Application of Scientific Machine Learning (SciML) for Manufacturing Processes

Machine Learning for Industry Forum 2021

August 10, 2021

Vic Castillo, LLNL

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LLNL-PRES-825564

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

Lawrence Livermore National Laboratory

U.S. Dept. Of Energy Labs are helping the Manufacturing Industry Sector

Photo: courtesy of ArcelorMittal USA

- The U.S. manufacturing sector uses approximately 25% of the nation’s energy.

  Energy is a significant cost in manufacturing

Source: DOE’s Advanced Manufacturing Office Multi-Year Program Plan for Fiscal Years 2017 through 2021

HPC4Mfg Program

We provide Scientific Machine Learning (SciML) tools *and* expertise to the manufacturing community

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Manufacturing Industry Needs

- Rapid prediction of current or future process states.
- Integration of production data and simulation output.
- Informed decision-making for capital investment (sensors, simulation, experiments)

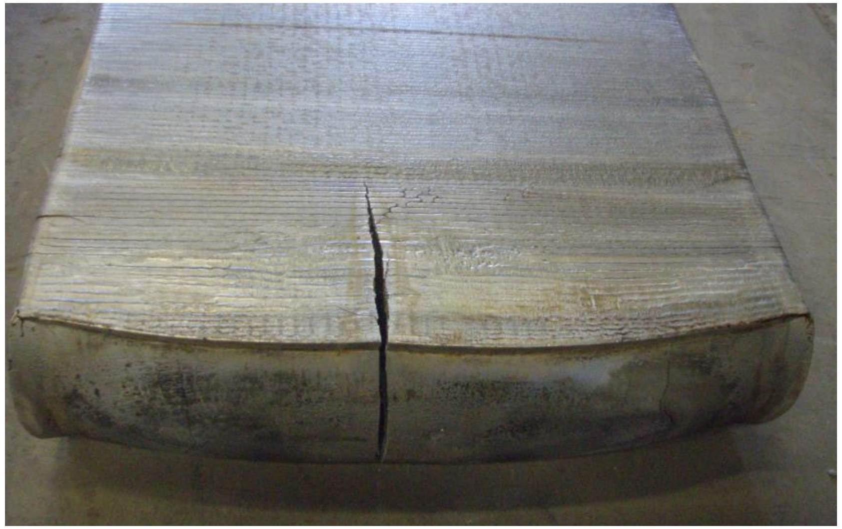


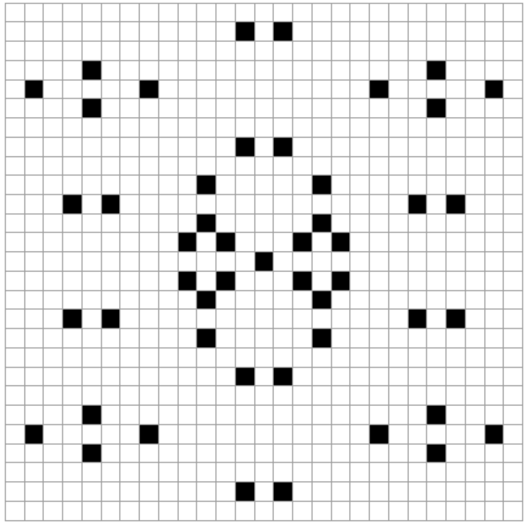
Photo: courtesy of Arconic Corporation

Photo: courtesy of Vitro Glass Corporation

How Machine Learning can help

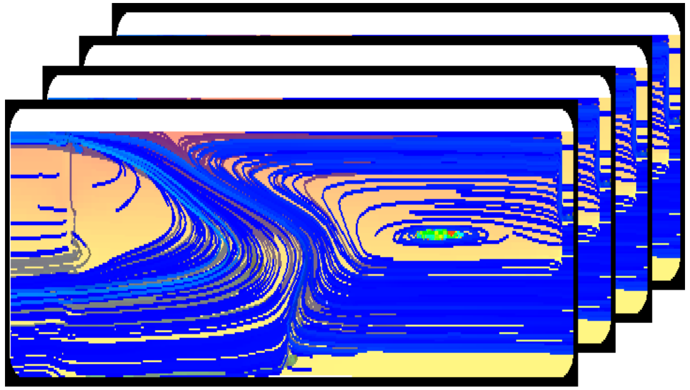
- Vision tools for quality control
- Predictive Maintenance
- Supply chain / Inventory optimization
- Process prediction and optimization
- Generative design
- Robotics

Scientific Simulation + ML (SciML) Workflow

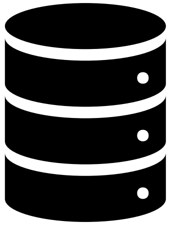


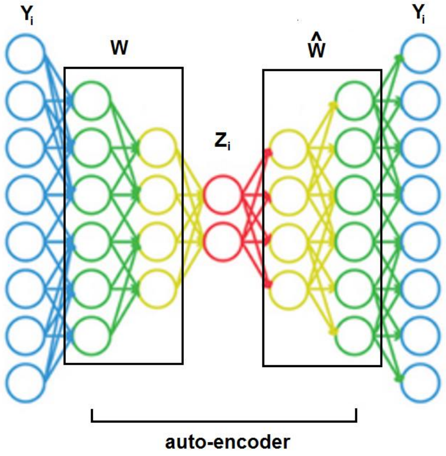
Design of Experiment (Parameter Study)

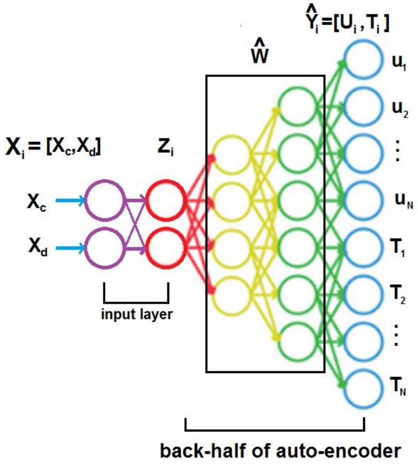
Simulations



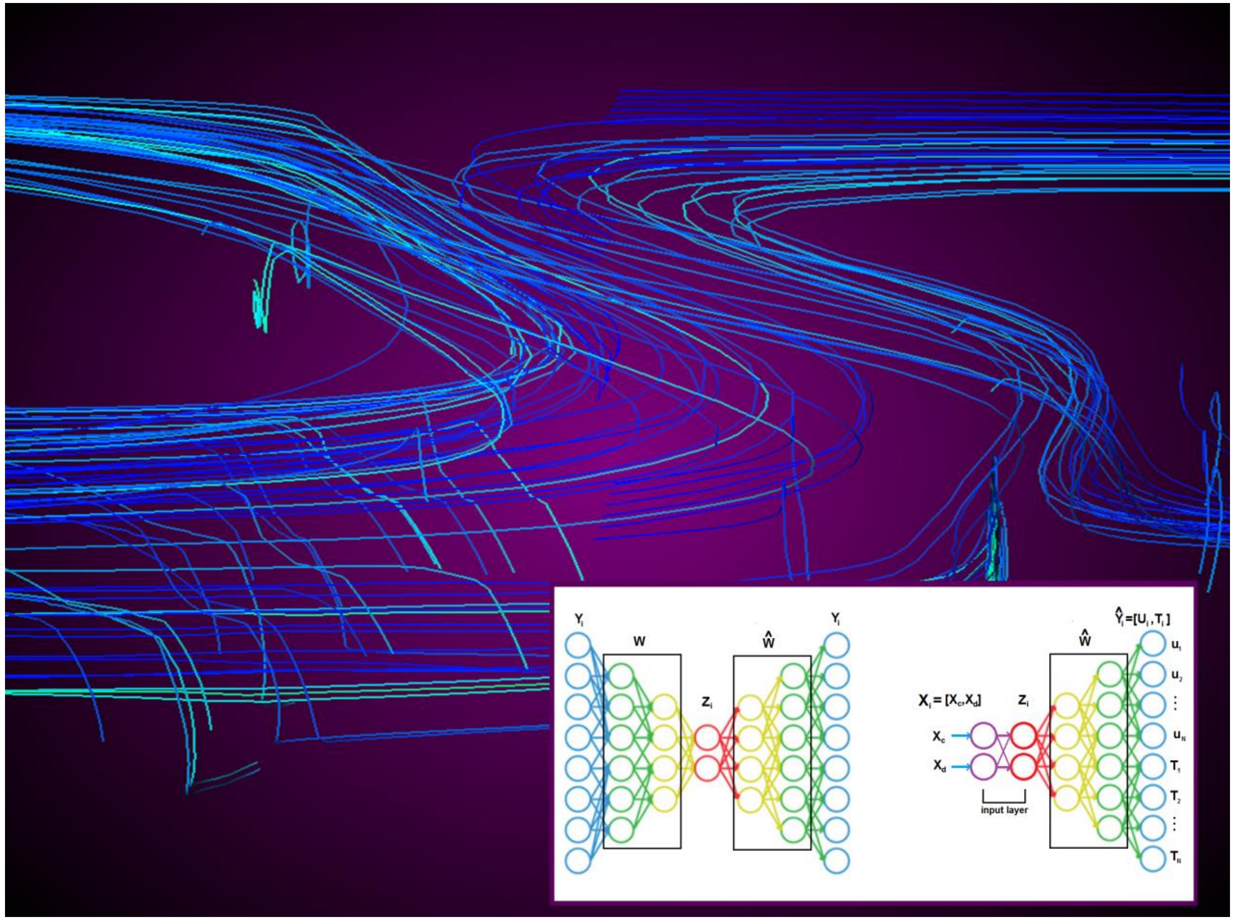
Data Curation







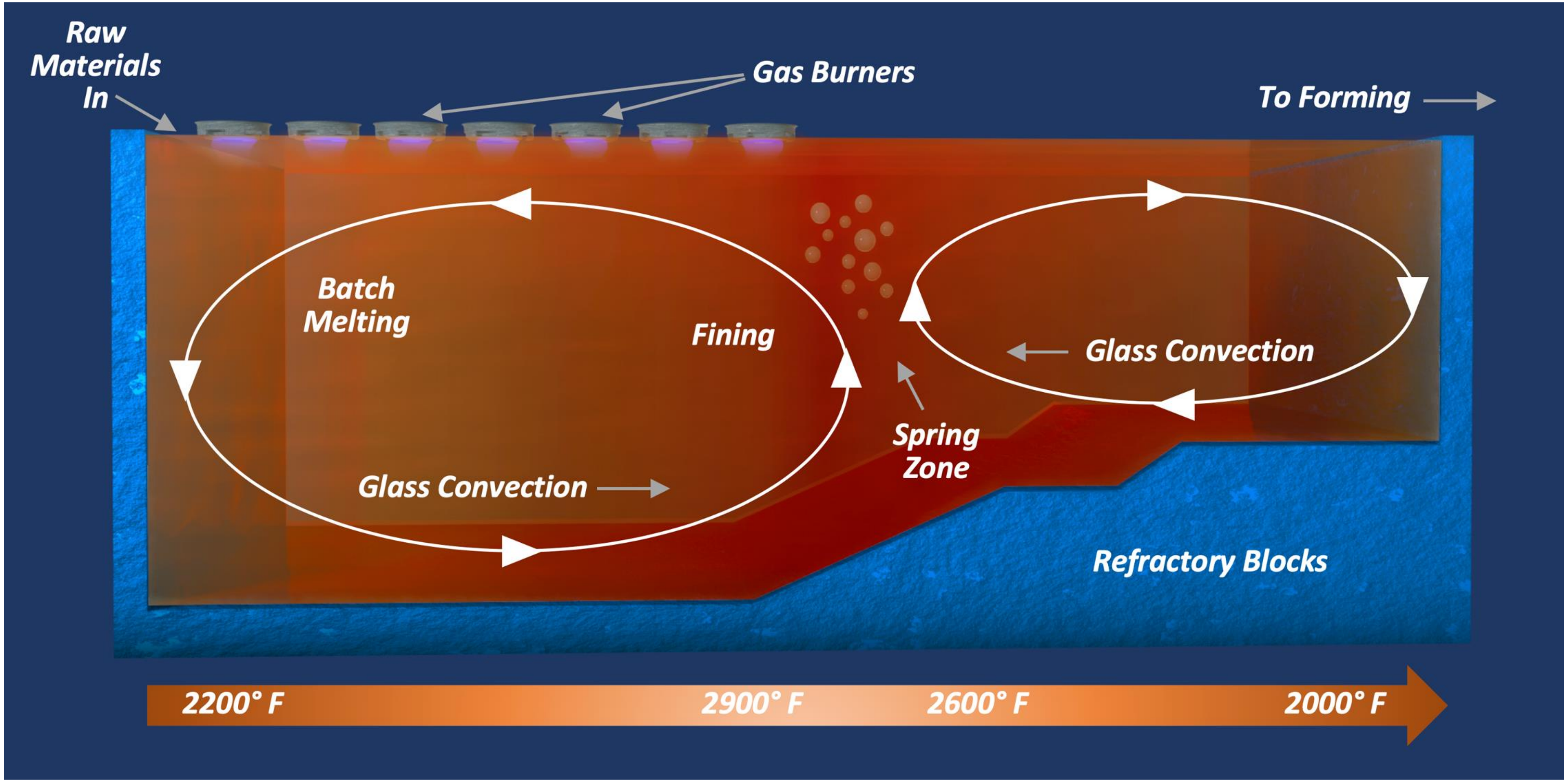
Example: Glass manufacturing



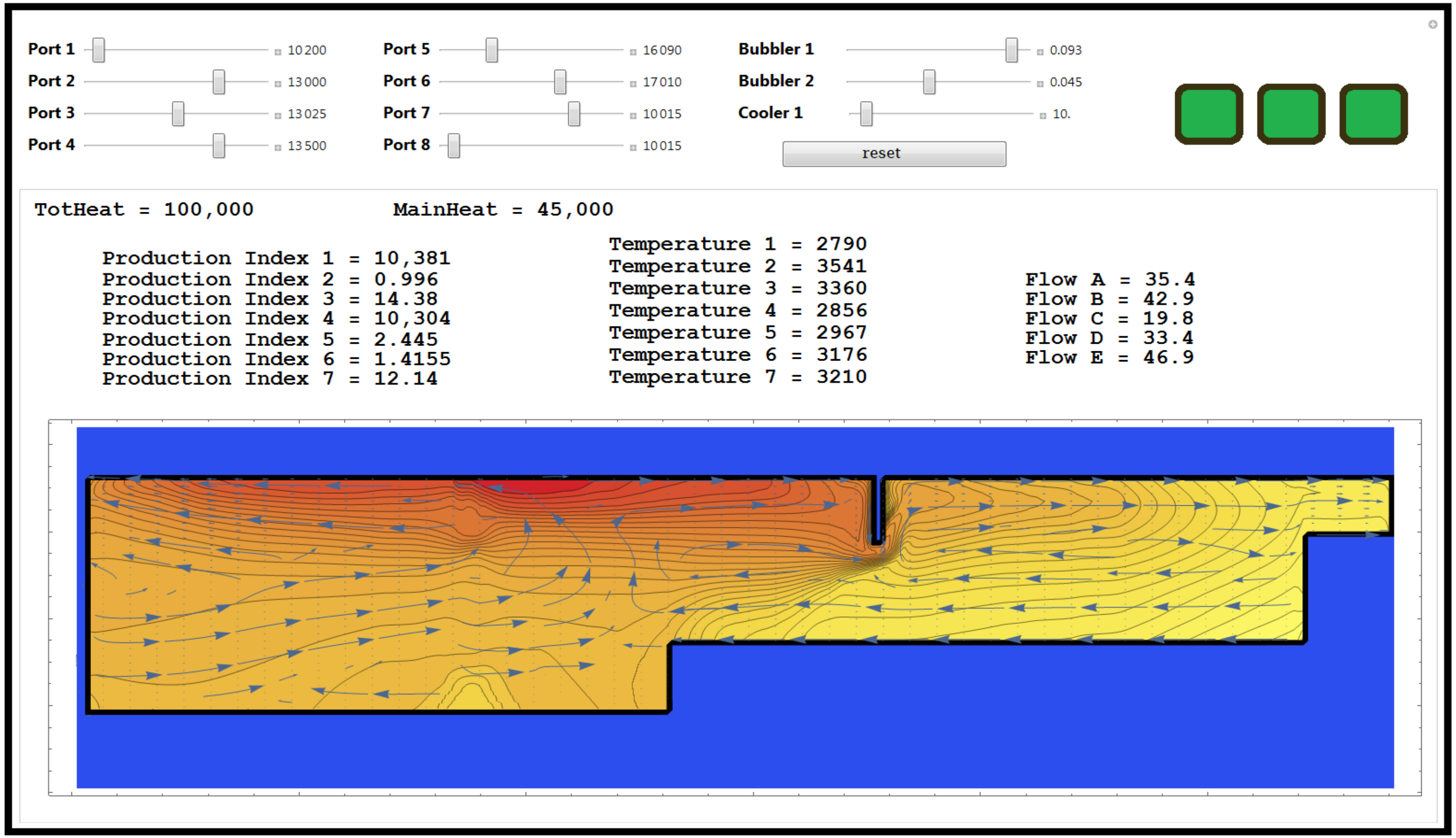
Streamlines in glass furnace. Inset: Autoencoder network

Photo: LLNL team at PPG Glass production facility

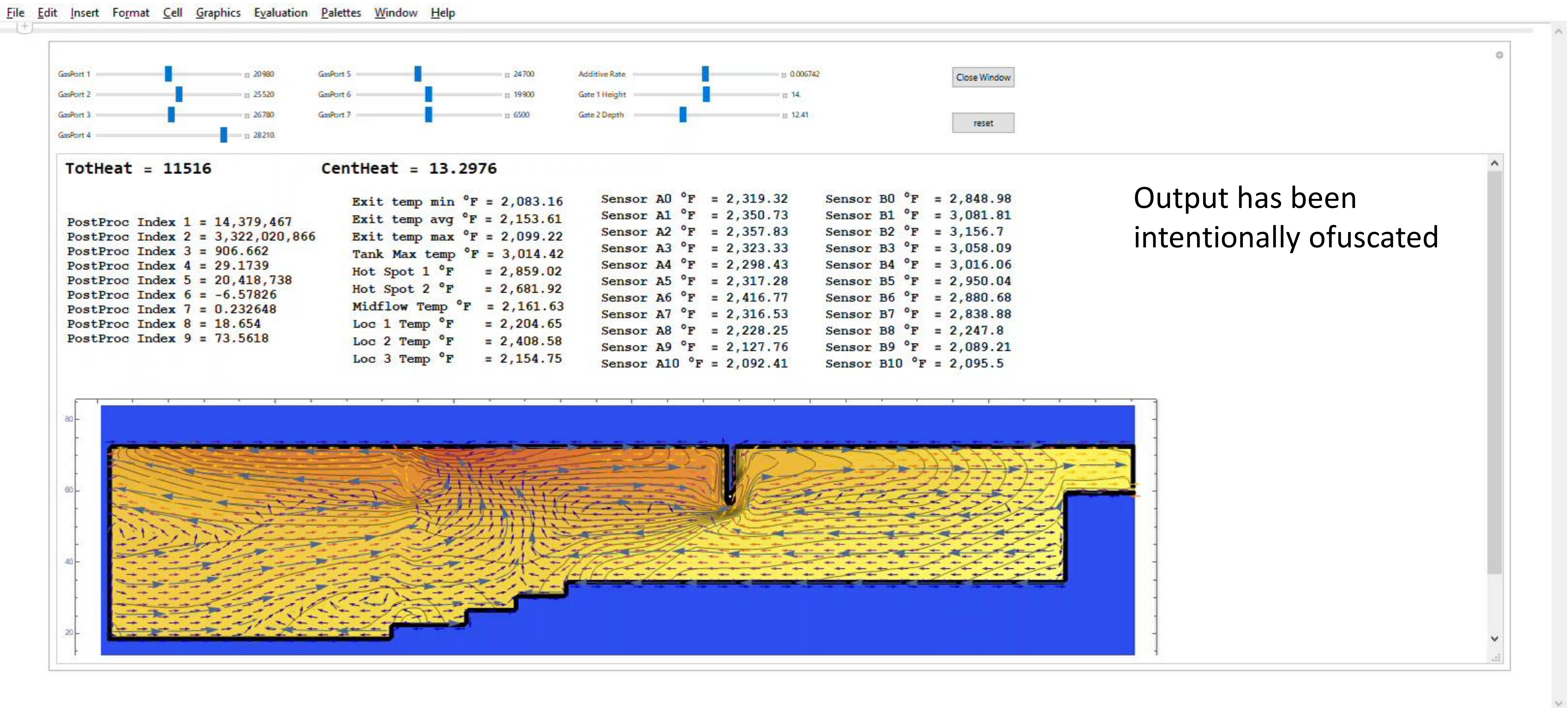
Issue: Molten Glass tank



Solution: Fast-running Emulator

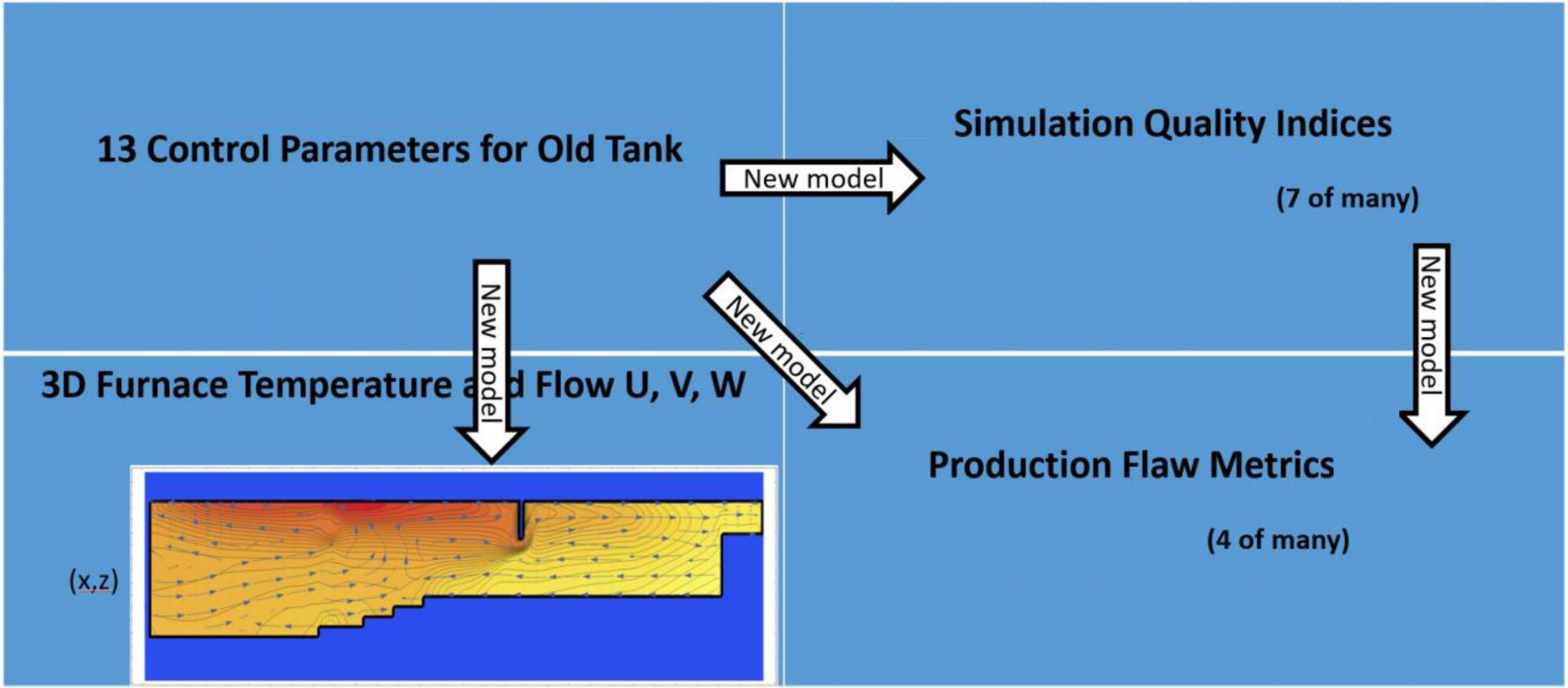


Solution: Fast-running Emulator



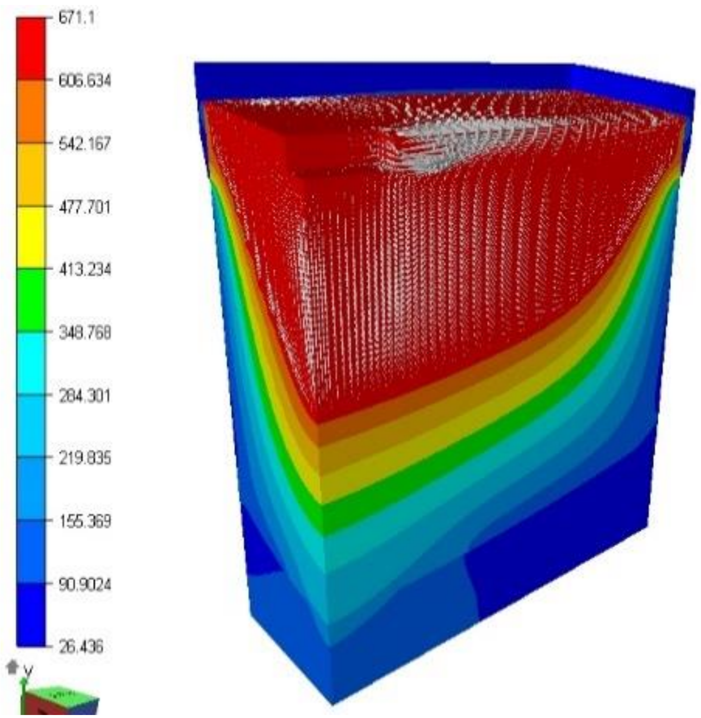
Output has been intentionally ofuscated

Simulation to Production data



Example: Aluminum Casting

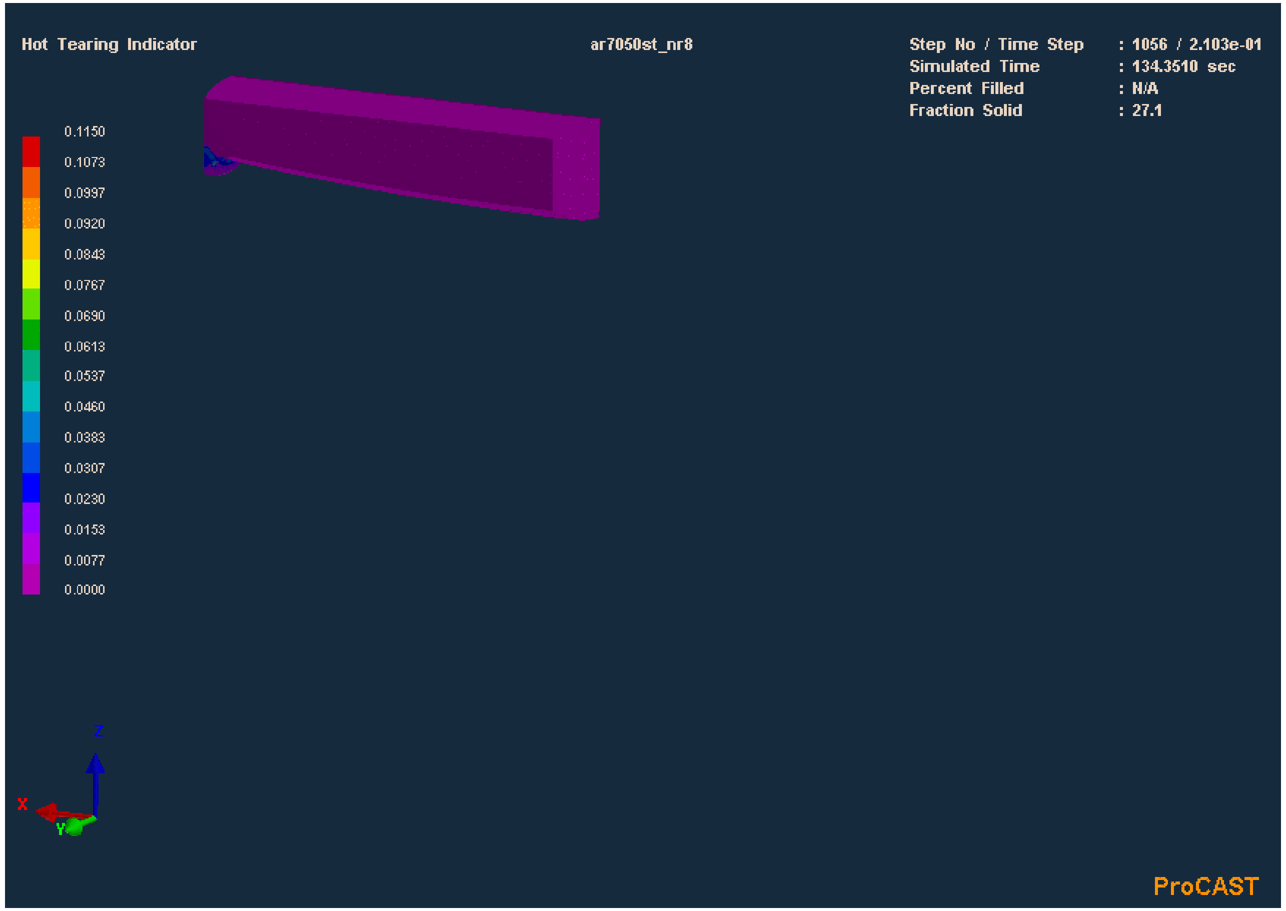
- Computer simulation – using commercial off-the-shelf tools to analyze potential for cracking
- Pilot-scale production experiments



Aluminum casting simulation

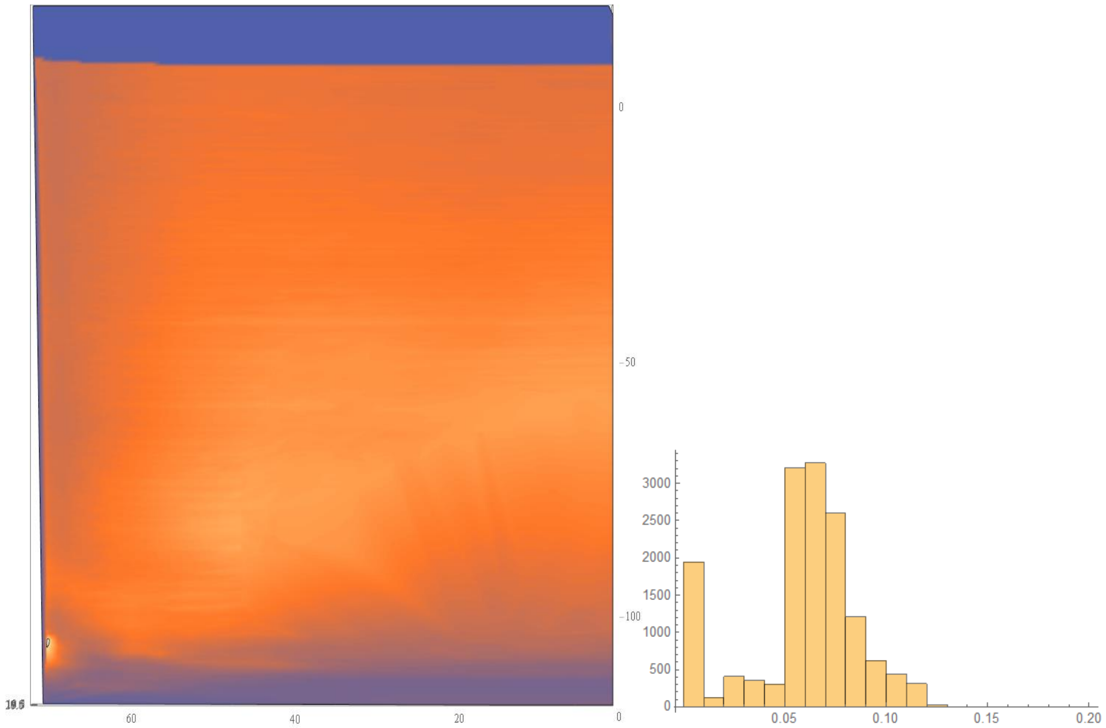
LLNL and ORNL team at Arconic R&D Center

Aluminum Casting:
COTS simulations developed (ProCAST)

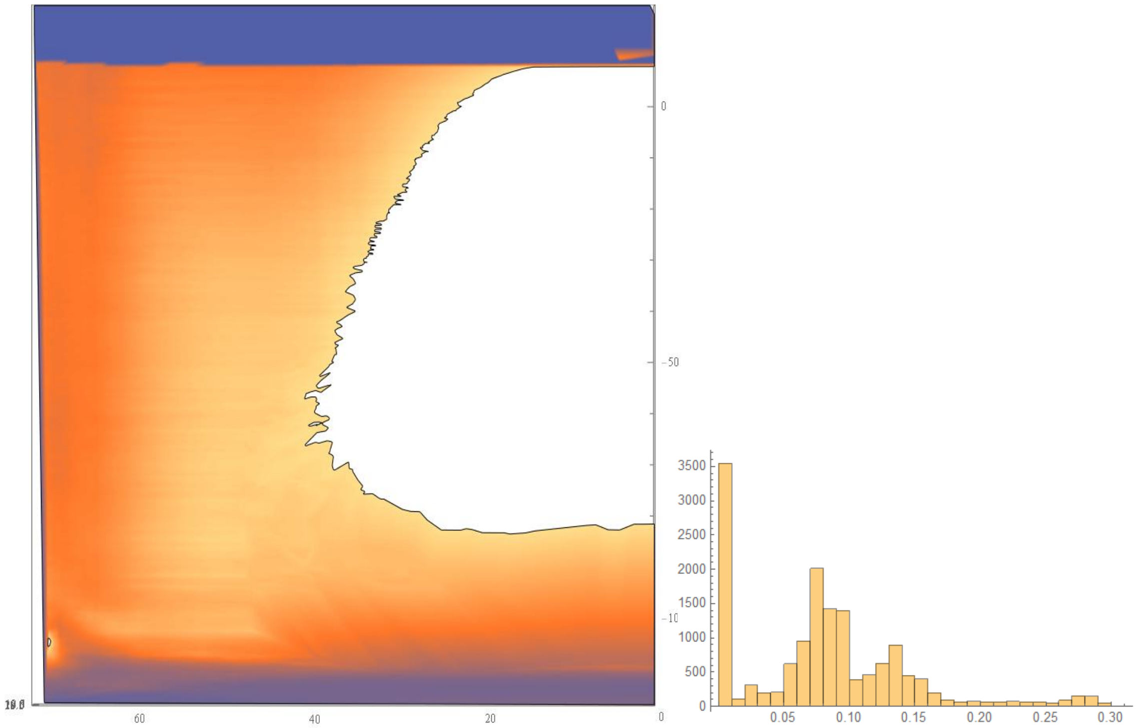


Aluminum Casting:
Fast-running Surrogate Model

- No Cracking



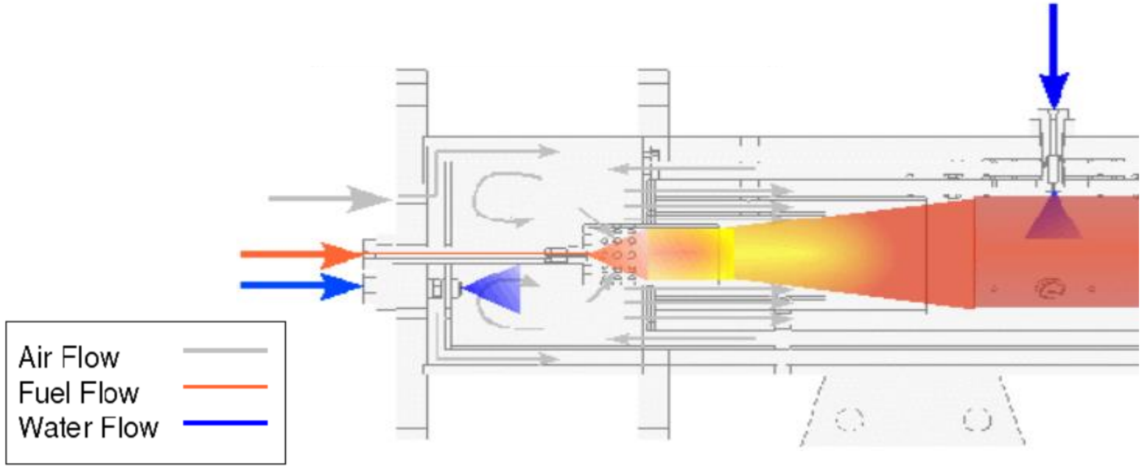
- Cracking



Innovating Startups: VAST Power Systems

VAST Power Systems' Gas Turbines

- ➢ Backup Power Vital for Wind and Solar
- ➢ Boost Power ~60% and Efficiency ~24%
- ➢ NO_x Below Limits without Catalysts



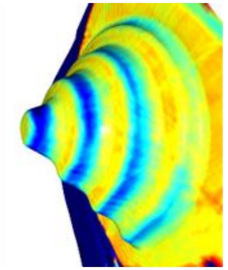
- Optimizing top 10 of >100 Design Parameters of VAST's proprietary combustor, with a chemistry set reduced from ~8,000 combustion reactions
- Design Parameters
  - Argonne NL HPC Modeled VAST Emissions
    - ➢ 1,000,000 Core Hours of Computational Fluid Dynamics (CFD)
  - Lawrence Livermore NL optimizing conditions using Reduced-order models
- DOE Phase II - Low NOx VAST Turbine Design. Expect Best in Class with Hydrogen, Ammonia

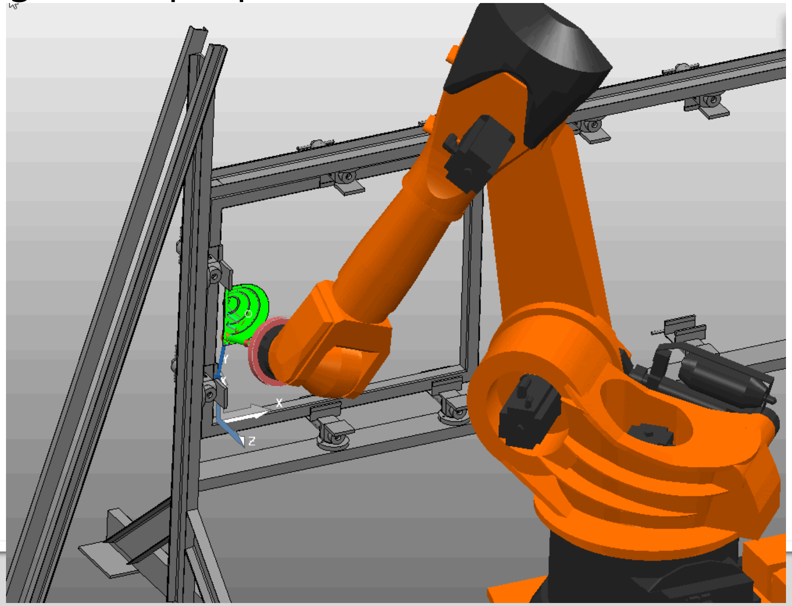
Innovating Startups: Machina Labs

AI & Robotics for on-demand Manufacturing

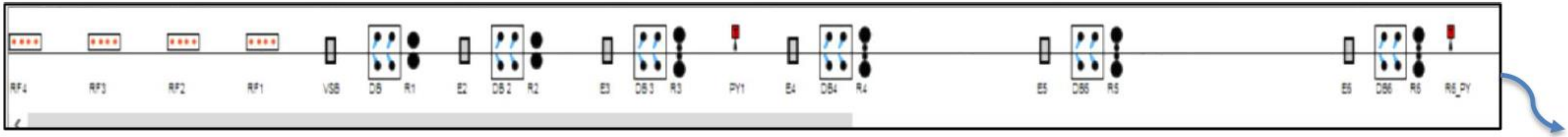
- Rapid deployment and scale-up
- Learning from data-driven models. Building towards autonomy for various geometries and alloys
- Enabling agile manufacturing of unique parts

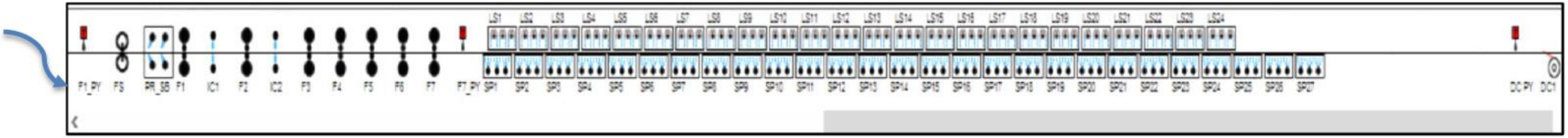
- Develop fast-running models for deformation of various materials.
- Develop reduced-order ML models for integration into autonomous path planning
- ML models will allow for better adaptive control

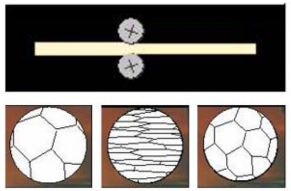


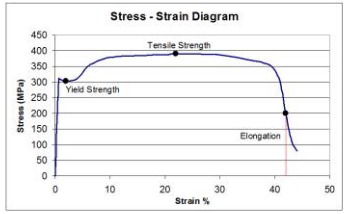



Sheet metal production (AK Steel / Cleveland Cliffs)

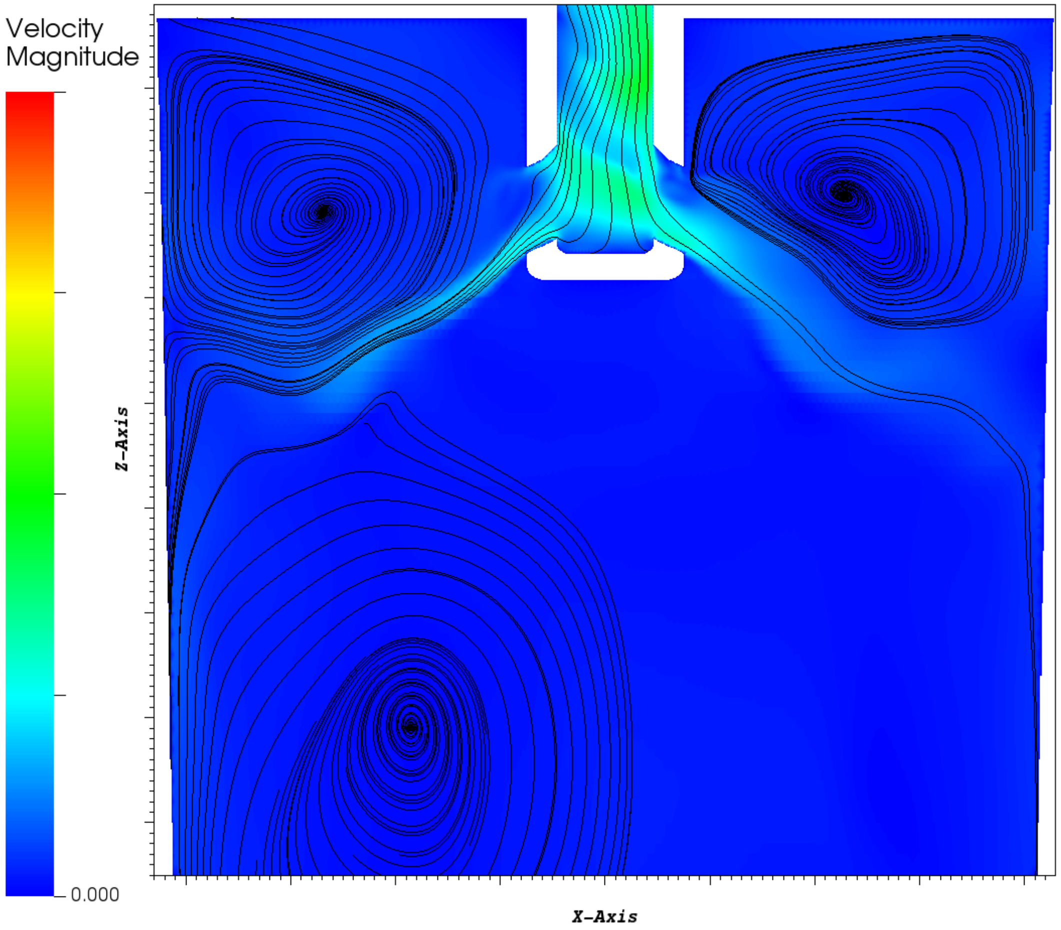


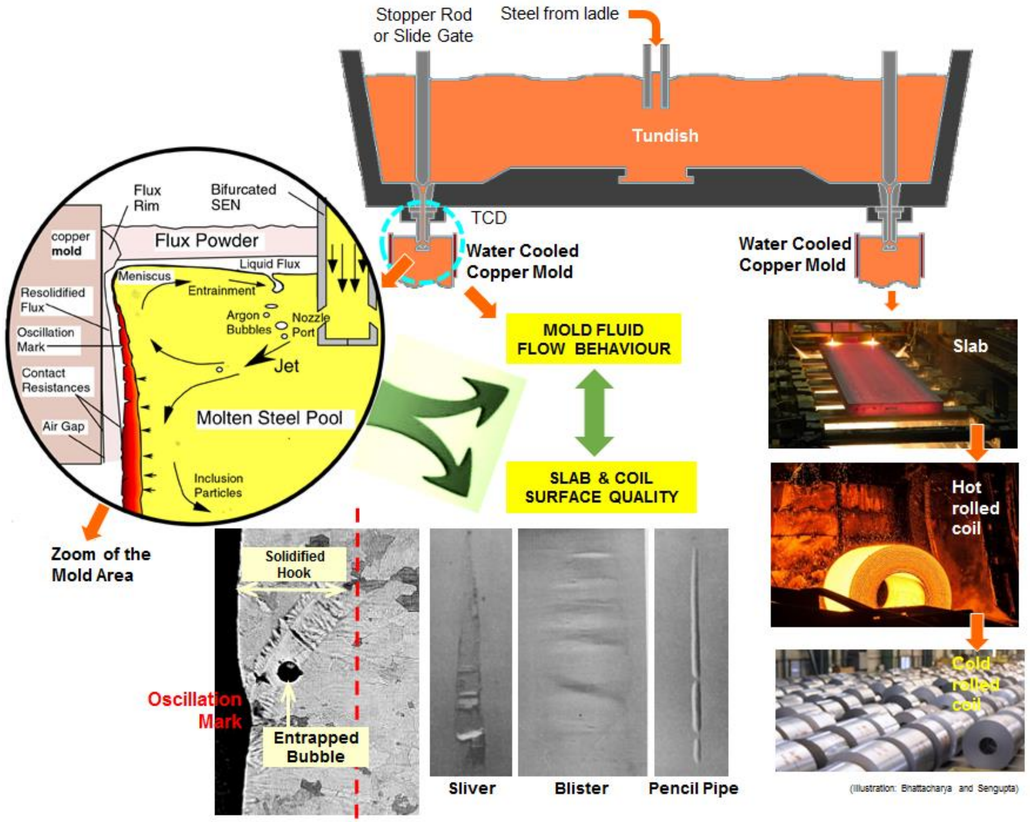




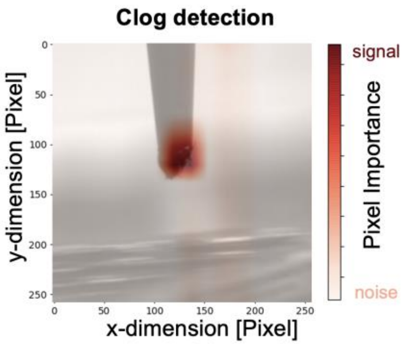


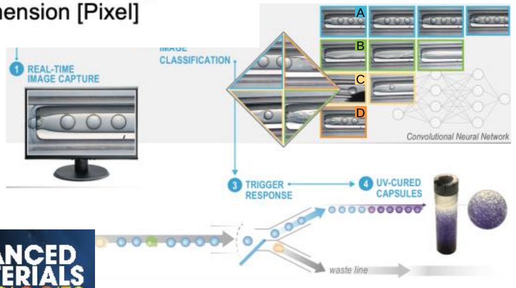
Steel production (ArcelorMittal-USA / Cleveland Cliffs)

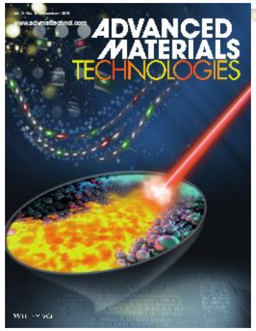




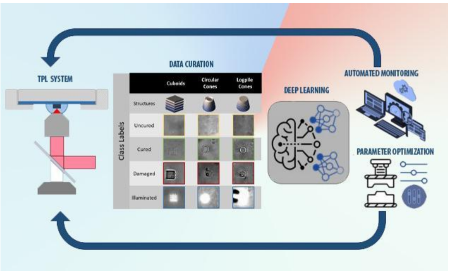
Technological Trajectory of Smart Advanced Manufacturing at LLNL



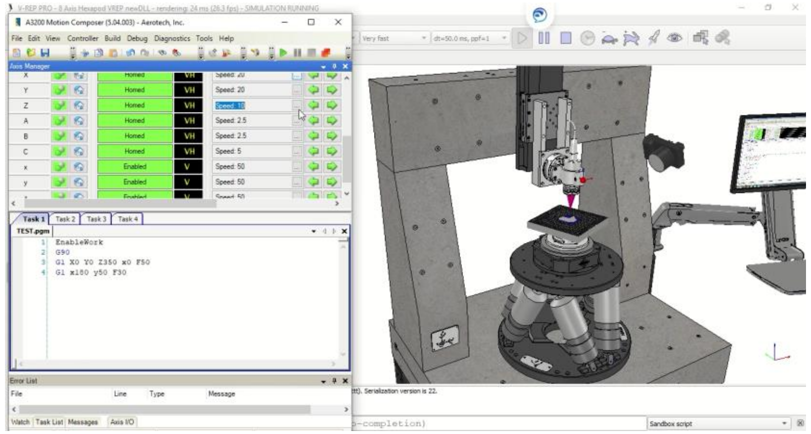




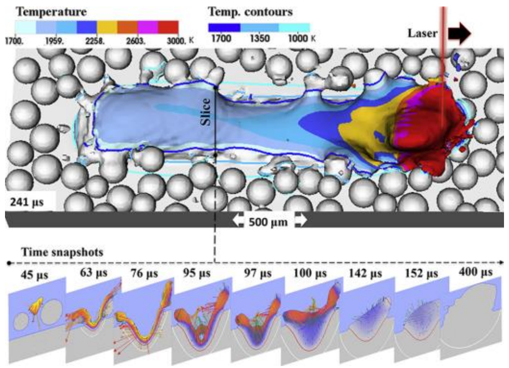
ML-based monitoring



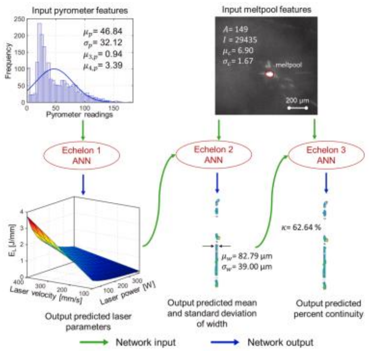
ML-based process control



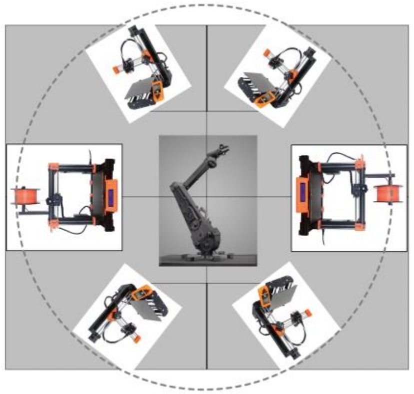
Machine-level digital twins



Real-time multi-scale modeling



Hybrid physics/ML-models



Production-level digital twins

Facility-level digital twins

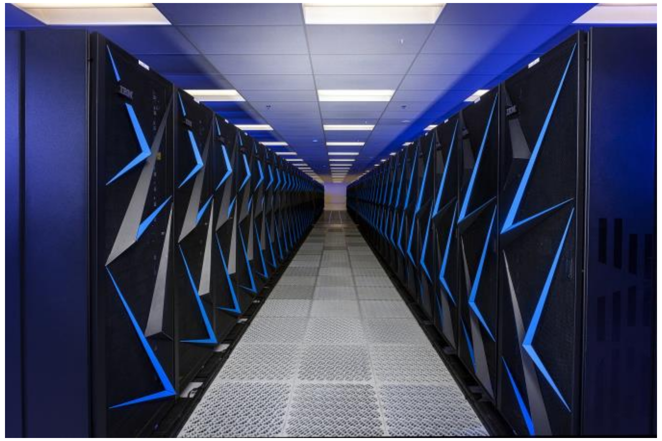
~3 years ago **Today** **10 years**

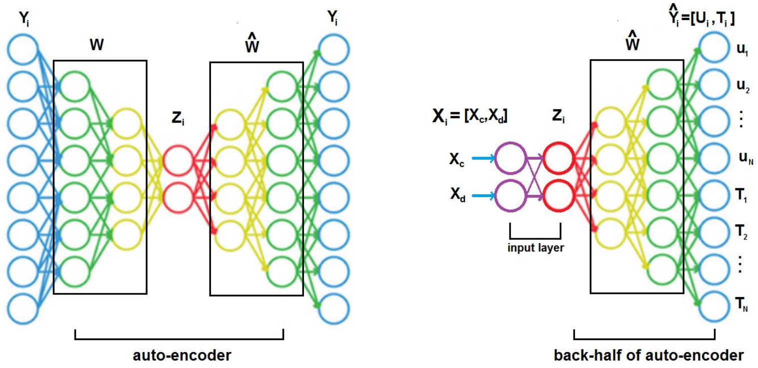
POC: Brian Giera, Adam Jaycox

Scientific Machine Learning

Scientific Machine Learning (SciML)

- **Using physical simulation for data (training)**
- **ML for fast surrogate model (inference)**
- **Simulations can be expensive**
  - Intelligent sampling
  - Speculative sampling

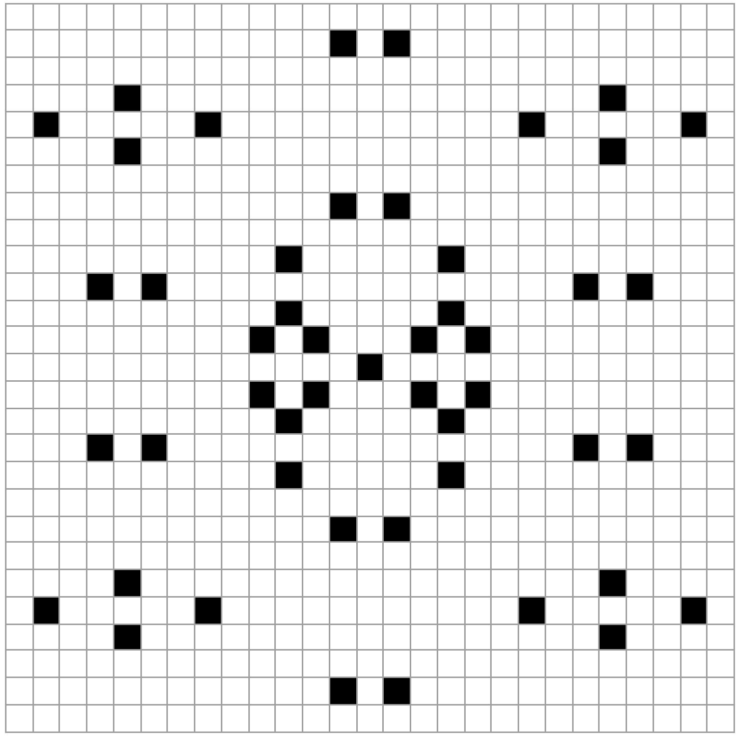




Concept – Design of Experiment

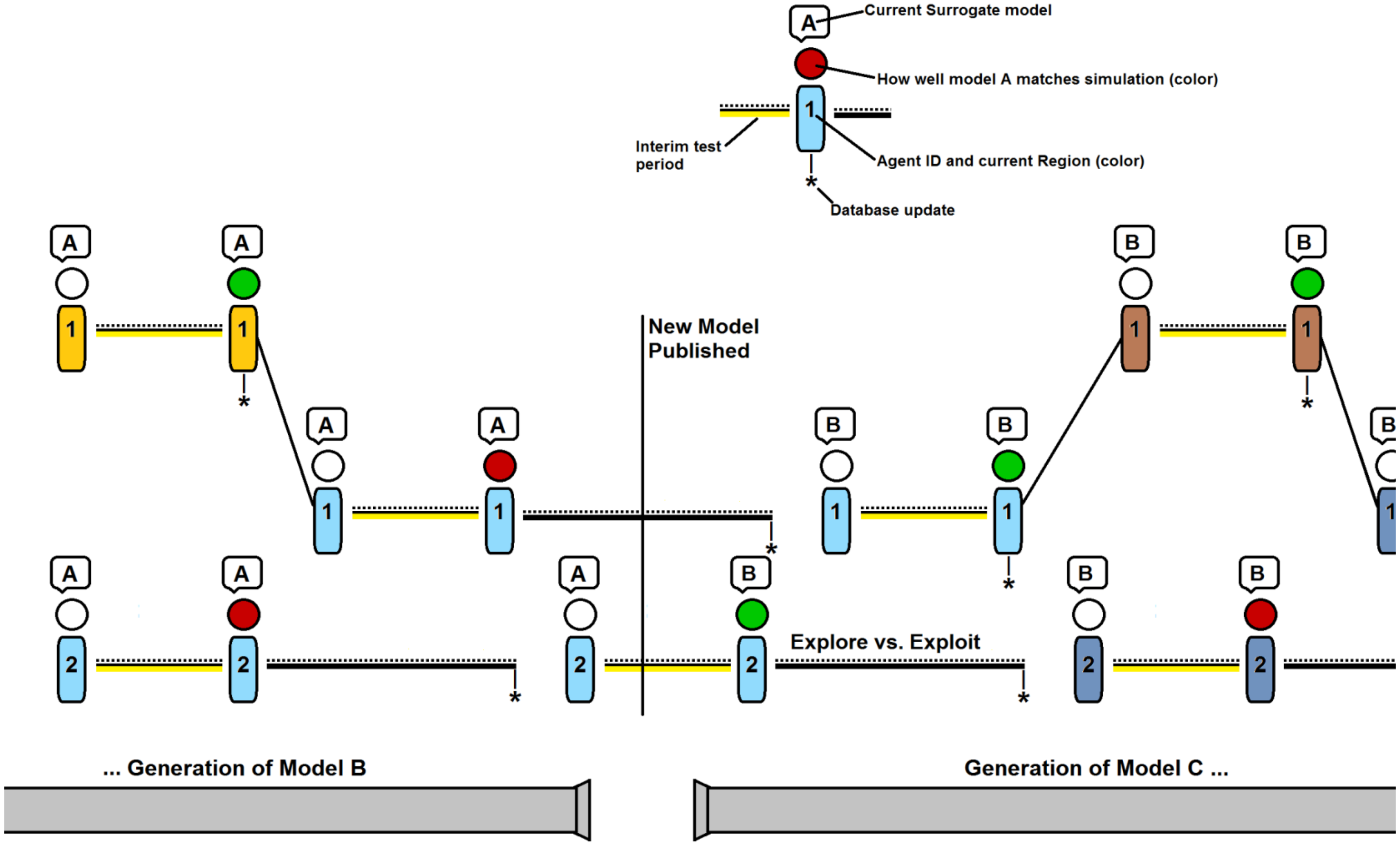
Design of Experiment

- **Used to cover design space efficiently**
- **Sampling can be rotated to leverage existing simulations**
- **Care must be taken to avoid unsuitable control configurations.**



2D mapping of 6 control variables: Box-Behnken sampling

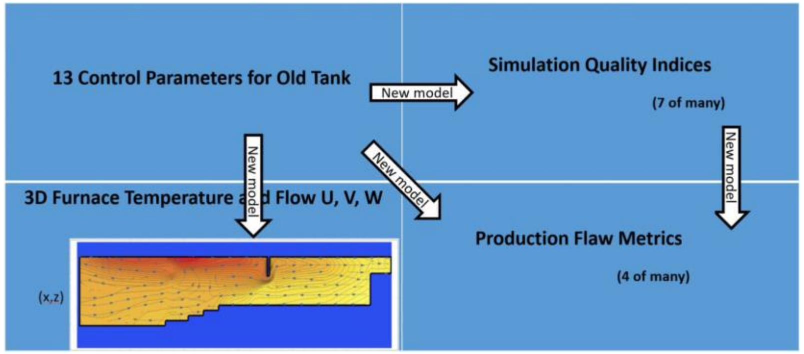
Concept – Active Learning

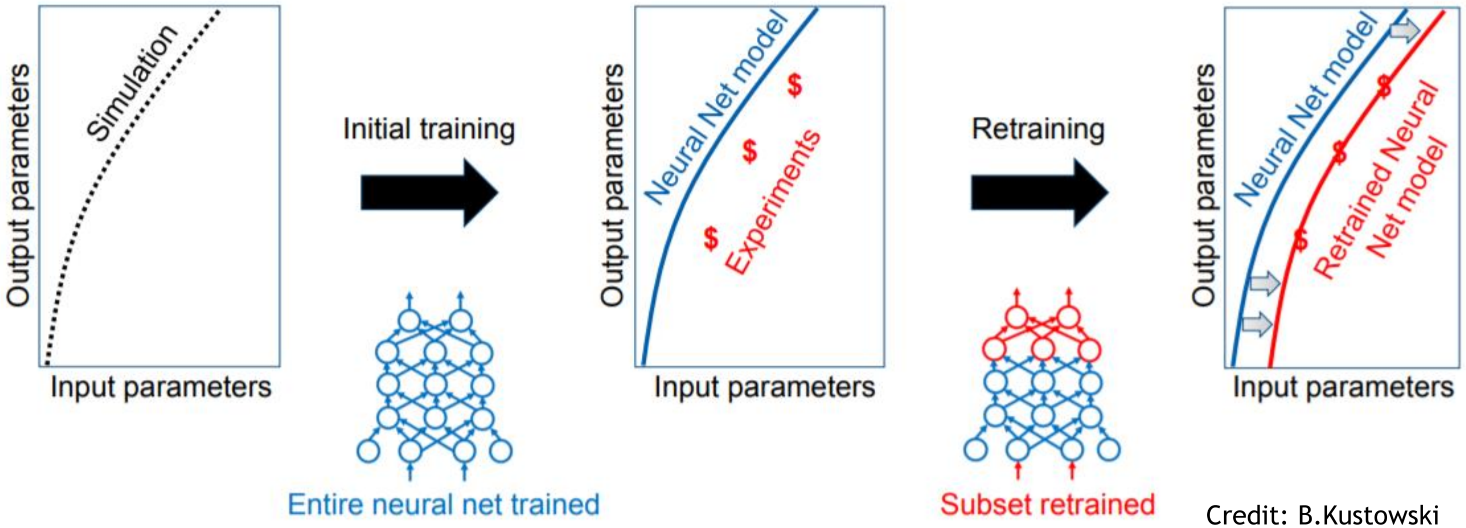


Concept – Transfer Learning

Transfer Learning

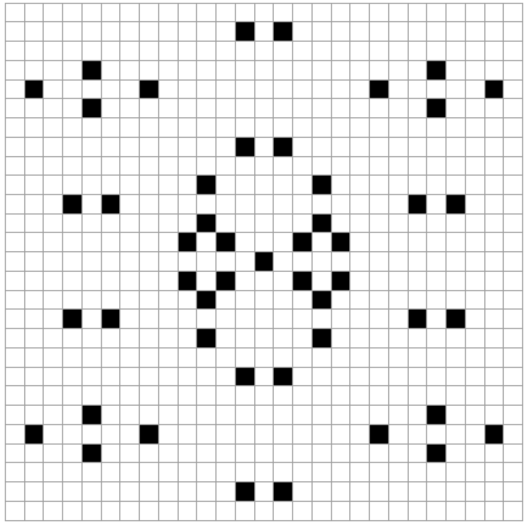
- **Elevates surrogate with production data**
- **Combines sensor data with physics**





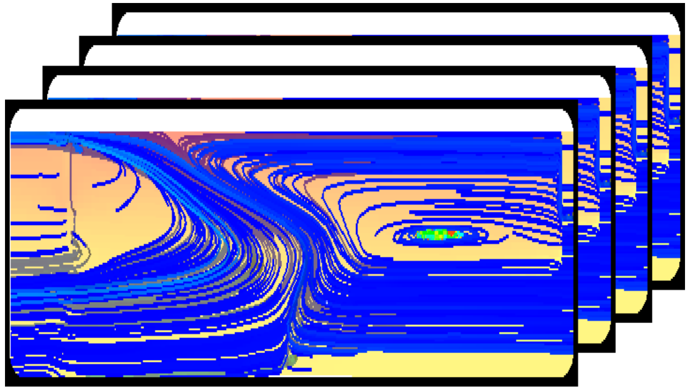
Credit: B.Kustowski

SciML Workflow

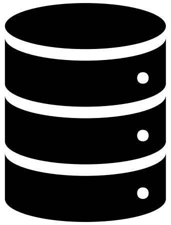


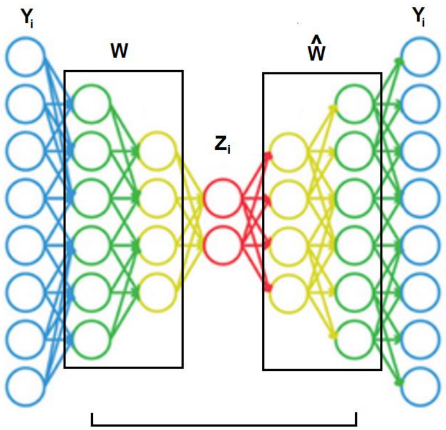
Design of Experiment (Parameter Study)

Simulations

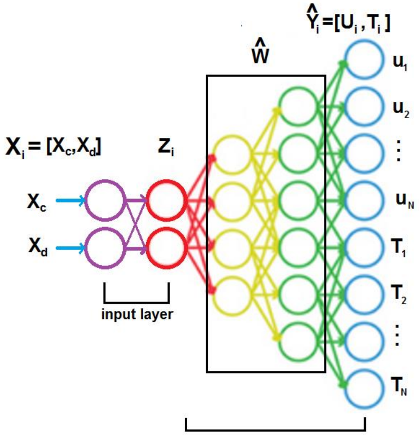


Data Curation



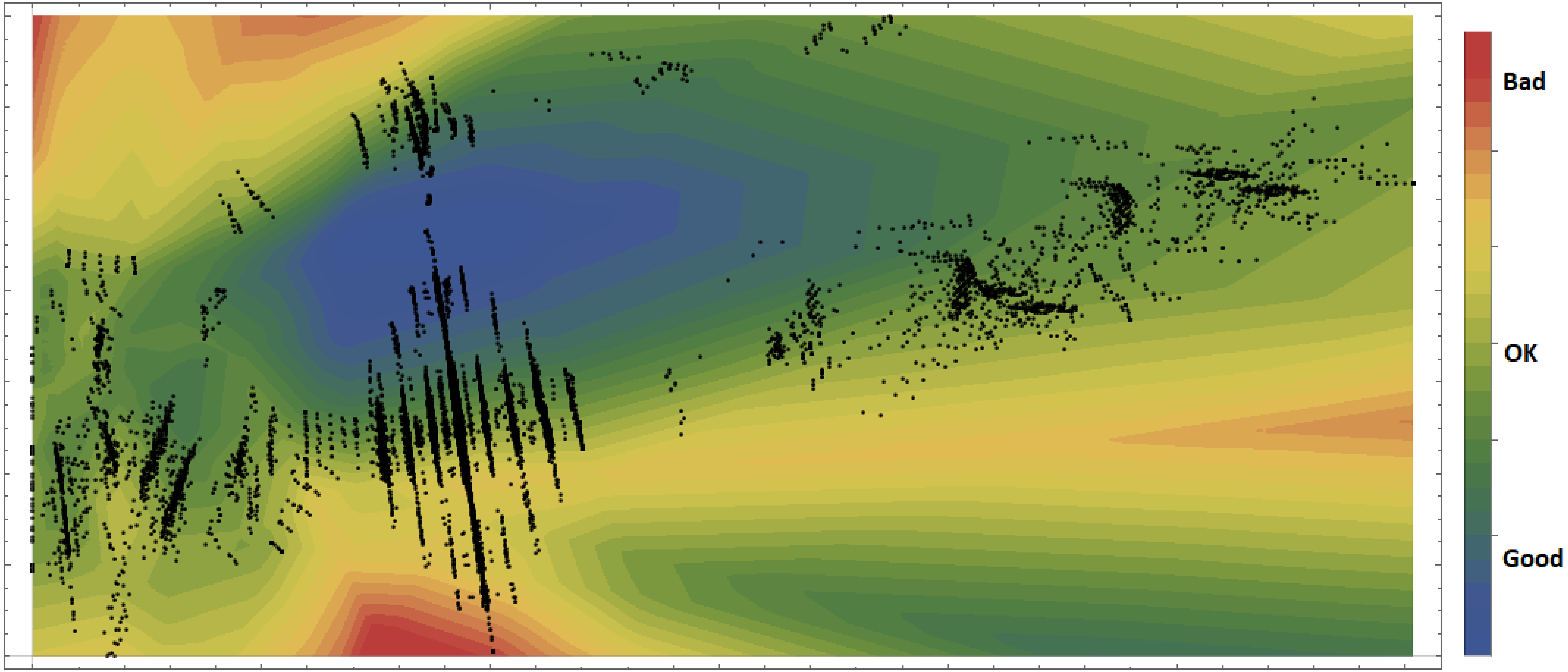


auto-encoder



back-half of auto-encoder

Typical Quality Map (X -> Z -> Y)



Key Points

- **Neural Networks** can learn and predict features of complex processes
- **Simulations** can provide training data
- **Physical experiments** and/or **production data** can be integrated into predictor model
- We have **tools and resources**

Impact: savings

- Reduced-order model saves days, weeks, or months when process is out of control limits.
- Data integration makes most of sensor data and simulation investment.
- Uncertainty quantification helps to avoid costly investments that don't inform.

Project Impact: company/industry

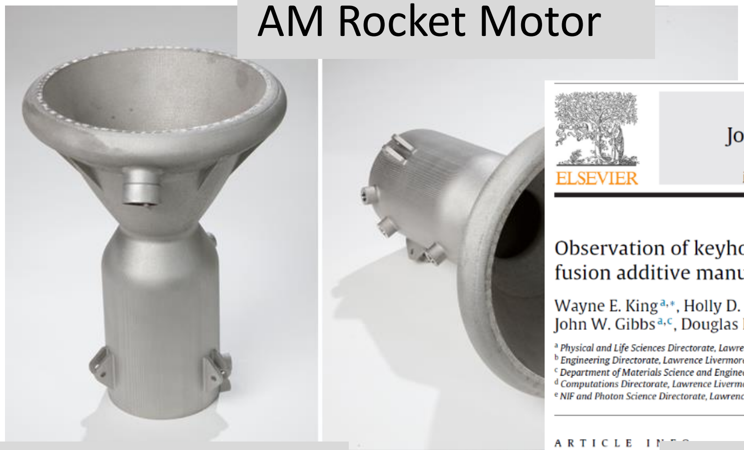
Company	Savings
PPG/Vitro (Glass)	Two weeks of production per year per furnace
U.S. Glass Industry	• Save ~2.5 TBTUs of energy • Avoid 130,000 metric tons of CO_2 emissions
Arconic/Alcoa (Aluminum)	$60M per year: if this technology can reduce the amount of reworked scrap by 50%
U.S. Primary Casting	$365M per year
VAST Power Systems	save ~1% of U.S. turbine fuel use
AK Steel / Cleveland Cliffs	>$1M per mill per year
ArcelorMittal / Cleveland Cliffs (steel casting)	$90M per year
U.S. Steel industry	3 PJ energy -> $30.5M per year

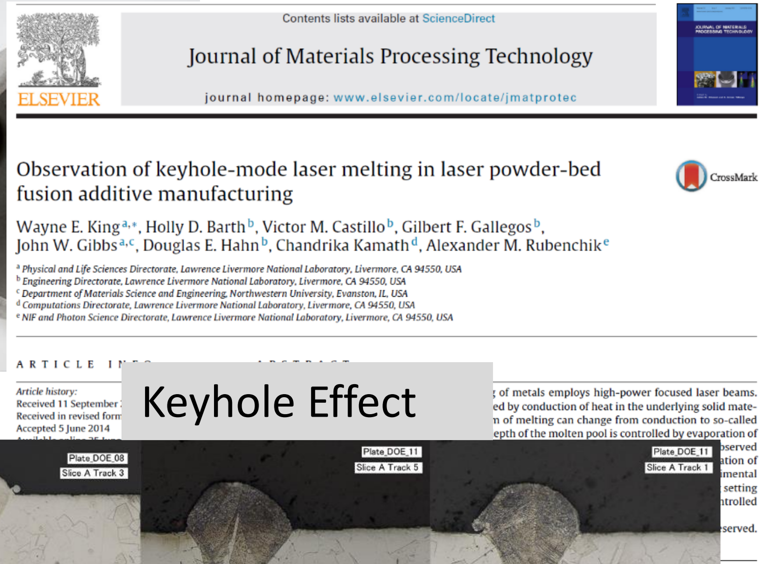
LLNL Metal Additive Manufacturing Data Curation, Distribution, and Documentation – Ethan Ahlquist, CED

DSSI Student Project: Curate, Publish, and Market metal additive manufacturing data from ACAMM LDRD Strategic Initiative.

Sophie and Vanessa

AM Rocket Motor





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Observation of keyhole-mode laser melting in laser powder-bed fusion additive manufacturing

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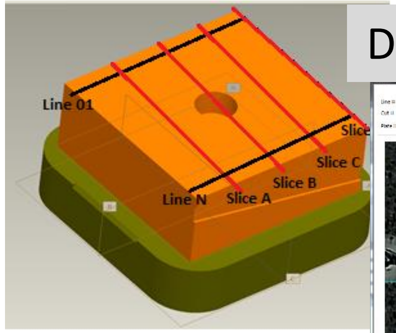
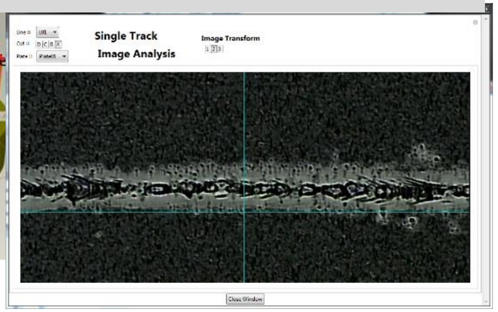
Article history:
Received 11 September
Received in revised form
Accepted 5 June 2014

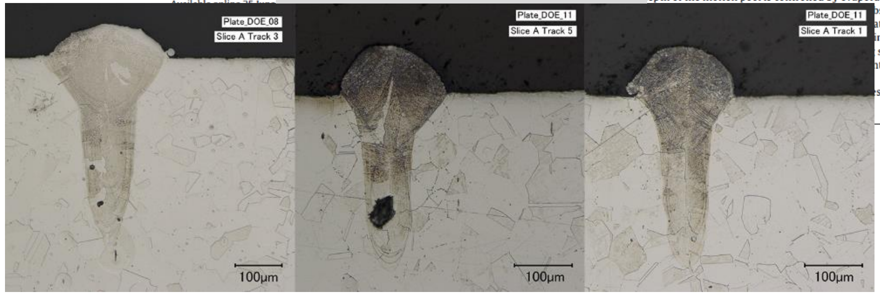
g of metals employs high-power focused laser beams.
ed by conduction of heat in the underlying solid mate-
n of melting can change from conduction to so-called
epth of the molten pool is controlled by evaporation of

Design of Experiment





Keyhole Effect



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