PAIRS: Physics-Enabled AI for Real-Time Simulations Surrogates

Zeinab Alfaytarouni[1] and Hamza Ben Ammar[1]

[1]Capgemini Engineering (France)

Contact email: zeinab.alfaytarouni@capgemini.com

hamza.ben-ammar @capgemini.com

Dr. Zeinab Alfaytarouni

zeinab.alfaytarouni@capgemini.com

Dr. Hamza Ben-Ammar

hamza.ben-ammar@capgemini.com

Zeinab Alfaytarouni received a Master’s degree in Medical Physics from the Lebanese University in 2019, followed by a Ph.D. in Physics from the University of Strasbourg in 2023. Throughout this academic journey, she developed expertise in deep learning and simulation technologies. She currently works at Capgemini Engineering as a Scientific Expert on the RT-SIM (Real-Time Simulation) internal research project. Her work focuses on developing tools that assist engineers in designing and managing the lifecycle of surrogate models, based on both artificial intelligence and physical principles, to replace complex simulation models.

Hamza Ben-Ammar obtained in March 2019 his doctoral degree after defending his Ph.D entitled "On Models for Performance Evaluation and Cache Resources Placement in Multi-Cache Networks". In May 2019, he started at L3i laboratory a post-doctoral fellowship to work on resource-adaptive IoT service placement on the 5G edge. In January 2022, he joined Orange Innovation to work on topologies aggregations for large scale virtual networks infrastructure. Since September 2023, he works at Capgemini Engineering and is currently a Scientific Expert in the R&I project RT-SIM, which aims to create assets and tools to develop simulation infrastructure templates for diverse applications. His research interests are mostly in the area of networking and distributed systems and especially on future Internet architectures, network resources management, modeling and simulation, etc.

RT-SIM: Generic Real-Time Simulation Platform

Motivation : **Can we develop common simulation infrastructure templates for diverse applications?**

The internal research project RT-SIM at Capgemini Engineering develops assets and tools to realise this objective keeping in mind different sectors such as aerospace, orbital vehicles, rail transportation, etc.

Current Focus Areas :

- Development of a space simulator
- Development of an avionics simulator
- Accelerating and facilitating the development of hybrid AI-based surrogate models to replace complex, time consuming simulations.

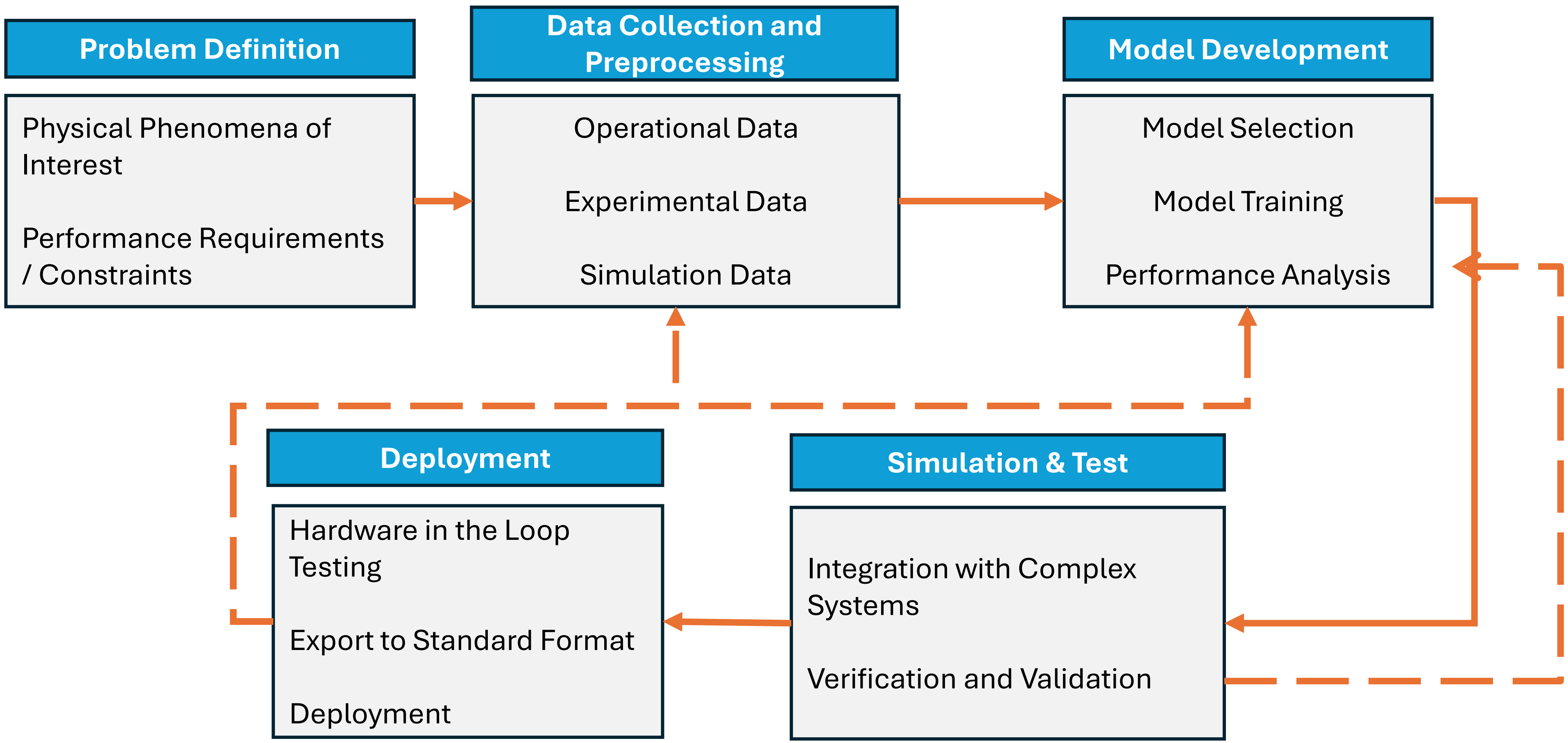
Physics-Enabled AI simulations Surrogates

Why use AI surrogate models to replace simulations of multi-physics/engineering systems?

Simulations of multi-physics / engineering systems	AI based Surrogate Models
Time and resource consuming	Efficiency and Reduced Computational Load
Accurate but often inflexible	Offers a good balance of accuracy and flexibility
Challenging in situations where the underlying physics is poorly understood	Particularly useful in situations where the underlying physics is poorly understood or complex
High-fidelity models are too slow for real-time	Fast enough for real-time simulations

- Physics-Enabled AI : A Hybrid Solution
  - It combines AI speed with physical laws, enhancing their accuracy, generalization and interpretability, while also reducing data requirements.

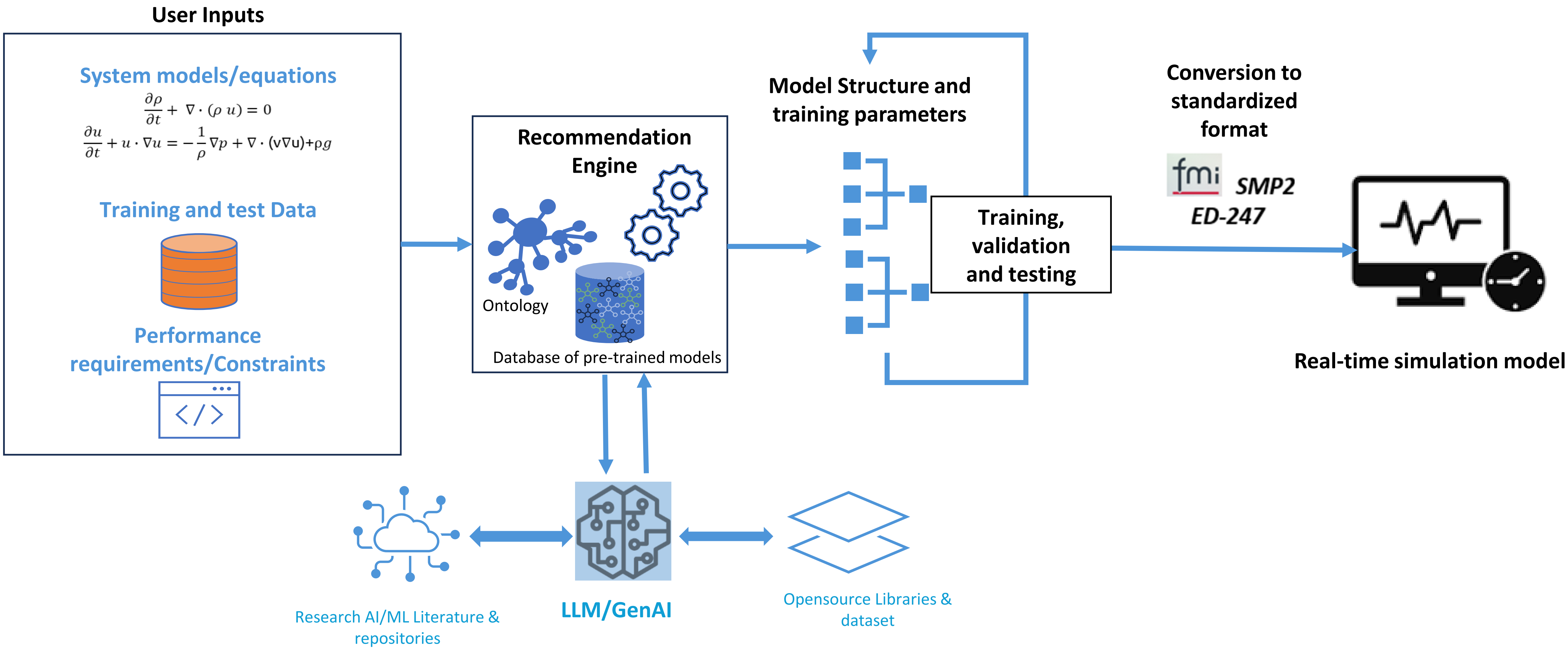
Process of developing surrogate models



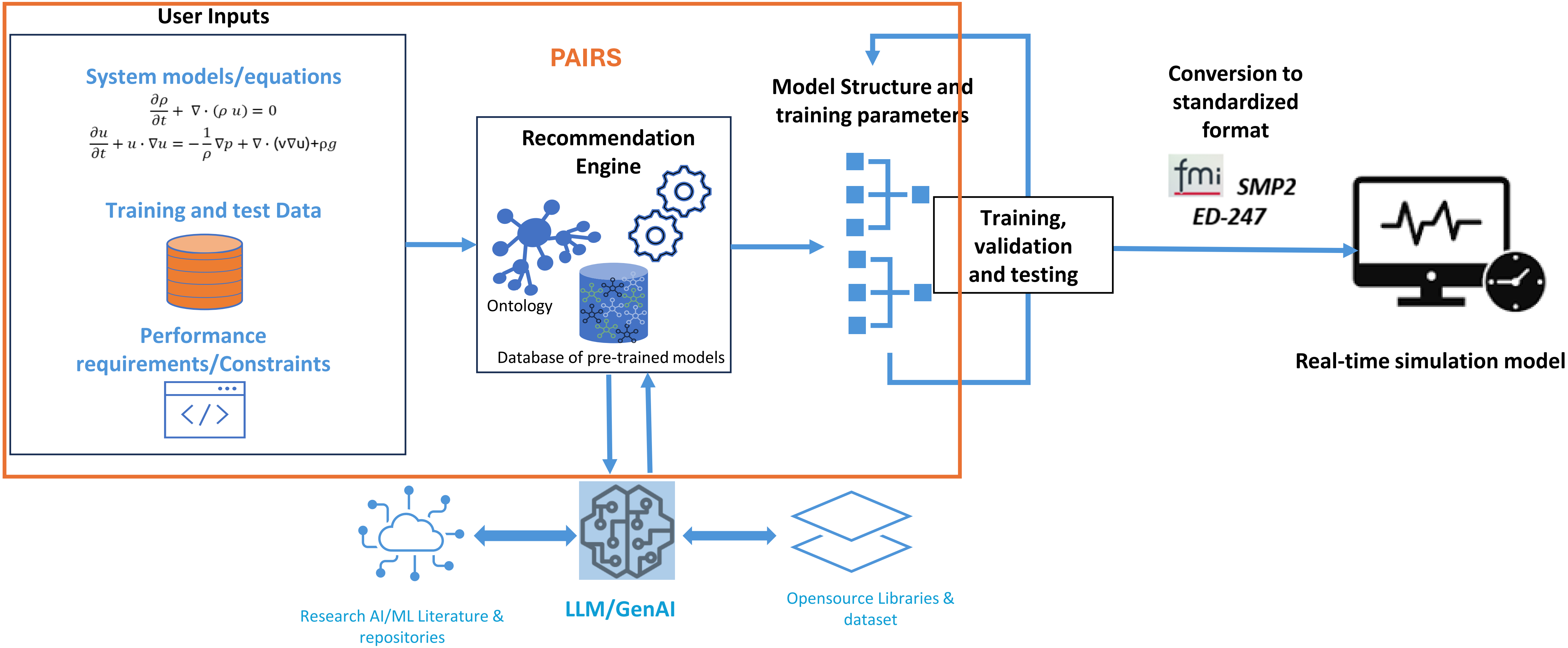
Developing surrogate models is a complex, time-consuming and effort-intensive process that necessitates collaboration among multidisciplinary teams

- Need for a tool that can help streamline this process and continuously update itself

Proposed Workflow for Managing the Lifecycle of Surrogate Models in Complex Simulations



Focus of This Presentation : PAIRS “Physics-Enabled AI for Real-Time Simulations Surrogates”

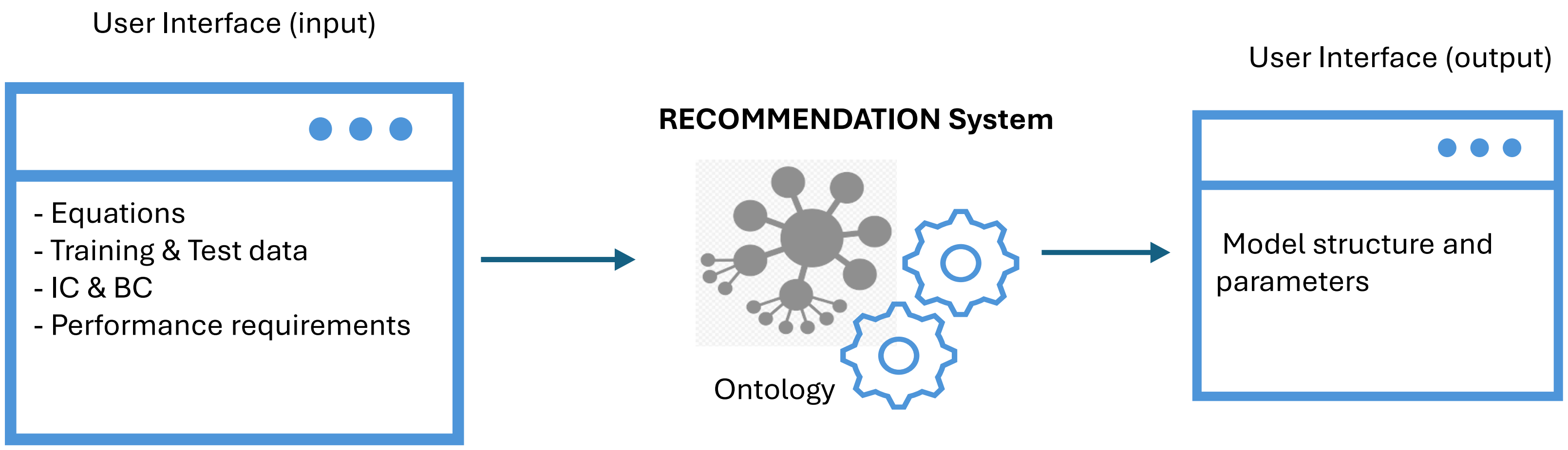


Selecting the Right AI Model for Surrogate Simulation of Complex Engineering Systems

Challenge : Choosing the optimal neural network architecture and parameters is difficult due to the multitude of available options.

Solution : A recommendation system powered by an Ontology that connects:

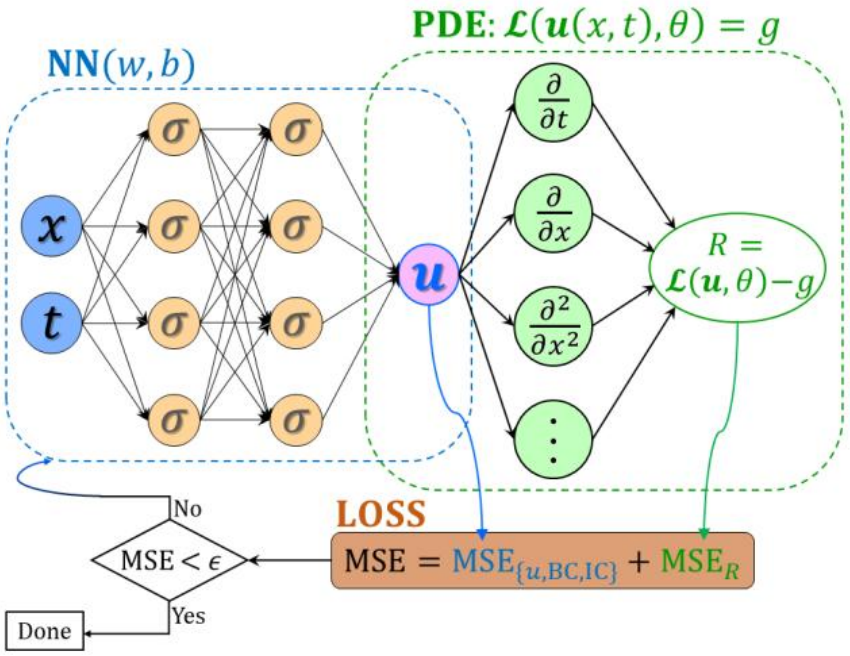
- Physics-Informed Neural Network architectures
- Specific tasks or requirements
- Data types and characteristics



Ontology of Physics-Informed Neural Networks

Physics-Informed Neural Networks (PINNs):

- Embed physical laws (e.g., PDEs) into the training process to ensure physically consistent predictions.
- Require less data and remain robust even when data is noisy or incomplete.

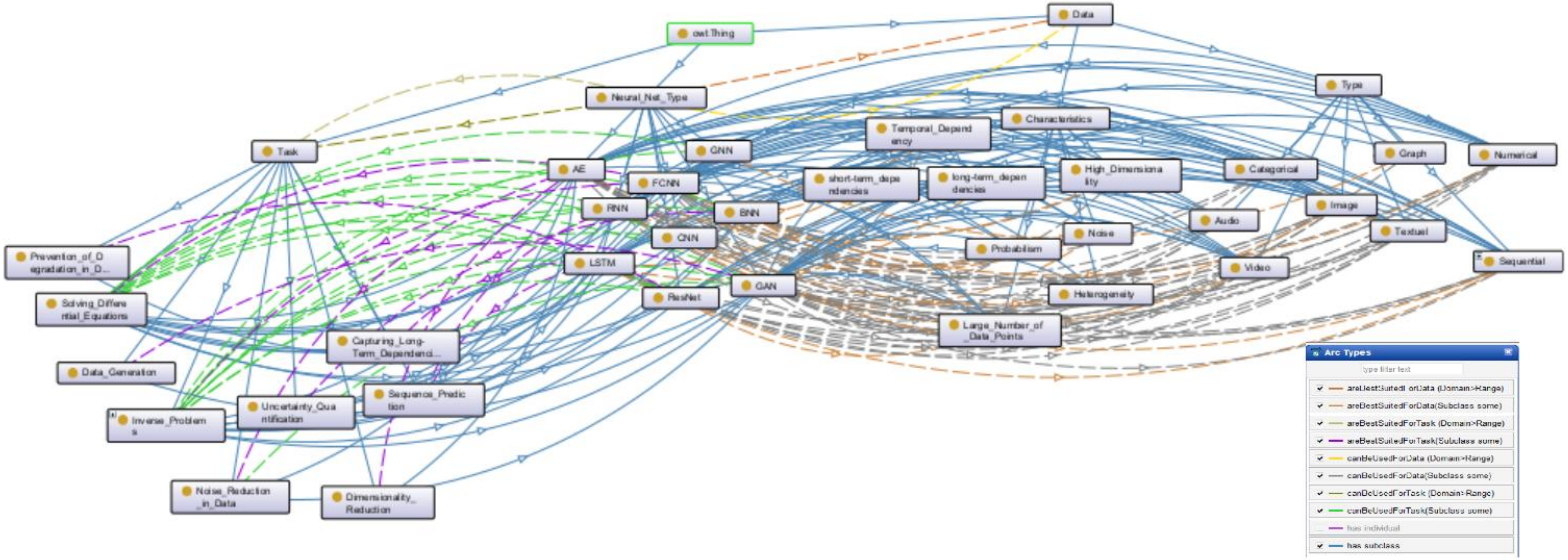


Structure of PINNs:

- A Neural Network
- A Physics-Informed Module
- An Optimization Module

Ontology of PINNs

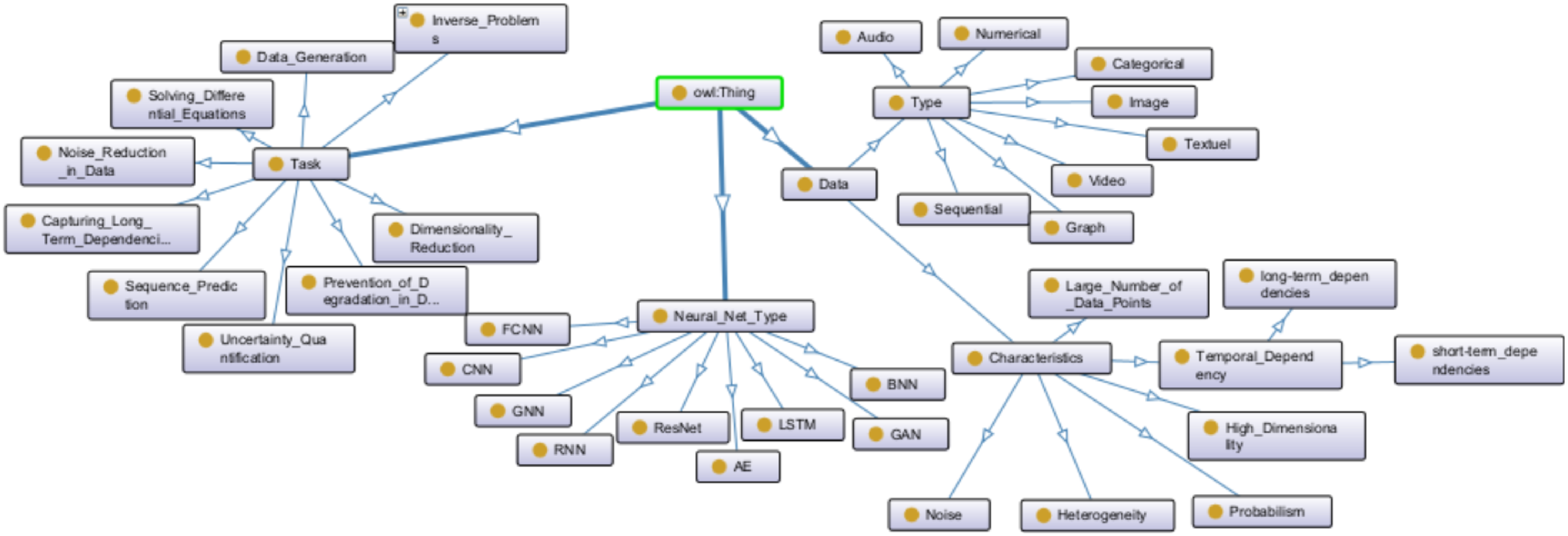
- The ontology is developed using the Protégé open-source ontology editor.
- This ontology reduces exploration time and facilitates model selection by guiding users toward suitable neural network configurations.



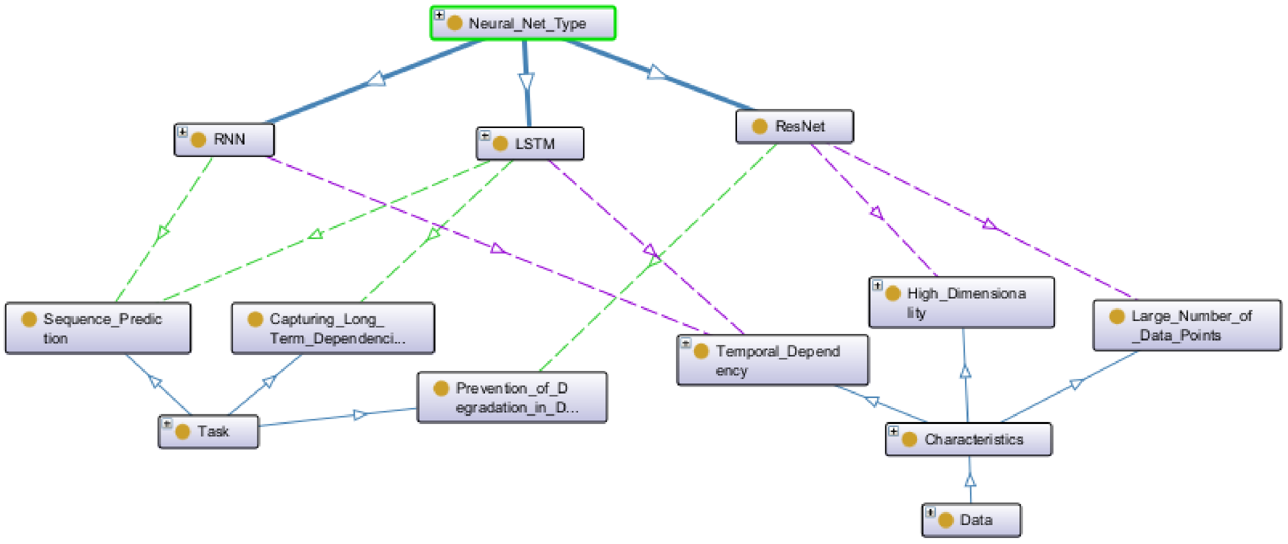
Ontology of PINNs Visualized with OntoGraph

Ontology of PINNs

Ontology class diagram generated with OntoGraf, showing the main concepts: Data Types and Characteristics, Tasks, and Neural Network Types, along with their respective subclasses.

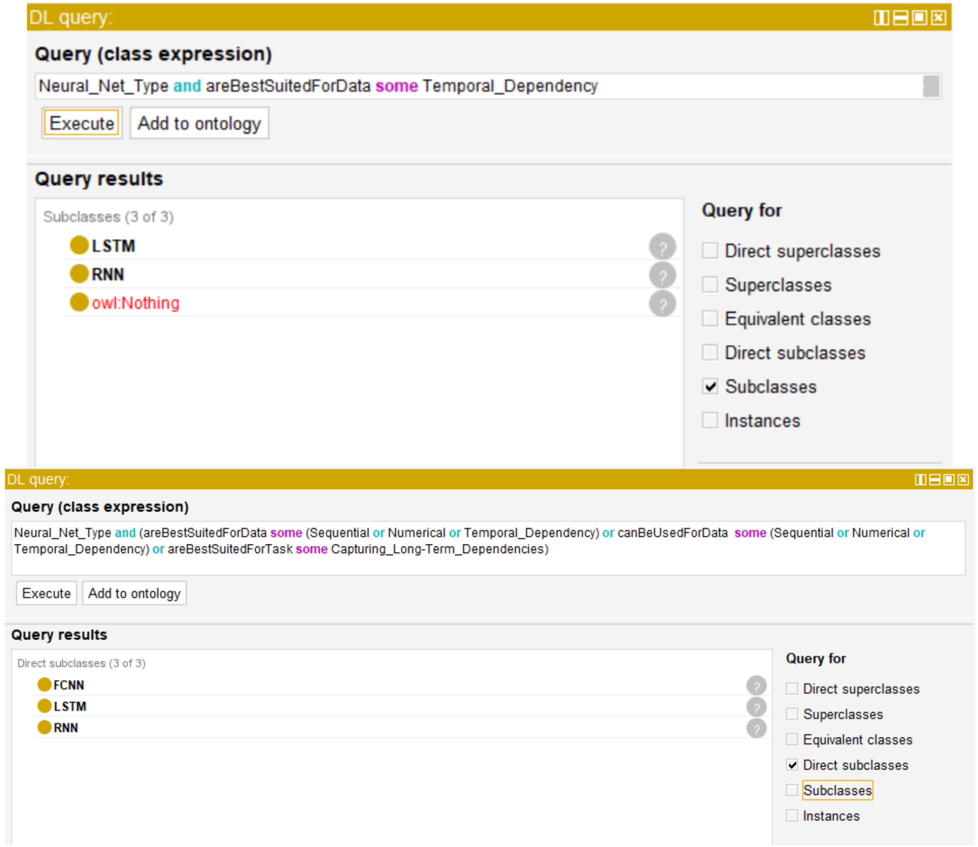


Ontology of PINNs



A graph showing three types of neural networks and the links between these networks, data characteristics, and tasks.

Example of queries used to test the ontology

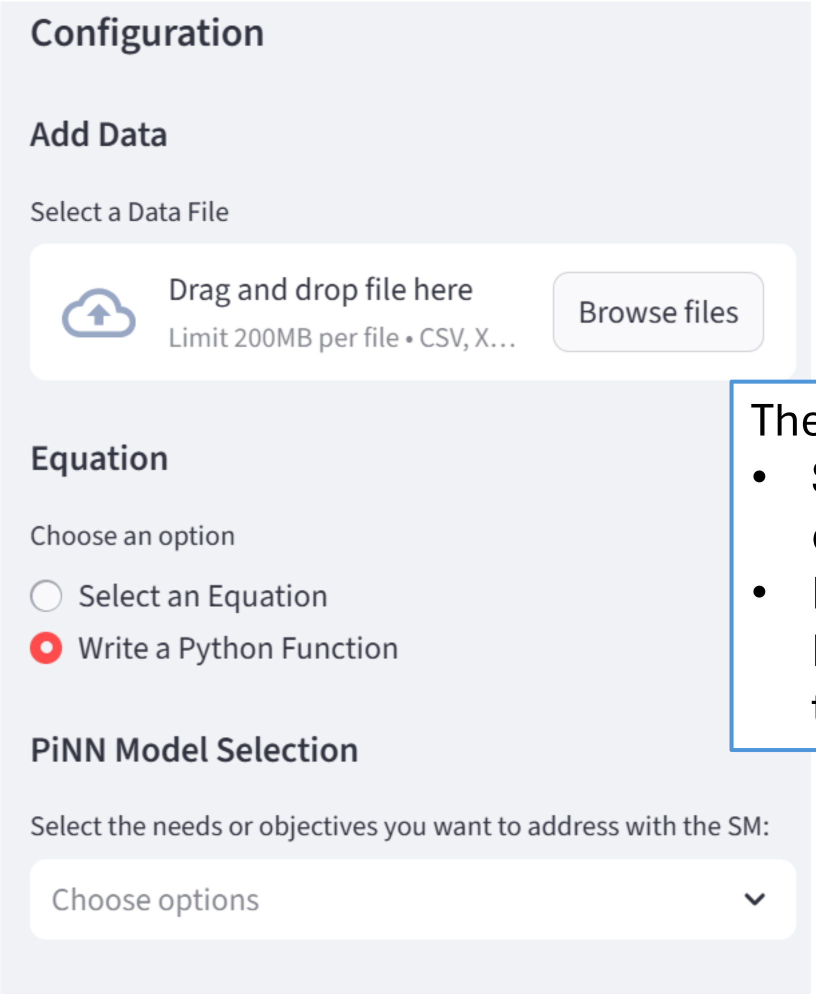


The queries performed on the ontology returned the expected results.

PAIRS Web Application: Model Recommendation

- PAIRS is a web-based interactive application built with Streamlit.
- It helps users explore, configure, and train PINNs model through a guided interface.
- The Recommendation System (RS) component uses the PINN ontology developed in Protégé.
- The recommendation system uses the OWL ontology via the owlready2 Python library to query and match relevant neural network models.
- Based on the data type and selected task, PAIRS recommends suitable PINN models with descriptions to support informed decision-making.

PAIRS Web Application: Model Recommendation

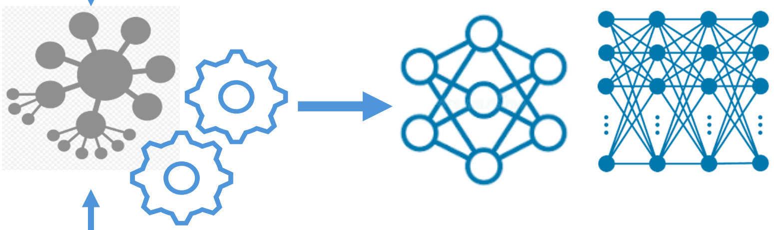


The data file uploaded by the user is automatically analyzed to detect its type

The user can either:

- Select from predefined equation examples, or
- Define a custom equation using Python in a dedicated editor window that appears upon selection.

The user chooses one or more tasks



The system recommends suitable PINN models

PAIRS Web Application: Model Building, Training, and Testing

Parameter Configuration → Model Building & Training → Model Evaluation, Saving & Comparison

Parameter Configuration

- Start after model selection.
- Set parameters:
  - Use recommended defaults or custom values.
  - Choose from ranges (e.g., learning rate, neurons, etc.).
- Select search strategy:
  - Manual / Grid / Random

Model Building & Training

- Build model with selected parameters.
- Use user-defined equations in physics loss.
- Define input bounds → generate collocation points.
- Show dynamic loss plot during training.
- Apply early stopping at threshold.

Model Evaluation, Saving & Comparison

- After training:
  - Test on unseen data (actual vs. predicted).
  - Save models with configs.
  - Compare multiple models.

PyTorch

Conclusion & Perspectives

Purpose & Impact of PAIRS

- PAIRS Provides a streamlined solution for building physics-informed AI surrogate models, an efficient alternative to traditional, resource-intensive simulations.
- Offers a no-code/low-code interface, empowering engineers and researchers to develop models without deep expertise in AI.
- Designed to be scalable and adaptable: the ontology can be updated to include new models, tasks, and data types.
- PAIRS bridges the gap between simulation expertise and machine learning, making advanced modeling more accessible.

Future Directions

- Automatic ontology updates using Generative AI to keep pace with evolving architectures.
- Creation of a pretrained model database to accelerate deployment.
- Integration of AI agents to assist users in model selection, configuration, and training.
- Expansion beyond PINNs to cover a broader range of physics-informed ML models.