# LA-UR-23-24119

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Title: Code Demonstration: Approximation of nearly-periodic symplectic maps

via structure-preserving neural networks

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**Intended for:** Demonstration of our neural network implementation through a notebook

and as a presentation.

**Issued:** 2023-04-20









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# Code Demonstration: Approximation of nearly-periodic symplectic maps via structure-preserving neural networks

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This notebook presents a simplified version of the code used to generate some of the numerical results presented in our paper [Duruisseaux et al., 2022].

The notebook was performed on jupyter.nersc.gov using NERSC's CPU nodes

Acknowledgments. This research was supported by the U.S. Department of Energy (DOE), the Office of Science and the Office of Advanced Scientific Computing Research (ASCR). Specifically, we acknowledge funding support from ASCR for DOE-FOA-2493 "Data-intensive scientific machine learning and analysis". This research used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility located at Lawrence Berkeley National Laboratory, operated under Contract No. DE-AC02-05CH11231 using NERSC award ASCR-ERCAP0020162.

# Introduction

In this notebook, we use the symplectic gyroceptron architecture from [Duruisseaux et al., 2022] to learn a surrogate map for the nearly-periodic symplectic flow map associated to a nearly-periodic Hamiltonian system composed of two nonlinearly coupled oscillators, where one of them oscillates significantly faster than the other:

$$\begin{cases} \dot{q}_1 = p_1 & \dot{p}_1 = -q_1 - \varepsilon \partial_{q_1} U(q_1, q_2) \\ \dot{q}_2 = \varepsilon p_2 & \dot{p}_2 = -\varepsilon q_2 - \varepsilon \partial_{q_2} U(q_1, q_2) \end{cases}$$

These equations of motion are the Hamilton's equations associated to the Hamiltonian

$$H_{\varepsilon}(q_1, q_2, p_1, p_2) = \frac{1}{2}(q_1^2 + p_1^2) + \frac{1}{2}\varepsilon(q_2^2 + p_2^2) + \varepsilon U(q_1, q_2)$$

# 1 Imports

```
import os
import time
import numpy as np
import matplotlib.pyplot as plt
os.environ['TF_CPP_MIN_LOG_LEVEL'] = '2'

import tensorflow as tf
from tensorflow import keras
from tensorflow.keras import Model
from tensorflow.keras import layers
from tensorflow.keras.layers import Dense
tf.keras.backend.set_floatx('float32')
```

### 2 Parameters

### 2.1 Problem Parameters

```
[2]: # Near-periodicity parameter
epsilon = 0.01

# Step size
rk4_step = 0.0005

# Number of steps per iteration
n_steps_per_rk4_eval = 100
```

### 2.2 Symplectic Gyroceptron Parameters

```
[3]: # Number and shape of layers in Henon Network psi
HenonLayersShape = []
for i in range(10):
    HenonLayersShape.append(8)

# Number and shape of layers in Near-Identity Henon Network I_epsilon
NIHenonLayersShape = []
for i in range(8):
    NIHenonLayersShape.append(6)
```

### 2.3 Training Parameters

```
[4]: # Loss Function (Weighhed MSE)
    def custom_loss(y_true, y_pred):
         diff = (y_true - y_pred)**2
         Oscillator1_Loss = epsilon * (tf.math.reduce_sum(diff[:,0]) + tf.math.reduce_sum(diff[:,2]))
         Oscillator2_Loss = tf.math.reduce_sum(diff[:,1]) + tf.math.reduce_sum(diff[:,3])
         return Oscillator1_Loss + Oscillator2_Loss
     # Optimizer
    Optim = keras.optimizers.Adam(learning_rate = 0.1, clipnorm = 0.1)
     # Either train from scratch, or upload weights from previous training
     train = True
    if train:
         initial_epoch = 0
         # Number of data points to learn from
             # In general Window
        n_general_points = 20000
             # In small window near orbits on the right
        n_points_small_right_orbits = 20000
             # In small window near orbits on the left
        n_points_small_left_orbits = 20000
         number\_data\_points = n\_general\_points + n\_points\_small\_right\_orbits + n\_points\_small\_left\_orbits
```

```
# Batch Size
my_batch_size = 512

# Number of epochs
n_epochs = 5600

# Save every how many epochs ?
n_epochs_before_save = n_epochs

# Define scheduler
scheduler = tf.keras.callbacks.ReduceLROnPlateau(monitor='loss', factor=0.8, patience=8, mode='min')

else:
    # Location of saved weights
    SavedWeights = "./TrainingWeights/my_saved_weights.ckpt"
```

### 2.4 Prediction Parameters

```
[5]: # Number of iterations computed in the final predictions
n_pred_steps = 40000

# Number of trajectories to evolve in the final predictions
n_ics = 7

# Initial conditions
q1_ic = 1.5*np.ones((n_ics,1))
p1_ic = np.zeros((n_ics,1))
q2_ic = np.array([0.0, 0.15, 0.3, 0.4, 1.0, 1.45, 1.55]).reshape([n_ics,1])
p2_ic = np.zeros((n_ics,1))

z_ic = np.hstack([q1_ic,q2_ic,p1_ic,p2_ic])
```

### 3 Potential and Vector Field

Here the potential is taken to be

$$U(q_1, q_2) = q_1 q_2 \sin(2q_1 + 2q_2)$$

and the equations of motion are

$$\begin{cases} \dot{q}_1 = p_1 & \dot{p}_1 = -q_1 - \varepsilon \partial_{q_1} U(q_1, q_2) \\ \dot{q}_2 = \varepsilon p_2 & \dot{p}_2 = -\varepsilon q_2 - \varepsilon \partial_{q_2} U(q_1, q_2) \end{cases}$$

```
[6]: # Potential U and its partial derivatives

def Potential(q1,q2):
    return q1*q2*tf.math.sin(2*q1+2*q2)

def dUdq1(q1,q2):
    return q2*tf.math.sin(2*q1+2*q2) + 2*tf.math.cos(2*q1+2*q2)*q1*q2

def dUdq2(q1,q2):
    return q1*tf.math.sin(2*q1+2*q2) + 2*tf.math.cos(2*q1+2*q2)*q1*q2
```

```
# Takes set of z=(q1,p1,q2,p2) points, and returns array of corresponding values of zdot
Outf.function
def zdot(z,epsilon):
    n = z.shape[0]
    q1 = z[:,0]
    q2 = z[:,1]
    p1 = z[:,2]
    p2 = z[:,3]

q1dot = tf.reshape(p1, [n,1])
    q2dot = tf.reshape(epsilon*p2, [n,1])
    p1dot = tf.reshape(-q1-epsilon*dUdq1(q1,q2), [n,1])
    p2dot = tf.reshape(- epsilon*q2 - epsilon*dUdq2(q1,q2) , [n,1])
return tf.concat([q1dot, q2dot, p1dot, p2dot], 1)
```

To simulate the reference trajectories and create the dataset, we use the classical Runge-Kutta 4 method with very small time-steps

```
[7]: # RK4 integration for n_steps
def rk4(z0,time_step,epsilon,n_steps):
    h = time_step
    z = z0
    for i in range(n_steps):
        k1 = zdot(z,epsilon)
        k2 = zdot(z + 0.5*h*k1,epsilon)
        k3 = zdot(z + 0.5*h*k2,epsilon)
        k4 = zdot(z + h * k3,epsilon)
        z = z + (1.0/6.0) * h * (k1 + 2*k2 + 2*k3 + k4)
    return z
```

# 4 Generate Data and Labels for Training

```
[8]: if train:
         # Points in full [-0.9, 1.6]x[-1.1, 1.1] window for oscillator 2
         q1_data1 = -1.6 + 3.2*tf.random.uniform((n_general_points,1), dtype=tf.dtypes.float32)
         q2_data1 = -0.9 + 2.5*tf.random.uniform((n_general_points,1), dtype=tf.dtypes.float32)
         p1_data1 = -1.6 + 3.2*tf.random.uniform((n_general_points,1), dtype=tf.dtypes.float32)
         p2_data1 = -1.1 + 2.2*tf.random.uniform((n_general_points,1), dtype=tf.dtypes.float32)
         # More points for smaller right orbits in [0.6,1.5]x[-0.5,0.5] for oscillator 2
         q1_data2 = -1.6 + 3.2*tf.random.uniform((n_points_small_right_orbits,1), dtype=tf.dtypes.float32)
         q2_data2 = 0.6 + 0.9*tf.random.uniform((n_points_small_right_orbits,1), dtype=tf.dtypes.float32)
         p1_data2 = -1.6 + 3.2*tf.random.uniform((n_points_small_right_orbits,1), dtype=tf.dtypes.float32)
         p2_data2 = -0.5 + 1.0*tf.random.uniform((n_points_small_right_orbits,1), dtype=tf.dtypes.float32)
         # More points for smaller left orbits in [-0.75, 0.75]x[-0.75, 0.75] for oscillator 2
         q1_data3 = -1.6 + 3.2*tf.random.uniform((n_points_small_left_orbits,1), dtype=tf.dtypes.float32)
         p1_data3 = -1.6 + 3.2*tf.random.uniform((n_points_small_left_orbits,1), dtype=tf.dtypes.float32)
         q2_data3 = -0.8 + 1.6*tf.random.uniform((n_points_small_left_orbits,1), dtype=tf.dtypes.float32)
         p2_data3 = -0.8 + 1.6*tf.random.uniform((n_points_small_left_orbits,1), dtype=tf.dtypes.float32)
         # Concatenate all the data
         data = tf.concat([tf.concat([q1_data1, q1_data2, q1_data3], 0),
                           tf.concat([q2_data1, q2_data2, q2_data3], 0),
                           tf.concat([p1_data1, p1_data2, p1_data3], 0),
                           tf.concat([p2_data1, p2_data2, p2_data3], 0)], 1)
         # Evolve the data using RK4 to generate the labels
         labels = rk4(data,rk4_step,epsilon, n_steps_per_rk4_eval)
```

# 5 Neural Network Architecture

## 5.1 Henon map, Henon layer, and HenonNet

We first define the near-identity Henon map

$$H_{\varepsilon}[V,\eta] \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} y+\eta \\ -x+\varepsilon \nabla V(y) \end{pmatrix}$$

which reduces to the regular Henon Map when  $\varepsilon = 1$ .

In our network, we will take

$$V(y) = W_{out}^{\top} \tanh \left( W_{in}^{\top} y + b_{in} \right)$$

for some weight matrices  $W_{in}, W_{out}$  and bias  $b_{in}$ 

```
[9]: def HenonMap(X,Y,W_in,W_out,b_in,eta,epsilon=1):
    with tf.GradientTape() as tape:
        tape.watch(Y)
        V = tf.linalg.matmul(tf.math.tanh(tf.linalg.matmul(Y, W_in) + b_in),W_out)
        X_out= Y + eta
        Y_out= -X + epsilon*tape.gradient(V,Y)
        return X_out, Y_out
```

We then define a Henon layer as the composition of 4 copies of a Henon map

$$L_{\varepsilon}[V,\eta] = H_{\varepsilon}[V,\eta]^4$$

```
[10]: class HenonLayer(layers.Layer):
         def __init__(self,ni,epsilon =1):
             super(HenonLayer, self).__init__()
             self.dim = 2  # half of the dimension of the full space
             self.epsilon = epsilon
              # Initialize weights
              init = tf.initializers.GlorotNormal()
              init_zero = tf.zeros_initializer()
             W_in_init = init(shape=[self.dim,ni], dtype = tf.float32)
             W_out_init = init(shape=[ni,1], dtype = tf.float32)
             b_in_init = init(shape=[1,ni], dtype = tf.float32)
              eta_init = init(shape=[1,self.dim], dtype = tf.float32)
             self.W_in = tf.Variable(W_in_init, dtype = tf.float32)
             self.W_out = tf.Variable(W_out_init, dtype = tf.float32)
             self.b_in = tf.Variable(b_in_init, dtype = tf.float32)
             self.eta = tf.Variable(eta_init, dtype = tf.float32)
          def call(self,z):
             xnext,ynext=HenonMap(z[:,0:self.dim],z[:,self.dim:],
                                   self.W_in,self.W_out,self.b_in,self.eta,self.epsilon)
             xnext,ynext=HenonMap(xnext,ynext,self.W_in,self.W_out,self.b_in,self.eta,self.epsilon)
             xnext,ynext=HenonMap(xnext,ynext,self.W_in,self.W_out,self.b_in,self.eta,self.epsilon)
             xnext,ynext=HenonMap(xnext,ynext,self.W_in,self.W_out,self.b_in,self.eta,self.epsilon)
             return tf.concat([xnext,ynext], axis =1)
```

### 5.2 Inverse Henon Map and Henon Layer

Next we define the inverse of the Henon map

$$H_{\varepsilon}[V,\eta] \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} y+\eta \\ -x+\varepsilon \nabla V(y) \end{pmatrix}$$

which is given by

$$H_{\varepsilon}^{-1}[V,\eta] \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \varepsilon \nabla V(x-\eta) - y \\ x - \eta \end{pmatrix}$$

```
def InverseHenonMap(X,Y,W_in,W_out,b_in,eta,epsilon=1.):
    Y_out = X - eta
    with tf.GradientTape() as tape:
        tape.watch(Y_out)
        V = tf.linalg.matmul(tf.math.tanh(tf.linalg.matmul(Y_out, W_in) + b_in),W_out)

X_out = epsilon*tape.gradient(V,Y_out) - Y
    return X_out, Y_out
```

The inverse Henon layer is then the composition of 4 copies of the inverse Henon map

```
[11]: def InverseHenonLayer(z, original_layer):
    # The original Henon layer is an input

# Get parameter values and weights of the original Henon layer
    epsilon = original_layer.epsilon
    dim = original_layer.dim
    W_in = original_layer.W_in
    W_out = original_layer.W_out
    b_in = original_layer.b_in
    eta = original_layer.eta

# Evaluate the inverse Henon layer Map
    xnext,ynext=InverseHenonMap(z[:,0:dim],z[:,dim:],W_in,W_out,b_in,eta,epsilon)
    xnext,ynext=InverseHenonMap(xnext,ynext,W_in,W_out,b_in,eta,epsilon)
    xnext,ynext=InverseHenonMap(xnext,ynext,W_in,W_out,b_in,eta,epsilon)
    xnext,ynext=InverseHenonMap(xnext,ynext,W_in,W_out,b_in,eta,epsilon)
    return tf.concat([xnext,ynext], axis =1)
```

### 5.3 Circle Action Layer

The circle action is

$$\Phi_{\theta}(q_1, q_2, p_1, p_2) = \begin{pmatrix} \cos \theta & 0 & \sin \theta & 0 \\ 0 & 1 & 0 & 0 \\ -\sin \theta & 0 & \cos \theta & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \\ p_1 \\ p_2 \end{pmatrix}$$

This corresponds to clockwise circular rotation of the the components  $(q_1, p_1)$  in phase space

```
[12]: class CircleActionLayer(layers.Layer):
          def __init__(self):
              super(CircleActionLayer, self).__init__()
              init = tf.initializers.GlorotNormal()
              theta0_init = init(shape=[1,1], dtype = tf.float32)
              self.theta0 = tf.Variable(theta0_init, dtype = tf.float32)
          def call(self,z):
              theta0 = self.theta0
              q1 = z[:,0:1]
              q2 = z[:,1:2]
              p1 = z[:,2:3]
              p2 = z[:,3:]
              # Last columns for p2 values
              r_{out} = p2
              # Add 3rd column for new values of p1
              r_out = tf.concat([tf.cos(theta0)*p1-tf.sin(theta0)*q1, r_out], 1)
              # Add 2nd column for new values of q2
              r_{out} = tf.concat([q2, r_{out}], 1)
              # Add 1st column for new values of q1
              r_out = tf.concat([tf.cos(theta0)*q1+tf.sin(theta0)*p1, r_out], 1)
              return r_out
```

### 5.4 Symplectic Gyroceptron

The symplectic gyroceptron is defined as the composition

$$I_{\varepsilon} \circ \psi \circ \Phi_{\theta} \circ \psi^{-1}$$

where

- $I_{\varepsilon}$  is a neural network capable of learning near-identity symplectic maps
- $\psi$  is a neural network capable of learning symplectic maps
- $\Phi_{\theta}$  is a circle action.

Here we choose  $I_{\varepsilon}$  to be a near-identity Henon network and  $\psi$  to be a Henon network.

These networks are defined as compositions of near-identity Henon layers and Henon layers

```
class SymplecticGyroceptron(Model):

    def __init__(self,NIHenon_unit_list,Henon_unit_list,eps):
        super(SymplecticGyroceptron, self).__init__()

    self.N_Henon = len(Henon_unit_list)
        self.N_NI_Henon = len(NIHenon_unit_list)
        self.psi_layers = []
        self.NI_layers = []
        self.hlayers = []
        self.hlayers = eps
```

```
# Create Circle Action
hl = CircleActionLayer()
self.hlayers.append(hl)
# HenonNet psi
for i in range(self.N_Henon):
    # Get the number of neurons in i-th Henon layer
    ni = Henon_unit_list[i]
    # Create i-th Henon layer
    hl = HenonLayer(ni,epsilon=1.0)
    # Add i-th Henon layer
    self.psi_layers.append(hl)
    self.hlayers.append(hl)
# Near_Identity_Henon_Net
for i in range(self.N_NI_Henon):
    # Get the number of neurons in i-th Henon layer
    ni = NIHenon_unit_list[i]
    # Create and add the i-th Henon layer
    hl = HenonLayer(ni,epsilon=self.epsilon)
    self.hlayers.append(hl)
    self.NI_layers.append(hl)
```

```
@tf.function
def call(self, r):
    # Evaluate the HenonNet by passing the input r through each layer
    r_out = r

# First pass through psi inverse
NumberPsiLayers = self.psi_layers.__len__()
for i in range(NumberPsiLayers):
    r_out = InverseHenonLayer(r_out, self.psi_layers[NumberPsiLayers-i-1])

# Then pass through the other layers
NumberLayers = self.hlayers.__len__()
for i in range(NumberLayers):
    r_out = self.hlayers[i](r_out)
return r_out
```

### 6 Build and Train Model

### 6.1 Define Model

```
[14]: # Build model
SG = SymplecticGyroceptron(NIHenonLayersShape, HenonLayersShape, epsilon)

# Upload weights
if train == False:
    SG.load_weights(SavedWeights)

# Compile model
SG.compile(optimizer = Optim, loss = custom_loss)
```

```
[14]: # Evaluate Model Briefly to make sure it works and print its summary

SG.evaluate(tf.random.normal([10,4]),tf.random.normal([10,4]), batch_size=5)

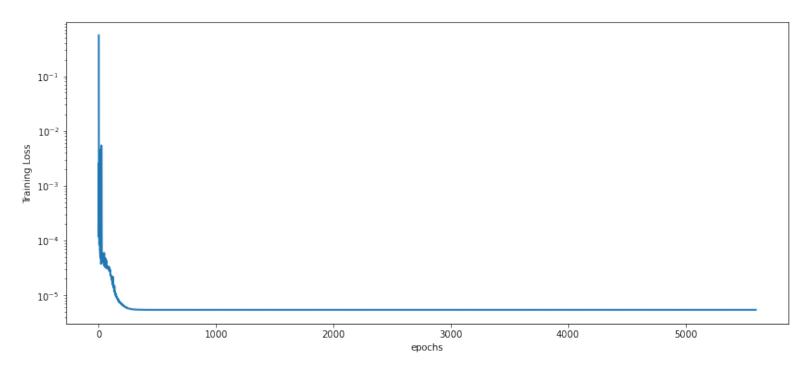
SG.summary()
```

2/2 [===================================				
Layer (type)	Output Shape	Param #		
henon_layer (HenonLayer)	multiple	34		
henon_layer_1 (HenonLayer)	multiple	34		
henon_layer_2 (HenonLayer)	multiple	34		
henon_layer_3 (HenonLayer)	multiple	34		
henon_layer_4 (HenonLayer)	multiple	34		
henon_layer_5 (HenonLayer)	multiple	34		
henon_layer_6 (HenonLayer)	multiple	34		
henon_layer_7 (HenonLayer)	multiple	34		
henon_layer_8 (HenonLayer)	multiple	34		
henon_layer_9 (HenonLayer)	multiple	34		

henon_layer_10 (	(HenonLayer)	multiple	26
henon_layer_11 (	(HenonLayer)	multiple	26
henon_layer_12 (	(HenonLayer)	multiple	26
henon_layer_13 (	(HenonLayer)	multiple	26
henon_layer_14 (	(HenonLayer)	multiple	26
henon_layer_15 (	(HenonLayer)	multiple	26
henon_layer_16 (	(HenonLayer)	multiple	26
henon_layer_17	(HenonLayer)	multiple	26
circle_action_la	ayer (CircleA	multiple	1
Total params: 54 Trainable params Non-trainable pa	s: 549		

### 6.2 Train Model

```
[15]: if train:
          # Callback to Save Weights
          checkpoint_path = "./TrainingWeights/epoch_{epoch:05d}.ckpt"
          saving_frequency = n_epochs_before_save*(int(number_data_points/my_batch_size)+1)
          callback_SaveWeights = tf.keras.callbacks.ModelCheckpoint(filepath=checkpoint_path,
                                                                    save_weights_only=True,
                                                                    save_freq=saving_frequency,
                                                                     verbose=0)
          # Training
         h = SG.fit(data, labels, batch_size=my_batch_size,
                     epochs=n_epochs, initial_epoch=initial_epoch,
                     callbacks=[scheduler, callback_SaveWeights],
                     verbose=1)
          plt.subplots(figsize=(14,6))
         plt.semilogy(h.history['loss'], linewidth=2)
         plt.xlabel("epochs")
         plt.ylabel("Training Loss")
```



# 7 Prediction

# 7.1 Symplectic Gyroceptron Prediction

```
[16]: # Initialize model
NN_state_model = tf.convert_to_tensor(z_ic, dtype = tf.float32)

# Initialize arrays collecting predictions
NN_model = np.zeros([n_ics,4,n_pred_steps+1])

start = time.time()
for i in range(n_pred_steps+1):
    # Collect Results
    NN_model[:,:, i] = NN_state_model.numpy()[:,:]
    # Evolve solutions
    NN_state_model = SG(NN_state_model)
end = time.time()

print('Symplectic Gyroceptron Prediction took {} seconds'.format(end-start))
```

Symplectic Gyroceptron Prediction took 48.89636421203613 seconds

# 7.2 RK4 Reference Prediction

```
[17]: # Initialize Model state and RK state
    rk_state_model = tf.convert_to_tensor(z_ic, dtype = tf.float32)
    # Initialize arrays collecting predictions
    rk_model = np.zeros([n_ics,4,n_pred_steps+1])

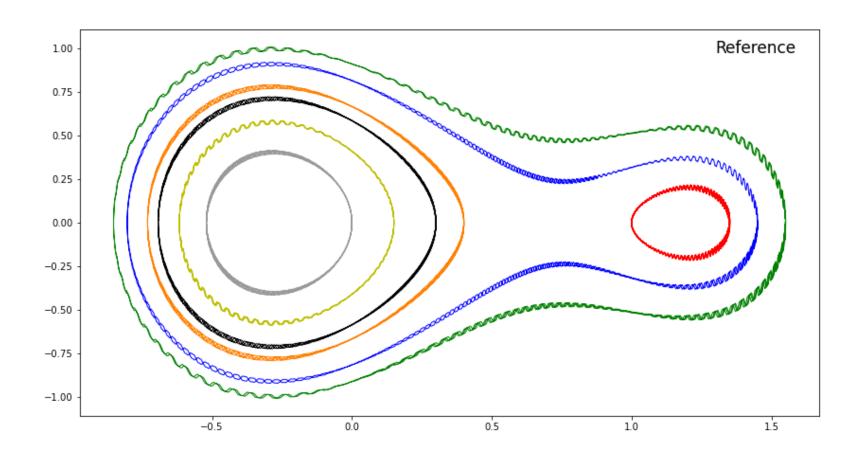
start = time.time()
    # Evolve the systems
for i in range(n_pred_steps+1):
        # Collect Results
        rk_model[:,:, i] = rk_state_model.numpy()[:,:]
        # Evolve solutions
        rk_state_model = rk4(rk_state_model,rk4_step,epsilon, n_steps_per_rk4_eval)
end = time.time()

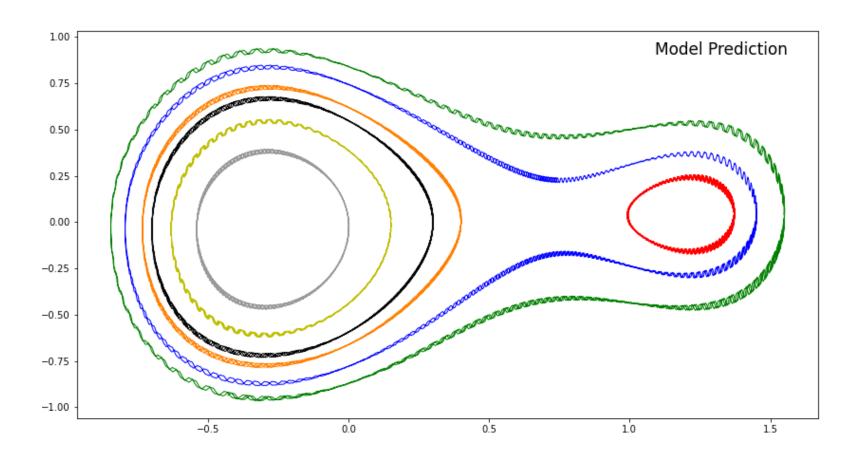
print('RK4 Prediction took {} seconds'.format(end-start))
```

RK4 Prediction took 2616.064284801483 seconds

### 7.3 Plotting Predictions

```
[18]: # RK4 Reference Plot for Oscillator 2
     fig3, ax3 = plt.subplots(figsize=(14,7.5))
     line3,=ax3.plot(rk_model[4,1,:],rk_model[4,3,:],'r',linewidth = 1)
     line3,=ax3.plot(rk_model[3,1,:],rk_model[3,3,:],color =[1, 0.5, 0],linewidth = 1)
     line3,=ax3.plot(rk_model[2,1,:],rk_model[2,3,:],'k',linewidth = 1)
     line3,=ax3.plot(rk_model[1,1,:],rk_model[1,3,:], 'v', linewidth = 1)
     line3,=ax3.plot(rk_model[0,1,:],rk_model[0,3,:],color=[0.6, 0.6, 0.6],linewidth = 1)
     line3,=ax3.plot(rk_model[5,1,:],rk_model[5,3,:],'b',linewidth = 1)
     line3,=ax3.plot(rk_model[6,1,:],rk_model[6,3,:],'g',linewidth = 1)
     textstr = "Reference"
     ax3.text(0.86,0.94,textstr,transform=ax3.transAxes,fontsize = 17)
     Filename = "Reference.png"
     plt.savefig(Filename, bbox_inches = 'tight', dpi = 500)
      # Symplectic Gyroceptron Plot for Oscillator 2
     fig4, ax4 = plt.subplots(figsize=(14,7.5))
     line4,=ax4.plot(NN_model[4,1,:],NN_model[4,3,:],'r',linewidth = 1)
     line4,=ax4.plot(NN_model[3,1,:],NN_model[3,3,:],color = [1, 0.5, 0],linewidth = 1)
     line4,=ax4.plot(NN_model[2,1,:],NN_model[2,3,:],'k',linewidth = 1)
     line4,=ax4.plot(NN_model[1,1,:],NN_model[1,3,:], 'y', linewidth = 1)
     line4,=ax4.plot(NN_model[0,1,:],NN_model[0,3,:],color=[0.6, 0.6, 0.6],linewidth = 1)
     line4,=ax4.plot(NN_model[5,1,:],NN_model[5,3,:],'b',linewidth = 1)
     line4,=ax4.plot(NN_model[6,1,:],NN_model[6,3,:],'g',linewidth = 1)
     textstr = "Model Prediction"
     ax4.text(0.78,0.94,textstr,transform=ax4.transAxes,fontsize = 17)
     Filename = "Model_Prediction.png"
     plt.savefig(Filename, bbox_inches = 'tight', dpi = 500)
```





# References

[Duruisseaux et al., 2022] Duruisseaux, V., Burby, J. W., and Tang, Q. (2022). Approximation of nearly-periodic symplectic maps via structure-preserving neural networks.