Space Weather Simulation Summer School 2023

Instructor: Boris Kramer (http://kramer.ucsd.edu/)

Operator Inference for Space Weather Model Reduction

The goal of non-intrusive model reduction is to efficiently make physics-based predictions given high-fidelity simulation data. This tutorial explores learning a operator inference (https://willcox-research-group.github.io/rom-operator-inference-Python3/source/index.html) reduced order model for the conduction model (https://github.com/AetherModel/swsss2023/tree/main/day_06) taught earlier in the week.

Relevant literature:

1. Peherstorfer, B. and Willcox, K., *Data-driven operator inference for nonintrusive projection-based model reduction, Computer Methods in Applied Mechanics and Engineering*, Vol. 306, pp. 196-215, 2016.
2. Issan, O. and Kramer, B., *Predicting solar wind streams from the inner-heliosphere to Earth via shifted operator inference*, Journal of Computational Physics, Vol. 473, pp. 111689, 2023.

Necessary data for this exercise (ask from the intructor before proceeding):

1. *conduction_v6_data.npy* - simulation data of the temperature as a function of space and time.
2. *conduction_v6_alt.npy* - the altitude, i.e. x, grid in km.
3. *conduction_v6_time.npy* - the time, i.e. t, grid in hr.
4. *conduction_v6_lower_bc.npy* - the lower boundary condition as a function of time.

Exercise Questions:

1. It took 9.93 minutes to simulative the full order model data on MacBook Pro 2.3 GHz Quad-Core Intel Core i7 processor with 16 GB RAM. Assuming you are using a similar machine, how much faster was simulating the ROM? Discuss the motivation of using model reduction for space weather operational forecasting.
2. There are a few hyperparameters that can improve the ROM accuracy: the regularization parameter λ and the number of reduced basis r. Rigoursly test what happens when you increase the regularization parameter and/or the reduced basis dimension. Discuss your findings.

Full Order Model: As taught by Prof. Aaron Ridley, the governing equations are

$$\frac{\partial}{\partial t}\underbrace{q(x,t)}_{\text{temperature}} = \underbrace{c\frac{\partial^2}{\partial x^2}q(x,t)}_{\text{conduction term}} + \underbrace{u(x,t)}_{\text{source term}}.$$

Once discretized in space via finite differencing the semi-discrete form of the equations is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{q}(t) = \mathbf{A}\mathbf{q}(t) + \mathbf{B}\mathbf{u}(t)$$

where $\mathbf{q}(t) \in \mathbb{R}^n, \mathbf{A} \in \mathbb{R}^{n\times n}, \mathbf{B} \in \mathbb{R}^{n\times m}, \mathbf{u}(t) \in \mathbb{R}^m, m = 1, n = 8001$

Step 1: Import Python modules

Tip: Install the latest version of *opinf* package using pip (https://willcox-research-group.github.io/rom-operator-inference-Python3/source/opinf/installation.html).

In [1]:
```
# import modules: numpy, scipy, opinf, matplotlib
import numpy as np
import scipy.linalg as la
import scipy.sparse as sparse
import opinf
import matplotlib.pyplot as plt
import matplotlib
font = {'family' : 'serif',
        'size'   : 12}

matplotlib.rc('font', **font)
matplotlib.rc('xtick', labelsize=12)
matplotlib.rc('ytick', labelsize=12)
```

Step 2: Read in training data

The training data is provided as *conduction_v6_data.npy* file

In [2]:
```
# load simulation data using numpy
data = np.load("conduction_v6_data.npy")
# use 100 snapshots for training and 43 for testing
Q_train = data[:, :100]
Q_test = data[:, 100:]
print("shape of the simulation data = ", np.shape(data))
print("shape of the training simulation data = ", np.shape(Q_train))
print("shape of the testing simulation data = ", np.shape(Q_test))
```

```
shape of the simulation data =  (8001, 143)
shape of the training simulation data =  (8001, 100)
shape of the testing simulation data =  (8001, 43)
```

In [3]:
```
# altitude in km
x = np.load("conduction_v6_alt.npy")/1000
dx = x[1] - x[0]
print(f"Spatial step size δx = {dx} km")
```

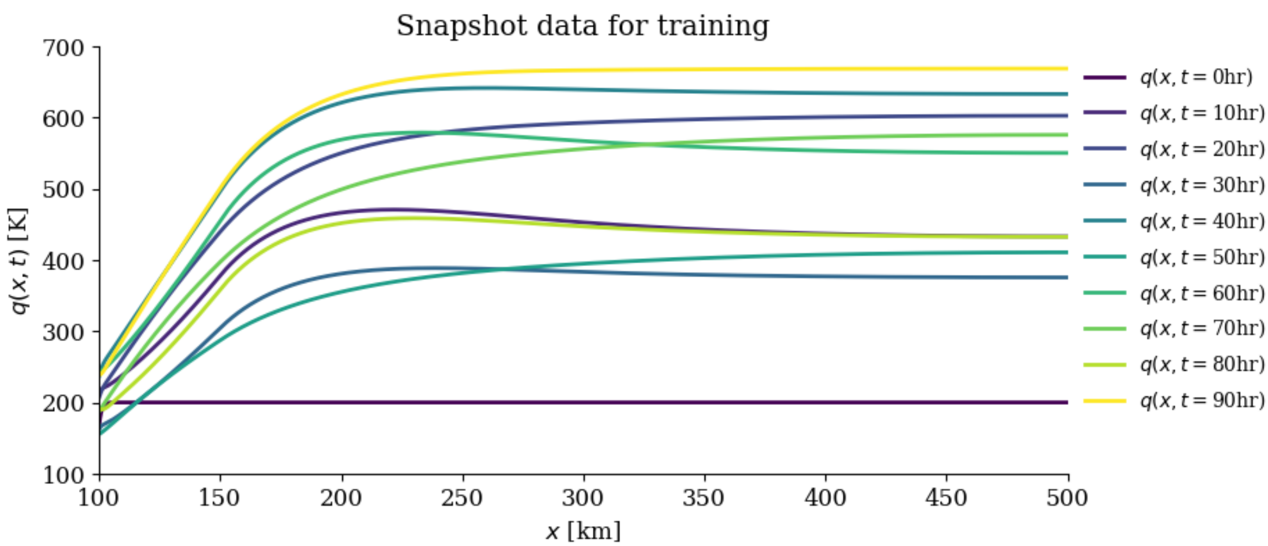
```
Spatial step size δx = 0.04999999999999716 km
```

In [4]:
```
# time in hr
time = np.load("conduction_v6_time.npy")[:-1]
dt = time[1] - time[0]
print(f"Temporal step size δt = {dt} hr")
```

```
Temporal step size δt = 1.0 hr
```

In [5]:
```
# inputs
inputs = np.load("conduction_v6_lower_bc.npy")[:-1]
```

In [6]:
```
colors = plt.cm.viridis(np.linspace(0, 1, 10))
# plot the training data
fig, ax = plt.subplots(figsize=(9, 4))
# plot up to noon
for ii, tt in enumerate(np.arange(0, 100, 10)):
    ax.plot(x, Q_train[:, tt], linewidth=2, label="$q(x, t=$" + str(int(time[tt])) + "hr)", color=colo

# hide axis
ax.spines['right'].set_visible(False)
ax.spines['top'].set_visible(False)

# set axis limits
ax.set_xlim(100, 500)
ax.set_ylim(100, 700)

# axis legends
ax.set_xlabel("$x$ [km]")
ax.set_ylabel("$q(x, t)$ [K]")

# add legend
legend = ax.legend(ncols=1, fancybox=False, shadow=False, fontsize=10,  bbox_to_anchor=(1, 1))
legend.get_frame().set_alpha(0)

# add title
_= ax.set_title("Snapshot data for training")
```



Step 3: ROM construction & learning

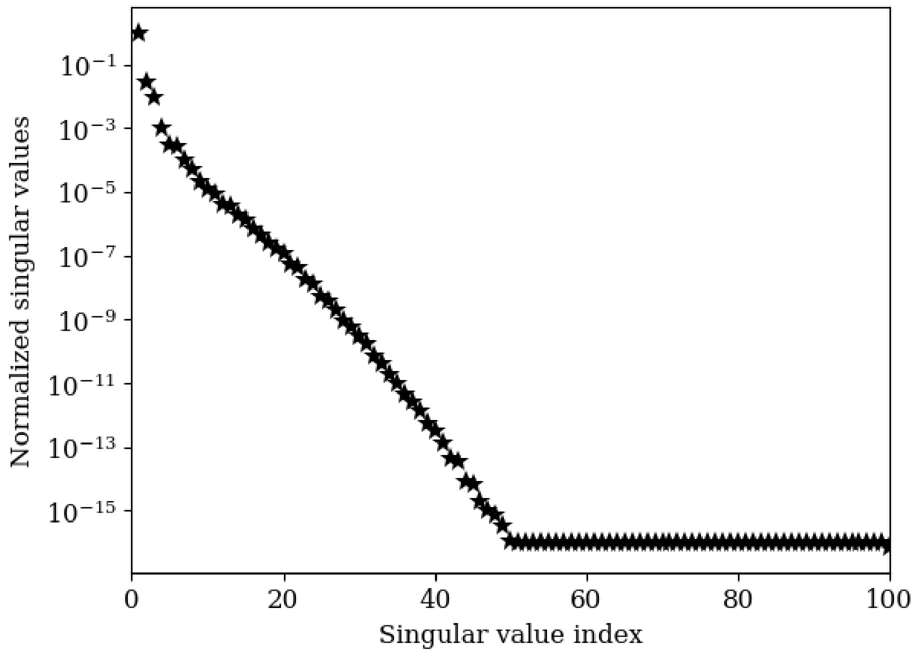
Now that we have our training data $\mathbf{Q} \in \mathbb{R}^{n \times k}$, we can construct a basis matrix $\mathbf{V}_r \in \mathbb{R}^{n \times r}$, where $n = 8001$ in our model and $r \ll n$. The basis matrix relates the high-dimensional state and low-dimensional state by $\mathbf{q}(t) \approx \mathbf{V}_r \widehat{\mathbf{q}}(t)$.

For operator inference, we use the proper orthogonal decomposition (POD) basis. The integer r, which defines the dimension of the reduced-order model to be constructed, is usually determined by how quickly the singular values of $\mathbf{Q}$ decay. In this example, we choose the minimal r such that the residual energy is less than a given tolerance ε, i.e.,

$$\frac{\sum_{j=r+1}^{k} \sigma_j^2}{\sum_{j=1}^{k} \sigma_j^2} < \varepsilon,$$

In [14]:
```
# Compute the POD basis, using the residual energy tolerance to select r.
basis = opinf.pre.PODBasis().fit(Q_train, residual_energy=1e-18)
print(basis)

# Check the decay of the singular values.
_ = basis.plot_svdval_decay()
```

```
PODBasis
Full-order dimension    n = 8001
Reduced-order dimension r = 23
```



In [8]:
```
# based on the cirteria above we set
basis.r = 23
```

In [9]:
```
# approximate the dx/dt using forward euler finite differencing
training_data_ddt = (Q_train[:, 1:] - Q_train[:, :-1])/dt
```

In [24]:
```
# learn reduced model.
rom = opinf.ContinuousOpInfROM("AB")
rom.fit(basis=basis, states=Q_train[:, :-1], ddts=training_data_ddt, regularizer=1, inputs=inputs[1:10
```

Out[24]:
```
<ContinuousOpInfROM object at 0x7fb2a520ee20>
Reduced-order model structure: dq / dt = Aq(t) + Bu(t)
Full-order dimension    n = 8001
Input/control dimension m = 1
Reduced-order dimension r = 23
```

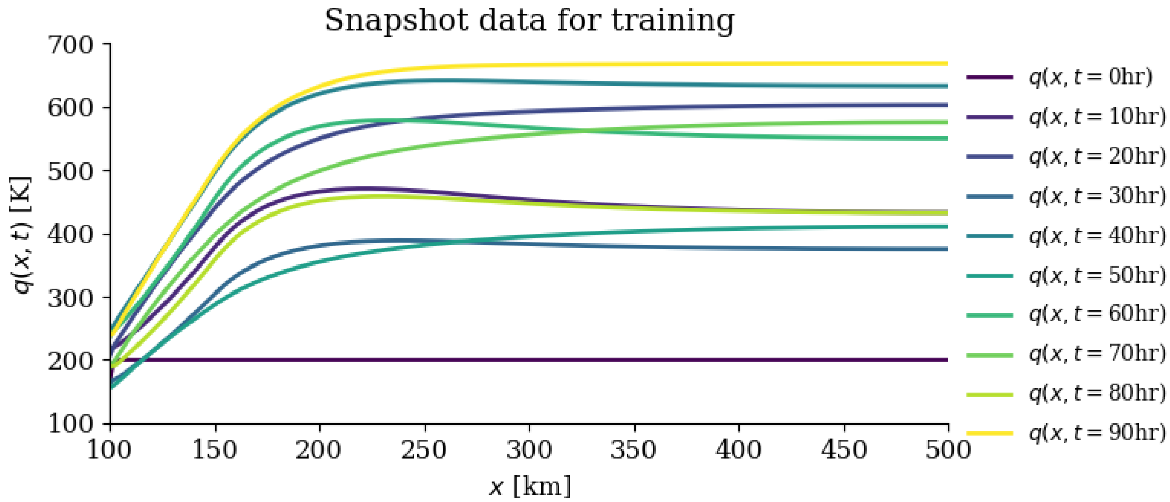
Step 4: ROM evaluation

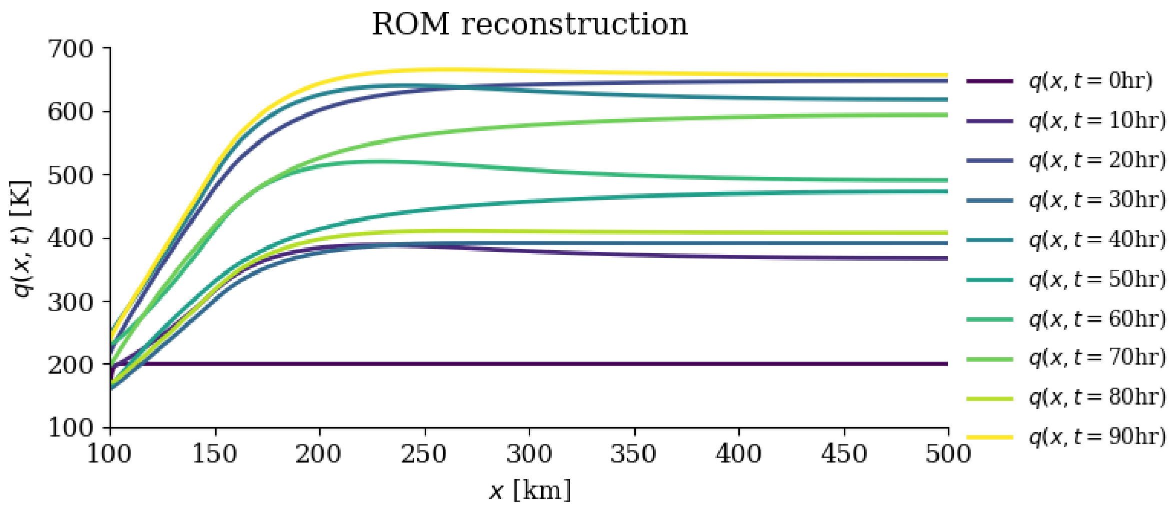
We integrate the learned ROM using the implicit Euler method, using the reduced-order operators $\widehat{\mathbf{A}}$ and the initial condition $\widehat{\mathbf{q}}_0 = \mathbf{V}^\top \mathbf{q}_0$. The resulting low-dimensional state vectors are decoded back to the full-dimensional space via $\mathbf{q}(t) = \mathbf{V}_r \widehat{\mathbf{q}}(t)$.

In [25]:
```
# Express the initial condition in the coordinates of the basis.
q0_ = rom.encode(Q_train[:, 0])

# Solve the reduced-order model using BDF
Q_ROM = rom.predict(state0=q0_, t=time, decode=True, input_func=inputs)
```

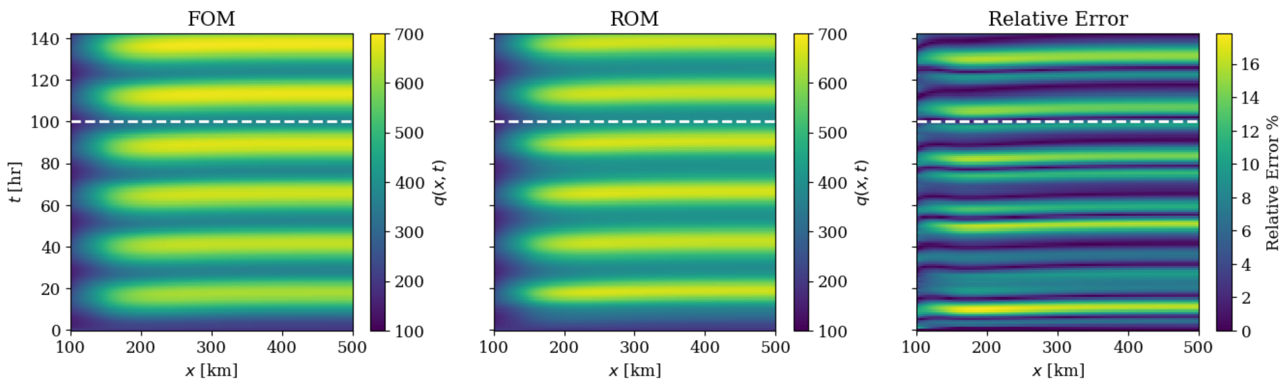
In [26]:

```
# plot the training data
fig, ax = plt.subplots(nrows=2, figsize=(8, 7))
# plot up to noon
for ii, tt in enumerate(np.arange(0, 100, 10)):
    ax[0].plot(x, Q_train[:, tt], linewidth=2, label="$q(x, t=$" + str(tt) + "hr)", color=colors[ii])
    ax[1].plot(x, Q_ROM[:, tt], linewidth=2, label="$q(x, t=$" + str(tt) + "hr)", color=colors[ii])
# hide axis
ax[0].spines['right'].set_visible(False)
ax[0].spines['top'].set_visible(False)
ax[1].spines['right'].set_visible(False)
ax[1].spines['top'].set_visible(False)

# set axis limits
ax[0].set_xlim(100, 500)
ax[1].set_xlim(100, 500)
ax[0].set_ylim(100, 700)
ax[1].set_ylim(100, 700)

# axis legends
ax[0].set_xlabel("$x$ [km]")
ax[0].set_ylabel("$q(x, t)$ [K]")
ax[1].set_xlabel("$x$ [km]")
ax[1].set_ylabel("$q(x, t)$ [K]")

# add legend
legend = ax[0].legend(ncols=1, fancybox=False, shadow=False, fontsize=10,  bbox_to_anchor=(1, 1))
legend.get_frame().set_alpha(0)
legend = ax[1].legend(ncols=1, fancybox=False, shadow=False, fontsize=10,  bbox_to_anchor=(1, 1))
legend.get_frame().set_alpha(0)


# add title
_= ax[0].set_title("Snapshot data for training")
_= ax[1].set_title("ROM reconstruction")
plt.tight_layout()
```


Snapshot data for training
700
600
500
400
300
200
100
$q(x, t)$ [K]
100
150
200
250
300
350
400
450
500
x [km]
$q(x, t = 0\text{hr})$
$q(x, t = 10\text{hr})$
$q(x, t = 20\text{hr})$
$q(x, t = 30\text{hr})$
$q(x, t = 40\text{hr})$
$q(x, t = 50\text{hr})$
$q(x, t = 60\text{hr})$
$q(x, t = 70\text{hr})$
$q(x, t = 80\text{hr})$
$q(x, t = 90\text{hr})$


ROM reconstruction
700
600
500
400
300
200
100
$q(x, t)$ [K]
100
150
200
250
300
350
400
450
500
x [km]
$q(x, t = 0\text{hr})$
$q(x, t = 10\text{hr})$
$q(x, t = 20\text{hr})$
$q(x, t = 30\text{hr})$
$q(x, t = 40\text{hr})$
$q(x, t = 50\text{hr})$
$q(x, t = 60\text{hr})$
$q(x, t = 70\text{hr})$
$q(x, t = 80\text{hr})$
$q(x, t = 90\text{hr})$

In [27]:
```
fig, ax = plt.subplots(ncols=3, sharey=True, figsize=(16, 4))
pos = ax[0].pcolormesh(x, time, data.T, vmin=100, vmax=700)
cbar = fig.colorbar(pos)
cbar.ax.set_ylabel('$q(x, t)$', rotation=90)
pos = ax[1].pcolormesh(x, time, Q_ROM.T, vmin=100, vmax=700)
cbar = fig.colorbar(pos)
cbar.ax.set_ylabel('$q(x, t)$', rotation=90)

pos = ax[2].pcolormesh(x, time, 100*np.abs(data.T - Q_ROM.T)/np.abs(data.T))
cbar = fig.colorbar(pos)
cbar.ax.set_ylabel(r"Relative Error %", rotation=90)

ax[0].axhline(time[100], linewidth=2, color="white", linestyle="--")
ax[1].axhline(time[100], linewidth=2, color="white", linestyle="--")
ax[2].axhline(time[100], linewidth=2, color="white", linestyle="--")
ax[0].set_xlabel("$x$ [km]")
ax[1].set_xlabel("$x$ [km]")
ax[2].set_xlabel("$x$ [km]")
ax[0].set_ylabel("$t$ [hr]")

_ = ax[0].set_title("FOM")
_ = ax[1].set_title("ROM")
_ = ax[2].set_title("Relative Error")
```



In [ ]:

In [ ]:

In [ ]: