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Scientific Machine Learning using MOOSE

July 2023

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Changing the World's Energy Future

Idaho National Laboratory

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Advances in Scientific Machine Learning in MOOSE

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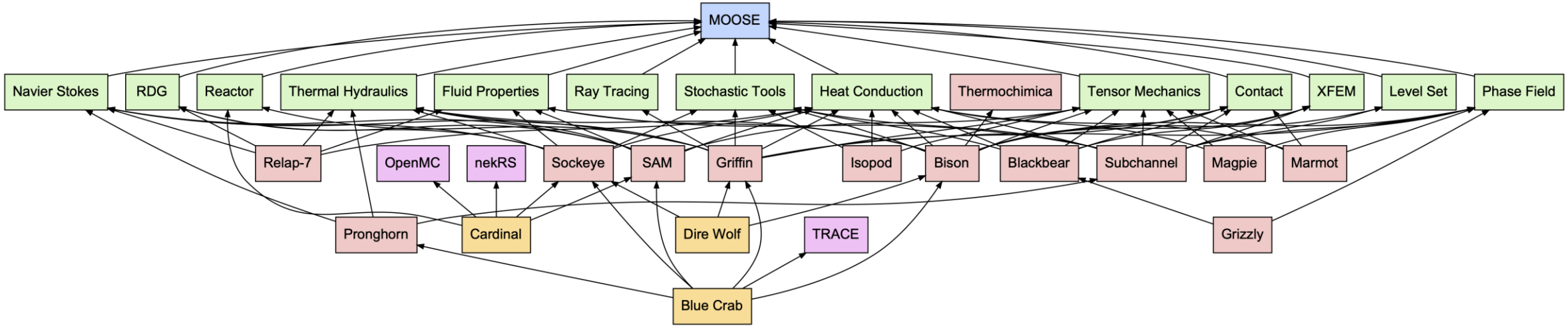
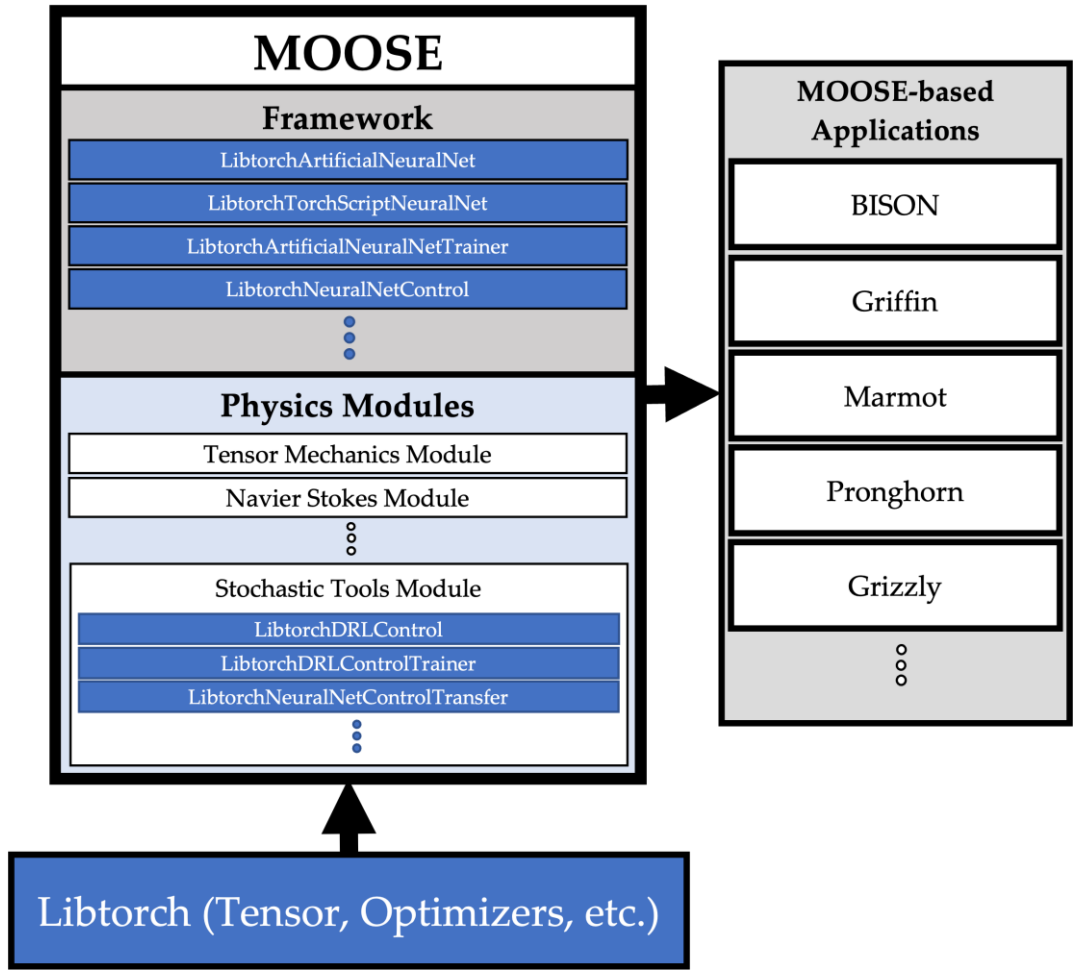
Multiphysics Object-Oriented Simulation Environment (MOOSE)

- MOOSE [1] has a modular structure:
  - Framework
  - Physics modules: Fluid dynamics, elasticity, heat conduction
  - Applications: Nuclear fuel performance (BISON), reactor physics (Griffin)
- LGPL 2.1 license (very permissive)
- https://github.com/idaholab/moose



How can we harvest machine learning in MOOSE?

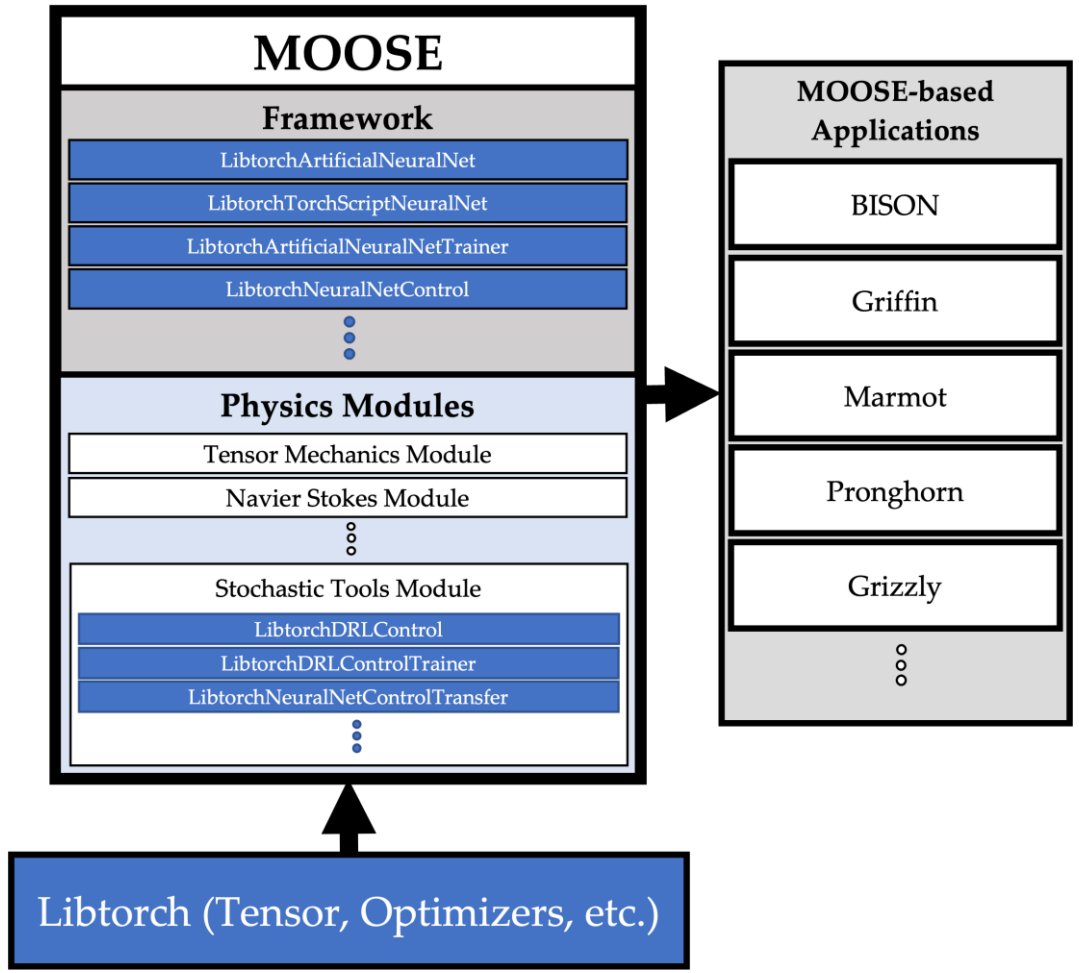
- High-fidelity simulations can be accelerated or (partially) replaced by machine learning models
- Creation of machine-learning-based (ML) controllers for complex multiphysics systems—which is extremely challenging using traditional model-based control—relies on the control system and all existing physics modules in MOOSE
- Could be used to train fast surrogates on the fly to act as predictors in transient problems
- Could be used to train fast surrogates to accelerate sensitivity analysis and uncertainty quantification on complex multiphysics problems



Linking with Libtorch (C++ front end of Pytorch [2])

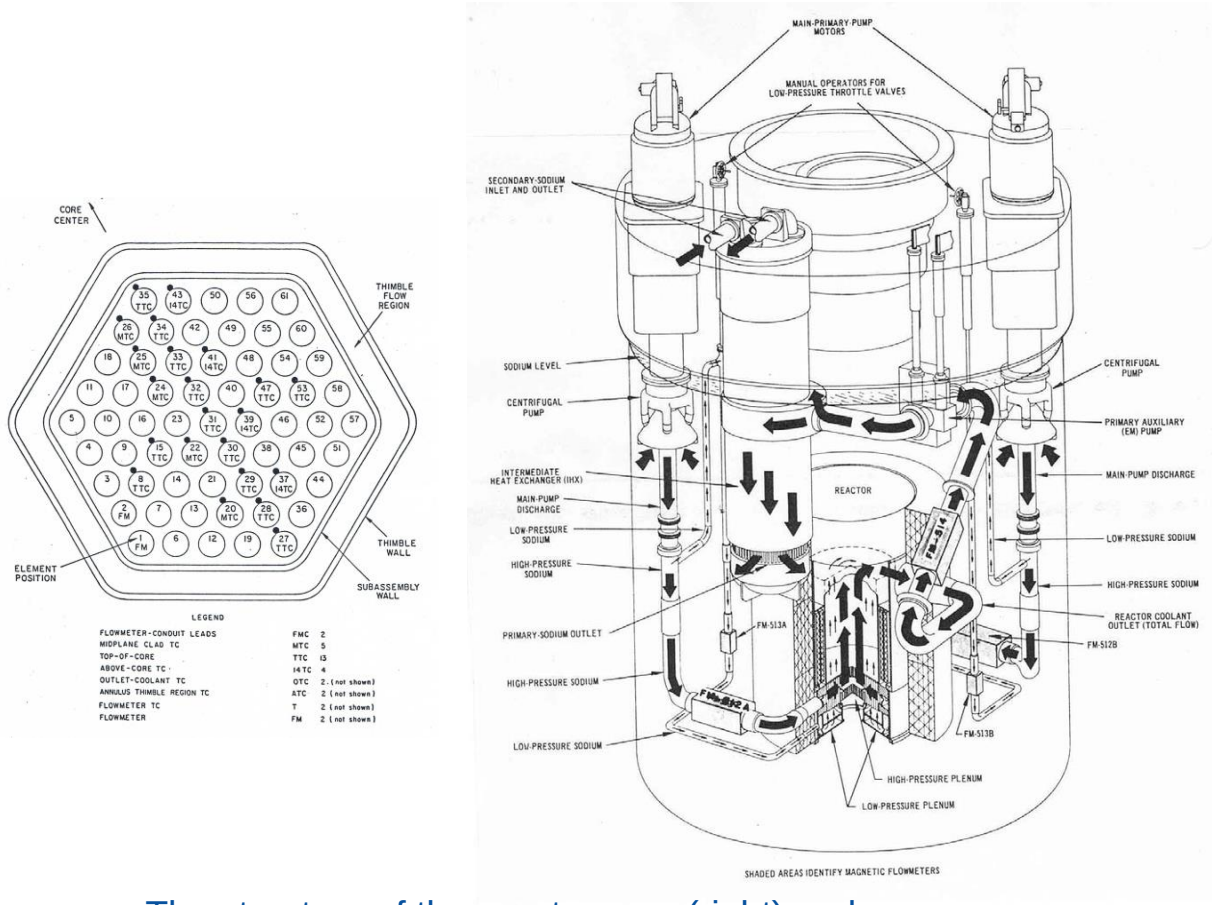
New capabilities

- Framework:
  - General Neural Net (NN) interfaces
  - Enables using networks trained using the python API by reading TorchScript files
  - Implements basic neural net-based controllers
- Stochastic Tools Module
  - Uses NNs for surrogate generation (for sensitivity and uncertainty studies)
  - Enables the use of Proximal Policy Optimization-based Deep Reinforcement Learning [3]



Surrogate generation for flow in nuclear fuel assemblies

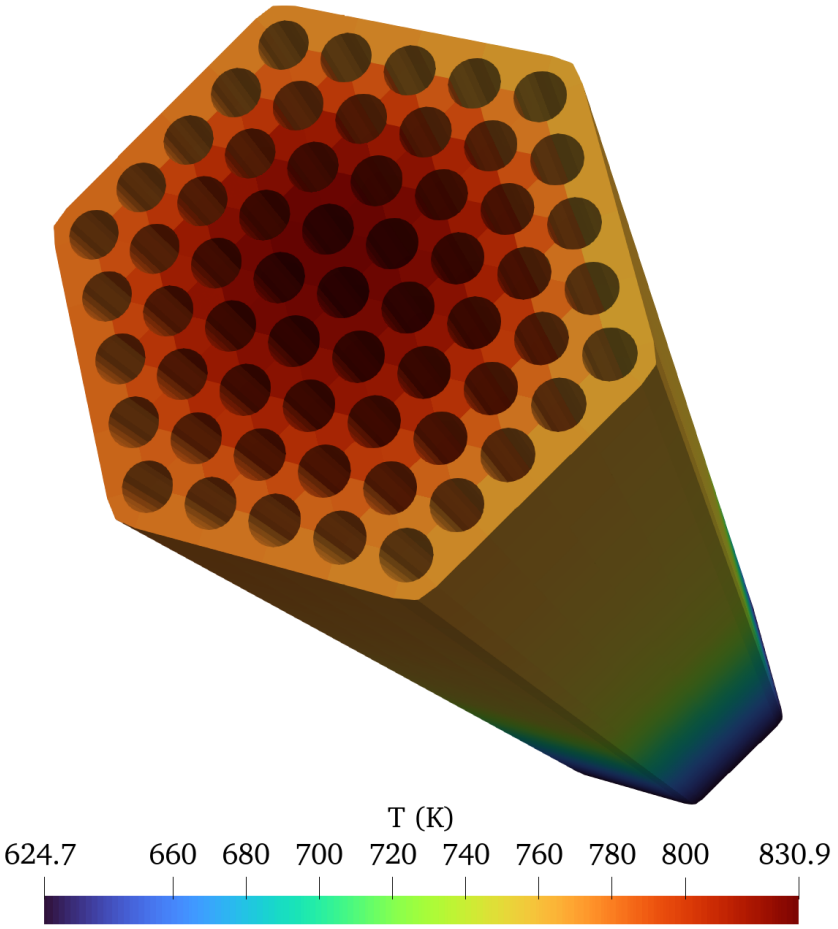
- Experimental Breeder Reactor II (EBR-II) [4] assembly flow simulations
- Quantities of interest:
  - Minimum and maximum temperatures
- Simulation tool: Pronghorn-Subchannel [5]
- Depend on many input parameters:
  - Power tilt factor
  - Power magnitude
  - Inlet mass flow rate
  - Turbulent mixing factor
- Goal: Carry out global sensitivity analysis for the quantities of interest (compute Sobol indices)
- Assumes that the input parameters can change in a +/-15% interval around the expected value



The structure of the reactor core (right) and a fuel assembly (left) of EBR-II [4]

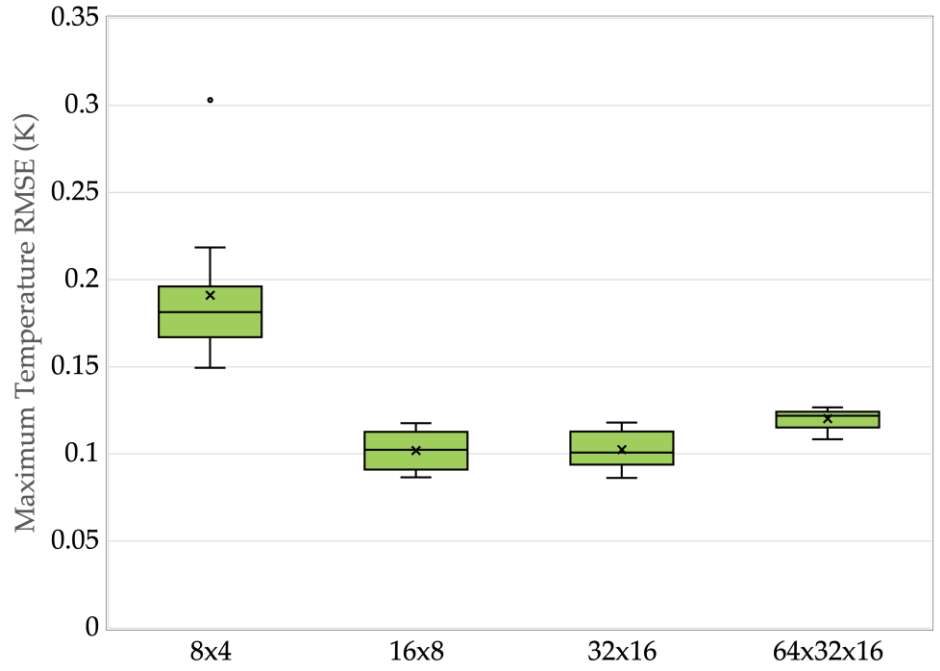
Surrogate generation for flow in nuclear fuel assemblies

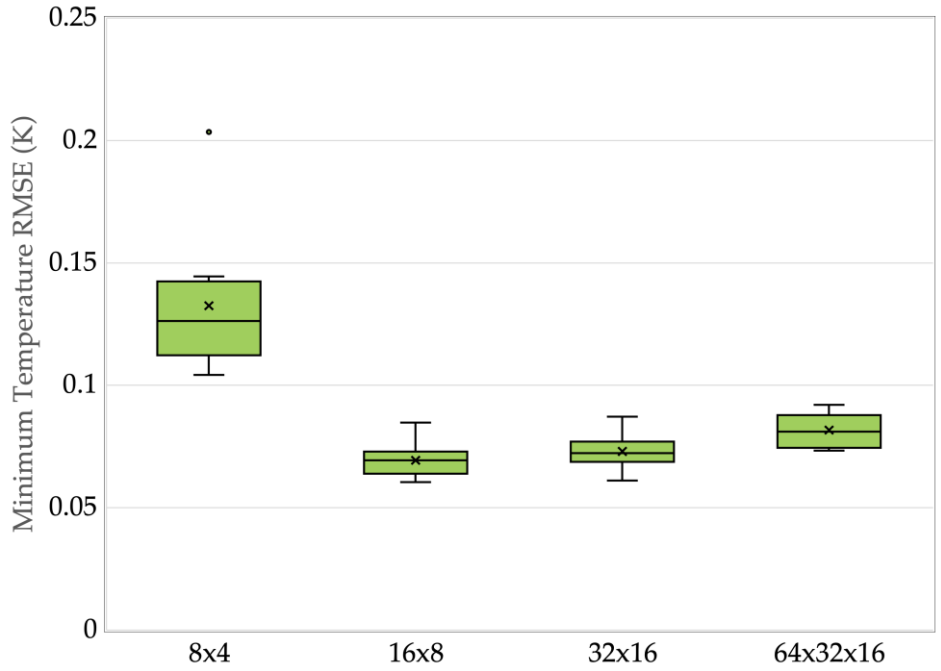
- Issues:
  - For acceptable statistics, one would require a large number of samples
  - One run is relatively expensive (~10^6 degrees of freedom)
- Solution:
  - Build NN-based surrogate → carry out sensitivity study with surrogates
- Using the Stochastic Tools Module
  - 2,000 samples for training, data normalization
  - Train neural networks with different architectures
  - Use three-fold cross-validation for approximating test accuracy (minimize approximation and overfitting errors)



Surrogate generation for flow in nuclear fuel assemblies

- Root Mean Squared Error (RMSE) for different architectures (based on 10 repeated three-fold tests):

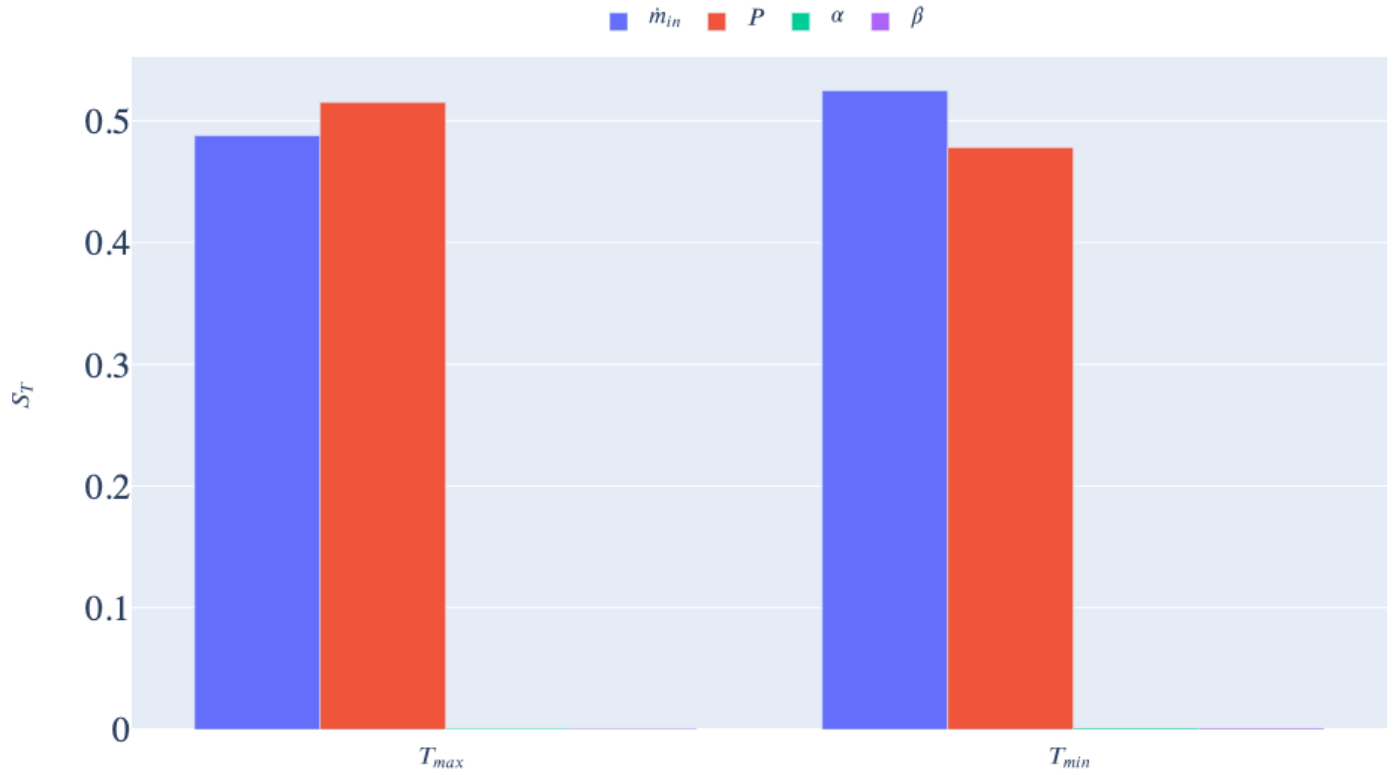




- Simple solution surface, 16 x 8 neural network generalizes well with good accuracy
- Beyond 16 x 8 some overfitting is visible

Surrogate generation for flow in nuclear fuel assemblies

- Total Sobol indices generated using 10^6 samples



- Maximum and minimum temperatures are most sensitive to the inlet mass flow rate and the power

Surrogate generation for flow in nuclear fuel assemblies

- Streamlined input file (plug and play with MOOSE-based models)

```
[Distributions]
  [alpha]
    type = Uniform
    lower_bound = '${fparse 1.8012*0.85}'
    upper_bound = '${fparse 1.8012*1.15}'
  []
  [beta]
    type = Uniform
    lower_bound = '${fparse 0.006*0.85}'
    upper_bound = '${fparse 0.006*1.15}'
  []
  [mass_in]
    type = Uniform
    lower_bound = '${fparse 2.45*0.85}'
    upper_bound = '${fparse 2.45*1.15}'
  []
  [power]
    type = Uniform
    lower_bound = '${fparse 486200*0.85}'
    upper_bound = '${fparse 486200*1.15}'
  []
[]
```

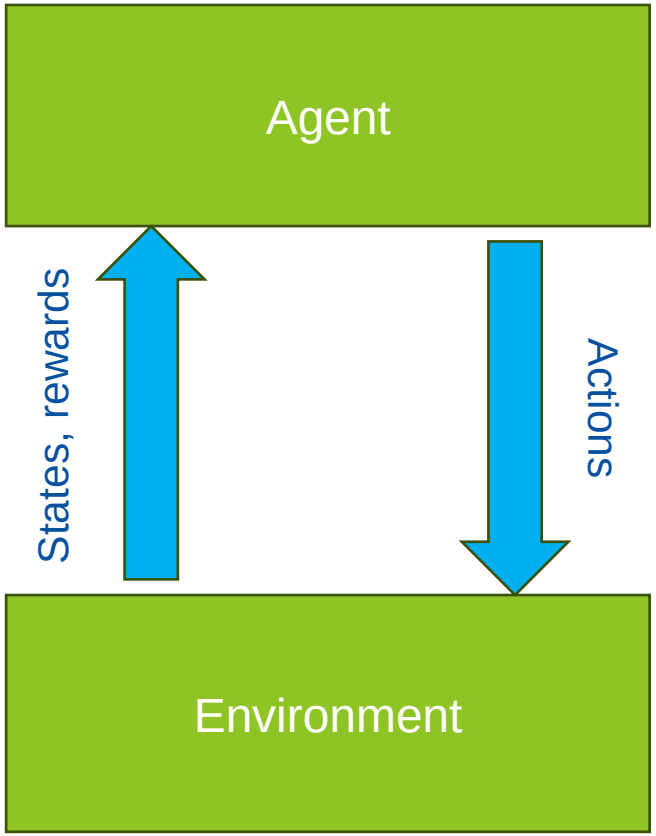
```
[Trainers]
  [nn_max]
    type = LibtorchANNTrainer
    sampler = sample
    response = "results_train/T_max_out:value"
    num_neurons_per_layer = '16 8'
    activation_function = 'relu relu'
    nn_filename = 'weights_max.pt'
    read_from_file = false
    num_epochs = 15000
    num_batches = 20
    learning_rate = 5e-5
    print_epoch_loss = 10
  []
[]
```

```
[Surrogates]
  [nn_max]
    type = LibtorchANNSurrogate
    filename = "train_nn_trainer_nn_max.rd"
  []
[]
```

```
[Samplers]
  [sample]
    type = MonteCarlo
    distributions = 'mass_in power alpha beta'
    num_rows = 200000000
    seed = 0
  []
[]
```

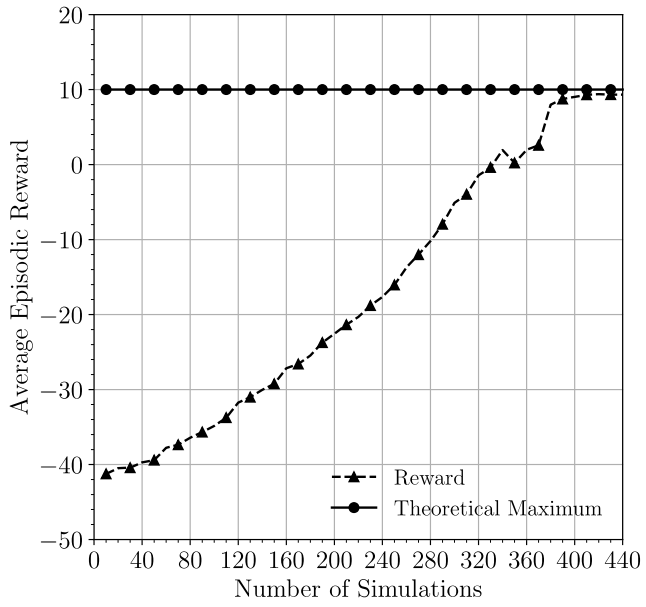
Process control with Deep Reinforcement Learning

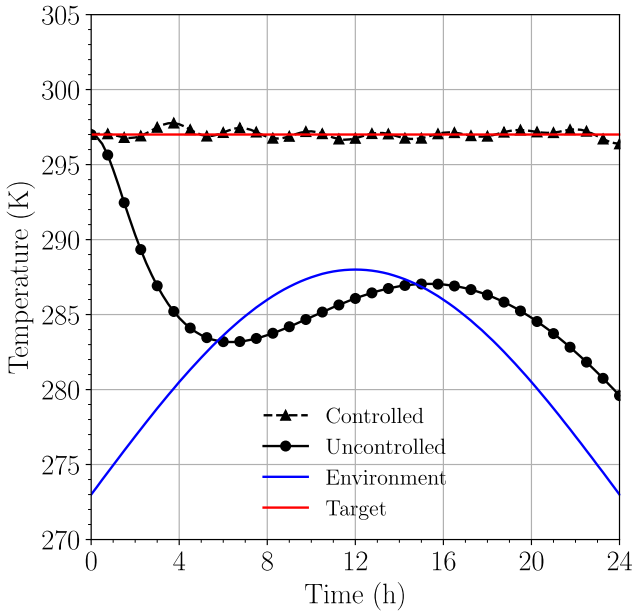
- Proximal Policy Optimization [3]:
  - Agent uses 2 neural networks:
    - Actor (controller)
    - Critic (value-estimator)
- Try to maximize the reward
- Probabilistic action (policy), help with exploration and the reduction of overfitting
- Exercise the environment and see if the actions resulted in higher rewards (if we have an advantage)
- Use the advantage and the probability of the actions to update the controller
- Use clipping for the update to be conservative

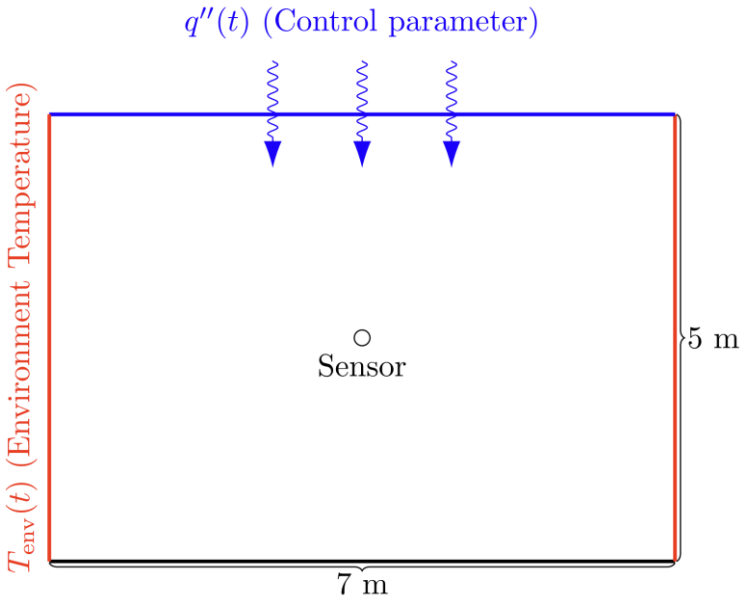


Process control with Deep Reinforcement Learning

- Simple heat conduction problem
  - Try to keep the temperature at the sensor constant
  - Using the heat flux on the top boundary
  - Side boundaries follow the environmental temperature







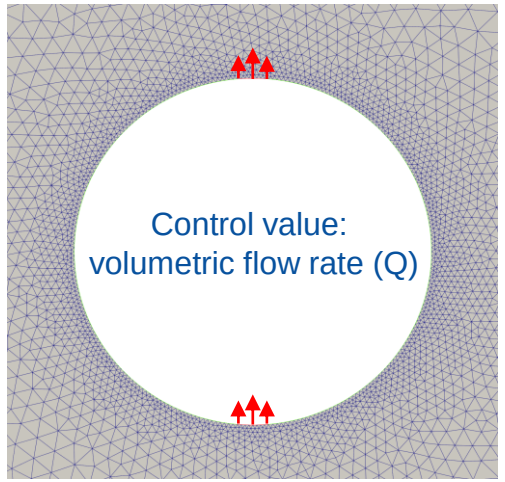
Process control with Deep Reinforcement Learning

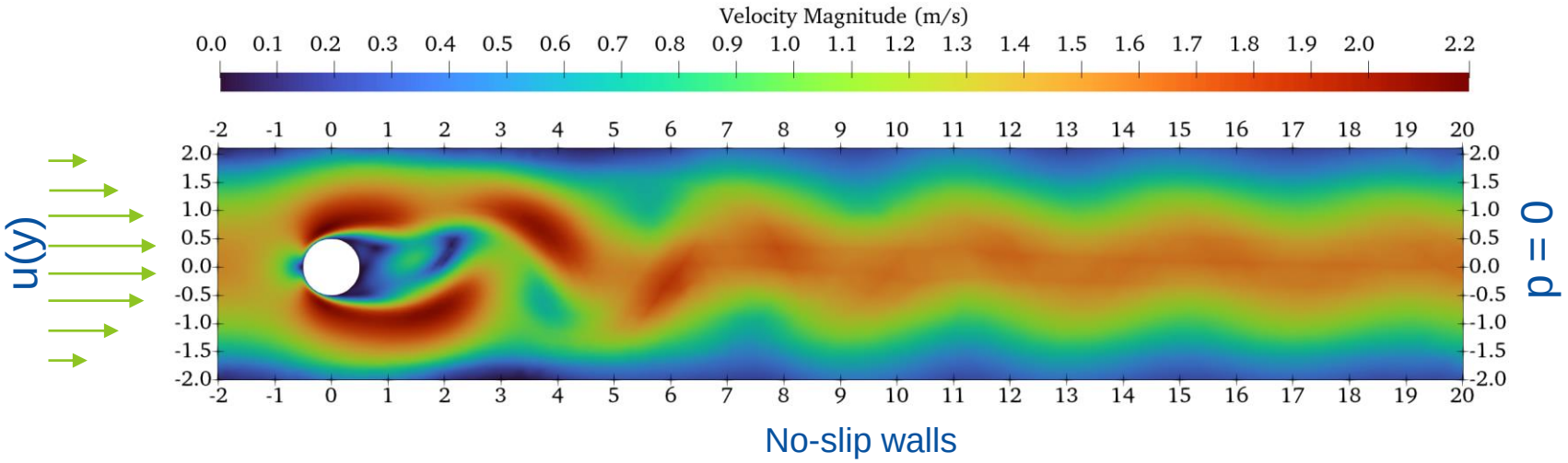
```
[Trainers]
  [nn_trainer]
    type = LibtorchDRLControlTrainer
    response = 'results/center_temp results/env_temp'
    control = 'results/top_flux'
    log_probability = 'results/log_prob_top_flux'
    reward = 'results/reward'

    num_epochs = 1000
    update_frequency = 10
    decay_factor = 0.0

    loss_print_frequency = 10

    critic_learning_rate = 0.0001
    num_critic_neurons_per_layer = '64 27'

    control_learning_rate = 0.0005
    num_control_neurons_per_layer = '16 6'

    # keep consistent with LibtorchNeuralNetControl
    input_timesteps = 2
    response_scaling_factors = '0.03 0.03'
    response_shift_factors = '290 290'
    action_standard_deviations = '0.02'

    standardize_advantage = true

    read_from_file = false
  []
[]
```

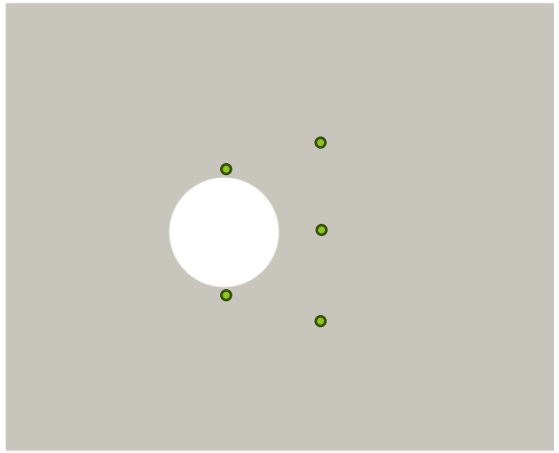
```
[Controls]
  [src_control]
    type = LibtorchDRLControl
    parameters = "BCs/top_flux/value"
    responses = 'center_temp_tend env_temp'

    # keep consistent with LibtorchDRLControlTrainer
    input_timesteps = 2
    response_scaling_factors = '0.03 0.03'
    response_shift_factors = '290 290'
    action_standard_deviations = '0.02'
    action_scaling_factors = 200

    execute_on = 'TIMESTEP_BEGIN'
  []
[]
```

Flow control with Deep Reinforcement Learning

- Benchmark case from [6], uncontrolled case validated using data from [7]
- Fluid dynamics solver: MOOSE Navier Stokes Module
- Mesh: GMSH (~9,300 elements)
- Goal: Minimize the drag without considerable increase in the lift using the small jets on the surface of the body
- Sensors: Five sensors recording pressure and velocity

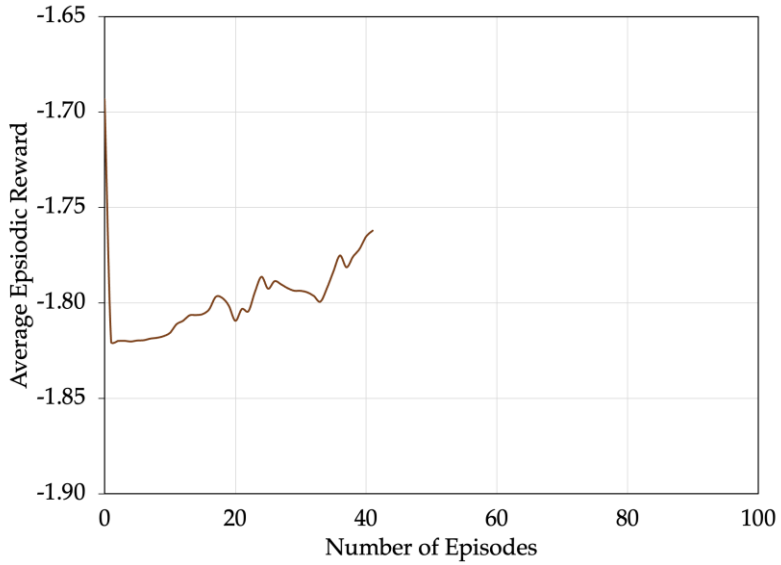


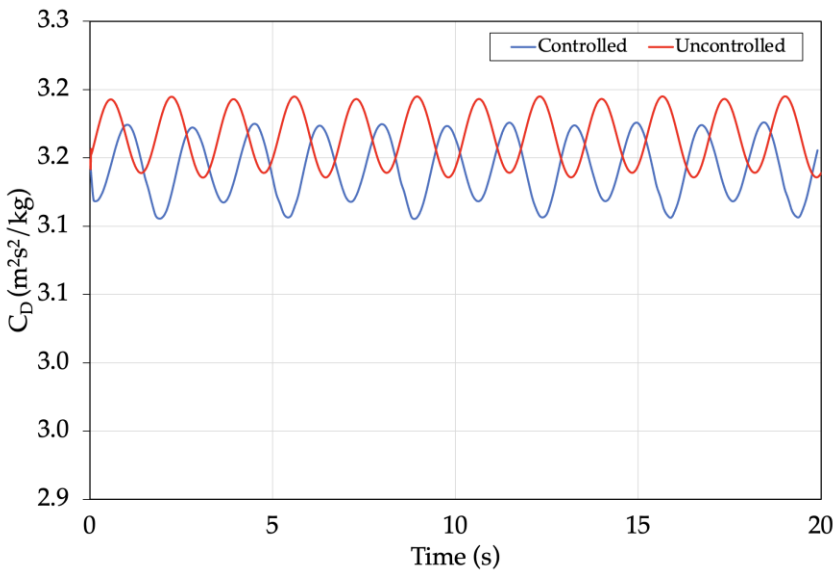




Sensor locations

Flow control with Deep Reinforcement Learning





- Reward function: $r = -\langle C_D \rangle_T - 0.2\langle C_L \rangle_T$ (average quantities over one period)
- Tricks (adapted from [6]):
  - Relax the change in the control value in the Q by $Q^n = Q^{n-1} + 0.2(a - Q^{n-1})$, where a is the action determined by the controller
  - Action a changes every 25 time steps (no quick changes in a)
  - Limit the maximum control value to $0.06\,Q^*$, where Q^* is the volumetric flow rate intercepting the cylinder

Summary

- New Libtorch interface is readily available in MOOSE and any MOOSE-based application
- Can be used for:
  - Surrogate generation for Uncertainty Quantification and Sensitivity Analysis
    - Example provided for EBR-II fuel assembly computations
  - Reinforcement learning for physics controllers
    - Example provided for control aimed at reducing drag
- Future (ongoing) work:
  - Reinforcement learning for additive manufacturing
  - Advanced material models for plasticity

References

[1] Lindsay, A. D., et al. 2020. “2.0-MOOSE: Enabling massively parallel multiphysics simulation.” *SoftwareX* 20: 101202. https://doi.org/10.1016/j.softx.2022.101202.

[2] Paszke, A., et al. 2019. “Pytorch: An imperative style, high-performance deep learning library.” *Advances in Neural Information Processing Systems* 32. https://doi.org/10.48550/arXiv.1912.01703

[3] Schulman, J., et al. 2017. “Proximal Policy Optimization Algorithms.” *https://doi.org/10.48550/arXiv.1707.06347*.

[4] Lentz, G. L., H. W. Buschman, and R. N. Smith. 1985. “EBR-II: twenty years of operating experience.” CONF-850722-1, Argonne National Laboratory. https://www.osti.gov/servlets/purl/5434129.

[5] Kyriakopoulos, V., M. E. Tano, and J. C. Ragusa. 2022. “Development of a Single-Phase, Transient, Subchannel Code, within the MOOSE Multi-Physics Computational Framework.” *Energies* 15(11): 3948. https://doi.org/10.3390/en15113948.

[6] Rabault, J., et al. 2019. "Artificial neural networks trained through deep reinforcement learning discover control strategies for active flow control." *Journal of Fluid Mechanics* 865: 281–302. https://doi.org/10.1017/jfm.2019.62.

[7] Schäfer, M., S. Turek, F. Durst, E. Krause, and R. Rannacher. 1996. “Benchmark computations of laminar flow around a cylinder.” In Hirschel, E.H. (eds) Flow Simulation with High-Performance Computers II. Vieweg+Teubner Verlag. https://doi.org/10.1007/978-3-322-89849-4_39.

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Surrogate generation for flow in nuclear fuel assemblies

- Sobol expansion:

$$Y = f(X_1, X_2, \dots, X_k) = f_0 + \sum_{i}^{k} f_i(X_i) + \sum_{i} \sum_{j<i} f_{ij}(X_i, X_j) + \cdots + f_{12\dots k}(X_1, X_2, \dots, X_k)$$

- If each term has a zero mean
  - The functions are pair-wise orthogonal
  - The terms can be determined using conditional expectations from low to high orders
  - The total variance can be expressed as:

$$\mathrm{Var}(f) = \sum_{i}^{k} \mathrm{Var}(f_i) + \sum_{i} \sum_{j<i} \mathrm{Var}(f_{ij}) + \cdots + \mathrm{Var}(f_{12\dots k})$$

- Sobol indices:
  - First order: $S_i = \frac{\mathrm{Var}(f_i)}{\mathrm{Var}(f)}$
  - Total: $S_{T,i} = S_i + \sum_{j}^{k} S_{ij} + \cdots + S_{ij\dots k}$
- Compute these using Saltelli's Monte Carlo methods

Saltelli, Andrea, et al. *Sensitivity analysis in practice: a guide to assessing scientific models*. Vol. 1. New York: Wiley, 2004.