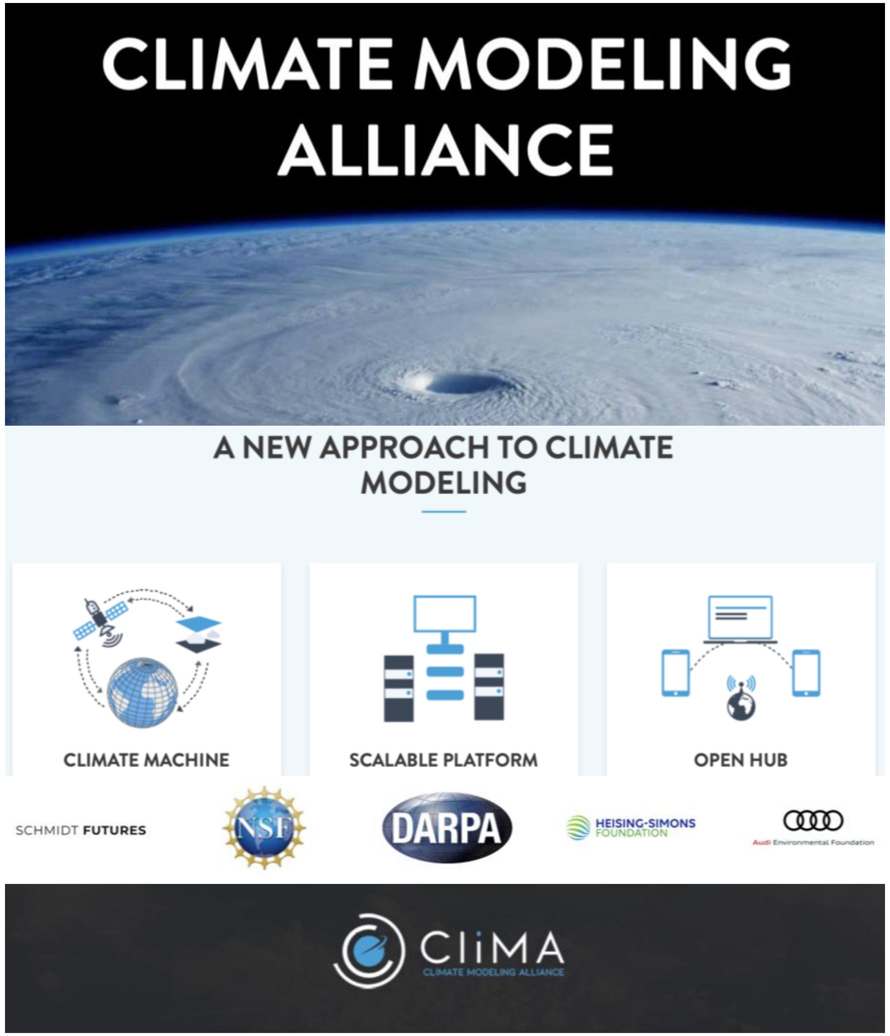
Published online: 22 July 2024

Dmitrii Kochkov[1,6] ✉, Janni Yuval[1,6] ✉, Ian Langmore[1,6], Peter Norgaard[1,6], Jamie Smith[1,6], Griffin Mooers[1], Milan Klöwer[2], James Lottes[1], Stephan Rasp[1], Peter Düben[3], Sam Hatfield[3], Peter Battaglia[4], Alvaro Sanchez-Gonzalez[4], Matthew Willson[4], Michael P. Brenner[1,5] & Stephan Hoyer[1,6] ✉

Differentiating a GPU-enabled climate model in Julia

DJ4Earth

Building on CliMA



Harness next-gen. compute architecture

TOOLBOX

JULIA: COME FOR THE SYNTAX, STAY FOR THE SPEED

Researchers often find themselves coding algorithms in one programming language, only to have to rewrite them in a faster one. An up-and-coming language could be the answer.

1 AUGUST 2019 | VOL 572 | NATURE

SIAM REVIEW
Vol. 59, No. 1, pp. 65–98

Julia: A Fresh Approach to Numerical Computing*

ClimaOcean.jl:

Ocean model component of the *Climate Model Alliance (CliMA) model*

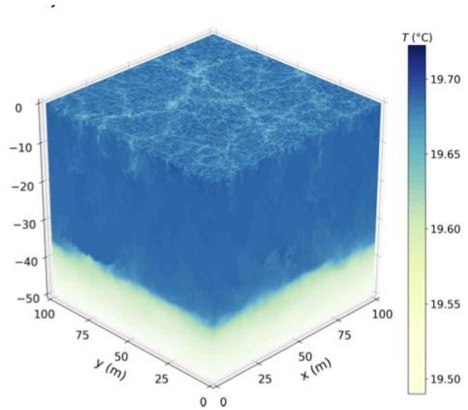
The Journal of Open Source Software

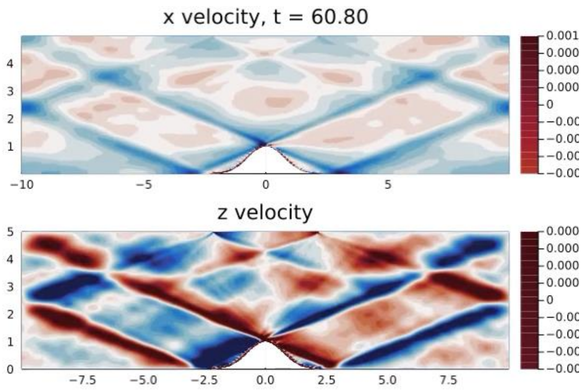
Oceananigans.jl: Fast and friendly geophysical fluid dynamics on GPUs

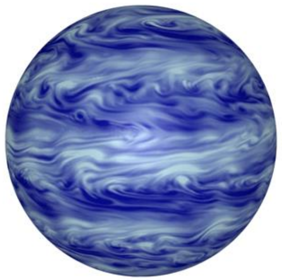
Ali Ramadhan[1], Gregory LeClaire Wagner[1], Chris Hill[1], Jean-Michel Campin[1], Valentin Churavy[1], Tim Besard[2], Andre Souza[1], Alan Edelman[1], Raffaele Ferrari[1], and John Marshall[1]

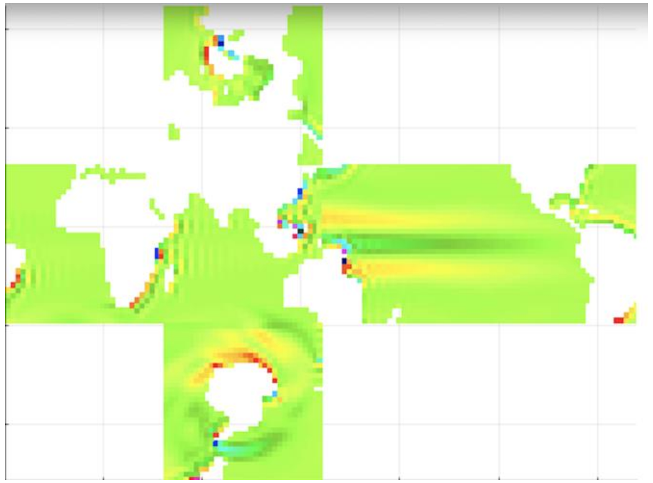
1 Massachusetts Institute of Technology **2** Julia Computing, Inc.

- Finite volume, rotating, stratified fluids model for geophysical fluid dynamics (GFD).
- Written from scratch in Julia
- Multiple simulation options.
- GPU and CPU via kernel abstractions
- Parallelize using MPI.jl and multi-threading









https://github.com/clima/Oceananigans.jl

Differentiable programming for full-model / end-to-end learning

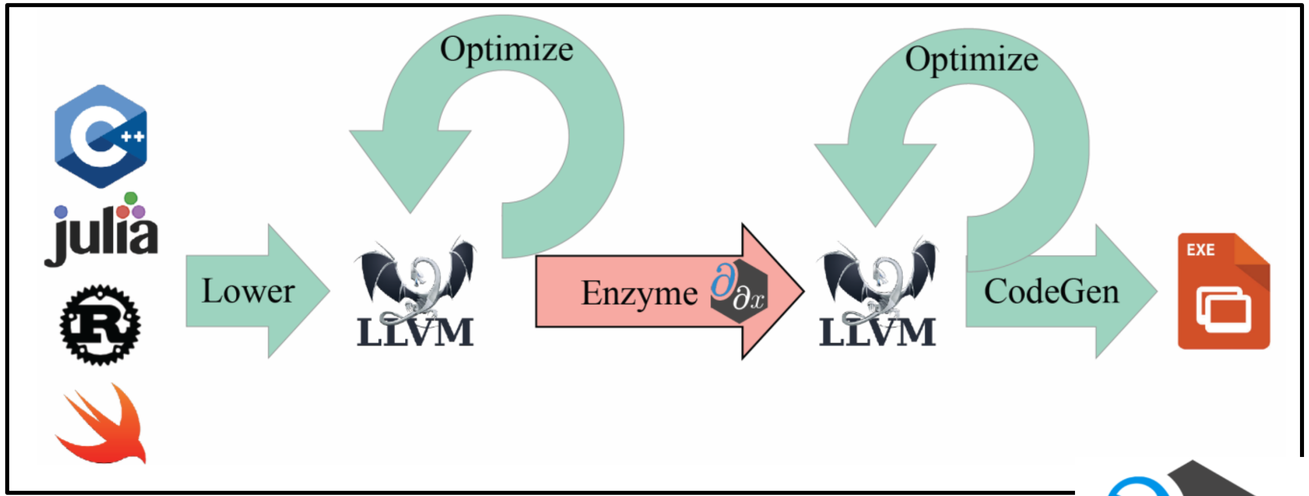
Differentiating GPU-enabled ocean model
in Julia via the AD tool ***Enzyme.jl***

DJ4Earth

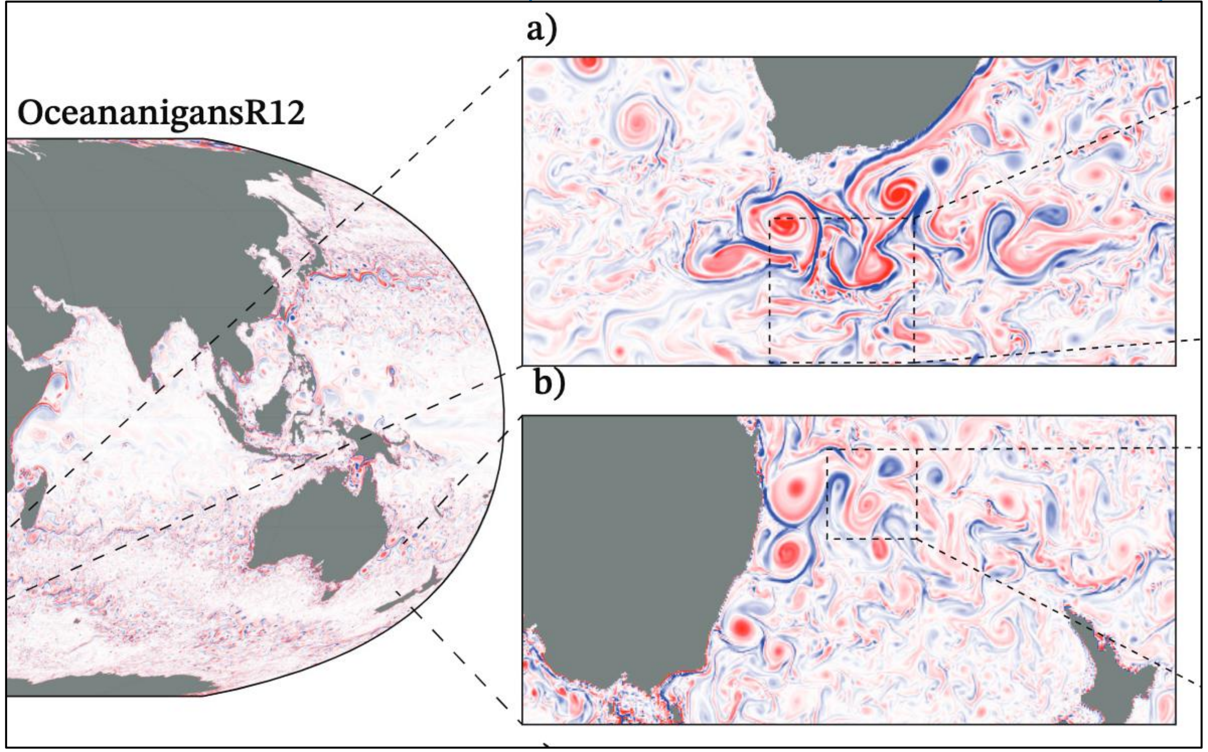
CliMA CLIMATE MODELING ALLIANCE

Oceananigans.jl

(Silvestri et al., arXiv, 2024)



Moses, Churavy, et al., SC'21



Three initial Earth system applications

DJ4Earth

Ocean

S. Williamson

J. Kump

N. Loose

Sea ice

S. Silvestri

G. Wagner

C. Hill

Ice sheets

M. Morlighem

C. Gong

- Bringing together concepts from …
  - … **big data science** & **sparse data science**
  - … **computer science** & **computational science**
  - … **scientific machine learning** & **simulation-based science**
- Sensitivity/gradient information is a powerful ingredient; obtained via
  - **differentiable programming**
  - **general-purpose automatic differentiation (AD)**

Ocean Predict

In partnership with

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Intergovernmental Oceanographic Commission

2021 2030 United Nations Decade of Ocean Science for Sustainable Development

SYMPOSIUM OP'24

ADVANCING OCEAN PREDICTION SCIENCE FOR SOCIETAL BENEFITS

Thank you!