Machine-Learning
Augmented HPC Workflow
for Physics-based
Analysis in the Cloud
Presenter Biography

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- Solutions Architect, Rescale
- 5+ years in HPC
- MS in Physics(almost), with a focus on Numerical Relativity and Computational Physics
Vision > Single Platform to Run HPC Simulations on Cloud

Rescale ScaleX Platform

- Enterprise big compute
- Innovation acceleration
- User-first platform
- Security and admin controls

FULLY INTEGRATED STACK OF ENTERPRISE DEPLOYMENT TOOLS
Future of Computing

AI-AUGMENTED HPC: THE FUTURE OF COMPUTING
Algorithms and Simulation Will Define Our Future

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- Digital Twin
- Model Based Engineering
- Personalized Healthcare
- Autonomous Vehicle

POWERED BY

Intelligent Algorithms + Simulation

Predict & Accelerate
The Two Pillars of the Rescale Artificial Intelligence Strategy

AI-Enabled HPC Workflow

AI-Augmented HPC Decision Support

- Input
- Software
- Post Processing
- Hardware Settings
- Output
- Filters
AI-Augmented HPC Engineering workflow ScaleX Platform
AI can enhance all steps of a simulation workflow

Typical workflow

AI-enhanced workflow

Engineering Hours

Geometr y Import

Geometry Defeaturing

Meshing

Model Setup

Solver

Results Analysis

Design Optimization

Automatic geometry cleanup

AI-enabled automatic meshing

Automatic Boundary Conditioning

AI-enabled hardware tuning

AI-enabled feature/anomaly detection

Pre-processing

Post-processing
Key Technical Components of Rescale AI strategy

Open Platform
- Multi-storage governance
- Data connectivity solution

Application Publication
- Bring your own container
- Container repository management
- Inference IOT publication

Workflow Orchestration
- Method builder
- Multi-cloud container execution orchestration

Data Analytics
- Data ingestion and visualization
AI-Enabled Workflow for Continuous Training and Deployment

**AI MODEL DEVELOPMENT**
- Automate with DOE framework
- Standardize ML Stack
- Scale
  - CPU
  - GPU/TPU
- Deep Learning for model training
- Model validation, inference and test

**EDGE DEPLOYMENT**
- Edge device
- Integrate IoT and Edge service
- Real time analysis
- GPU/TPU
- CPU
Key enablers of AI-enabled engineering simulations

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- GPU/TPU
- High Performance Storage
- DL/ML Software
- Engineers
Let’s design a T-junction pipe

Cold Inlet T = 250, …, 280 K

Hot Inlet T = 320, …, 350 K

Outlet Temperature?

T-junction Pipe CFD
How do we analyze this design?

Inputs:
- Hot inlet temp
- Cold inlet temp

Outputs:
- Outlet temp
What is a Design of Experiments?

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Test 1: T = 250K
Test 2: T = 251K
Test 3: T = 252K
Test n
Test 100: T = 349K

T_out = ?
T_out = ?
T_out = ?
T_out = ?
T_out = ?
T_out = ?
Combining DOE and AI on a Single Platform
The T-junction system is modeled by a NN with the following structure:

- **An input layer** of two units to ingest the data for the two features
- **Two fully-connected hidden layers** of 15 units with ReLU activation.
- **An output layer** of a single unit with linear activation.
- Training done over 96 CFD samples split to train/test/validate the model.

We used Tensorflow using Keras API to create and train this neural net.
Model + Software + Training on a Single Comprehensive Platform
An easy button on Rescale platform to training a model