



### Simone Venturi, Tiernan Casey

Extreme-Scale Data Science & Analytics (8739)

Part of the Code Documentation for Neural Networks for Reduced Order Modeling (ROMNet)





Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

### **Generating Data**

Run the Jupyter Notebook:

\$WORKSPACE\_PATH/ROMNet/romnet/scripts/generating\_data/PlasmaSystem/Generate\_Data\_1.py for generating simulation data

Run Jupyter Notebook:

\$WORKSPACE\_PATH/ROMNet/romnet/scripts/generating\_data/ PlasmaSystem/Generate\_Data\_2.ipynb for producing training and test data

# Test Case 1 Data-Driven Vanilla DeepONet in the Thermodynamic State Space

### **Test Case 1: Data-driven Vanilla DeepONet**

- 1.1. Copy \$WORKSPACE\_PATH/ROMNet/romnet/input/PlasmaSystem/DeepONet/PlasmaSystem\_TestCase1/ROMNet\_Input.py to \$WORKSPACE\_PATH/ROMNet/romnet/input/ROMNet\_Input.py
- 1.2. In \$WORKSPACE\_PATH/ROMNet/romnet/input/ROMNet\_Input.py, change: 1.2.1. "self.WORKSPACE\_PATH = ..."
- 1.3. Move to \$WORKSPACE\_PATH/ROMNet/romnet/app/
- 1.4. Run: "python3 ROMNet.py ../input/"
- 1.5. Postprocess results via: \$WORKSPACE\_PATH/ROMNet/romnet/scripts/postprocessing/PlasmaSystem/DeepONet/Predict\_DeepONet.ipynb



# Test Case 2 Data-Driven DeepONet with Frozen Trunks in the Thermodynamic State Space

6

### A Plasma System Test Case



### **Generating Data**

Run the python scrip:

\$WORKSPACE\_PATH/ROMNet/romnet/scripts/generating\_data/ScenarioAggregated\_ROMS/0DReactor/Generate\_Data.py for generating the trunks' modes.



### **Test Case 2: Data-driven DeepONet with Frozen Trunks**

#### **Train the Trunks:**

- 2.1. Run \$WORKSPACE\_PATH/ROMNet/romnet/input/ScenarioAggregated\_ROMs/PlasmaSytem/FNN/Trunk/Parallelize\_ROMNet.py
- 2.2 Postprocess with \$WORKSPACE\_PATH/ROMNet/romnet/scripts/postprocessing/ScenarioAggregated\_ROMS/PlasmaSystem/FNN/Predict\_FNN\_Trunk.ipynb

#### **Train the Rest of the DeepONet**

- 2.1. Copy \$WORKSPACE\_PATH/ROMNet/romnet/input/PlasmaSystem/DeepONet/PlasmaSystem\_TestCase2/ROMNet\_Input.py to \$WORKSPACE\_PATH/ROMNet/romnet/input/ROMNet\_Input.py
- 2.2. In \$WORKSPACE\_PATH/ROMNet/romnet/input/ROMNet\_Input.py, change: 2.2.1. "self.WORKSPACE\_PATH = ..."
- 2.3. Move to \$WORKSPACE\_PATH/ROMNet/romnet/app/
- 2.4. Run: "python3 ROMNet.py ../input/"
- 2.5. Postprocess results via: \$WORKSPACE\_PATH/ROMNet/romnet/scripts/postprocessing/Rect/DeepONet/Predict\_DeepONet.ipynb



# Test Case 3 Data-Driven flexDeepONet in the Thermodynamic State Space

### **Test Case 3: Data-driven FlexDeepONet**

- 3.1. Copy \$WORKSPACE\_PATH/ROMNet/romnet/input/PlasmaSystem/DeepONet/PlasmaSystem\_TestCase3/ROMNet\_Input.py to \$WORKSPACE\_PATH/ROMNet/romnet/input/ROMNet\_Input.py
- 3.2. In \$WORKSPACE\_PATH/ROMNet/romnet/input/ROMNet\_Input.py, change: 3.2.1. "self.WORKSPACE\_PATH = ..."
- 3.3. Move to \$WORKSPACE\_PATH/ROMNet/romnet/app/
- 3.4. Run: "python3 ROMNet.py ../input/"
- 3.5. Postprocess results via: \$WORKSPACE\_PATH/ROMNet/romnet/scripts/postprocessing/PlasmaSystem/DeepONet/Predict\_DeepONet.ipynb

# Test Case 4 Data-Driven MIONet in the Thermodynamic State Space

### **Generating Data**

Run the Jupyter Notebook:

\$WORKSPACE\_PATH/ROMNet/romnet/scripts/generating\_data/PlasmaSystem/Generate\_Data\_1.py for generating simulation data

Run Jupyter Notebook:

\$WORKSPACE\_PATH/ROMNet/romnet/scripts/generating\_data/ PlasmaSystem/Generate\_Data\_2.ipynb for producing training and test data





### **Test Case 4: Data-driven MIONet**

- 4.1. Copy \$WORKSPACE\_PATH/ROMNet/romnet/input/PlasmaSystem/MIONet/PlasmaSystem\_TestCase4/ROMNet\_Input.py to \$WORKSPACE\_PATH/ROMNet/romnet/input/ROMNet\_Input.py
- 4.2. In \$WORKSPACE\_PATH/ROMNet/romnet/input/ROMNet\_Input.py, change: 4.2.1. "self.WORKSPACE\_PATH = ..."
- 4.3. Move to \$WORKSPACE\_PATH/ROMNet/romnet/app/
- 4.4. Run: "python3 ROMNet.py ../input/"
- 4.5. Postprocess results via: \$WORKSPACE\_PATH/ROMNet/romnet/scripts/postprocessing/PlasmaSystem/ MIONet /Predict\_MIONet\_Orig\_UncertainParams.ipynb

### **Test Case 4: Data-driven DeepONet with Frozen Trunks**

- 4.1. Copy \$WORKSPACE\_PATH/ROMNet/romnet/input/PlasmaSystem/DeepONet/PlasmaSystem\_TestCase4/ROMNet\_Input.py to \$WORKSPACE\_PATH/ROMNet/romnet/input/ROMNet\_Input.py
- 4.2. In \$WORKSPACE\_PATH/ROMNet/romnet/input/ROMNet\_Input.py, change: 4.2.1. "self.WORKSPACE\_PATH = ..."
- 4.3. Move to \$WORKSPACE\_PATH/ROMNet/romnet/app/
- 4.4. Run: "python3 ROMNet.py ../input/"
- 4.5. Postprocess results via: \$WORKSPACE\_PATH/ROMNet/romnet/scripts/postprocessing/Rect/DeepONet/Predict\_DeepONet.ipynb