

The Eviden logo is rendered in a white, stylized, outlined font. The letters are spaced out and have a modern, geometric feel. The background of the slide features a dark teal color with a large, abstract graphic on the right side consisting of several overlapping, concentric, rounded rectangular shapes that create a tunnel-like or spiral effect, receding towards the center.

CEPP AI4Sim

Leveraging AI for numerical simulation

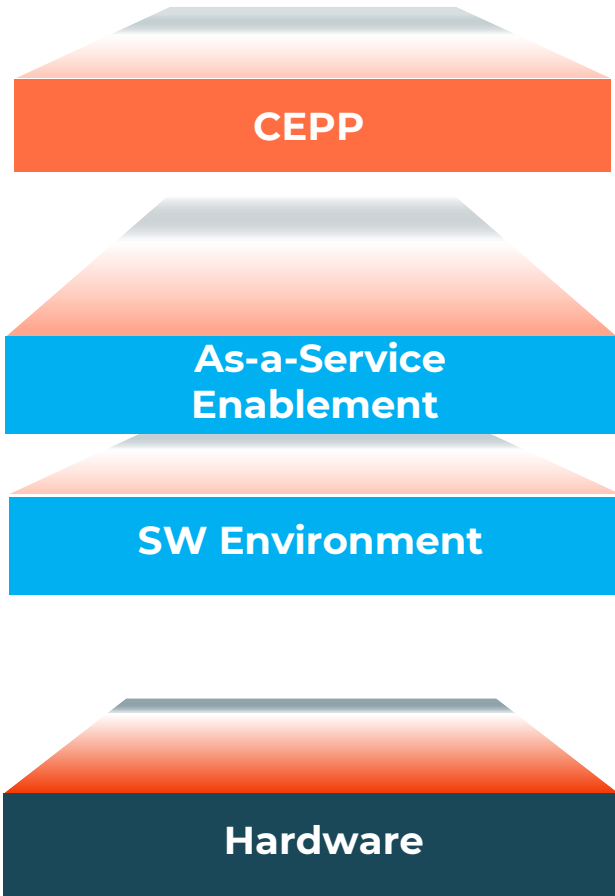
Mikaël Jacquemont
AI Technical Consultant
21/01/2026

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an atos business

Eviden CEPP – Center for Excellence in Performance Programming

Accelerate workload, give value to simulation!

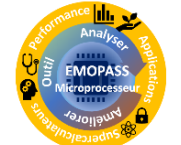


Institutions
 Science research funded projects where CEPP does HPC services & co-design

IT Partners
 Focus on key IT partners in HPC, AI & Quantum

Customers
 Taylor-made solutions on customer KEY applications and topics

R&D
 Co-design and co-creation between R&D for applications



CEPP AI4Sim

AI for numerical simulation

- Project-based activity
- Use cases focused
- Collaborative framework
 - Academic partners
- European projects
 - Public partners



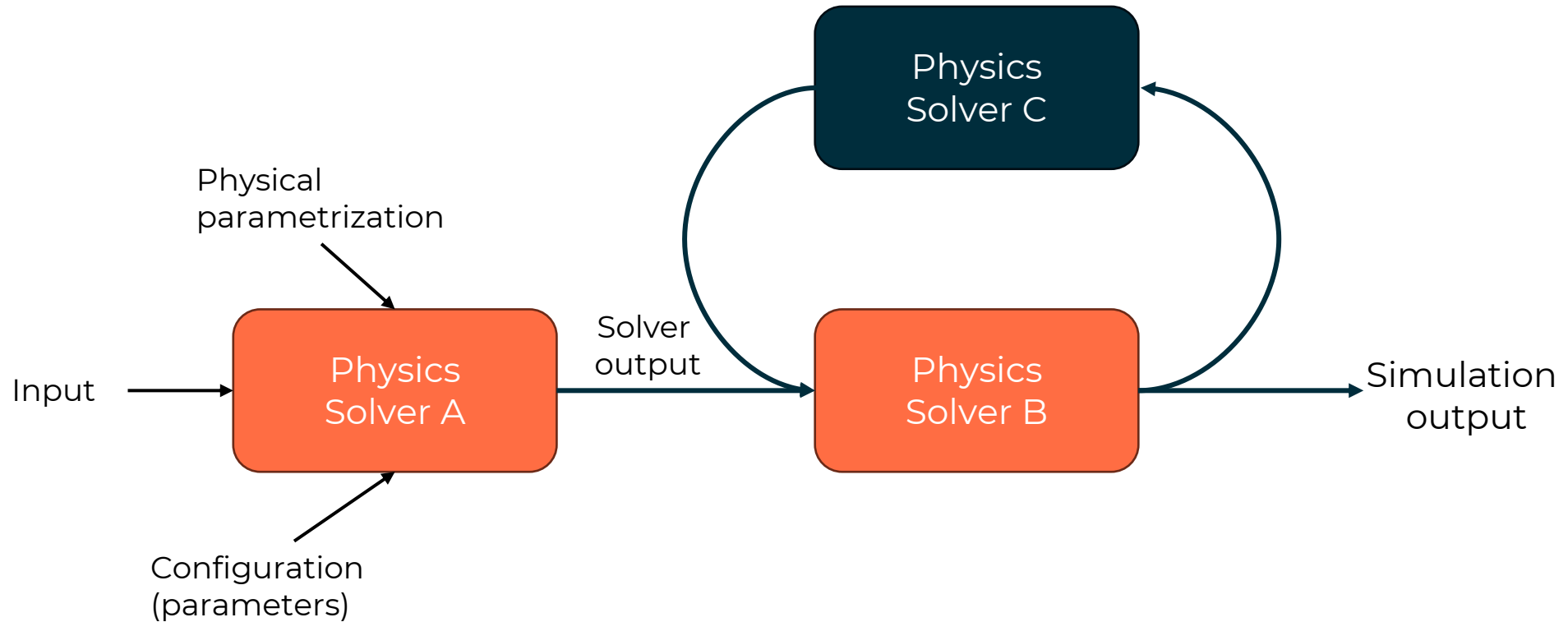
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AI for numerical simulation

CEPP AI4Sim

AI for numerical simulation

- Complex numerical simulation workflow

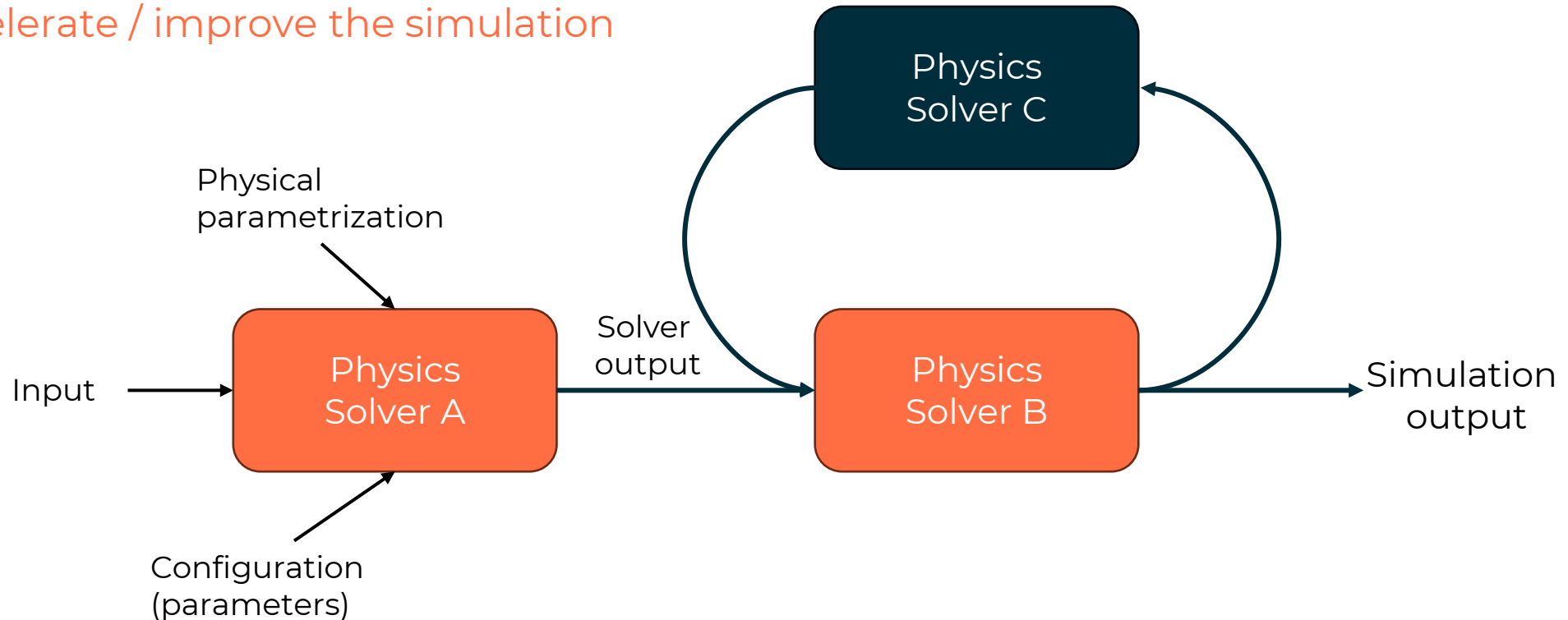


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AI for numerical simulation

- Complex numerical simulation workflow

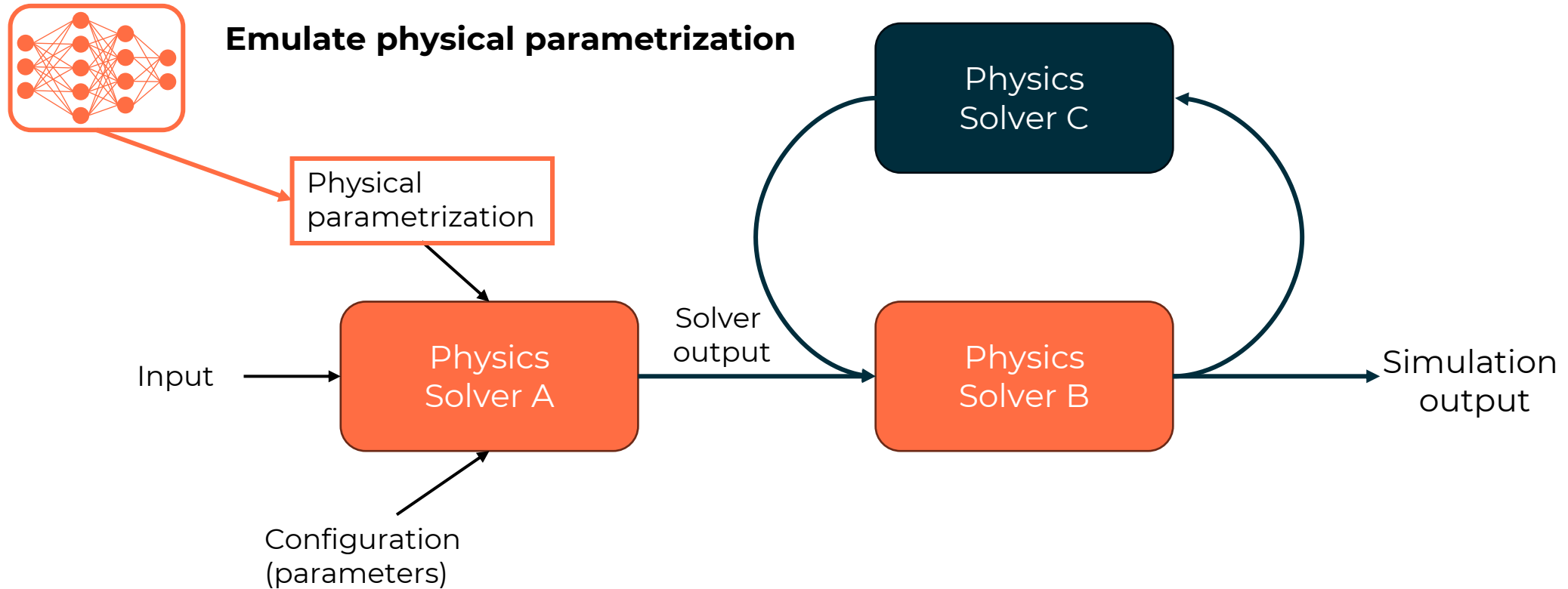
→ accelerate / improve the simulation



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AI for numerical simulation

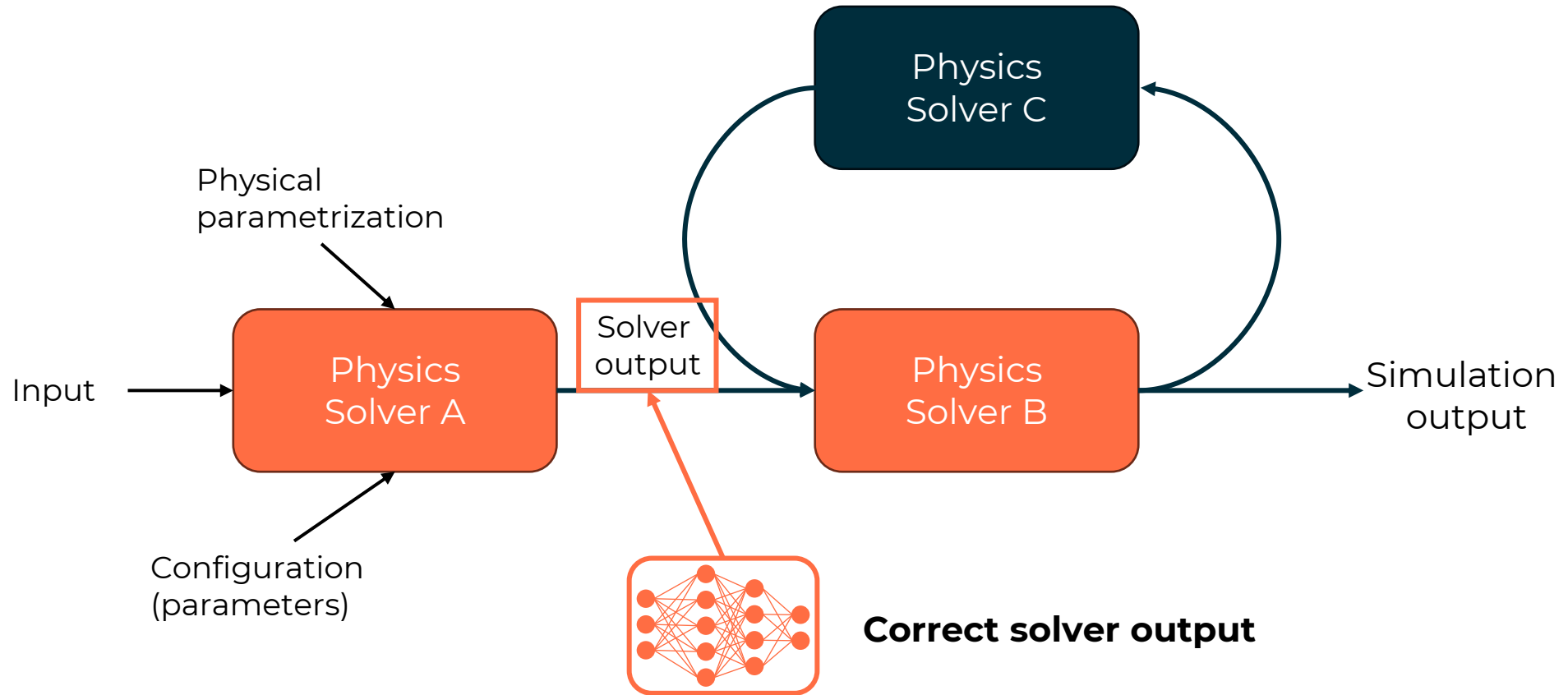
- Complex numerical simulation workflow



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AI for numerical simulation

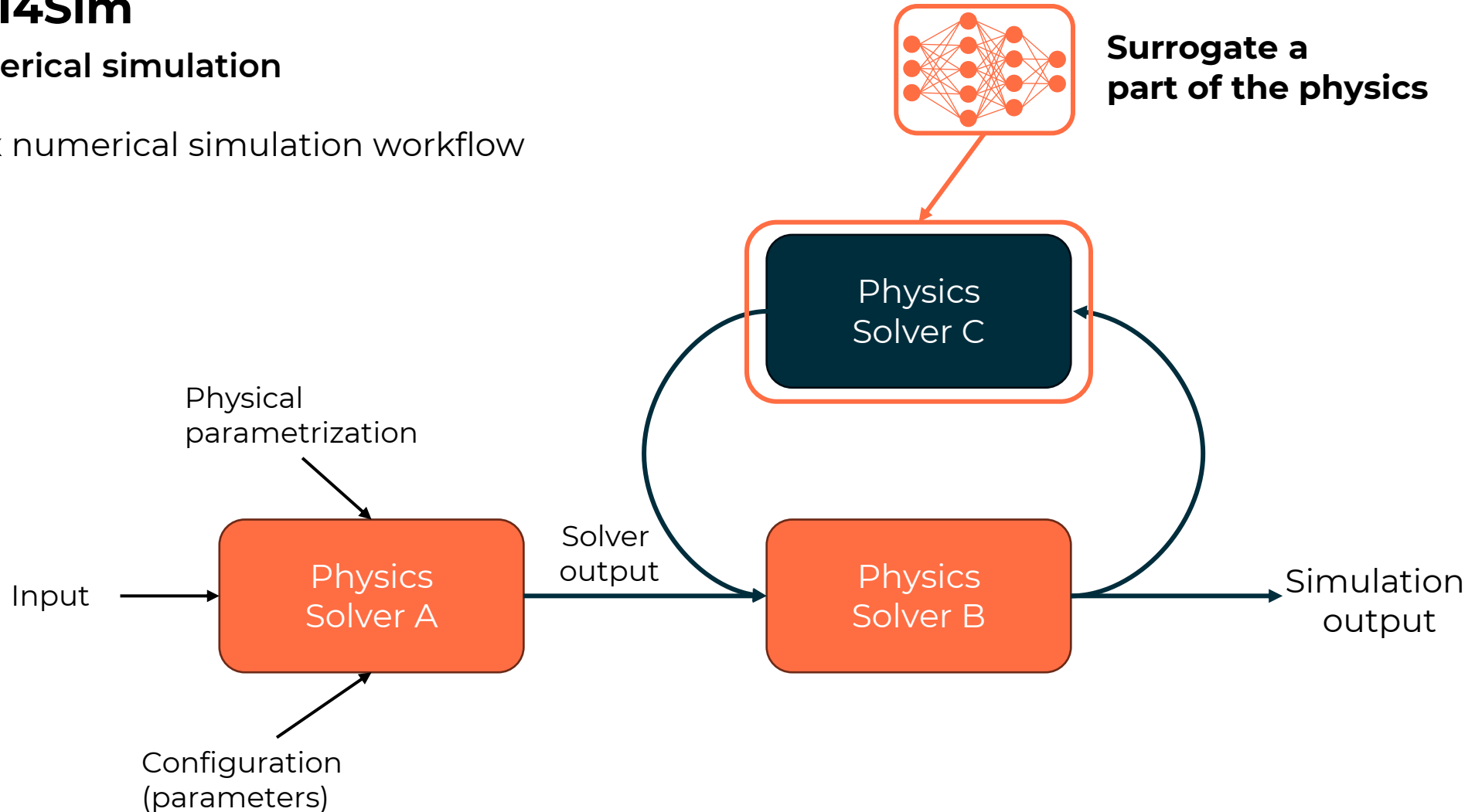
- Complex numerical simulation workflow



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AI for numerical simulation

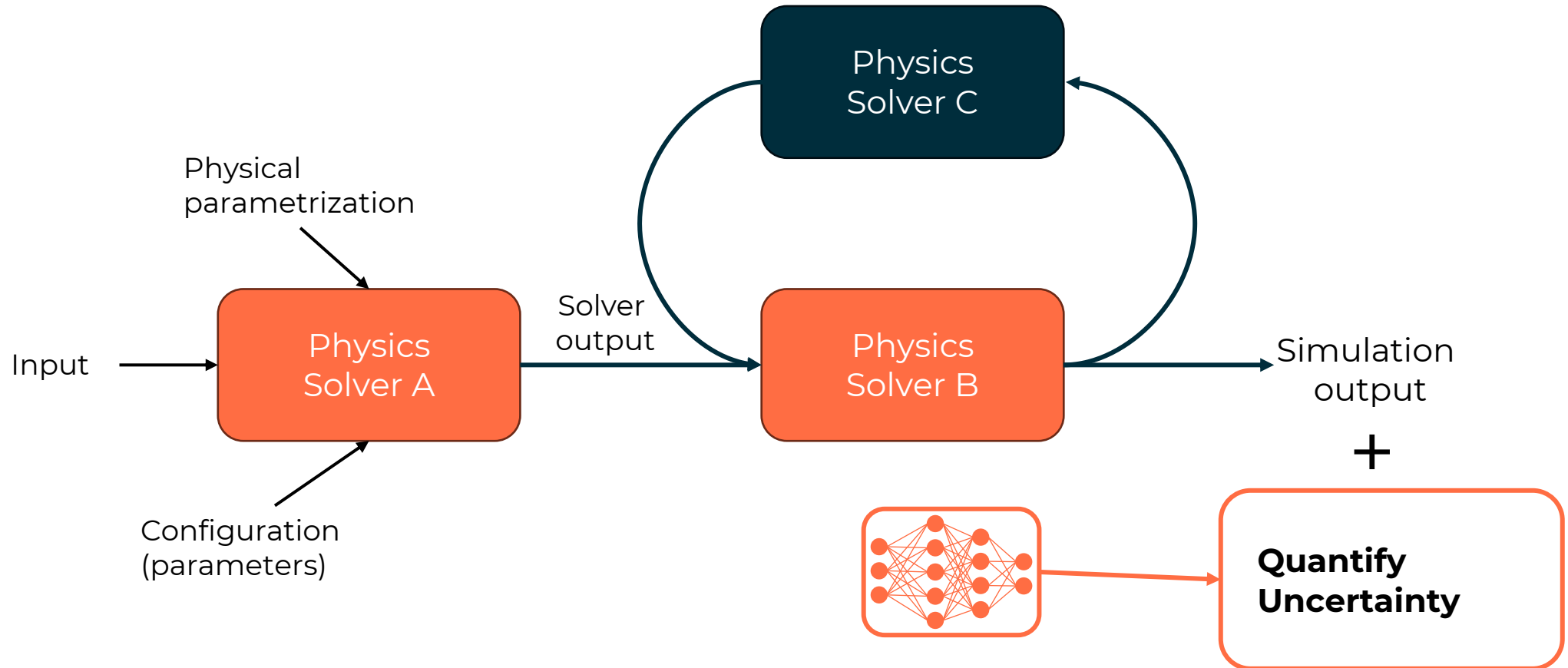
- Complex numerical simulation workflow



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AI for numerical simulation

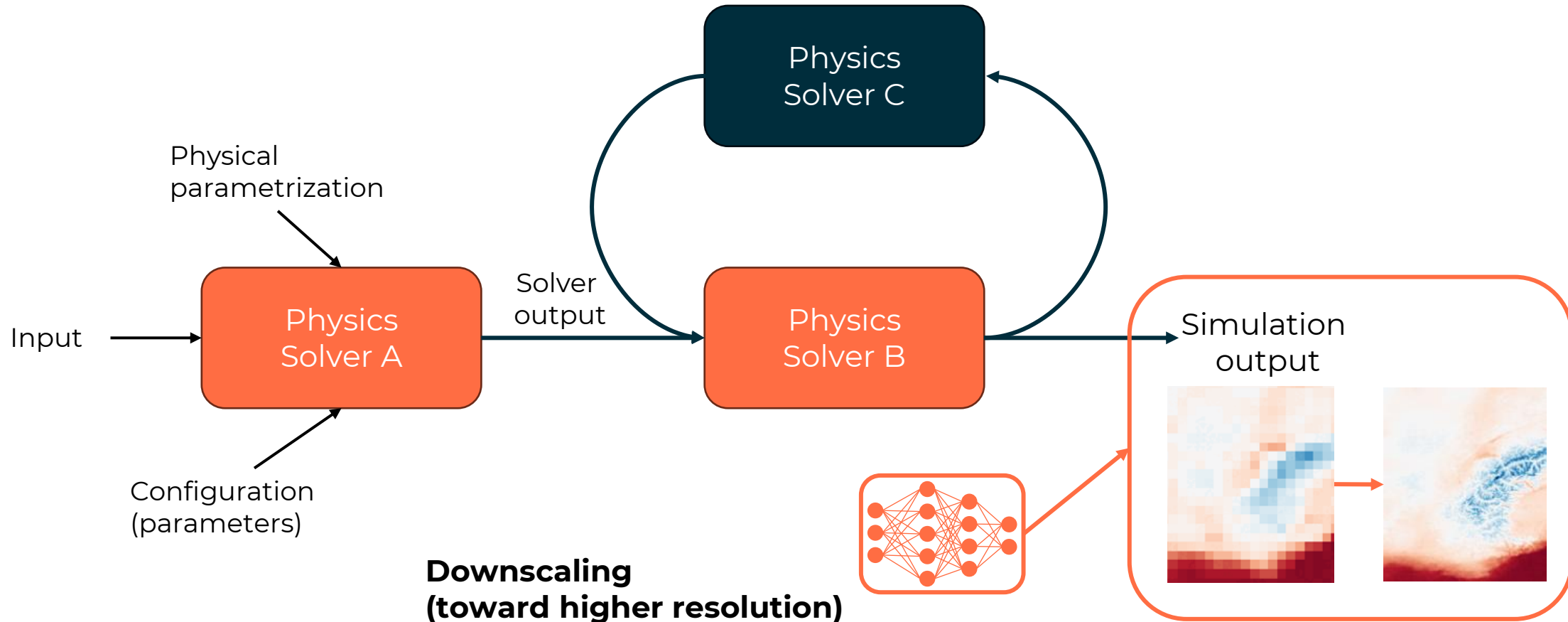
- Complex numerical simulation workflow



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AI for numerical simulation

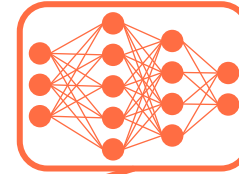
- Complex numerical simulation workflow



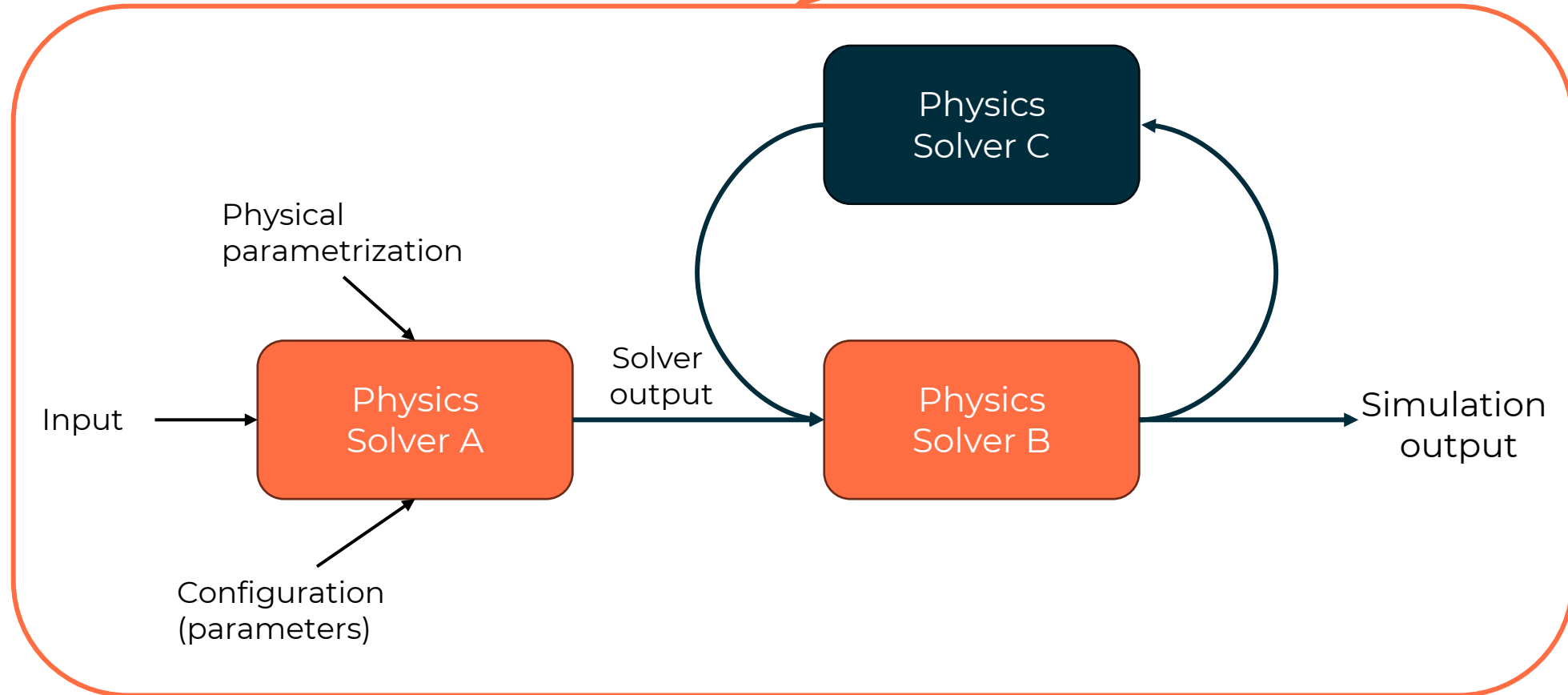
CEPP AI4Sim

AI for numerical simulation

- Complex numerical simulation workflow



Surrogate the full solver



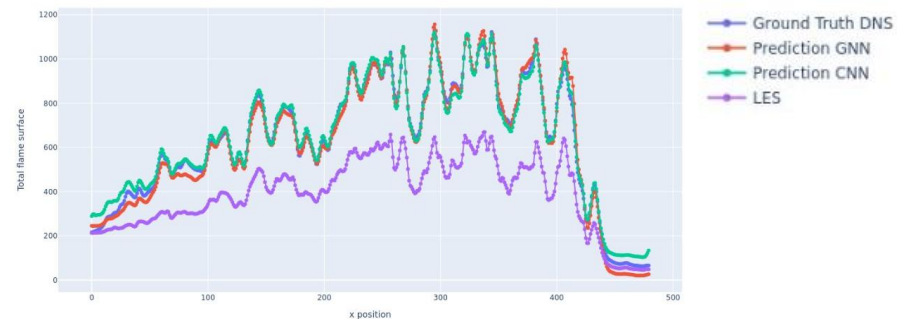
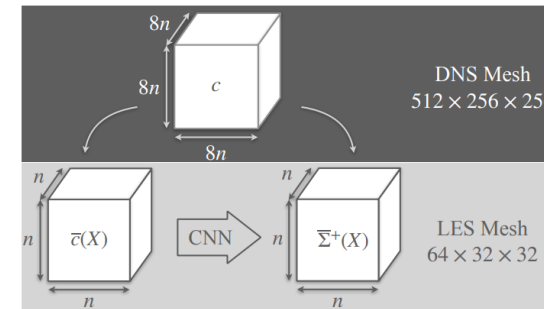
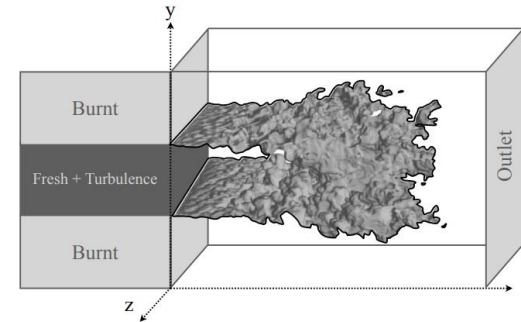
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CEPP AI4Sim projects

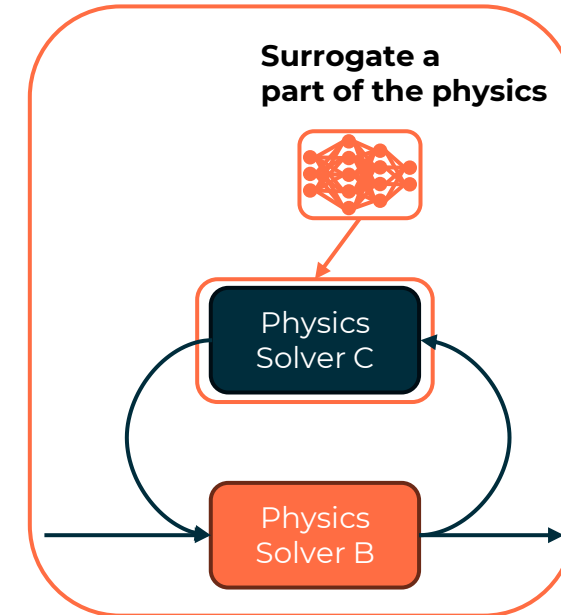
CEPP AI4Sim

Reactive flow: Surrogating sub-grid scale physics to improve LES-like simulations

- **Context:** RAISE H2020 European project
- **Problem:** Reactive flow simulation is challenging
 - It requires to resolve:
 - The fluid dynamics (CFD)
 - The chemistry (burnt/unburnt gas)
 - DNS + chemistry is **too costly** in practice
 - Reduced-order space (*LES-like*) simulations are challenging (chemistry)
- **Solution:** Use a NN to learn the flame surface density ($\bar{\Sigma}^+$) from a filtered progress variable (\bar{c})
- **Results**
 - GNN (tackles irregular grids)
 - 48% improved accuracy
 - 4 X faster than previous Sota CNN



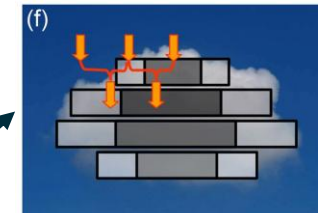
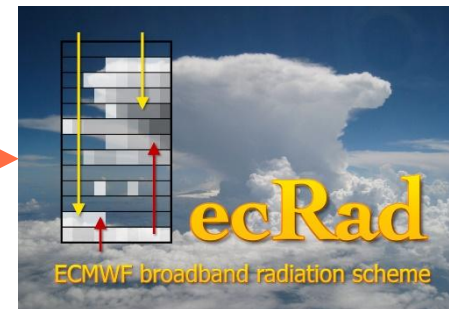
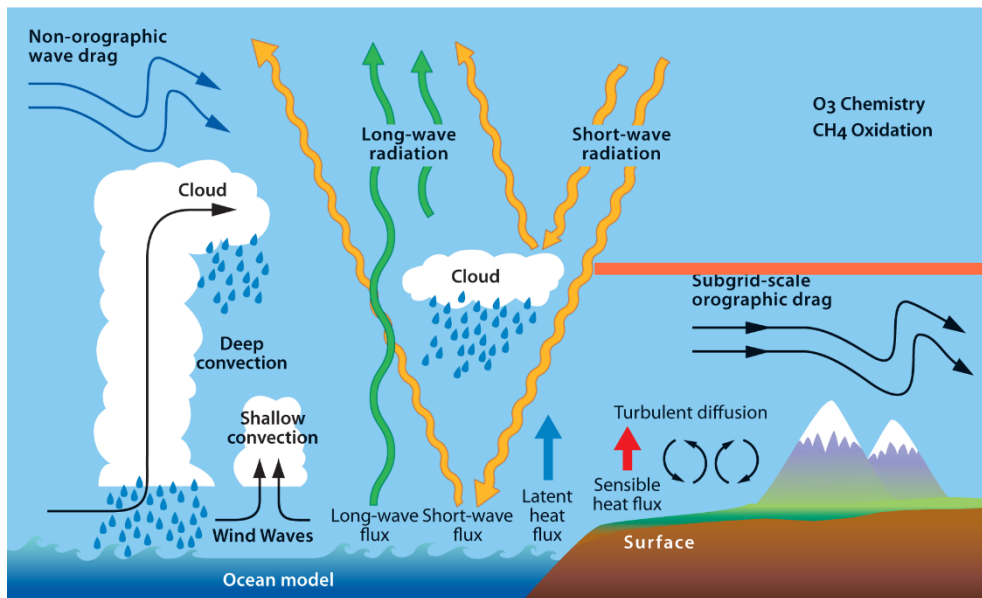
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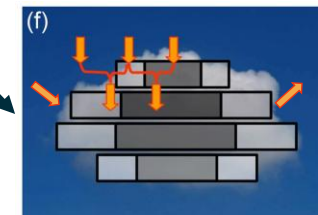
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Weather forecast: Enhancing the radiative scheme to reflect 3D cloud effect

- **Context:** Center of Excellence ECMWF - Eviden
- **Problem:** 3D cloud effect in the radiative scheme is too costly
 - IFS is composed of several solvers, including ecRad
 - Tripleclouds is used in production
 - SPARTACUS \approx Tripleclouds + 3D effect



Tripleclouds

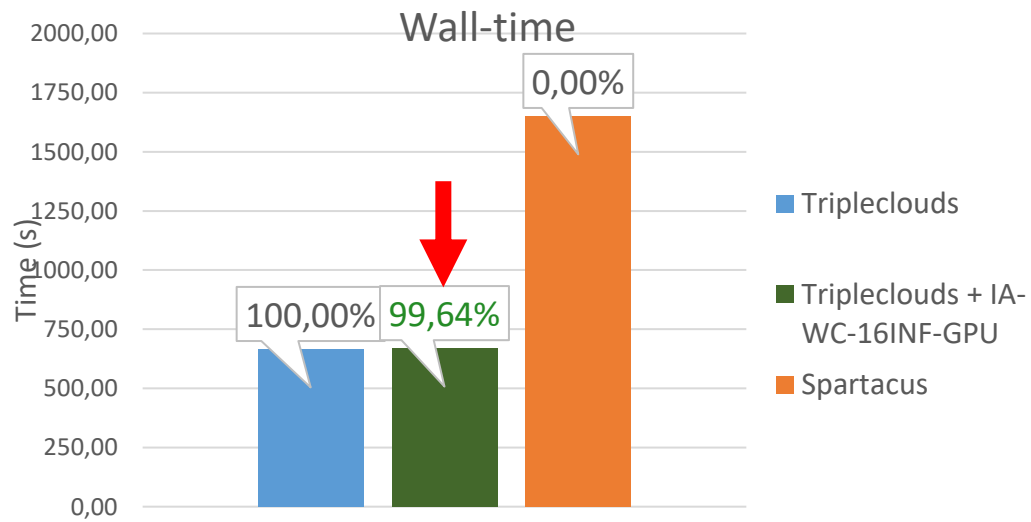
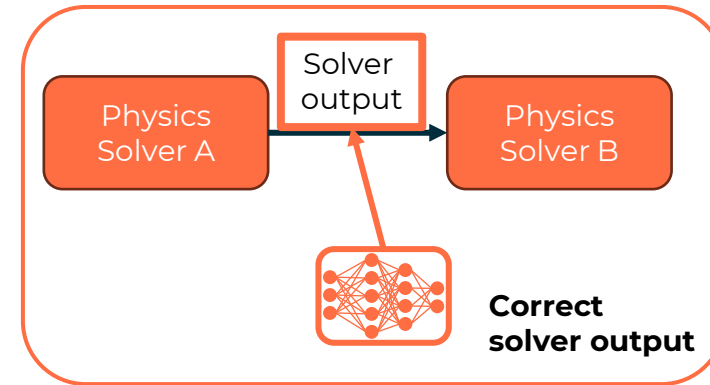


SPARTACUS
= Tripleclouds
+ 3D effects

CEPP AI4Sim

Weather forecast: Enhancing the radiative scheme to reflect 3D cloud effect

- **Solution:** Train NN to reduce the difference between the output of Tripleclouds and SPARTACUS
- **Results:**
 - RNN + coupling solutions
 - 97 % accuracy
 - A fraction of Spartacus running time

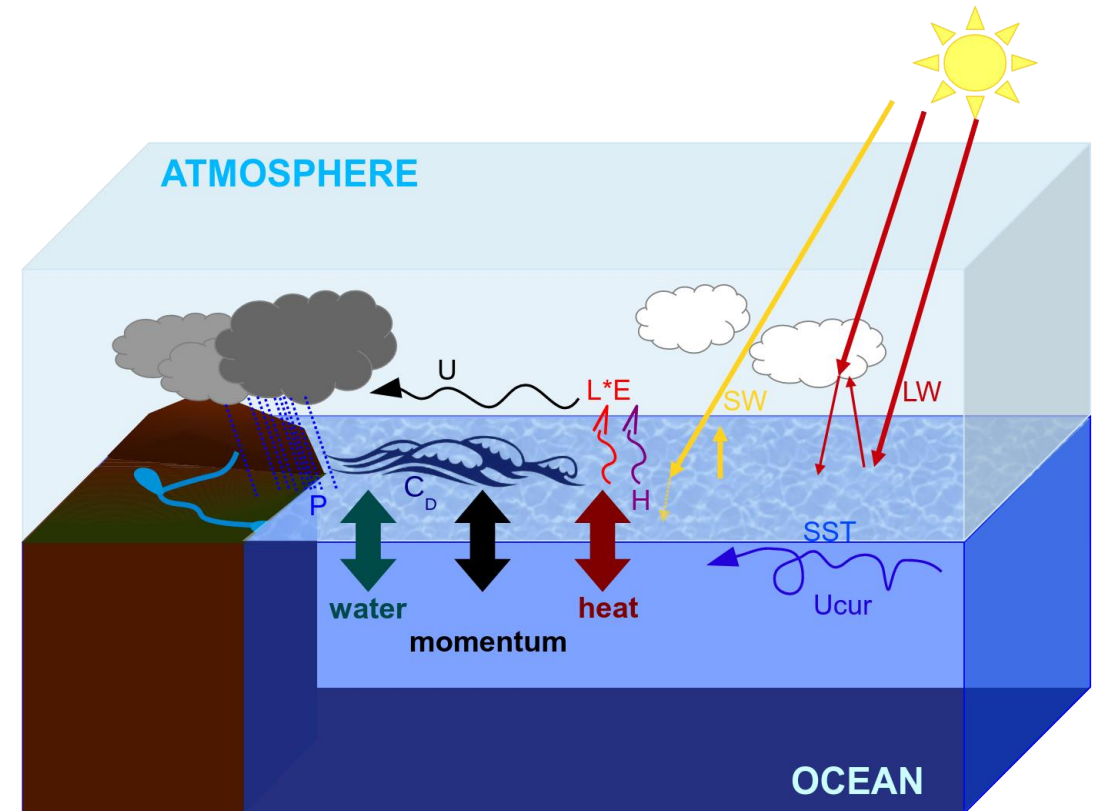


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Ocean-atmosphere interactions: Accelerating coupled simulations



- **Context:** Collaboration with AIRSea (Inria) and Shom
- **Problem:** High-quality ocean simulations require costly atmospheric ones
 - Atmospheric surface fluxes influence ocean dynamics and vice-versa
 - These exchanges are essential for realistic ocean modeling



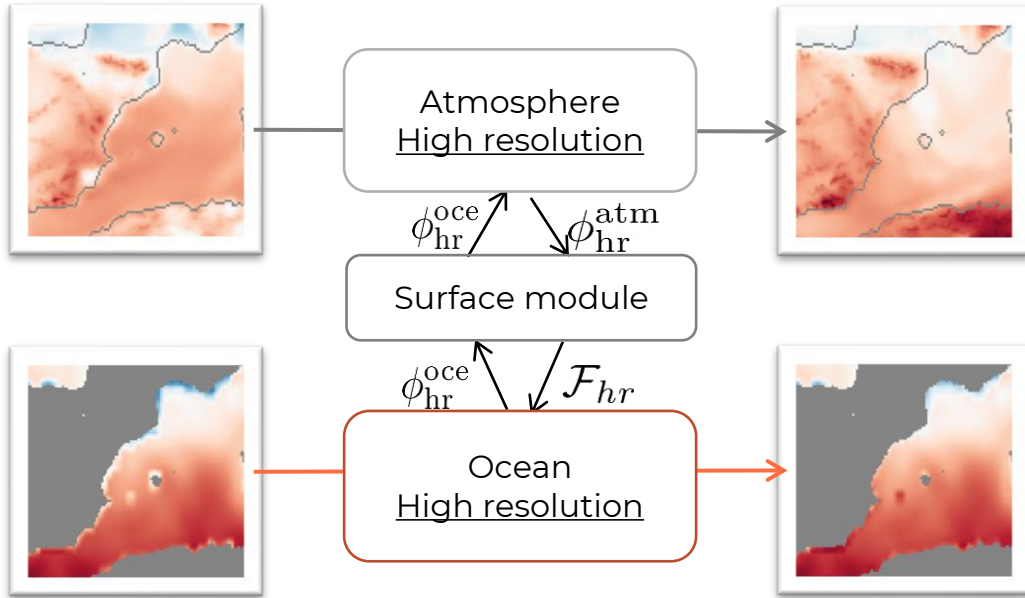
CEPP AI4Sim

Ocean-atmosphere interactions: Accelerating coupled simulations



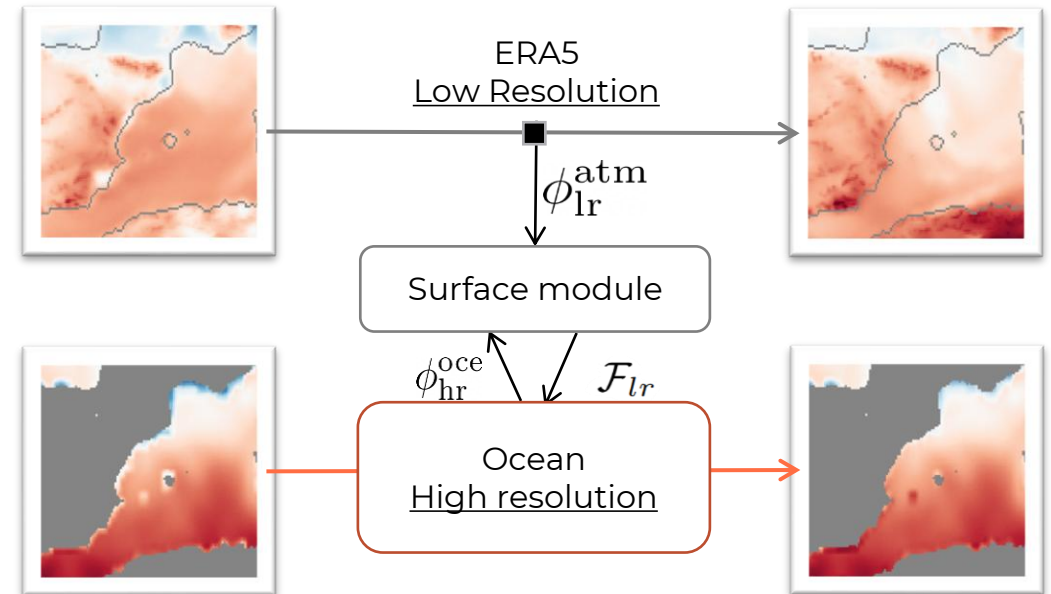
- **Problem:** High-quality ocean simulations require costly atmospheric ones
 - Currently, 2 strategies

Fully-Coupled Strategy



- ⊕ Best numerical accuracy
- ⊖ Resource greedy (2,9 kcpu.h for 6-day simulation)
- ⊖ Most of the atmospheric data is useless

Forced Strategy



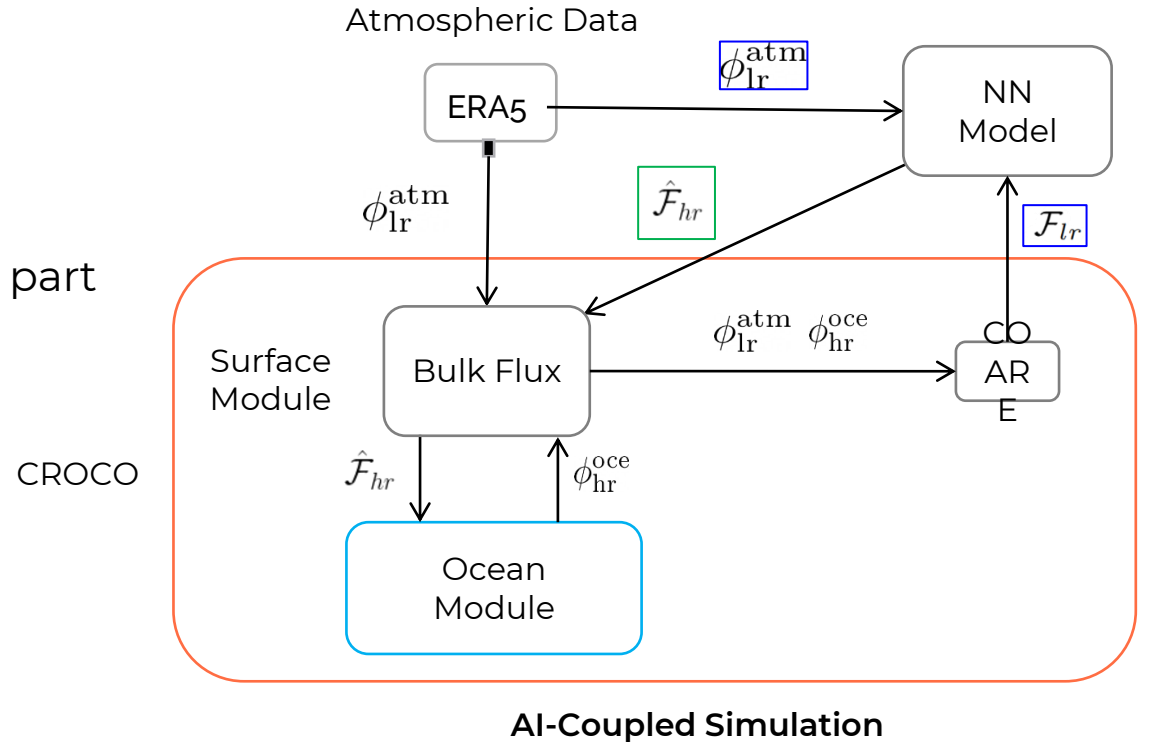
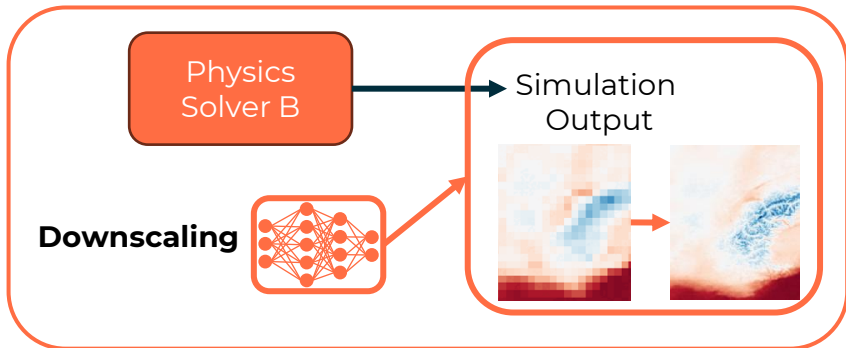
- ⊖ Poor numerical resolution impacting the model accuracy
- ⊕ Less resource required (88 cpu.h for 6-day simulation)

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Ocean-atmosphere interactions: Accelerating coupled simulations



- **Solution:** Train a NN to enhance the atmospheric data spatially and temporally
- **Results:** PhD running
 - Objectives
 - Physical results close to fully-coupled runs
 - Wall-time close to forced runs
 - Limited additional resources required to run the ML part

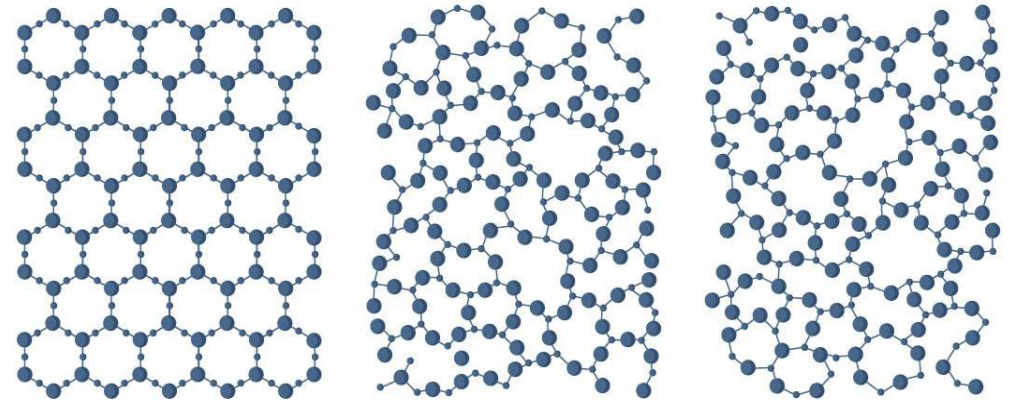


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Glass dynamics: Toward accurate and interpretable simulations



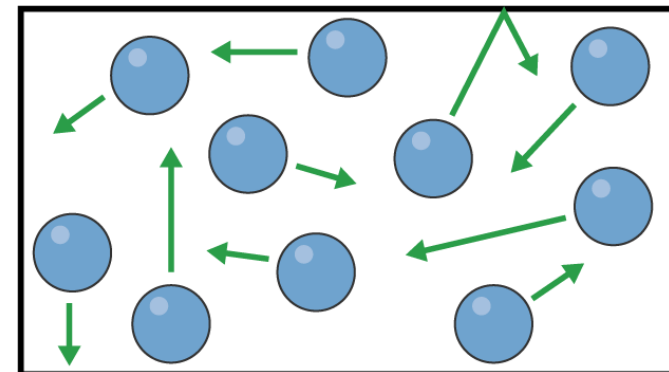
- **Context:** Collaboration with LIPhy
- **Problem:** Understanding glass dynamics is a long-standing challenge in physics
 - Glass has disordered molecules like liquid yet is rigid
 - Glass transition is very slow, and simulations are highly costly (even with 1k particles)
 - Simulations are accurate, but we lack knowledge about the origin of the transition
- **Solution:** Train a (quite) interpretable NN to predict glass particle mobility at different time steps
- **Results:**
 - SE(3)-equivariant GNN + attention
 - Explainability analysis



Crystal

Liquid

Glass

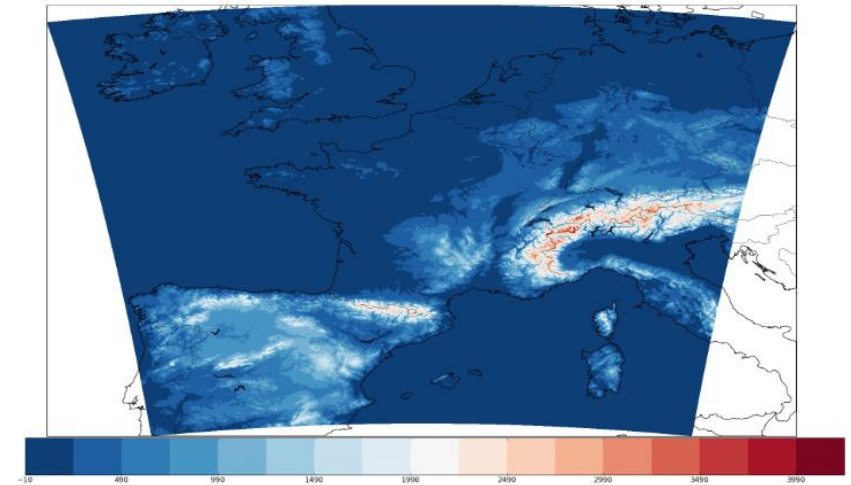


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Weather forecast: Emulating Arome ensemble with Machine Learning

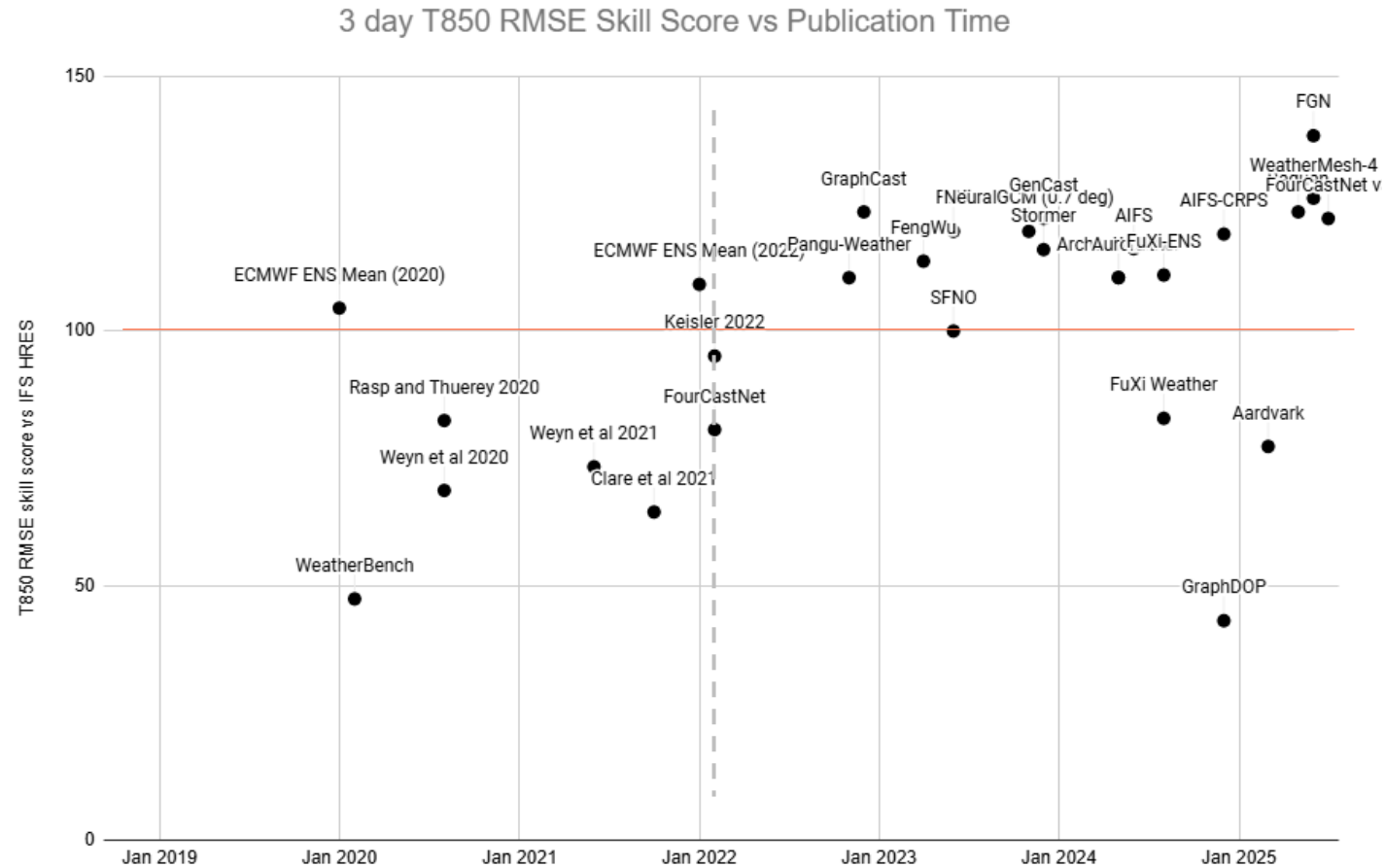


- **Context:** Collaboration with Météo France
- **Problem:** Weather forecast including uncertainty estimation is highly costly
 - Deterministic simulations are already costly e.g., 6 kcpu.h for 48-hour prediction, run every 3 hours
 - Uncertainty estimation is usually obtained with ensemble simulations
 - distribution prediction
 - Resource needed X members in the ensemble
 - Arome is a limited area model



CEPP AI4Sim

Weather forecast: Emulating Arome ensemble with Machine Learning



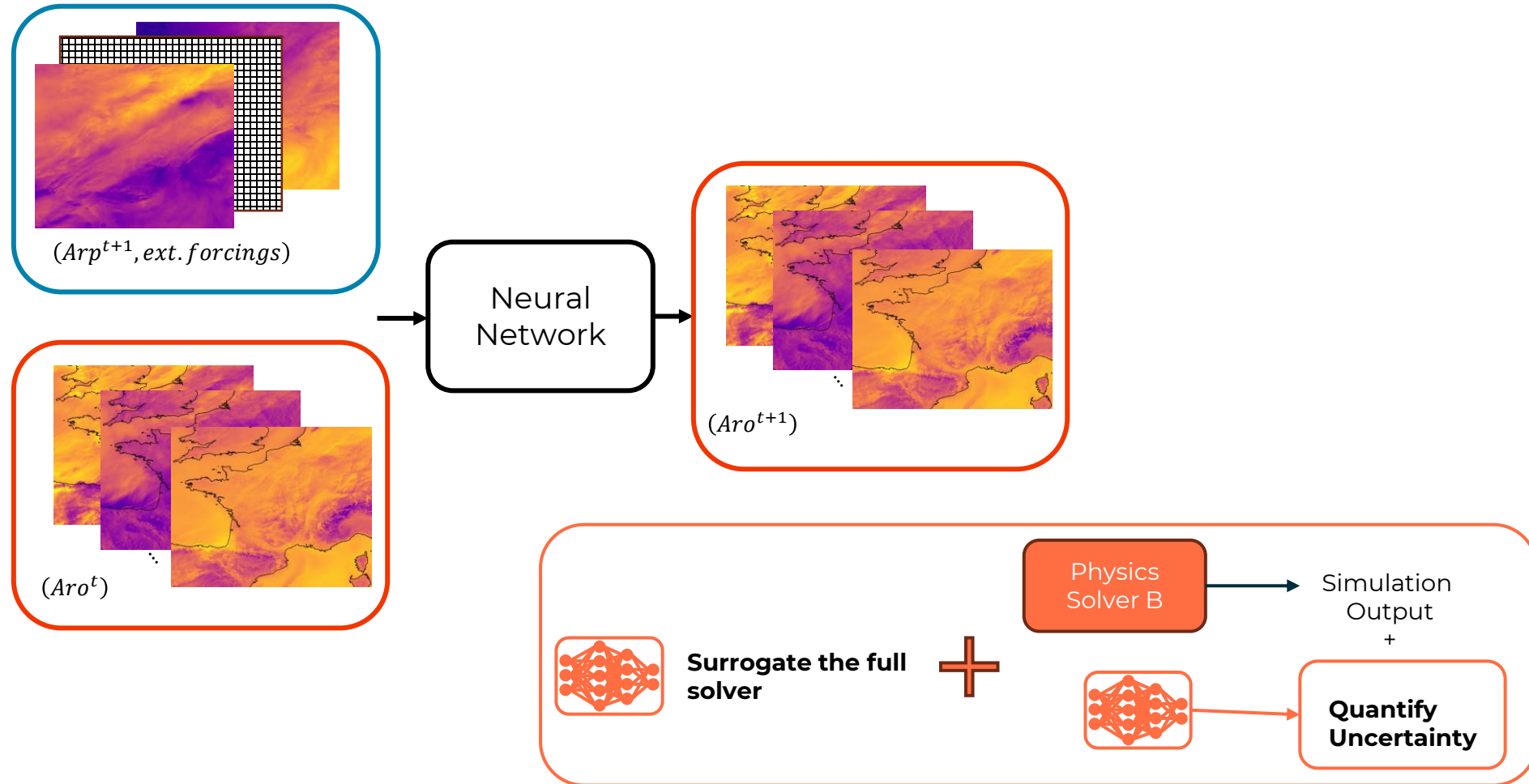
Rasp, Stephan (2024). AI-Weather SotA vs Time. figshare. Dataset. <https://doi.org/10.6084/m9.figshare.28083515.v1>

CEPP AI4Sim

Weather forecast: Emulating Arome ensemble with Machine Learning



- **Solution:** Train a NN to directly predict distribution for each variable
- **Results:** PhD running



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Thank you!

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<https://github.com/AI4SIM/model-collection>

