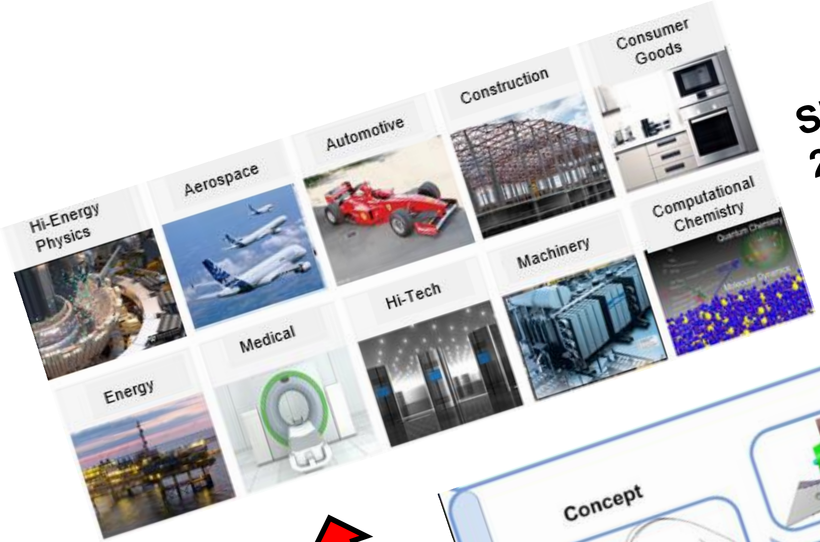
Physics Informed Neural Networks

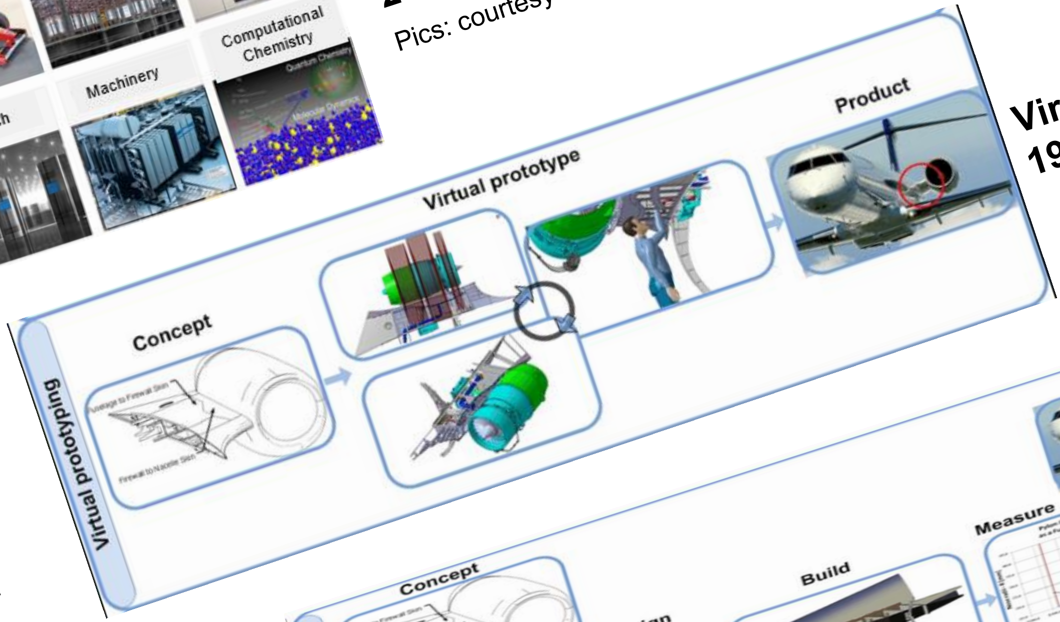
Convergence of HPC & AI domains

- Sanjay Choudhry
NVIDIA

Simulations in Product Development



Simulation is Ubiquitous
2000s-Today
Pics: courtesy Ansys



Virtual Prototyping
1980s-90s

Set-Based Prototyping with Digital Mock-Up Technologies

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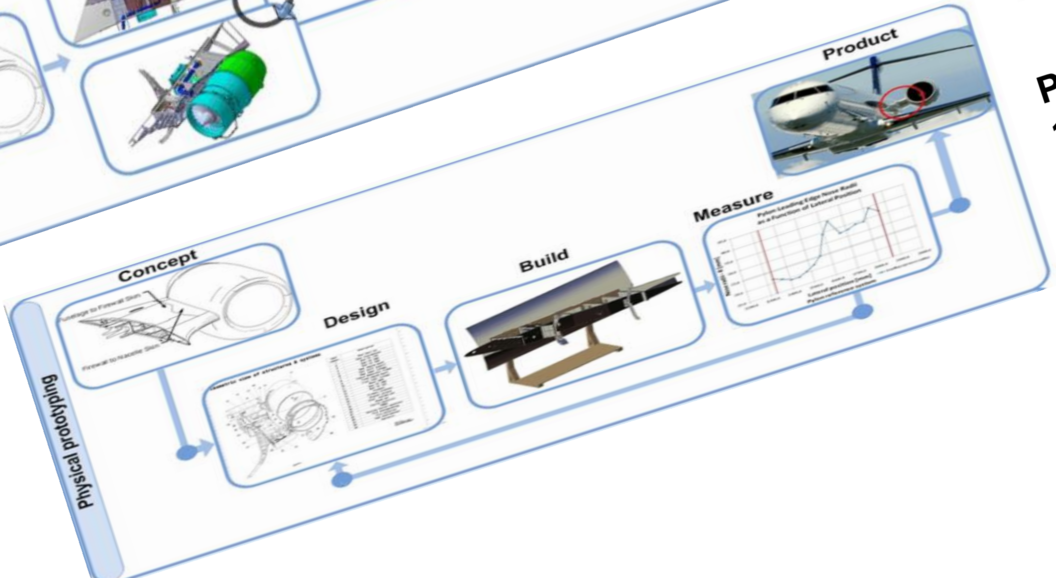
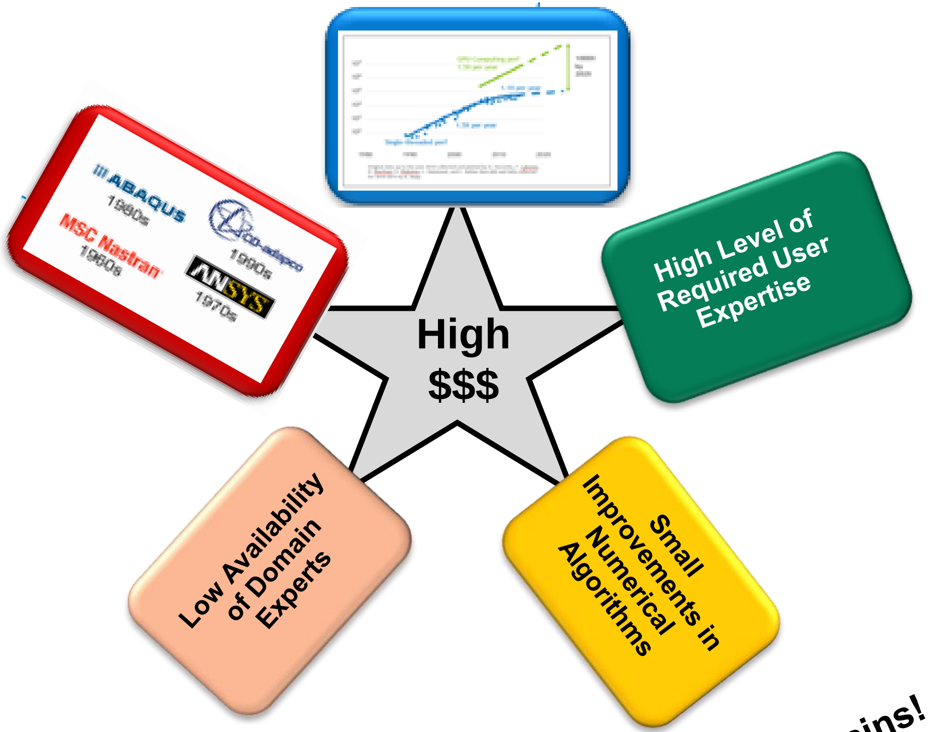
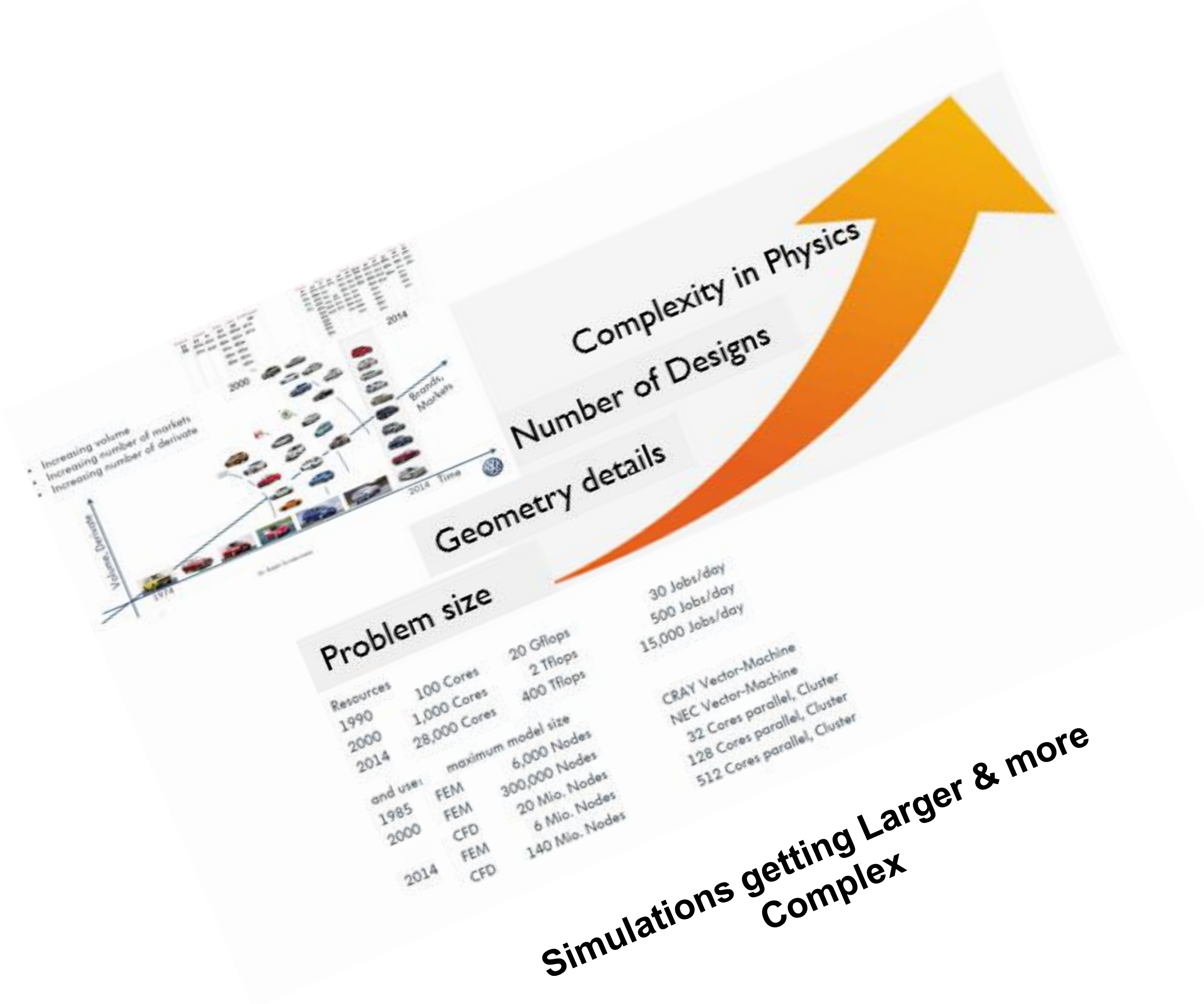


Physical Prototyping
1960s-70s

Saturating Performance Gains with Traditional HPC

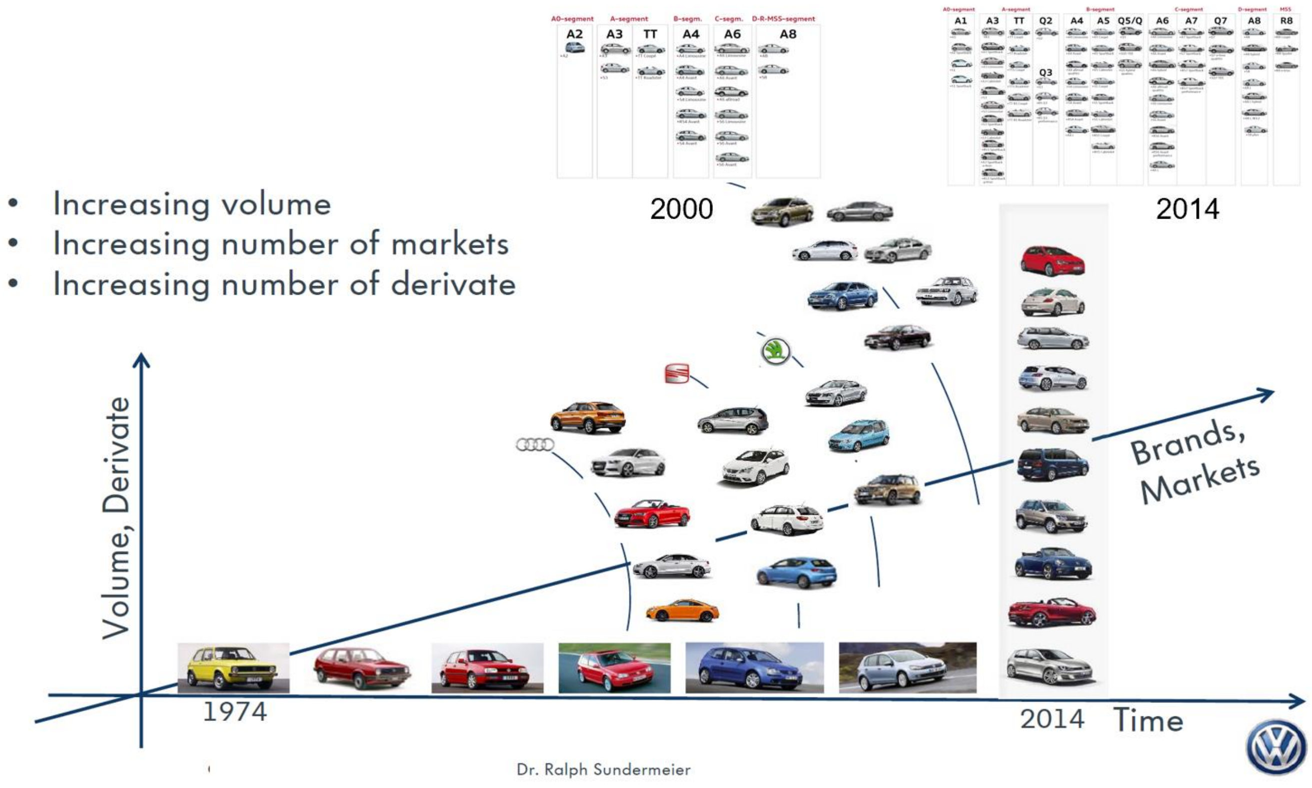


No More Easy Performance Gains!

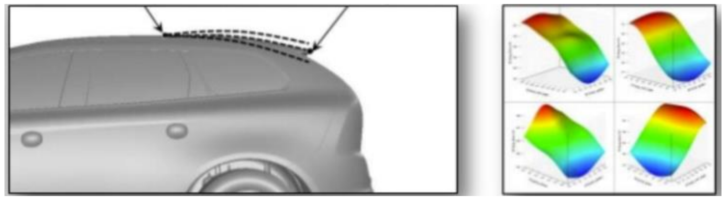


Simulations getting Larger & more Complex

Motivation: Evolving Platform with Mass Customization

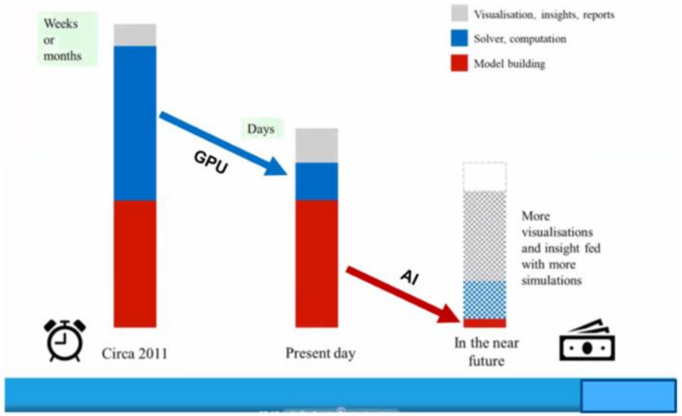


Customized Developments for Audi's OpenFOAM Processes, Richard Borris, Audi AG, Oct. 2016



CFD Aerodynamics Optimization: Computationally Intensive

Answer: AI powered Simulations!



AI in Computational Mechanics & Sciences

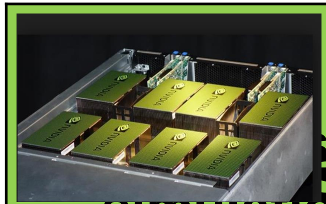
AI Powered Computational Domains

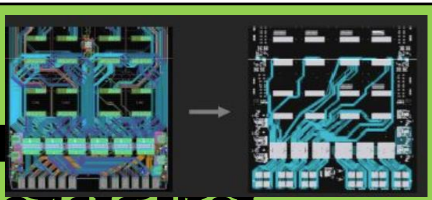
Computational Mechanics	Earth Sciences	Life Sciences	Computational Physics	Computational Chemistry
Solid Mechanics	Climate Modeling	Genomics	Particle Science	Quantum Chemistry
Fluid Mechanics	Weather Modeling	Proteomics	Astrophysics	Molecular Dynamics
Electromagnetics	Ocean Modeling			
Thermal	Seismic Interpretation			
Acoustics				
Optics				
Multi-body Dynamics				
Systems				
Electrical				
Designer Materials				

AI benefits in Computational Mechanics & Sciences

Primary Driver

Physics



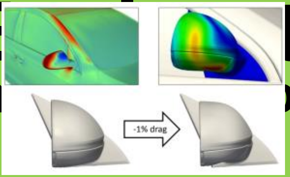


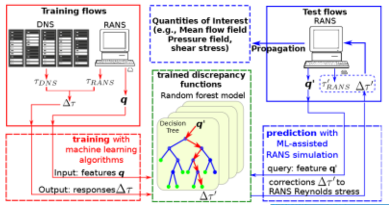
Design: AI simulation surrogate that allows ... ping of many ... optimization

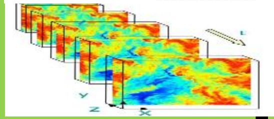
Design Exploration

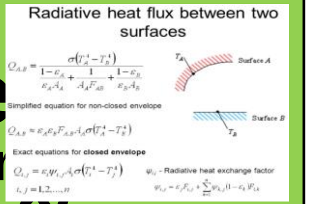
Heat Sink

Vias on a PCB









Improve accuracy ... of empiri... ... works ... rate ... periments

Physics

Turbulence

Radiation

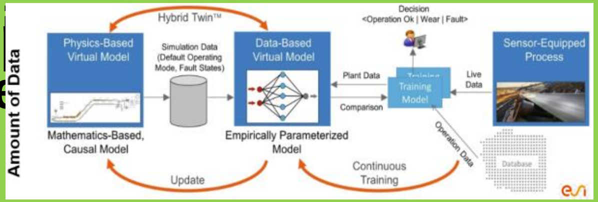
Data

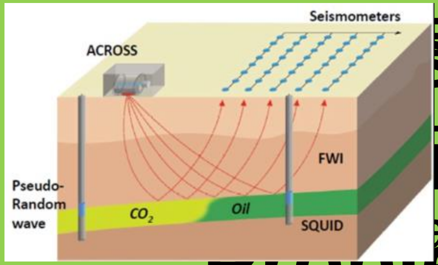
Reduced Time to Decision: Rapid results for a single model ... trained ne...

Real Time Si...

Digital Twin - IoT/Simulation

Robotics





Expert ... Quant...n: ... y ... from ... observation with calculations

... Problems

Full Wave Inversion

Aneurysm

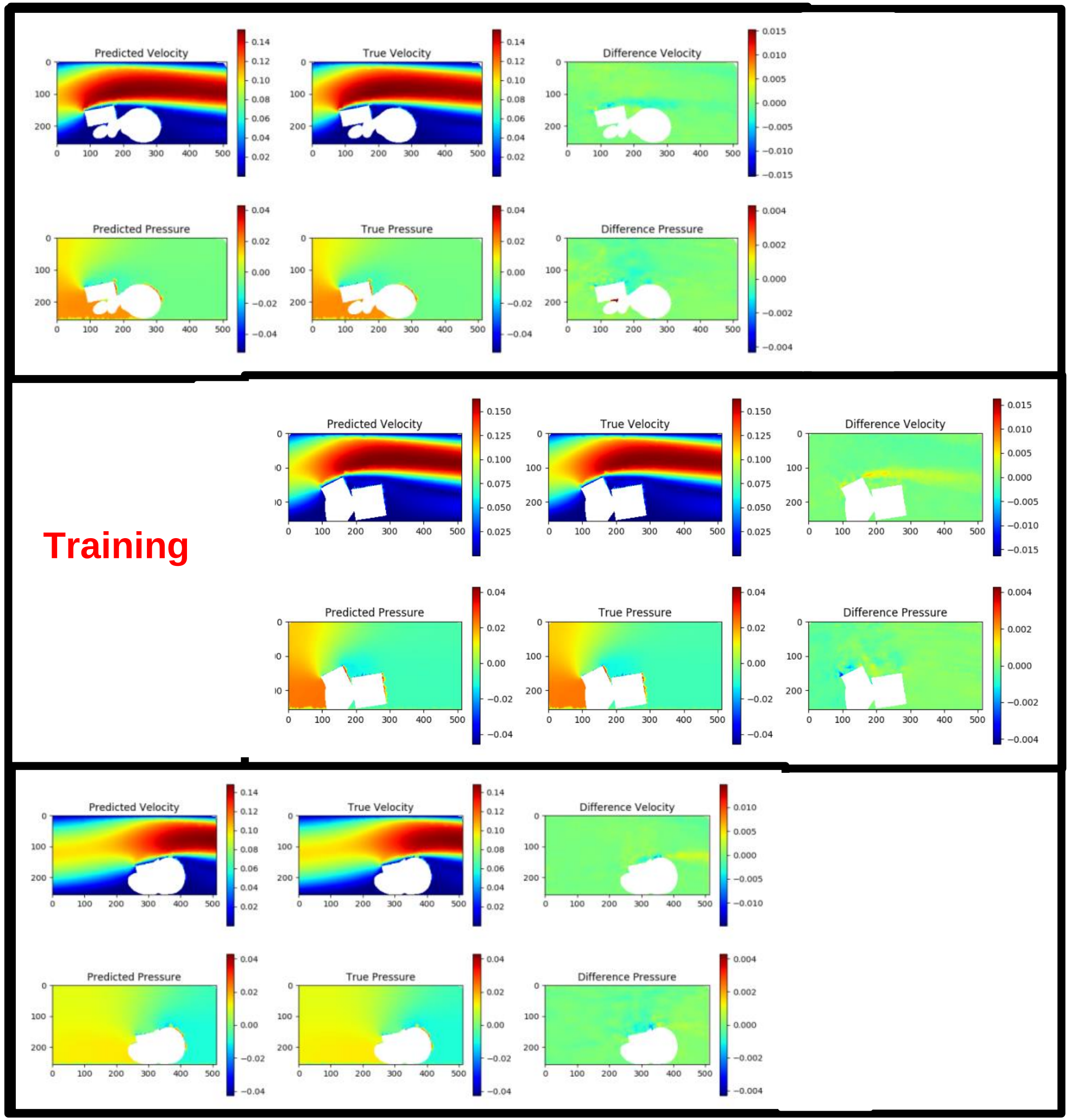
Large to Very Large

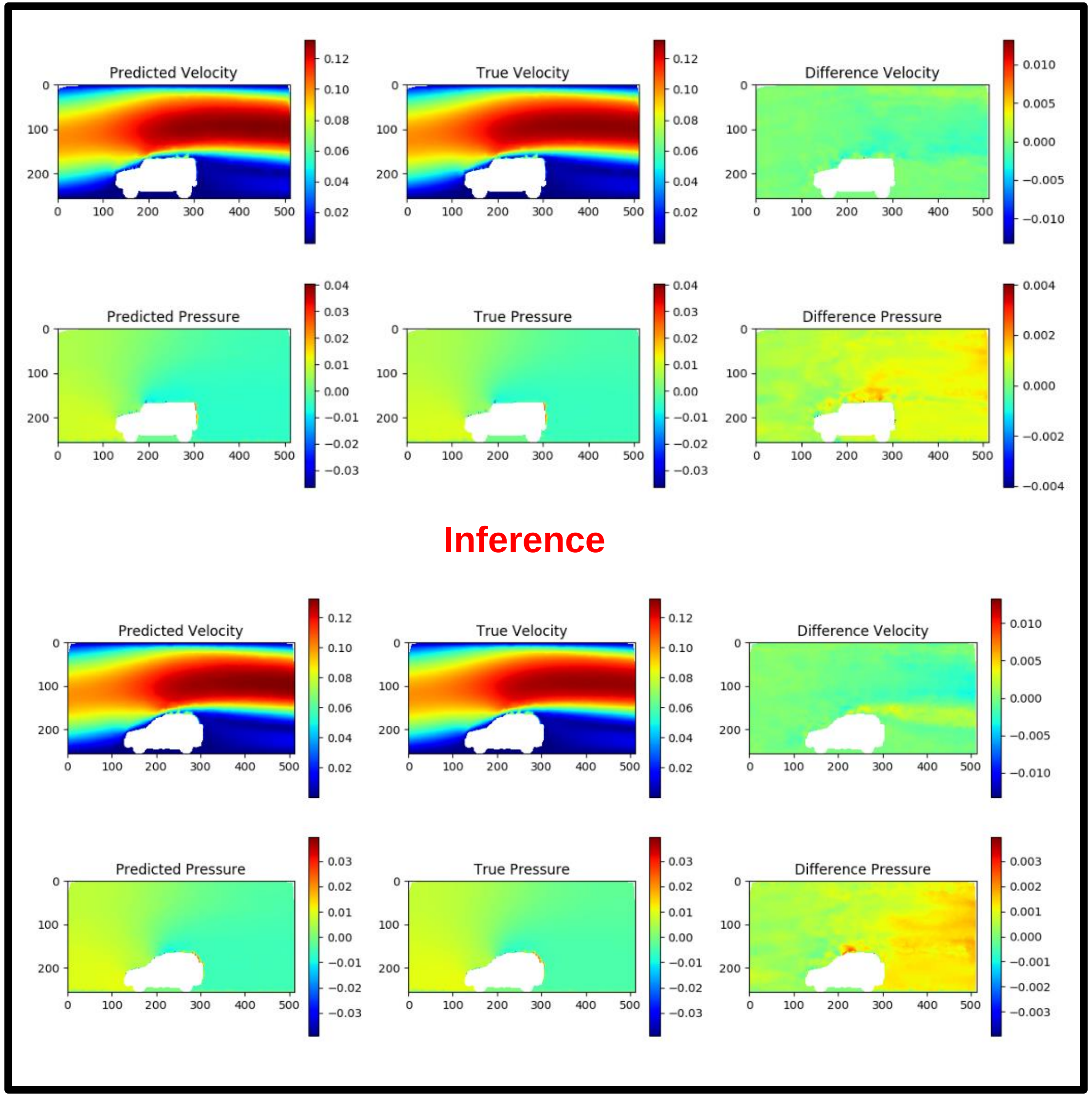
Training Data

Small to Medium

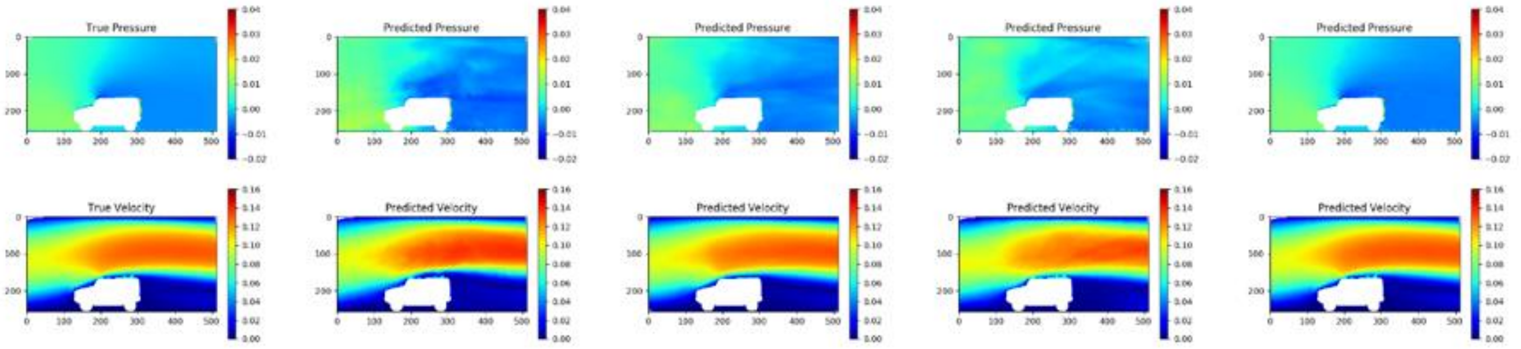
Data Driven Neural Networks (DDNNs)

Automotive Aerodynamics

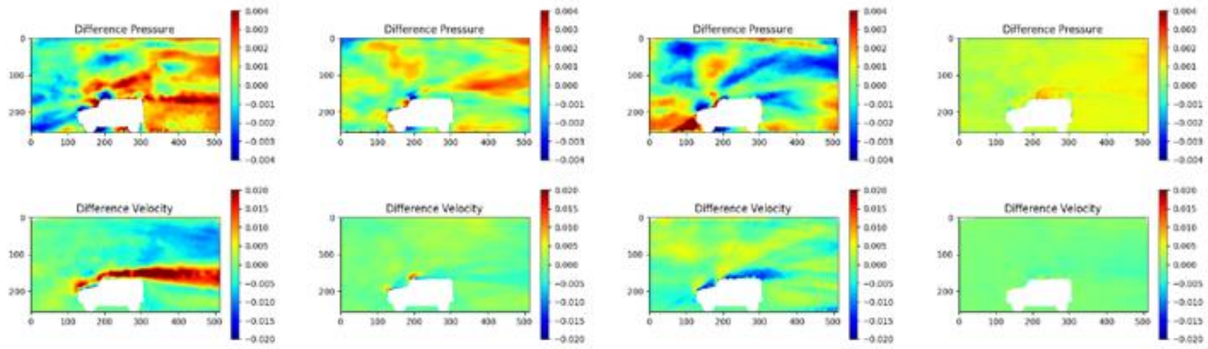




Comparisons of various Point Cloud based NN



(a) Ground Truth (b) PointNet++ (c) PointNet++ B.O. (d) DGCNN (e) DGN



(a) PointNet++ (b) PointNet++ B.O. (c) DGCNN (d) DGN

Data Driven Methods

- Need to generate a lot of Simulations
- No Physics Awareness
- Not very efficient for Complex 3D Geometries/Curved Surfaces
- Interpolation/Extrapolation Errors

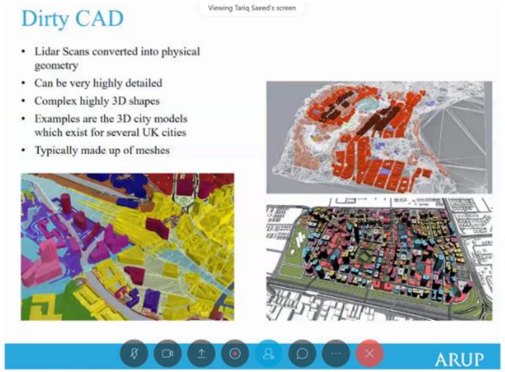
+ Not dependent on Physics

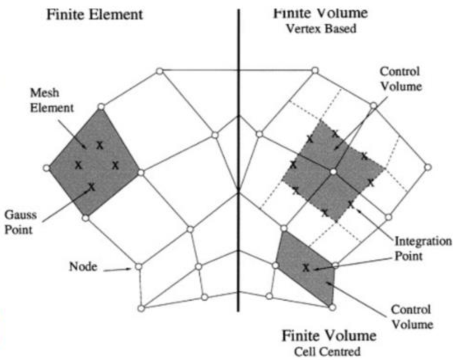
Physics Informed Neural Networks (PINNs)

Physics Informed Neural Nets: Architecture

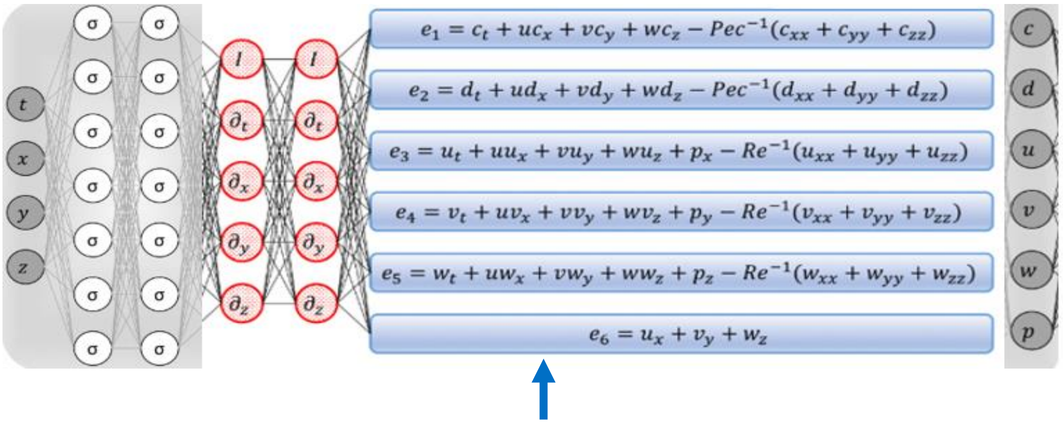
A Neural Network Architecture for Computational Mechanics/Physics problems

- ❑ **Point Cloud for 3D Geometries & Meshes (Fixed/Moving, Deforming, Structured & Unstructured)**
- ❑ **Physics Driven & Physics Aware Networks (respects the governing PDEs, Multi-disciplinary)**
- ❑ **Performance optimized for GPU tensor cores**





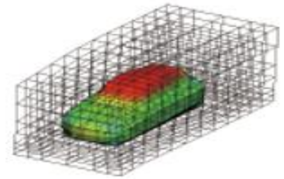
Point Cloud representation of Computational Domain & Data on 3D Geometries



PINN - Physics Informed Neural Networks

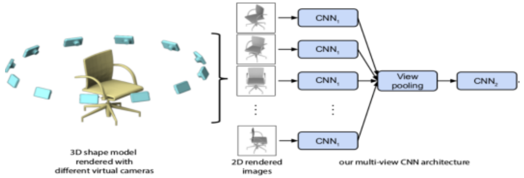
Shape Parameterization

- **Voxels**



- Good for CNNs but memory intensive for high resolution and inefficient due to unoccupied voxels.
- Introduces quantization effects for inter- & extrapolation when using CNN, accuracy for Physics problems is questionable

- **Multi-View**



- Unable to capture fine geometry details & gradients and completely unsuitable for Physics problems

✓ **Point Cloud**

Input: 3D Scene Point cloud

- One-to-one correspondence with analysis data format.
- Works for LIDAR based geometry or uneven density and unstructured meshes. Perfect for Physics problems

- **Poly Cube**

level-1

- Will require integration into CAD tools in order to regenerate uniform mesh and then invoke CNN structure
- Will retain the deficiencies of Voxel based CNNs
- Does not address legacy analysis results

Loss and Output

Physics laws present constraints –

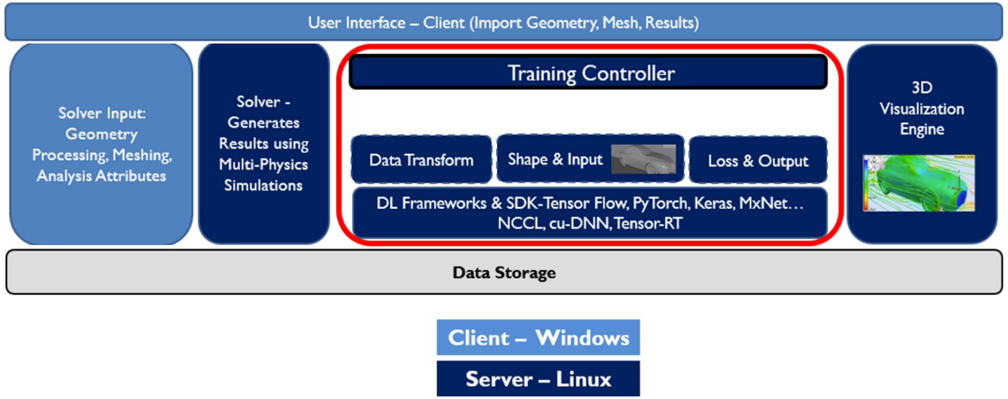
- Governing differential equations
- Constitutive models

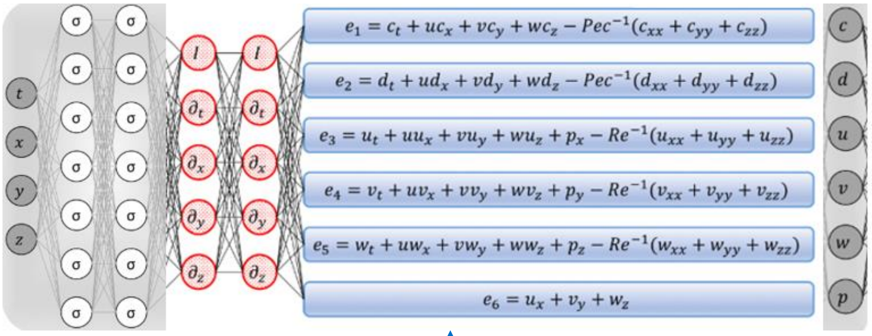
Loss Function

✓ Physics based: Conservation of Mass, Momentum & Energy, Strain Energy etc.)

$$f_{obj} = \sum_i w_i \left\{ \nabla \cdot \left(u_t^\star - \frac{1}{\rho} \nabla \hat{p}_t \right) \right\}_i^2$$

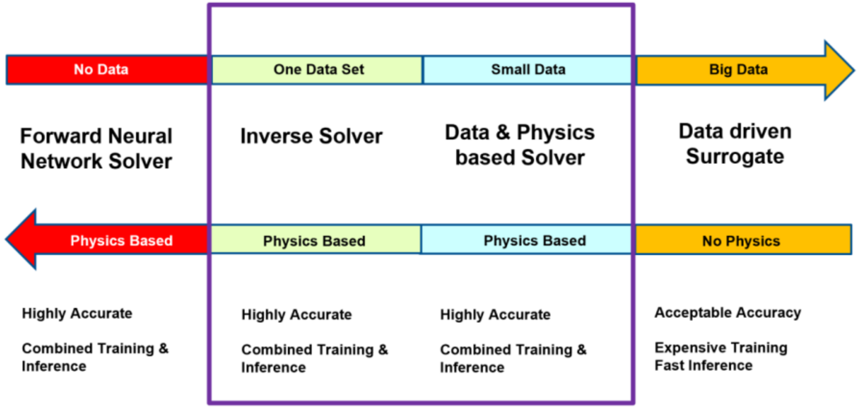
Workflow –





PINN - Physics Informed Neural Networks

Discovering Hidden Physics



Hidden Physics Models in CFD:
Infer hidden quantities of interest fields from spatial-temporal visualizations of a passive scaler (e.g., dye or smoke) leveraging the underlying Physics laws (i.e., mass, momentum & energy)

Mass conservation:

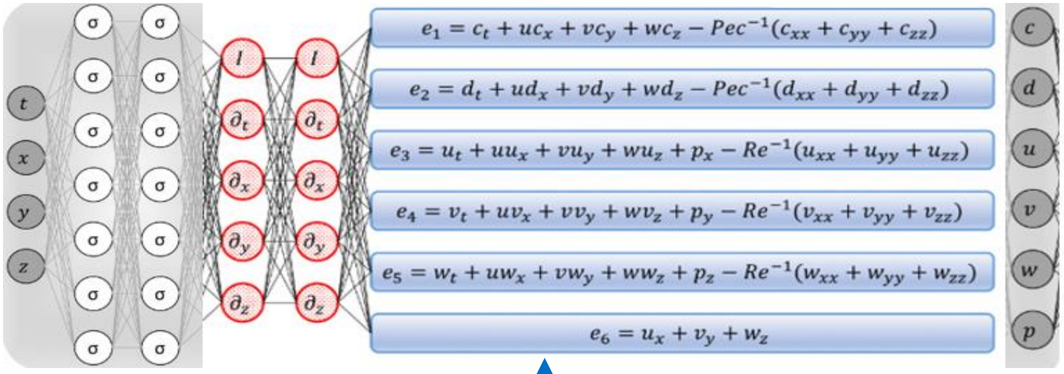
$$u_x + v_y + w_z = 0.$$

Momentum conservation:

$$u_t + uu_x + vu_y + wu_z = -p_x + \mathrm{Re}^{-1}(u_{xx} + u_{yy} + u_{zz})$$
$$v_t + uv_x + vv_y + wv_z = -p_y + \mathrm{Re}^{-1}(v_{xx} + v_{yy} + v_{zz})$$
$$w_t + uw_x + vw_y + ww_z = -p_z + \mathrm{Re}^{-1}(w_{xx} + w_{yy} + w_{zz})$$

Transport:

$$c_t + uc_x + vc_y + wc_z = \mathrm{Pec}^{-1}(c_{xx} + c_{yy} + c_{zz})$$

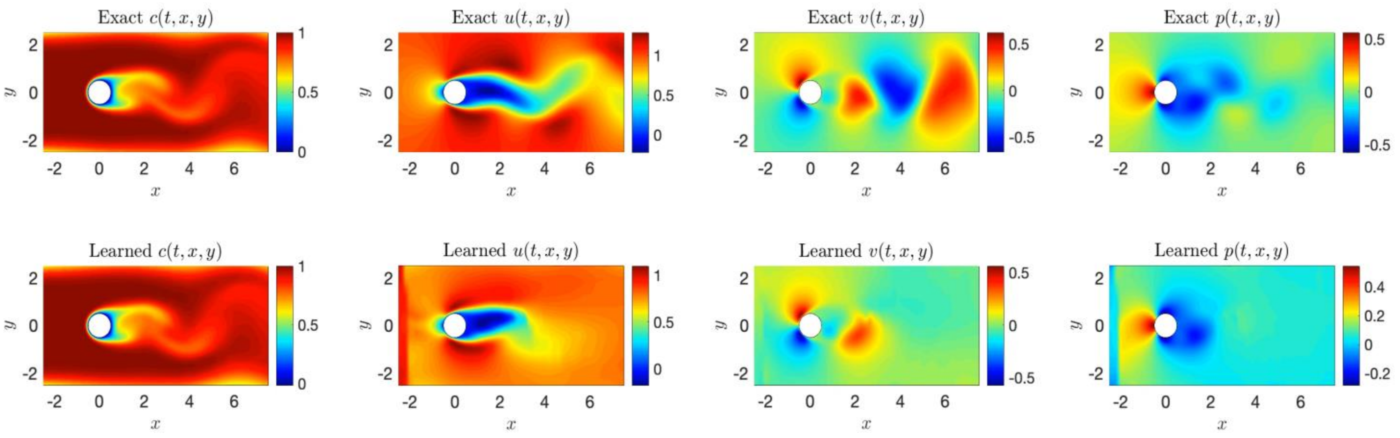


PINN - Physics Based Neural Networks

External Flow past a Cylinder - Learnt vs. Ground Truth

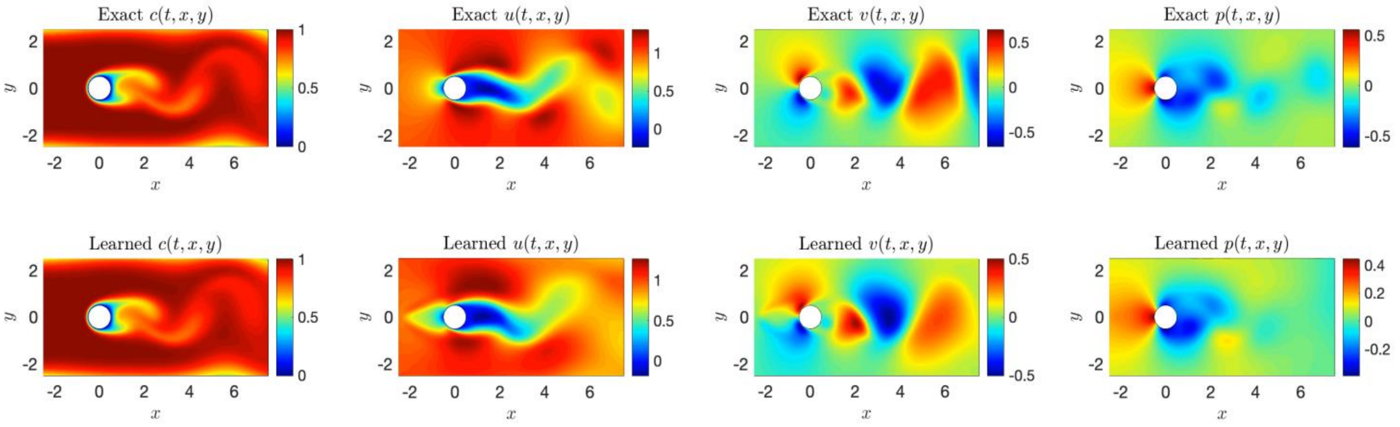
CFD Simulation of an **External Flow over a Cylinder** with OpenFOAM –

A user error was incidentally discovered by the PINNs that presented itself as a mismatch between the Simulation & AI result !!!

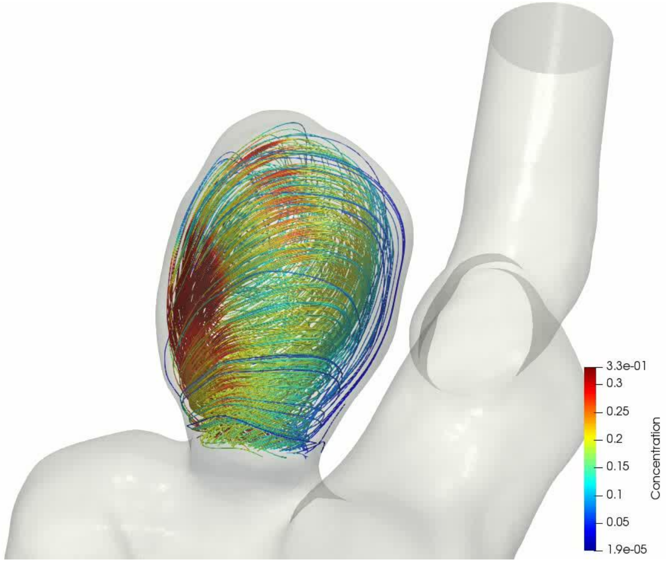


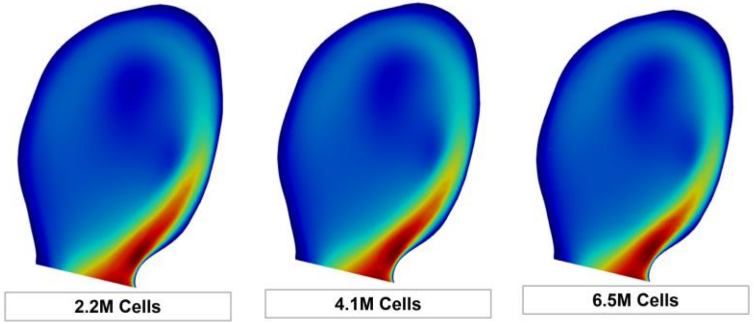
Correct CFD Simulation Results with OpenFOAM (Ground Truth)

Correct Predictions

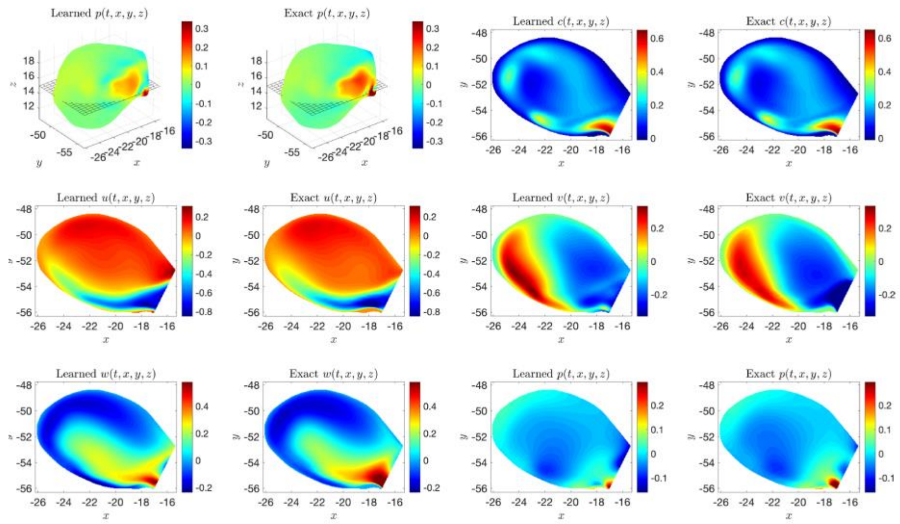


Intracranial Cerebral Aneurysm (ICA)

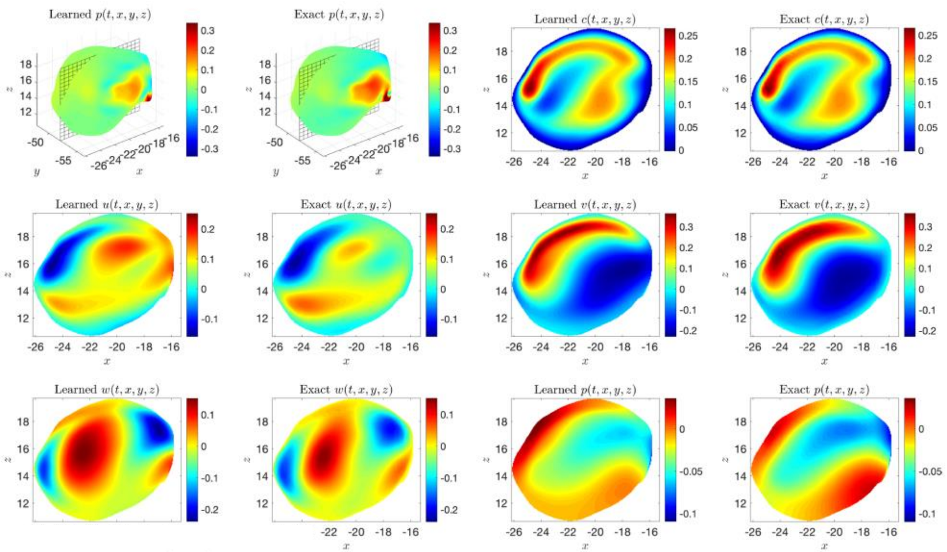




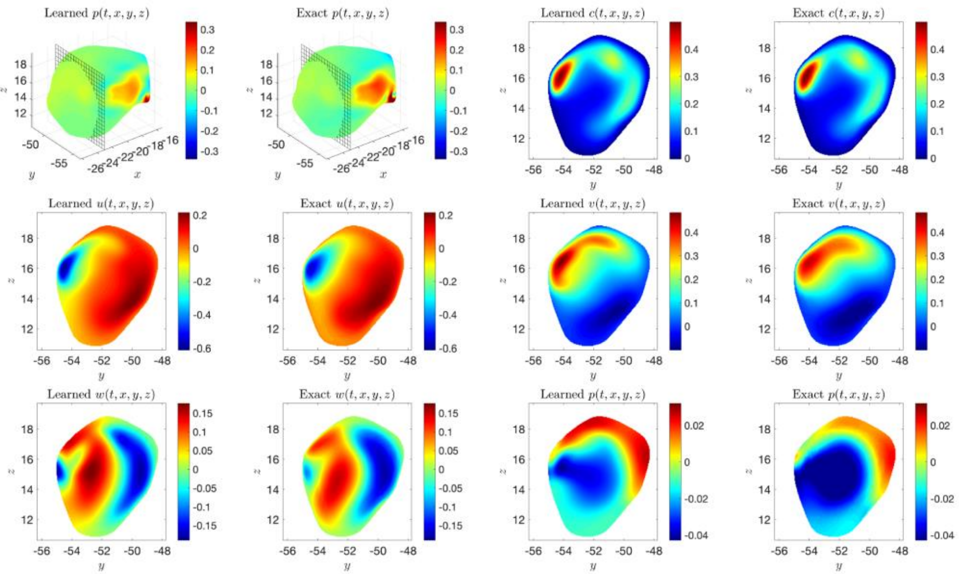
ICA - Comparison between Simulation & NN



Cut along Z-Plane

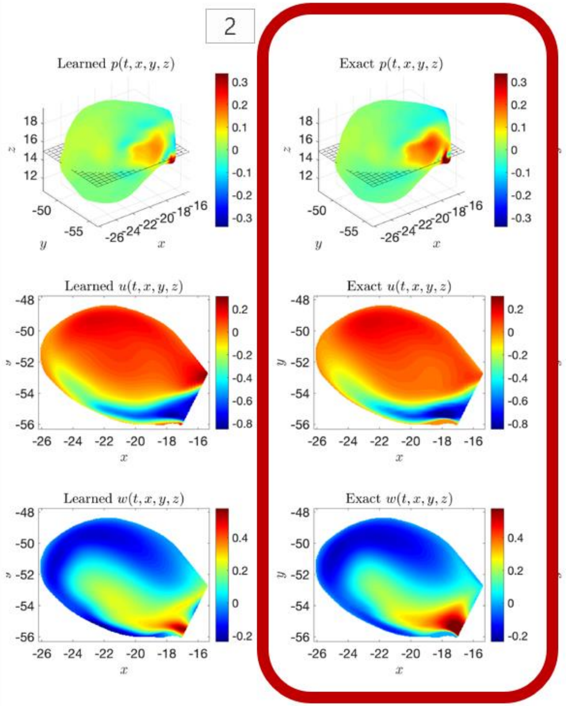


Cut along Y-Plane

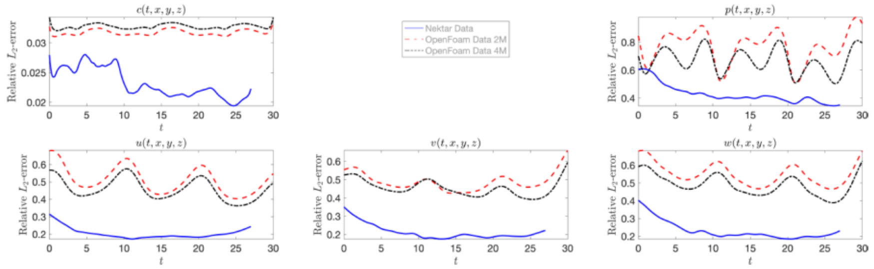


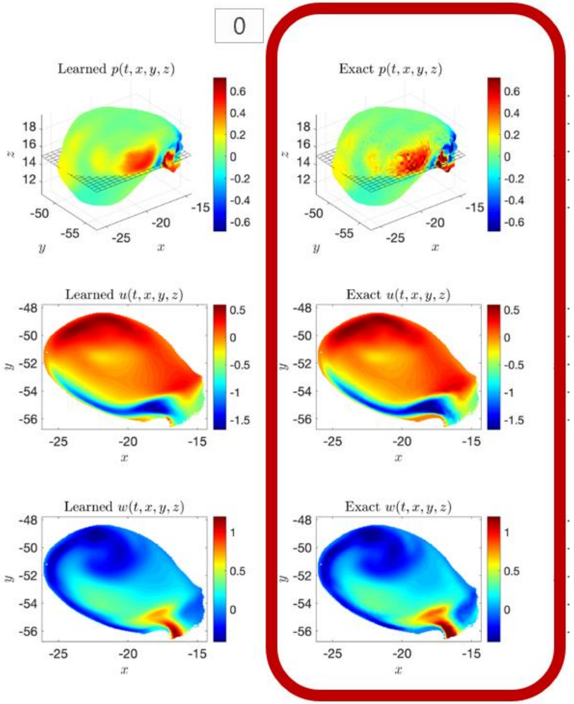
Cut along X-Plane

ICA – Comparison between two CFD Solvers



OpenFOAM v/s Neural Networks





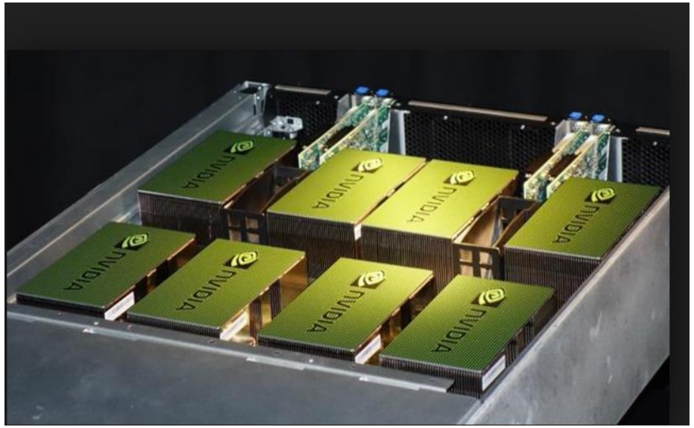
Nektar++ v/s Neural Networks

- **Nektar++ is a higher fidelity solver (implicit, h- & p- method based finite element CFD code) and provides higher quality results with less diffusion**

Heat Sink

Heat Sink –
* Temperatures to not exceed the design criteria

Objectives –
* Similar accuracy as the Solver
* Geometry representation with Point Clouds
* Multiple simultaneous parametrized &
  unparametrized geometries



Physics involved – CFD & Heat Transfer

Ansys IcePack used for Simulation (** we kindly acknowledge Ansys's support **)

Heat Sink - Conjugate Heat Transfer

$$MSE = \frac{1}{N}\sum_{i=1}^{N} |d(x_i, y_i) - d_i|^2.$$

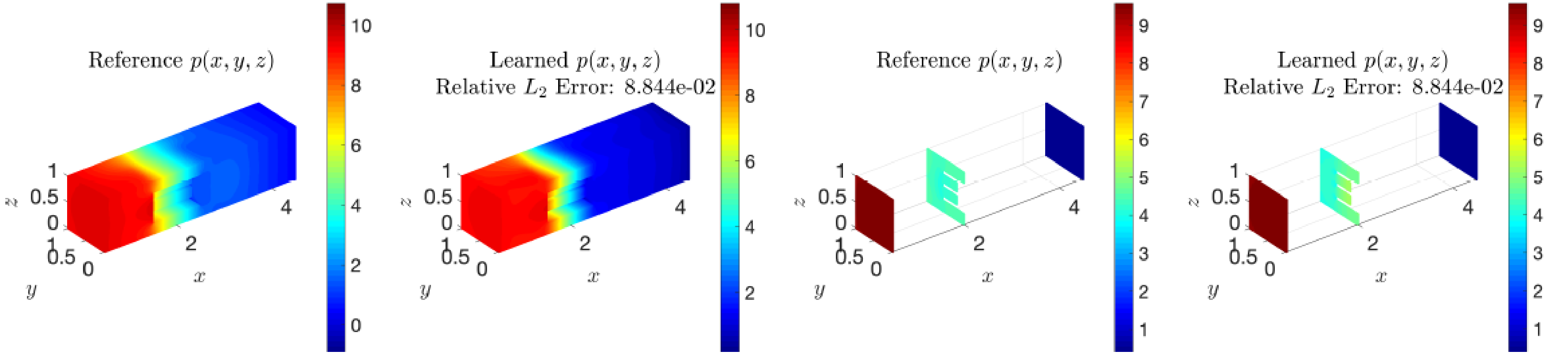
Mean Square Error

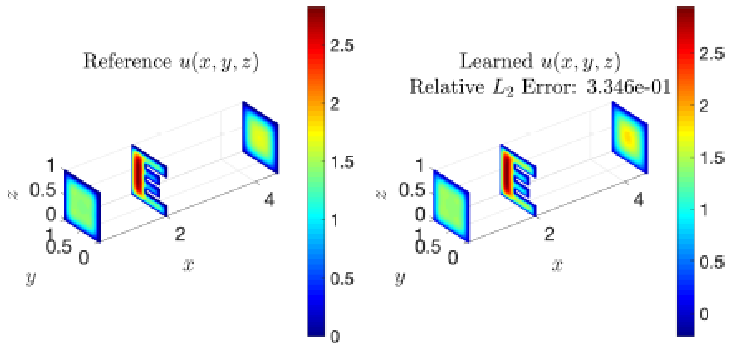
$$\begin{aligned}
e_1 &:= uu_x + vu_y + p_x - (\nu + \nu^t)(u_{xx} + u_{yy}) - 2(\nu^t_x s^{xx} + \nu^t_y s^{xy}),\\
e_2 &:= uv_x + vv_y + p_y - (\nu + \nu^t)(v_{xx} + v_{yy}) - 2(\nu^t_x s^{xy} + \nu^t_y s^{yy}),\\
e_3 &:= u_x + v_y,\\
e^f &:= u\theta^f_x + v\theta^f_y - (\kappa^f/c^f_p + \kappa^t/c^f_p)(\theta^f_{xx} + \theta^f_{yy}) - (1/c^f_p)(\kappa^t_x\theta^f_x + \kappa^t_y\theta^f_y),\\
e^s &:= -\alpha^s(\theta^s_{xx} + \theta^s_{yy}).
\end{aligned}$$

Loss

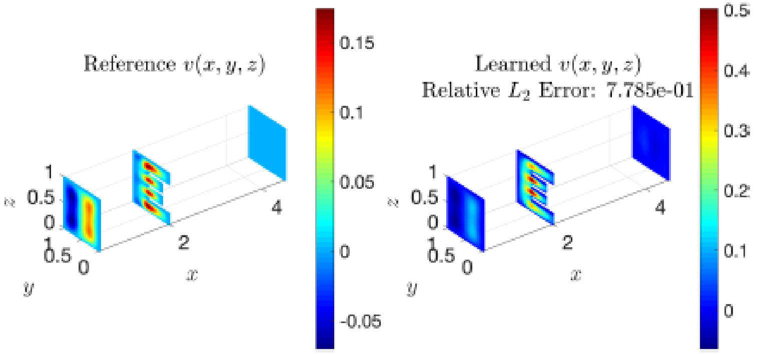
Point Clouds used for modeling Geometry

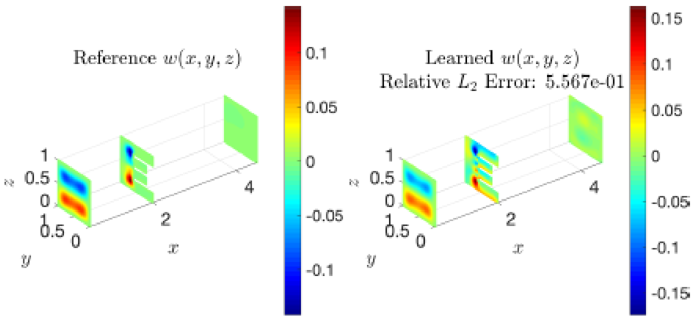
Heat Sink - Conjugate Heat Transfer





Turbulence modeled





Conclusion

Executive Summary

Neural network for simulation workflows:

- ✓ **Higher Performance:** gains on CPU are fast approaching saturation point. AI speeds up the “time-to-insight, design, manufacture and service”

- ✓ **Broader application areas:** Never before imagined scientific simulations use-cases are now possible with AI

- ✓ **Broader user base:** Increased ease-of-use and robustness in the simulation workflow will enable increased number of users with little simulation expertise