APRIL 26, 2022

Argonne NATIONAL LABORATORY 75 1946–2021

PYTHONFOAM WORKSHOP ARGONNE LEADERSHIP COMPUTING FACILITY

R. MAULIK[1], D. FYTANIDIS[1], S. PATEL[1], B. LUSCH[1], S. PAWAR[2]

1-ARGONNE NATIONAL LABORATORY, 2-OKLAHOMA STATE UNIVERSITY

Argonne NATIONAL LABORATORY 75 1946–2021

INFORMATION

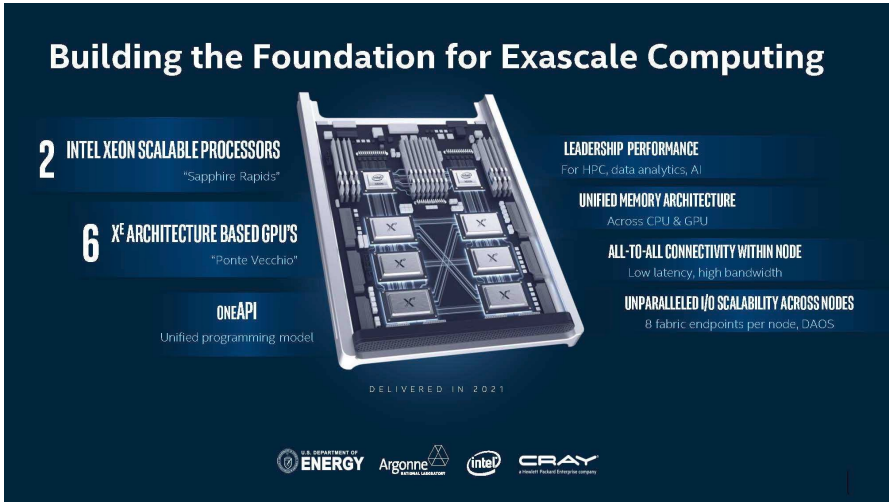
- Code with examples available on Github. Development environment available on Docker-hub.
- We will be using Slack for this workshop (and beyond). Instructors will be monitoring channels so do not hesitate to ask questions. Slack also has several instructions for attendees (Sign up link in reminder email).
- Use the #random channel in slack to introduce yourself/affiliation/any interesting problems you are working on.
- **Special thanks to Kathy, Julie, Linda for all the help with organization!**

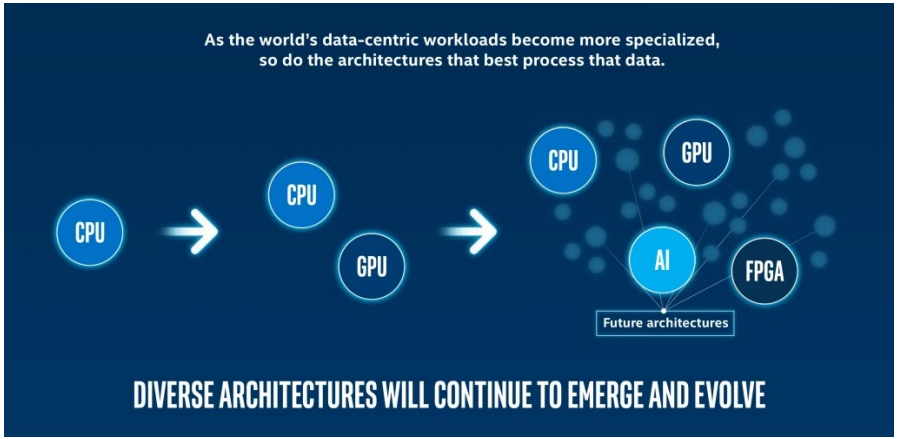
AGENDA

- Introduction/motivation/discussion of responses from survey.
- Case studies – in-situ modal analyses, surrogate modeling.
- A minimum working example for C++ and Python coupling.
- Working through and running PythonFOAM examples in Docker.
- Several breaks to encourage interaction between instructors and participants and time for participants to get hands dirty with code.

MOTIVATION

Hardware is no longer homogeneous
Simulation and AI coupling is gaining traction





Choose best simulations to launch

- Active learning: ones that improve ML model
- Or “experiment design”
- Diverse set?
- Ones likely to improve quantity of interest?
- If ML model degrading, collect more data?
- Sample space more effectively

Example:
“Machine Learning Inter-Atomic Potentials Generation Driven by Active Learning”
Sivaraman, et al.
https://arxiv.org/abs/1910.10254
https://github.com/argonne-lcf/active-learning-md

Surrogate modeling

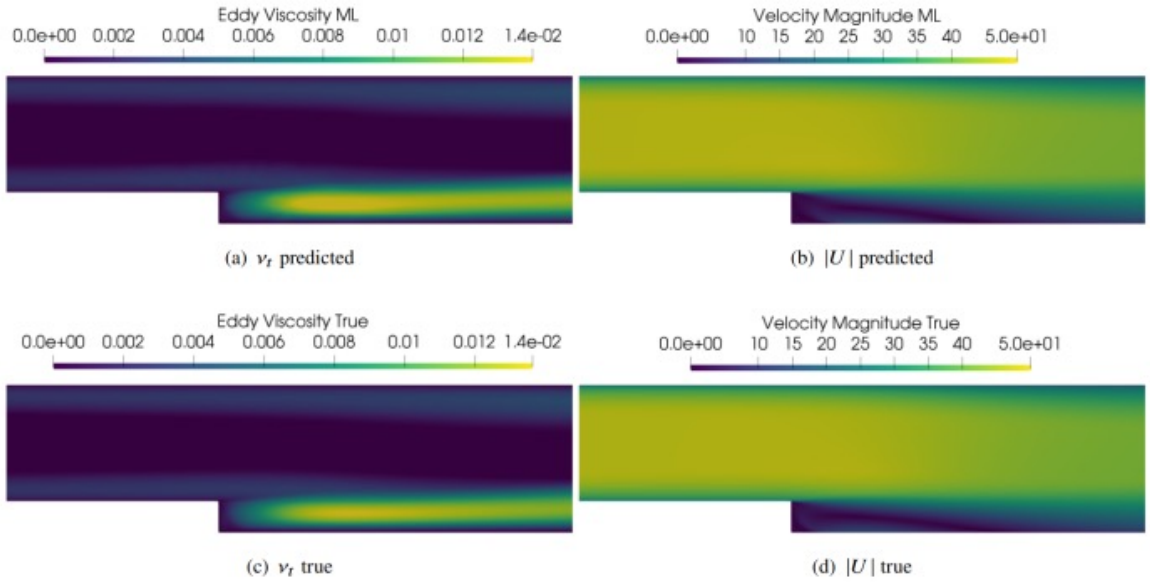
Replace *part* of simulation with ML surrogate model

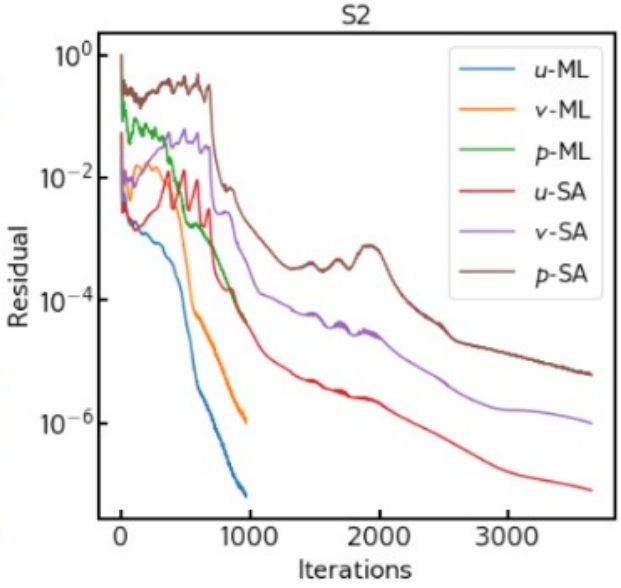
- Expensive part?
- Inaccurate part?

ML model output fed back into rest of simulation

Example:
“A turbulent eddy-viscosity surrogate modeling framework for RANS simulations”
By Maulik, et al.
https://doi.org/10.1016/j.compfluid.2020.104777
https://github.com/argonne-lcf/TensorFlowFoam

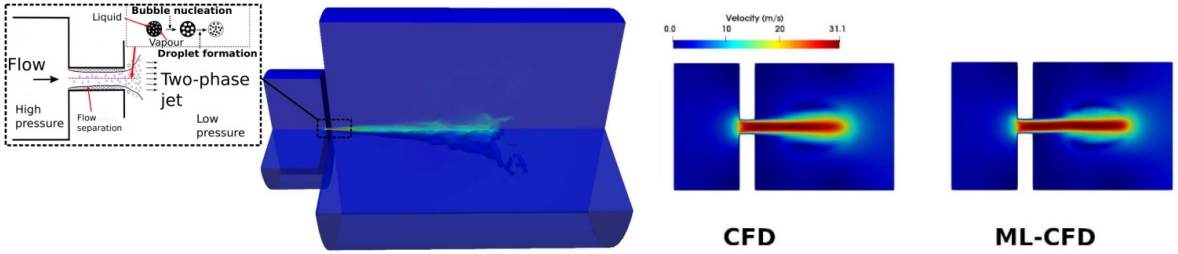
EXAMPLES: TURBULENCE MODELING

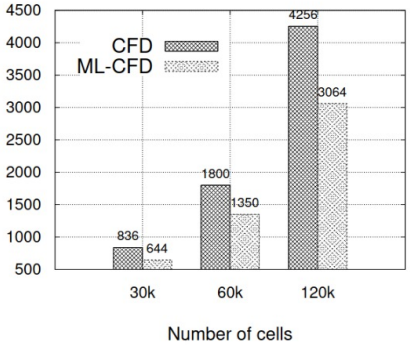


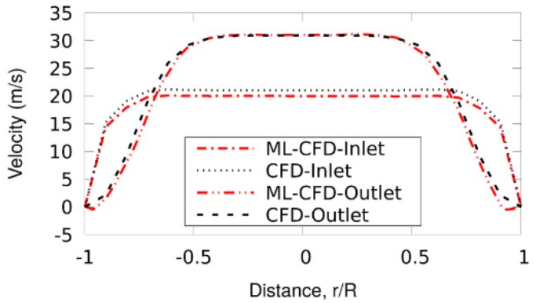


NN predicts steady state turbulent eddy-viscosity. Equations are solved to convergence – Maulik et al., Comput. Fluids, 2021

EXAMPLES: TURBULENCE MODELING







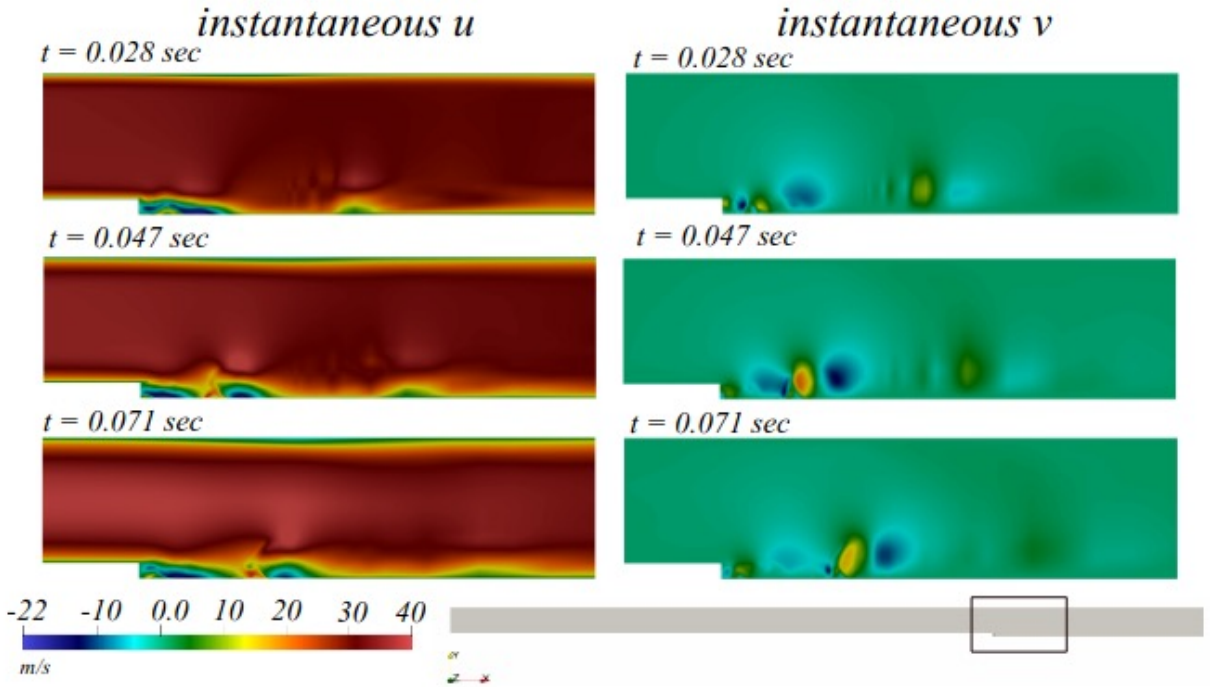
NN predicts transient turbulent eddy-viscosity – Schmidt, Maulik, and Lyras – Phys. Fluids - 33 (12), 127104

Reduce I/O

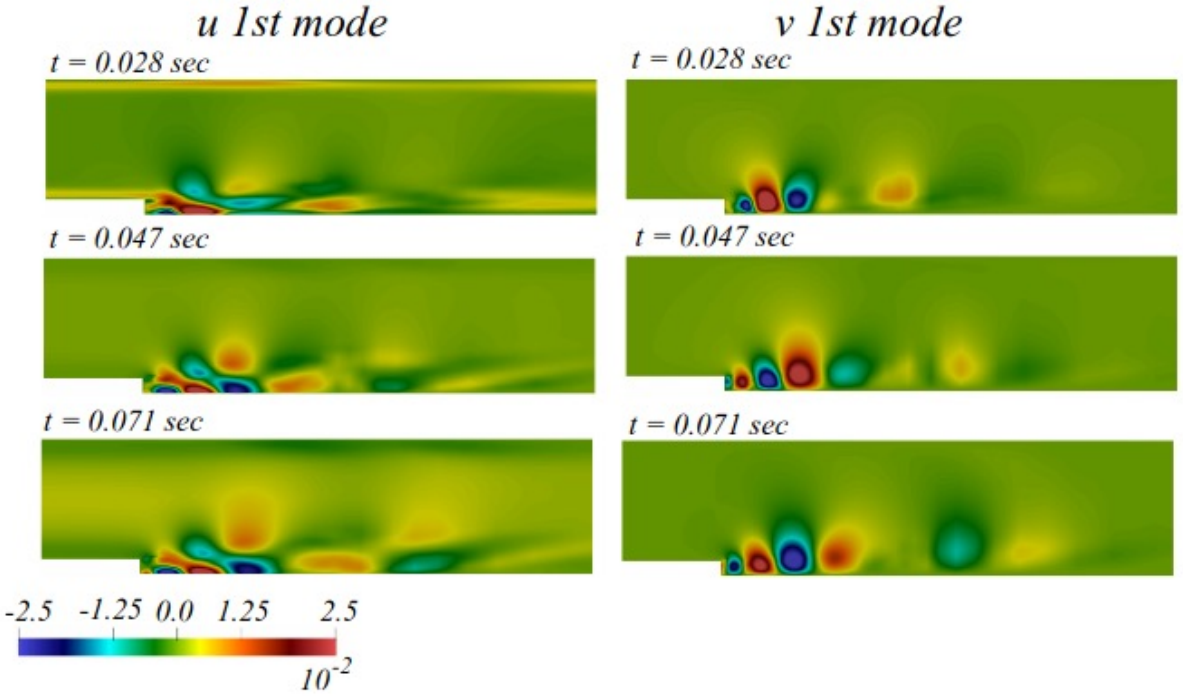
- Apply ML model to save compressed simulation results
- Train online during simulation (skip I/O bottleneck)
- *In situ* analysis giving feedback on simulations before completed
  - Need to adjust something?

Example:
“In Situ Compression Artifact Removal in Scientific Data Using DeepTransfer Learning and Experience Replay” by Madireddy, et al.
https://doi.org/10.1088/2632-2153/abc326

EXAMPLES: MODAL ANALYSES



EXAMPLES: MODAL ANALYSES



Control Simulation with ML

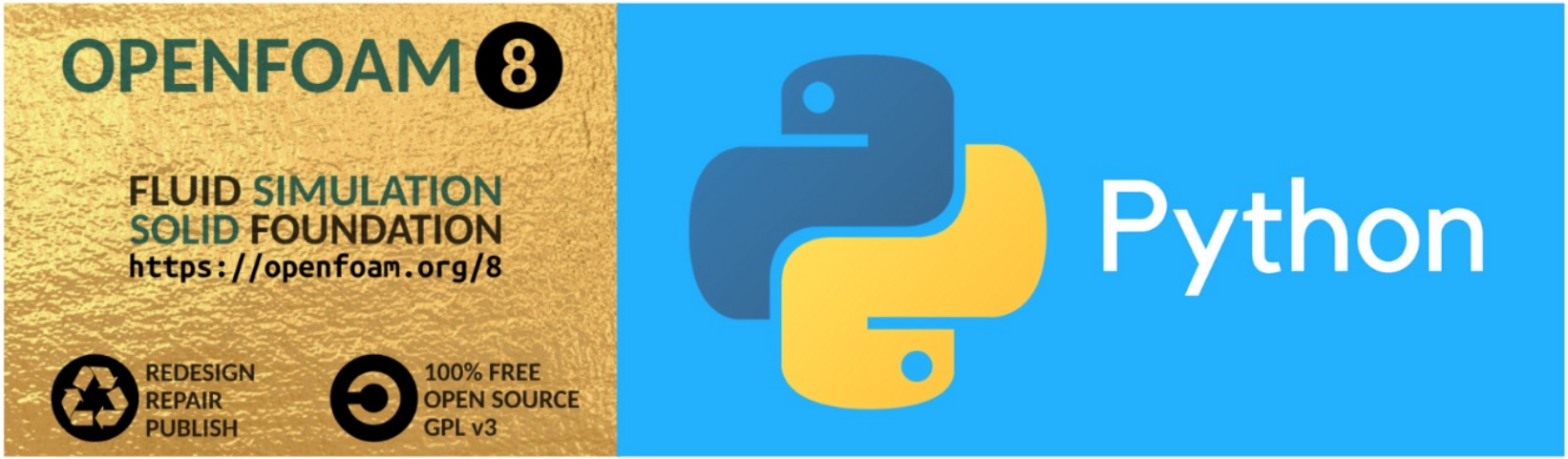
- Select simulation parameters
- Select numerical scheme

Example:
“Distributed Deep Reinforcement Learning for Simulation Control”
By Pawar & Maulik
Machine Learning: Science and Technology 2 (2), 025029
https://github.com/Romit-Maulik/PAR-RL

Other Use Cases

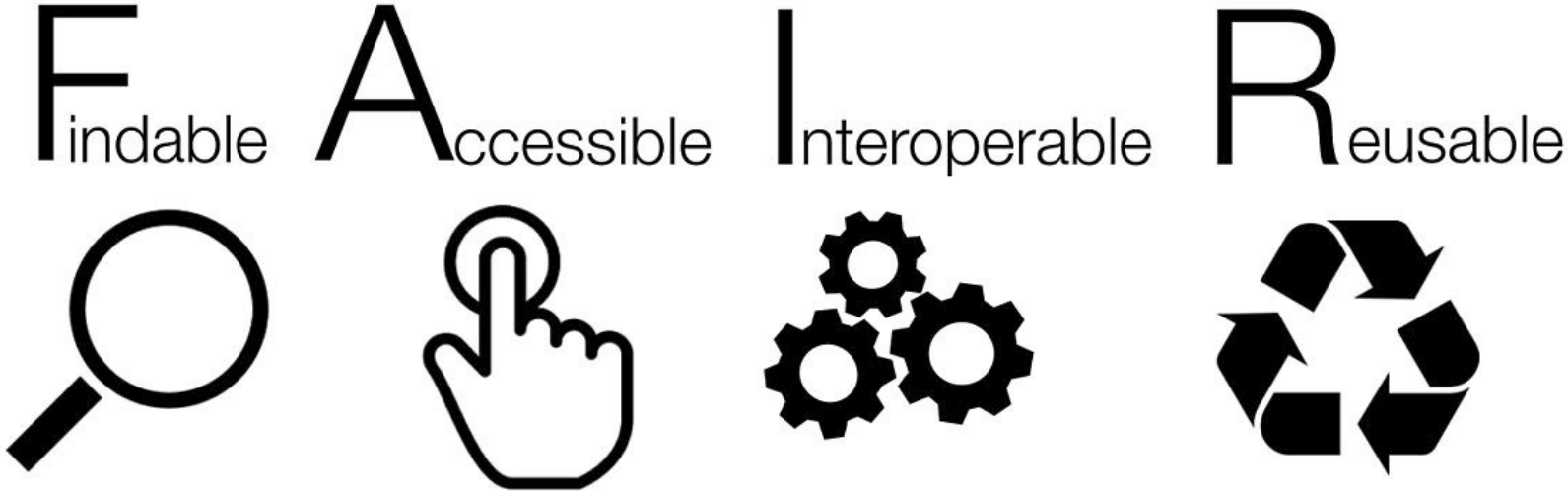
- Data assimilation
- Augmenting simulation with ML closure/discrepancy model
- Solver as part of ML loss function

MOTIVATION



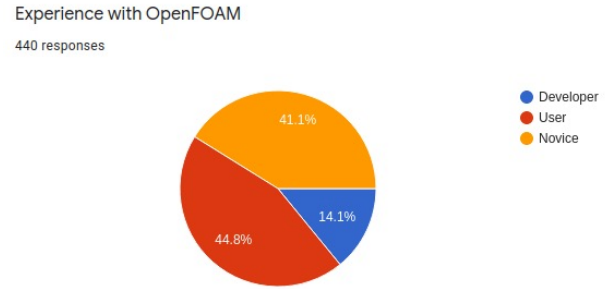
Our goal is to make **OpenFOAM** the **flagship** framework for data-science in computational fluid dynamics

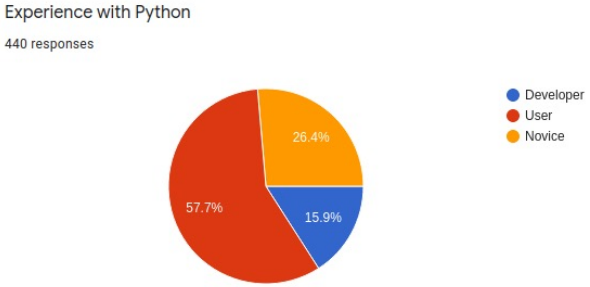
MOTIVATION



Our goal is to make **OpenFOAM** the **flagship** framework for data-science in computational fluid dynamics

OUR DEMOGRAPHIC





Some comments:
“I would like to explore the use of machine learning and deep learning to CFD. Since I have been using OpenFOAM for almost 5 years now, i believe that there is a great potential for that purpose”

“Nice idea for algorithm prototyping, especially for my working students who typically do not have experience with openfoam programming”

“I have been using openFOAM & python together for almost 2 years now, but more in a way where python would be my chef d'orchestre and openFOAM my orchestra. So I would be really interested to take it one step further.”

“Just for fun! I have been learning DL stuff on my own, maybe this will be helpful in the future”

“Honestly I'm just curious”

VISION

1. Setup a PythonFOAM community (extensively interact via slack and workshops).
2. In future editions of such workshops, invite presentations for test-cases where Python-OpenFOAM coupling enables science.
3. Encourage community contribution to our code/repository.

A request! To those proficient in OpenFOAM – please help out your fellow attendees via the Slack channel.