

CEPP AI4Sim Accelerate and improve numerical solvers with AI

Artificial Intelligence (AI) has spread into numerous domains, including computer vision, natural language processing, and more. Nowadays, AI has even ventured into the world of numerical simulations, offering invaluable assistance in tackling complex mathematical and physical challenges that traditional numerical solvers find daunting.

Al plays a multifaceted role in this context, from emulating parts of the physics within solvers and refining closure models to correcting solver biases, emulating parametrization, and quantifying uncertainties.



Key technological challenges

- Harnessing the power of AI for numerical simulations demands significant computational, storage, and networking resources. Training neural networks require vast volumes of data, and even when distributed across multiple nodes in an AI-ready High-Performance Computing (HPC) environment, it can last days, depending on data volume.
- After the training phase, a critical step is to combine the numerical solver and the neural network for inference, involving data transfer between both models. There is a possibility of network bottlenecks if the solver and the AI model are located on different computing nodes. In such cases, it is vital to have a robust coupling solution at the application level to connect the numerical solver and AI components and avoid any potential issues.
- To speed up training and inference phases, specialized processors like GPUs, TPUs, and IPUs are now integral parts of HPC, resulting in heterogeneous infrastructures. These powerful computational resources must be seamlessly interconnected with high-speed network infrastructure to fully leverage their potential for neural networks.

The integration of AI into numerical solvers can accelerate simulations while maintaining or even improving the level of detail during production. This makes AI a crucial asset for achieving Exascale and beyond in simulations.

The CEPP (Center for Excellence in Performing Programming) helps organizations worldwide tackle industrial and scientific challenges by leveraging the value of massive data. By combining deep HPC (High-Performance Computing) expertise, data sciences, and profound industry knowledge, **CEPP** accelerates HPC simulation, optimizes cluster performance and operation, and reduces cost-to-innovation. With a modular and flexible service offering, CEPP can customize its service to adapt to your goals with training, workshops, webinars, or dedicated resources for your specific project.



Eviden is at the forefront of HPC, providing teams with cuttingedge resources for exploring AI in numerical simulations to improve solver performance for customers. Eviden is a global leader in the HPC market and delivers the industry's most advanced and comprehensive HPC portfolio, including AI-HPC ready infrastucture.

Eviden experts and researchers are actively delving into the use of AI across various domains, including Computational Fluid Dynamics (CFD), weather forecasting, life sciences, and more. These skills are at our client's disposal, empowering them to enhance the precision and efficiency of their numerical simulations.

AI Evaluation Program:

Objective:	Evaluate the potential
Audience:	Businesses seeking an evaluation to accelerate or make a more accurate numerical solver using Al
Participants' prerequisite knowledge:	Field of expertise
Technical prerequisite:	Client's data

An Eviden data scientist will work together with the subject matter expert from the customer and use data from their numerical solver to evaluate how AI can improve it. They will explore a variety of potential enhancements, starting with the most straightforward solutions and moving on to more complex ones. Together, they will discuss and analyze the options for improving the numerical solver.

Objective	Description	Prerequisite
Correct bias from a solver:	Correct the output of a numerical solver with the output of an Al model trained on a more accurate numerical solver	Differentiate data between the existing numerical solver and an accurate numerical solver simulating the same phenomena with the same parametrization
Emulate parametrization:	Emulate a side numerical solver	Input and output data of the side solver
Surrogate a part of the physic in the numerical solver:	Surrogate a part of the kernel of the numerical solver	Input and output data related to the kernel of the numerical solver to replace
Create closure models (only for CFD):	AI can be used to create accurate closure models	Data from an accurate simulation (DNS)
Quantify uncertainties:	AI can be used to take into account the uncertainties at the different steps of the simulation in order to evaluate the confidence of the results	Need to be discussed with the experts
surrogate a complete numerical solver:	Replace the complete numerical solver with an Al model	Input and output data of the complete numerical solver

Al expertise program

Objective:	Provide AI expertise to the customer
Audience:	To end users with a need to improve the performance of a numerical simulation using AI (surrogate a part of the physic in a solver, create more precise closure models, correct bias from a solver, emulate parametrization, quantify uncertainties)
Participants' prerequisite knowledge:	Expertise in the targeted numerical solver
Technical prerequisite:	Client's data

Co-development

Co-development is a common practice in today's business world. We aim to create a remote task force of customer and Eviden experts who will work together to tackle a specific challenge. Our team will provide one or two experts who will closely collaborate with the customer's team for several weeks to find a solution.





Ask a Data Scientist

Creating an AI model for numerical simulations requires a deep understanding of the physics underlying the numerical solver.

The collaboration between Eviden's data science experts and a subject matter expert from the customer will drive the co-development of an AI solution, which will subsequently be seamlessly integrated into the numerical solver.

In established domains, AI models are typically developed following these steps:

Step

Initial assessment of the potential: This involves discussions between our data scientists and the client, a thorough understanding of the numerical solver's limitations, and exploring the potential for enhancement through AI.



Data analysis and architectural design: We conduct an in-depth analysis of the client's data and propose a suitable neural network architecture (such as CNN, GNN, Unet, etc.).

Step 3

Tailoring and meticulous refinement: We proceed with training and fine-tuning the neural network to achieve optimal performance. If the domain is not yet known from our data scientists, the "data analysis and architecture definition" step might be longer due to a need to step up on this new domain. The integration of the AI model with the numerical solver is up to the client.

" Eviden provided seamless AI and technical work, critical for bringing AI into the complex workflow of weather forecasting "



Matthew Chantry

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