NVIDIA MODULUS: AN AI FRAMEWORK FOR PHYSICS ML

MODULUS TALKS IN GTC NOV. '21

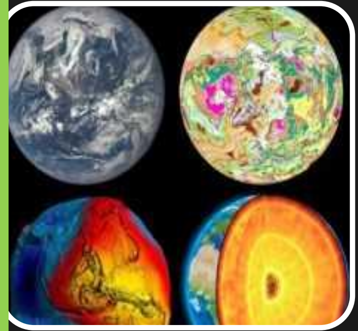
Physics-informed Neural Networks for Wave Propagation Using NVIDIA SimNet
[A31302]

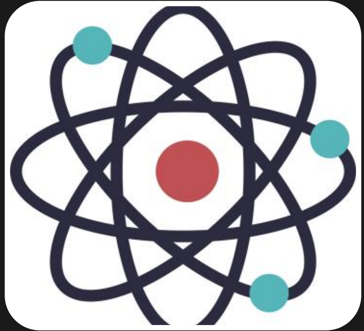
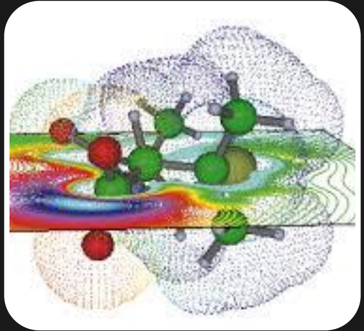
Toward Developing High Reynolds Number, Compressible, Reacting Flows in Modulus
[A31094]

Uncertainty Quantification for Transport in Porous Media Using Parameterized Physics Informed Neural Networks
[A31281]

Accelerate HPC simulations at scale with Physics-informed Neural Networks (PINNs) and NVIDIA GPUs on AWS
[A31724]

AI POWERED SCIENCE & ENGINEERING DOMAINS

Engineering Physics

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

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

Process/Product Design, Manufacturing, Testing, In-Service

AI IN COMPUTATIONAL SCIENCES

Primary Driver: Data vs. Physics

Physics | No Physics

Numerical Solvers

Neural Networks

No Data | Big Data

Forward Solution

Inverse Solution/ Data Assimilation

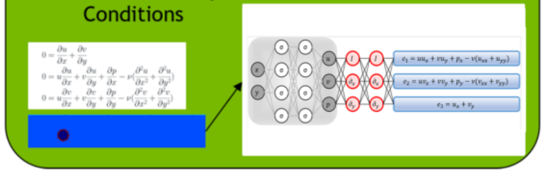
Data-Driven Solution

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

Unsupervised Physics Driven Approach

PDE and Boundary Conditions

Neural Network



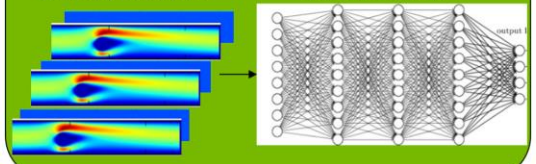
m*N layers (for m^{th} order PDE)

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

Supervised Data Driven Approach

Simulation Dataset

Neural Network

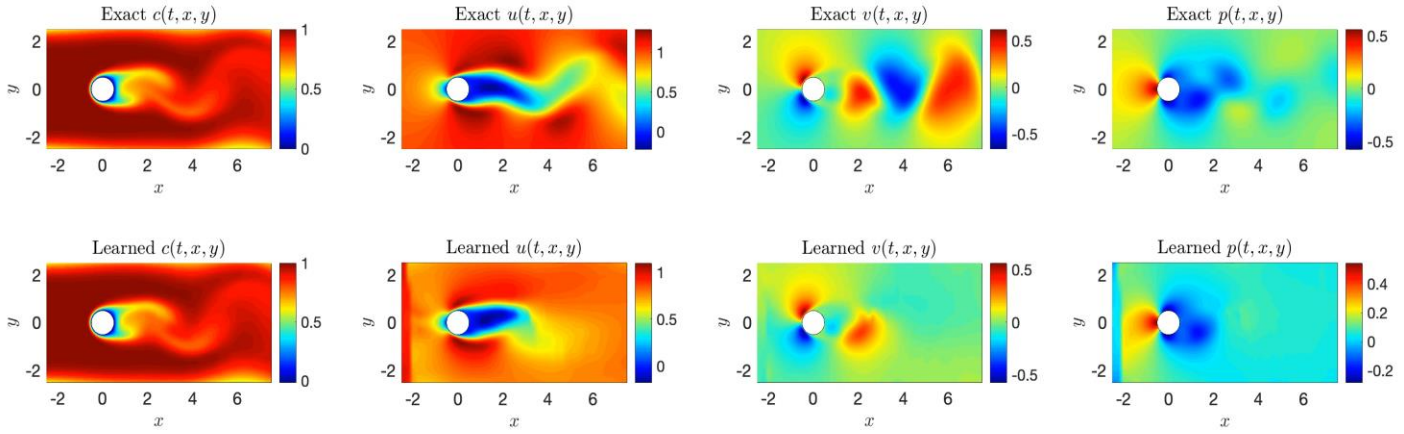


N layers

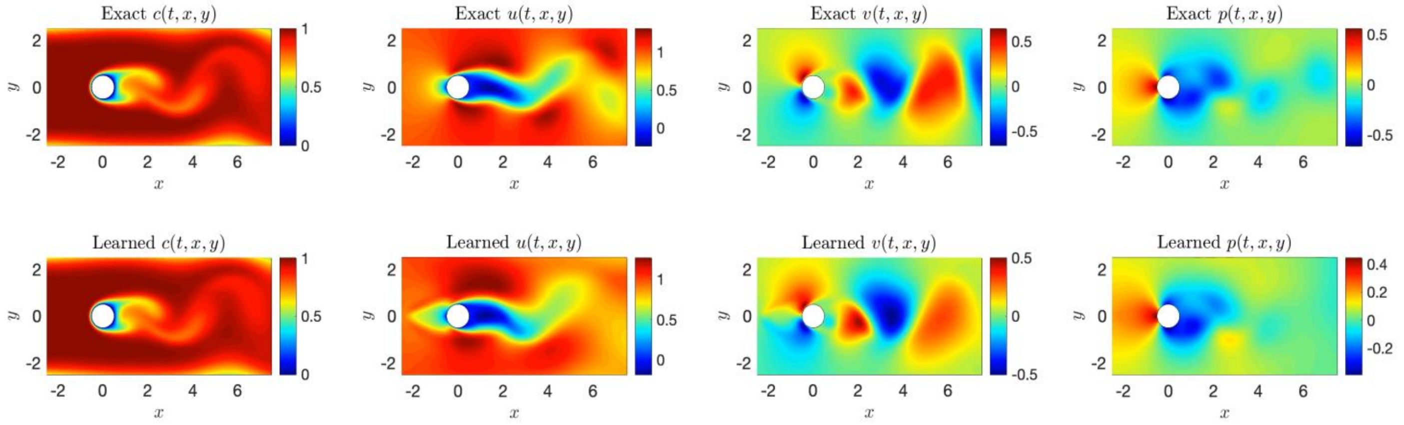
Data Driven Neural Networks

TRANSIENT: EXTERNAL FLOW PAST A 2D CYLINDER

CFD Simulation of an External Flow over a Cylinder

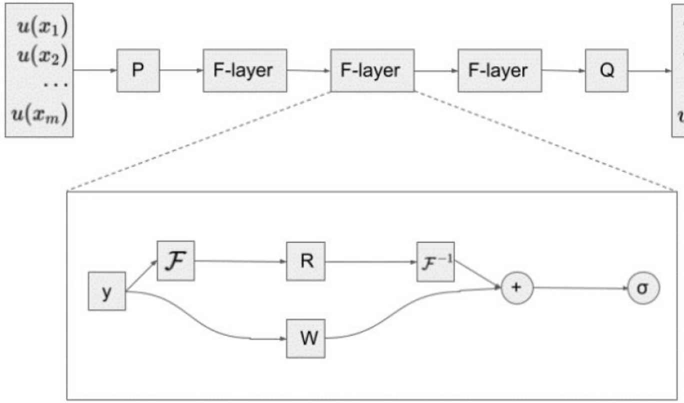


Corrected CFD Simulation Results (Ground Truth)



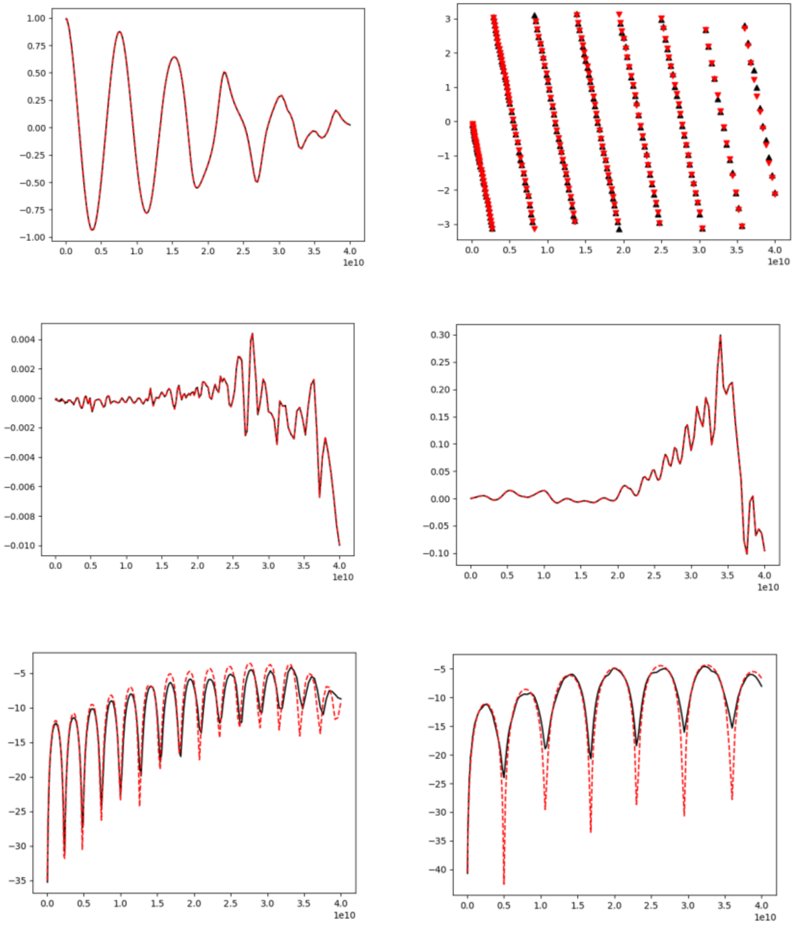
AUTOMATED DETECTION OF SI HOTSPOTS

Nvidia GeForce Boards



Fourier Neural Operator

Return loss (RL) → launch at 1; observation at 1
Insertion loss (IL) → launch at 1; observation at 2
Near end crosstalk (NEXT) → launch at 1; observation at 3
Far end crosstalk (FEXT) → launch at 1; observation at 4



Insertion Loss

Cross-Talk

Return Loss

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

Modulus

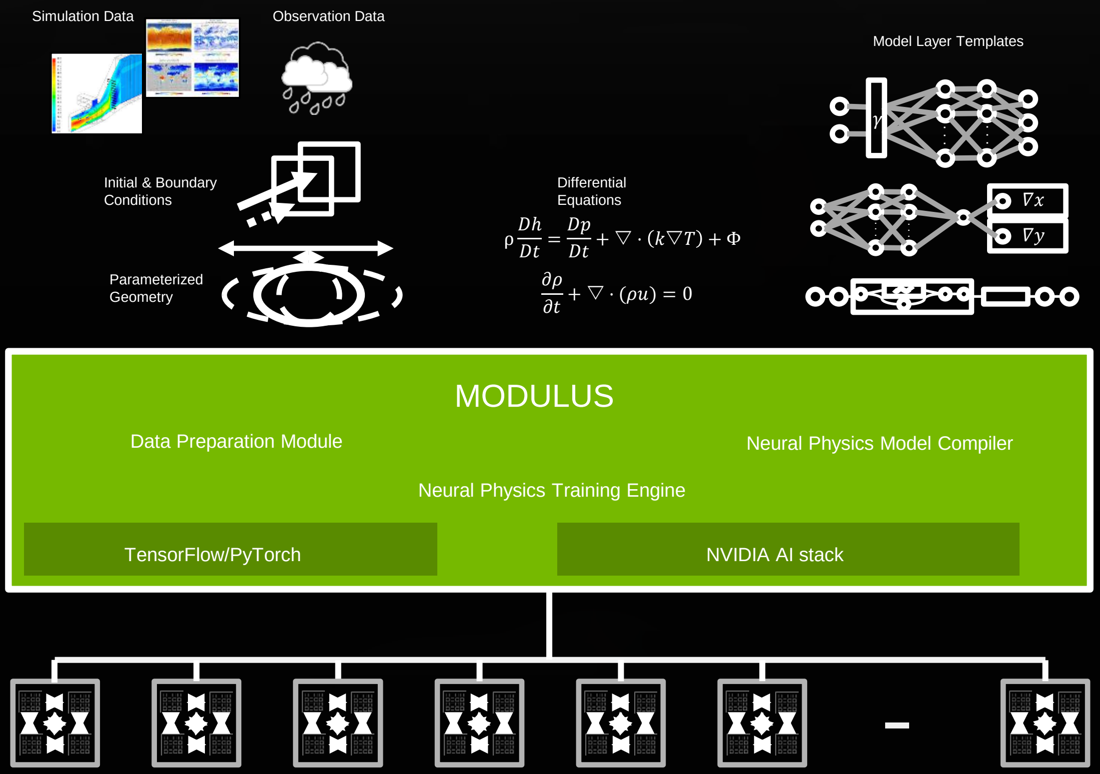
WHAT IS MODULUS?

NVIDIA MODULUS

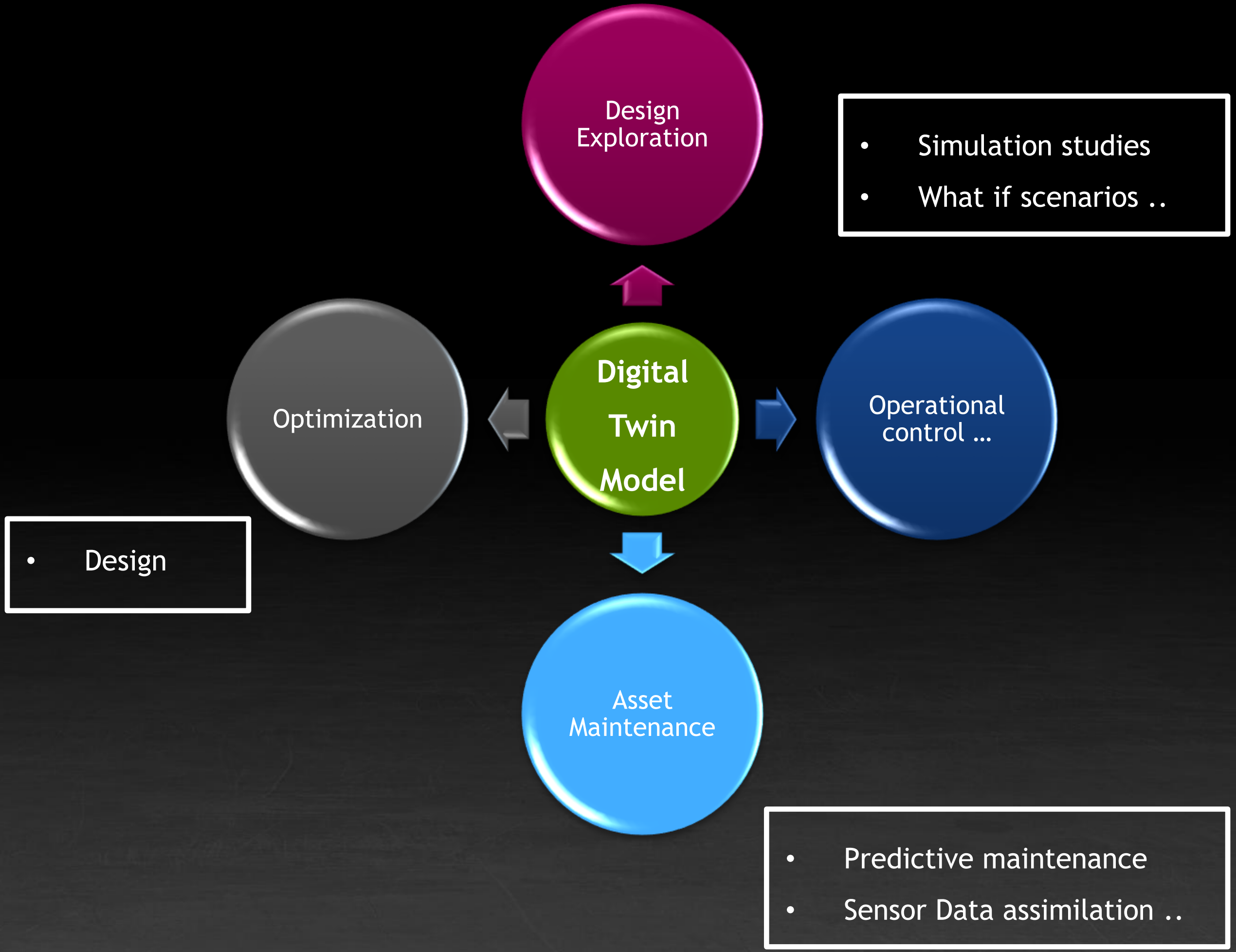
Framework for Developing Physics ML Models - AI framework for Science & Engineering problems

Use simulation and observation data and governing physics equations to generate a robust Digital Twin model

What its not? Not a Solver, Not a Simulation platform



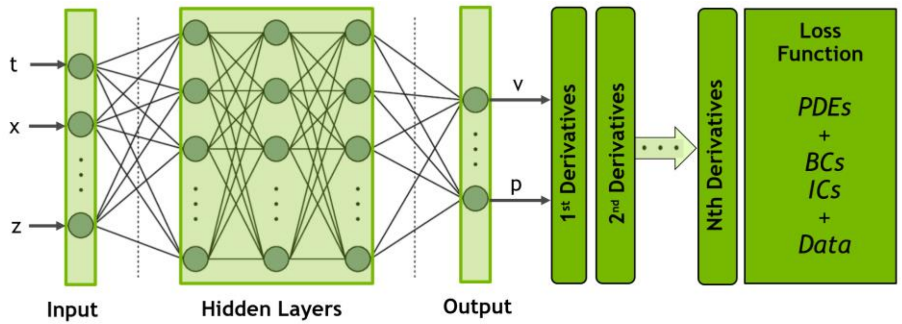
WHY MODULUS?


Design Exploration
Simulation studies
What if scenarios ..
Optimization
Design
Digital Twin Model
Operational control …
Asset Maintenance
Predictive maintenance
Sensor Data assimilation ..

MODULUS FUNCTIONALITY

Physics Based Neural Network: Architectures & Features

Architectures:



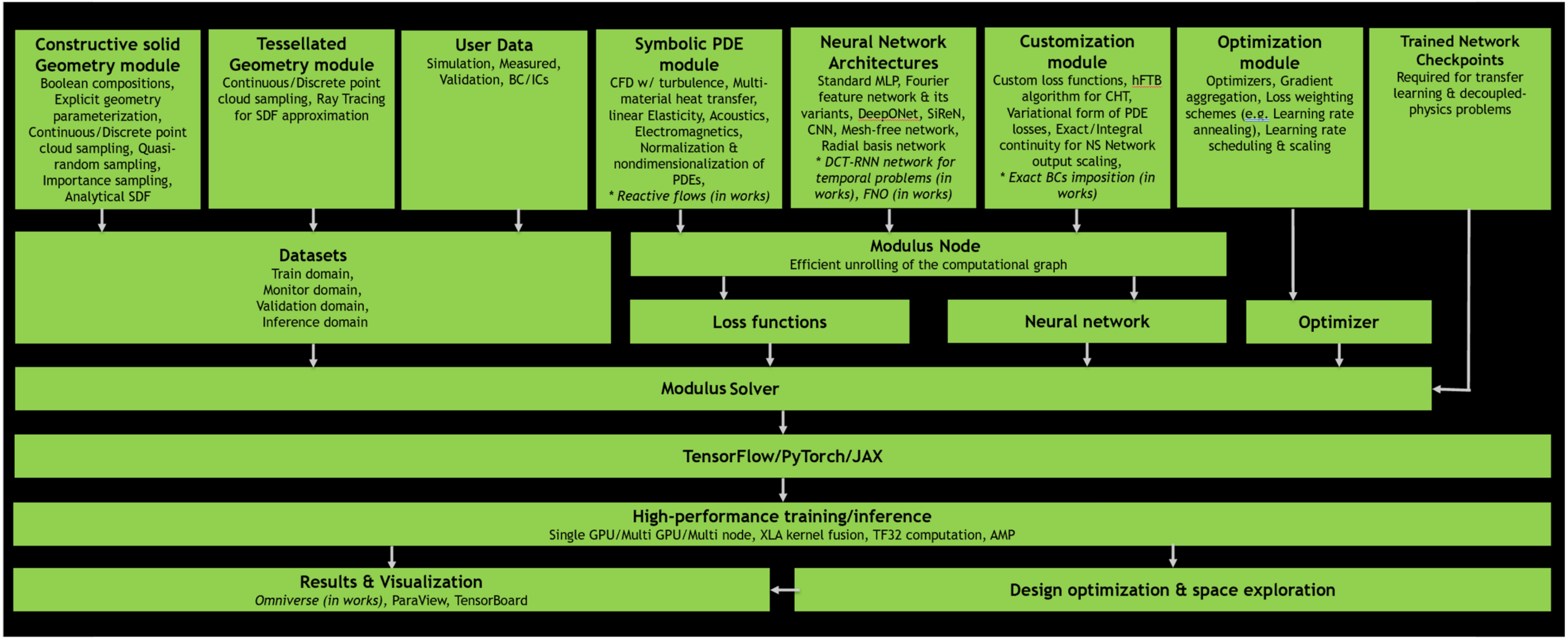
- Fully Connected (FC)
- Fourier Features (FN) – Axis, Partial, Full or Random Spectrum, Positional & Gaussian Encodings, Multi-Scale
- Sinusoidal Representation (SiReNs)
- Modified Fourier Features (mFN)
- Deep Galerkin Method (DGM)
- Modified Highway Networks
- Multiplicative Filter Networks

Features:

- CFD, Thermal, Electromagnetics, Solids, Acoustics
- Geometry Modules: STL or Parametrized CSG
- Differential & Variational treatment of PDEs
- Time stepping schemes for Transient Problems
- Homoscedastic task uncertainty quant. for loss wt.
- hFTB algorithm for conjugate heat transfer problems
- Global & Local Learning Rate Annealing
- Global Activation Functions
- Halton Sequences for Low-Discrepancy Point Cloud
- SDF weighting of Losses
- Integral & Exact Continuity (Mass Balance)
- Quasi-Random/Continuous Sampling of Point Cloud
- Importance Sampling
- Gradient Aggregation
- Transfer Learning
- Polynomial Chaos Expansion
- Performance: XLA, Multi-GPU/Node Scaling, AMP, TF32

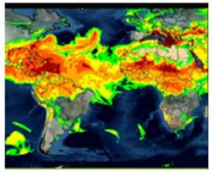
MODULUS CODE FLOW

http://developer.nvidia.com/Modulus



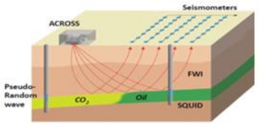
AI IN SCIENCE & ENGINEERING

Inverse & Data Assimilation Problems

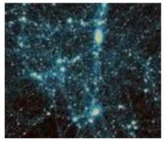


Climate

Medical Imaging

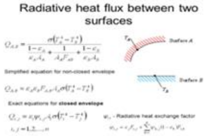


Oil & Gas

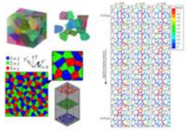


High Energy/ Nuclear Physics

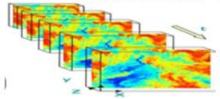
Improved Physics & Predictions



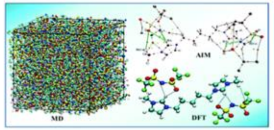
Radiation



Micro-mechanical Material Model



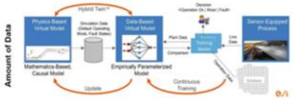
Turbulence



Molecular Dynamics

Real Time Simulations

Robotics

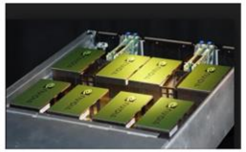


Digital Twin

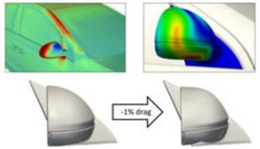
Autonomous Ride & Handling

Games

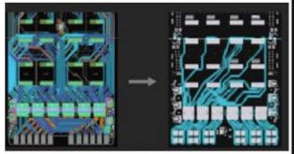
Digital Design & Manufacturing



Heat Sink



Aerodynamics



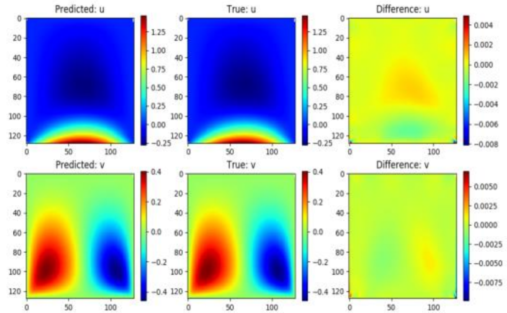
Vias on a PCB

Physics & Data - No Traditional Solver

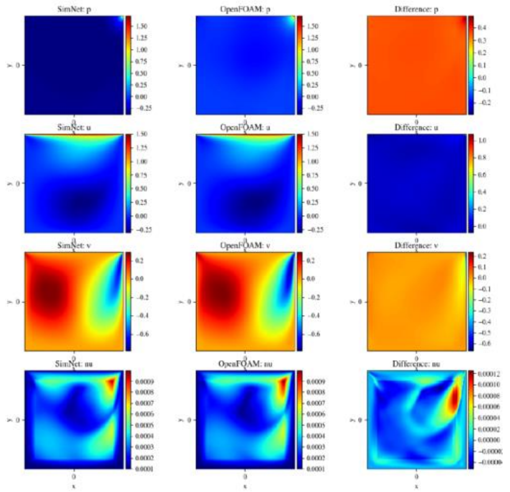
Physics - Traditional Solver (Speed is a limitation)

MODULUS FRAMEWORK - VERIFICATION

CFD

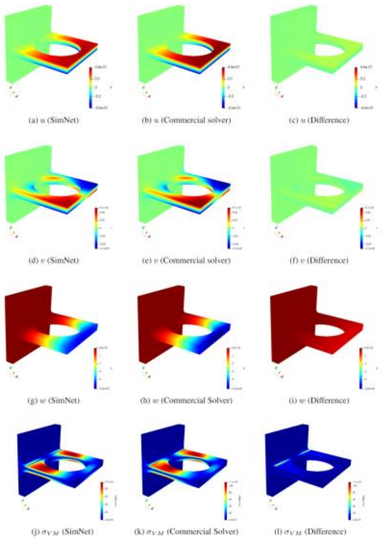


Laminar



Turbulent

Solid Mechanics

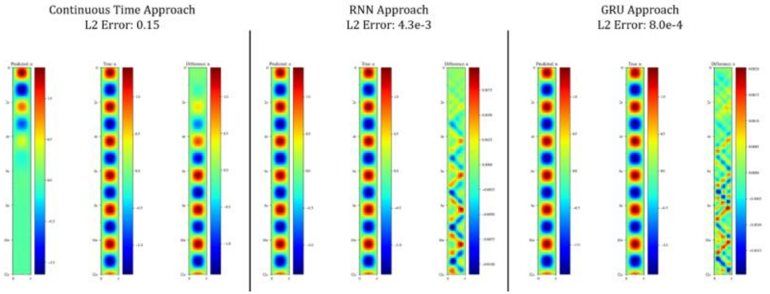


Equilibrium: $\sigma_{ji,j} + f_i = 0,$

Stress-Strain: $\sigma_{ij} = \lambda \epsilon_{kk} \delta_{ij} + 2\mu\epsilon_{ij},$

Strain-Displacement: $\epsilon_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right).$

Acoustics



$$
\begin{aligned}
u_{tt} &= c^2 u_{xx} \\
u(0,t) &= 0, \\
u(\pi,t) &= 0, \\
u(x,0) &= \sin(x), \\
u_t(x,0) &= \sin(x).
\end{aligned}
$$

MODULUS FRAMEWORK - VERIFICATION

Electromagnetics

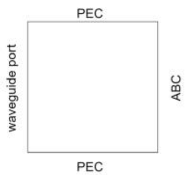


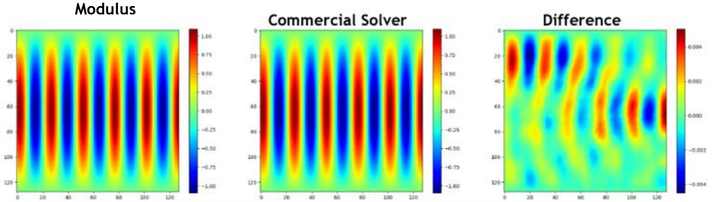
Figure 42: Domain of 2D waveguide

In this example we will solve this waveguide problem by transverse-magnetic (TM_z) mode, so that our unknown variable is $E_z(x, y)$. The governing equation in Ω is

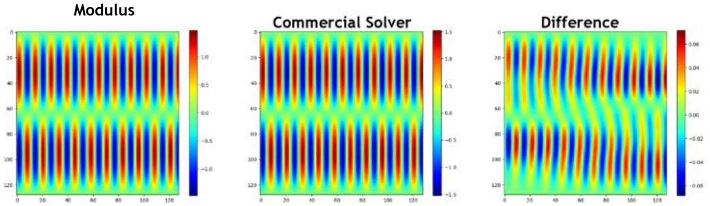
$$\Delta E_z(x, y) + k^2 E_z(x, y) = 0,$$

where k is the wavenumber. Notice in 2D scalar case, the PEC and ABC will be simplified in the following form, respectively:

$$E_z(x, y) = 0 \text{ on top and bottom boundaries, } \frac{\partial E_z}{\partial y} = 0 \text{ on right boundary.}$$



Wave Number = 16, Eigen Mode = 1



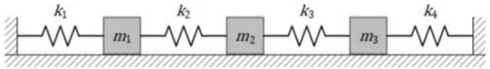
Wave Number = 32, Eigen Mode = 2

Vibrations

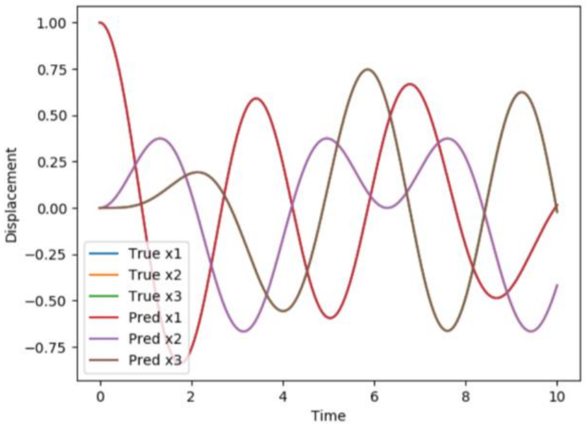
$$\begin{aligned}
m_1 x_1''(t) &= -k_1 x_1(t) + k_2(x_2(t) - x_1(t)),\\
m_2 x_2''(t) &= -k_2(x_2(t) - x_1(t)) + k_3(x_3(t) - x_2(t)),\\
m_3 x_3''(t) &= -k_3(x_3(t) - x_2(t)) - k_4 x_3(t).
\end{aligned}$$

$$\begin{aligned}
[m_1, m_2, m_3] &= [1, 1, 1],\\
[k_1, k_2, k_3, k_4] &= [2, 1, 1, 2],\\
[x_1(0), x_2(0), x_3(0)] &= [1, 0, 0],\\
[x_1'(0), x_2'(0), x_3'(0)] &= [0, 0, 0].
\end{aligned}$$

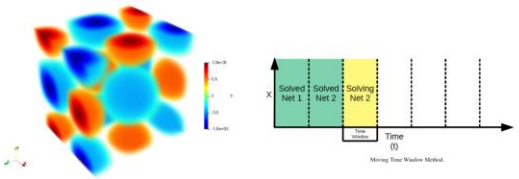
Modulus



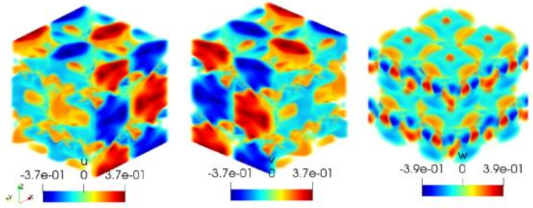
Three masses connected by four springs on a friction-less surface

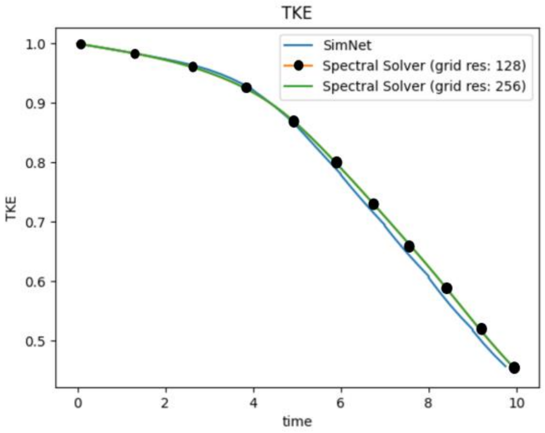


Turbulence



Taylor-Green vortex initial conditions.

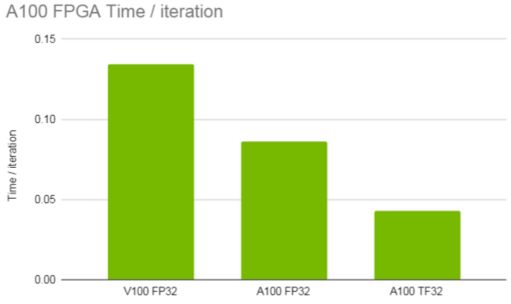




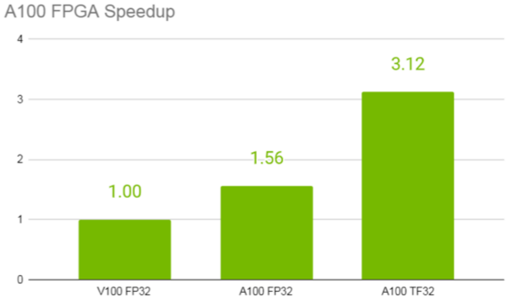
Taylor-Green Trubulent kinetic energy decay.

MODULUS FRAMEWORK - PERFORMANCE

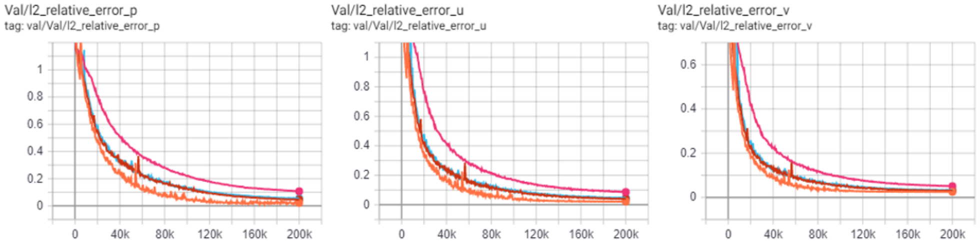
SINGLE GPU: Tensor Core Speed-up for PDEs



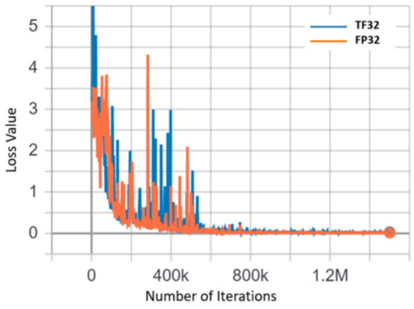
(a) Time per iteration



(b) Speed-up



Case Description	P_{drop} (Pa)	Compute Time (hrs)
Fully Connected Networks with FP32	29.24	86.9
Fully Connected Networks with TF32	29.13	39.5



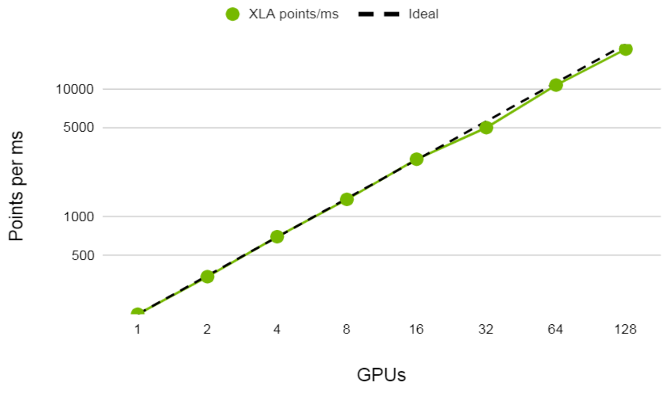
Second-order formulation	100 mins
First-order formulation	68 mins
First-order formulation + AMP	53 mins

A100 FP32 vs. TF32: Results, Compute Time, Loss

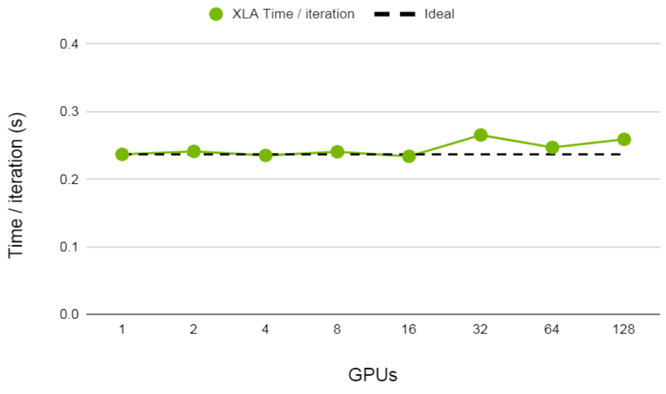
AMP

MODULUS FRAMEWORK - PERFORMANCE

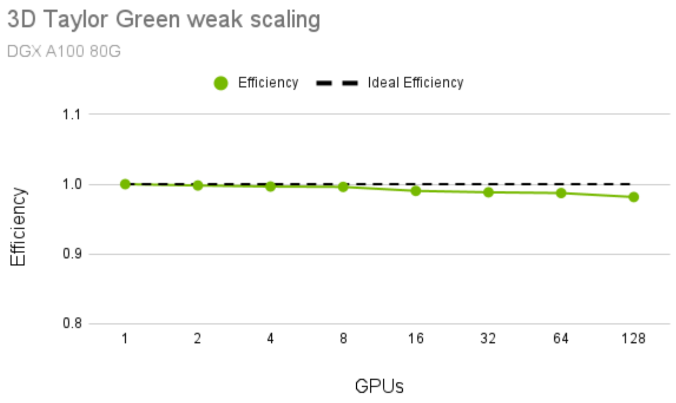
MULTI-GPU/NODE Scalability

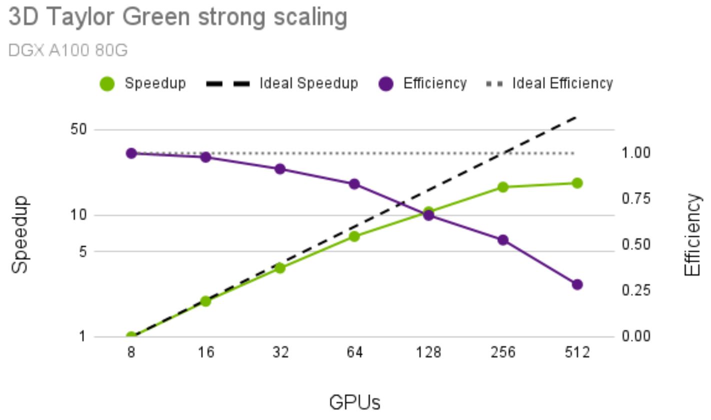


(a) Points per ms



(b) Time per iteration





Digital Twins

NVIDIA®

DIGITAL TWIN OF AIRCRAFT CABIN PANELS

University of Central Florida (Prof. Felipe Vianna)

https://www.phmsociety2020.com/corporate-sponsors/nvidia

Use case (synthetic data):

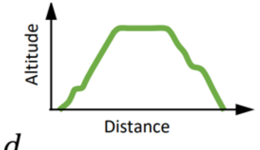
- Monitoring fatigue crack growth on the corner of a window (Al 2024)
- Fleet of 300 aircraft
- 5 flights per day
- 3 to 5 years of operation

Modulus:

- PINN model for stress as a function of pressure differential
- Reduced-order model:
    - Linear elastic analysis
    - Simply supported sides and far-field hoop stresses defining boundary conditions

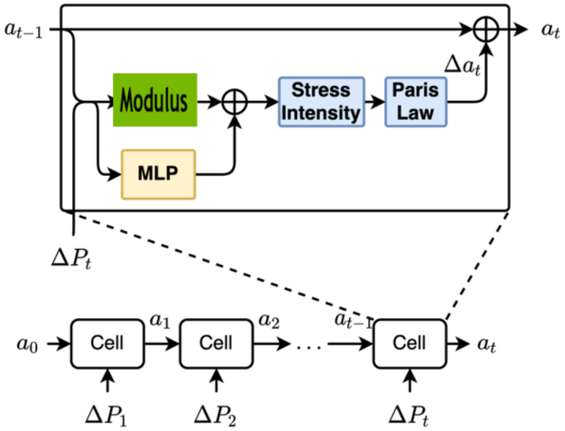
PINN-CDM

- Perform damage accumulation
- Adjust local stresses



$$\sigma_{HOOP} = \frac{\Delta P \times d}{2t}$$

- d : external diameter
- t : thickness
- ΔP: pressure differential (function of altitude)

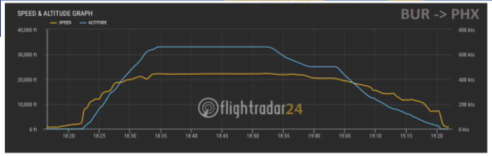


Crack growth:

$\frac{da}{dN} = C\Delta K^m$ and $\Delta K = F\Delta S\sqrt{\pi a}$

$F = 1.122$ **(assumed)**

$F = f(a)$ **(reality)**



Short
Max Alt: 33000 ft
(20 min)

Medium
Max Alt: 40000 ft
(60 min)

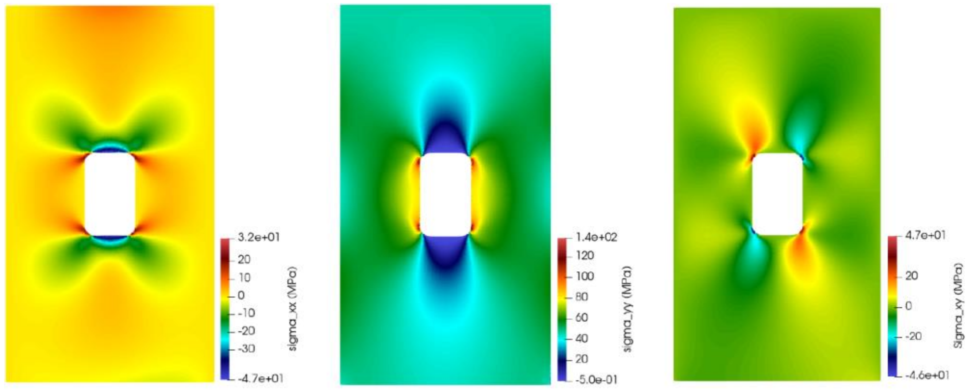
Long
Max Alt: 40000 ft
(120 min)

DIGITAL TWIN OF AIRCRAFT CABIN PANELS

University of Central Florida (Prof. Felipe Vianna)

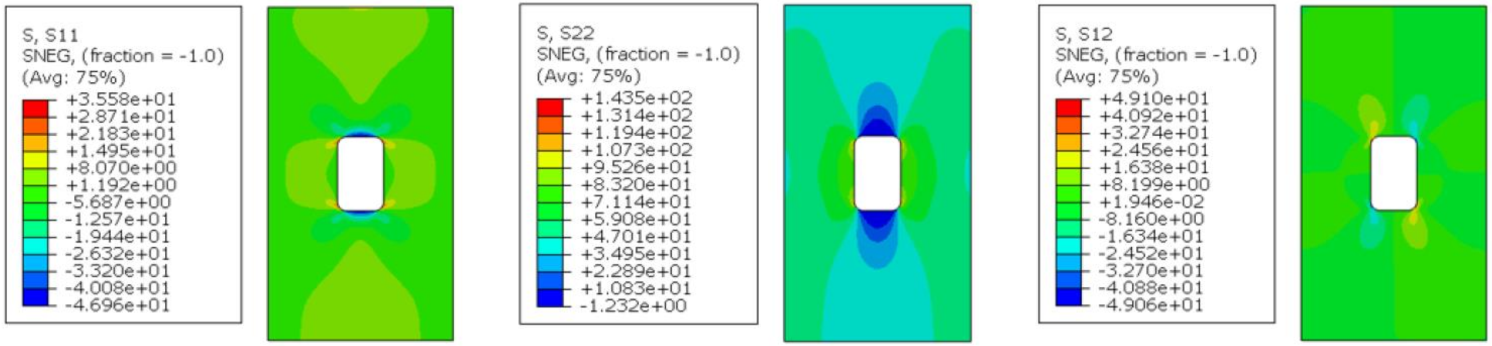
https://www.phmsociety2020.com/corporate-sponsors/nvidia

Modulus



(a) σ_{xx} (b) σ_{yy} (c) σ_{xy}

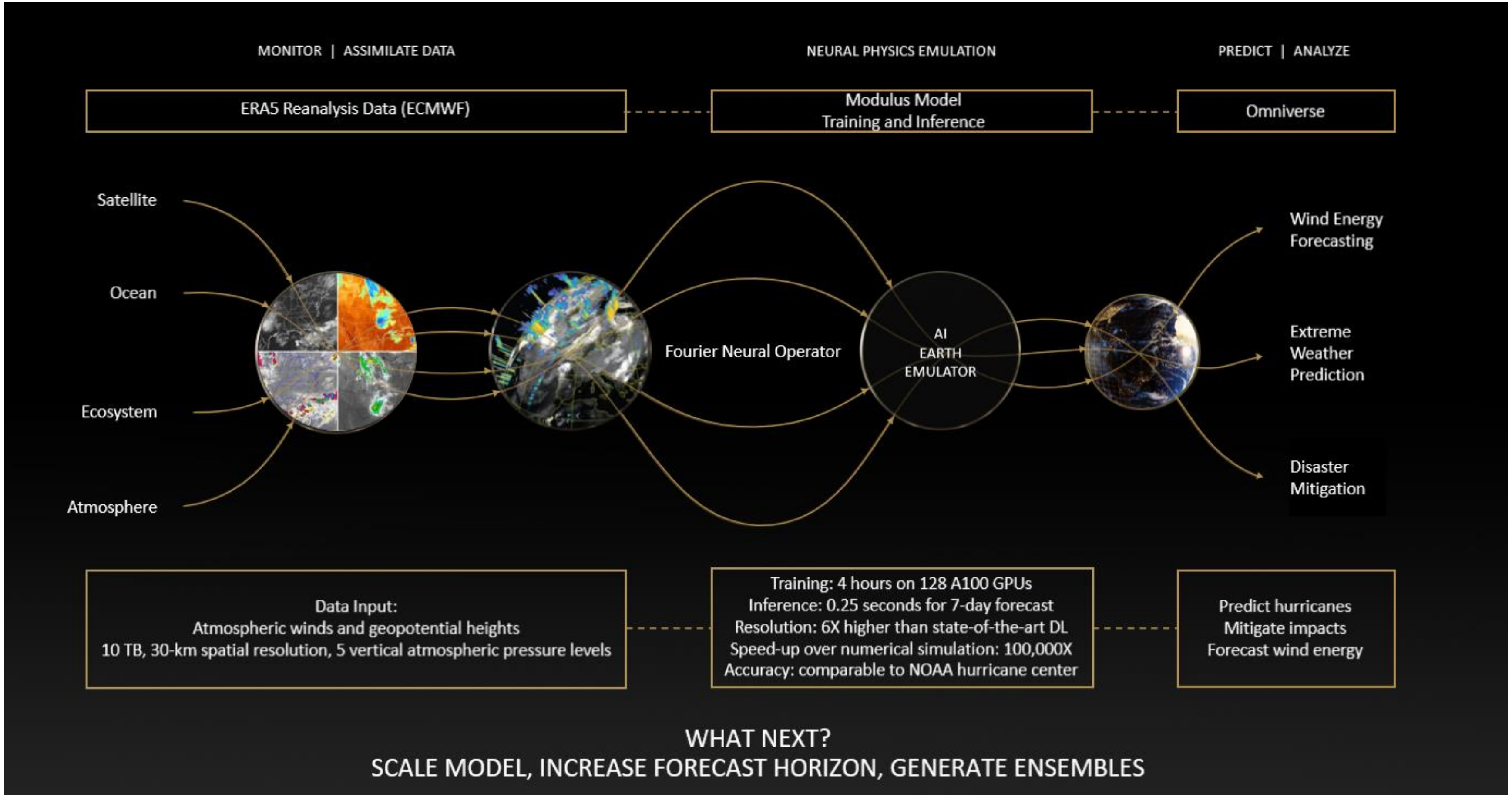
Commercial Solver



(a) σ_{xx} (b) σ_{yy} (c) σ_{xy}

NVIDIA MODULUS FOR EARTH DIGITAL TWIN

Unprecedented Resolution, Speed & Accuracy enables Real-Time Prediction of Extremes



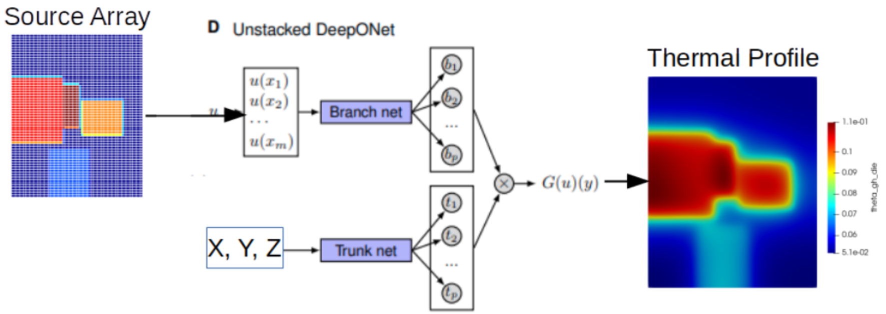
Design Optimization

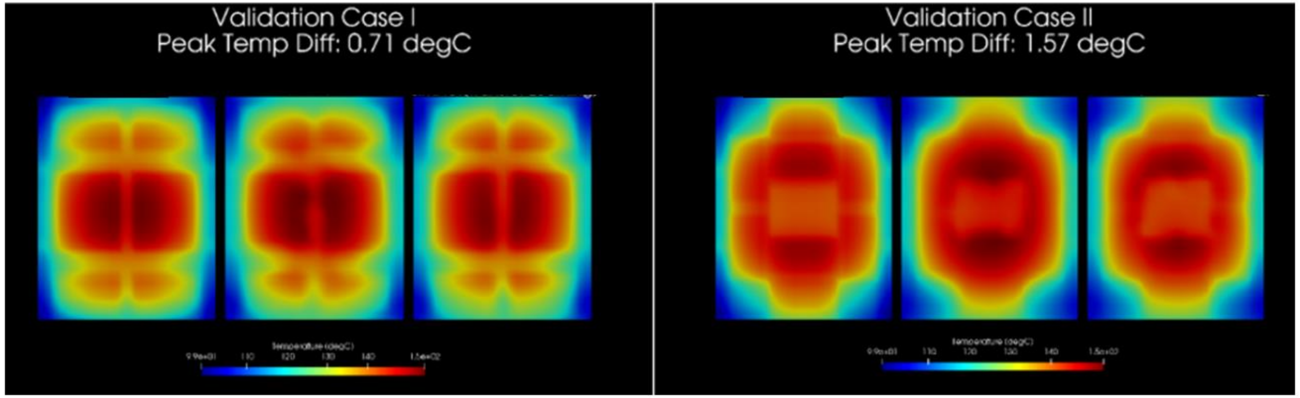
NVIDIA®

NVIDIA GPU FLOOR PLANNING

Thermal Design

Floor Planning with DeepONet





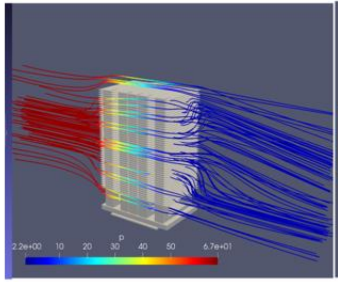
Goals:

1. Instant Thermal Profile
2. Best Layout for Thermal Offset

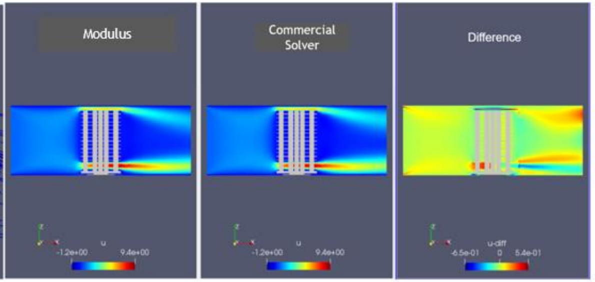
NVIDIA DGX-A100 NVSWITCH HEAT SINK

Validation/Verification of single geometry results with CFD solvers

Nvidia DGX A100 Heatsink



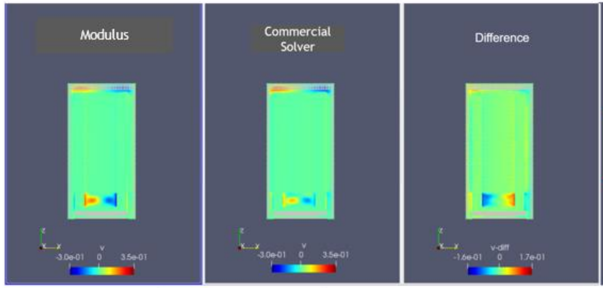
Pressure color coded flow streamlines



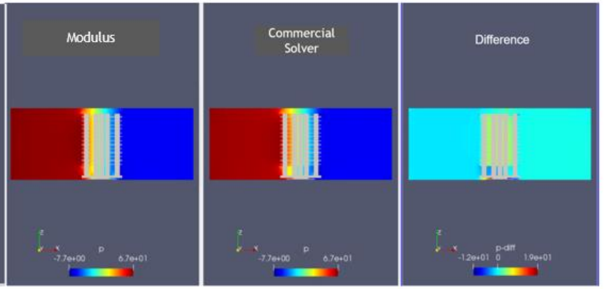
U-velocity (transverse direction) comparison

Commercial solver mesh refinement results for NVSwitch pressure drop and peak temperature.

Mesh element size	Commercial solver pressure drop (Pa)	Modulus pressure drop (Pa)	Absolute difference (%)	Commercial solver peak temperature ($^\circ C$)	Modulus temperature ($^\circ C$)	Absolute difference (%)
22.4 M	81.27	150.25	84.88	97.40	97.35	0.05
24.7 M	111.76	150.25	34.44	95.50	97.35	1.94
26.9 M	122.90	150.25	22.25	95.10	97.35	2.36
30.0 M	132.80	150.25	13.14	-	-	-
32.0 M	137.50	150.25	9.27	-	-	-



V-velocity (transverse direction) comparison



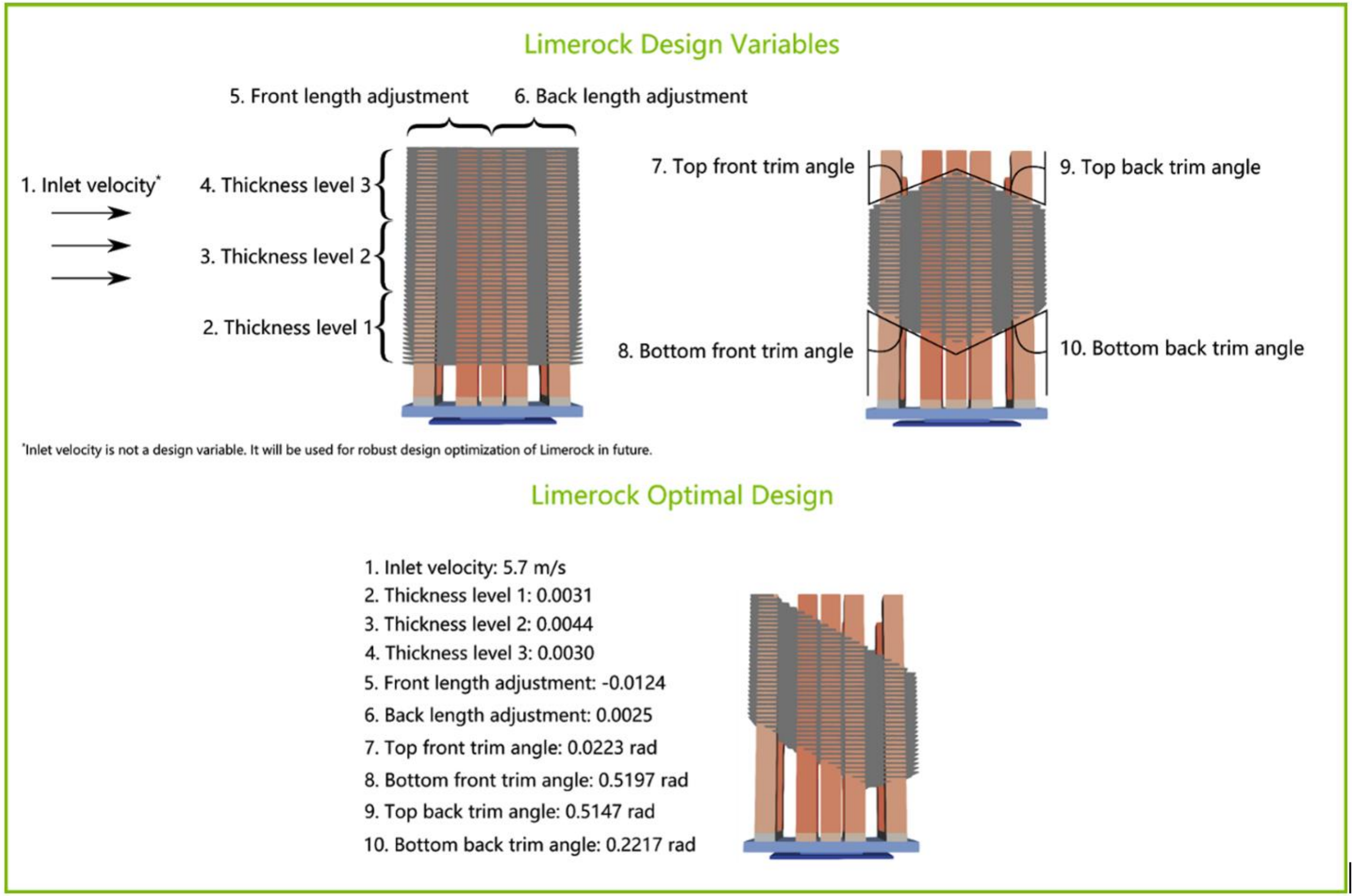
Pressure comparison

A comparison for the solver and SimNet results for NVSwitch pressure drop and peak temperature.

Property	OpenFOAM	Commercial Solver	Modulus
Pressure Drop (Pa)	133.96	137.50	150.25
Peak Temperature ($^\circ C$)	93.41	95.10	97.35

PARAMETERIZED DGX-A100 NVSWITCH HEAT SINK

10,000x faster !!!



Computational Times (10 parameters, 3 values per parameter)	
Modulus (Training Time)	10,800 V100 GPU hrs.
Traditional Solver (OpenFOAM) 59,049 separate runs (26 wall hours on 12 CPU cores)	18.4 Million CPU hrs.

Improved Physics & Predictions

IMPROVED PREDICTIONS WITH MODULUS

Solution Accuracy Studies

Just channel with no heatsink

Mesh Size and details	Elements	Modulus P drop	Commercial Solver P drop	% diff.
Base mesh	8.5 M	4.45	3.80	17.04
1.3x refinement	14 M	4.45	3.88	14.64
2.7x refinement	23 M	4.45	3.89	14.36
1.2x refinement + Wall refinement	10 M	4.45	4.32	2.95
2.4x refinement + Wall refinement	20 M	4.45	4.40	1.23

FPGA heatsink

Mesh Size and details	Elements	Modulus P drop	Commercial Solver P drop	% diff.
Base mesh + Wall refinement	15 M	27.45	25.23	8.81
1.7x refinement + Wall refinement	25 M	27.45	26.16	4.94

FLOW & TRANSPORT IN A POROUS MEDIA

Stanford University (Cedric G. Fraces)

Buckley-Leverett Equation:

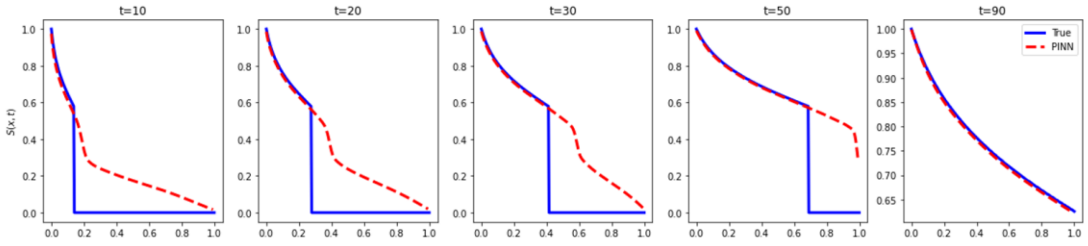
$$\frac{\partial S}{\partial t} + \frac{\partial f(S)}{\partial x} = 0$$

Where the fractional flow f is a nonlinear equation defined as:

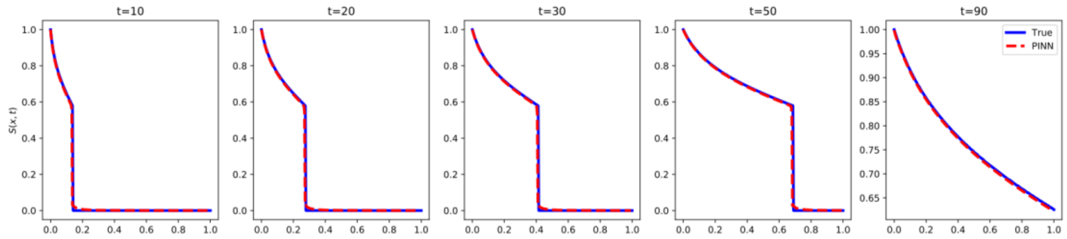
$$f(S) = \frac{(S - S_{wc})^2}{(S - S_{wc})^2 + (1 - S - S_{or})^2/M}$$

subject to constant boundary and initial conditions:

$$\begin{aligned} S(x=0,t) &= S_{inj} \\ S(x,t=0) &= S_{wc} \end{aligned}$$



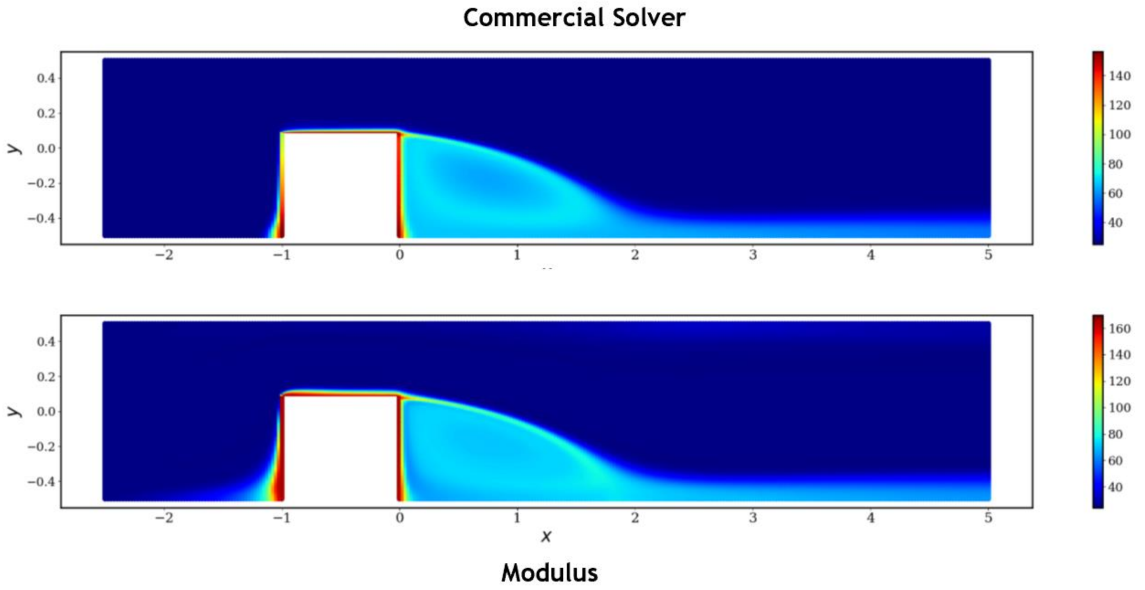
Fuks & Tchelpi (PINNs)



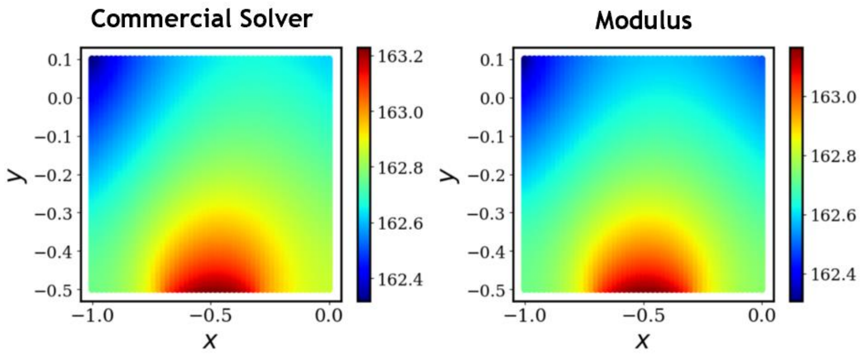
Gasmi & Tchelpi (using Modulus)

MULTI-PHYSICS SIMULATION

Conjugate Heat Transfer – No Training Data!



Fluid Temperature



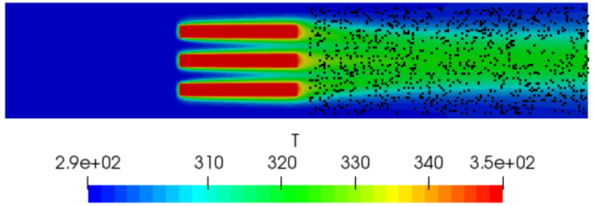
Solid Temperature

Inverse & Data Assimilation Problems

NVIDIA®

INVERSE PROBLEM

Finding Unknown Coefficients of a PDE: Heat Sink



Fluid Heat Convection:

$$0 = \nabla \cdot (D_{fluid} \nabla \theta_{fluid}) - \nabla \cdot (U \theta_{fluid}) \qquad D_{fluid} = \frac{k_{fluid}}{\rho_{fluid} c_{pfluid}}$$

Solid Heat Conduction:

$$0 = \nabla \cdot (k_{solid} \nabla \theta_{solid}) \qquad D_{solid} = \frac{k_{solid}}{\rho_{solid} c_{psolid}}$$

Interface Conditions:

$$\theta_{solid} = \theta_{fluid}$$

$$k_{solid}(N \cdot \nabla \theta_{solid}) = k_{fluid}(N \cdot \nabla \theta_{fluid})$$

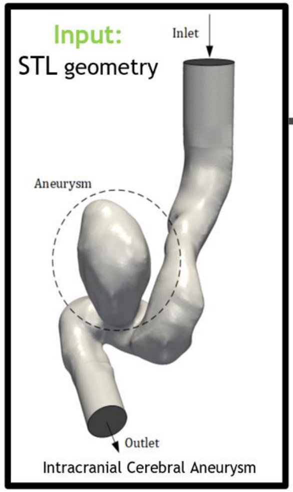
Results:

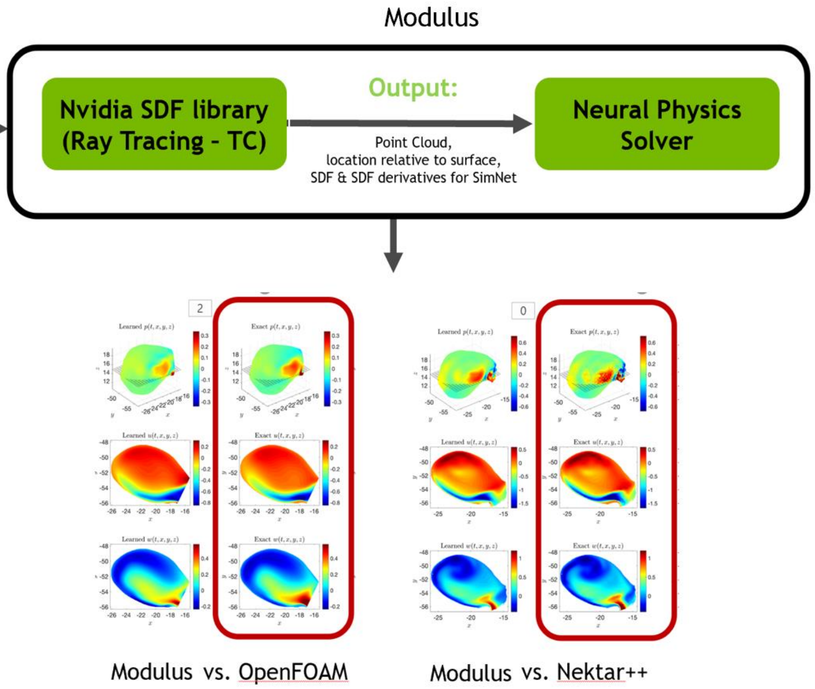
Property	OpenFOAM (True)	Modulus (Predicted)
Kinematic Viscosity (m^2/s)	1.00×10^{-2}	1.03×10^{-2}
Thermal Diffusivity (m^2/s)	2.00×10^{-3}	2.19×10^{-3}

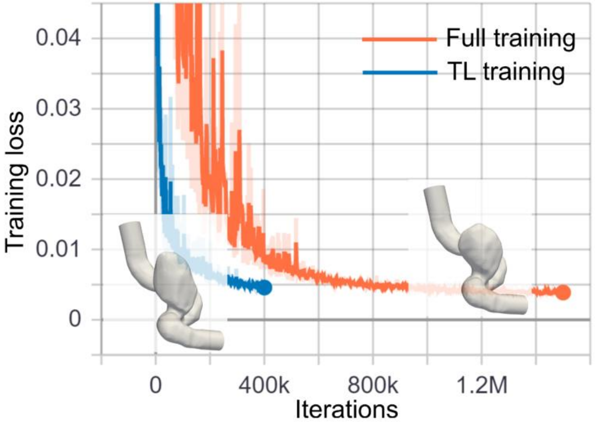
SURGICAL PLANNING

Medical Imaging of an Intra-Cranial Aneurysm

https://www.youtube.com/watch?v=QjY_8xFjsgE





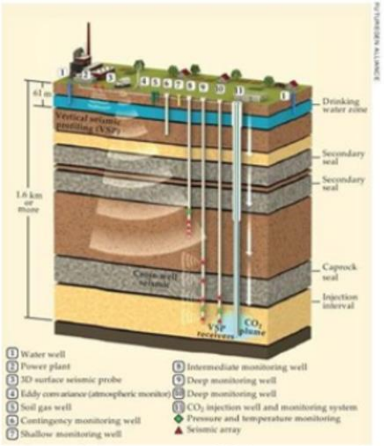


GEOPHYSICS APPLICATION

Seismic Wave Simulations

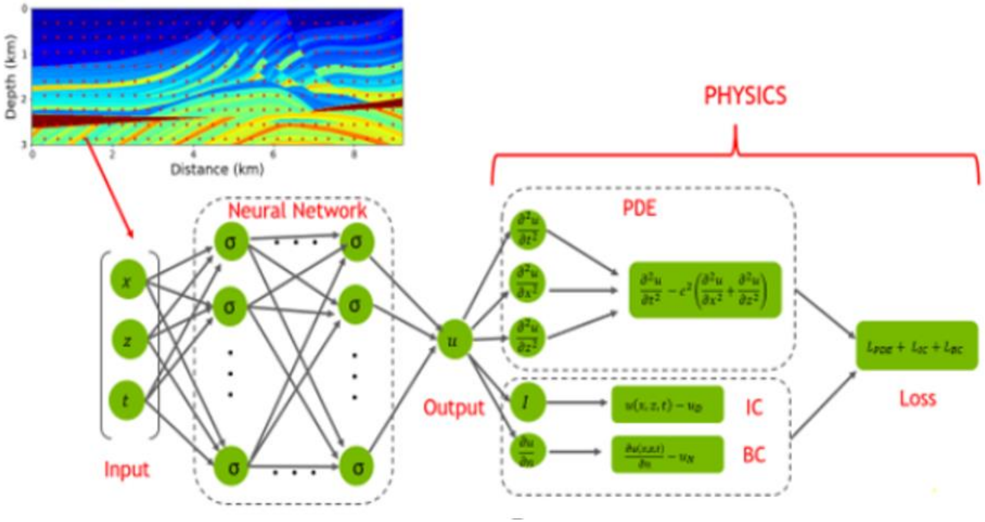
Seismic Imaging:

- An Intense sound source is directed into ground to evaluate subsurface conditions and contamination.
- Receivers called geophones , analogous to microphones, pickup echoes that come back from ground record the intensity and timing of these echoes on computers.
- The data collected is finally processed and turned into images of geologic structure (like MRI scan of brain)



https://geospatial.blogs.com/

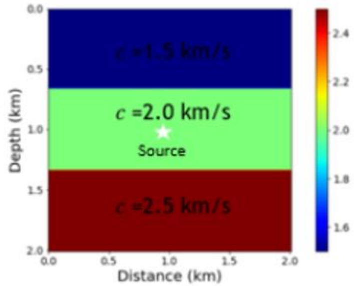
PINN Input : Point cloud representation of subsurface.
PINN Output : Seismic wave



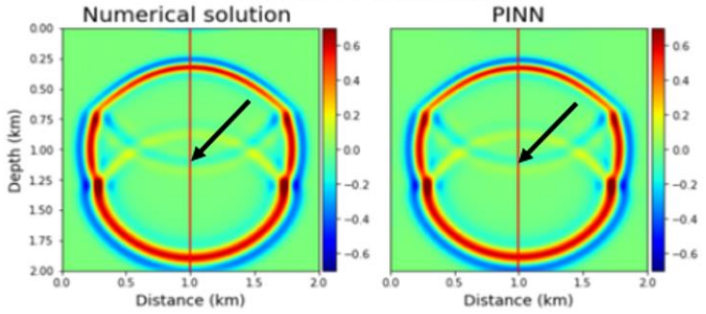
GEOPHYSICS APPLICATION

Seismic Wave Simulations

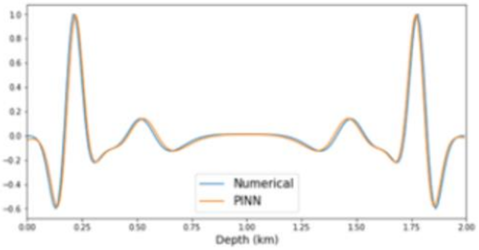
Subsurface model 1:



Seismic wavefields



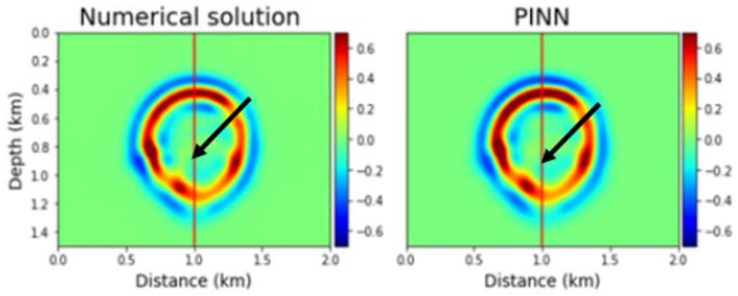
Closer look at the vertical red line:



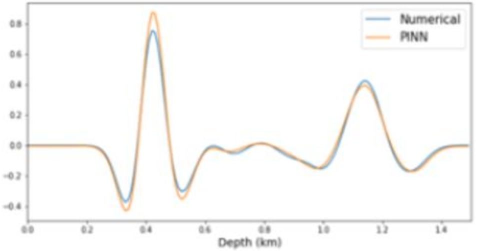
Subsurface model 2:

Source

Seismic wavefields



Closer look at the vertical red line:



CONCLUSION

- Modulus – a framework for Physics based ML
  http://developer.nvidia.com/Modulus
  - Release Notes
  - Installation Notes
  - User Guide
    - Theory
    - Examples
  - API Manual
  - Source Code
  - Example Data Sets

- Continued Development with 3-4 Releases/year

- Contributions from Scientific Community are welcome!