

Accelerating NSUF studies with Artificial Intelligence and Machine Learning at Partner Facilities

Kevin G. Field^{1,2*}

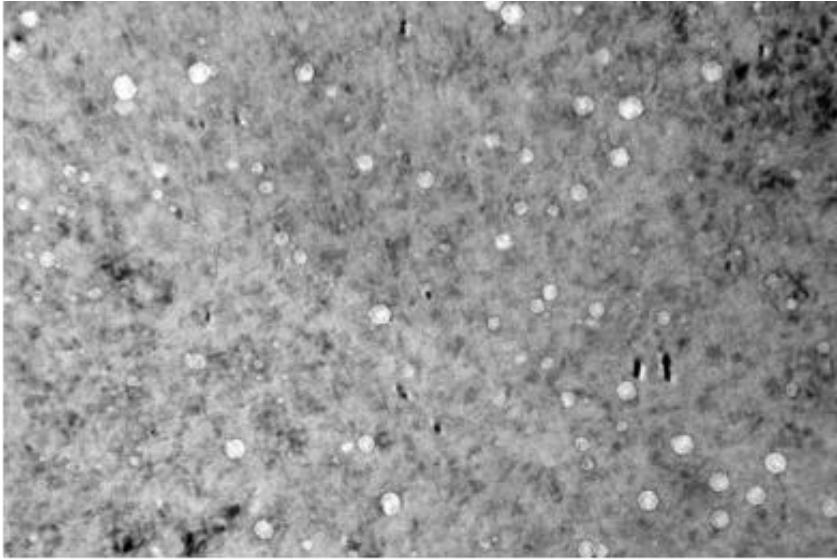
¹ University of Michigan, Ann Arbor, MI 48109

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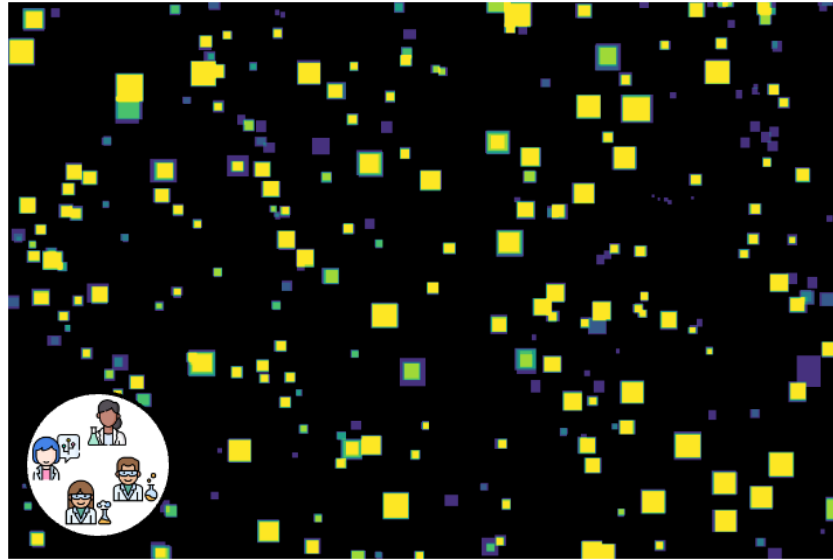
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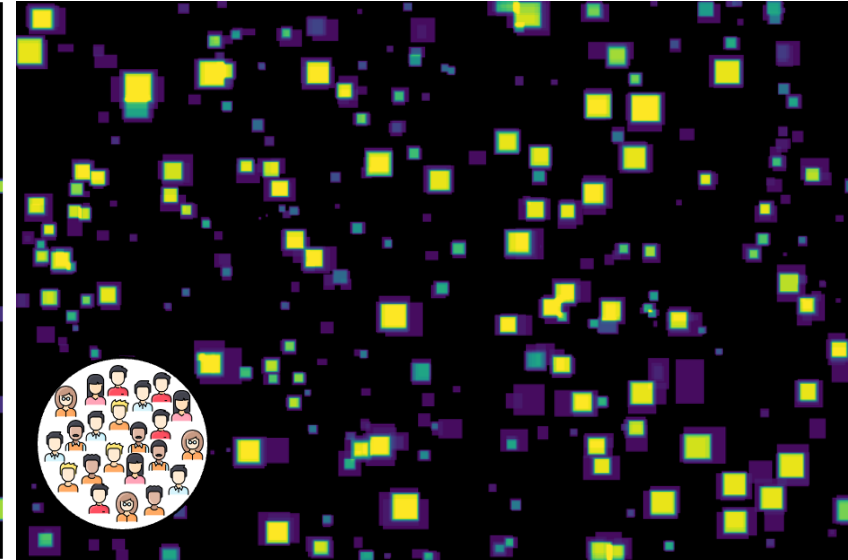
Applying machine learning can increase the quality and consistency of NSUF user data



Original Image



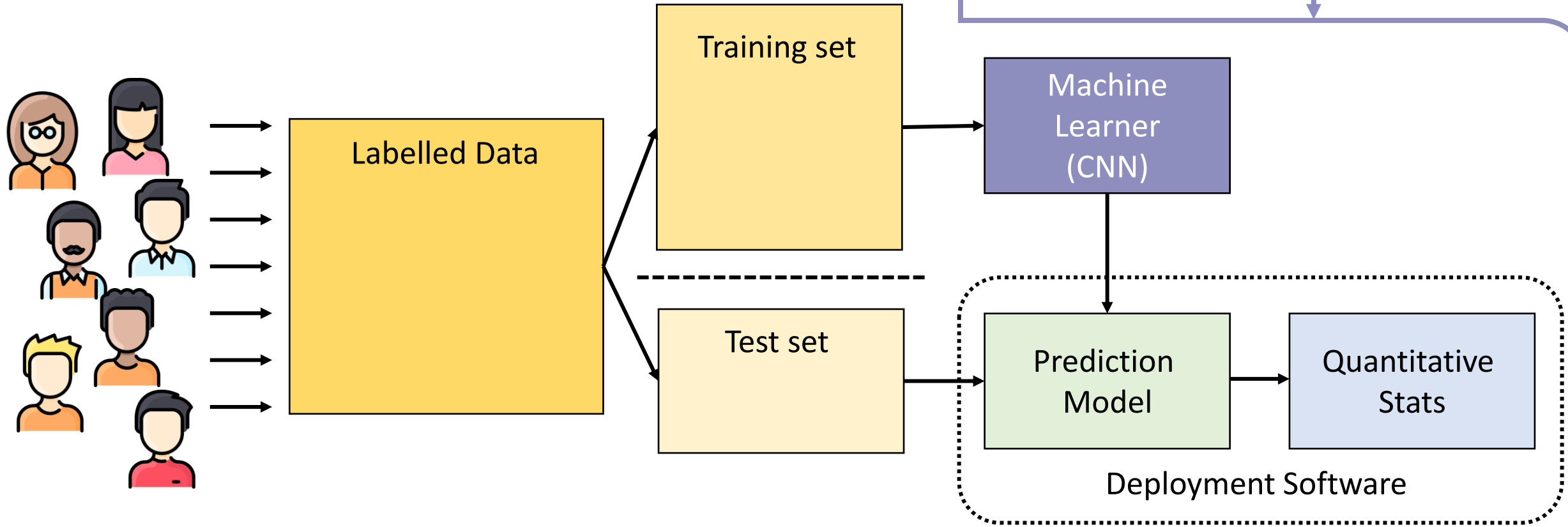
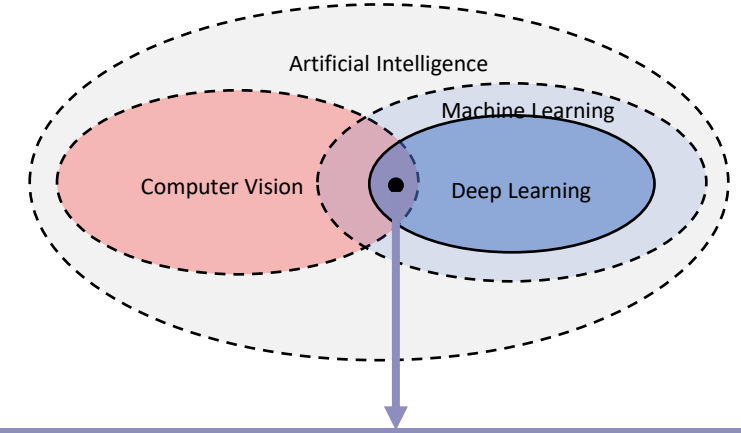
6 Experts



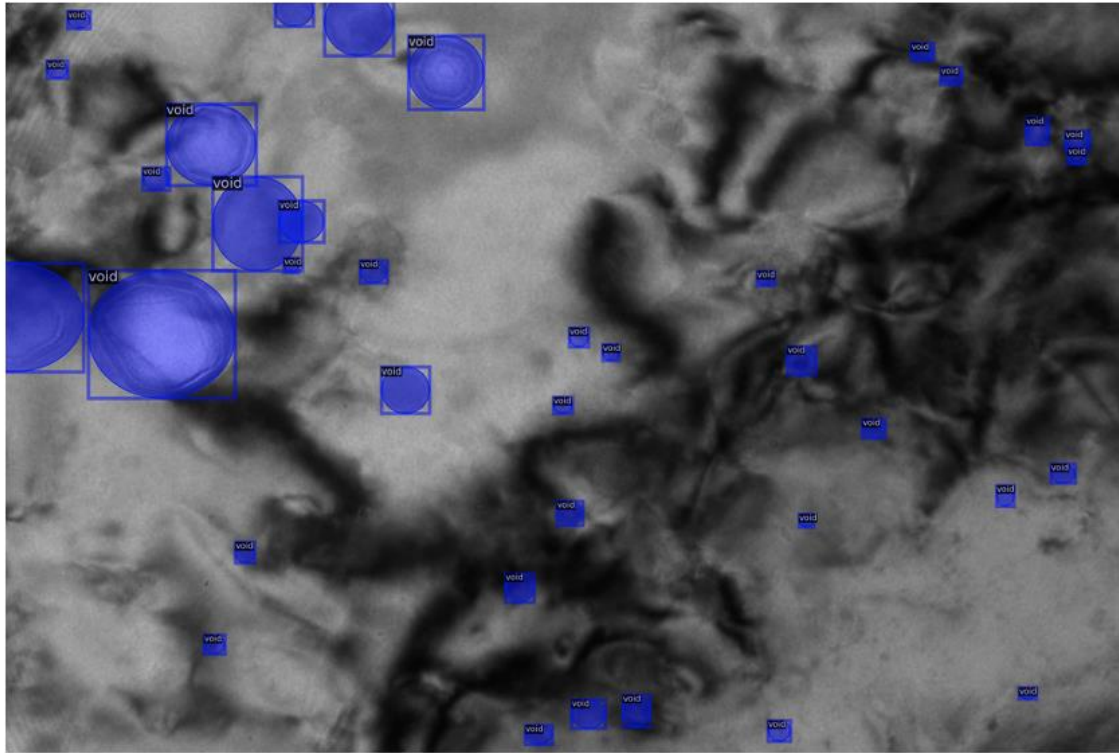
33 Non-Experts

- Only in rare instances are users likely to quantify a complex image the same
- ML methods like object detection will provide the same answer on the same image everytime

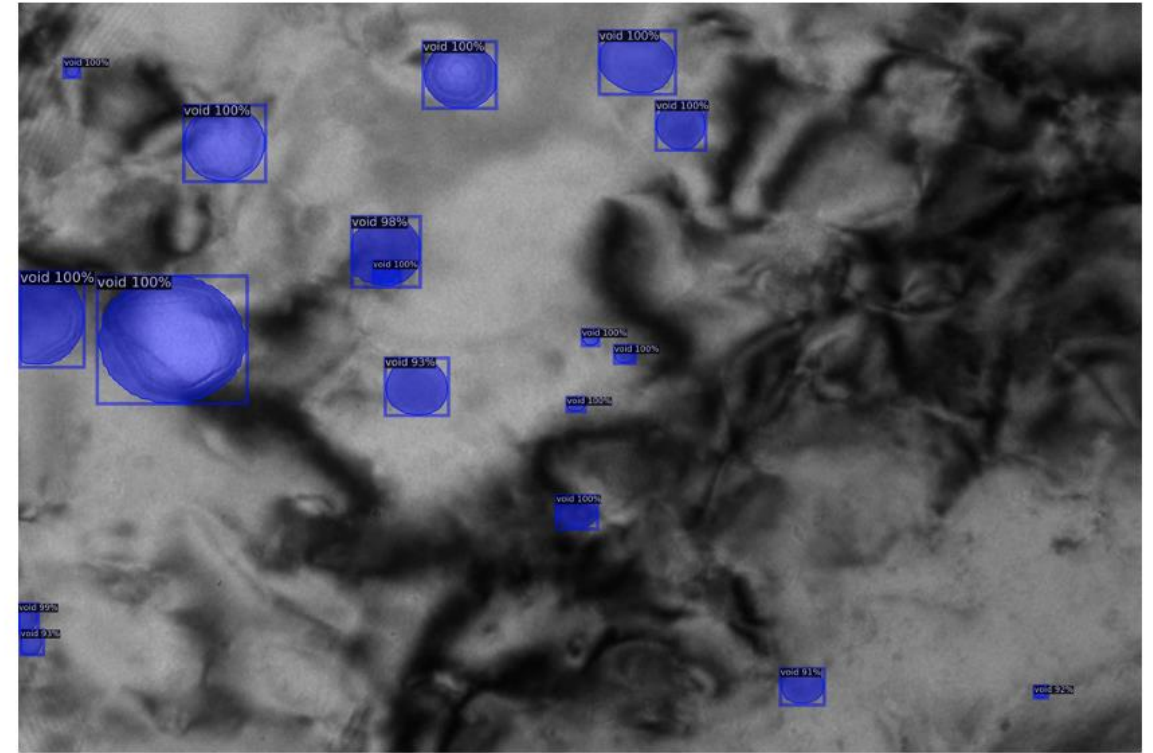
Our ML approach uses supervised learning (requires labelled data)



Example of our best Mask R-CNN detection model for cavities in irradiated materials

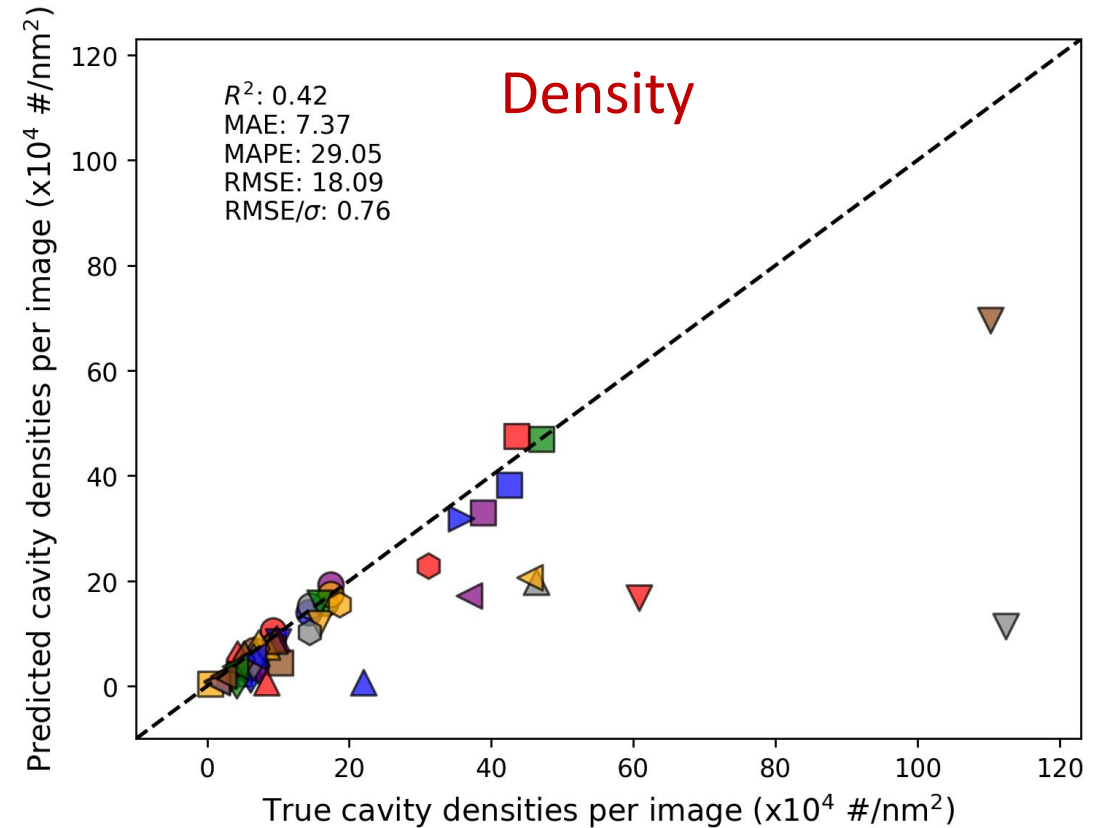
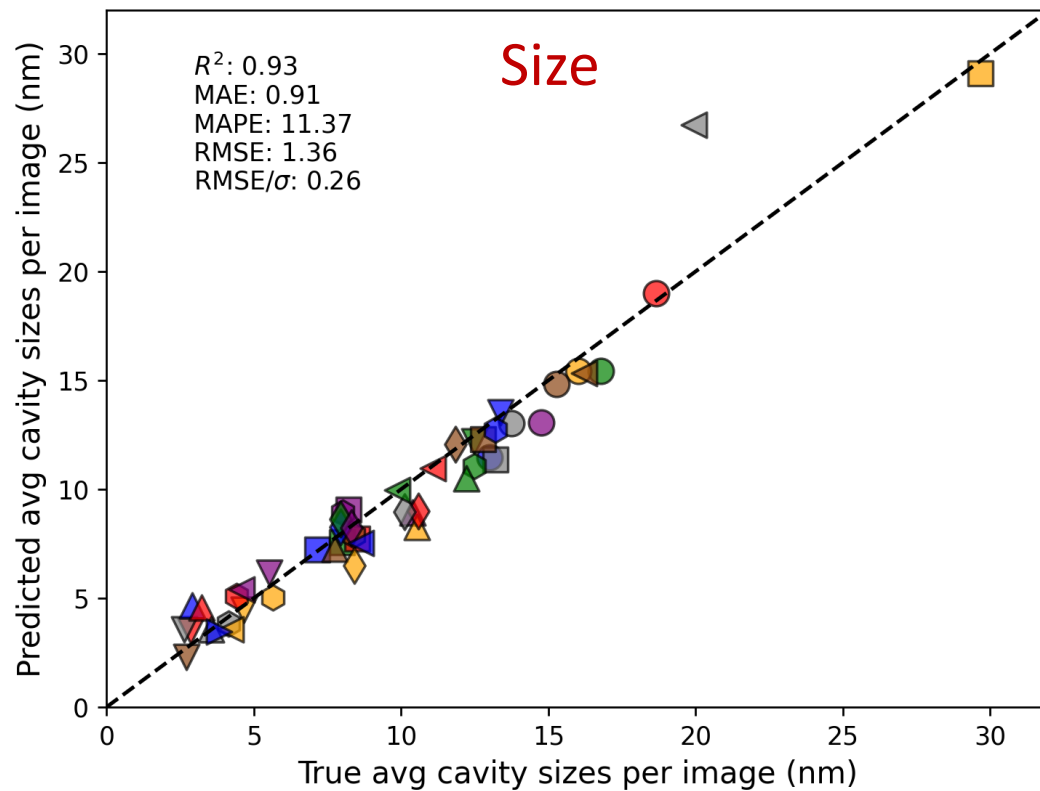


Human Expert

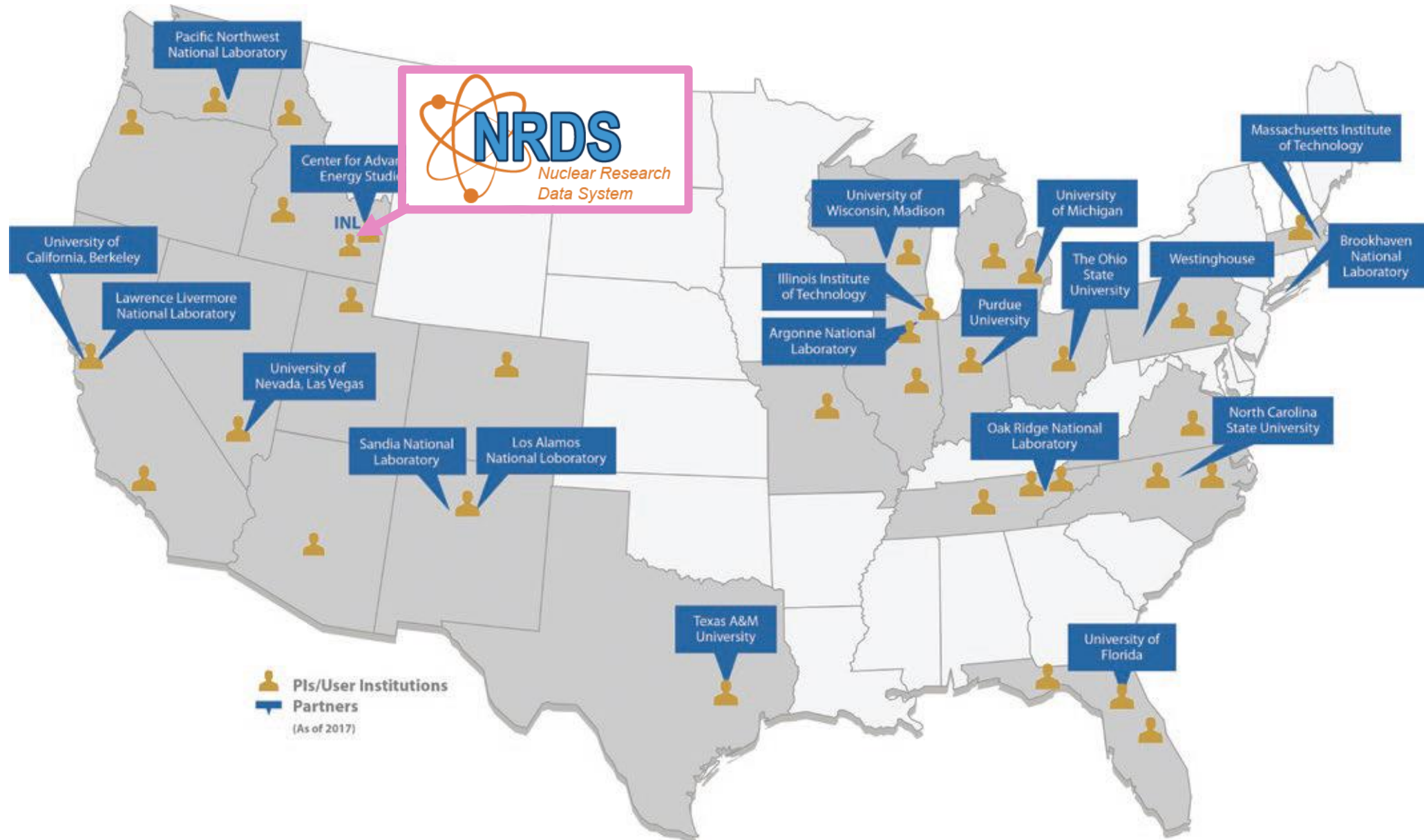


Mask R-CNN

ML-based object detection using convolutional neural networks (CNNs) enable human-like quantification in less than a second



Theiascope™ systems are now at several partner facilities



Welcome to NRDS

The Nuclear Research Data Search (NRDS) site is a public-facing, long-term data storage solution and science data gateway featuring integrated compute resources such as artificial intelligence enabled hardware, and access to graphics processing units (GPUs). Operated out of the US Department of Energy Office of Nuclear Energy's Nuclear Science User Facilities (NSUF) program, NRDS takes publicly funded data from NSUF research and makes it accessible to the public without requiring a paywall or account and ensure all data meets the pFAIR criteria.

Advanced Test Reactor



Search data



Current AI Analysis Features

Super Resolution - Low resolution to high resolution photos

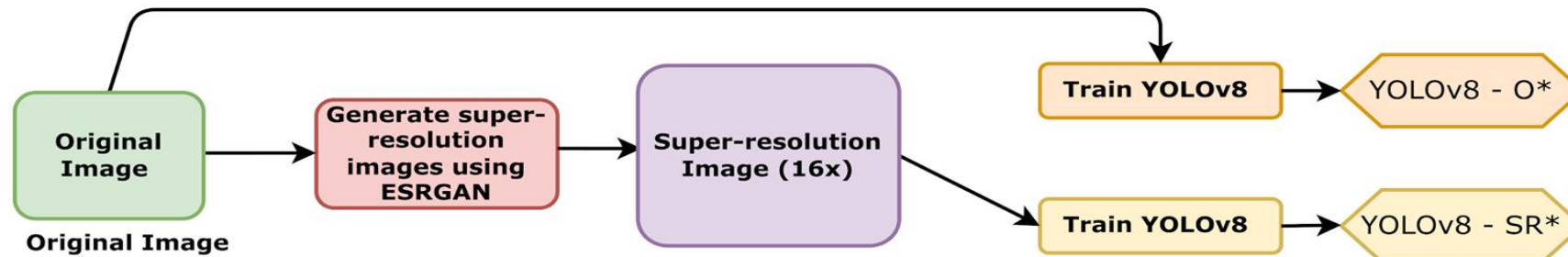
Activity Detection - Locating temporal activities within a video

Dislocation Segmentation - Segment dislocation loop and line defects in an image

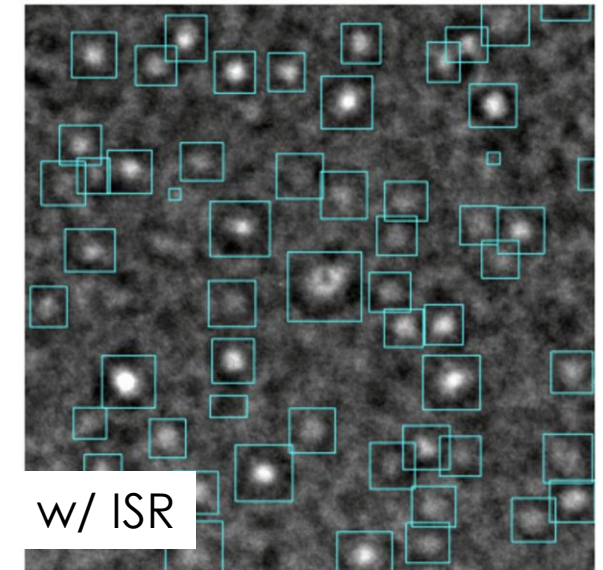
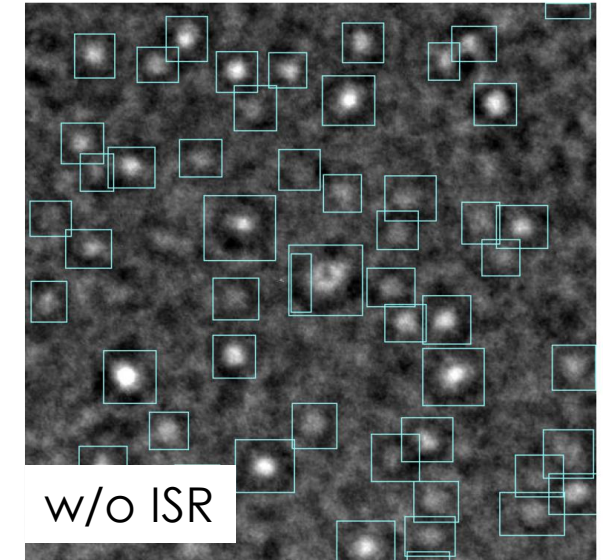
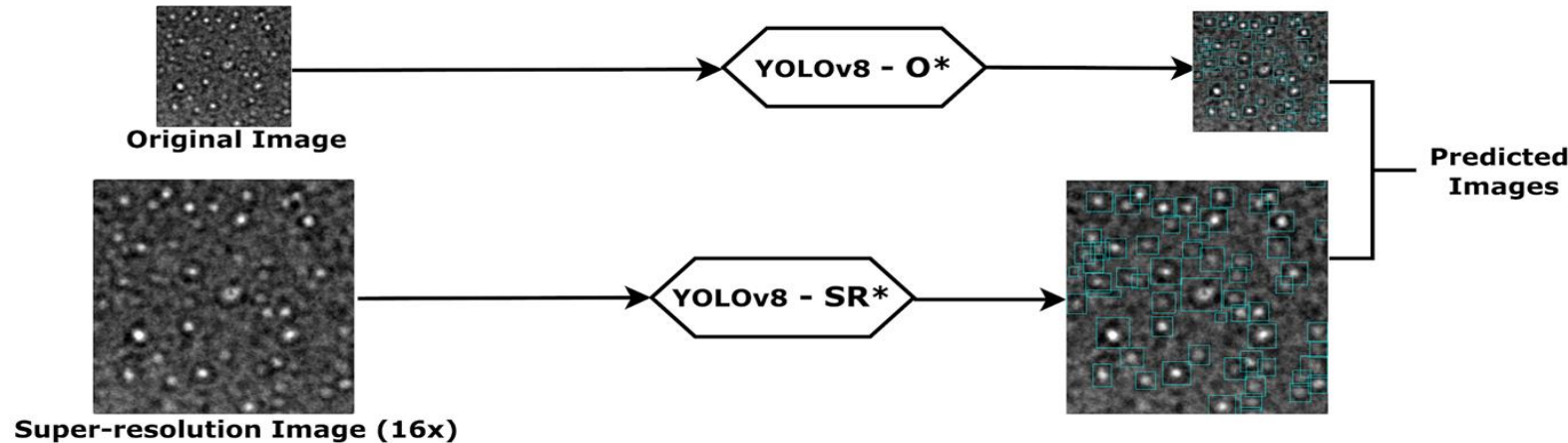
Dislocation Lines - Overlay dislocation lines on an image

Application of image super-resolution (ISR) like in NRDS can improve machine learning object detection

Training (using the original training dataset and generated super-resolution dataset, respectively.)



Testing (using the original testing dataset, and generated super-resolution dataset, respectively.)



Application of image super-resolution (ISR) like in NRDS can improve machine learning object detection

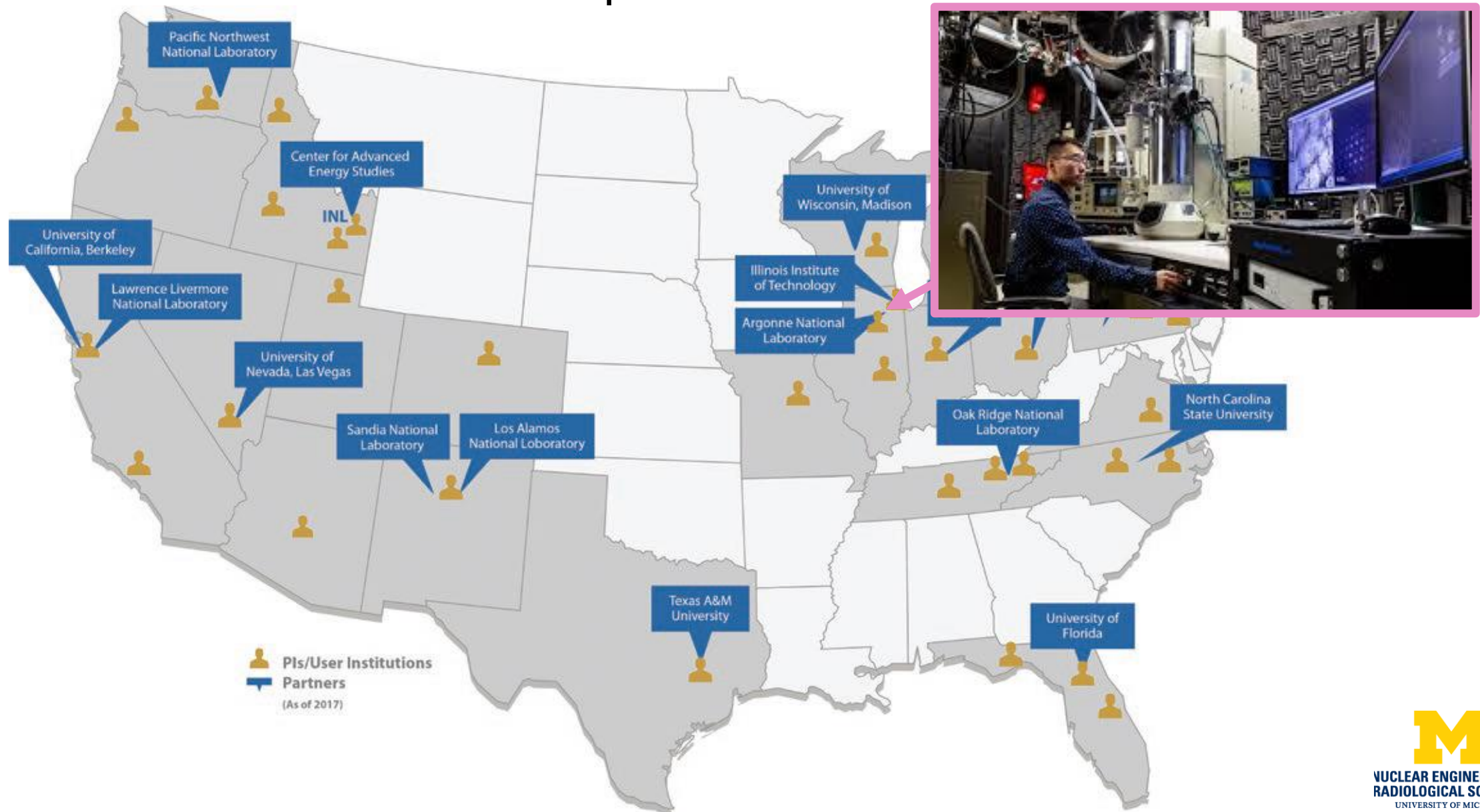
	Model O-M	Model SR-M
Total Predictions	4775	3768
Total ground-truth	4259	4259
True Positives	2607	2475
False Positives	2168	1293
False Negatives	1652	1784
Precision	0.5459	0.6568
Recall	0.6121	0.5811
F1	0.5772	0.6167

*** **Model O-M:** YOLOv8 model trained on original dataset and tested on original dataset for all modalities

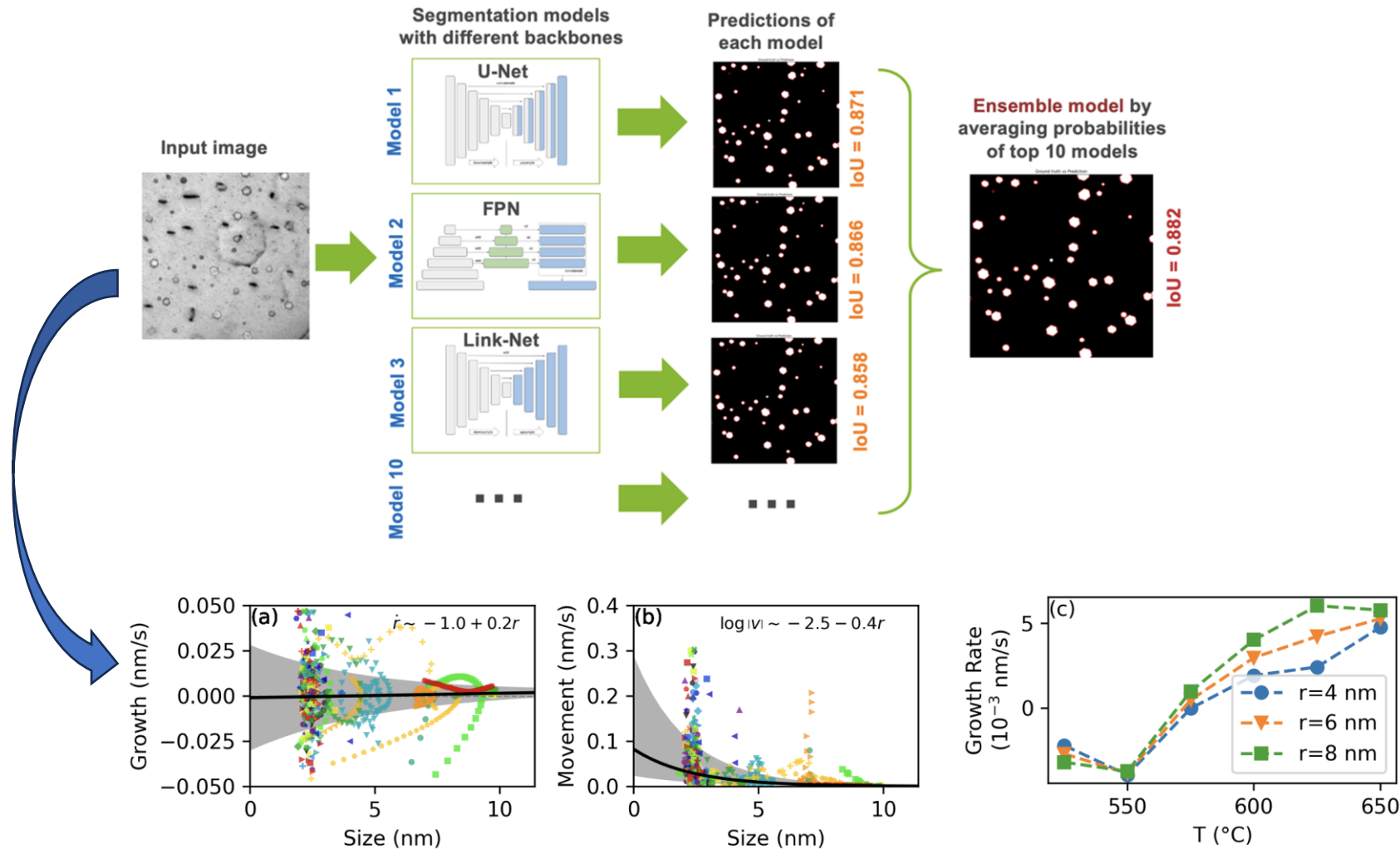
*** **Model SR-M:** YOLOv8 model trained on super-resolution dataset and tested on super-resolution dataset for all modalities

- **Super-Resolution (ISR) enhances precision (+20.5%)** by improving image clarity, making detections more reliable
- **A minor trade-off occurs with recall (-5.1%),** meaning some true cavities might be overlooked.
- **F1-score (+6.8%) confirms an overall performance boost,** making ISR a valuable enhancement for cavity detection
- **False positives are drastically reduced (-40.3%),** proving that ISR refines detection accuracy

Development of DSCNNs and SORT-based tracking has been under development at ORNL



IVEM has developed machine learning methods that enable cavity tracking and extraction of cavity growth rates

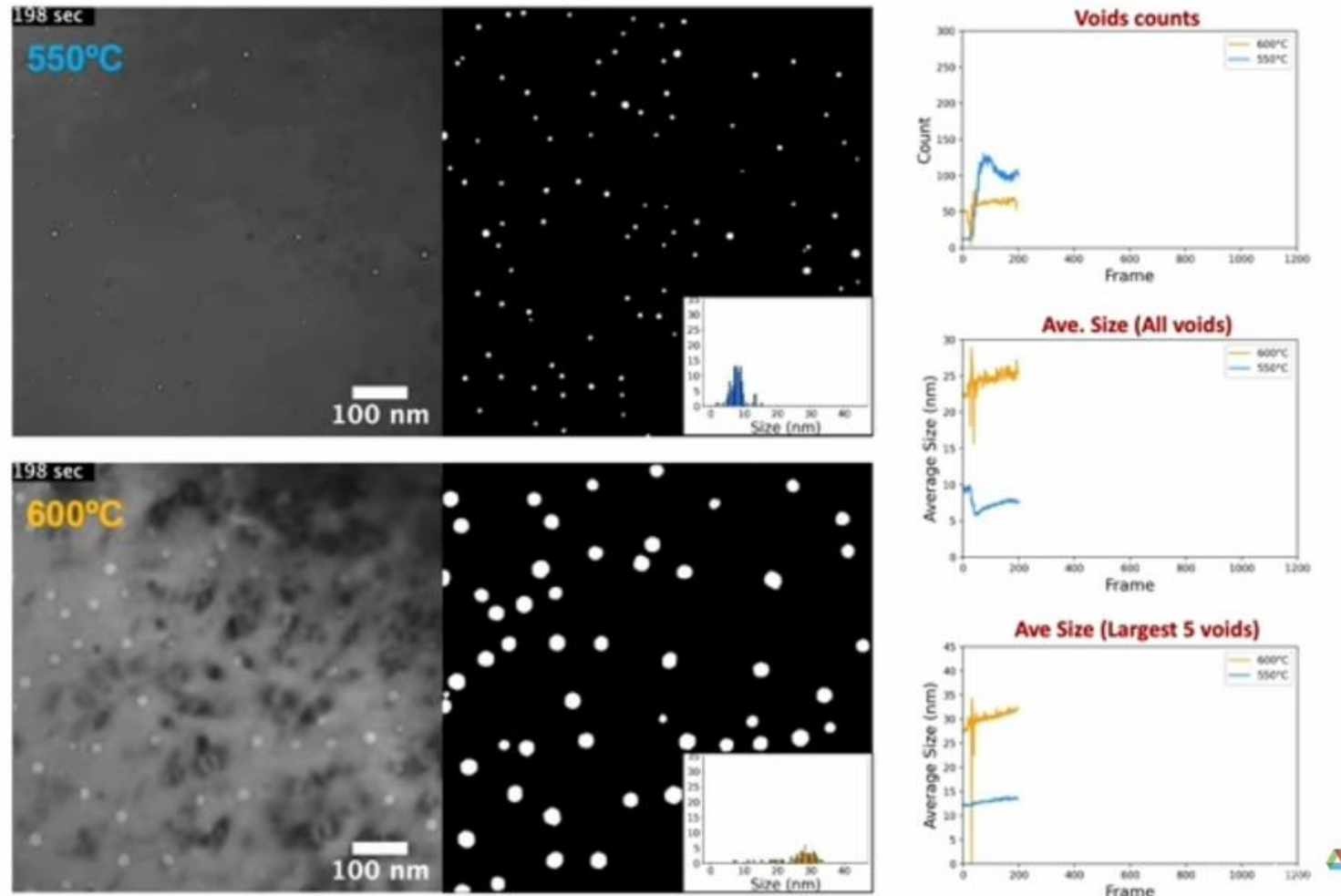


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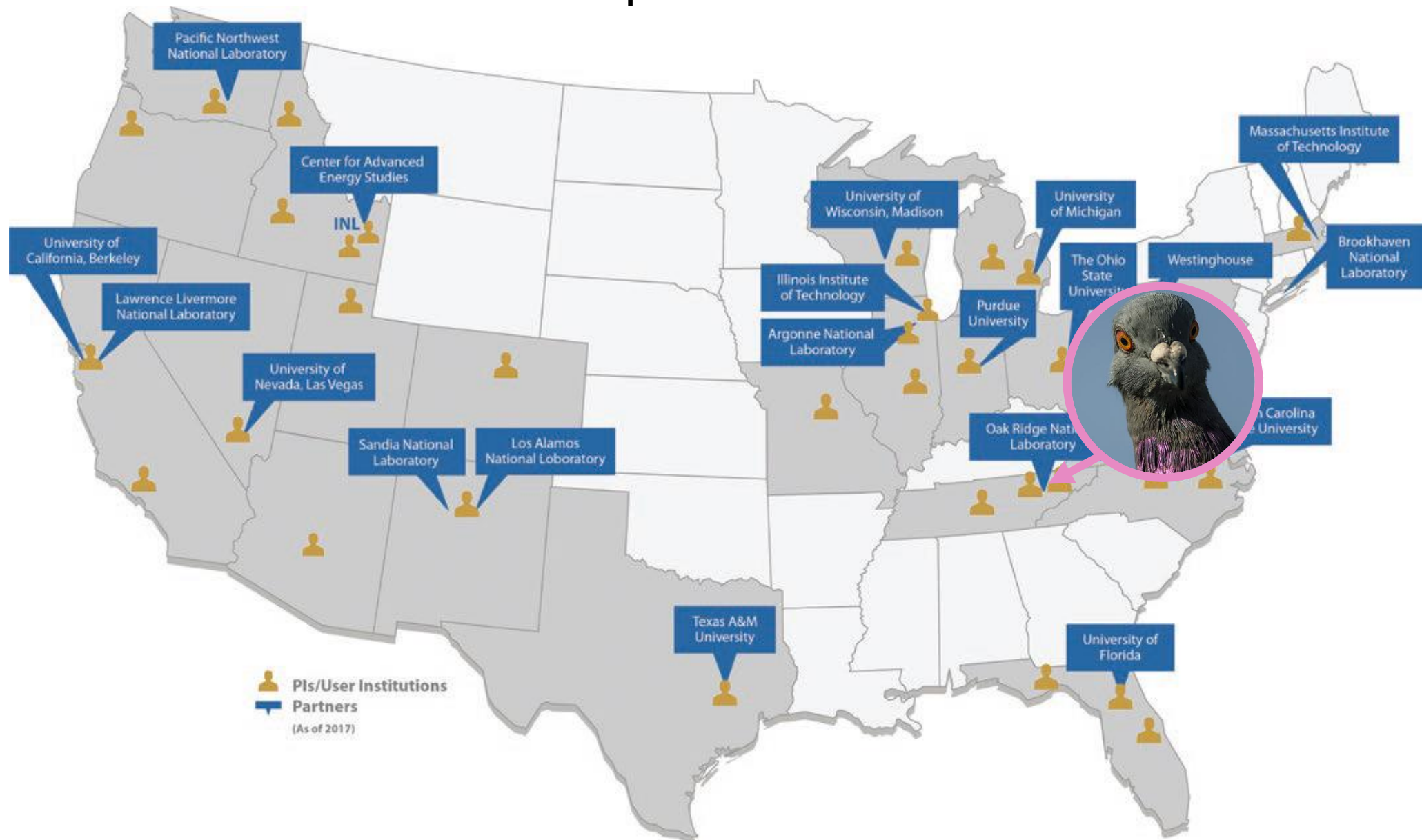
IVEM-Tandem Facility at Argonne National Laboratory

Automatic Segmentation of *in-situ* video by computer vision

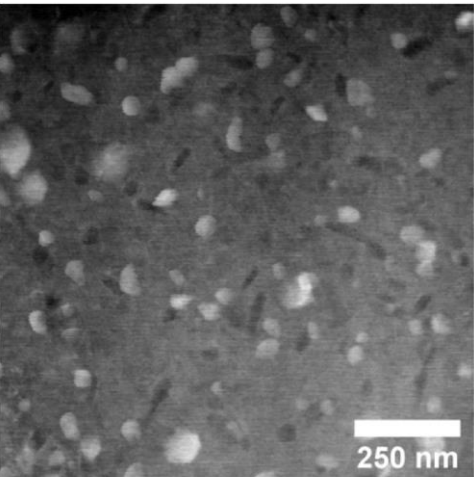
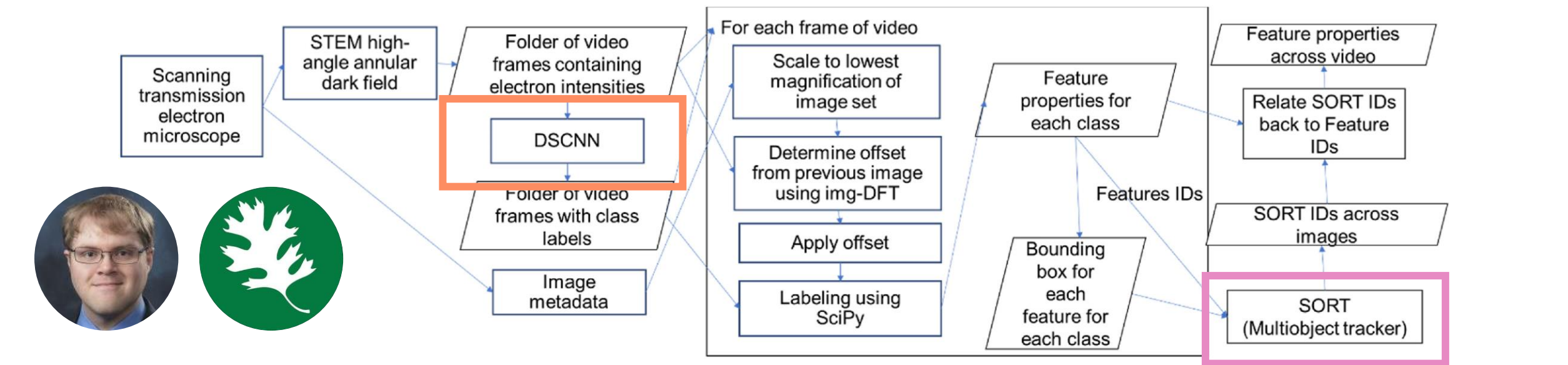
Nickel under *in-situ* 1 MeV Kr ion irradiation from 0.7 dpa to 1.9 dpa



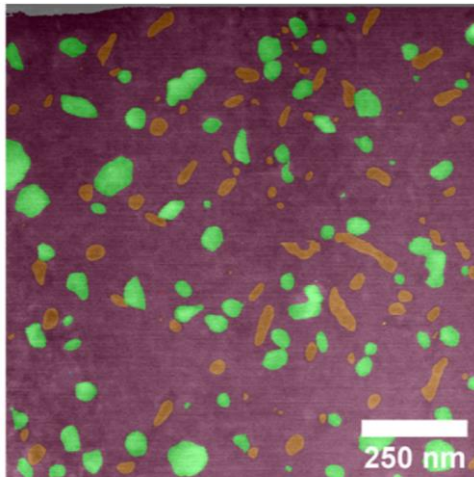
Development of DSCNNs and SORT-based tracking has been under development at ORNL



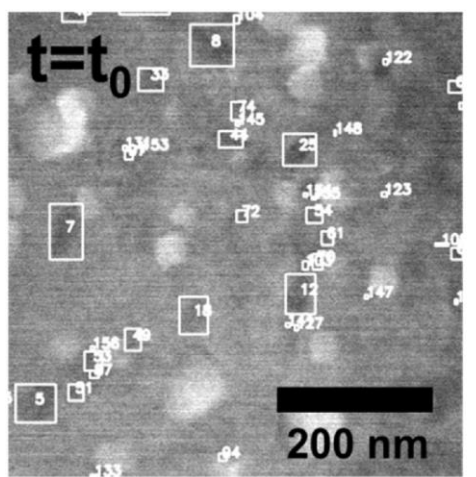
Other users of MiTEM are developing their own frameworks built on Convolutional Neural Networks and SORT algorithms



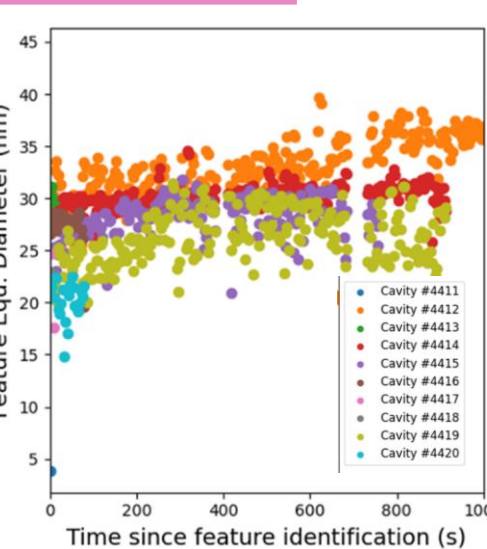
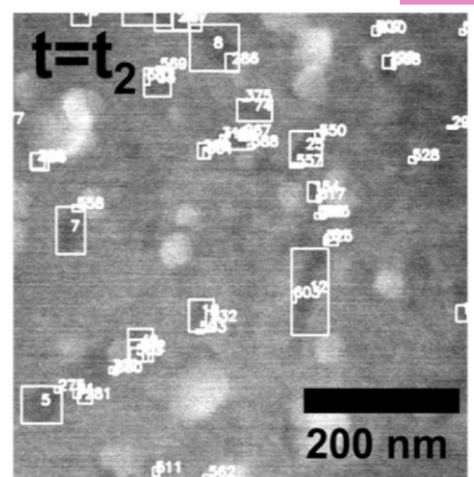
In-Situ STEM Irr. of IN718



Semantic Segmentation of Phases



SORT based tracking of cavities in HAADF

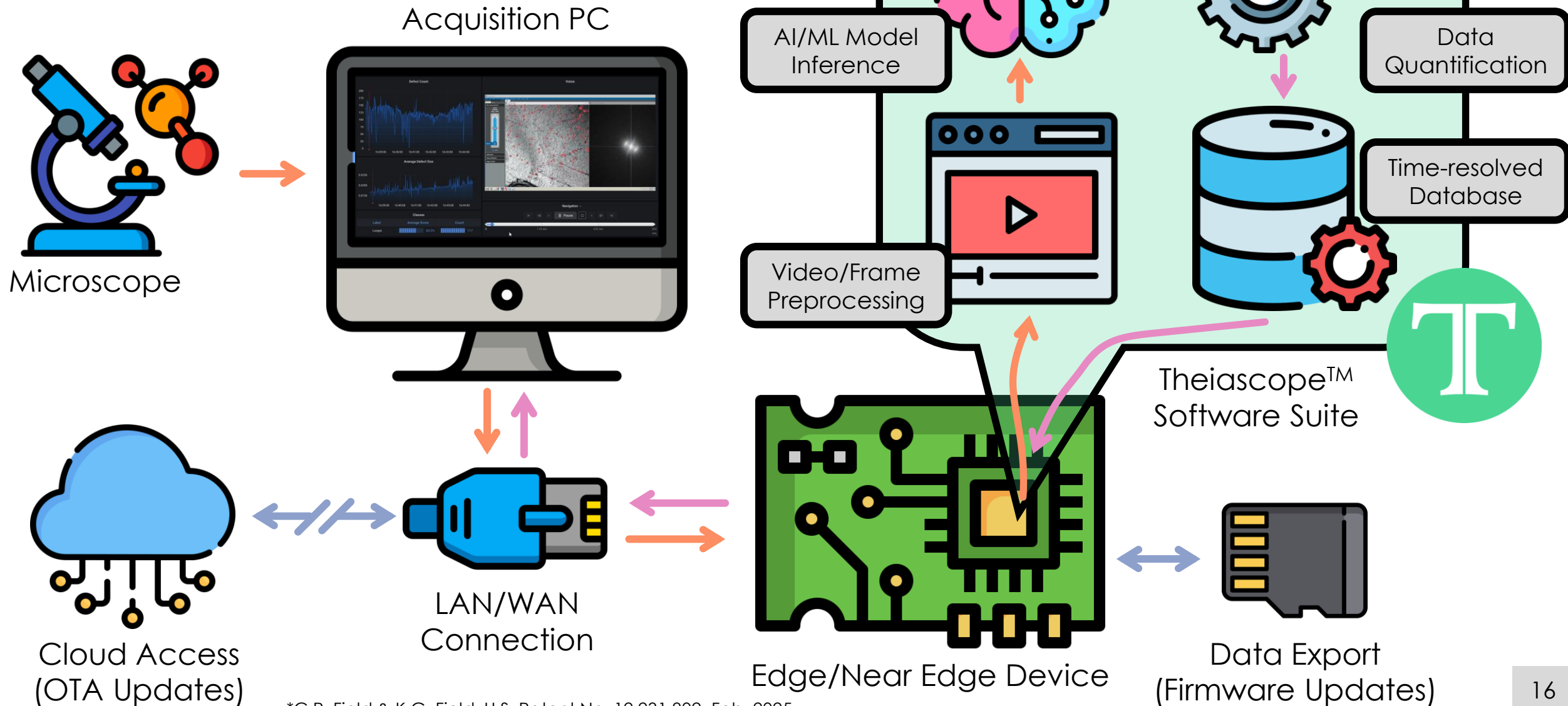


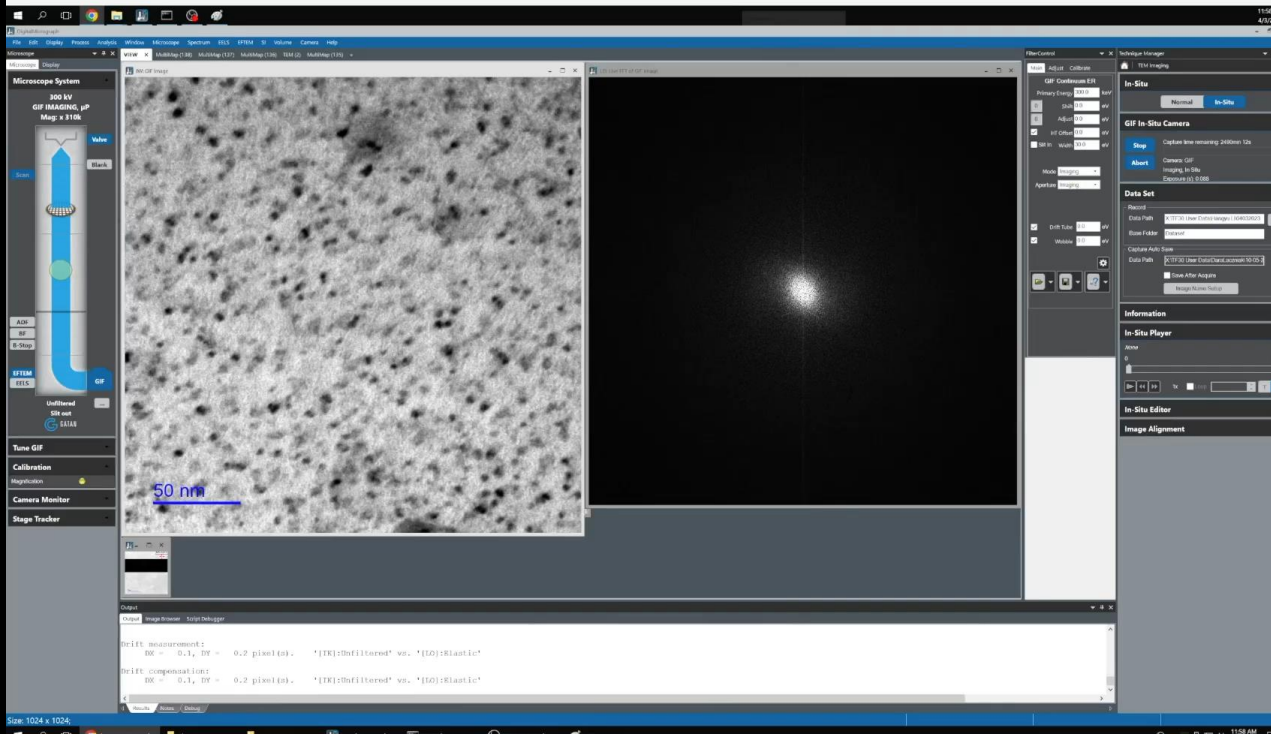
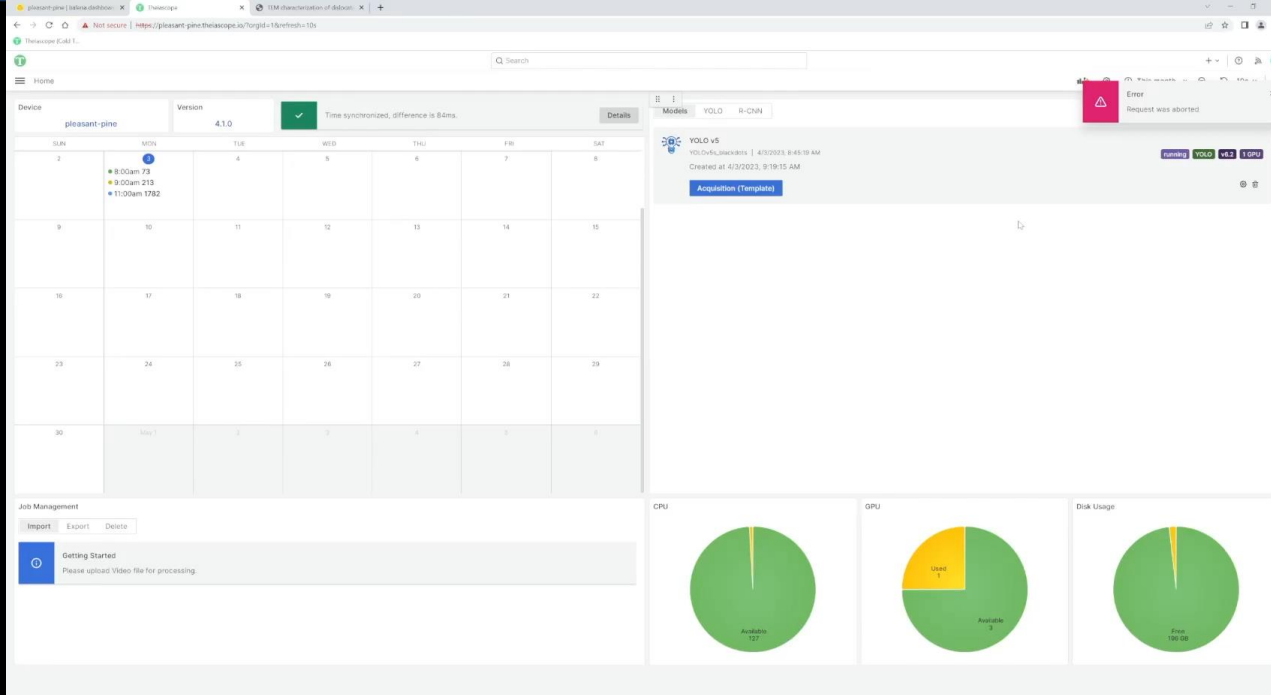
CNN+SORT based quantification

Theiascope™ systems are now at several partner facilities



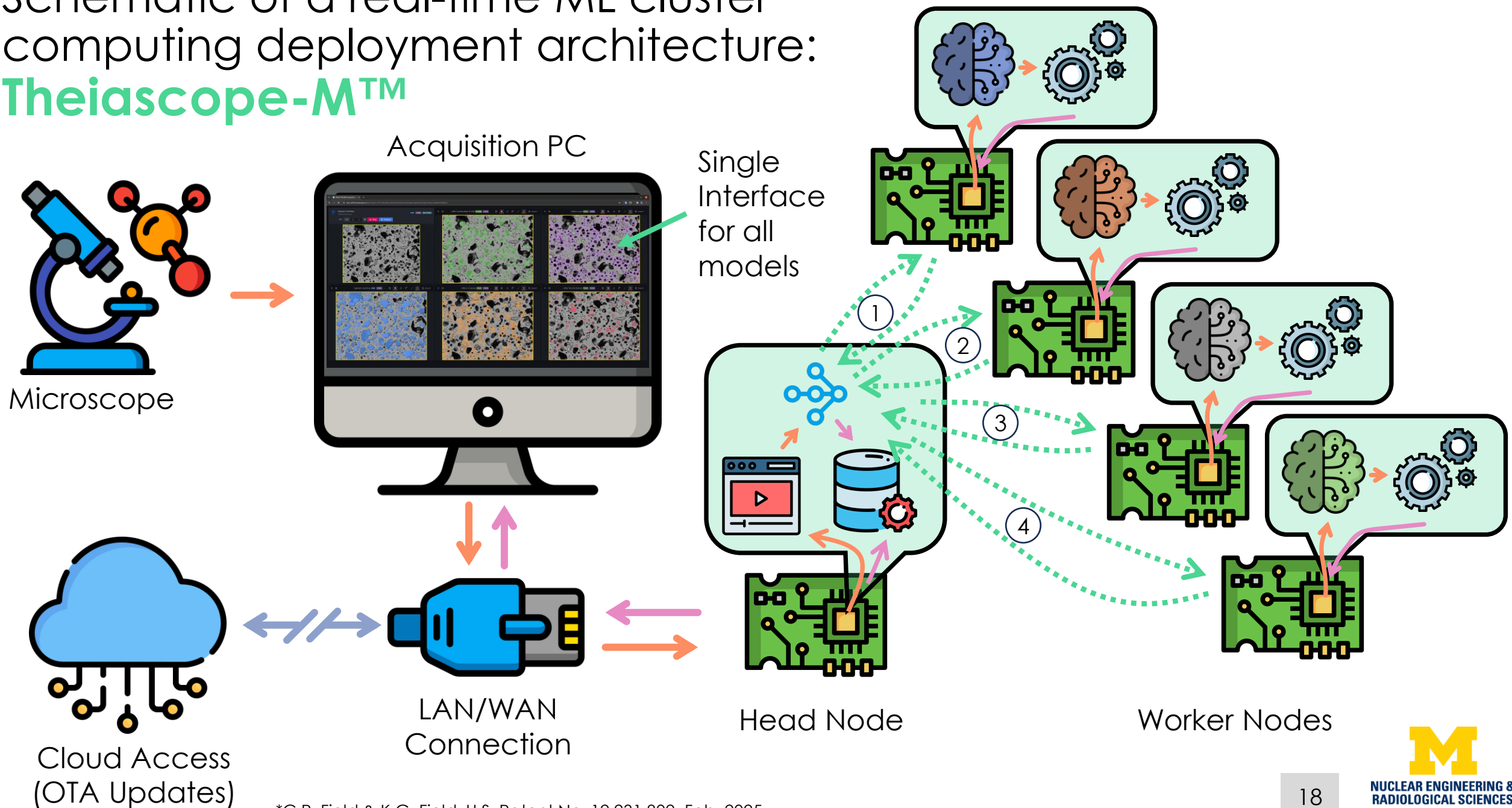
We have deployed a Theiascope™ to enable **real-time ML quantification** of in-situ irradiations



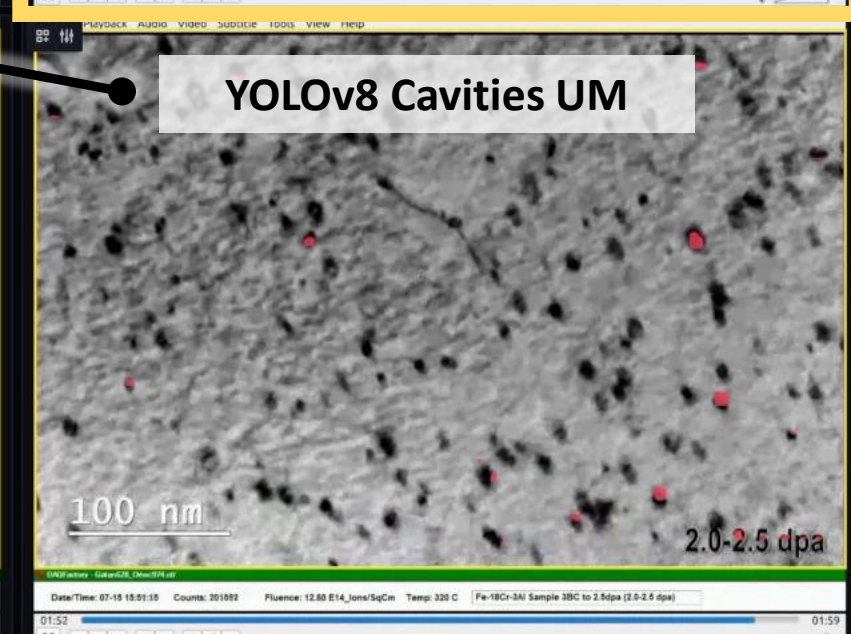
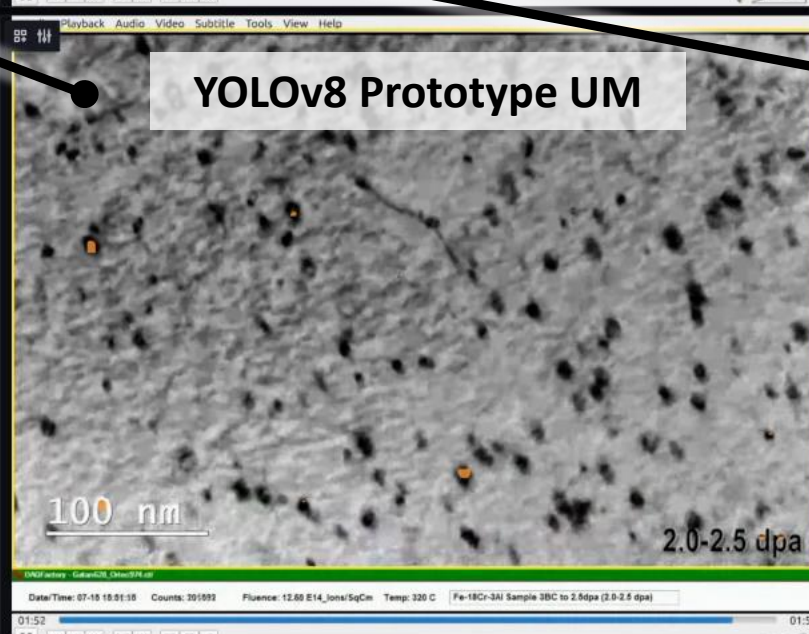
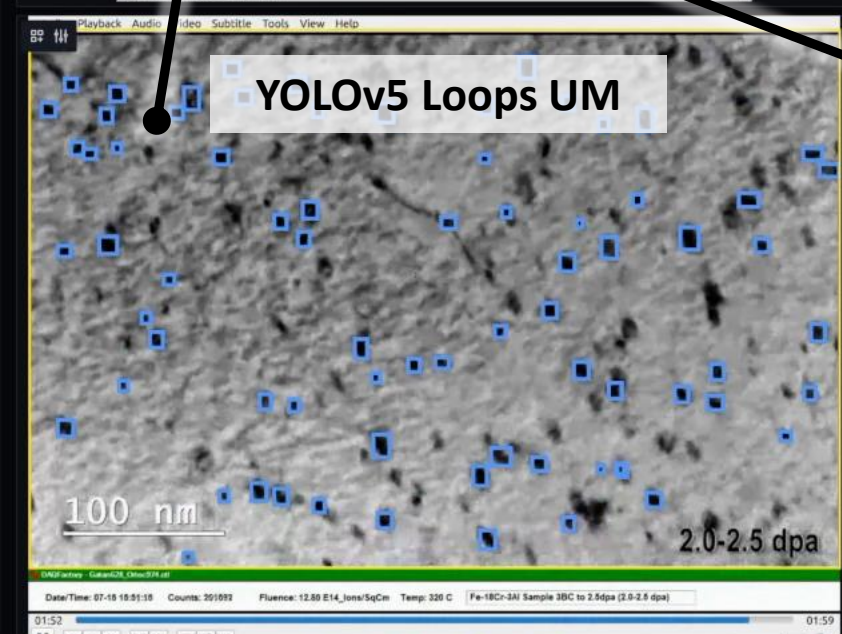
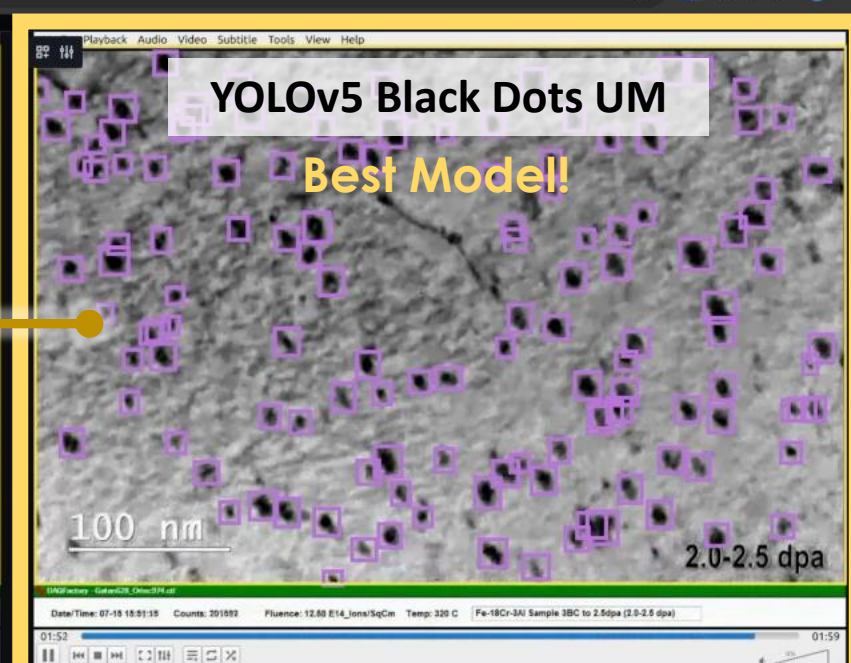
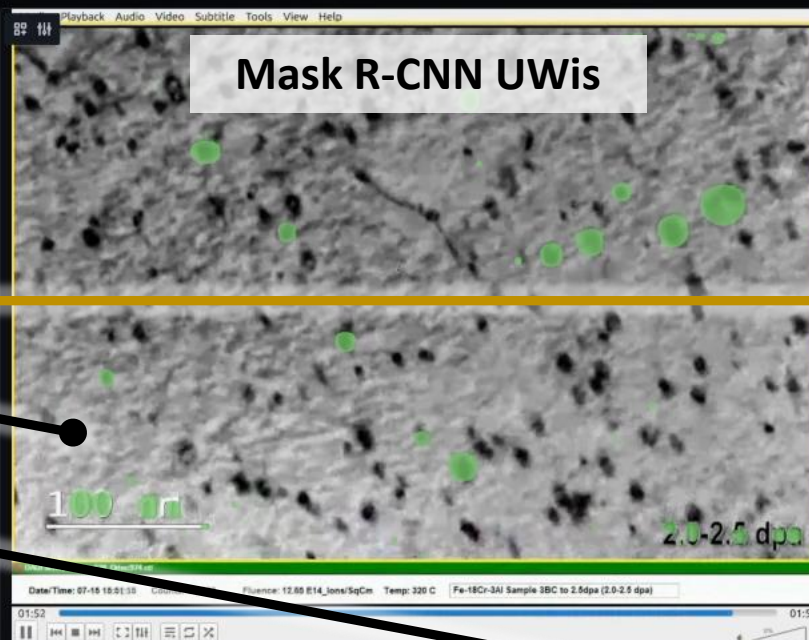
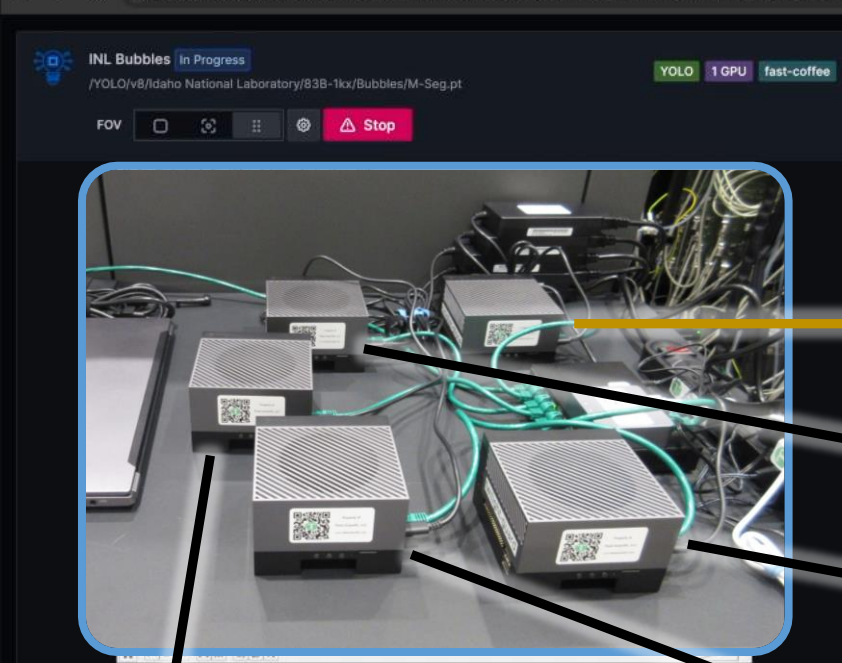


**In-situ TEM irradiation of an FeCrAl alloy
in MIBL-(MC)²**
Results courtesy of K. Sun and H. Li (UM)

Schematic of a real-time ML cluster computing deployment architecture: **Theiascope-M™**



*C.R. Field & K.G. Field, U.S. Patent No. 12,231,802, Feb. 2025



4 Model Acquisition

f362224e55164694347f80290f72bab4.balena-devices.com/d/c3dc83be-5bc2-40aa-a52b-c157b88e2ca9/4-model-acquisition?orgId=1&refresh=2s&var-modelId=31&kiosk

UWis Cavities Mask R-CNN

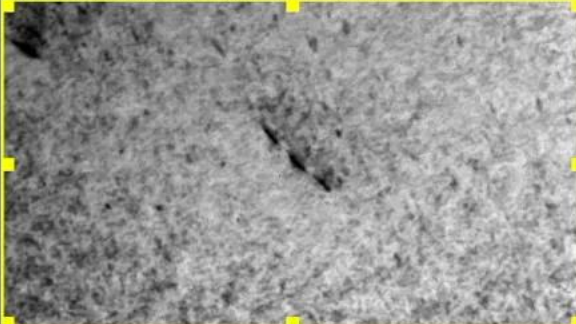
In Progress

R-CNN 1 GPU pleasant-pine

FOV

Stop

Media Playback Audio Video Subtitle Tools View Help



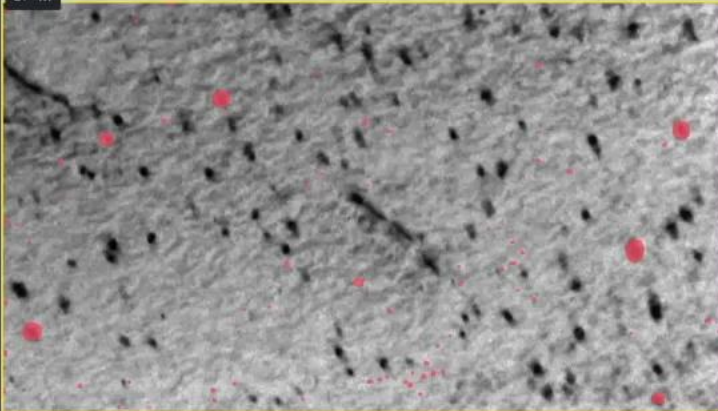
0.5 μm0 - 0.1 dpa

00:01

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UWis Mask R-CNN Cavities

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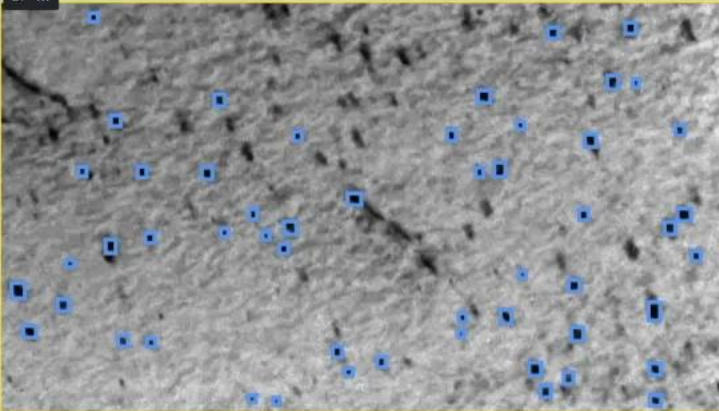
100 nm1.5-2.0 dpa

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UMich YOLOv5 3 Classes Loops

Playback Audio Video Subtitle Tools View Help



100 nm1.5-2.0 dpa

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UWis Mask R-CNN Cavities

72

UMich YOLOv5 3 Classes Loops

52

JHU YOLOv5 Emily

240

UMich YOLOv5 Blackdots

93

UWis Mask R-CNN Cavities

7.69

UMich YOLOv5 3 Classes Loop

62.6

UWis YOLOv8 Defects

100 nm1.5-2.0 dpa

INL YOLOv8 Bubbles

100 nm1.5-2.0 dpa

JHU YOLOv5 Emily

65.8

UMich YOLOv5 Blackdots

78.8

UWis Mask R-CNN Cavities

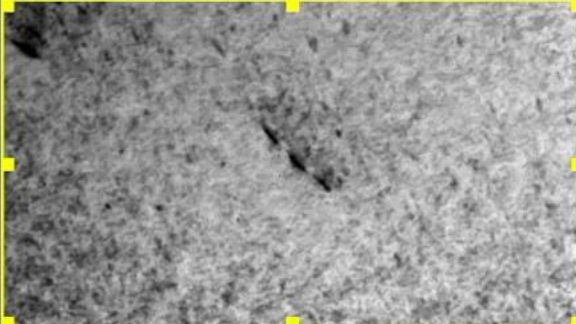
In Progress

R-CNN 1 GPU pleasant-pine

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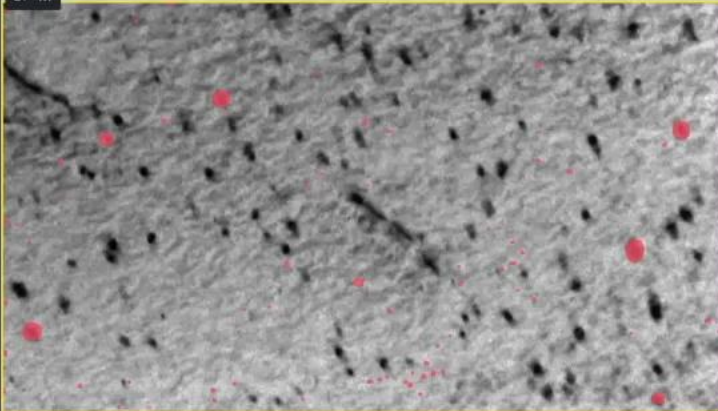
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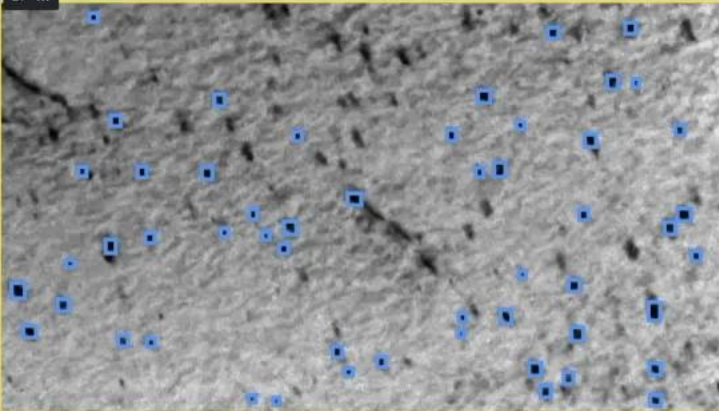
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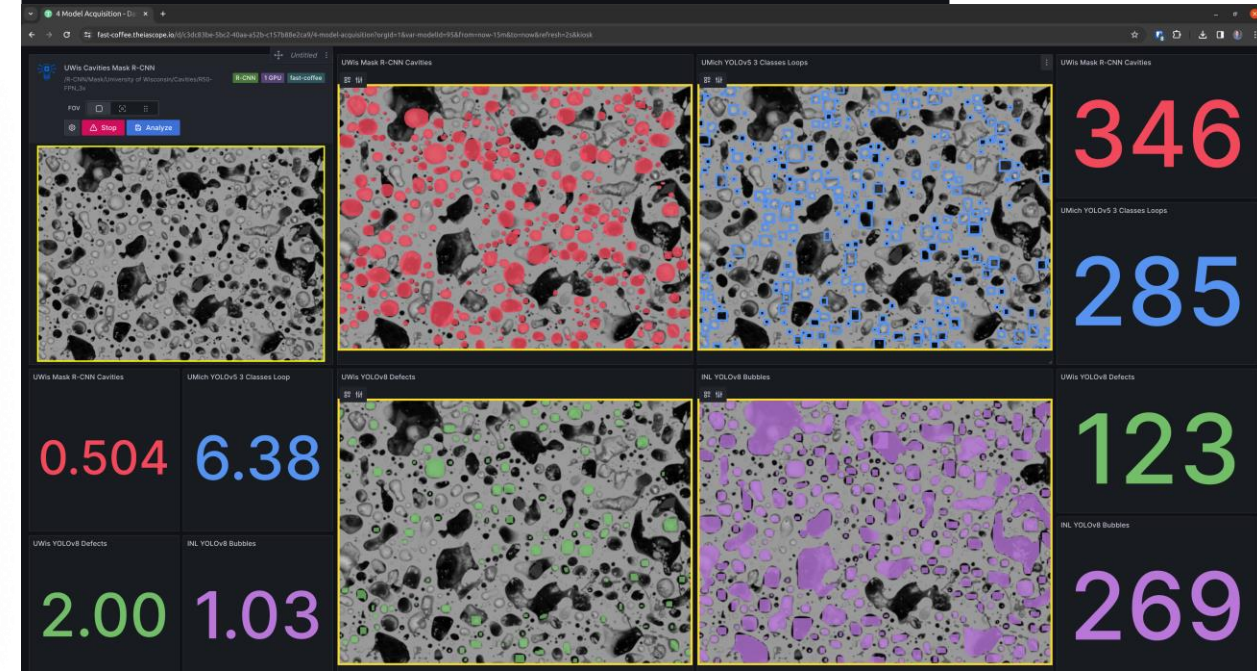
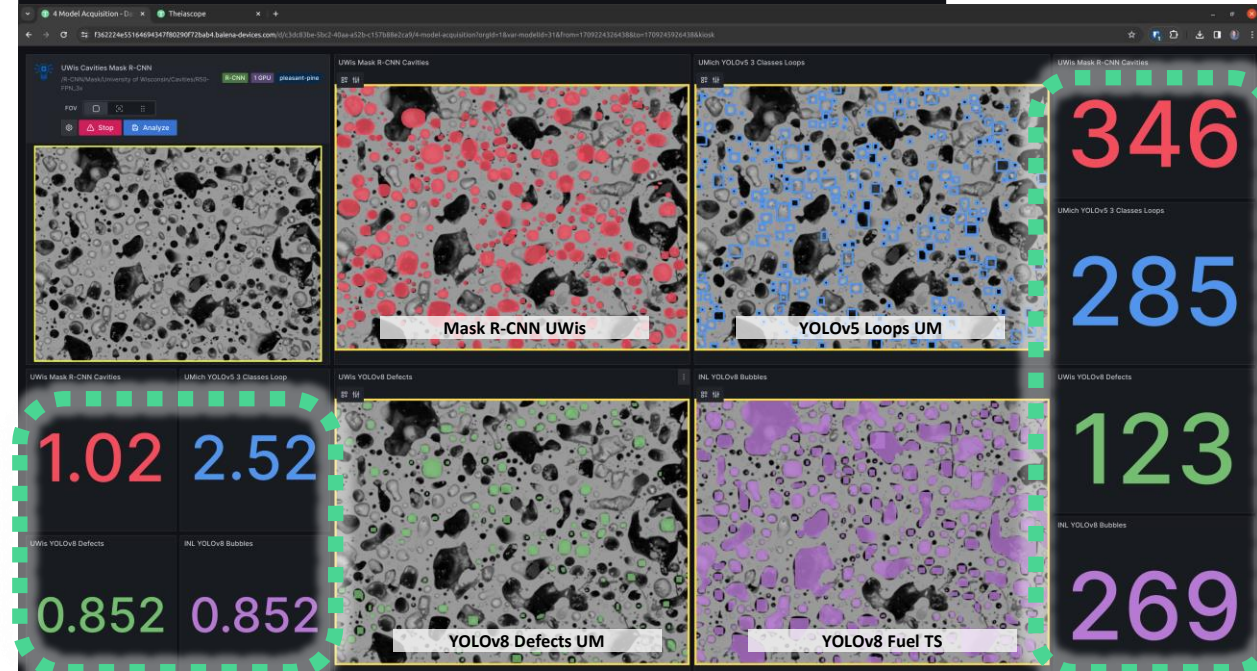
78.8

The new architecture enables a **fully scalable** ad-hoc heterogeneous cluster for **real-time ML**-enable microscopy

4 GPU-enabled edge-computing devices with intra-node data dispatching



1 Near-edge workstation with 4 GPUs and inter-GPU data dispatching

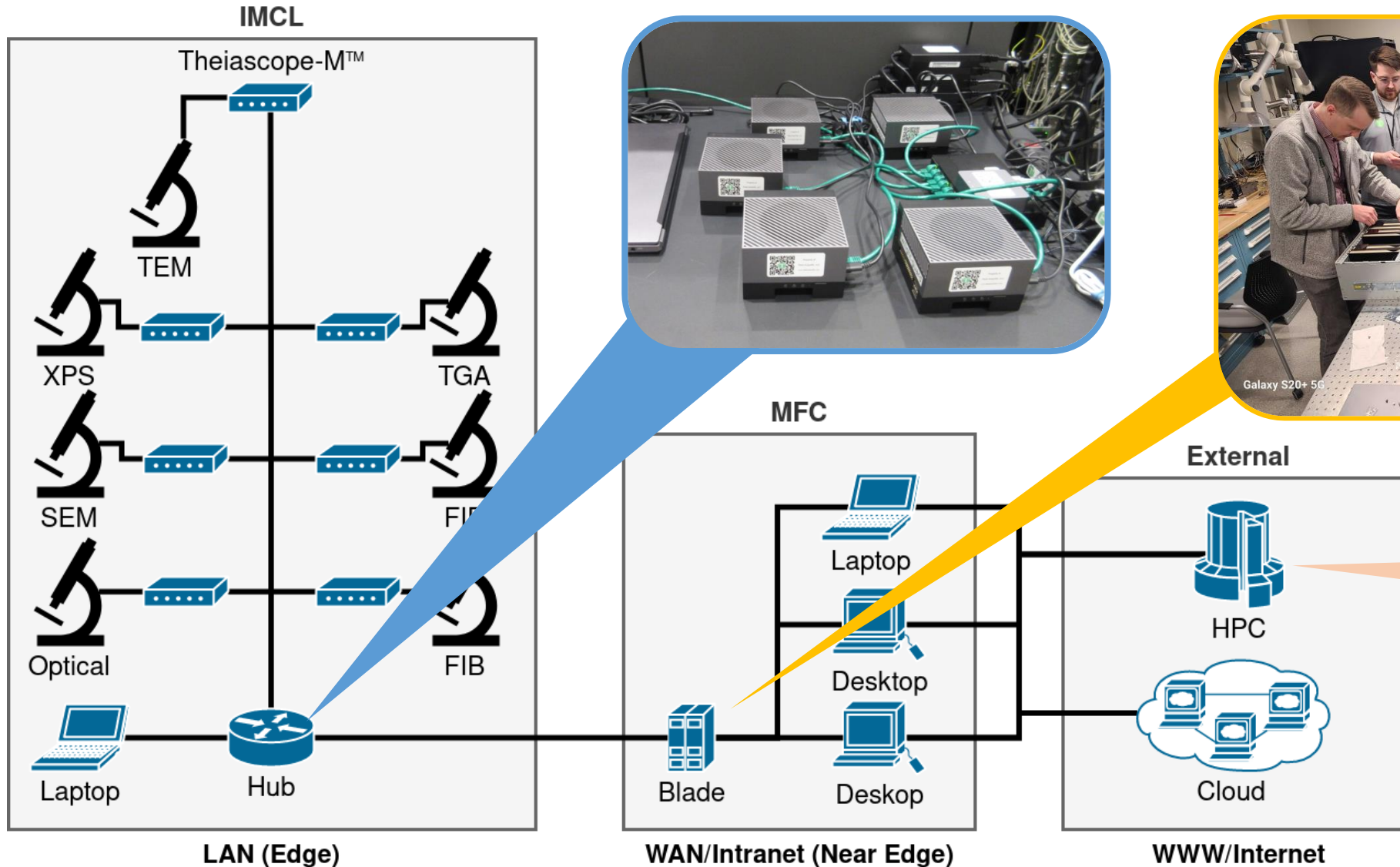


ML Model
FPS

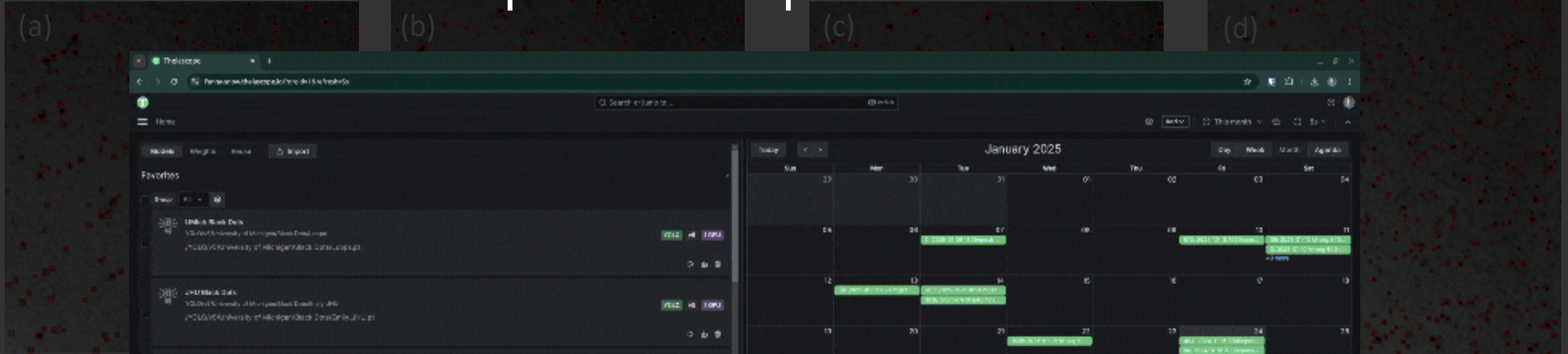
Feature
Count

Identical Response!

The **Theiascope-M™** is currently available to users at Idaho National Laboratory after successful install at MFC

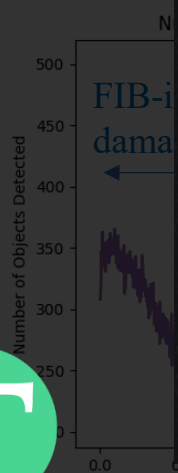


Can you run your algorithms on the Theiascope™ at partner facilities?



2-Beam BF im

model FeCrAl alloy
tively.



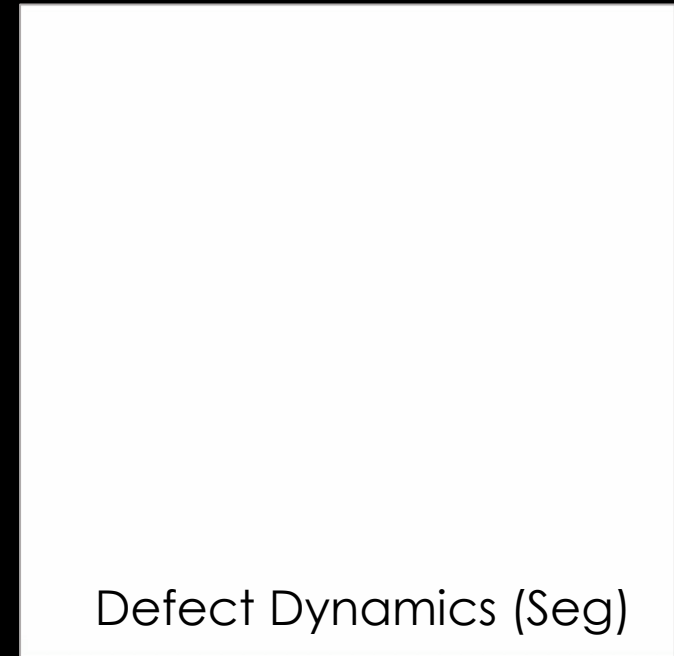
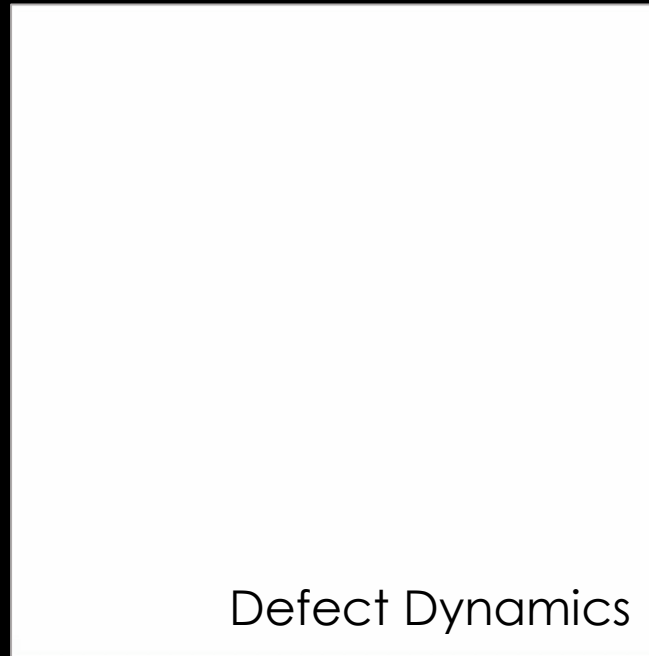
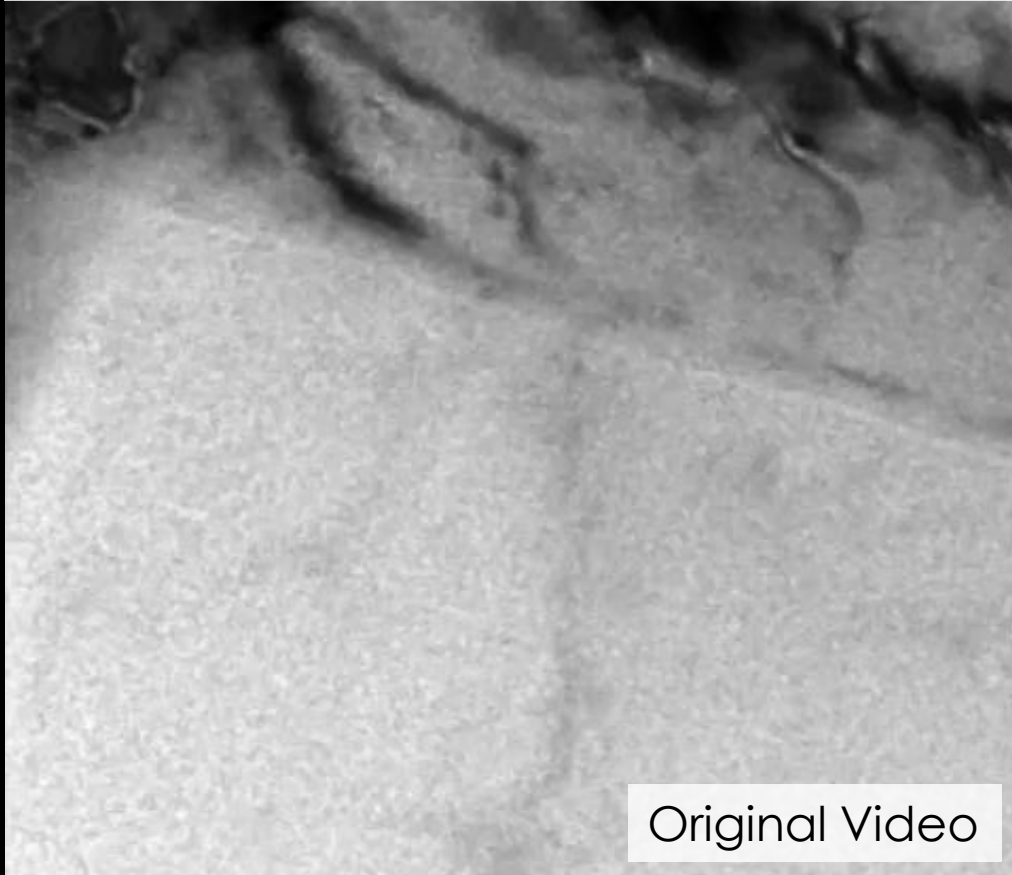
On-Board Jupyter Notebook

al dose to
nucleation in
ML-based



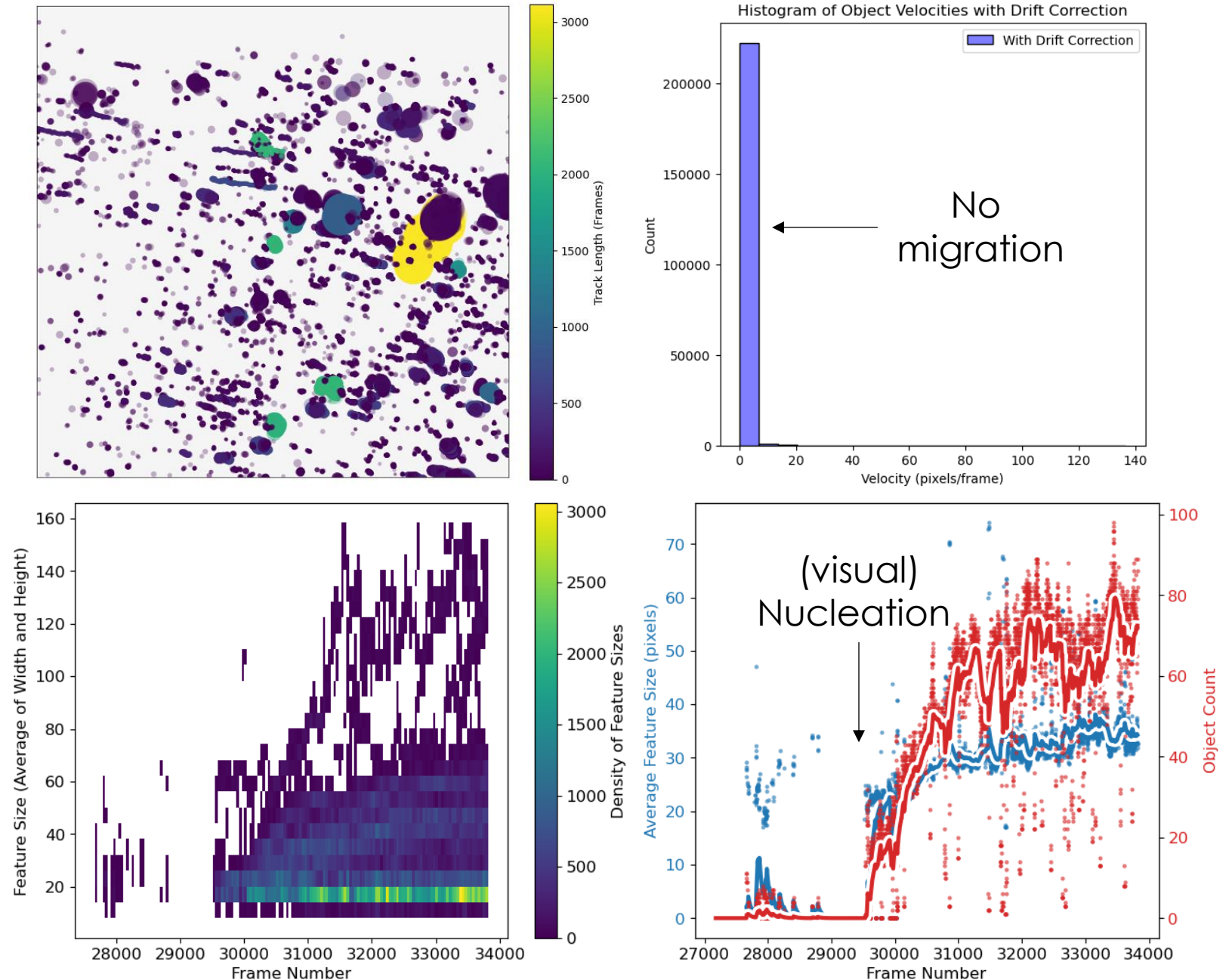
TRACS+SAHI with the Theiascope™ facilitates **dynamic quantification and drift correction** during in-situ TEM investigations at MIBL

316L implanted with 100 appm He and annealed at 500°C for 1 hr



TRACS + SAHI provided **high temporal and spatial fidelity** on cavity evolution

- Cavities under annealing in 316L did not migrate → only ‘movement’ was **preferential directional growth**
- Cavities nucleated and grew with limit additional nucleation after initial growth



Post-acquisition ML quantification and ***real-time ML microscopy*** is now available to NSUF users through NRDS, the user community, and through the Theiascope™ systems existing at NSUF partner facilities

