AI/ML and Simulation in the Context of Product Innovation

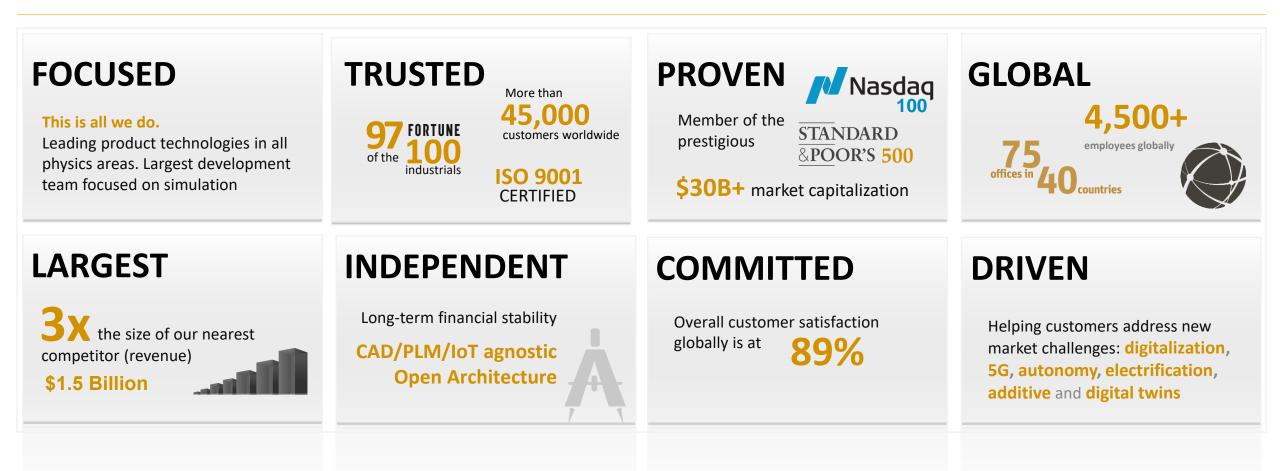
Prith Banerjee, Ph.D. Chief Technology Officer, Ansys

November 4, 2020

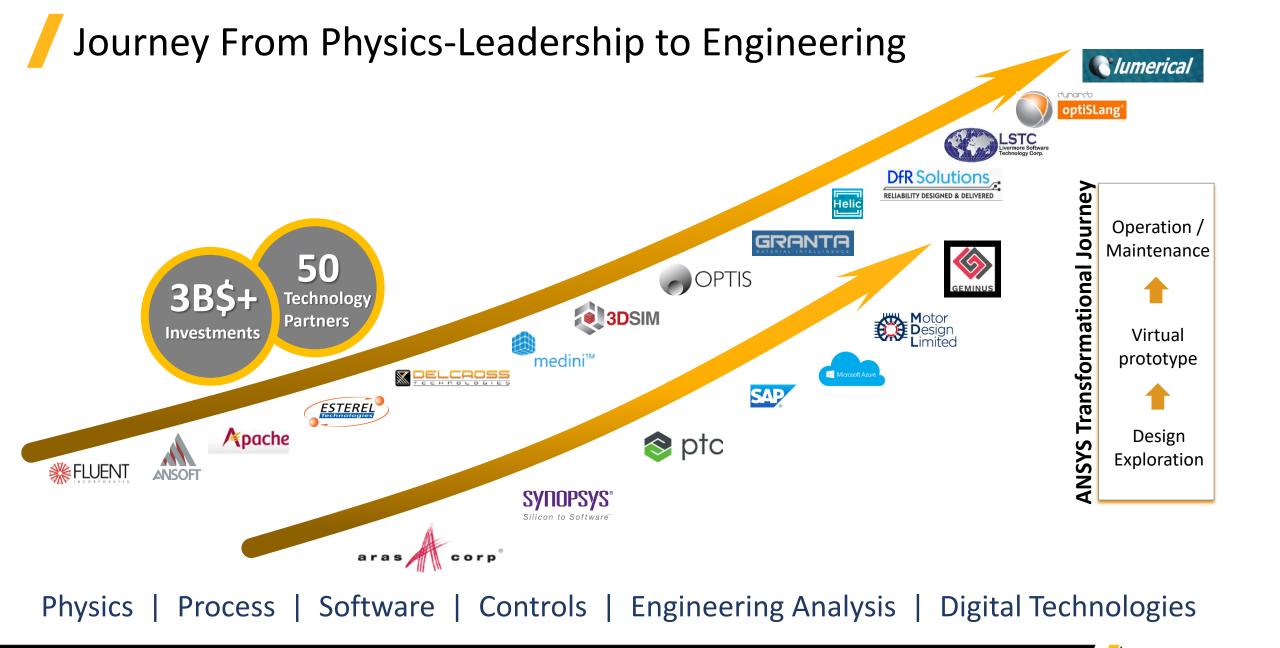


Ansys is the Simulation Leader

MISSION: Empower our customers to design and deliver transformational products



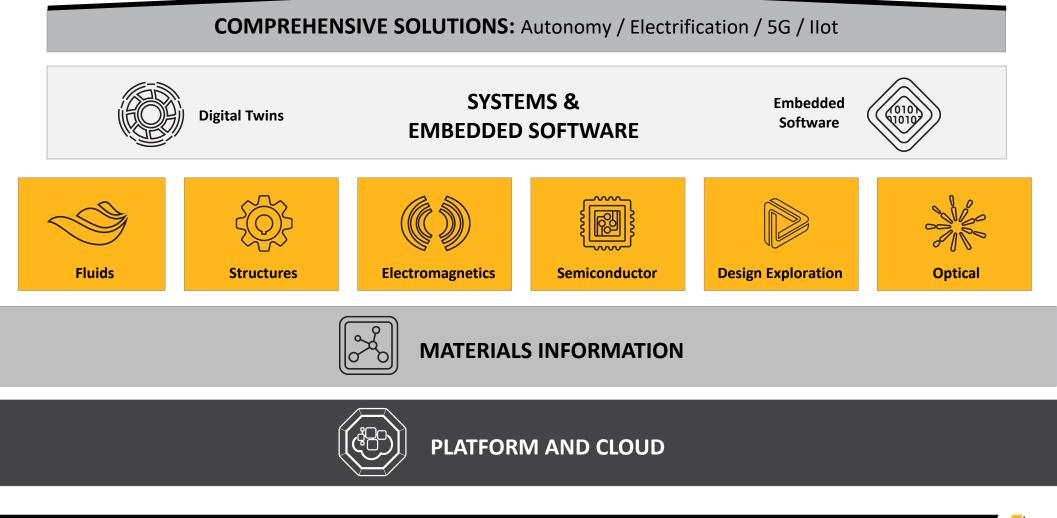






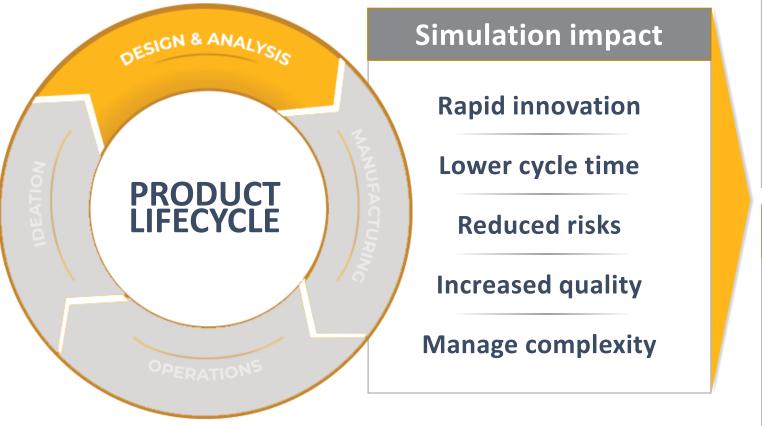
Ansys

Ansys Offers the Only True Simulation Platform





Simulation Impacts Top-Line Growth And Bottom-Line Savings



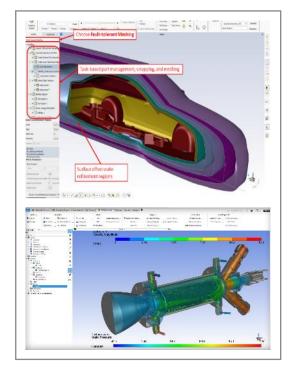
Revenue growth Offer more products Launch right products **Faster time to market Cost savings** Improved R&D efficiency

Fewer physical prototypes

Lower warranty costs

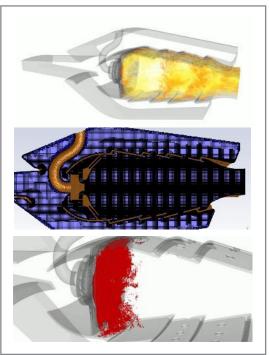


Fluids R&D directions



PRODUCTIVITY

- Workflows
- Customer driven
- Speed and robustness
- GPU based post processing
- Usability and repeatability



GAS TURBINES

- Combustion physics
- Numerics
- Spray physics
- Turbulence
- Best practices

EXTERNAL AERODYNAMICS

- Speed
- Accuracy
- Robustness
- Hypersonic physics
- Multiphase flows

ELECTRIFICATION

- Conjugate Heat Transfer Electro-Chemistry
- Battery Life
- Capacity fade
- Process and Chemical Industries



Structures R&D Directions

APPLICATION SPECIFIC

- Medical Initiative: heart simulation
- Electrophysiology, Incompressible flow, FSI, Adv. Mat.
- Additive Manufacturing
- Machine learning for faster thermal solutions
- Microstructure & property predictions
- Battery modeling in crash analysis

MATERIALS

- Multiscale Data Driven framework, Short fibers
- Crystal plasticity
- Elastomers fatigue, inelastic fracture
- Thermo mechanical fatigue with damage
- ICME

EQUATION SOLVERS

- Data driven means to assess resource needs
- Low Rank meth. for acoustic wave equations
- Efficient scheduling for HPC performance

AUTOMOTIVE APPLICATIONS

- Streamlined Welding for Automotive Chassis
- New Meshing and geometry Enable Optimization Workflows

ELECTRONICS RELIABILITY

- Best-in-class pre-processing for seamless model exchange
- Coupling Ansys Mechanical and Sherlock

MORPHING-BASED OPTIMIZATION

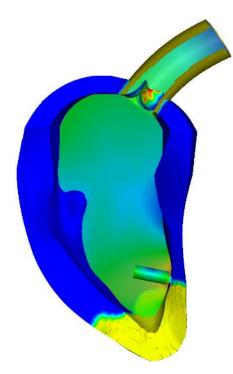
- Better topology optimization
- Automatic creation of clean CAD

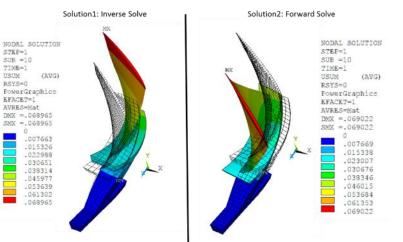
SOLVER METHODS

- Iso Geometric Analysis (IGA)
- Inverse methods
- Dual Lagrange Multiplier methods for contact
- Manufacturing constraints in Topo Optimization

SOFTWARE

- DCS:
- Distributed Log Service
- HPC 2.0 HPC on demand
- System Coupling for multi-physics







Electromagnetics R&D Directions

AUTOMATION AND PERFORMANCE

- Streamlined electronics workflows for package and board
- Integration with thermo-mechanical for new applications

ANTENNA

• Advances in phased array antenna analysis with scalable HPC.

SEMICONDUCTORS

- RaptorH combines Helic's RaptorX with Ansys HFSS,
- Gold standard verification for sensitive 5G integrated circuits

ELECTRIFICATION – RELIABILITY AND NVH

• New thermal and vibrational analysis coupled with Maxwell

ANSYS HFSS

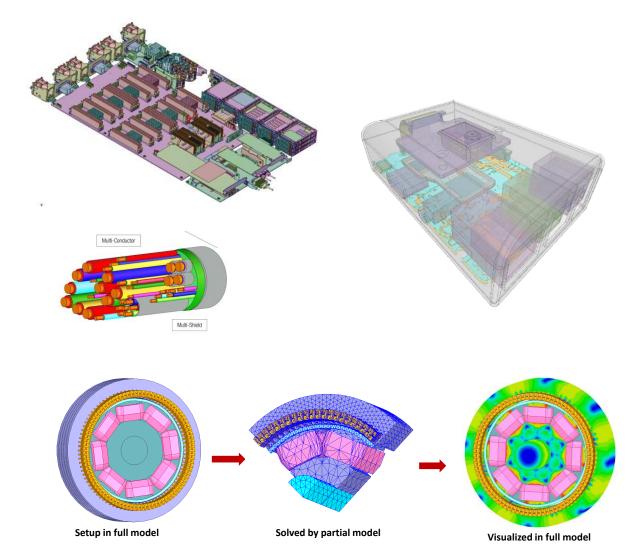
- Enhanced distributed direct matrix solver available on Cloud.
- Significantly reduced memory
- Scales to 100's of cores.

NEW ANSYS EMA 3D PRODUCT

• Models EMI/EMC between complex cables

NEW CAPABILITIES IN ANSYS MAXWELL

• Speeds simulation by creating/solving model for rotating machines.





Ansys Long-Term Technology Strategy Dimensions



ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING

- Simulation used to train AI methods
- Al used to improve simulation



DIGITAL AND PHYSICAL WORLDS

- AR/VR for Simulation brings digital world to physical
- IOT and Connectedness brings physical world to digital



PLATFORM FOR MULTIPHYSICS SIMULATION

- Robust Multiphysics, Multi-disciplinary Optimization
- Micro-services for simulation



DIGITAL TRANSFORMATION

- Digital Threads, Digital Continuity, Digital Twins
- Model Based Systems Engineering



HYPERSCALE SIMULATION, COLLABORATION ON CLOUD

- GPU, SMP, MPI, task based
- Quantum computing



COMPUTATIONAL METHODS IN NEW AREAS

- Integrated Computational Materials Engineering
- Computational Chemistry, Biology, Healthcare, Photonic IC



PREDICTIVE AND ROBUST DESIGN

- High accuracy, adaptive numerical methods
- Materials variation and uncertainties



FUTURE OF SIMULATION

- ML based PDE -Solver, generative design
- Integrated synthesis and verification
- Automated mixed mode (0D-4D), MF, MS simulation

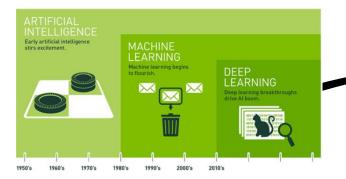


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AI/Machine Learning and Simulation

Machine Learning, defined by Arthur Samuel, 1959:

"Field of study that gives computers the ability to learn without being explicitly programmed".



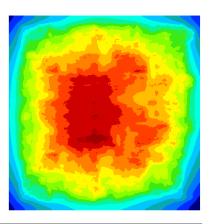
Machine Learning Methods

- Supervised Learning
- Unsupervised Learning
- Semi-supervised Learning
- Reinforcement Learning



AI/ML Use Cases

- Customer Productivity
- Augmented Simulation
- Engineering Design
- Business Intelligence



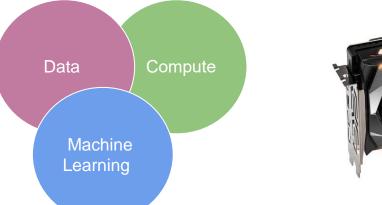
Engg. Simulation Methods

- Geometry/Meshing
- 3D/4D Finite Element/Volume
- Physical/Math Models
- Reduced Order & System Models, Digital Twins
- Postprocessing/Visualization



Why is Machine Learning Relevant today?

- Data storage is cheap
- Almost infinite compute capacity with rise in GPUs/TPUs







Open source datasets which accelerated the pace of research

- Open source and ML Frameworks and datasets
- Growing community through top AI/ML conferences







Top ML conferences



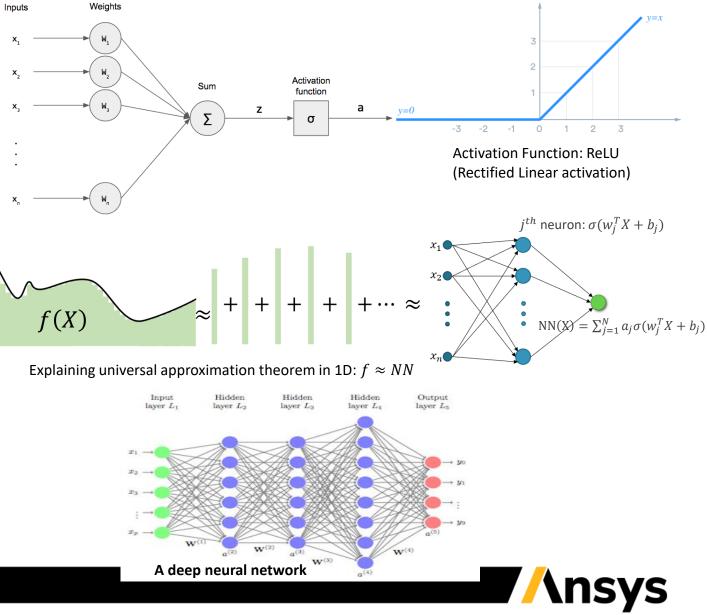
Open source ML frameworks that survived test of time



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How does Deep Learning Work?

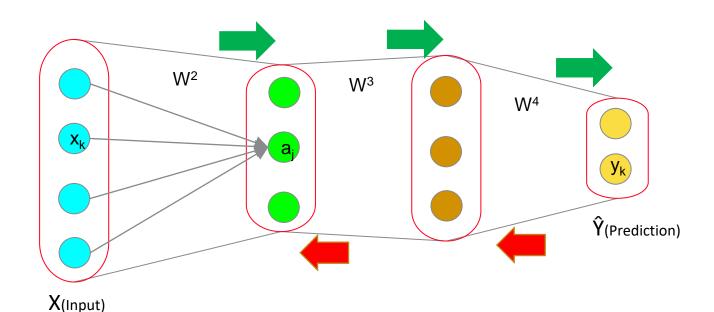
- Single neuron
 - Outputs an activation(a) of weighted sum of input (x)
 - Simplest activation: ReLU
- Universal Approximation Theorem (Cybenko, 1989):
 - A neural network with one hidden layer containing a finite number of neurons can approximate *any* continuous function to a reasonable accuracy.
 - >1D, no problem, but must increase neurons
- If we increase the numbers of layers
 - Can <u>approximately represent</u> many complex functions, say one function per layer
 - Can handle any non-linearity through ReLU
 - Why didn't we have perfect learning systems?



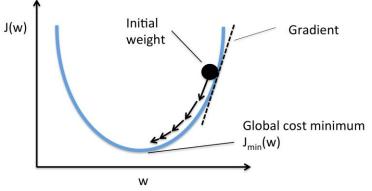
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How does Deep Learning Work?

- Is there a relationship between input X and observation Y?
- Yes, Given pairs(X,Y), Neural Network tries to fit a function $\mathcal{F}()$, which is parameterized by weights(w), such that : $\hat{Y} = \mathcal{F}(w, X)$.



- Key Steps
 - Initialize weights randomly or transfer from a previous learned task of a similar network
 - 🛑 Feed Forward:
 - In this step NN predicts the \hat{Y} based on the current weights w and inputs.
 - Calculate Error($\mathcal{J}(w)$) = Norm of (Y- \hat{Y})
 - **Here** Backpropagation:
 - Based on the Error(\mathcal{J}), gradient of Error w.r.t. weights i.e. $\nabla(\mathcal{J}(w))$ is calculated.
 - *Gradient Descent:* $w = w \alpha$. $\nabla(\mathcal{J}(w))$, where α is learning rate



AI/Machine Learning at Ansys

Build internal expertise and support organic R&D

- Hired a small team of AI/ML software developers and leader in the Office of the CTO
- Working with a distributed team of AI/ML software developers in the Business Units
- Support, complement, accelerate BU projects short term
- Canonical customer use cases, drive results across BUs long term
 - Customer Productivity
 - Augmented Simulation
 - Engineering Design
 - Business Intelligence

Use partnerships to augment:

- Larger companies
- Startups
- Universities





Hicrosoft Azure











AI/ML for Engineering Simulation **R&D** Projects in BUs

CTO Office

- ML based PDE Solver (Augmented simulation)
- Physics Informed Neural Network (Augmented sim) ٠
- Optimization for AMG Solver (Customer productivity) ٠
- ML Framework as a service ((Customer productivity) ٠

Mechanical BU

•Auto-identification of contacts (**Customer productivity**) •Google: Reinforcement Learning with Py-ANSYS

(Customer productivity)

 ML based surrogate modeling for VVUQ (Augmented) simulation)

Fluids BU

- Geminus: Turbulence model tuning using ML (Customer productivity)
- AI/ML-enabled flow solver (Augmented simulation) ٠

Electronics BU

 Runtime Predictor (Business intelligence) Auto-identify HFSS 3D regions in Slwave (Customer productivity)

Design BU

Fast Topology Optimization (Revolutionizing design)

- Materials BU
- ML Analysis for Additive Manufacturing data (Revolutionizing design)
- ML methods in Granta Materials (Customer productivity) ٠

Semiconductor BU

- Data-driven fast static/transient thermal solver (Augmented simulation) ٠
- Nvidia: Physics Informed Neural Network Solvers (Augmented ٠ simulation)
- AutoML for SI and PI tools (Customer productivity) ٠

System and Platform BU

- Automated ROM Creation for non-linear systems (Augmented simulation)
- Creation of Path Planners for autonomous vehicles (Customer productivity)
- Geminus: Augmented flow for Twinbuilder (Augmented simulation)

Cloud and Platform BU

Resource prediction compute and storage on cloud (Business intelligence) ٠

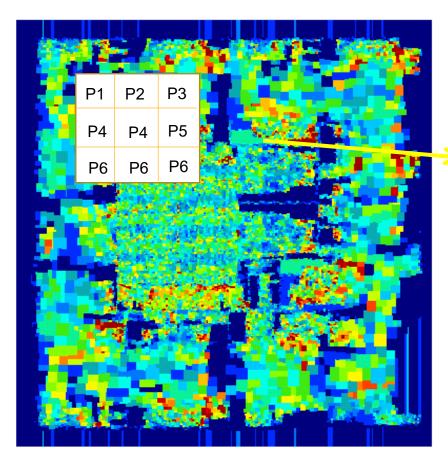
ACE

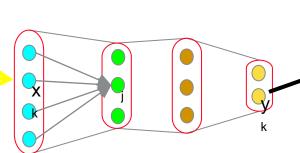
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- Virtual Validation: Fusion modeling + less tests (Augmented simulation)
 - Generative design for OEM Concept modeling (**Revolutionizing design**)

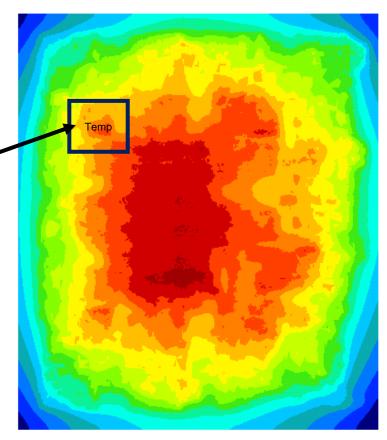
Augmented Simulation: Data-Driven Fast On-Chip Thermal Solver

Providing Inferencing by Striding Templates with One Tile for Predicting Temperature at all Tile Locations



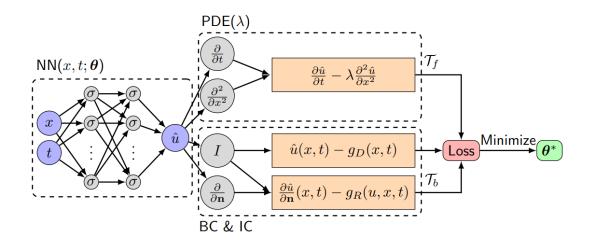


For each tile location, a set of tile powers and Theta-JA are input to the trained DeltaT Predictor to predict the temperature at the corresponding tile and added to the Temp from rough thermal profile

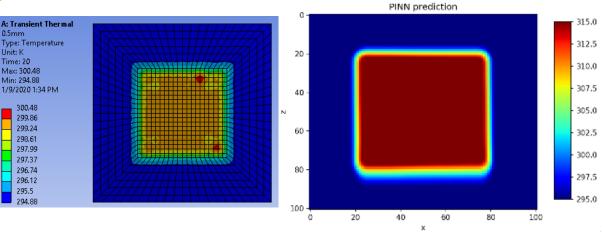




Augmented Simulation: Physics-Informed Neural Nets (PINN)

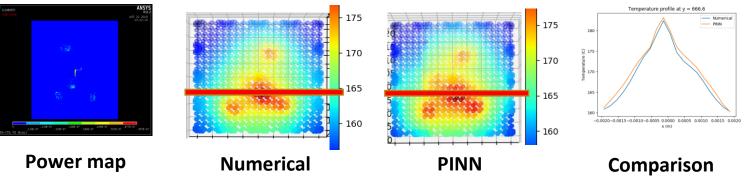






² 2D heat transfer on a chip with nonlinear power map

- PINN uses upfront inference modeling
- Runtimes in fractions of seconds (100X)



Augmented Simulation: ML-Based Partial Differential Equation Solver

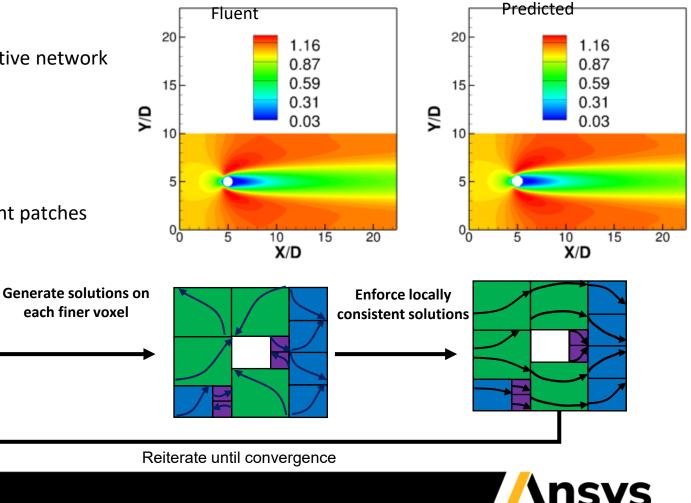
- Motivation:
 - Geometries and physics have lots of patterns.
 - Do we need to solve from scratch?
 - No! Create solution instances on patches using a generative network
- Key insights:
 - Take a general domain and voxelize into patches
 - Decide boundary conditions for each patch
 - "Solve" for the latent vectors on each patch.
 - Requires learning a consistency condition between adjacent patches

Divide into finer voxel

Each voxel can be 8*8*8 point voxels or more

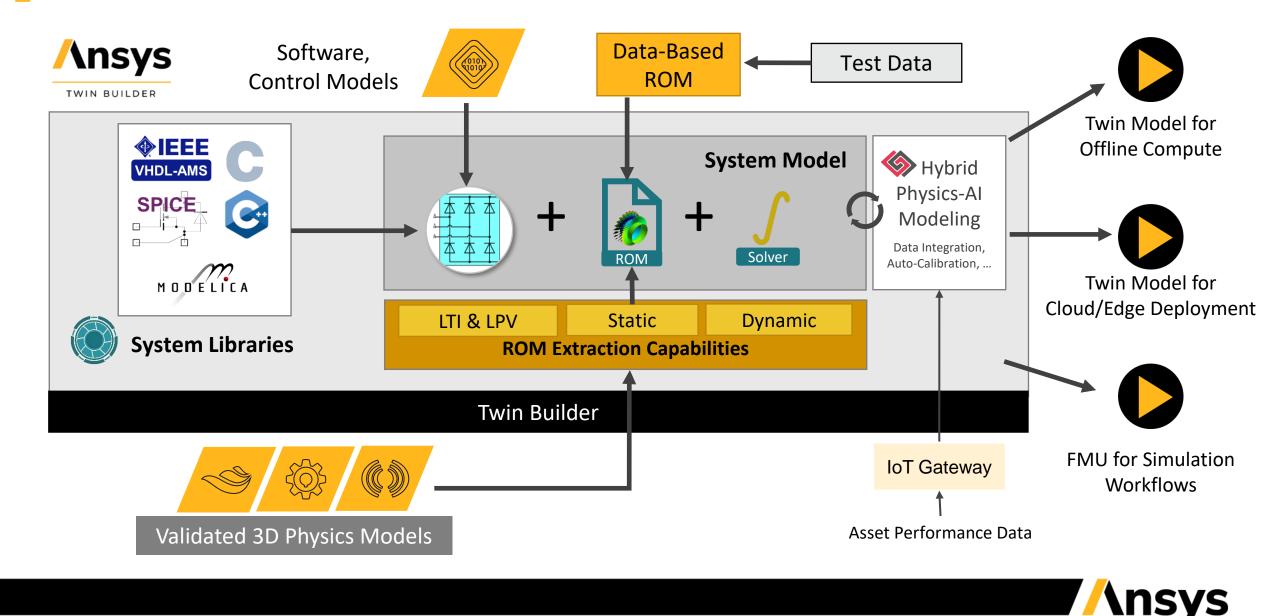
- More than 100X speedup in time to solution

Example Results: Flow over cylinder: Velocity



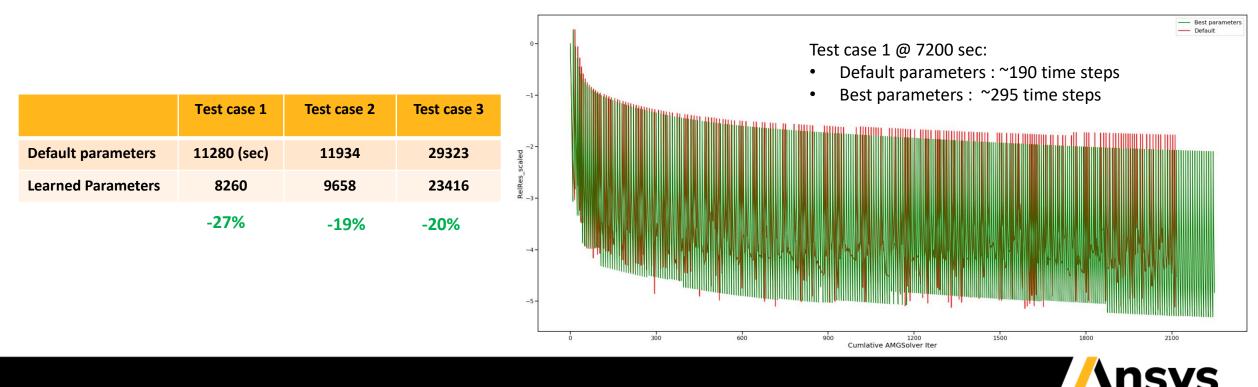
Voxelize

Augmented Simulation: Hybrid Physics AI Digital Twin Architecture and Workflow



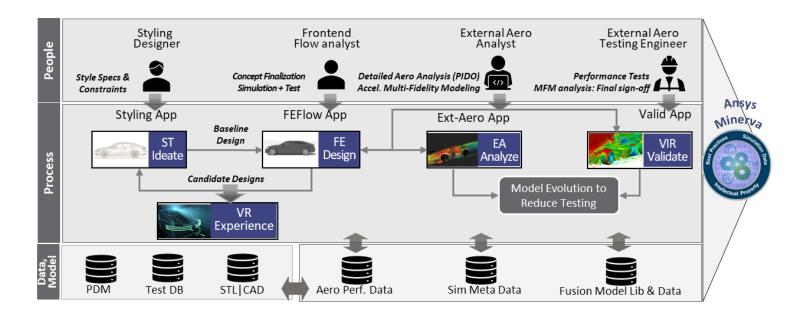
Customer Productivity : Using AI/ML to Improve Convergence

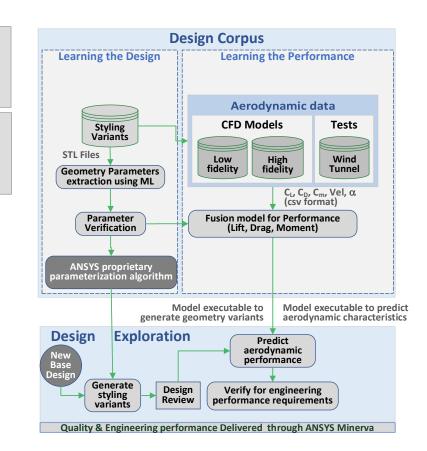
- Problem:
 - Solution convergence takes a lot of time and applicable to all solvers
 - Can we learn from the history of convergence to find the ideal control parameters?
- Solution:
 - We applied Bayesian optimization to a linear solver such as AMG
 - Results shown below



Engineering Design: Machine Learning-Driven Generative Design

Le	earning the Designs	 <i>Embeddings:</i> Prior designs are parameterized Future design style changes embodied in parametric design space Variant designs are constructed from the parametrized model
	earning the erformance	 Using Fusion Modeling technique, prior CAE and test data are fused to fast and accurate surrogate model Surrogate models are used for rapid evaluation of design variants









- Engineering simulation solves laws of physics in our world
 - Physics captured by equations (Navier Stokes' equations for fluids, Maxwell's equations for electro-magnetics)
 - Equations solved using numerical methods such as finite element analysis and finite difference
- Artificial Intelligence has progressed from Expert Systems to Machine Learning to Deep Learning
- Discussed the use of AI/ML to improve engineering simulation around four use cases:
 - Improving Customer Productivity
 - Augmented Simulation
 - Revolutionizing engineering design
 - Business Intelligence.
- Highlighted six AI/ML applications in engineering simulation
 - Data-driven thermal solver
 - Physics informed neural network for simulation
 - Machine learning based PDE solvers
 - Hybrid AI and Physics based Digital Twins
 - Using AI/ML to Improve Convergence
 - ML based Generative networks



