



Sandia
National
Laboratories

Test Cases for the Moving Rectangle

Simone Venturi, Tiernan Casey

Extreme-Scale Data Science & Analytics (8739)

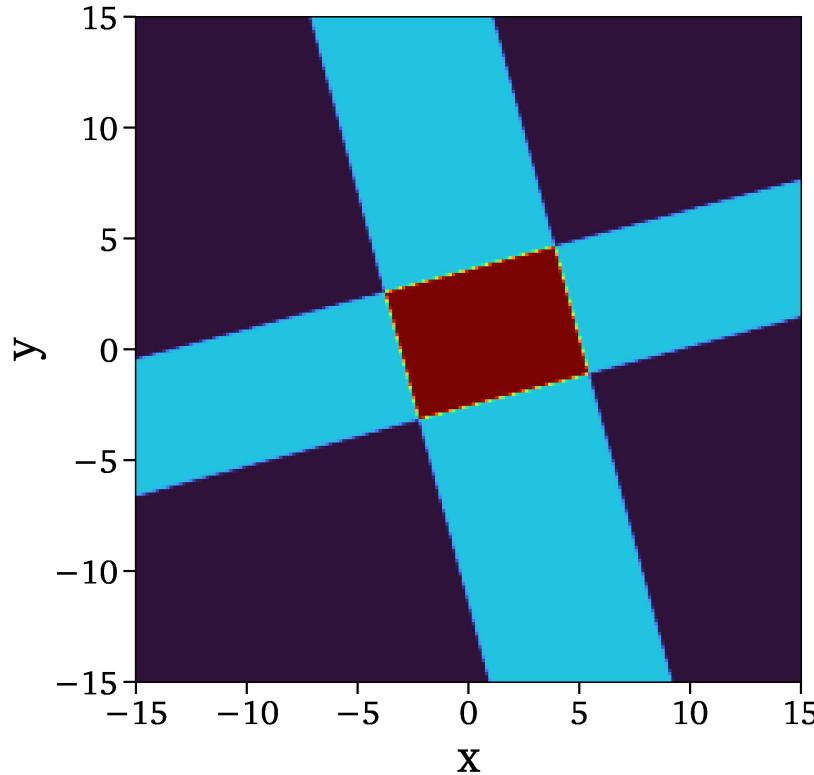
**Part of the Code Documentation for
Neural Networks for Reduced Order Modeling (ROMNet)**



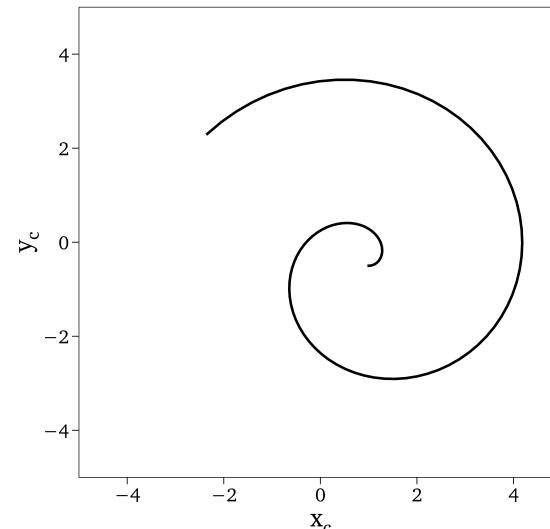
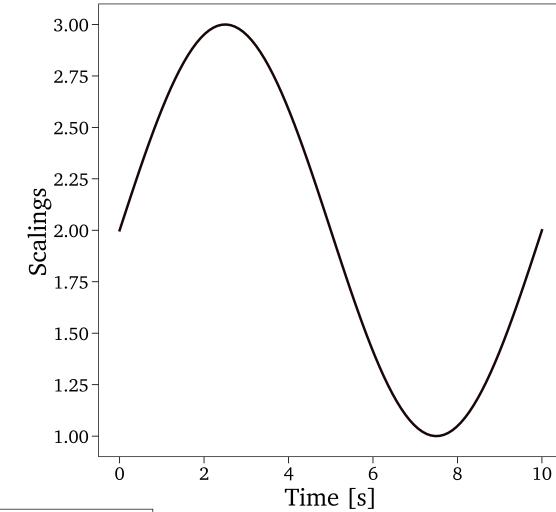
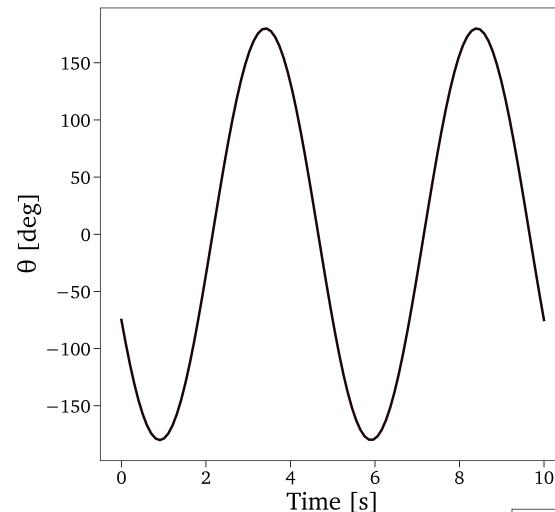
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

A Moving Rectangle Test Case

200 time snapshots of [200×200] x and y grid points



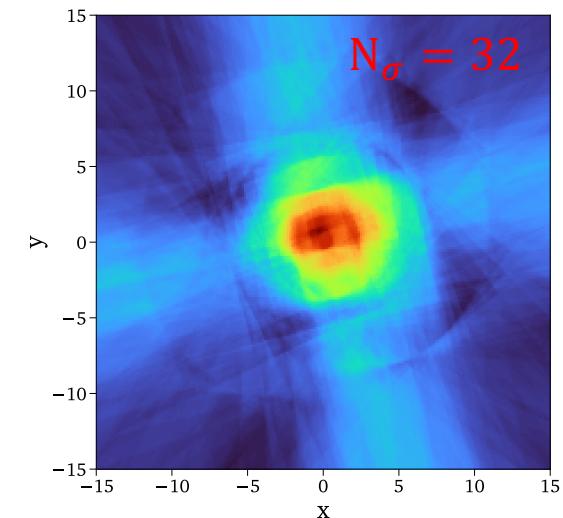
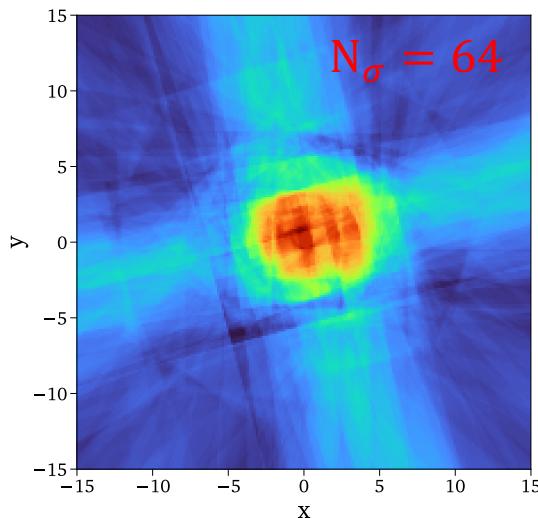
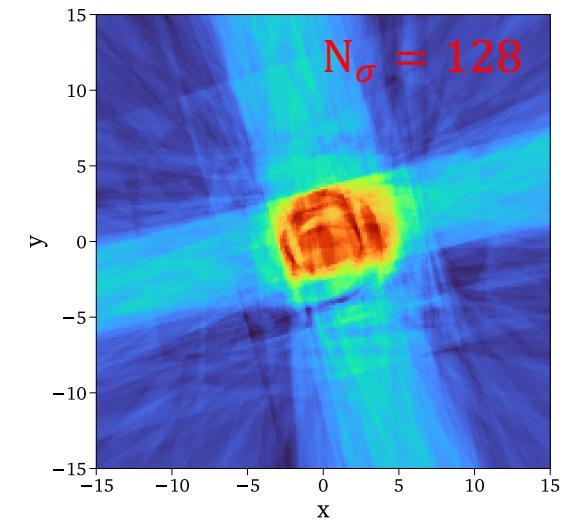
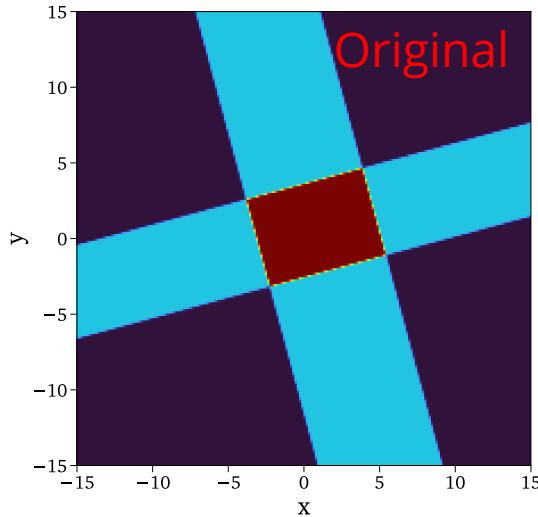
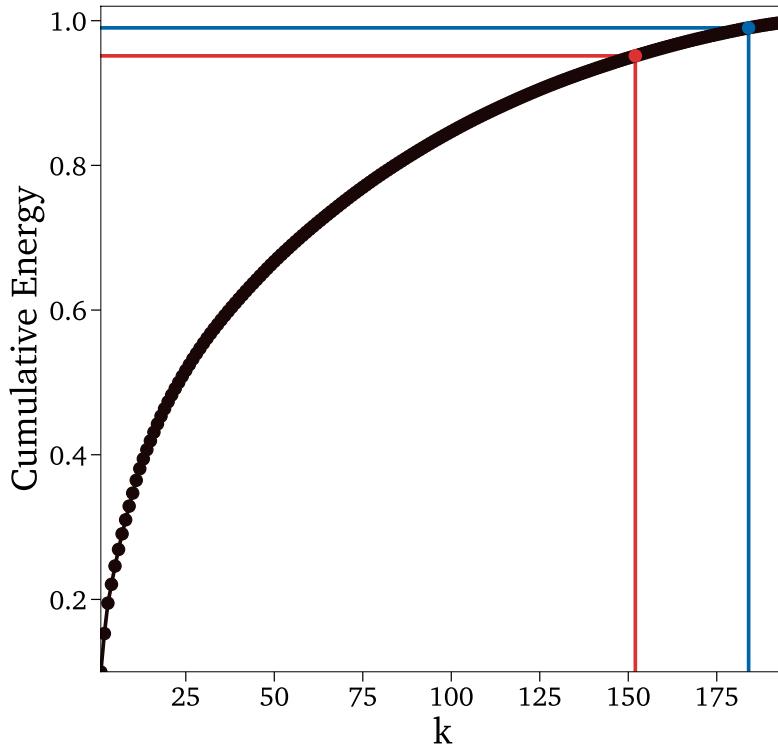
Rectangle (cross) rotating, scaling and shifting



A Moving Rectangle Test Case



SVD of the time-aggregated snapshot matrix (i.e., POD style)





A Moving Rectangle Test Case

Run Jupyter Notebook:

`$WORKSPACE_PATH/ROMNet/romnet/scripts/generating_data/Rect/Generate_Data_1.ipynb`
for generating training and test data

A Moving Rectangle Test Case



Constructing surrogate models via DeepONet:

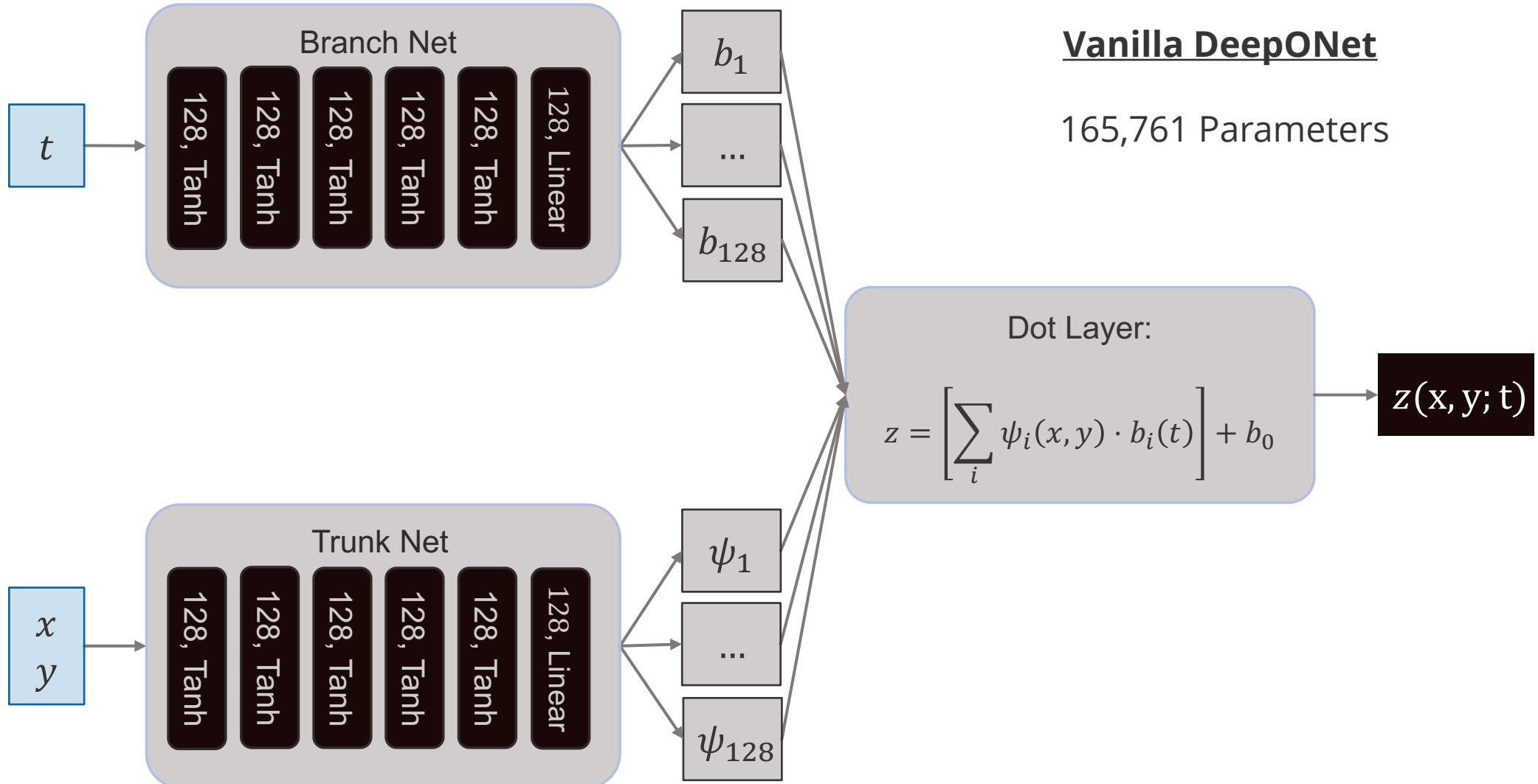
- Randomizing data points in x, y and t
- Less data points (1,000,000 rather than 8,000,000)
- Sampling x, y in a $[-10,10] \times [-10,10]$ window, rather than $[-15,15] \times [-15,15]$

A Moving Rectangle Test Case

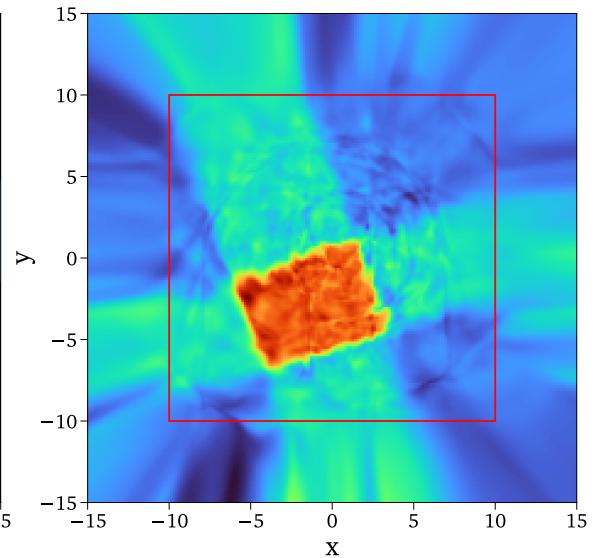
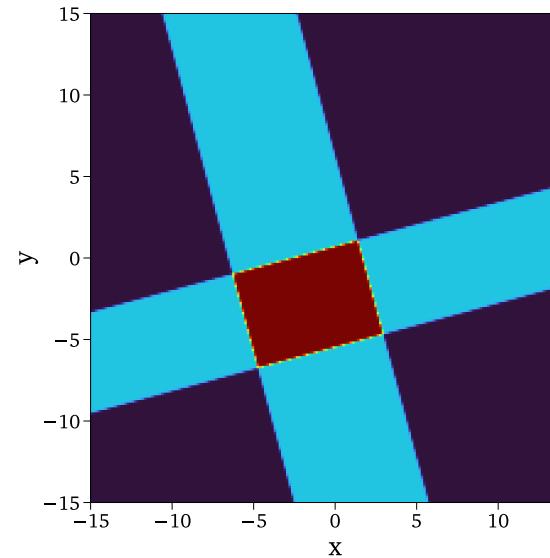
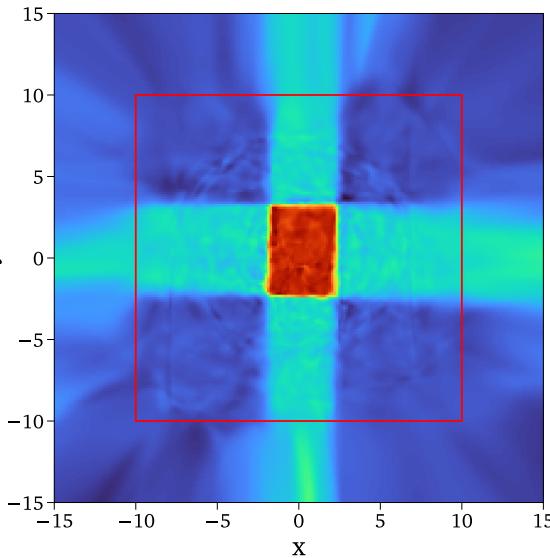
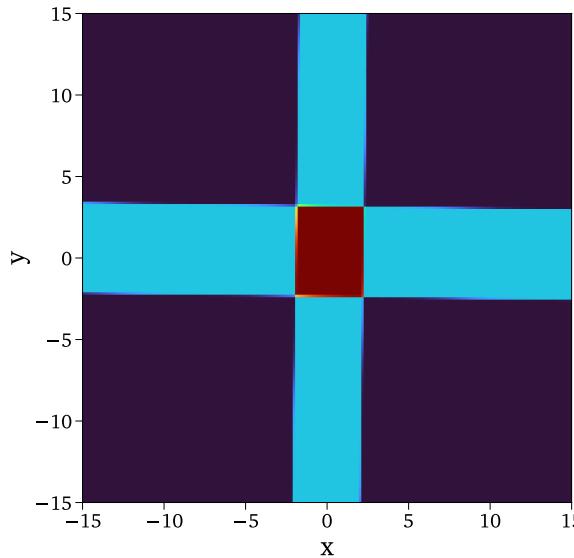
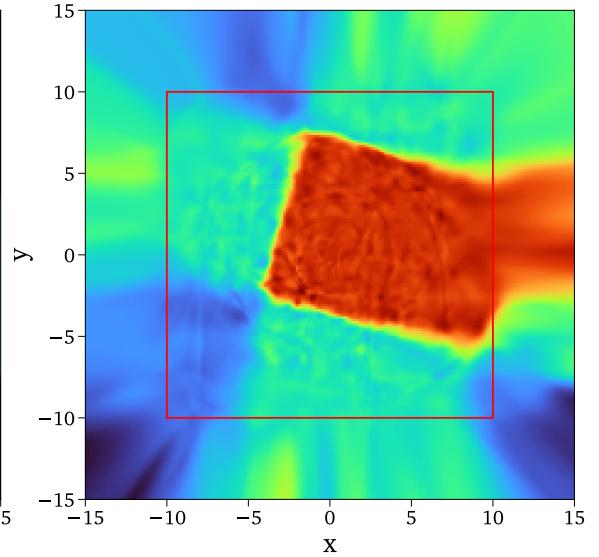
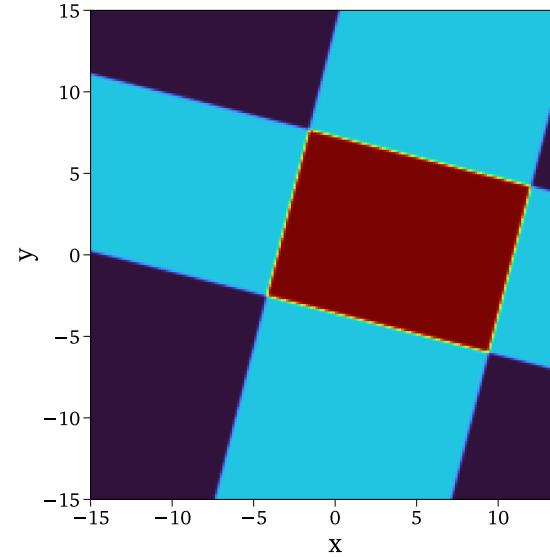
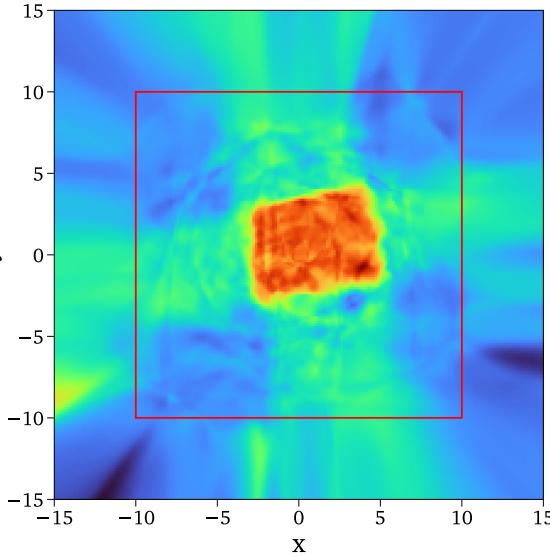
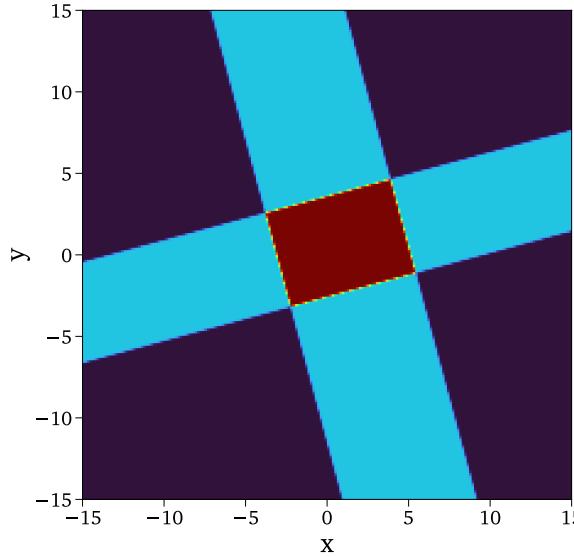


Test Case 1

A Moving Rectangle Test Case



A Moving Rectangle Test Case



A Combustion Chemistry in Isobaric Reactor Test Case



Test Case 1: Data-driven vanilla DeepONet

- 1.1. Copy \$WORKSPACE_PATH/ROMNet/romnet/input/0DReact/DeepONet/Rect_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/Rect/DeepONet/Predict_DeepONet.ipynb

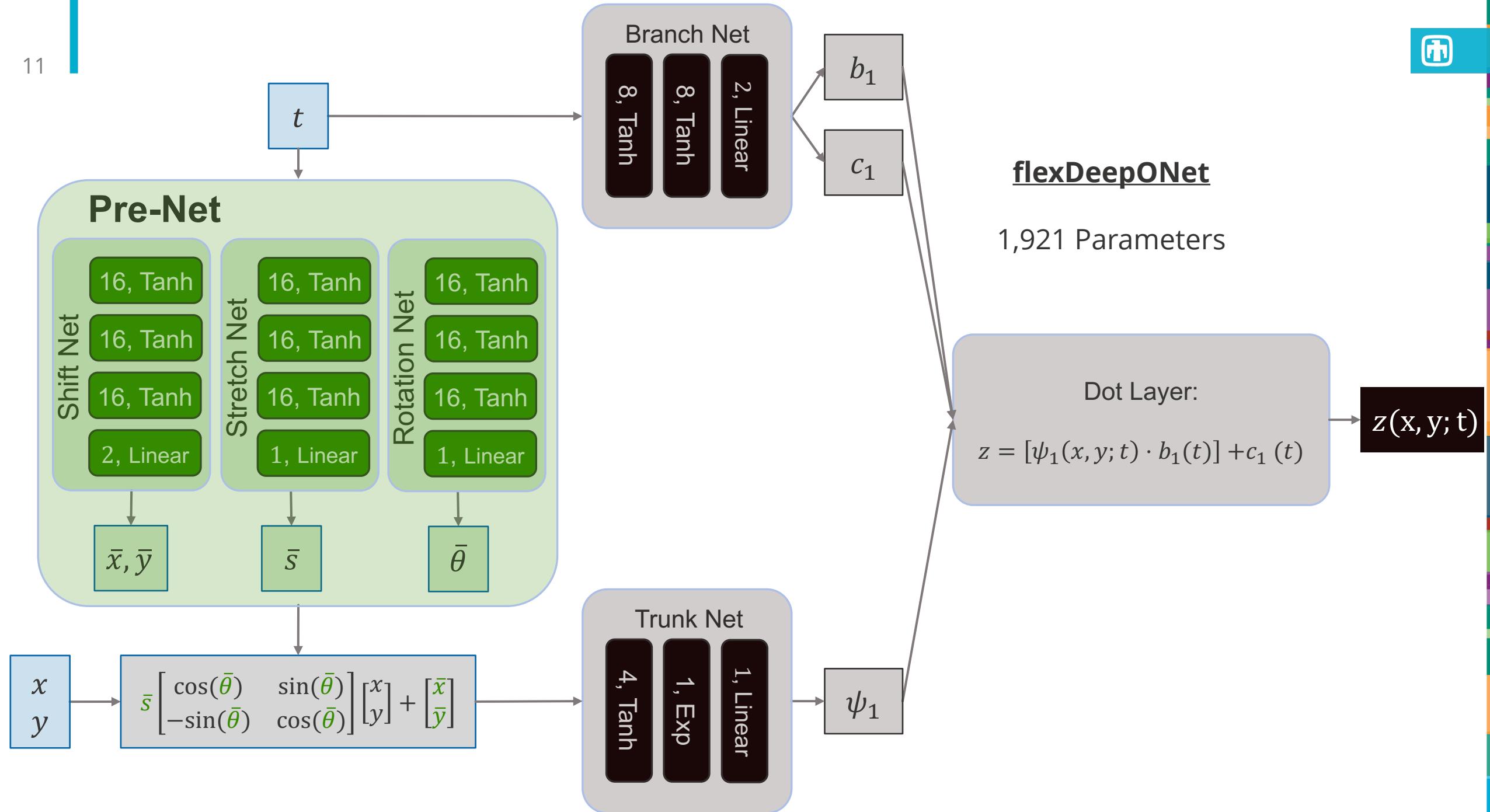
A Moving Rectangle Test Case



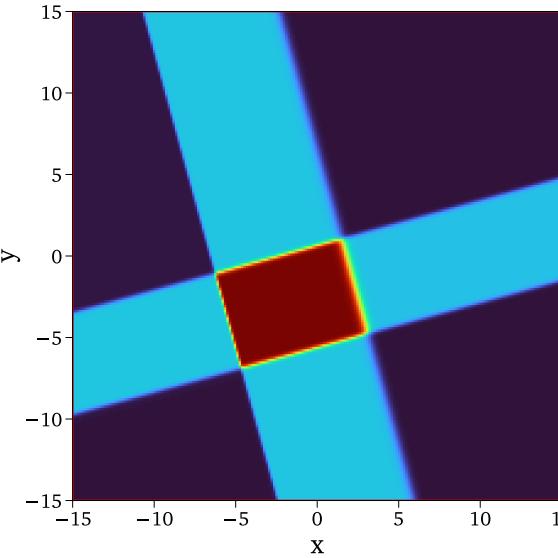
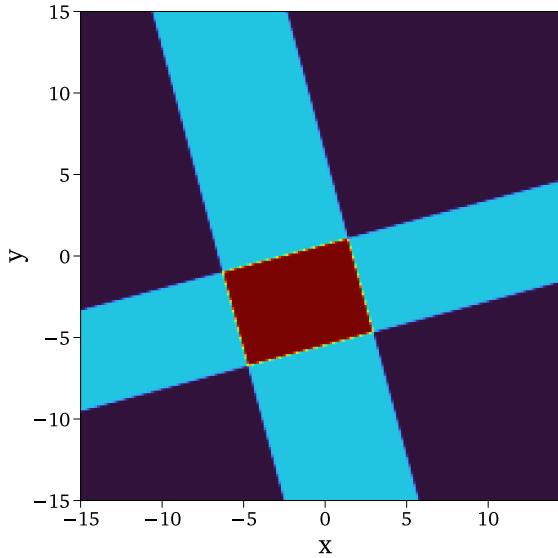
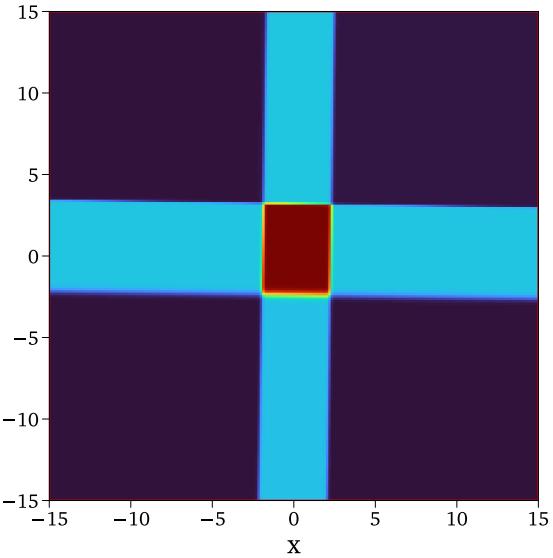
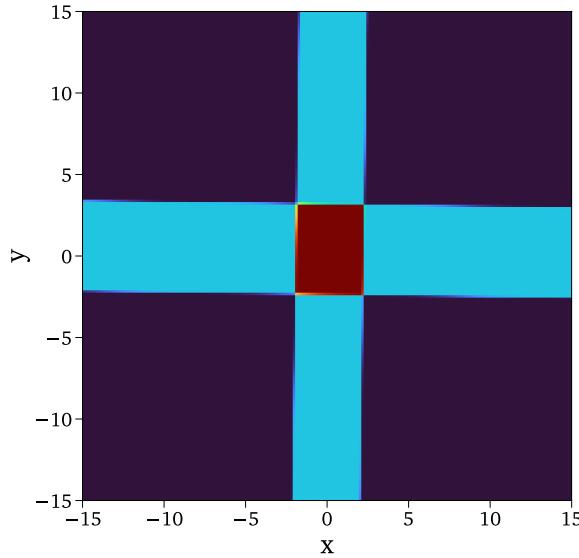
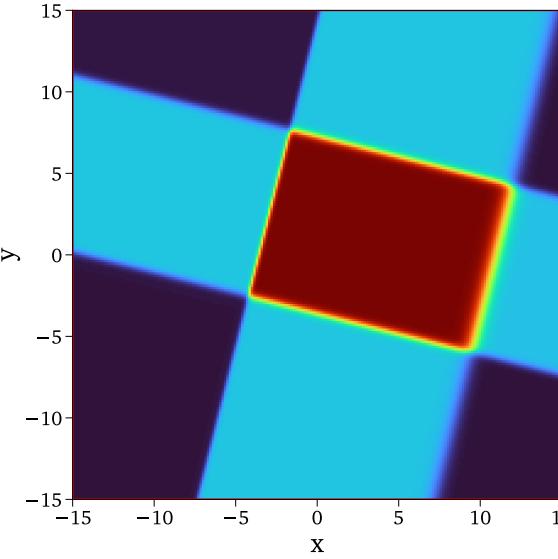
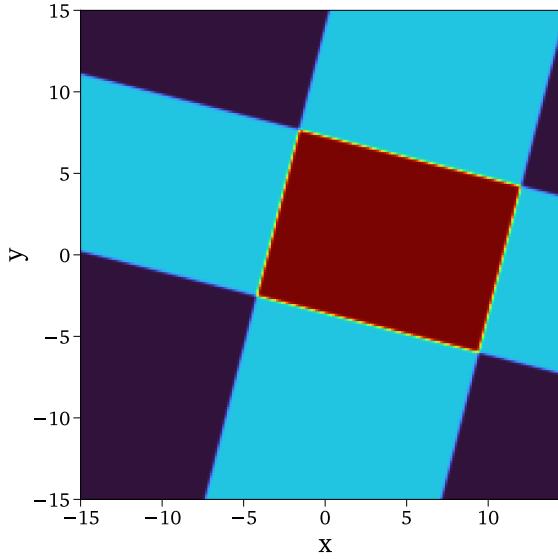
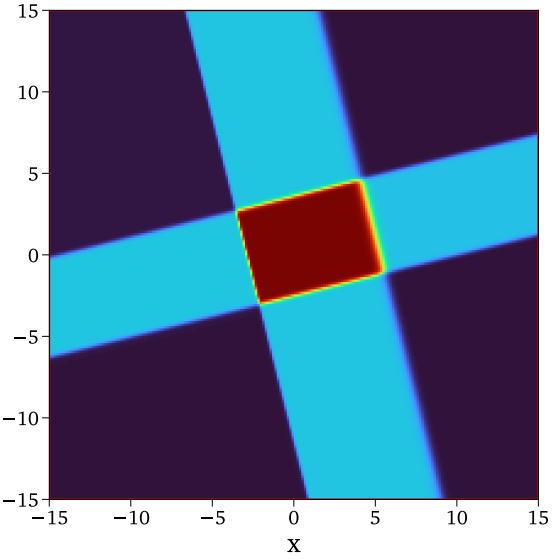
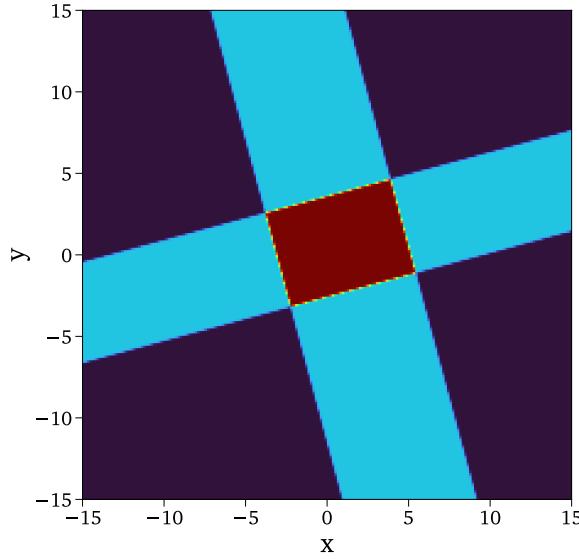
Test Case 5

flexDeepONet

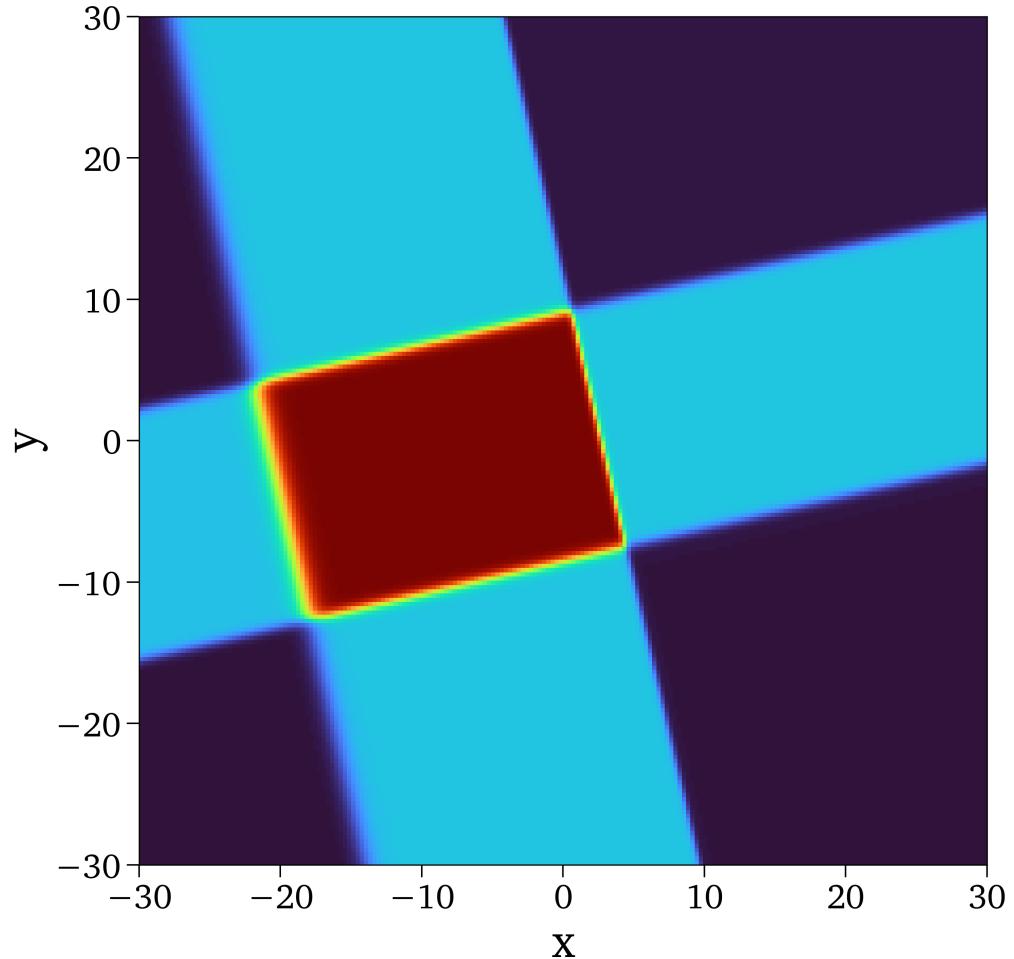
1,921 Parameters



A Moving Rectangle Test Case



A Moving Rectangle Test Case

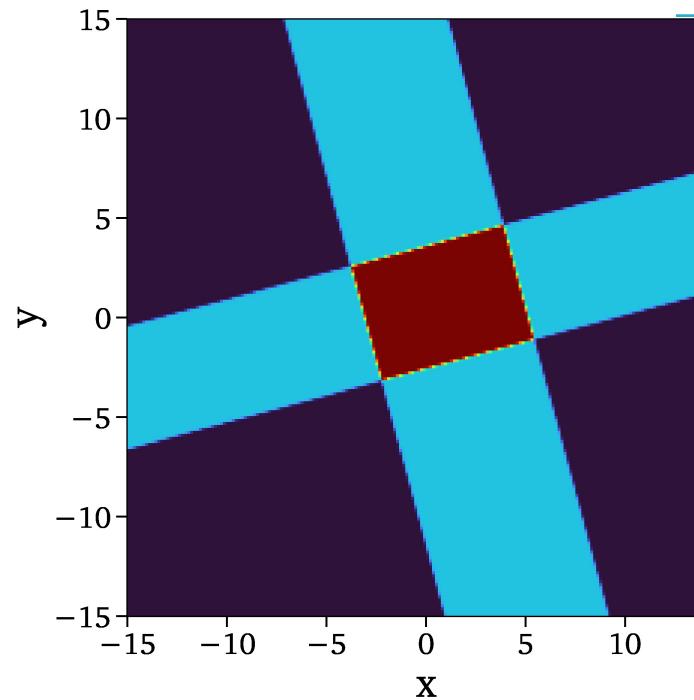


Trunk's Output (i.e., mode)

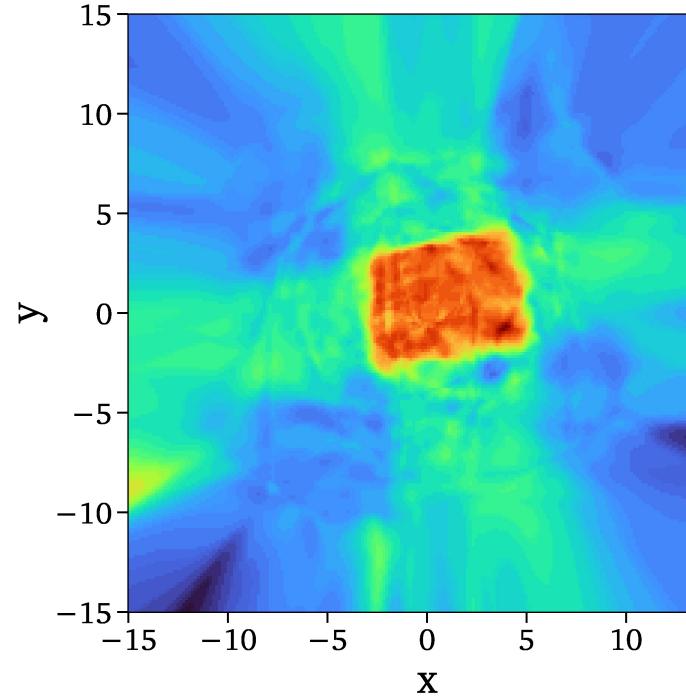
A Moving Rectangle Test Case



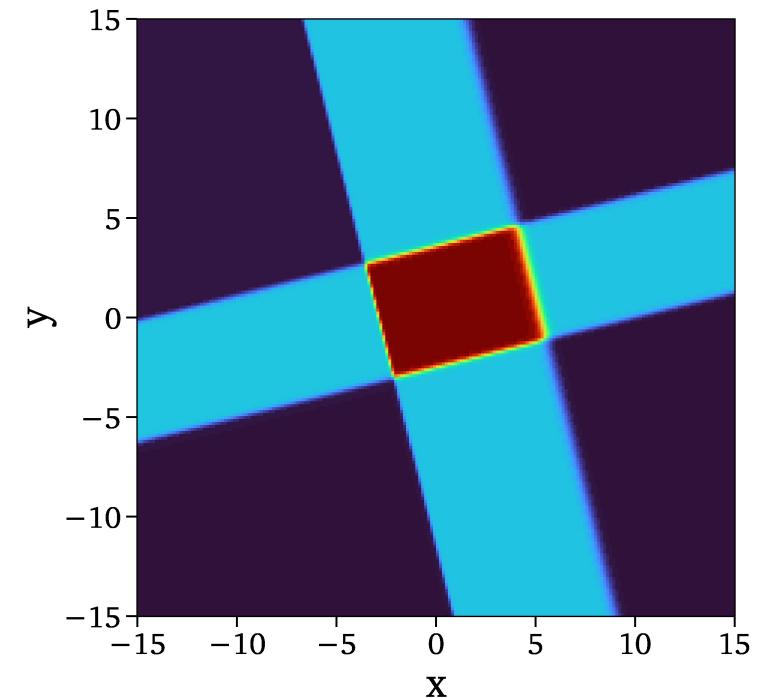
Original



Vanilla DeepONet



flexDeepONet



A Combustion Chemistry in Isobaric Reactor Test Case



Test Case 5: Data-driven flexDeepONet

- 5.1. Copy \$WORKSPACE_PATH/ROMNet/romnet/input/0DReact/DeepONet/Rect_TestCase5/ROMNet_Input.py to \$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py
- 5.2. In \$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py, change:
 - 5.2.1. "self.WORKSPACE_PATH = ..."
- 5.3. Move to \$WORKSPACE_PATH/ROMNet/romnet/app/
- 5.4. Run: "python3 ROMNet.py ..//input/"
- 5.5. Postprocess results via: \$WORKSPACE_PATH/ROMNet/romnet/scripts/postprocessing/Rect/DeepONet/Predict_DeepONet.ipynb