AI+HPC
利用 NVIDIA Modulus 實踐 AI 於物理模擬

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AGENDA – DAY 1

09:15-10:15: Review DL Fundamentals

10:30-11:00: Introduce Data Driven and Physics Inspired/Driven

11:00-12:00: Data Driven Lab: Solving Steady State Flow using Neural Networks

AGENDA – DAY 2

09:30-10:20: Introduce Modulus

10:30-11:20: Physics Inspired Lab 0: Solve a Darcy flow problem using Fourier Neural Operators

11:30-12:00: Physics Driven Lab 1: Solve Partial Differential Equations using PINN approach

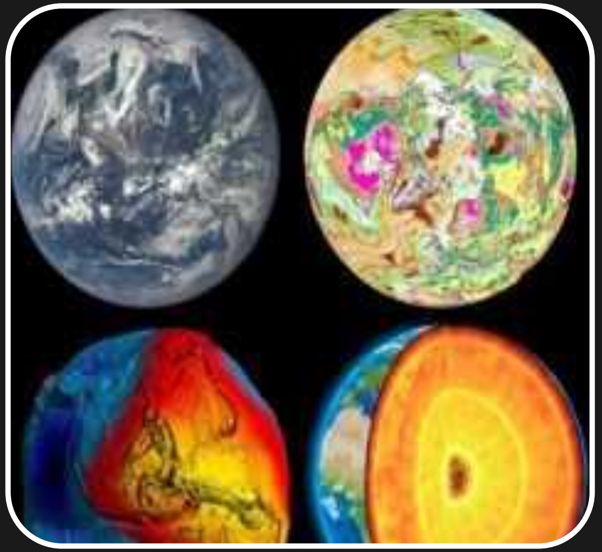
12:00-13:00: Launch Break

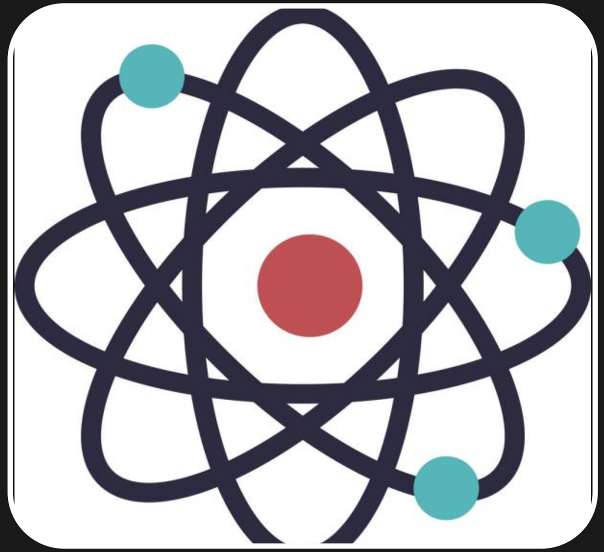
13:00-13:50: Physics Driven Lab 1: Solve Partial Differential Equations using PINN approach

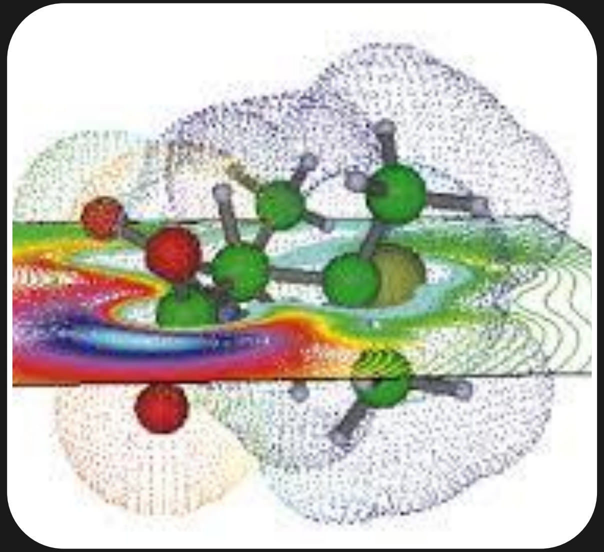
14:00-14:50: Physics Driven Lab 2: Solve transient problems and inverse problems

15:00-16:00: Physics Driven Challenge: Solve a fluid mechanics problem

COMPUTATIONAL DOMAINS







Computational Eng.

Solid & Fluid Mechanics,
Electromagnetics,
Thermal, Acoustics,
Optics, Electrical,
Multi-body Dynamics,
Design Materials

Earth Sciences

Climate Modeling,
Weather Modeling,
Ocean Modeling,
Seismic Interpretation

Life Sciences

Genomics,
Proteomics

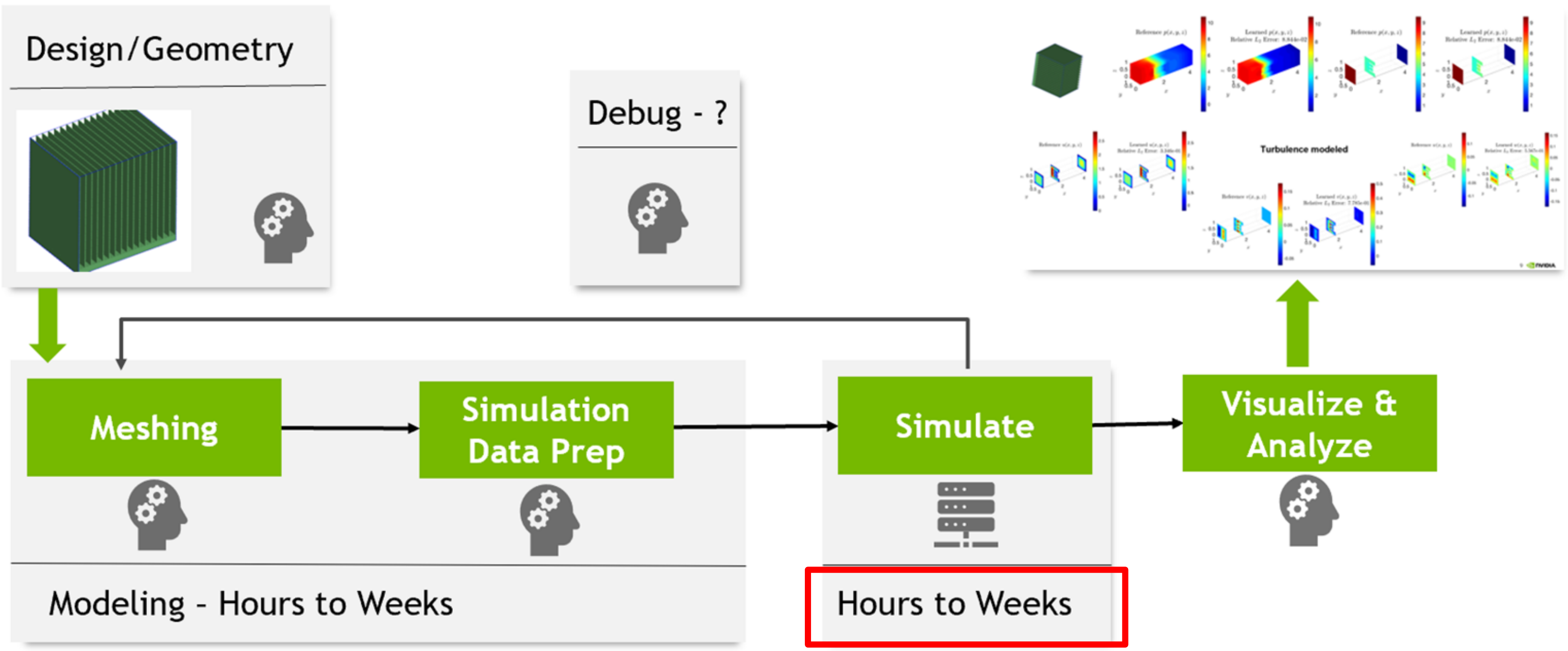
Computational Physics

Particle Science,
Astrophysics

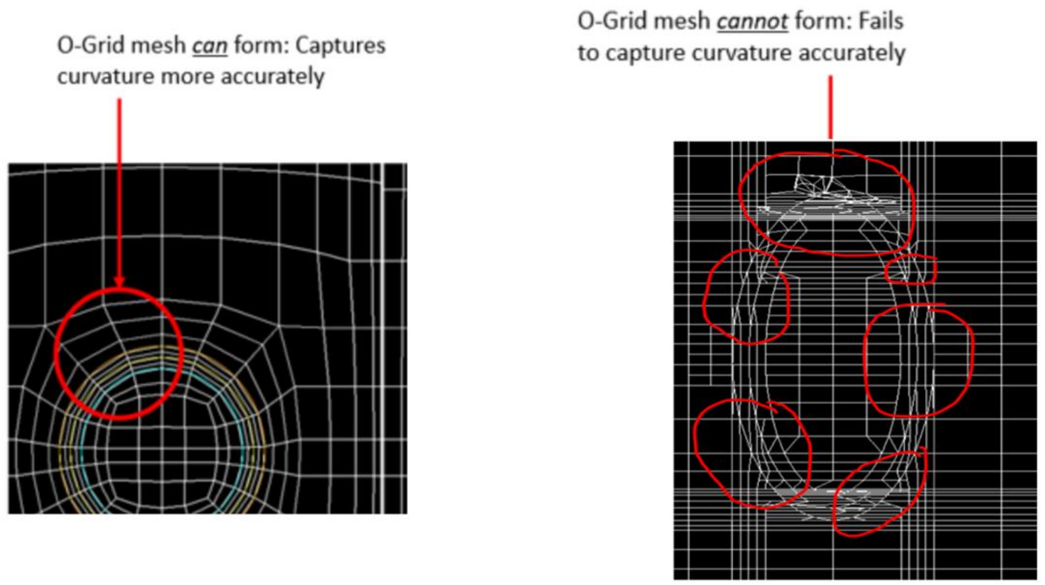
Computational Chemistry

Quantum Chemistry,
Molecular Dynamics

ISSUES IN TRADITIONAL SIMULATIONS



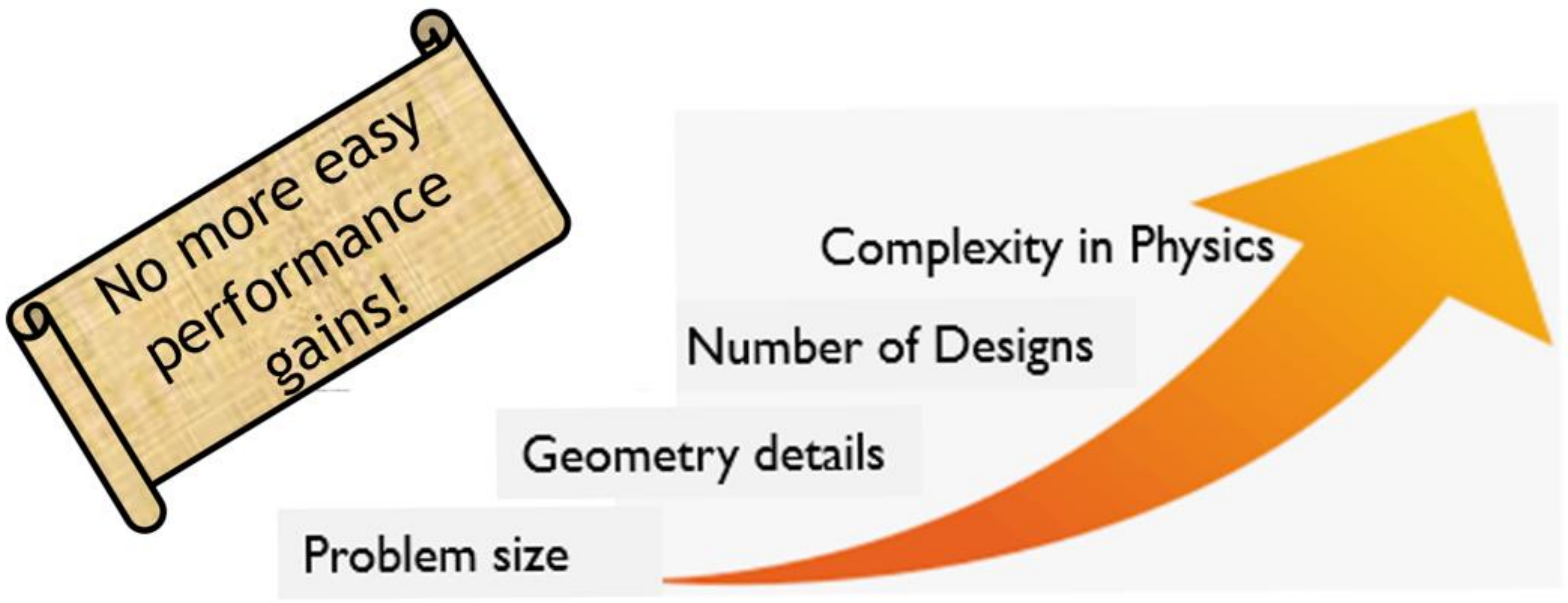
- Meshing Accuracy



- Limited Scope & Applicability
- Computational Speed Bottleneck

SATURATING PERFORMANCE IN TRADITIONAL HPC

Simulations are getting larger & more complex

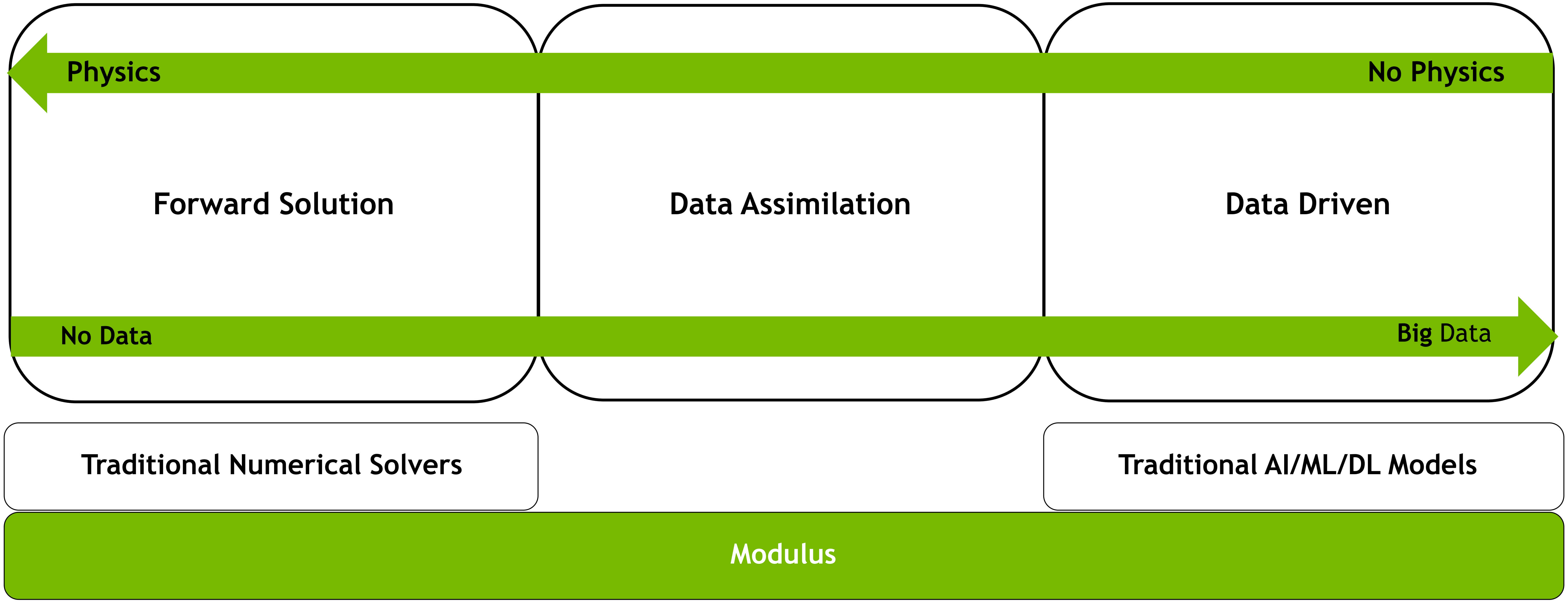


Traditional simulation methods are:

- Computationally expensive
- Demand ever-increasing resolution
- Plagued by domain discretization techniques
- Not suitable for data-assimilation or inverse problems

AI IN COMPUTATIONAL SCIENCES

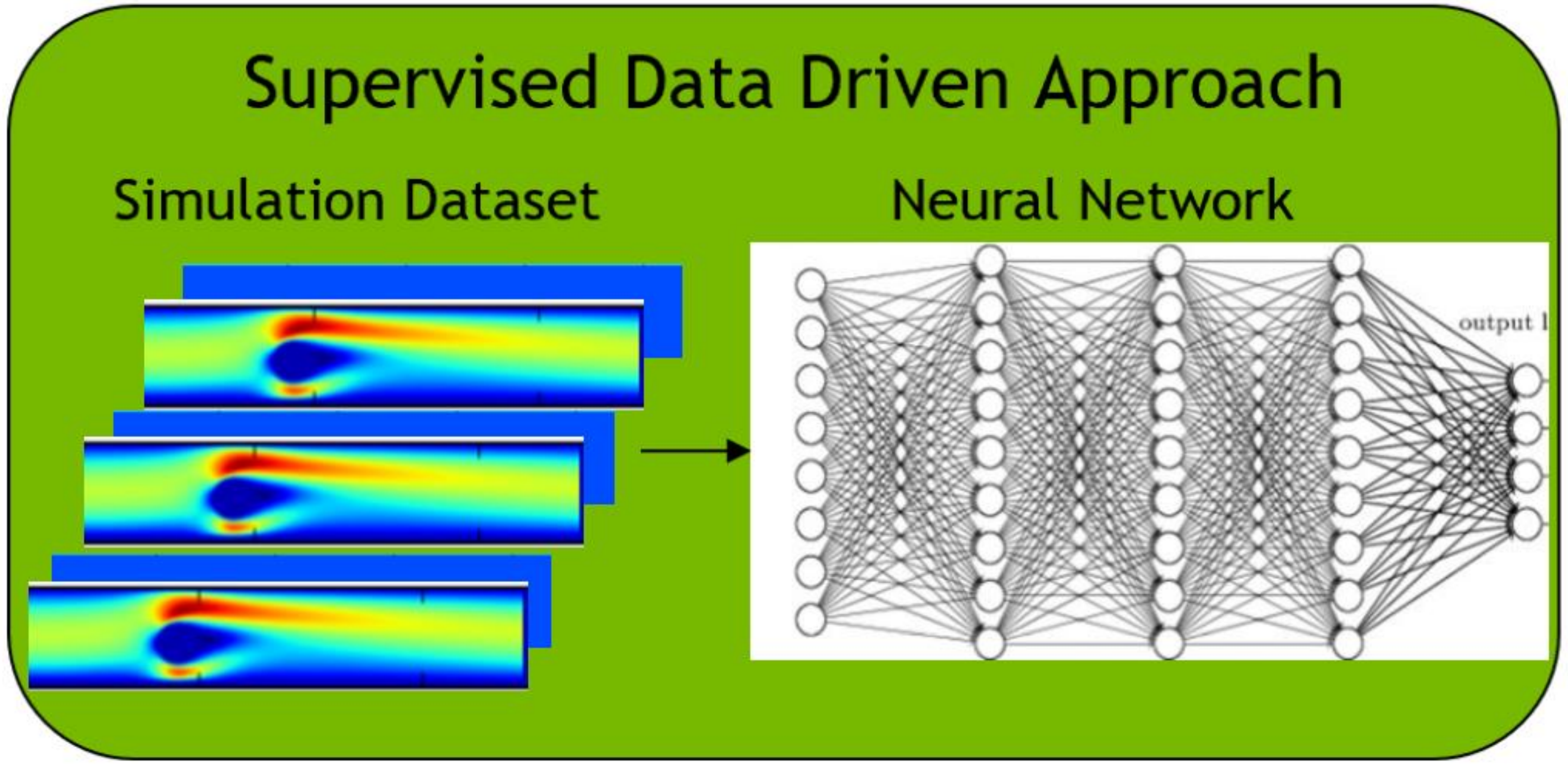
Primary Driver: Data vs. Physics

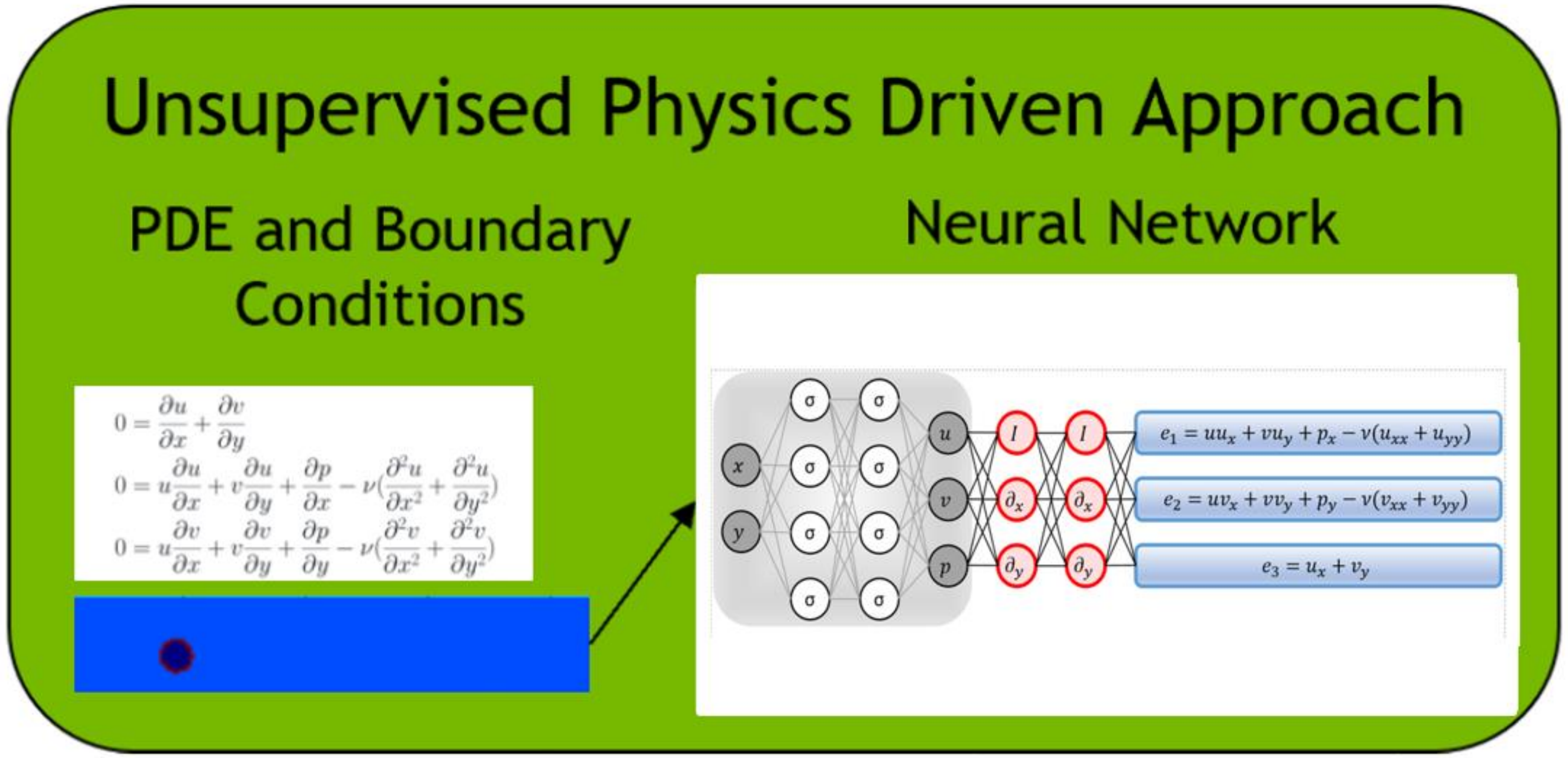


SOLVING PDES WITH NEURAL NETWORKS

A **Data Driven Neural Network** requires training data

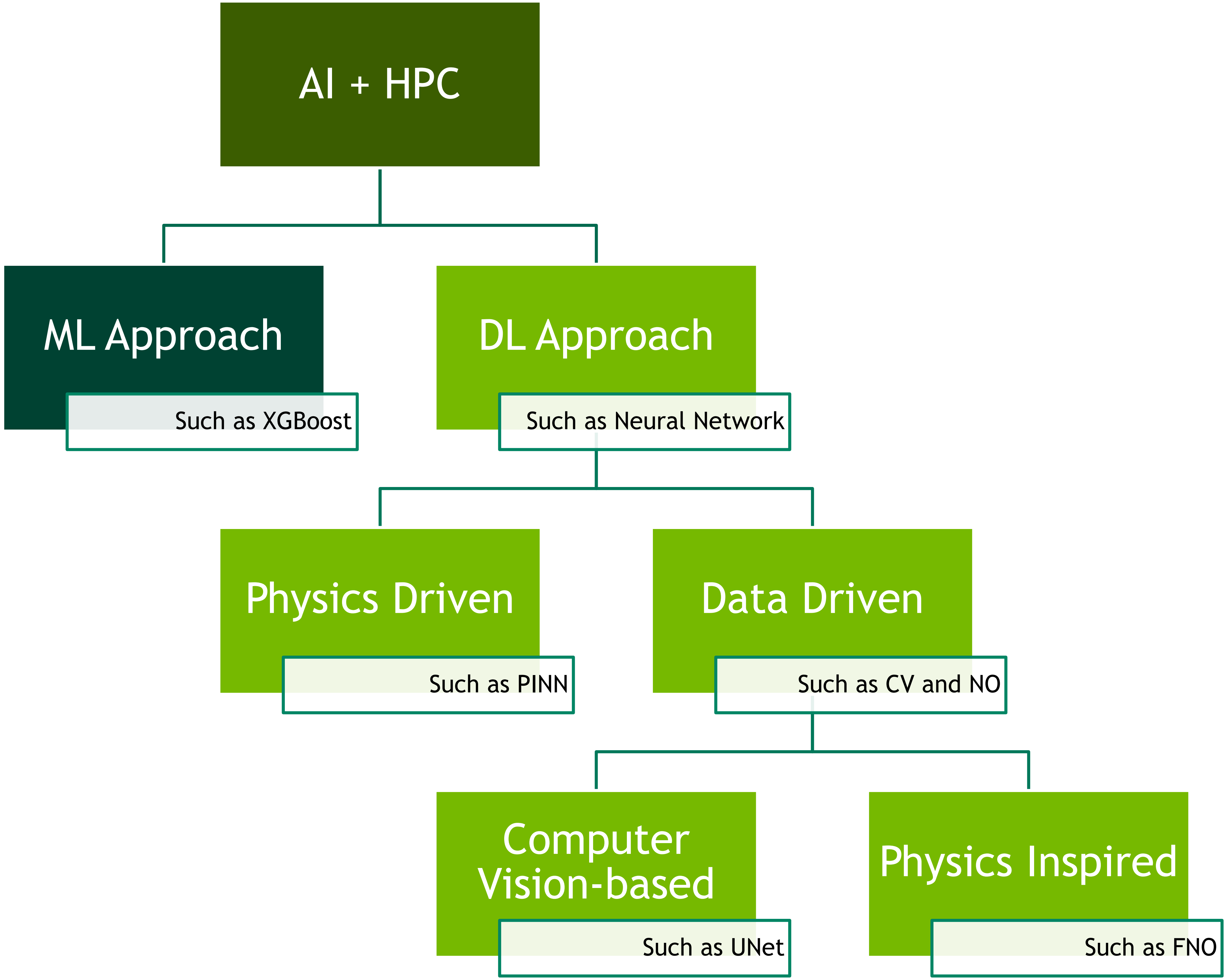
A **Physics Driven Neural Network** solver does **NOT** require training data





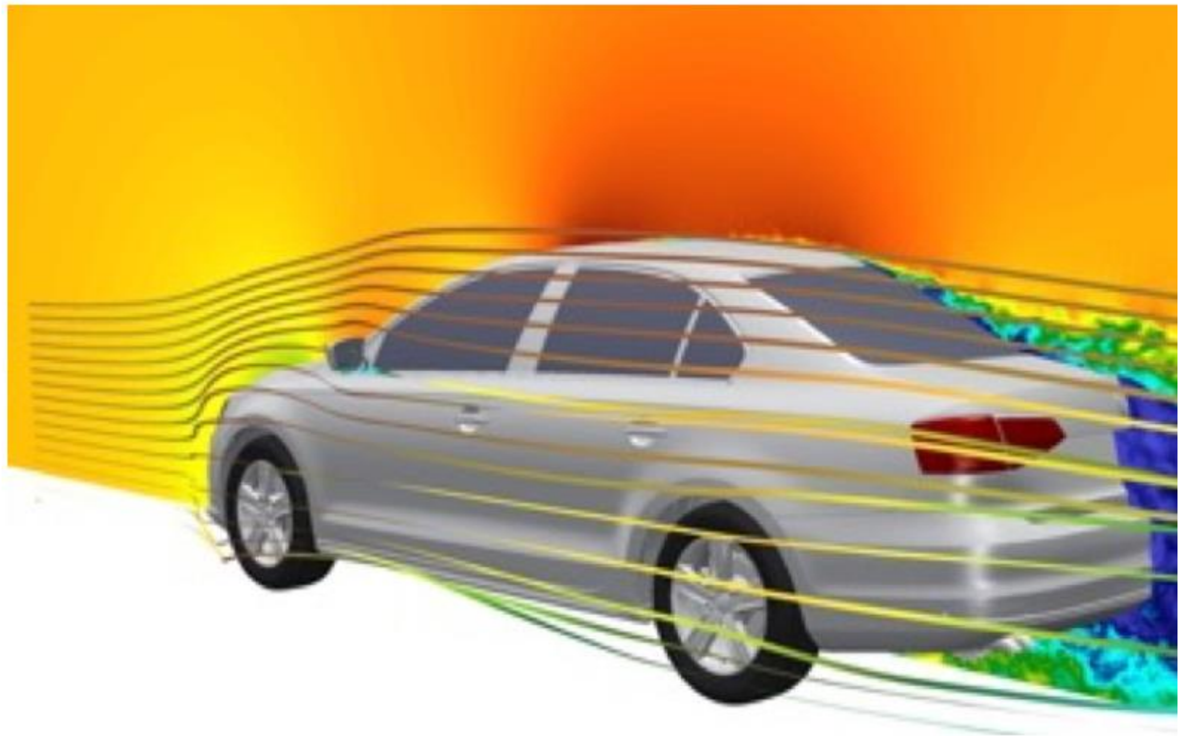
N layers

m*N layers (for m^{th} order PDE)


AI + HPC
ML Approach
Such as XGBoost
DL Approach
Such as Neural Network
Physics Driven
Such as PINN
Data Driven
Such as CV and NO
Computer Vision-based
Such as UNet
Physics Inspired
Such as FNO

DATA DRIVEN METHODS

Strengths
Measured/observed data along with Physics laws provides the most accurate representation of state
Data enables discovering of trends even when Physics is not known or too complex to model
Weaknesses
No Physics awareness
If measured/observed data is not available then time-consuming simulations are needed to generate the data.
Accuracy is dependent on the simulation code and user expertise
Lower Generalizability
Modeling complex 3D geometries/curved surfaces may be error probe

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