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

Presenter Biography

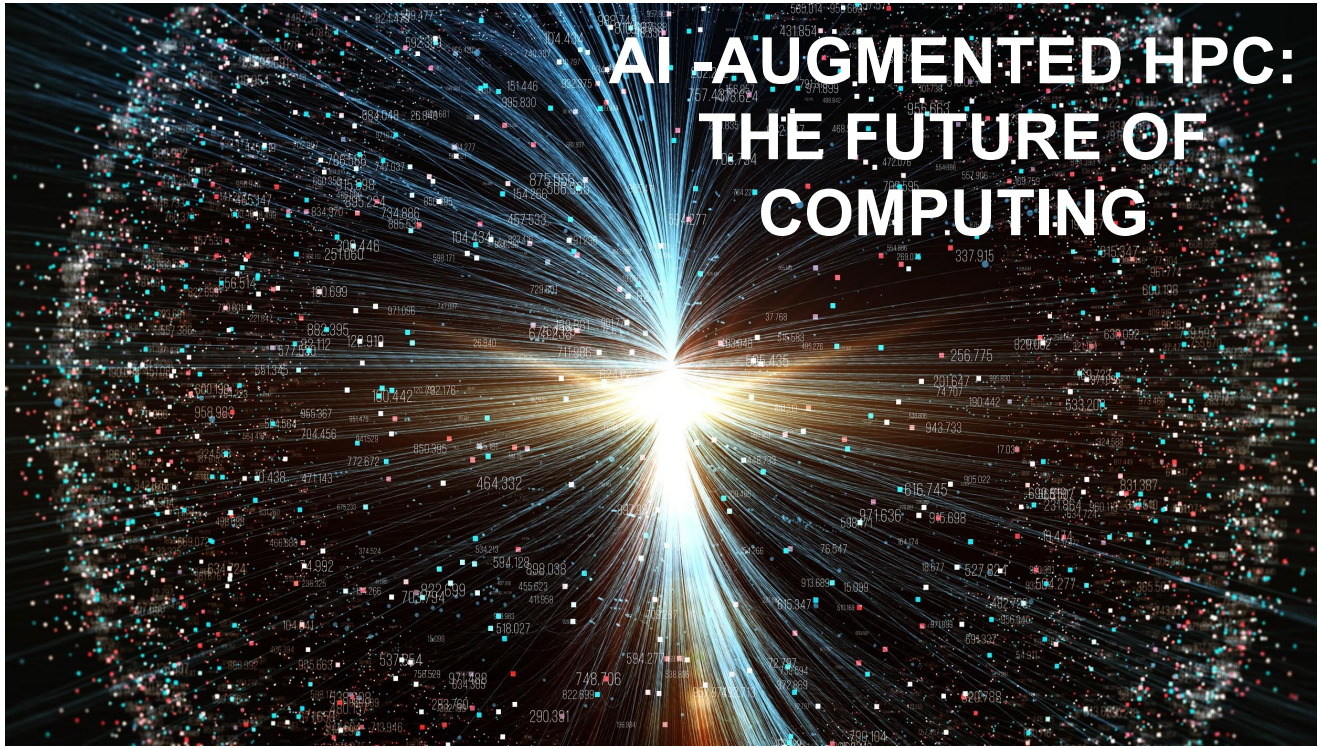
- **Solutions Architect, Rescale**
- **5+ years in HPC**
- **MS in Physics(almost), with a focus on Numerical Relativity and Computational Physics**

Vision > Single Platform to Run HPC Simulations on Cloud

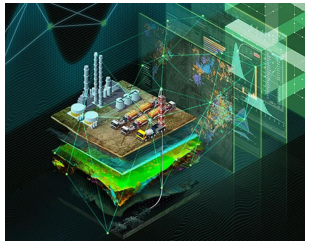
FULLY INTEGRATED STACK OF ENTERPRISE DEPLOYMENT TOOLS

Rescale ScaleX Platform

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


AI -AUGMENTED HPC:
THE FUTURE OF
COMPUTING

Algorithms and Simulation Will Define Our Future



Digital Twin

Model Based Engineering

Personalized Healthcare

Autonomous Vehicle

POWERED BY

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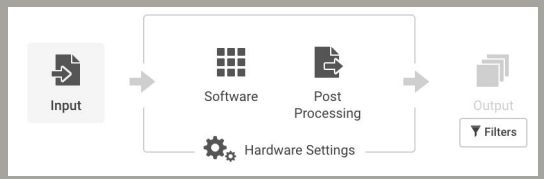
Intelligent Algorithms + Simulation

Predict & Accelerate

The Two Pillars of the Rescale Artificial Intelligence Strategy

AI-Enabled HPC Workflow



AI-Augmented HPC Decision Support

AI-Augmented HPC Engineering workflow ScaleX Platform

AI can enhance all steps of a simulation workflow

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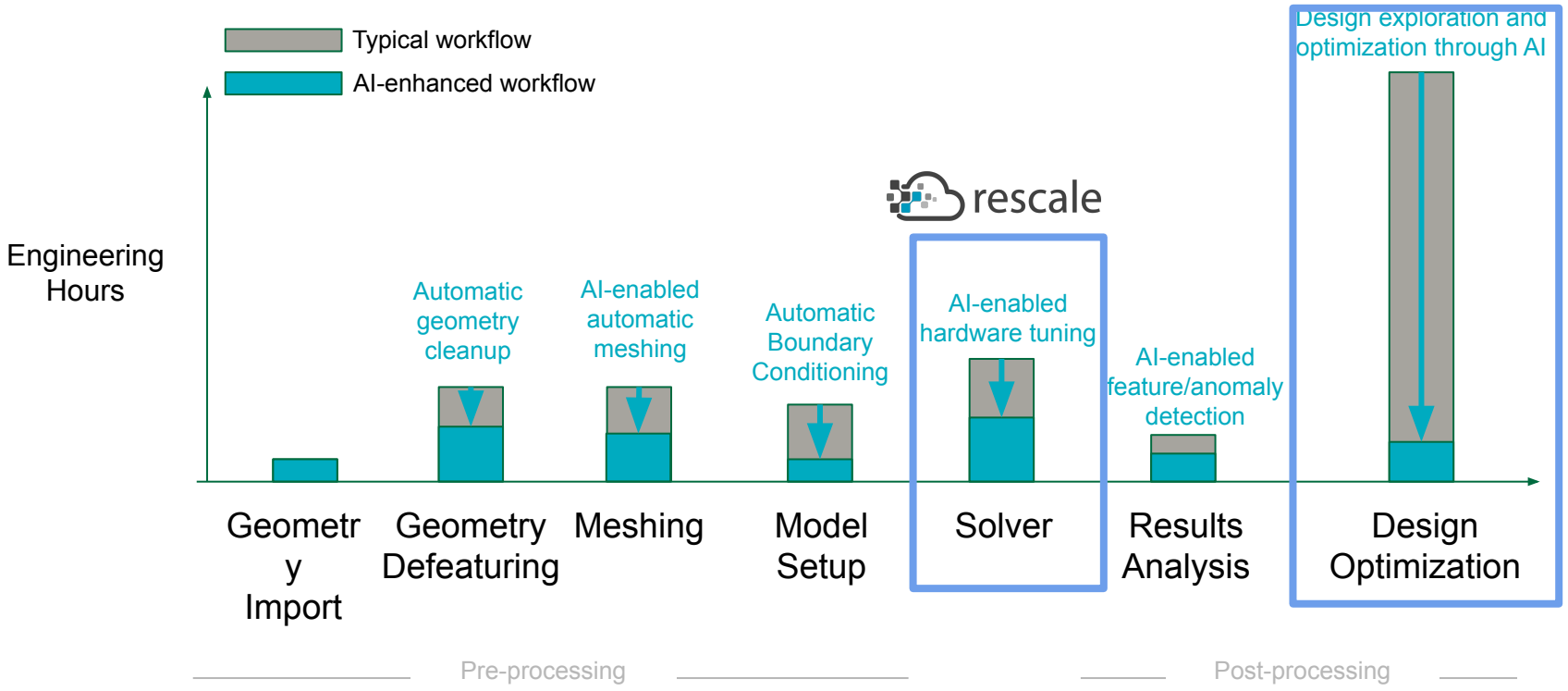


Key Technical Components of Rescale AI strategy

Open Platform

- *Multi-storage governance*
- *Data connectivity solution*

Application Publication

- *Bring your own container*
- *Container repository management*
- *Inference IOT publication*

Workflow Orchestration

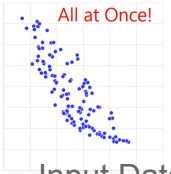
- *Method builder*
- *Multi-cloud container execution orchestration*

Data Analytics

- *Data ingestion and visualization*

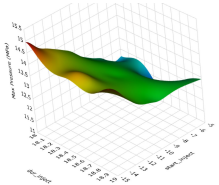
AI-Enabled Workflow for Continuous Training and Deployment

AI MODEL DEVELOPMENT



Input Data Generation

Deep Learning for model training

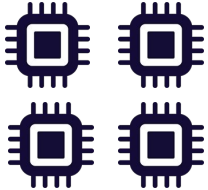


Model validation, inference and test

Automate with DOE framework

CPU

Standardize ML Stack



GPU/TPU

Scale

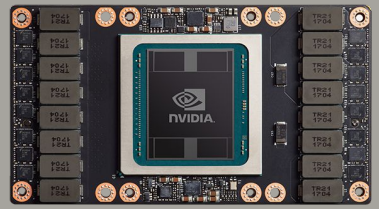
EDGE DEPLOYMENT

Edge device

Integrate IOT and Edge service

Real time analysis

Key enablers of AI-enabled engineering simulations



GPU/TPU

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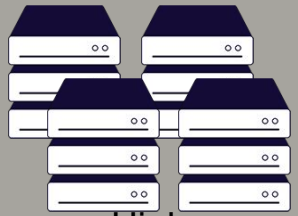
TensorFlow

DL/ML Software



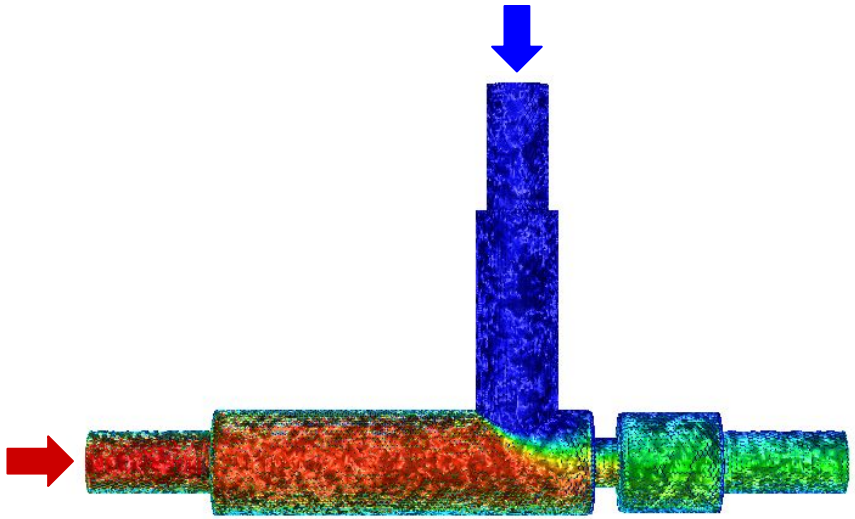
High Performance Storage

Engineers

Let’s design a T-junction pipe

Cold Inlet T = 250, …, 280 K

Hot Inlet T = 320, …, 350 K



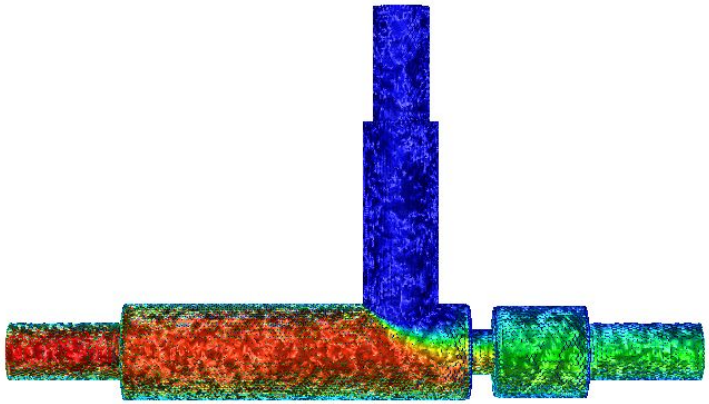
Outlet Temperature?

T-junction Pipe CFD

How do we analysis this design?

Inputs:

Hot inlet temp
Cold inlet temp



Outputs:

Outlet temp

What is a Design of Experiments?

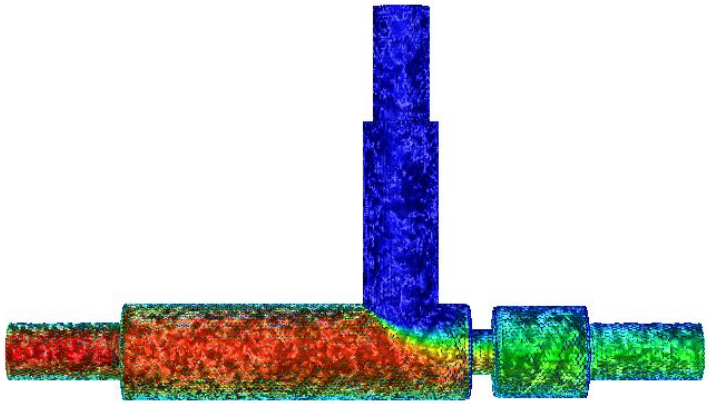
Test 1:
T = 250K

Test 2:
T = 251K

Test 3:
T = 252K

Test n

Test 100:
T = 349K



T_out = ?

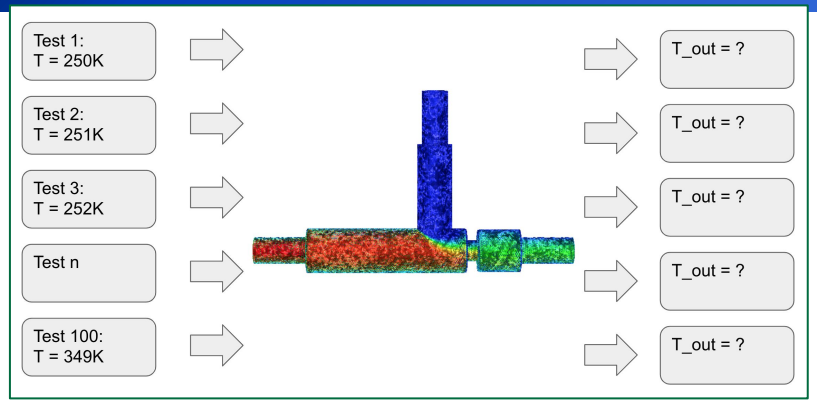
T_out = ?

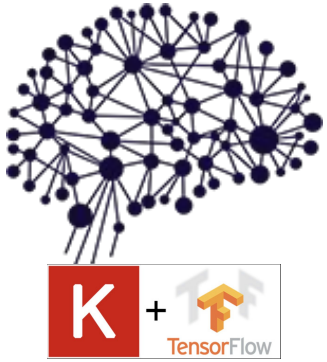
T_out = ?

T_out = ?

T_out = ?

Combining DOE and AI on a Single Platform

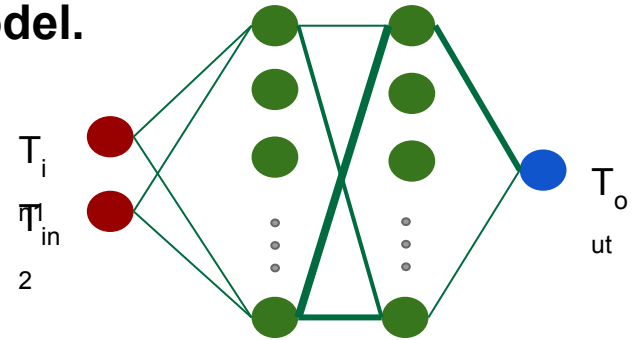




Neural Net Structure

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

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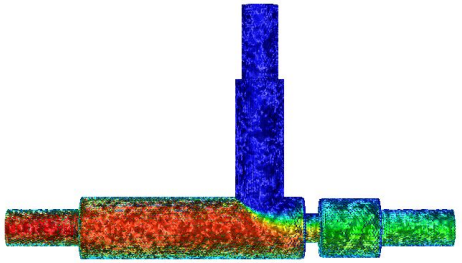
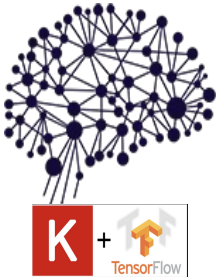
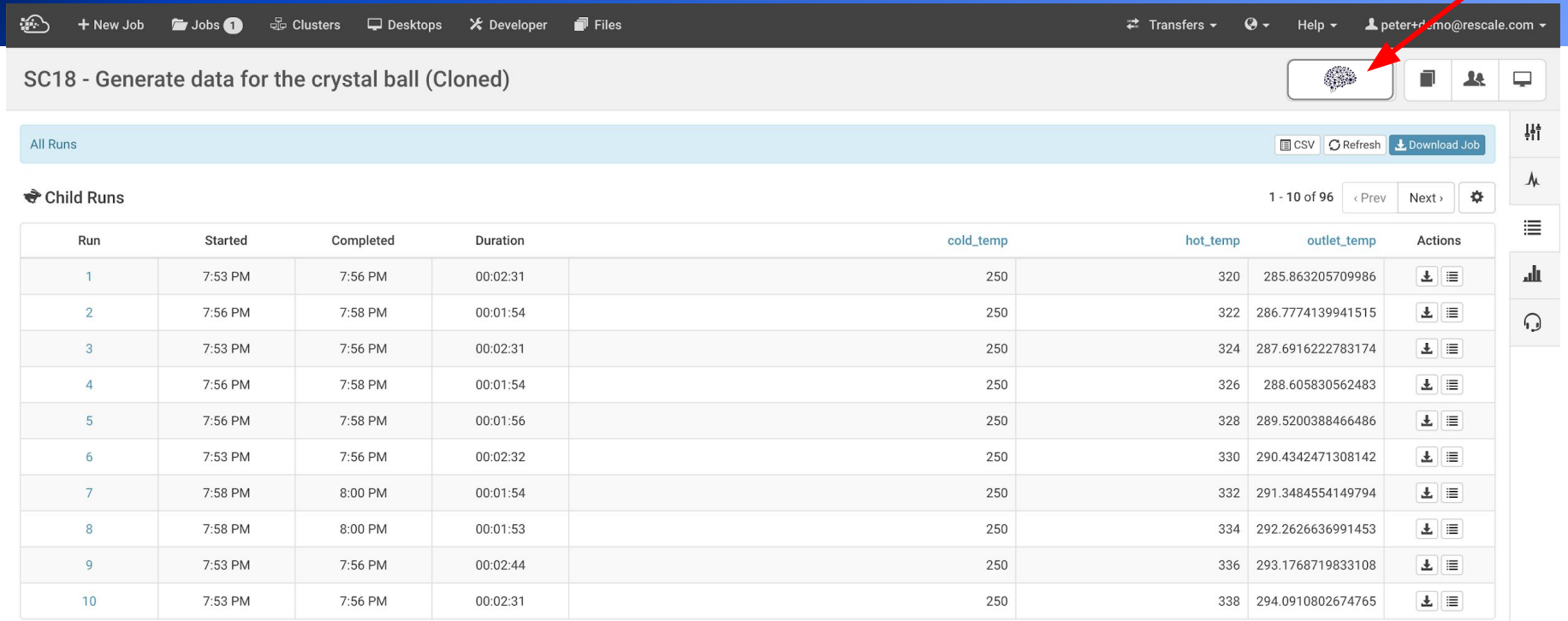




An easy button on Rescale platform to training a model



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3	7:53 PM	7:56 PM	00:02:31	250	324	287.6916222783174	
4	7:56 PM	7:58 PM	00:01:54	250	326	288.605830562483	
5	7:56 PM	7:58 PM	00:01:56	250	328	289.5200388466486	
6	7:53 PM	7:56 PM	00:02:32	250	330	290.4342471308142	
7	7:58 PM	8:00 PM	00:01:54	250	332	291.3484554149794	
8	7:58 PM	8:00 PM	00:01:53	250	334	292.2626636991453	
9	7:53 PM	7:56 PM	00:02:44	250	336	293.1768719833108	
10	7:53 PM	7:56 PM	00:02:31	250	338	294.0910802674765	