In [1]:
```
import os
import pathlib
import time
import re
import pickle
import numpy as np
import pandas as pd
import matplotlib
import matplotlib.pyplot as plt
import seaborn as sns
import tensorflow as tf
from tensorflow import keras
from tensorflow.keras import layers
print(tf.__version__)

# plotting style options
font = {'size': 18}
matplotlib.rc('font', **font)
sns.set_theme()
sns.set(font_scale = 1.2)
%matplotlib inline
```

```
2.7.0
```

Contents

The notebook is structured as follows:

1. Introduction

1.1. Problem statement

- Two opposing robots, R1 and R2, apply pressure onto a metal sheet to deform it.
- Each robot can move in x, y, z, and (roll, pitch, yaw) a, b, c.
- R1 (the "forming robot") pushes into the sheet (z) while moving along a path in x/y-plane, parallel to the sheet metal surface.
- R2 (the opposing "support robot") pushes into the sheet from the other side.
- Both robots experience forces at the tool-tip in x, y, and z directions.
- Positions, angles, and tool-tip forces are captured for each robot.

Deliverables:

- Develop a model to predict forces experienced by tool-tips for any path traveled by the robot arms
- Provide a Jupyter notebook that includes all the steps

1.2. Proposed solution

The problem is to find a function G to predict tool-tip forces from position coordinates:

$$\vec{f} = G(x, y, z, a, b, c)$$

Models like these could be solved using a parametrized dynamical model with Lagrange or Newton-Euler methods assuming rigid body motion. However, instead of doing that, I'm going to **approximate G with a neural network**.

Here are a few sources I looked at for inspiration:

- http://www.scholarpedia.org/article/Robot_dynamics
- https://ethz.ch/content/dam/ethz/special-interest/mavt/robotics-n-intelligent-systems/rsl-dam/documents/RobotDynamics2016/6-dynamics.pdf
- https://towardsdatascience.com/approximating-dynamic-models-of-industrial-robots-with-neural-networks-2474d1a2eecd
- https://www.nature.com/articles/s41598-021-97003-1.pdf

- https://www.tensorflow.org/tutorials/keras/regression
- https://www.tensorflow.org/guide/keras/rnn

2. Exploration of the dataset

Before training a model, it is always good to look at the data. Let's have a look at time series plots, histograms, and correlations.

Import the datasets into pd.DataFrame

In [2]:
```
workdir = pathlib.Path("./")


# create a timestamp for tagging saved models
timestamp = time.strftime("%Y%m%d_%H%M")

# output directory for saved models, plots, etc.
output_dir = workdir / 'olsson_solution_{}'.format(timestamp)
output_dir.mkdir(parents=True, exist_ok=True)

dataset_filenames = ["Test1", "Test2", "Test4"]

# list of dataframes
datasets = list()
print("loading datasets:")
for filename in dataset_filenames:
    print("-", workdir / str(filename+'.csv'))
    datasets.append(pd.read_csv(workdir / str(filename+'.csv')))
```

```
loading datasets:
- Test1.csv
- Test2.csv
- Test4.csv
```

Look at a summary of what's in the dataframe

In [3]:
```
print("First five entries: \n", datasets[0].head(5).T)
```

```
First five entries:
                      0             1             2             3             4
t         1.636580e+09  1.636580e+09  1.636580e+09  1.636580e+09  1.636580e+09
a_enc_1  -4.951100e+00 -4.951100e+00 -4.951100e+00 -4.951100e+00 -4.951100e+00
b_enc_1   1.830000e-02  1.830000e-02  1.830000e-02  1.830000e-02  1.830000e-02
c_enc_1  -7.190000e-02 -7.190000e-02 -7.190000e-02 -7.190000e-02 -7.190000e-02
x_enc_1   2.136337e+02  2.136337e+02  2.136337e+02  2.136337e+02  2.136337e+02
y_enc_1   3.241015e+02  3.241015e+02  3.241015e+02  3.241015e+02  3.241015e+02
z_enc_1   8.953528e+02  8.953528e+02  8.953528e+02  8.953528e+02  8.953528e+02
a_enc_2  -1.549772e+02 -1.549772e+02 -1.549772e+02 -1.549772e+02 -1.549772e+02
b_enc_2   2.023000e-01  2.024000e-01  2.024000e-01  2.024000e-01  2.024000e-01
c_enc_2  -1.798798e+02 -1.798798e+02 -1.798798e+02 -1.798798e+02 -1.798798e+02
x_enc_2   2.232210e+01  2.232040e+01  2.232040e+01  2.232040e+01  2.232040e+01
y_enc_2   7.831761e+02  7.831754e+02  7.831754e+02  7.831754e+02  7.831754e+02
z_enc_2  -7.725771e+02 -7.725771e+02 -7.725771e+02 -7.725771e+02 -7.725771e+02
fx_1     -2.326357e+00 -2.192611e+00 -2.103594e+00 -1.869649e+00 -2.336206e+00
fy_1      9.639795e+00  9.531656e+00  9.776526e+00  9.100982e+00  9.058406e+00
fz_1     -3.264595e+01 -3.307391e+01 -3.143578e+01 -3.171914e+01 -3.232948e+01
```

```
fx_2     1.180561e+01  1.169716e+01  1.166217e+01  1.141468e+01  1.122329e+01
fy_2     1.865609e+01  1.846252e+01  1.860119e+01  1.848982e+01  1.795298e+01
fz_2    -1.283101e+01 -1.225022e+01 -1.145559e+01 -1.253816e+01 -1.042543e+01
```

In [4]:
```
print("\ndescribe():\n", datasets[0].describe().T[['count', 'mean', 'std', 'min'
```

```
describe():
            count          mean          std           min           max
t         20091.0  1.636590e+09  5800.523780  1.636580e+09  1.636600e+09
a_enc_1   20091.0 -8.924334e+01     7.811876 -9.001034e+01 -4.951004e+00
b_enc_1   20091.0  8.760533e-04     0.002961 -1.604445e-02  2.338158e-02
c_enc_1   20091.0  1.884124e-03     0.007390 -7.199558e-02  2.159353e-02
x_enc_1   20091.0  4.578387e+02   197.669145  8.937531e+01  8.306894e+02
y_enc_1   20091.0  1.965825e+02   103.805836 -1.773652e+00  3.672685e+02
z_enc_1   20091.0 -6.500421e+01   100.980291 -1.767849e+02  8.953528e+02
a_enc_2   20091.0  8.804365e+01    22.349876 -1.783886e+02  1.789519e+02
b_enc_2   20091.0  1.449096e-03     0.029150 -2.199676e+00  1.164570e+00
c_enc_2   20091.0 -4.858466e+01   173.319815 -1.800000e+02  1.800000e+02
x_enc_2   20091.0  4.560382e+02   202.637762  2.231891e+01  8.318730e+02
y_enc_2   20091.0  1.995663e+02   120.025141 -3.800164e+00  7.831773e+02
z_enc_2   20091.0 -7.605120e+01    81.255998 -7.725771e+02 -6.817898e-01
fx_1      20091.0  3.084250e+01   681.262919 -1.919500e+03  1.876367e+03
fy_1      20091.0  9.071373e+01  1192.944410 -1.841587e+03  2.238735e+03
fz_1      20091.0  2.518588e+03   582.206105 -7.799607e+01  3.374799e+03
fx_2      20091.0 -2.917874e+01   441.132354 -1.488688e+03  1.233724e+03
fy_2      20091.0 -1.031784e+02   729.100519 -1.584797e+03  1.303751e+03
fz_2      20091.0 -7.406174e+02   302.882751 -2.315789e+03 -5.323892e+00
```

Make separate lists of input features (position coordinates and euler angles) and outputs (forces)

In [5]:
```
#features = [k for k in datasets[0].keys() if not re.search('^f', k) and 't' not
#outputs = [k for k in datasets[0].keys() if re.search('^f', k)]

features_1 = [i+'_enc_1' for i in 'xyzabc']
features_2 = [i+'_enc_2' for i in 'xyzabc']
outputs_1 = ['fx_1', 'fy_1', 'fz_1']
outputs_2 = ['fx_2', 'fy_2', 'fz_2']
features = features_1 + features_2
outputs = outputs_1 + outputs_2

print('features:', features)
print('outputs:', outputs)
```

```
features: ['x_enc_1', 'y_enc_1', 'z_enc_1', 'a_enc_1', 'b_enc_1', 'c_enc_1', 'x_
enc_2', 'y_enc_2', 'z_enc_2', 'a_enc_2', 'b_enc_2', 'c_enc_2']
outputs: ['fx_1', 'fy_1', 'fz_1', 'fx_2', 'fy_2', 'fz_2']
```

2.1. Correlations

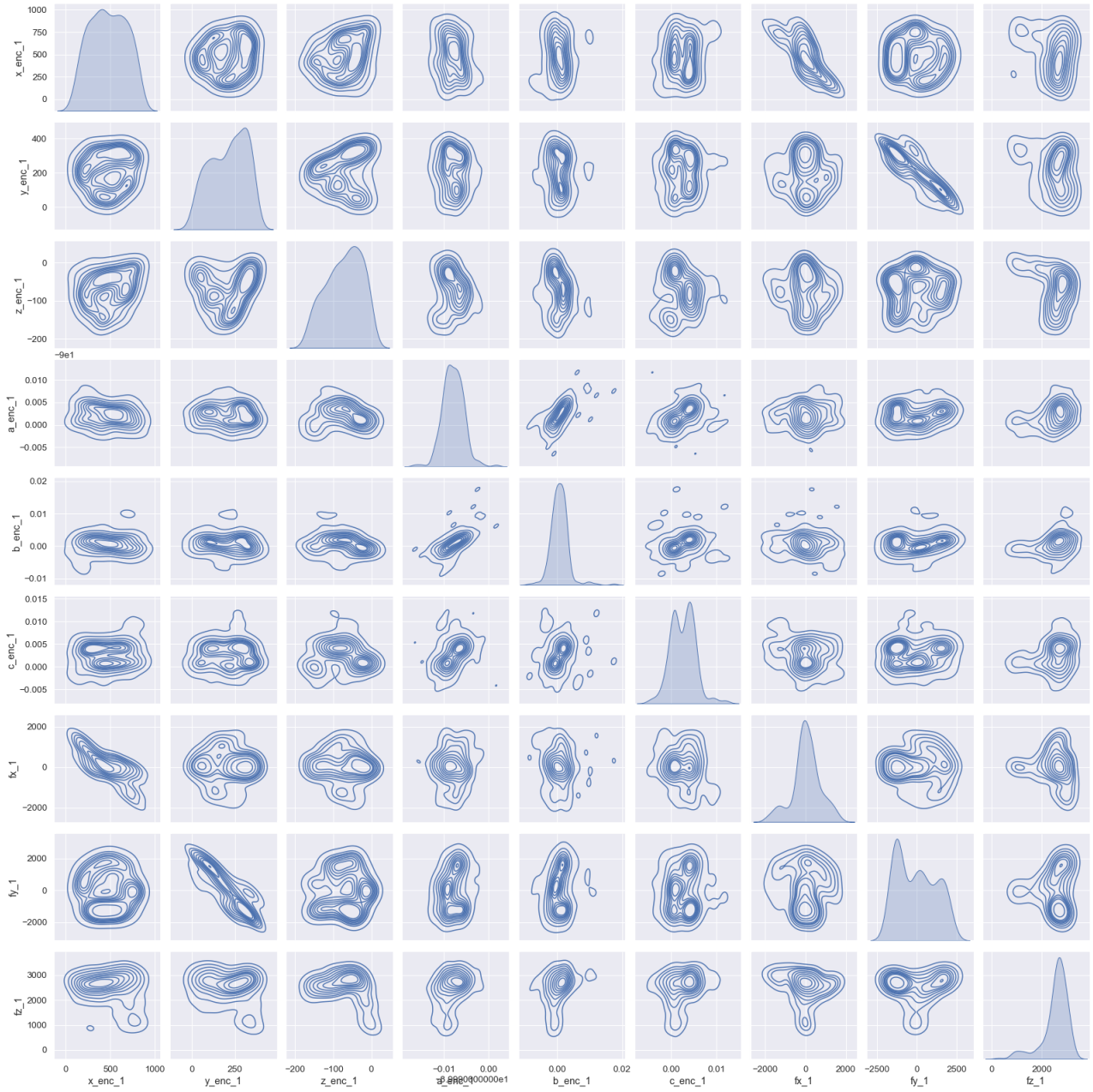
First look at correlations for R1 and R2 separately, for simplicity

seaborn.pairplot can be helpful to get an idea of correlations

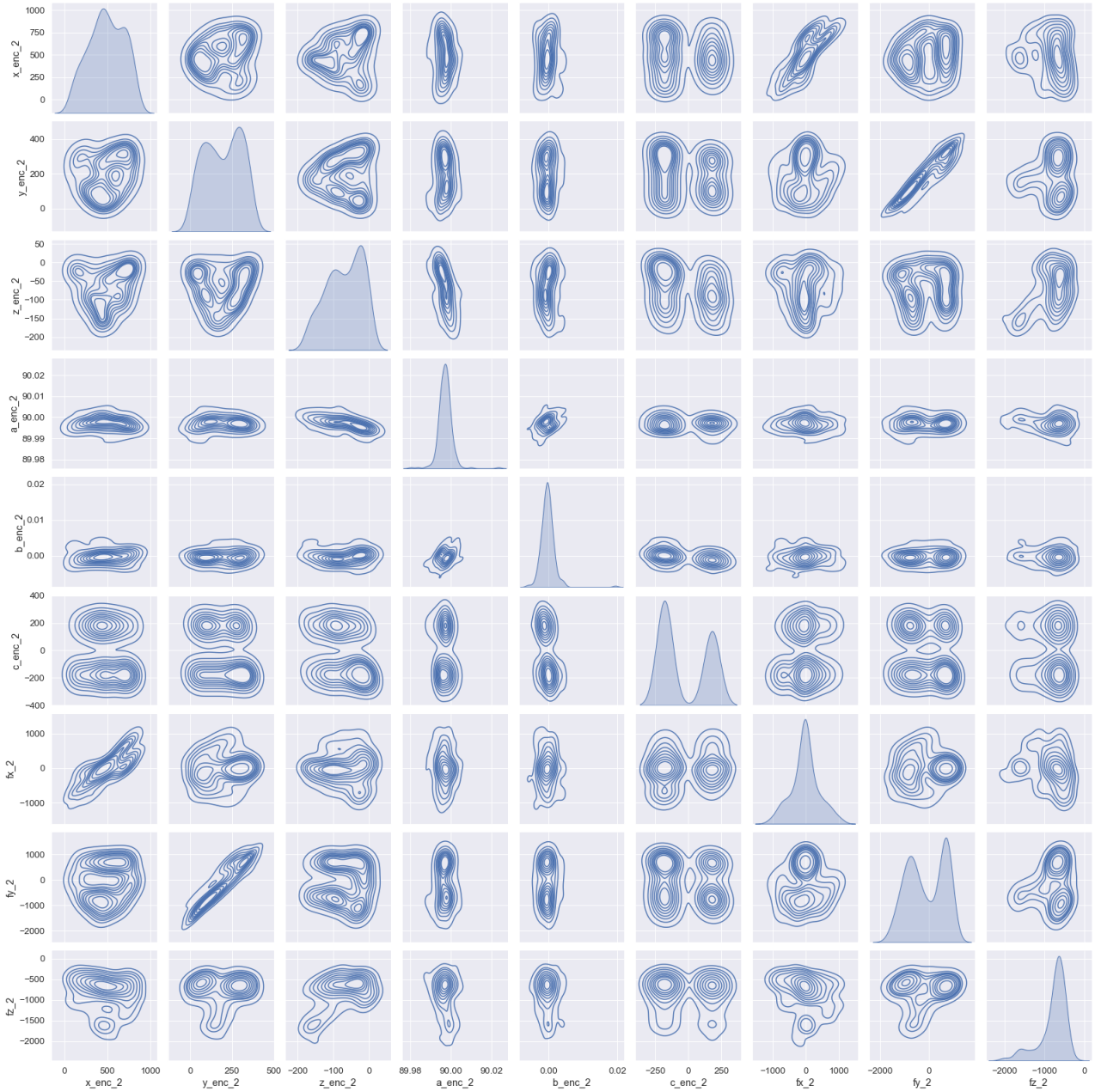
In [6]:
```
# pair plots (slow...)
labels = [features_1+outputs_1, features_2+outputs_2]
for robot_idx in range(2):
    fig = plt.figure(figsize=(20, 20))
```

```
    sns.pairplot(datasets[0].sample(200)[labels[robot_idx]], kind='kde')
    plt.savefig(output_dir/'pairplot_robot{}.pdf'.format(robot_idx+1))
```

```
<Figure size 1440x1440 with 0 Axes>
```



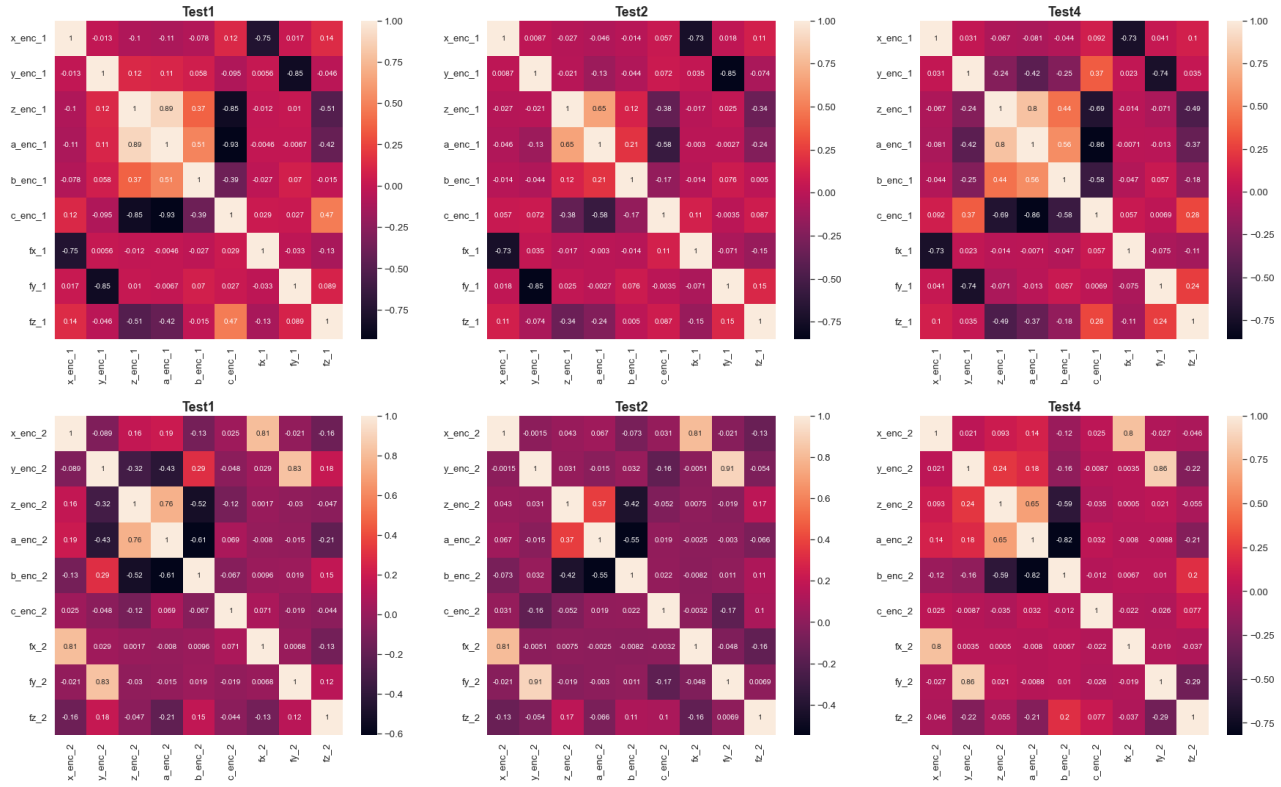

```
<Figure size 1440x1440 with 0 Axes>
```



Plot correlation matrices

In [7]:

```
sns.set_style("whitegrid")
labels = [features_1+outputs_1, features_2+outputs_2]
for robot_idx in range(2):
    fig = plt.figure(figsize=(10*len(datasets), 8))
    for i,df in enumerate(datasets):
        corr = df[labels[robot_idx]].corr()
        ax = fig.add_subplot(1, len(datasets), i+1)
        ax.set_title(dataset_filenames[i], weight='bold').set_fontsize('18')
        sns.heatmap(corr, annot=True)
    plt.savefig(output_dir/'corr_robot{}.pdf'.format(robot_idx+1))
```



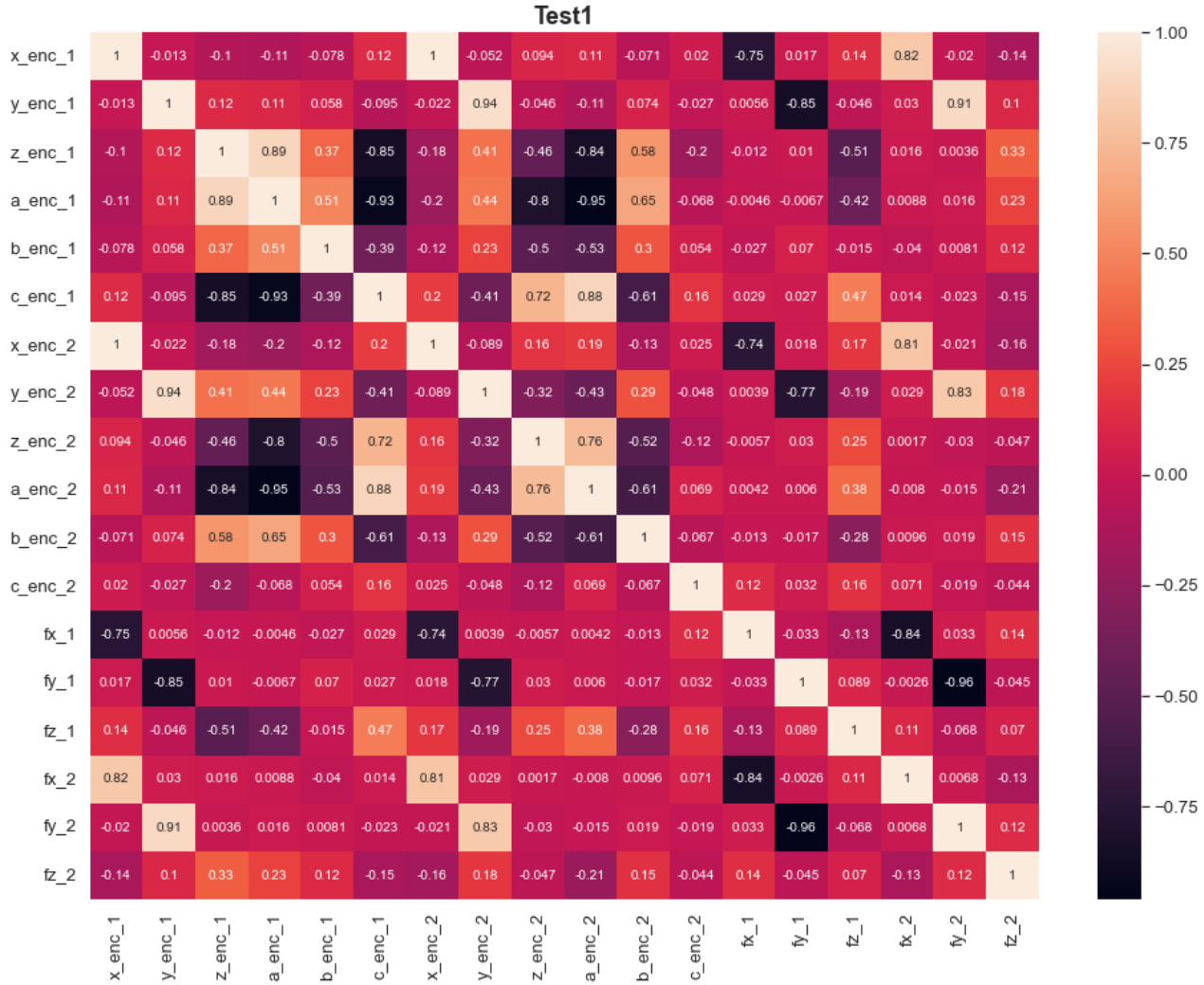
Observations:

- Forces f_x and f_y are strongly correlated with positions x and y respectively and relatively weakly related to anything else.
- f_z is mainly correlated to z, but also quite strongly correlated with a (roll) and c (yaw), especially for R1.

Now let's look at correlations between R1 and R2

In [8]:

```
dataset_idx = 0 # Test1
labels = features_1+features_2+outputs_1+outputs_2
fig = plt.figure(figsize=(16, 12))
corr = datasets[dataset_idx][labels].corr()
ax = fig.add_subplot(111)
ax.set_title(dataset_filenames[dataset_idx], weight='bold').set_fontsize('18')
sns.set_style("whitegrid")
sns.heatmap(corr, annot=True)
plt.savefig(output_dir/'corr_{}_both_robots.pdf'.format(dataset_filenames[datase
```



Observations:

- Strong correlations between x_1, x_2, f_{x_1}, and f_{x_2} and between y_1, y_2, f_{y_1}, and f_{y_2} which seems reasonable given the motion of the two robots.
- Relatively weak correlation between f_{z_1} and f_{z_2}. Forces in z have quite strong correlation to a, b, and c.

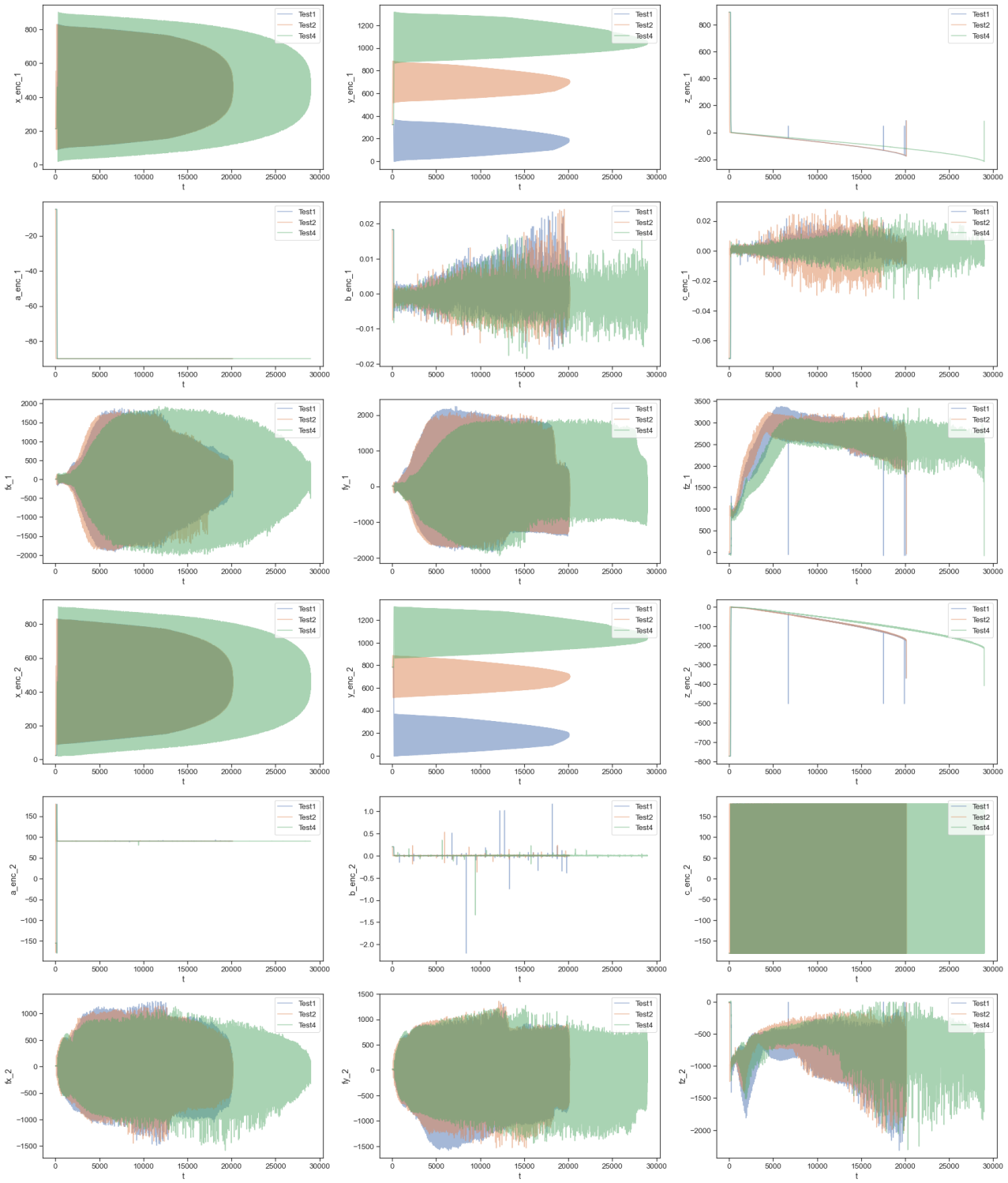
2.2. Time series plots

Plot varables in dataset to see what things look like

In [9]:

```
sns.set_style("ticks")
variables_to_plot = [i+'_enc' for i in 'xyzabc'] + ['fx', 'fy', 'fz']
for robot_idx in range(2):
    fig = plt.figure(figsize=(30,18))
    for i,k in enumerate(variables_to_plot):
        k += '_{}'.format(robot_idx+1)
        ax = fig.add_subplot(3,3, i+1)
        for j in range(len(datasets)):
            # shift 't' to start at 0 for each dataset
            ax.plot(datasets[j]['t']-min(datasets[j]['t']), datasets[j][k], labe
        ax.set_xlabel('t', y=0.5)
        ax.set_ylabel(k, y=0.5)
```

```
        ax.legend(loc=1)
    fig.savefig(output_dir/'1d_variables_vs_time_robot{}.pdf'.format(robot_idx+1
```

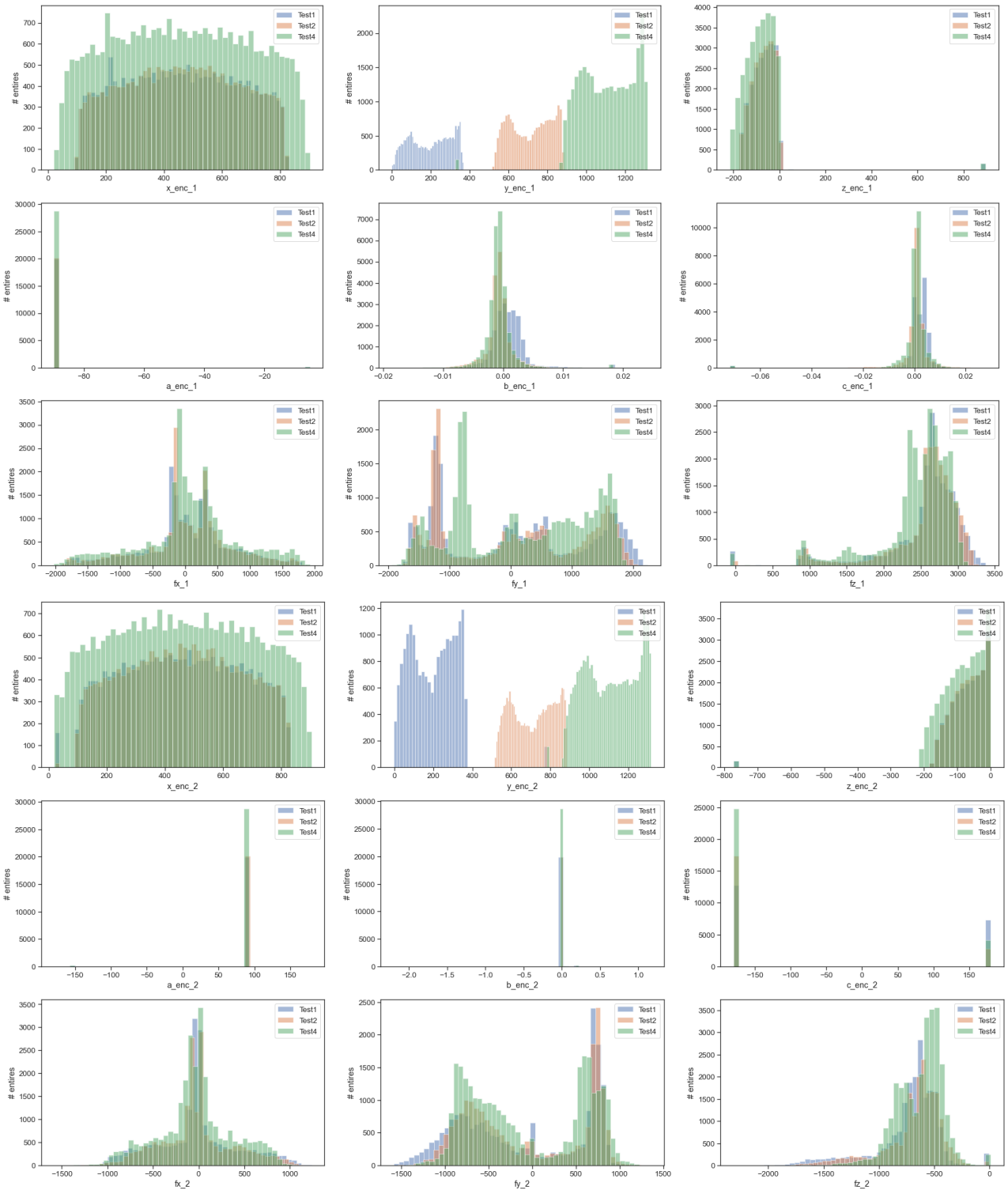


2.3. Histograms

Make histograms of varables in dataset

In [10]:
```
sns.set_style("ticks")
variables_to_plot = [i+'_enc' for i in 'xyzabc'] + ['fx', 'fy', 'fz']
for robot_idx in range(2):
    fig = plt.figure(figsize=(30,18))
```

```
    for i,k in enumerate(variables_to_plot):
        k += '_{}'.format(robot_idx+1)
        ax = fig.add_subplot(3,3, i+1)
        for j in range(len(datasets)):
            ax.hist(datasets[j][k], label=dataset_filenames[j], bins=50, alpha=0
        ax.set_xlabel(k, y=0.5)
        ax.set_ylabel('# entires', y=0.5)
        ax.legend(loc=1)
    fig.savefig(output_dir/'1d_hists_robot{}.pdf'.format(robot_idx+1))
```



3. Pre-processing

3.1. Addition of higher-order derivatives of input features

I noticed that the models could more accurately predict forces from motion in datasets not seen during training when adding higher-order derivatives of the position coordinates as input features.

First (velocity) and second (acceleration) order derivatives had a notable effect on the performance (more about that in section 4). I also tried to include up to 6th order derivatives (3rd=jerk, 4th=snap, 5th=crackle, 6th=pop) [1]. These had a smaller impact but did help in some cases.

[1] https://en.wikipedia.org/wiki/Fourth,_fifth,_and_sixth_derivatives_of_position

In [11]:
```
# differentiate variables in dataframe
def add_gradients(df, keys_to_diff, nth_order=1):
    for k in keys_to_diff:
        df['d'+str(nth_order)+'_'+re.sub('d\d_','', k)] = np.gradient(df[k])
```

In [12]:
```
# add derivatives of position and euler angles:
# 1=velocity, 2=acceleration, 3=jerk, 4=snap, 5=crackle, 6=pop
nth_order = 6
features_to_diff = features
for n in range(1, nth_order+1):
    for df in datasets:
        add_gradients(df, features_to_diff, n)
    features_to_diff = [k for k in datasets[0].keys() if re.search('^d{:d}'.form
```

Create feature lists

In [13]:
```
# x-axis only
features_x1 = ['x_enc_1'] + ["d{:d}_x_enc_1".format(i) for i in range(1,7)]
features_x2 = ['x_enc_2'] + ["d{:d}_x_enc_2".format(i) for i in range(1,7)]
outputs_x1 = ['fx_1']
outputs_x2 = ['fx_2']
```

In [14]:
```
def generate_feature_list(arm_idx, nth_order=6):
    features = []
    for i in 'xyzabc':
        features.append('{}_enc_{}'.format(i, arm_idx))
    for i in 'xyzabc':
        for j in range(1,nth_order+1):
            features.append('d{}_{}_enc_{}'.format(j, i, arm_idx))
    return features
```

In [15]:
```
# up to 6th order derivatives (velocity, acceleration, jerk, snap, crackle, pop)
features_1_nth = generate_feature_list(1, nth_order)
features_2_nth = generate_feature_list(2, nth_order)

# up to 2nd order derivatives (velocity, acceleration)
features_1_2nd = generate_feature_list(1, 2)
```

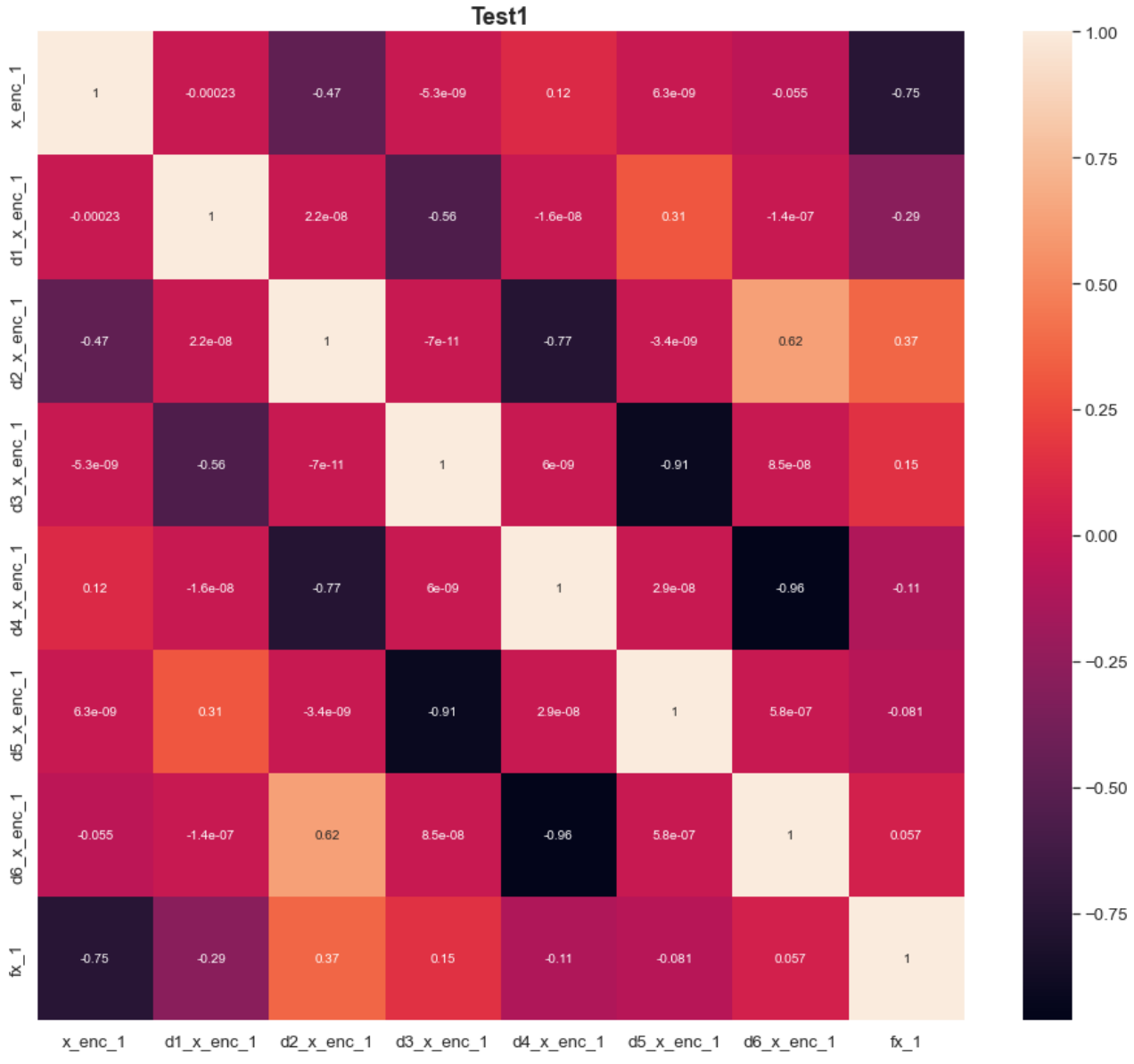
```
features_2_2nd = generate_feature_list(2, 2)

outputs_1 = ['fx_1', 'fy_1', 'fz_1']
outputs_2 = ['fx_2', 'fy_2', 'fz_2']
```

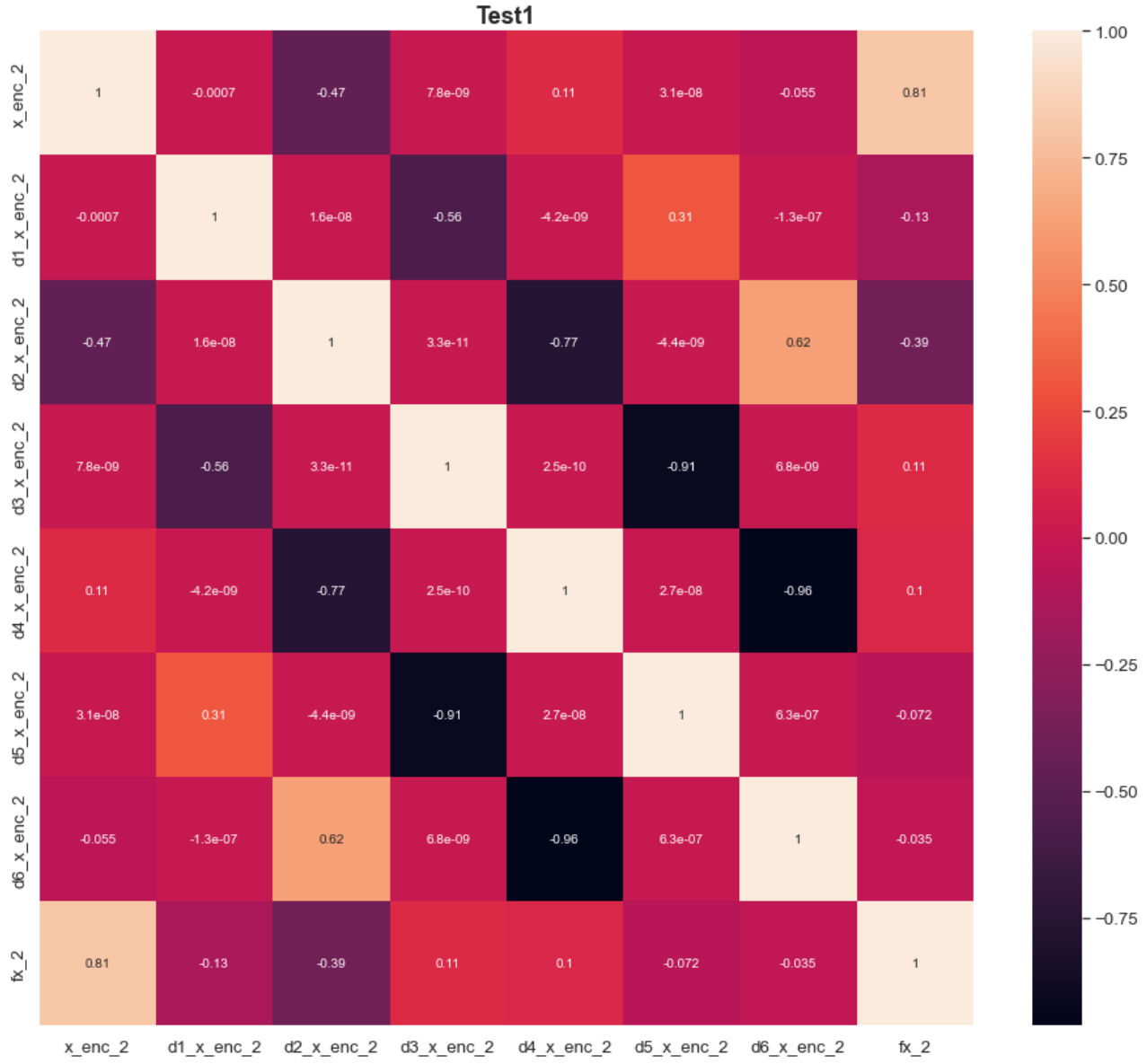
Correlations to higher order derivatives

x-axis only

In [16]:

```
idx = 0 # Test1
labels = [features_x1+outputs_x1, features_x2+outputs_x2]
sns.set_style("whitegrid")
for robot_idx in range(2):
    fig = plt.figure(figsize=(16, 14))
    corr = datasets[idx][labels[robot_idx]].corr()
    ax = fig.add_subplot(111)
    ax.set_title(dataset_filenames[idx], weight='bold').set_fontsize('18')
    sns.heatmap(corr, annot=True)
    plt.savefig(output_dir/'corr_derivatives_x_robot{}.pdf'.format(robot_idx+1))
```

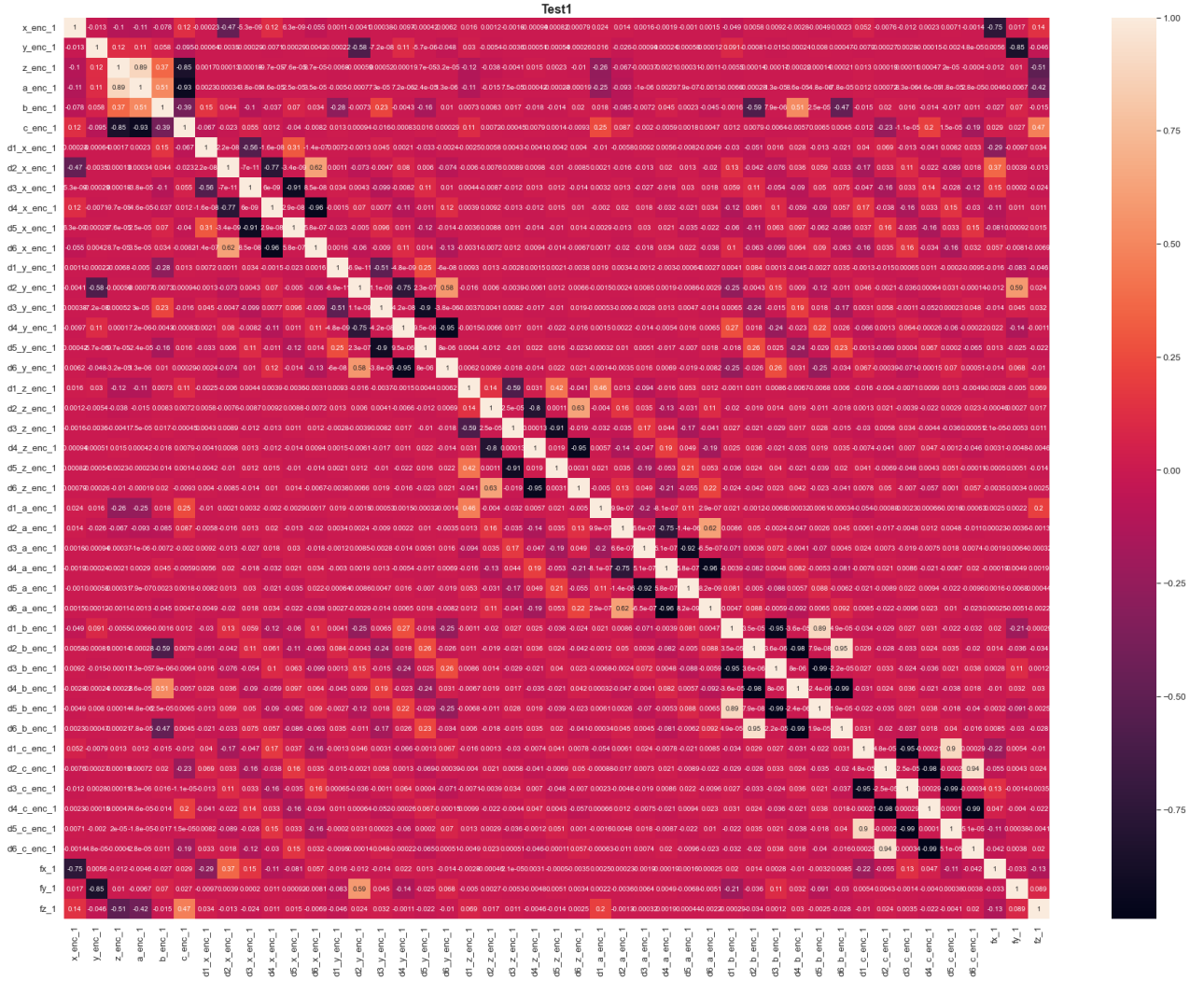


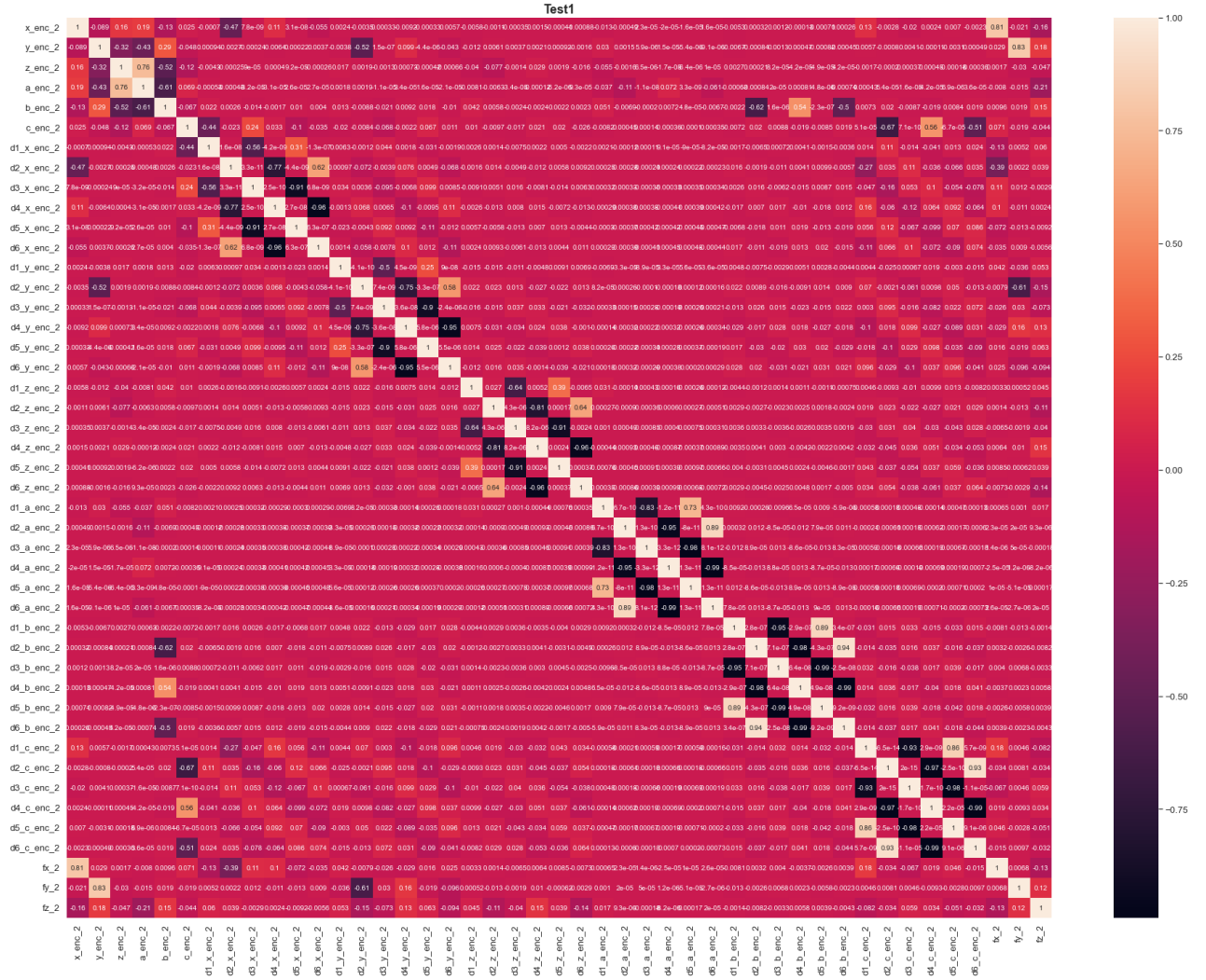


All coordinates

In [17]:

```
idx = 0 # Test1
labels = [features_1_nth+outputs_1, features_2_nth+outputs_2]
sns.set_style("whitegrid")
for robot_idx in range(2):
    fig = plt.figure(figsize=(32, 24))
    corr = datasets[idx][labels[robot_idx]].corr()
    ax = fig.add_subplot(111)
    ax.set_title(dataset_filenames[idx], weight='bold').set_fontsize('18')
    sns.heatmap(corr, annot=True)
    plt.savefig(output_dir/'corr_derivatives_all_robot{}.pdf'.format(robot_idx+1
```


Test1
x_enc_1
y_enc_1
z_enc_1
a_enc_1
b_enc_1
c_enc_1
d1_x_enc_1
d2_x_enc_1
d3_x_enc_1
d4_x_enc_1
d5_x_enc_1
d6_x_enc_1
d1_y_enc_1
d2_y_enc_1
d3_y_enc_1
d4_y_enc_1
d5_y_enc_1
d6_y_enc_1
d1_z_enc_1
d2_z_enc_1
d3_z_enc_1
d4_z_enc_1
d5_z_enc_1
d6_z_enc_1
d1_a_enc_1
d2_a_enc_1
d3_a_enc_1
d4_a_enc_1
d5_a_enc_1
d6_a_enc_1
d1_b_enc_1
d2_b_enc_1
d3_b_enc_1
d4_b_enc_1
d5_b_enc_1
d6_b_enc_1
d1_c_enc_1
d2_c_enc_1
d3_c_enc_1
d4_c_enc_1
d5_c_enc_1
d6_c_enc_1
fx_1
fy_1
fz_1
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75



3.2. Scaling of input features and outputs

Specify which datasets to use

Hold out 'Test2' for testing of model trained on data from 'Test1' and 'Test4'.

In [18]:
```
df1 = datasets[0] # Test1
df2 = datasets[1] # Test2
df4 = datasets[2] # Test4
df = df1.copy()
#df = df.append(datasets[1])
df = df.append(datasets[2])
```

Split dataframe into X (features) and Y (outputs)

In [19]:
```
features_nth = features_1_nth + features_2_nth
features_2nd = features_1_2nd + features_2_2nd
X = df[features_nth].to_numpy()
Y = df[outputs].to_numpy()
print(X.shape, Y.shape)
```

```
(49078, 84) (49078, 6)
```

Feature scaling

Both MinMaxScaler and StandardScaler were tried, the former gave slightly more robust performance.

In [20]:
```
from sklearn.preprocessing import StandardScaler, MinMaxScaler
#scaler_x = StandardScaler()
#scaler_y = StandardScaler()
scaler_x = MinMaxScaler()
scaler_y = MinMaxScaler()
X_normed = scaler_x.fit_transform(X)
Y_normed = scaler_y.fit_transform(Y)
```

In [21]:
```
# sanity check
print(X[0:5,0])
print(X_normed[0:5,0])
print(scaler_x.inverse_transform(X_normed)[0:4,0])
```

```
[213.6337 213.6337 213.6337 213.6337 213.6337]
[0.21954808 0.21954808 0.21954808 0.21954808 0.21954808]
[213.6337 213.6337 213.6337 213.6337]
```

3.3. Preparing input features for RNN training

Including multiple time steps of the input features and training an RNN to predict forces improved the performance over using a DNN. After some experimentation, I concluded that about 20 timesteps worked pretty well.

In [22]:
```
def split_sequences(X, Y, n_steps):
    X_seq, Y_seq = list(), list()
    for i in range(len(X)):
        end_i = i + n_steps
        if end_i > len(X):
            break
        Xi, yi = X[i:end_i, :], Y[end_i-1, :]
        X_seq.append(Xi)
        Y_seq.append(yi)
    return (np.array(X_seq), np.array(Y_seq))
```

In [23]:
```
# prepare sequences for RNN with 20 time steps
n_steps = 20
X_seq, Y_seq = split_sequences(X_normed, Y_normed, n_steps)
print(X_seq.shape, Y_seq.shape)
```

```
(49059, 20, 84) (49059, 6)
```

3.4. Splitting of data into train/validation/test sets

In [24]:
```
from sklearn.model_selection import train_test_split
# if False: keep last events for testing
shuffle = True
# 70-10-20 train-validation-test split
```

```
train_frac = 0.7
val_frac = 0.1

# for dnn
X_train, X_val_test, Y_train, Y_val_test = train_test_split(X_normed, Y_normed,
X_val, X_test, Y_val, Y_test = train_test_split(X_val_test, Y_val_test, test_siz

print(X_train.shape, Y_train.shape)
print(X_val.shape, Y_val.shape)
print(X_test.shape, Y_test.shape)

# for rnn
X_seq_train, X_seq_val_test, Y_seq_train, Y_seq_val_test = train_test_split(X_se
X_seq_val, X_seq_test, Y_seq_val, Y_seq_test = train_test_split(X_seq_val_test,

print(X_seq_train.shape, Y_seq_train.shape)
print(X_seq_val.shape, Y_seq_val.shape)
print(X_seq_test.shape, Y_seq_test.shape)
```

```
(34354, 84) (34354, 6)
(4907, 84) (4907, 6)
(9817, 84) (9817, 6)
(34341, 20, 84) (34341, 6)
(4905, 20, 84) (4905, 6)
(9813, 20, 84) (9813, 6)
```

Create train/val/test sets with 12 (positions and angles) and 36 input features (positions, angles, and up to 2nd order derivatives)

In [25]:

```
# sanity check
print(features)
print(features_2nd)
print(outputs)
```

```
['x_enc_1', 'y_enc_1', 'z_enc_1', 'a_enc_1', 'b_enc_1', 'c_enc_1', 'x_enc_2', 'y
_enc_2', 'z_enc_2', 'a_enc_2', 'b_enc_2', 'c_enc_2']
['x_enc_1', 'y_enc_1', 'z_enc_1', 'a_enc_1', 'b_enc_1', 'c_enc_1', 'd1_x_enc_1',
'd2_x_enc_1', 'd1_y_enc_1', 'd2_y_enc_1', 'd1_z_enc_1', 'd2_z_enc_1', 'd1_a_enc_
1', 'd2_a_enc_1', 'd1_b_enc_1', 'd2_b_enc_1', 'd1_c_enc_1', 'd2_c_enc_1', 'x_enc
_2', 'y_enc_2', 'z_enc_2', 'a_enc_2', 'b_enc_2', 'c_enc_2', 'd1_x_enc_2', 'd2_x_
enc_2', 'd1_y_enc_2', 'd2_y_enc_2', 'd1_z_enc_2', 'd2_z_enc_2', 'd1_a_enc_2', 'd
2_a_enc_2', 'd1_b_enc_2', 'd2_b_enc_2', 'd1_c_enc_2', 'd2_c_enc_2']
['fx_1', 'fy_1', 'fz_1', 'fx_2', 'fy_2', 'fz_2']
```

In [26]:

```
# indices of 12 position input features
feature_idx = [df[features_nth].columns.get_loc(col) for col in features]
# indices of position, velocity, and acceleration input features
feature_idx_2nd = [df[features_nth].columns.get_loc(col) for col in features_2nd
# indices of all features
feature_idx_nth = [df[features_nth].columns.get_loc(col) for col in features_nth
```

In [27]:

```
# sanity check
print(df[features][4000:4001].to_numpy())
print(scaler_x.inverse_transform(X_normed)[:,feature_idx][4000:4001,:])
```

```
[[ 7.01138030e+02  9.05163185e+01 -2.66579203e+01 -8.99984769e+01
  -4.16576996e-04  2.06331677e-03  7.04664055e+02  8.46991898e+01
  -2.02531592e+01  8.99942266e+01 -2.56791472e-04 -1.79998530e+02]]
```

```
[[ 7.01138030e+02  9.05163185e+01 -2.66579203e+01 -8.99984769e+01
  -4.16576996e-04  2.06331677e-03  7.04664055e+02  8.46991898e+01
  -2.02531593e+01  8.99942266e+01 -2.56791472e-04 -1.79998530e+02]]
```

In [28]:

```
# select 12 input features: x,y,z,a,b,c for robots 1 and 2
X_train_12 = X_train[:,feature_idx]
X_val_12 = X_val[:,feature_idx]
X_test_12 = X_test[:,feature_idx]

X_seq_train_12 = X_seq_train[:,:,feature_idx]
X_seq_val_12 = X_seq_val[:,:,feature_idx]
X_seq_test_12 = X_seq_test[:,:,feature_idx]

# select 36 input features: x,y,z,a,b,c + 1st and 2nd order derivatives for robo
X_train_36 = X_train[:,feature_idx_2nd]
X_val_36 = X_val[:,feature_idx_2nd]
X_test_36 = X_test[:,feature_idx_2nd]

X_seq_train_36 = X_seq_train[:,:,feature_idx_2nd]
X_seq_val_36 = X_seq_val[:,:, feature_idx_2nd]
X_seq_test_36 = X_seq_test[:,:,feature_idx_2nd]
```

In [29]:

```
# sanity check
print(X_train_12.shape)
print(X_seq_train_12.shape)

print(X_train_36.shape)
print(X_seq_train_36.shape)
```

```
(34354, 12)
(34341, 20, 12)
(34354, 36)
(34341, 20, 36)
```

4. Modeling

Finally, we're getting to the exciting part of training some neural nets.

In [30]:

```
# function to plot loss, to be used several times below
def plot_loss(history, name, title=''):
    fig = plt.figure(figsize=(24,10))
    fig.suptitle(title)

    # full range
    ax = fig.add_subplot(121)
    ax.plot(history.history['loss'], label='loss')
    ax.plot(history.history['val_loss'], label='val_loss')
    ax.set_xlabel('Epoch')
    ax.set_ylabel('Error')
    ax.legend()
    ax.grid(True)

    # last 30 percent of epochs
    zoom_frac = 0.7
    nepochs = len(history.history['loss'])
    ax = fig.add_subplot(122)
```

```
    ax.plot(history.history['loss'], label='loss')
    ax.plot(history.history['val_loss'], label='val_loss')
    xmin = int(zoom_frac*nepochs)
    xmax = nepochs
    ax.set_xlim([xmin, xmax])
    ymin = 0.99*np.min(history.history['loss'][int(zoom_frac*nepochs):]
                       + history.history['val_loss'][int(zoom_frac*nepochs):])
    ymax = 1.01*np.max(history.history['loss'][int(zoom_frac*nepochs):]
                       + history.history['val_loss'][int(zoom_frac*nepochs):])
    ax.set_ylim([ymin, ymax])
    ax.set_xlabel('Epoch')
    ax.set_ylabel('Error')
    ax.legend()
    ax.grid(True)

    plt.savefig(output_dir/name)
```

In [31]:
```
# for comparing test results of different models
test_results = dict()
```

4.1. Linear Regression

Let's start with a simple linear regression.

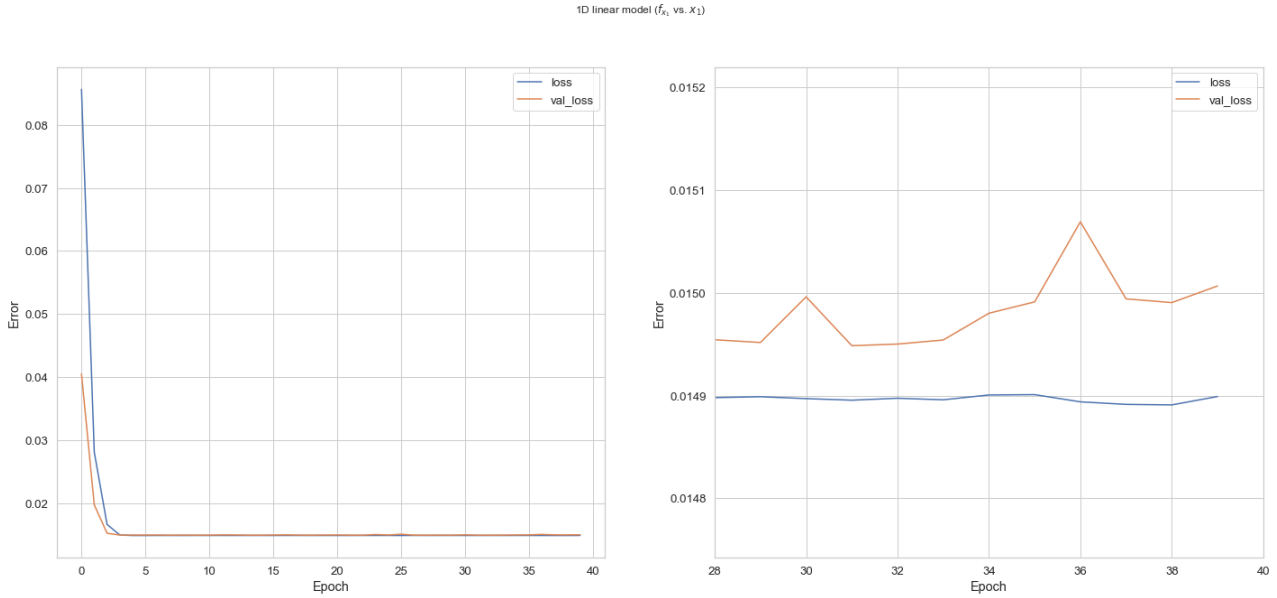
Predict f_{x_1} from x_1

In [32]:
```
x1_train = X_train[:,0].reshape(len(X_train),1)
fx1_train = Y_train[:,0].reshape(len(Y_train),1)
x1_val = X_val[:,0].reshape(len(X_val),1)
fx1_val = Y_val[:,0].reshape(len(Y_val),1)
x1_test = X_test[:,0].reshape(len(X_test),1)
fx1_test = Y_test[:,0].reshape(len(Y_test),1)
```

In [33]:
```
linear_model_x1 = keras.experimental.LinearModel()
linear_model_x1.compile(optimizer='adam', loss='mean_squared_error')
history_linear_x1 = linear_model_x1.fit(
    x1_train, fx1_train,
    validation_data=(x1_val, fx1_val),
    batch_size = 32,
    epochs=40,
    verbose=0)
with open(output_dir/'history_linear_x1.pickle', 'wb') as f:
    pickle.dump(history_linear_x1.history, f)
```

Plot loss vs. epoch

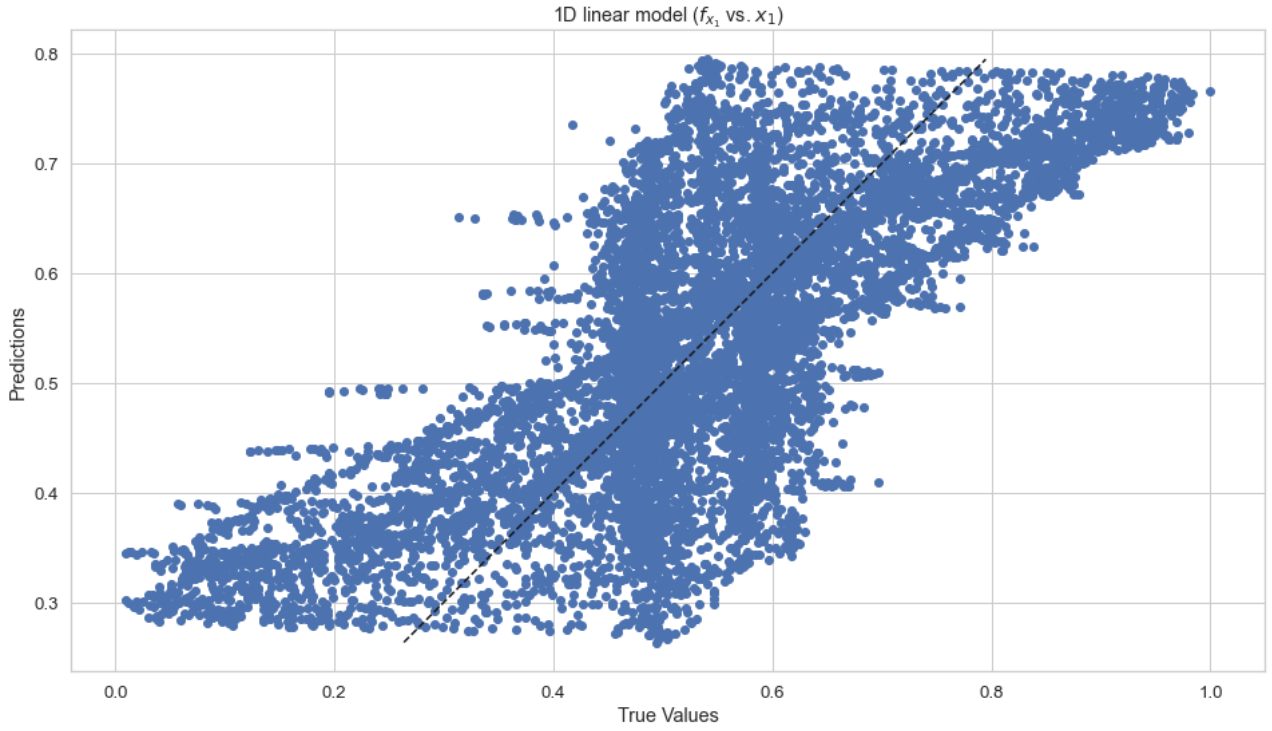
In [34]:
```
plot_loss(history_linear_x1, 'loss_linear_x1.pdf', '1D linear model ($f_{x_1}$ v
```



In [35]:
```
# save model loss on test set for evaluation section below
test_results['linear_x1'] = linear_model_x1.evaluate(x1_test, fx1_test, verbose=
```

Plot predictions vs. true values

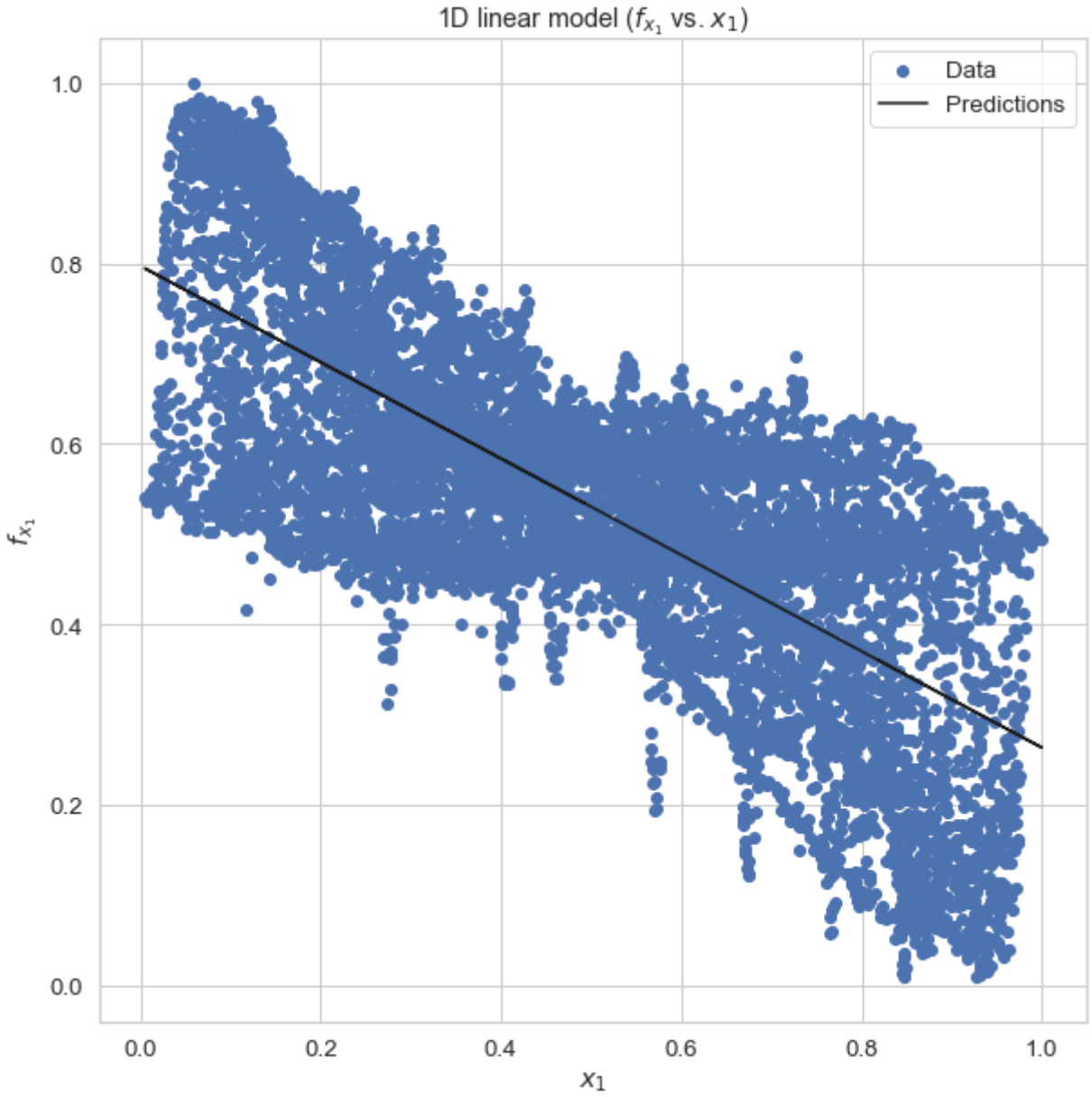
In [36]:
```
fx1_test_pred = linear_model_x1.predict(x1_test)
fig = plt.figure(figsize=(16,10))
ax = fig.add_subplot(111, aspect='equal')
ax.scatter(fx1_test, fx1_test_pred)
ax.plot([np.min(fx1_test_pred), np.max(fx1_test_pred)], [np.min(fx1_test_pred),
#ax.plot([0.2, 0.8], [0.2, 0.8], linestyle='dashed', label='Predictions', color=
ax.set_xlabel('True Values')
ax.set_ylabel('Predictions')
ax.set_title('1D linear model ($f_{x_1}$ vs. $x_1$)')
plt.savefig(output_dir/'pred_vs_true_linear_x1.pdf')
```



Plot f_{x_1} vs. x_1 (scaled)

In [37]:

```
fig = plt.figure(figsize=(16,10))
ax = fig.add_subplot(111, aspect='equal')
ax.scatter(x1_test, fx1_test, label='Data')
ax.plot(x1_test, fx1_test_pred, label='Predictions', color='k')
ax.set_xlabel('$x_{1}$')
ax.set_ylabel('$f_{x{_1}}$')
ax.set_title('1D linear model ($f_{x_1}$ vs. $x_1$)')
ax.legend()
plt.savefig(output_dir/'linear_fx1_vs_x1.pdf')
```

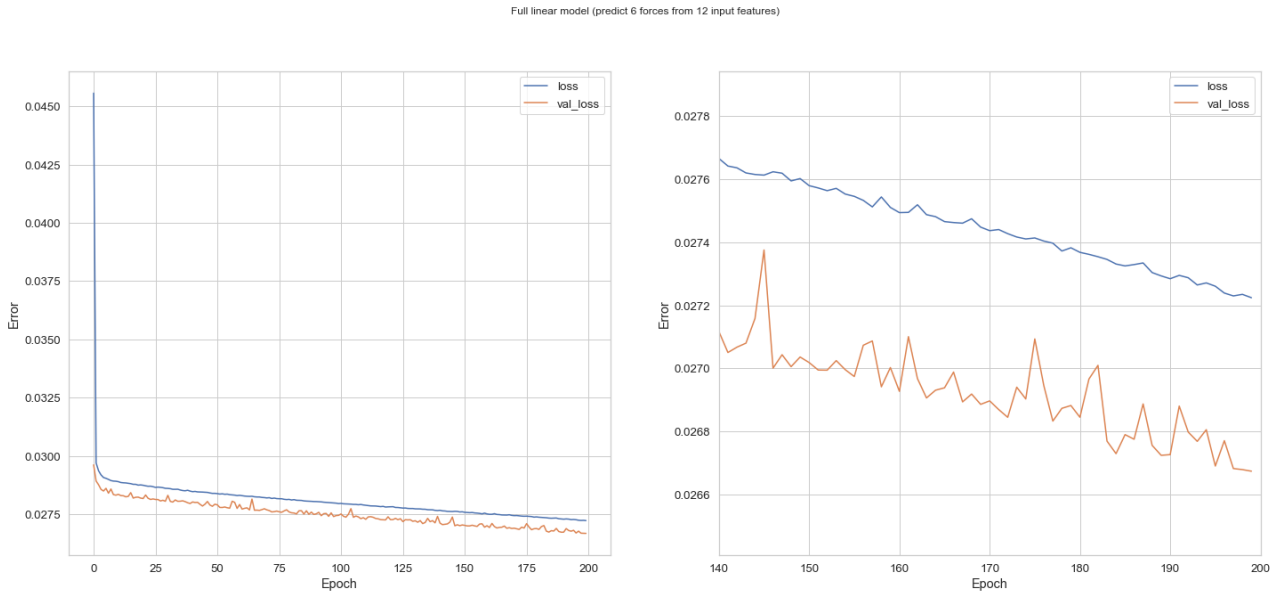


Predict all 6 forces from 12 input features

In [38]:
```
linear_model_12 = keras.experimental.LinearModel(units=6)
linear_model_12.compile(optimizer='adam', loss='mean_squared_error')
history_linear_12 = linear_model_12.fit(
    X_train_12, Y_train,
    validation_data=(X_val_12, Y_val),
    batch_size = 32,
    epochs=200,
    verbose=0)
with open(output_dir/'history_linear_12.pickle', 'wb') as f:
    pickle.dump(history_linear_12.history, f)
```

Plot loss vs. epoch

In [39]:
```
plot_loss(history_linear_12, 'loss_linear_12.pdf', 'Full linear model (predict 6
```

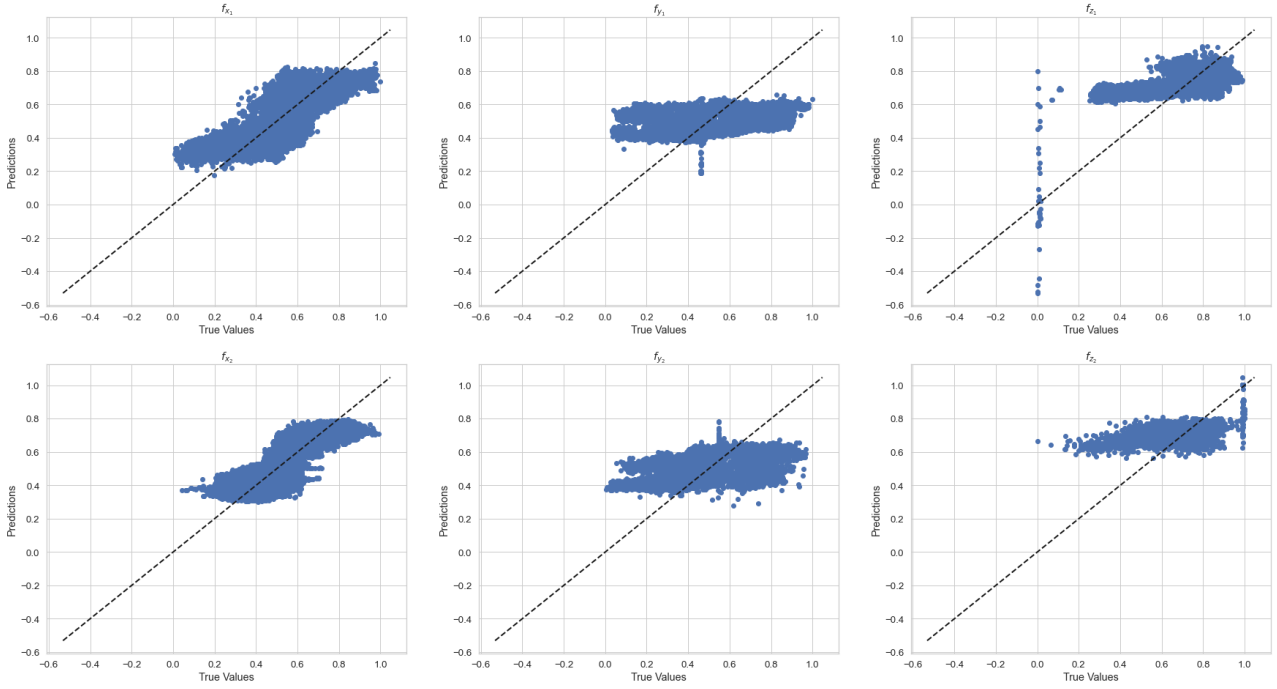


In [40]:
```
# save model loss on test set for evaluation section below
test_results['linear_12'] = linear_model_12.evaluate(X_test_12, Y_test, verbose=
```

Plot predictions vs. true values

In [41]:
```
def plot_pred_vs_true(pred, true, name, titles=None):
    fig = plt.figure(figsize=(30,16))
    for i in range(len(pred.T)):
        ax = fig.add_subplot(2,3,i+1)
        ax.scatter(true.T[i], pred.T[i])
        ax.plot([np.min(pred), np.max(pred)],[np.min(pred), np.max(pred)], lines
        ax.set_xlabel('True Values')
        ax.set_ylabel('Predictions')
        if len(titles)>=len(pred.T):
            ax.set_title(titles[i])
    plt.savefig(output_dir/'pred_vs_true_{}.pdf'.format(name))
```

In [42]:
```
Y_test_pred_linear_12 = linear_model_12.predict(X_test_12)
plot_pred_vs_true(Y_test_pred_linear_12, Y_test, 'pred_vs_true_linear_12', title
```



4.2. DNN regression

I experimented by varying the number of layers, dropout rate, learning rate, batch size, and adding batch normalization layers—the model below achieves pretty good performance.

In [43]:
```
# The Sequential model will do just fine here
# (functional API is more flexible though)

def setup_dnn_model(n_outputs):
  model = keras.Sequential([
      #layers.BatchNormalization(),
      layers.Dense(100, activation='relu'),
      layers.Dropout(0.05),
      layers.Dense(100, activation='relu'),
      layers.Dropout(0.05),
      layers.Dense(100, activation='relu'),
      layers.Dropout(0.05),
      layers.Dense(100, activation='relu'),
      layers.Dropout(0.05),
      layers.Dense(100, activation='relu'),
      layers.Dense(n_outputs)
  ])

  model.compile(loss='mean_squared_error',
                optimizer=tf.keras.optimizers.Adam(learning_rate=1e-3, decay=5e-
  return model
```

In [44]:
```
# dnn config
dnn_tag = "dnn_100x5_05dropout"
dnn_epochs = 1000
dnn_batch_size = 32
```

Predict all 6 forces from 12 input features

In [45]:
```
dnn_model_12 = setup_dnn_model(Y_train.shape[-1])
dnn_model_12_tag = "{}_12features".format(dnn_tag)
```

In [46]:
```
%%time

early_stop = tf.keras.callbacks.EarlyStopping(monitor='val_loss', patience=20)
save_every_epoch = tf.keras.callbacks.ModelCheckpoint(output_dir/'dnn_12_tmp.h5'

history_dnn_12 = dnn_model_12.fit(
    X_train_12, Y_train,
    validation_data=(X_val_12, Y_val),
    batch_size = dnn_batch_size,
    epochs=dnn_epochs,
    callbacks=[save_every_epoch],
    #callbacks=[early_stop, save_every_epoch],
    verbose=0
    )
dnn_model_12.summary()
with open(output_dir/'history_dnn_12.pickle', 'wb') as f:
    pickle.dump(history_dnn_12.history, f)
```

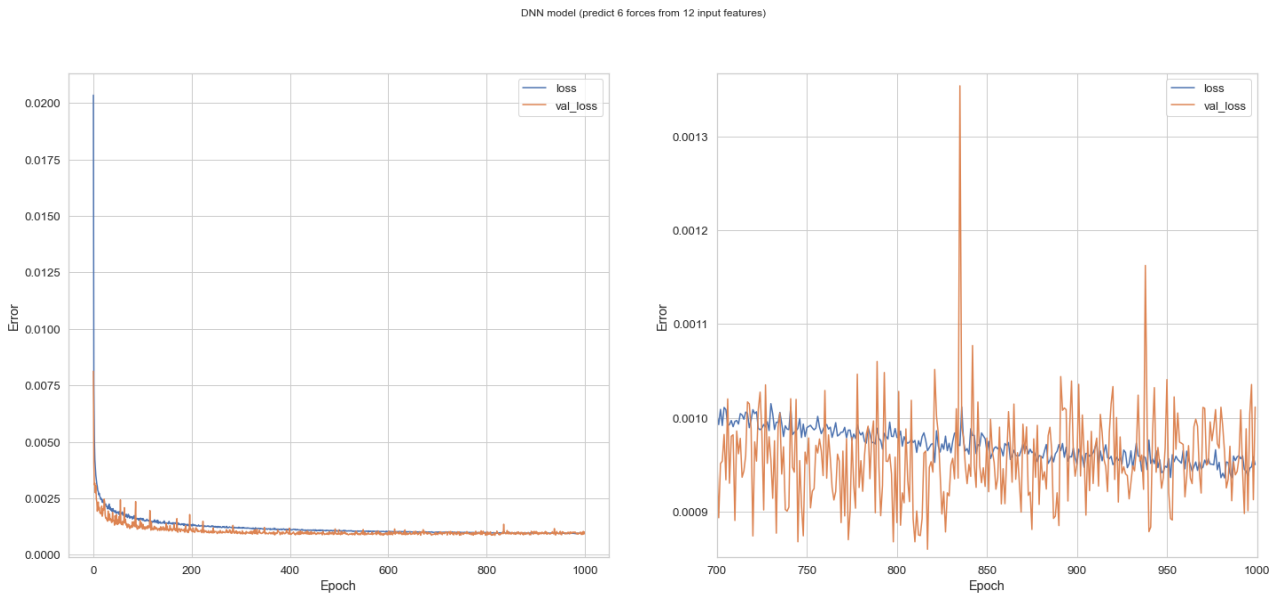
```
Model: "sequential"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense (Dense)               (None, 100)               1300

 dropout (Dropout)           (None, 100)               0

 dense_1 (Dense)             (None, 100)               10100

 dropout_1 (Dropout)         (None, 100)               0

 dense_2 (Dense)             (None, 100)               10100

 dropout_2 (Dropout)         (None, 100)               0

 dense_3 (Dense)             (None, 100)               10100

 dropout_3 (Dropout)         (None, 100)               0

 dense_4 (Dense)             (None, 100)               10100

 dense_5 (Dense)             (None, 6)                 606

=================================================================
Total params: 42,306
Trainable params: 42,306
Non-trainable params: 0
_________________________________________________________________
CPU times: user 49min, sys: 28min 52s, total: 1h 17min 53s
Wall time: 23min 54s
```

Save DNN model

In [47]:
```
dnn_model_12.save(output_dir/"{}_{}.h5".format(dnn_model_12_tag, timestamp))
```

Plot loss vs. epoch

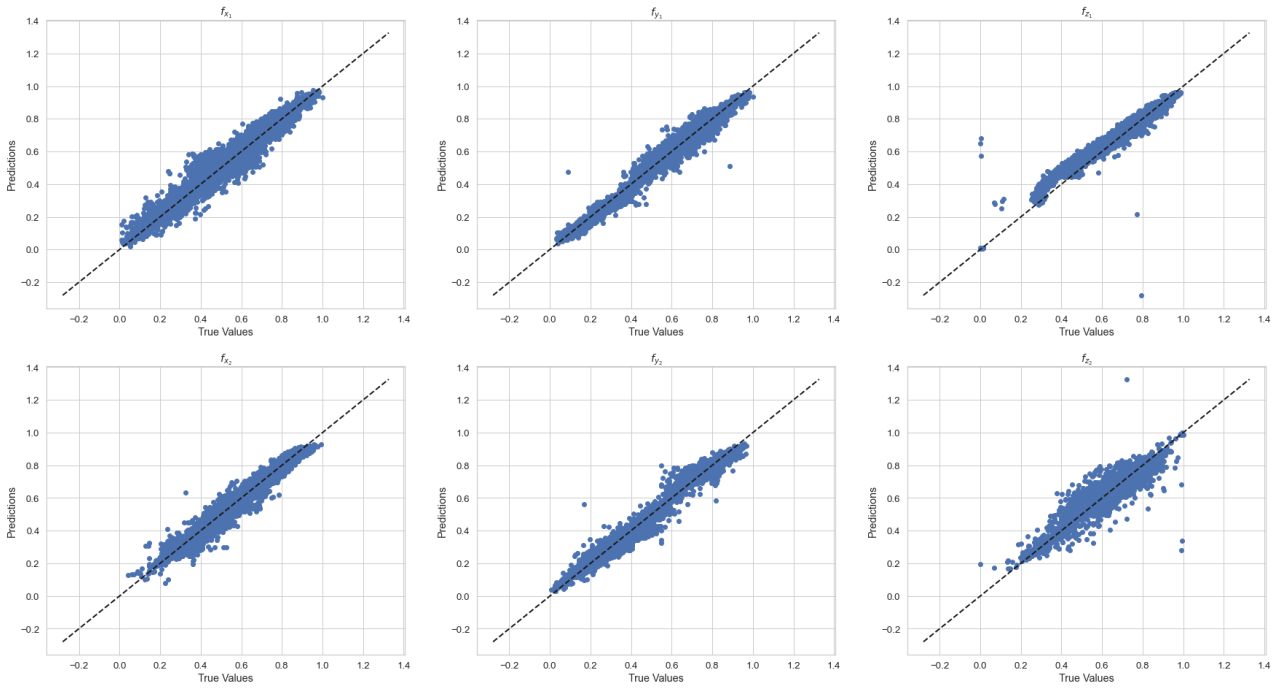
In [48]:
```
plot_loss(history_dnn_12, 'loss_{}.pdf'.format(dnn_model_12_tag), 'DNN model (pr
```



In [49]:
```
# save model loss on test set for evaluation section below
test_results['dnn_12'] = dnn_model_12.evaluate(X_test_12, Y_test, verbose=0)
```

Compare prediction vs. true values for the test set

In [50]:
```
Y_test_pred_dnn_12 = dnn_model_12.predict(X_test_12)
plot_pred_vs_true(Y_test_pred_dnn_12, Y_test, 'pred_vs_true_{}'.format(dnn_model
```



Predict all 6 forces from 36 input features (12+2x12)

Up to 2nd order derivatives for 12 input features.

In [51]:
```
dnn_model_36 = setup_dnn_model(Y_train.shape[-1])
```

```
dnn_model_36_tag = "{}_36features".format(dnn_tag)
```

In [52]:

```
%%time

early_stop = tf.keras.callbacks.EarlyStopping(monitor='val_loss', patience=20)
save_every_epoch = tf.keras.callbacks.ModelCheckpoint(output_dir/'dnn_36_tmp.h5'

history_dnn_36 = dnn_model_36.fit(
    X_train_36, Y_train,
    validation_data=(X_val_36, Y_val),
    batch_size = dnn_batch_size,
    epochs=dnn_epochs,
    callbacks=[save_every_epoch],
    #callbacks=[early_stop, save_every_epoch],
    verbose=0
    )
dnn_model_36.summary()
with open(output_dir/'history_dnn_36.pickle', 'wb') as f:
    pickle.dump(history_dnn_36.history, f)
```

```
Model: "sequential_1"
_________________________________________________________________
 Layer (type)                 Output Shape              Param #
=================================================================
 dense_6 (Dense)              (None, 100)               3700

 dropout_4 (Dropout)          (None, 100)               0

 dense_7 (Dense)              (None, 100)               10100

 dropout_5 (Dropout)          (None, 100)               0

 dense_8 (Dense)              (None, 100)               10100

 dropout_6 (Dropout)          (None, 100)               0

 dense_9 (Dense)              (None, 100)               10100

 dropout_7 (Dropout)          (None, 100)               0

 dense_10 (Dense)             (None, 100)               10100

 dense_11 (Dense)             (None, 6)                 606

=================================================================
Total params: 44,706
Trainable params: 44,706
Non-trainable params: 0
_________________________________________________________________
CPU times: user 51min 19s, sys: 31min 34s, total: 1h 22min 54s
Wall time: 24min 45s
```

Save DNN model

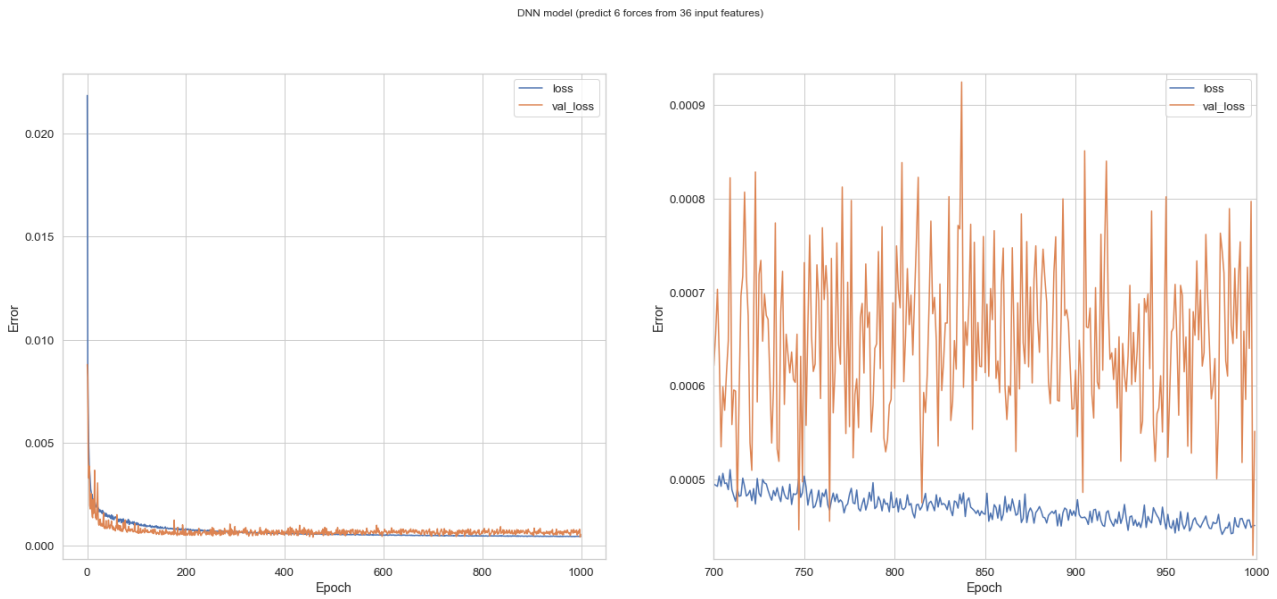
In [53]:

```
dnn_model_36.save(output_dir/"{}_{}.h5".format(dnn_model_36_tag, timestamp))
```

Plot loss vs. epoch

In [54]:

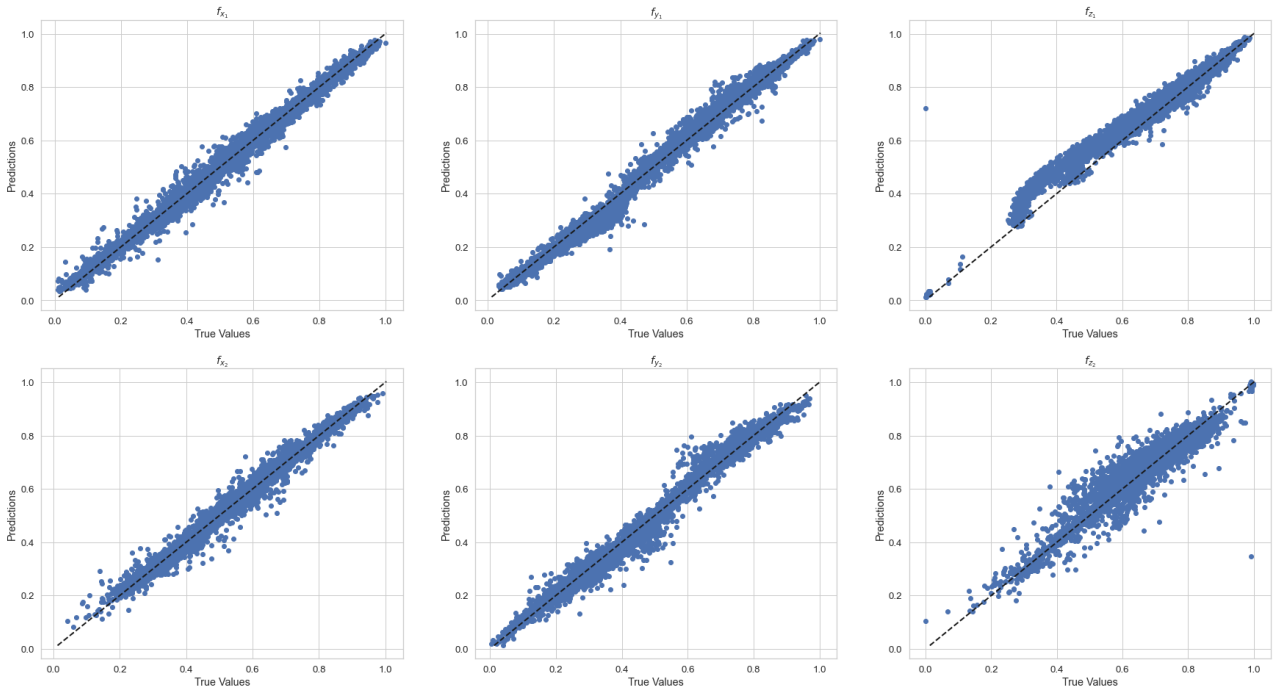
```
plot_loss(history_dnn_36, 'loss_{}.pdf'.format(dnn_model_36_tag), 'DNN model (pr
```



In [55]:
```
# save model loss on test set for evaluation section below
test_results['dnn_36'] = dnn_model_36.evaluate(X_test_36, Y_test, verbose=0)
```

Compare prediction vs. true values for the test set

In [56]:
```
Y_test_pred_dnn_36 = dnn_model_36.predict(X_test_36)
plot_pred_vs_true(Y_test_pred_dnn_36, Y_test, 'pred_vs_true_{}'.format(dnn_model
```



Predict all 6 forces from 84 input features (12+6x12)

Up to 6th order derivatives for 12 input features.

In [57]:
```
dnn_model_84 = setup_dnn_model(Y_train.shape[-1])
```

```
dnn_model_84_tag = "{}_84features".format(dnn_tag)
```

In [58]:

```
%%time

early_stop = tf.keras.callbacks.EarlyStopping(monitor='val_loss', patience=20)
save_every_epoch = tf.keras.callbacks.ModelCheckpoint(output_dir/'dnn_84_tmp.h5'

history_dnn_84 = dnn_model_84.fit(
    X_train, Y_train,
    validation_data=(X_val, Y_val),
    batch_size = dnn_batch_size,
    epochs=dnn_epochs,
    callbacks=[save_every_epoch],
    #callbacks=[early_stop, save_every_epoch],
    verbose=0
    )
dnn_model_84.summary()
with open(output_dir/'history_dnn_84.pickle', 'wb') as f:
    pickle.dump(history_dnn_84.history, f)
```

```
Model: "sequential_2"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense_12 (Dense)            (None, 100)               8500

 dropout_8 (Dropout)         (None, 100)               0

 dense_13 (Dense)            (None, 100)               10100

 dropout_9 (Dropout)         (None, 100)               0

 dense_14 (Dense)            (None, 100)               10100

 dropout_10 (Dropout)        (None, 100)               0

 dense_15 (Dense)            (None, 100)               10100

 dropout_11 (Dropout)        (None, 100)               0

 dense_16 (Dense)            (None, 100)               10100

 dense_17 (Dense)            (None, 6)                 606

=================================================================
Total params: 49,506
Trainable params: 49,506
Non-trainable params: 0
_________________________________________________________________
CPU times: user 50min 52s, sys: 30min 41s, total: 1h 21min 34s
Wall time: 24min 48s
```

Save DNN model

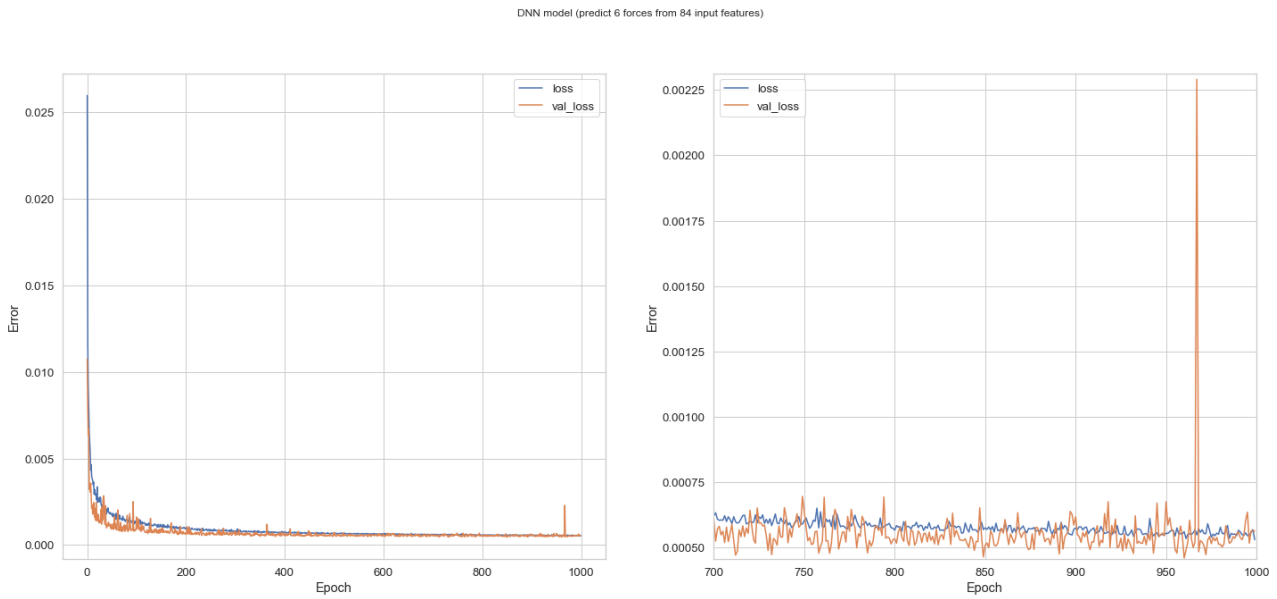
In [59]:

```
dnn_model_84.save(output_dir/"{}_{}.h5".format(dnn_model_84_tag, timestamp))
```

Plot loss vs. epoch

In [60]:

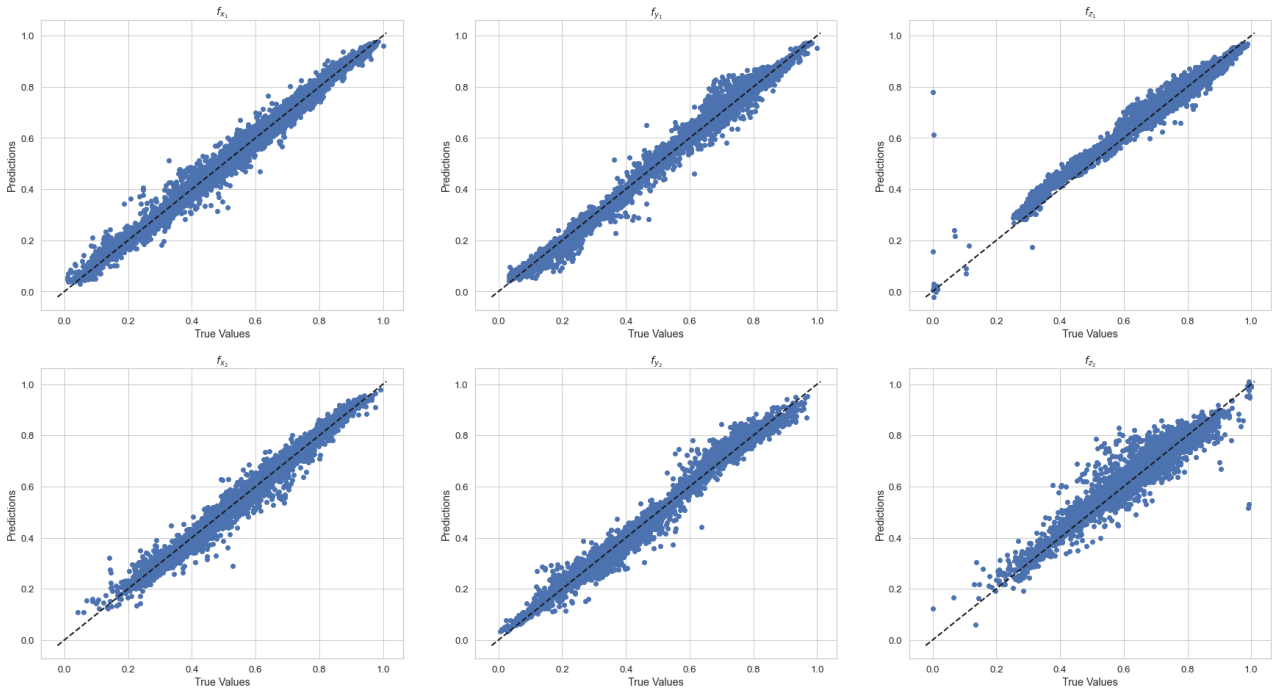
```
plot_loss(history_dnn_84, 'loss_{}.pdf'.format(dnn_model_84_tag), 'DNN model (pr
```



In [61]:
```
# save model loss on test set for evaluation section below
test_results['dnn_84'] = dnn_model_84.evaluate(X_test, Y_test, verbose=0)
```

Compare prediction vs. true values for the test set

In [62]:
```
Y_test_pred_dnn_84 = dnn_model_84.predict(X_test)
plot_pred_vs_true(Y_test_pred_dnn_84, Y_test, 'pred_vs_true_{}'.format(dnn_model
```



4.3 RNN regression

I experimented with LSTM, GRU, and SimpleRNN layers. Performance was relatively similar, but the LSTM seemed to do slightly better.

As is shown in section 5, an RNN did a significantly better job predicted unseen data than a DNN, especially for the dataset not seen during training.

In [63]:
```
def setup_rnn_model(n_outputs):
  model = keras.Sequential([
      #layers.BatchNormalization(),
      layers.LSTM(100, activation='relu', return_sequences=True),
      #layers.SimpleRNN(100, activation='relu', return_sequences=True),
      #layers.GRU(100, activation='relu', return_sequences=True),
      layers.Dropout(0.05),
      layers.LSTM(100, activation='relu', return_sequences=False),
      #layers.SimpleRNN(100, activation='relu', return_sequences=False),
      #layers.GRU(100, activation='relu', return_sequences=False),
      layers.Dropout(0.05),
      layers.Dense(100, activation='relu'),
      layers.Dense(n_outputs)
  ])

  model.compile(loss='mean_squared_error',
                optimizer=tf.keras.optimizers.Adam(learning_rate=1e-3, decay=5e-
  return model
```

In [64]:
```
# rnn config
rnn_tag = "rnn_lstm100x2_dense100x1_0p5drop"
rnn_epochs = 300
rnn_batch_size = 32
```

In [65]:
```
rnn_model_12 = setup_rnn_model(Y_seq_train.shape[-1])
rnn_model_12_tag = "{}_12features".format(rnn_tag)
```

In [66]:
```
rnn_model_36 = setup_rnn_model(Y_seq_train.shape[-1])
rnn_model_36_tag = "{}_36features".format(rnn_tag)
```

In [67]:
```
rnn_model_84 = setup_rnn_model(Y_seq_train.shape[-1])
rnn_model_84_tag = "{}_84features".format(rnn_tag)
```

In [68]:
```
%%time

early_stop = tf.keras.callbacks.EarlyStopping(monitor='val_loss', patience=20)
save_every_epoch = tf.keras.callbacks.ModelCheckpoint(output_dir/'rnn_12_tmp.h5'

history_rnn_12 = rnn_model_12.fit(
    X_seq_train_12, Y_seq_train,
    validation_data=(X_seq_val_12, Y_seq_val),
    batch_size = rnn_batch_size,
    epochs=rnn_epochs,
    callbacks=[save_every_epoch],
    #callbacks=[early_stop, save_every_epoch],
    verbose=0
    )
rnn_model_12.summary()
```

```
with open(output_dir/'history_rnn_12.pickle', 'wb') as f:
    pickle.dump(history_rnn_12.history, f)
```

```
Model: "sequential_3"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 lstm (LSTM)                 (None, 20, 100)           45200

 dropout_12 (Dropout)        (None, 20, 100)           0

 lstm_1 (LSTM)               (None, 100)               80400

 dropout_13 (Dropout)        (None, 100)               0

 dense_18 (Dense)            (None, 100)               10100

 dense_19 (Dense)            (None, 6)                 606

=================================================================
Total params: 136,306
Trainable params: 136,306
Non-trainable params: 0
_________________________________________________________________
CPU times: user 3h 38min 59s, sys: 51min, total: 4h 29min 59s
Wall time: 1h 19min 46s
```

In [69]:

```
%%time

early_stop = tf.keras.callbacks.EarlyStopping(monitor='val_loss', patience=20)
save_every_epoch = tf.keras.callbacks.ModelCheckpoint(output_dir/'rnn_36_tmp.h5'

history_rnn_36 = rnn_model_36.fit(
    X_seq_train_36, Y_seq_train,
    validation_data=(X_seq_val_36, Y_seq_val),
    batch_size = rnn_batch_size,
    epochs=rnn_epochs,
    callbacks=[save_every_epoch],
    #callbacks=[early_stop, save_every_epoch],
    verbose=0
    )
rnn_model_36.summary()
with open(output_dir/'history_rnn_36.pickle', 'wb') as f:
    pickle.dump(history_rnn_36.history, f)
```

```
Model: "sequential_4"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 lstm_2 (LSTM)               (None, 20, 100)           54800

 dropout_14 (Dropout)        (None, 20, 100)           0

 lstm_3 (LSTM)               (None, 100)               80400

 dropout_15 (Dropout)        (None, 100)               0

 dense_20 (Dense)            (None, 100)               10100

 dense_21 (Dense)            (None, 6)                 606

=================================================================
```

```
Total params: 145,906
Trainable params: 145,906
Non-trainable params: 0
_________________________________________________________________
CPU times: user 3h 45min 18s, sys: 51min 8s, total: 4h 36min 27s
Wall time: 1h 20min 40s
```

In [70]:

```
%%time

early_stop = tf.keras.callbacks.EarlyStopping(monitor='val_loss', patience=20)
save_every_epoch = tf.keras.callbacks.ModelCheckpoint(output_dir/'rnn_84_tmp.h5'

history_rnn_84 = rnn_model_84.fit(
    X_seq_train, Y_seq_train,
    validation_data=(X_seq_val, Y_seq_val),
    batch_size = rnn_batch_size,
    epochs=rnn_epochs,
    callbacks=[save_every_epoch],
    #callbacks=[early_stop, save_every_epoch],
    verbose=0
    )
rnn_model_84.summary()
with open(output_dir/'history_rnn_84.pickle', 'wb') as f:
    pickle.dump(history_rnn_84.history, f)
```

```
Model: "sequential_5"
_________________________________________________________________
 Layer (type)                 Output Shape              Param #
=================================================================
 lstm_4 (LSTM)                (None, 20, 100)           74000

 dropout_16 (Dropout)         (None, 20, 100)           0

 lstm_5 (LSTM)                (None, 100)               80400

 dropout_17 (Dropout)         (None, 100)               0

 dense_22 (Dense)             (None, 100)               10100

 dense_23 (Dense)             (None, 6)                 606

=================================================================
Total params: 165,106
Trainable params: 165,106
Non-trainable params: 0
_________________________________________________________________
CPU times: user 4h 2min 23s, sys: 56min 19s, total: 4h 58min 42s
Wall time: 1h 25min 40s
```

Save RNN model

In [71]:

```
rnn_model_12.save(output_dir/"{}_{}.h5".format(rnn_model_12_tag, timestamp), sav
```

In [72]:

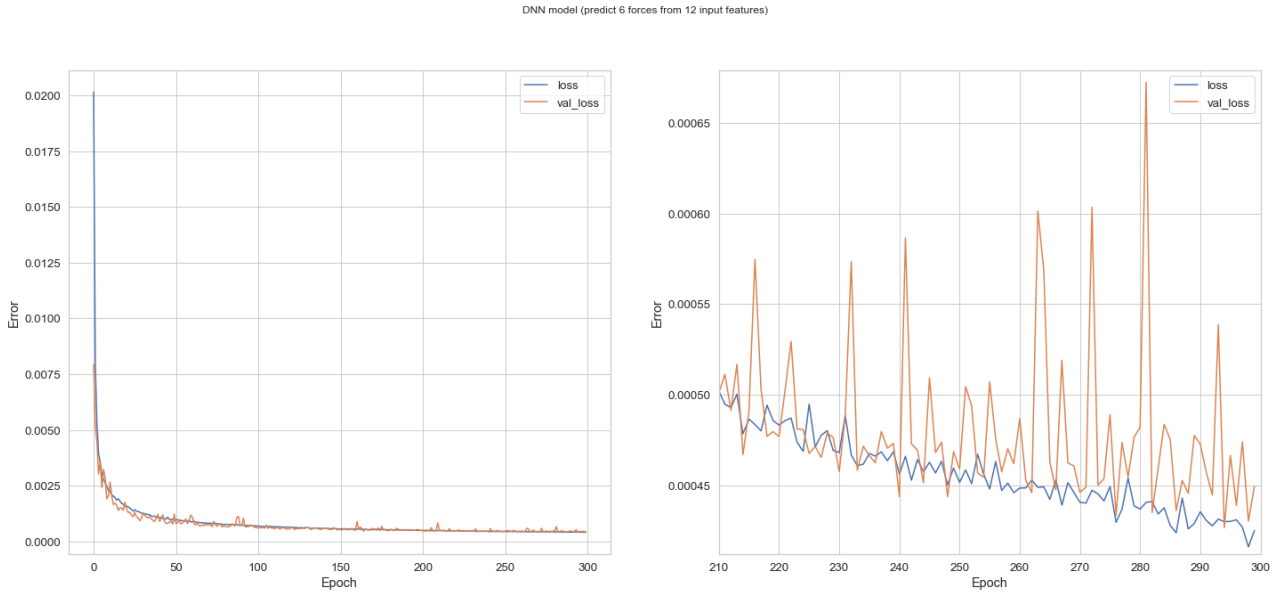
```
rnn_model_36.save(output_dir/"{}_{}.h5".format(rnn_model_36_tag, timestamp), sav
```

In [73]:

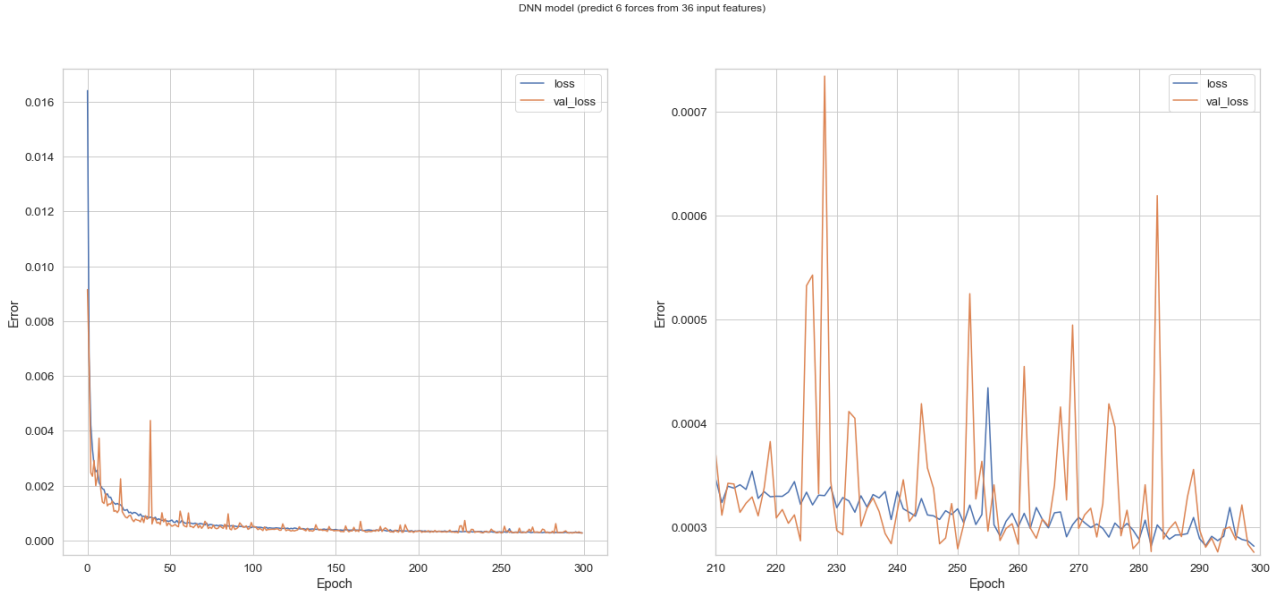
```
rnn_model_84.save(output_dir/"{}_{}.h5".format(rnn_model_84_tag, timestamp), sav
```

Plot loss vs. epoch

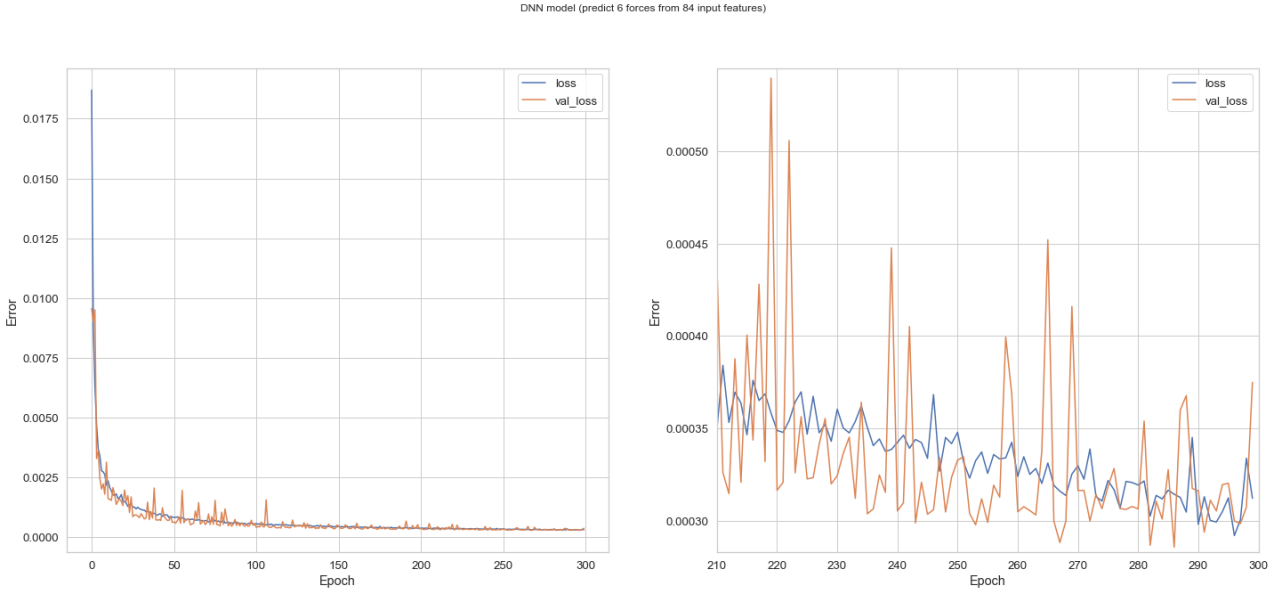
In [74]:
```
plot_loss(history_rnn_12, 'error_vs_epoch_{}.pdf'.format(rnn_model_12_tag), 'DNN
```



In [75]:
```
plot_loss(history_rnn_36, 'error_vs_epoch_{}.pdf'.format(rnn_model_36_tag), 'DNN
```



In [76]:
```
plot_loss(history_rnn_84, 'error_vs_epoch_{}.pdf'.format(rnn_model_84_tag), 'DNN
```



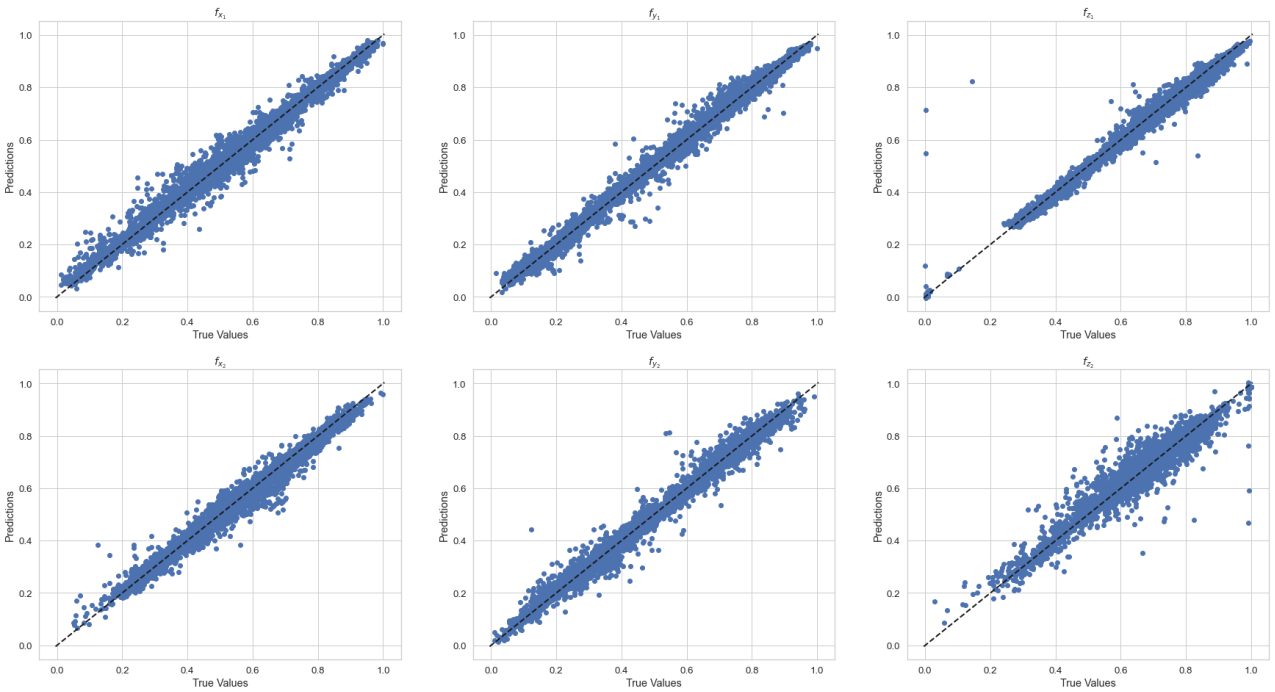
In [77]:
```
# save model loss on test set for evaluation section below
test_results['rnn_12'] = rnn_model_12.evaluate(X_seq_test_12, Y_seq_test, verbos
```

In [78]:
```
# save model loss on test set for evaluation section below
test_results['rnn_36'] = rnn_model_36.evaluate(X_seq_test_36, Y_seq_test, verbos
```

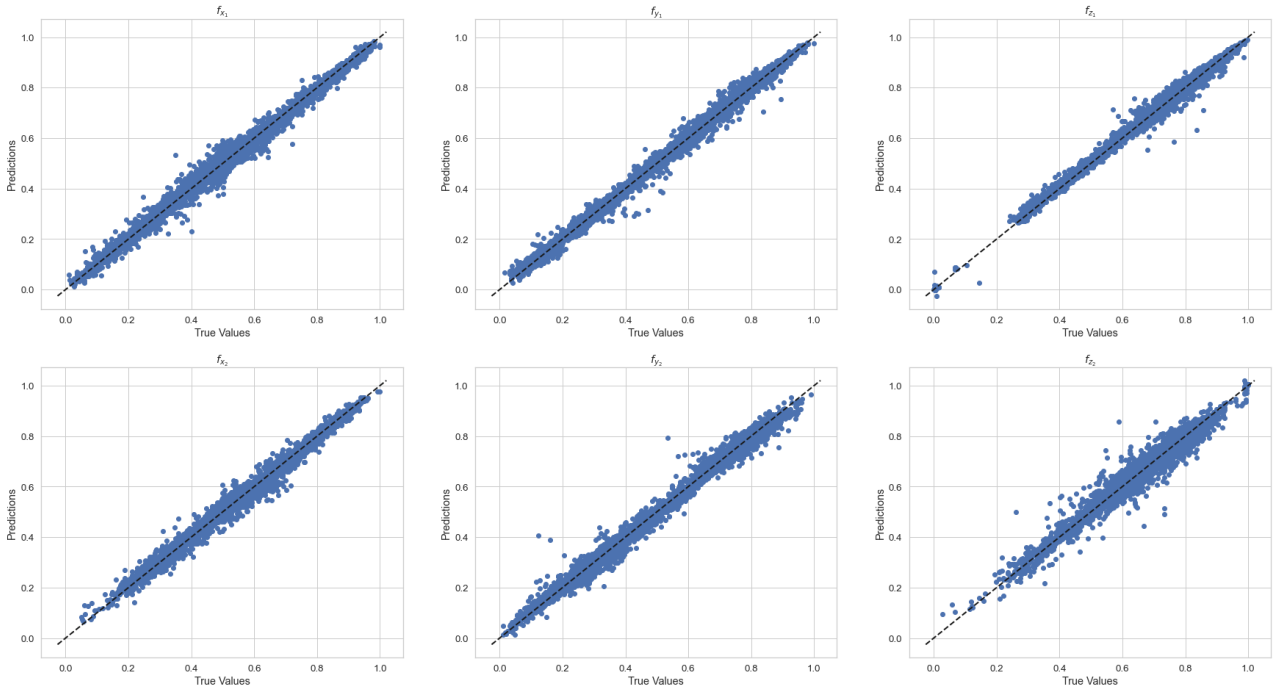
In [79]:
```
# save model loss on test set for evaluation section below
test_results['rnn_84'] = rnn_model_84.evaluate(X_seq_test, Y_seq_test, verbose=0
```

Compare prediction vs. true values for the test set

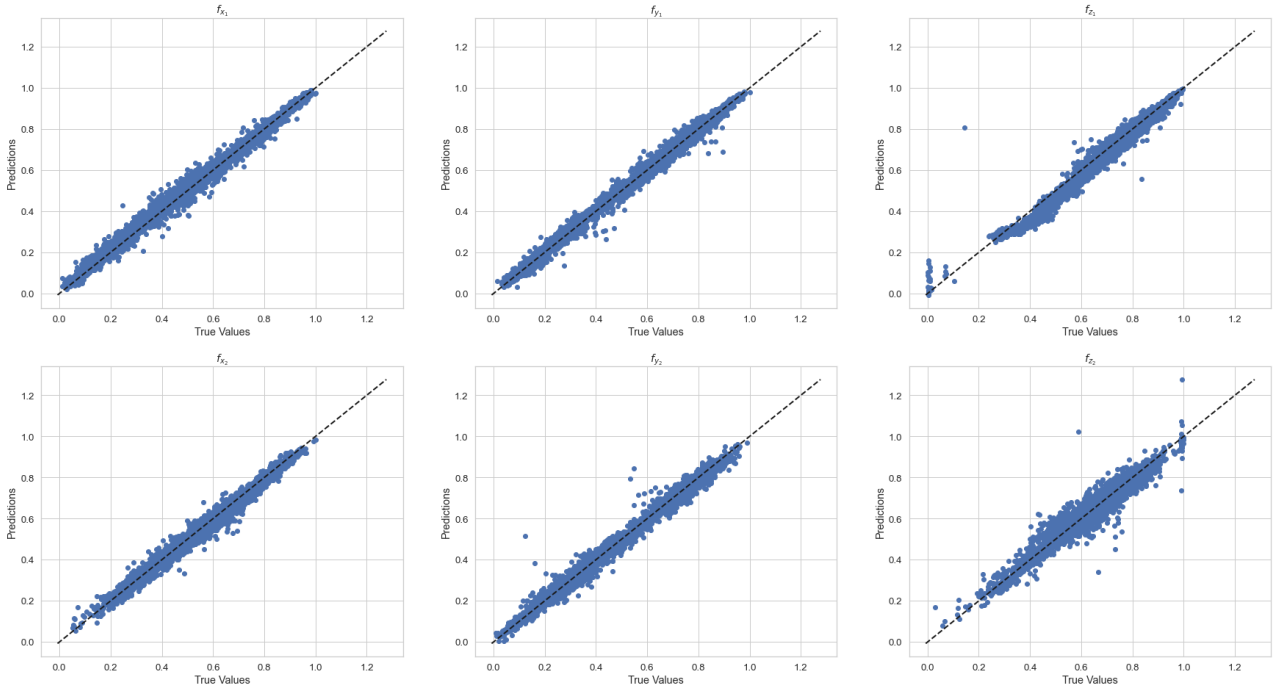
In [80]:
```
Y_seq_test_pred_12 = rnn_model_12.predict(X_seq_test_12)
plot_pred_vs_true(Y_seq_test_pred_12, Y_seq_test, 'pred_vs_true_{}'.format(rnn_m
```



In [81]:
```
Y_seq_test_pred_36 = rnn_model_36.predict(X_seq_test_36)
plot_pred_vs_true(Y_seq_test_pred_36, Y_seq_test, 'pred_vs_true_{}'.format(rnn_m
```



In [82]:
```
Y_seq_test_pred = rnn_model_84.predict(X_seq_test)
plot_pred_vs_true(Y_seq_test_pred, Y_seq_test, 'pred_vs_true_{}'.format(rnn_mode
```



5. Evaluation

5.1 Loss on test sets

In [83]:

```
print("loss on test sets:")
for key,val in test_results.items():
    print("- {}: {:.2e}".format(key,val))
```

```
loss on test sets:
- linear_x1: 1.49e-02
- linear_12: 2.68e-02
- dnn_12: 1.13e-03
- dnn_36: 5.88e-04
- dnn_84: 5.49e-04
- rnn_12: 4.86e-04
- rnn_36: 2.67e-04
- rnn_84: 3.92e-04
```

Linear models:

- linear_x1: 1.47e-02
- linear_12: 2.69e-02

Loss after 1000 and 300 epochs for DNN and RNN respectively:

DNN:

- Run 1: DNN-200x3-100x2
  - dnn_12: 8.80e-04
  - dnn_36: 3.78e-04
  - dnn_84: 4.47e-04
- Run 2: DNN-100x5
  - dnn_12: 1.13e-03
  - dnn_36: 5.88e-04
  - dnn_84: 5.49e-04

RNN:

- Run 1: LSTM-100x2-DNN-100x1
  - rnn_12: 3.96e-04
  - rnn_36: 2.87e-04
  - rnn_84: 3.88e-04
- Run 2: same architecture
  - rnn_12: 4.86e-04
  - rnn_36: 2.67e-04
  - rnn_84: 3.92e-04

Loss on Test1, Test2, Test4 (no data from Test2 was included in the training)

In [84]:

```
def create_separate_test_sets(df, features, outputs, n_steps=20, feature_idx=Non

    # select relevant features and outputs
    X = df[features].to_numpy()
    Y = df[outputs].to_numpy()
```

```
    # apply scaling
    X_normed = scaler_x.transform(X)
    Y_normed = scaler_y.transform(Y)

    # handle sequences
    X_seq, Y_seq = split_sequences(X_normed, Y_normed, n_steps)


    # select indices corresponding to desired feature
    if feature_idx:
        X = X[:,feature_idx]
        X_normed = X_normed[:,feature_idx]
        X_seq = X_seq[:,:,feature_idx]

    outputs = {
        'X': X, 'Y': Y,
        'X_normed': X_normed, 'Y_normed': Y_normed,
        'X_seq_normed': X_seq, 'Y_seq_normed': Y_seq,
        'Y_seq': scaler_y.inverse_transform(Y_seq)
        }

    # calculate model predictions
    if dnn_model:
        Y_pred_normed = dnn_model.predict(X_normed)
        Y_pred = scaler_y.inverse_transform(Y_pred_normed)
        outputs['Y_pred_normed'] = Y_pred_normed
        outputs['Y_pred'] = Y_pred
    if rnn_model:
        Y_seq_pred_normed = rnn_model.predict(X_seq)
        outputs['Y_seq_pred_normed'] = Y_seq_pred_normed
        Y_seq_pred = scaler_y.inverse_transform(Y_seq_pred_normed)
        outputs['Y_seq_pred'] = Y_seq_pred

    return outputs
```

In [85]:

```
tests_12 = dict()
for i,df in enumerate(datasets):
    tests_12[dataset_filenames[i]] = create_separate_test_sets(
        df, features_nth, outputs, n_steps, feature_idx=feature_idx,
        dnn_model=dnn_model_12, rnn_model=rnn_model_12)
```

In [86]:

```
tests_36 = dict()
for i,df in enumerate(datasets):
    tests_36[dataset_filenames[i]] = create_separate_test_sets(
        df, features_nth, outputs, n_steps, feature_idx=feature_idx_2nd,
        dnn_model=dnn_model_36, rnn_model=rnn_model_36)
```

In [87]:

```
tests_84 = dict()
for i,df in enumerate(datasets):
    tests_84[dataset_filenames[i]] = create_separate_test_sets(
        df, features_nth, outputs, n_steps, feature_idx=None,
        dnn_model=dnn_model_84, rnn_model=rnn_model_84)
```

In [88]:

```
print("Loss on full Test1, Test2, Test4 datasets:")
for filename in dataset_filenames:
```

```
    loss_dnn12 = dnn_model_12.evaluate(
        tests_12[filename]['X_normed'], tests_12[filename]['Y_normed'], verbose=
    loss_dnn36 = dnn_model_36.evaluate(
        tests_36[filename]['X_normed'], tests_36[filename]['Y_normed'], verbose=
    loss_dnn84 = dnn_model_84.evaluate(
        tests_84[filename]['X_normed'], tests_84[filename]['Y_normed'], verbose=
    loss_rnn12 = rnn_model_12.evaluate(
        tests_12[filename]['X_seq_normed'], tests_12[filename]['Y_seq_normed'],
    loss_rnn36 = rnn_model_36.evaluate(
        tests_36[filename]['X_seq_normed'], tests_36[filename]['Y_seq_normed'],
    loss_rnn84 = rnn_model_84.evaluate(
        tests_84[filename]['X_seq_normed'], tests_84[filename]['Y_seq_normed'],
    print("- {}:\n DNN-12: {:.2e}\n DNN-36: {:.2e}\n DNN-84: {:.2e}\n RNN-12: {:
        filename, loss_dnn12, loss_dnn36, loss_dnn84, loss_rnn12, loss_rnn36, lo
```

```
Loss on full Test1, Test2, Test4 datasets:
- Test1:
 DNN-12: 7.80e-04
 DNN-36: 4.62e-04
 DNN-84: 3.34e-04
 RNN-12: 2.22e-04
 RNN-36: 1.33e-04
 RNN-84: 2.40e-04
- Test2:
 DNN-12: 7.63e-02
 DNN-36: 2.86e-02
 DNN-84: 3.39e-02
 RNN-12: 6.12e-02
 RNN-36: 2.79e-03
 RNN-84: 4.41e-03
- Test4:
 DNN-12: 1.08e-03
 DNN-36: 5.42e-04
 DNN-84: 5.86e-04
 RNN-12: 4.43e-04
 RNN-36: 2.43e-04
 RNN-84: 3.44e-04
```

>> Note that no part of Test2 was included during training <<

Observations:

- The RNN does significantly better than any of the DNNs for all datasets. It has about an order of magnitude lower loss on Test2.
- DNN/RNN-84 does a bit worse than DNN/RNN-36, indicating that adding higher-order derivatives beyond acceleration makes learning harder. It may also not be worth it adding the additional derivatives. Perhaps training for more epochs could help.
- Comparing the loss on Test1 and Test4 (70 percent of Test1+Test4 was seen during training) w.r.t. loss on Test2, it is clear that all models struggled to generalize well to Test2. **There is room for improvement here.**

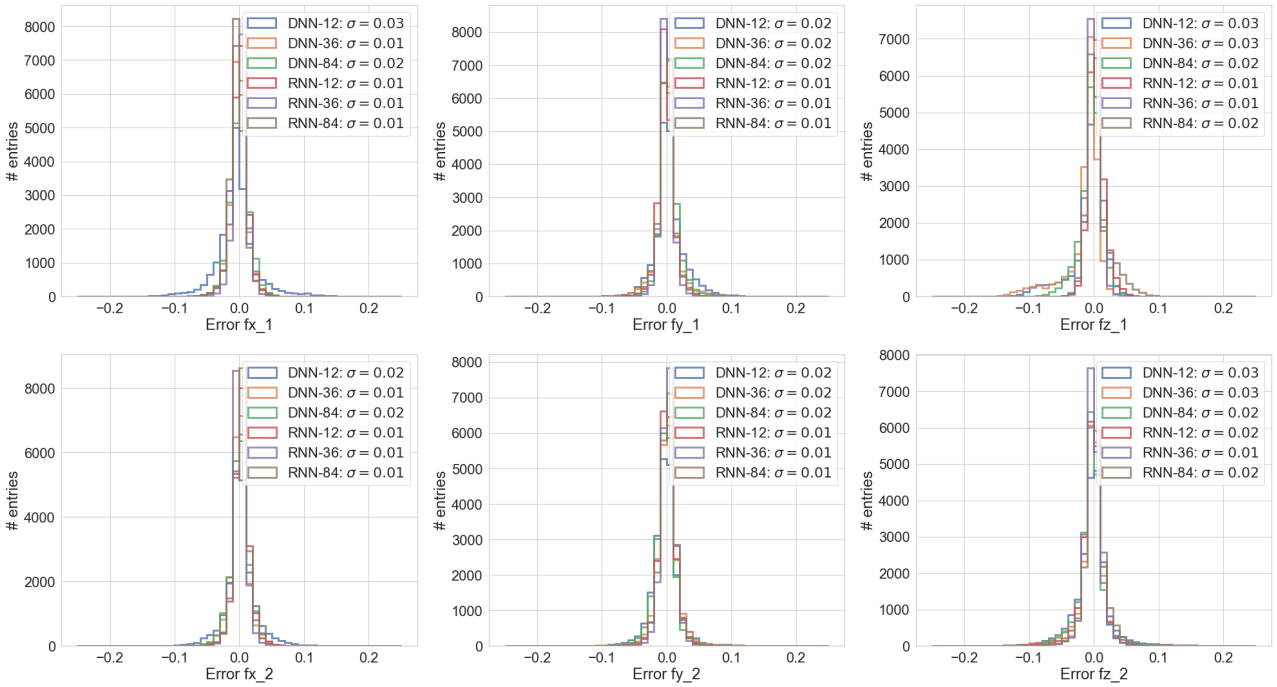
5.2. Prediction error

Model predictions on the different test sets

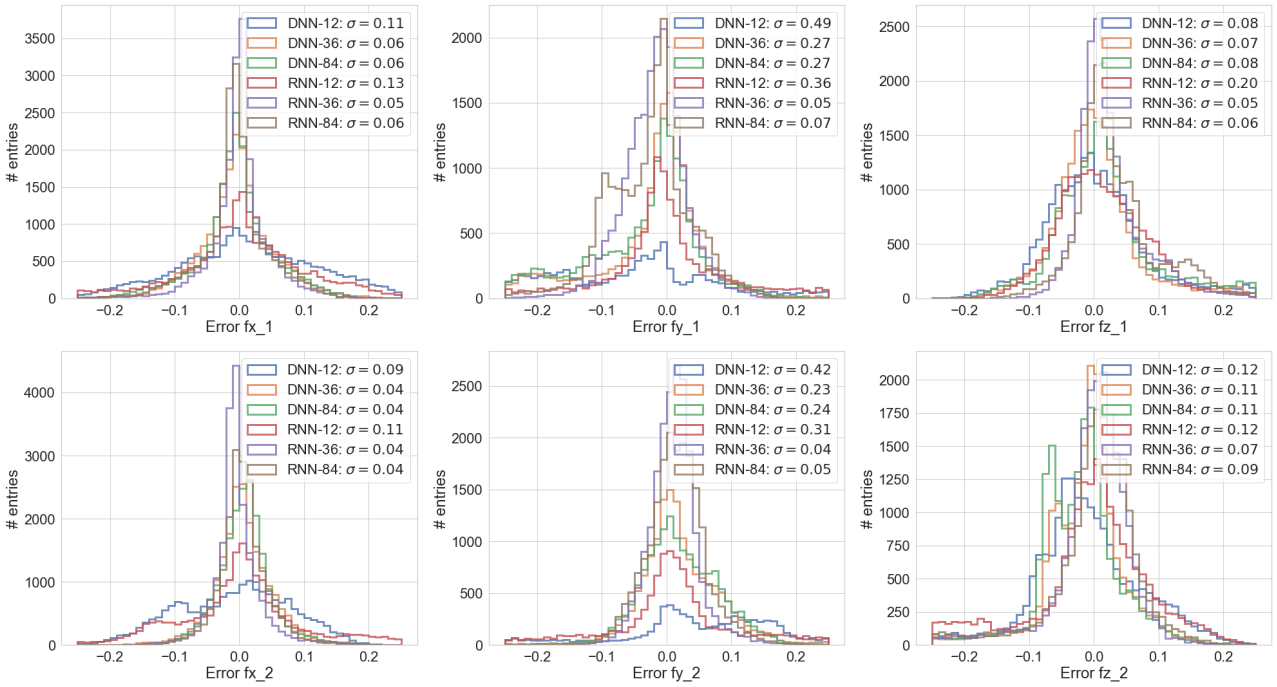
In [89]:
```
tmin = 0
```

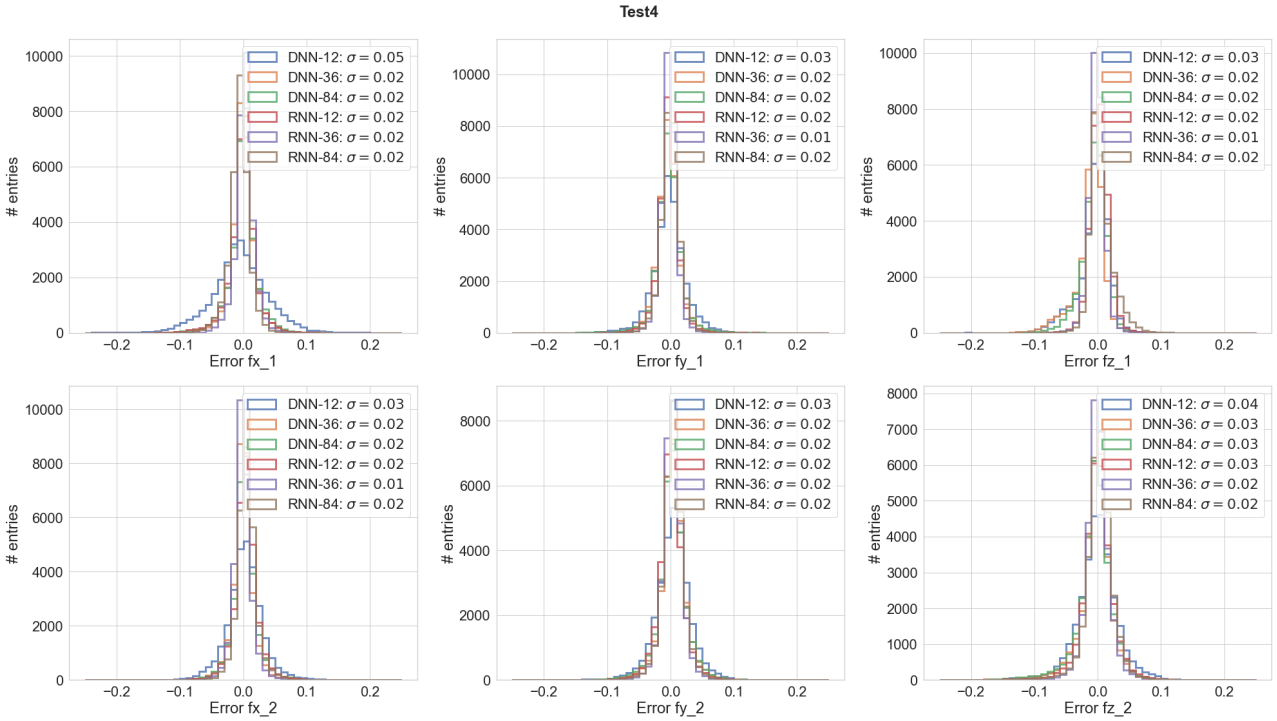
```
tmax = -1
bins=50
linewidth=3

sns.set(font_scale = 2)
sns.color_palette()
sns.set_style("whitegrid")
for filename in dataset_filenames:

    Y_err_12 = tests_12[filename]['Y_normed'] - tests_12[filename]['Y_pred_norme
    Y_err_36 = tests_36[filename]['Y_normed'] - tests_36[filename]['Y_pred_norme
    Y_err_84 = tests_84[filename]['Y_normed'] - tests_84[filename]['Y_pred_norme
    Y_seq_err_12 = tests_12[filename]['Y_seq_normed'] - tests_12[filename]['Y_se
    Y_seq_err_36 = tests_36[filename]['Y_seq_normed'] - tests_36[filename]['Y_se
    Y_seq_err_84 = tests_84[filename]['Y_seq_normed'] - tests_84[filename]['Y_se

    fig = plt.figure(figsize=(28,16))
    fig.suptitle(filename, weight='bold').set_fontsize('24')
    for i in range(len(outputs)):

        label_dnn12 = "DNN-12: $\sigma={:.2f}$".format(np.std(Y_err_12[:,i]))
        label_dnn36 = "DNN-36: $\sigma={:.2f}$".format(np.std(Y_err_36[:,i]))
        label_dnn84 = "DNN-84: $\sigma={:.2f}$".format(np.std(Y_err_84[:,i]))
        label_rnn12 = "RNN-12: $\sigma={:.2f}$".format(np.std(Y_seq_err_12[:,i])
        label_rnn36 = "RNN-36: $\sigma={:.2f}$".format(np.std(Y_seq_err_36[:,i])
        label_rnn84 = "RNN-84: $\sigma={:.2f}$".format(np.std(Y_seq_err_84[:,i])

        ax = fig.add_subplot(2,3,i+1)
        ax.hist(Y_err_12[:,i], bins=bins, range=(-0.25, 0.25), alpha=0.8, histty
        ax.hist(Y_err_36[:,i], bins=bins, range=(-0.25, 0.25), alpha=0.8, histty
        ax.hist(Y_err_84[:,i], bins=bins, range=(-0.25, 0.25), alpha=0.8, histty
        ax.hist(Y_seq_err_12[:,i], bins=bins, range=(-0.25, 0.25), alpha=0.8, hi
        ax.hist(Y_seq_err_36[:,i], bins=bins, range=(-0.25, 0.25), alpha=0.8, hi
        ax.hist(Y_seq_err_84[:,i], bins=bins, range=(-0.25, 0.25), alpha=0.8, hi
        ax.set_xlabel('Error {}'.format(outputs[i]))
        ax.set_ylabel('# entries')
        ax.legend()
    plt.tight_layout()
    plt.savefig(output_dir/'{}_error.pdf'.format(filename))
```

Test1


DNN-12: σ = 0.03
DNN-36: σ = 0.01
DNN-84: σ = 0.02
RNN-12: σ = 0.01
RNN-36: σ = 0.01
RNN-84: σ = 0.01
entries
Error fx_1
DNN-12: σ = 0.02
DNN-36: σ = 0.02
DNN-84: σ = 0.02
RNN-12: σ = 0.01
RNN-36: σ = 0.01
RNN-84: σ = 0.01
entries
Error fy_1
DNN-12: σ = 0.03
DNN-36: σ = 0.03
DNN-84: σ = 0.02
RNN-12: σ = 0.01
RNN-36: σ = 0.01
RNN-84: σ = 0.02
entries
Error fz_1
DNN-12: σ = 0.02
DNN-36: σ = 0.01
DNN-84: σ = 0.02
RNN-12: σ = 0.01
RNN-36: σ = 0.01
RNN-84: σ = 0.01
entries
Error fx_2
DNN-12: σ = 0.02
DNN-36: σ = 0.02
DNN-84: σ = 0.02
RNN-12: σ = 0.01
RNN-36: σ = 0.01
RNN-84: σ = 0.01
entries
Error fy_2
DNN-12: σ = 0.03
DNN-36: σ = 0.03
DNN-84: σ = 0.02
RNN-12: σ = 0.02
RNN-36: σ = 0.01
RNN-84: σ = 0.02
entries
Error fz_2

Test2


DNN-12: σ = 0.11
DNN-36: σ = 0.06
DNN-84: σ = 0.06
RNN-12: σ = 0.13
RNN-36: σ = 0.05
RNN-84: σ = 0.06
entries
Error fx_1
DNN-12: σ = 0.49
DNN-36: σ = 0.27
DNN-84: σ = 0.27
RNN-12: σ = 0.36
RNN-36: σ = 0.05
RNN-84: σ = 0.07
entries
Error fy_1
DNN-12: σ = 0.08
DNN-36: σ = 0.07
DNN-84: σ = 0.08
RNN-12: σ = 0.20
RNN-36: σ = 0.05
RNN-84: σ = 0.06
entries
Error fz_1
DNN-12: σ = 0.09
DNN-36: σ = 0.04
DNN-84: σ = 0.04
RNN-12: σ = 0.11
RNN-36: σ = 0.04
RNN-84: σ = 0.04
entries
Error fx_2
DNN-12: σ = 0.42
DNN-36: σ = 0.23
DNN-84: σ = 0.24
RNN-12: σ = 0.31
RNN-36: σ = 0.04
RNN-84: σ = 0.05
entries
Error fy_2
DNN-12: σ = 0.12
DNN-36: σ = 0.11
DNN-84: σ = 0.11
RNN-12: σ = 0.12
RNN-36: σ = 0.07
RNN-84: σ = 0.09
entries
Error fz_2



Observations:

- The RNN models outperforms the DNN models.
- The error is low (1-2% for RNN-36/84) on Test1 and Test4 (70% of Test1+Test4 was seen during training).
- The error is significantly higher (4-10%) for RNN-36/84 on Test2 (not seen during training).

R2 score

In [90]:
```
from sklearn.metrics import r2_score

print("R2 score on Test1, Test2, Test4 datasets:")
print("(" + " ".join(outputs) + ")")
for filename in dataset_filenames:

    r2_dnn12 = ['DNN-12:']
    r2_dnn36 = ['DNN-36:']
    r2_dnn84 = ['DNN-84:']
    r2_rnn12 = ['RNN-12:']
    r2_rnn36 = ['RNN-36:']
    r2_rnn84 = ['RNN-84:']
    for i in range(len(outputs)):
        r2_dnn12.append("{:.2f}".format(r2_score(tests_12[filename]['Y_normed'][
        r2_dnn36.append("{:.2f}".format(r2_score(tests_36[filename]['Y_normed'][
        r2_dnn84.append("{:.2f}".format(r2_score(tests_84[filename]['Y_normed'][
        r2_rnn12.append("{:.2f}".format(r2_score(tests_12[filename]['Y_seq_norme
        r2_rnn36.append("{:.2f}".format(r2_score(tests_36[filename]['Y_seq_norme
        r2_rnn84.append("{:.2f}".format(r2_score(tests_84[filename]['Y_seq_norme

    print("- {}:".format(filename))
    print("\t"+"\t".join(r2_dnn12))
    print("\t"+"\t".join(r2_dnn36))
    print("\t"+"\t".join(r2_dnn84))
    print("\t"+"\t".join(r2_rnn12))
```

```
    print("\t"+"\t".join(r2_rnn36))
    print("\t"+"\t".join(r2_rnn84))
```

```
R2 score on Test1, Test2, Test4 datasets:
(fx_1 fy_1 fz_1 fx_2 fy_2 fz_2)
- Test1:
        DNN-12: 0.97    0.99    0.97    0.98    0.99    0.94
        DNN-36: 0.99    1.00    0.96    0.99    0.99    0.96
        DNN-84: 0.99    1.00    0.98    0.99    1.00    0.97
        RNN-12: 0.99    1.00    0.99    0.99    1.00    0.98
        RNN-36: 1.00    1.00    1.00    1.00    1.00    0.99
        RNN-84: 0.99    1.00    0.98    0.99    1.00    0.98
- Test2:
        DNN-12: 0.57    -2.08   0.70    0.61    -2.13   -0.05
        DNN-36: 0.88    -0.09   0.78    0.90    -0.12   0.06
        DNN-84: 0.87    -0.32   0.67    0.91    -0.30   -0.09
        RNN-12: 0.46    -1.08   -1.13   0.45    -1.10   -0.11
        RNN-36: 0.92    0.97    0.85    0.93    0.97    0.61
        RNN-84: 0.89    0.94    0.75    0.91    0.96    0.35
- Test4:
        DNN-12: 0.94    0.99    0.97    0.96    0.98    0.85
        DNN-36: 0.99    0.99    0.97    0.98    0.99    0.89
        DNN-84: 0.98    0.99    0.98    0.98    0.99    0.88
        RNN-12: 0.99    0.99    0.99    0.98    0.99    0.92
        RNN-36: 0.99    1.00    0.99    0.99    0.99    0.95
        RNN-84: 0.99    1.00    0.98    0.99    0.99    0.94
```

The coefficient of determination (R2) is the proportion of the variation in the dependent variable (e.g., predicted forces) that is predictable from the independent variables (e.g., measured forces). The range is from negative infinity to +1.

- An R2 score of +1 indicates that the predictions match the observations perfectly.
- An R2 score of 0 indicates that the predictions are as good as random guesses around the mean of the observations.
- Negative R2 indicates that the predictions are worse than random.

Observations:

- All models do pretty well on Test1 and Test4, of which a significant fraction (70%) was seen during training.
- The RNN models does significantly better on Test2, which was not seen during training.
- Although it did better than the DNN models, even the RNN struggled to predict forces in the z-direction on the Test2 dataset (especially for R2).

Pearson corrrelation coefficient

In [91]:
```
def pearson(x, y):
   corr = np.corrcoef(x, y)
   return corr[0,1]
```

In [92]:
```
print("Pearson correlations for Test1, Test2, Test4 datasets:")
print("(" + " ".join(outputs) + ")")
for filename in dataset_filenames:

    pearson_dnn12 = ['DNN-12:']
```

```
    pearson_dnn36 = ['DNN-36:']
    pearson_dnn84 = ['DNN-84:']
    pearson_rnn12 = ['RNN-12:']
    pearson_rnn36 = ['RNN-36:']
    pearson_rnn84 = ['RNN-84:']
    for i in range(len(outputs)):
        pearson_dnn12.append("{:.2f}".format(pearson(tests_12[filename]['Y_norme
        pearson_dnn36.append("{:.2f}".format(pearson(tests_36[filename]['Y_norme
        pearson_dnn84.append("{:.2f}".format(pearson(tests_84[filename]['Y_norme
        pearson_rnn12.append("{:.2f}".format(pearson(tests_12[filename]['Y_seq_n
        pearson_rnn36.append("{:.2f}".format(pearson(tests_36[filename]['Y_seq_n
        pearson_rnn84.append("{:.2f}".format(pearson(tests_84[filename]['Y_seq_n

    print("- {}:".format(filename))
    print("\t"+"\t".join(pearson_dnn12))
    print("\t"+"\t".join(pearson_dnn36))
    print("\t"+"\t".join(pearson_dnn84))
    print("\t"+"\t".join(pearson_rnn12))
    print("\t"+"\t".join(pearson_rnn36))
    print("\t"+"\t".join(pearson_rnn84))
```

```
Pearson correlations for Test1, Test2, Test4 datasets:
(fx_1 fy_1 fz_1 fx_2 fy_2 fz_2)
- Test1:
        DNN-12: 0.98    1.00    0.99    0.99    1.00    0.97
        DNN-36: 1.00    1.00    0.99    1.00    1.00    0.98
        DNN-84: 1.00    1.00    0.99    1.00    1.00    0.98
        RNN-12: 1.00    1.00    1.00    1.00    1.00    0.99
        RNN-36: 1.00    1.00    1.00    1.00    1.00    0.99
        RNN-84: 1.00    1.00    0.99    1.00    1.00    0.99
- Test2:
        DNN-12: 0.78    -0.57   0.85    0.79    -0.60   0.29
        DNN-36: 0.94    0.49    0.89    0.95    0.47    0.45
        DNN-84: 0.94    0.44    0.85    0.95    0.42    0.40
        RNN-12: 0.68    -0.11   0.52    0.67    -0.11   0.35
        RNN-36: 0.96    0.98    0.94    0.96    0.99    0.79
        RNN-84: 0.95    0.97    0.91    0.96    0.98    0.61
- Test4:
        DNN-12: 0.97    0.99    0.99    0.98    0.99    0.92
        DNN-36: 0.99    1.00    0.99    0.99    1.00    0.95
        DNN-84: 0.99    1.00    0.99    0.99    0.99    0.94
        RNN-12: 0.99    1.00    0.99    0.99    1.00    0.96
        RNN-36: 1.00    1.00    1.00    0.99    1.00    0.98
        RNN-84: 1.00    1.00    0.99    0.99    1.00    0.97
```

The Pearson correlation coefficient (r) can range from -1 to +1.

- An r of -1 indicates a perfect negative linear correlation.
- An r of 0 indicates no correlation.
- An r of +1 indicates a perfect positive linear correlation.

Observations:

- Similar to the observations for the R2 score.

5.3. Time series plots of prediction vs. ground truth

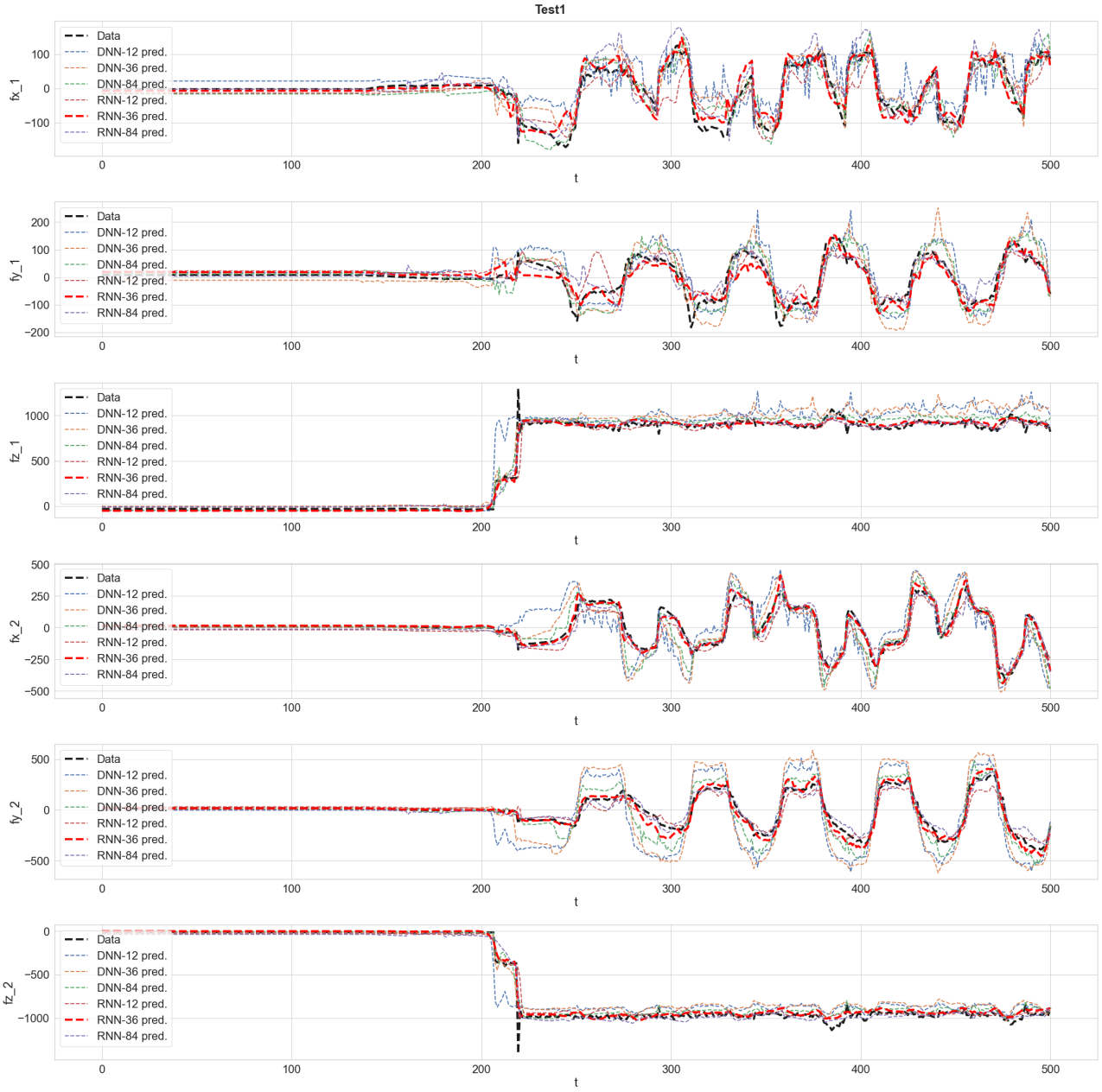
In [93]:

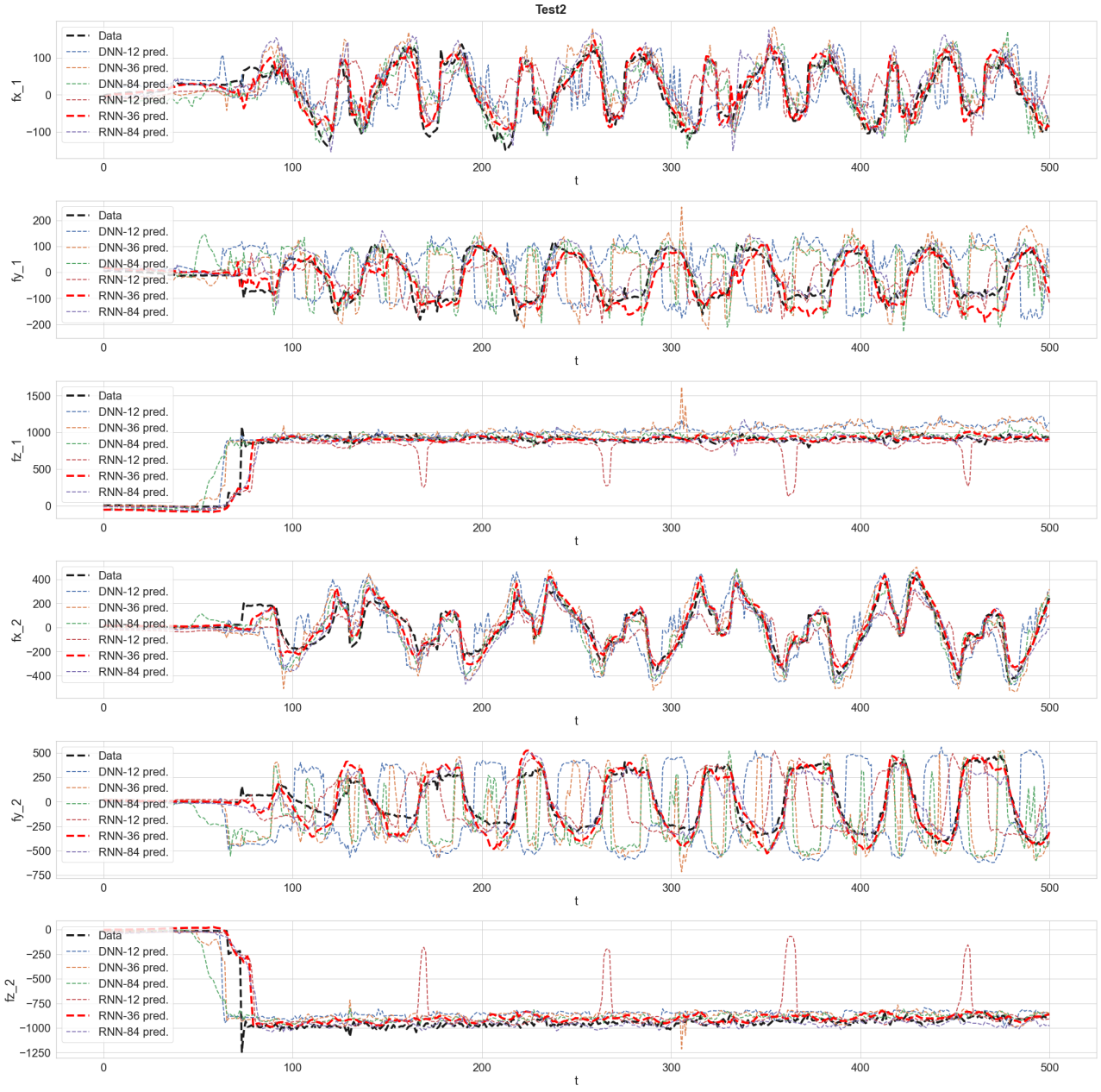
```
def plot_timeseries(tmin = 12000, tmax = 12500, linewidth=4):
```

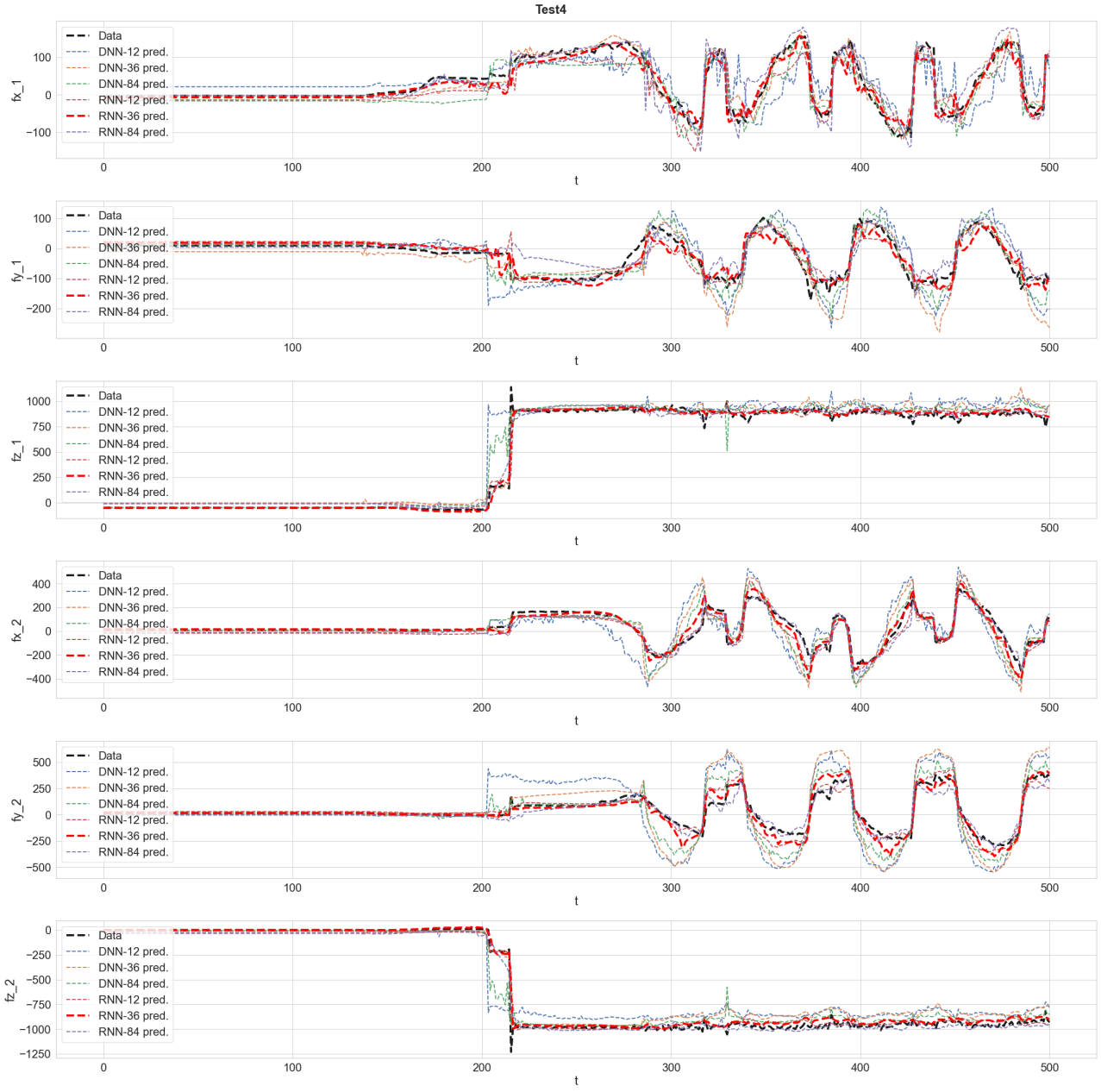
```
    t = np.linspace(tmin, tmax, tmax-tmin)
    sns.set(font_scale = 2)
    sns.color_palette()
    sns.set_style("whitegrid")
    for filename in dataset_filenames:

        fig = plt.figure(figsize=(30,30))
        fig.suptitle(filename, weight='bold').set_fontsize('24')
        for i in range(6):
            ax = fig.add_subplot(6, 1, i+1)
            ax.plot(t, tests_12[filename]['Y'].T[i][tmin+n_steps-1:tmax+n_steps-
            ax.plot(t, tests_12[filename]['Y_pred'].T[i][tmin+n_steps-1:tmax+n_s
            ax.plot(t, tests_36[filename]['Y_pred'].T[i][tmin+n_steps-1:tmax+n_s
            ax.plot(t, tests_84[filename]['Y_pred'].T[i][tmin+n_steps-1:tmax+n_s
            ax.plot(t, tests_12[filename]['Y_seq_pred'].T[i][tmin:tmax], label='
            ax.plot(t, tests_36[filename]['Y_seq_pred'].T[i][tmin:tmax], label='
            ax.plot(t, tests_84[filename]['Y_seq_pred'].T[i][tmin:tmax], label='
            ax.set_xlabel('t')
            ax.set_ylabel(outputs[i])
            ax.legend(loc=2)
        plt.tight_layout()
        plt.savefig(output_dir/'{}_timeseries_t{}to{}.pdf'.format(filename, tmin
```

In [94]:

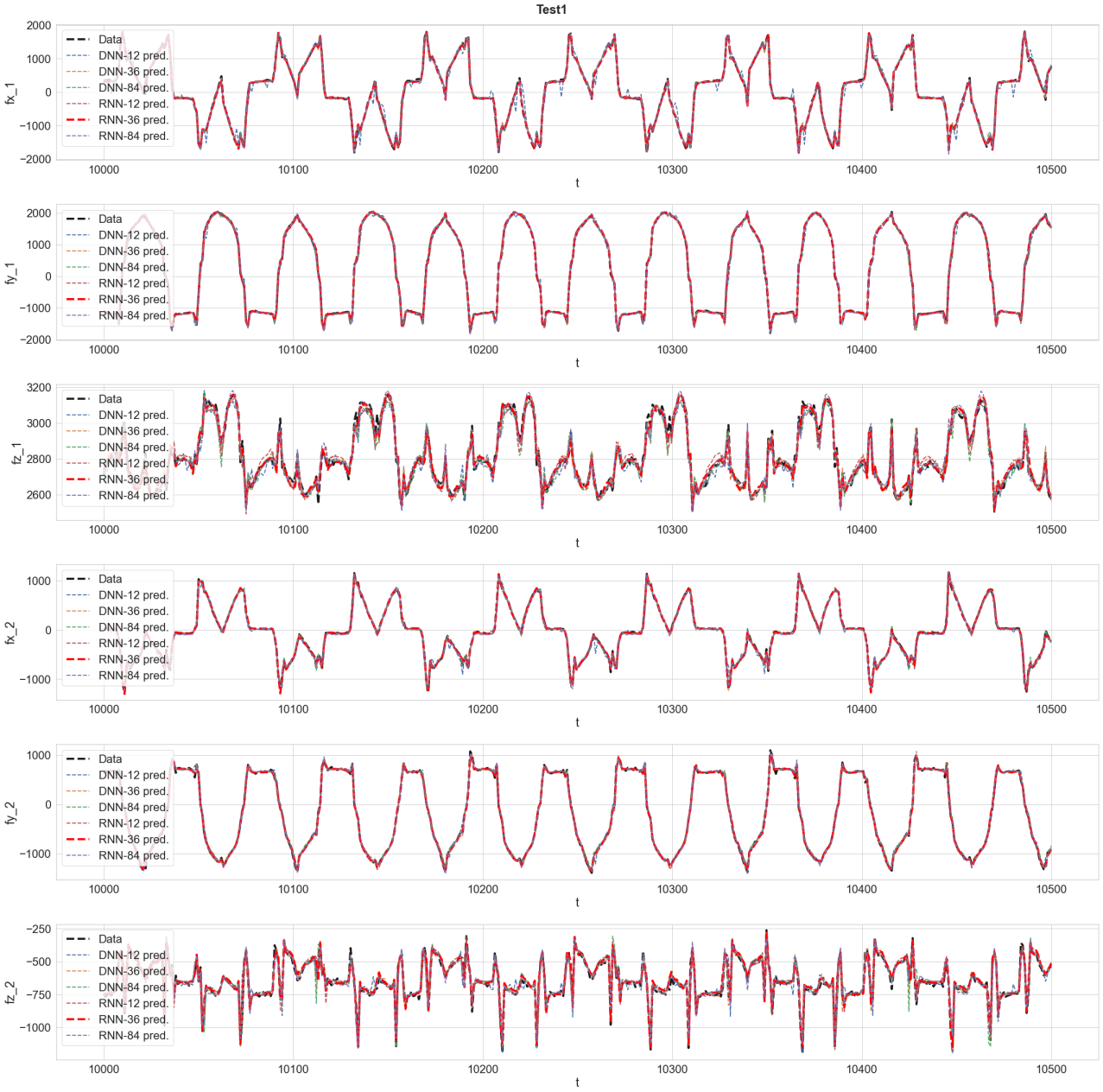
```
plot_timeseries(tmin=0, tmax=500)
```

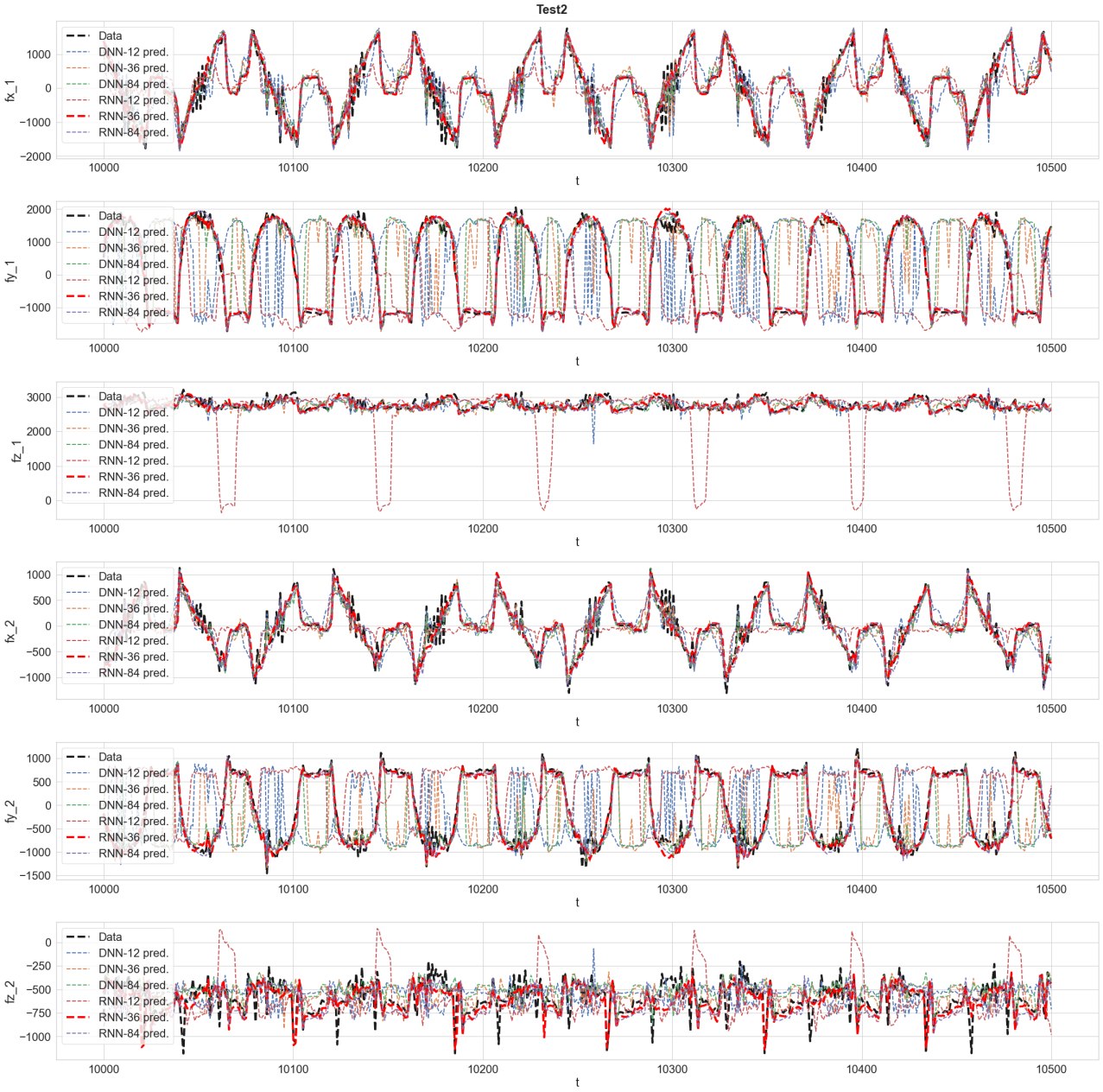

Test1
Data
DNN-12 pred.
DNN-36 pred.
DNN-84 pred.
RNN-12 pred.
RNN-36 pred.
RNN-84 pred.
fx_1
fy_1
fz_1
fx_2
fy_2
fz_2
t

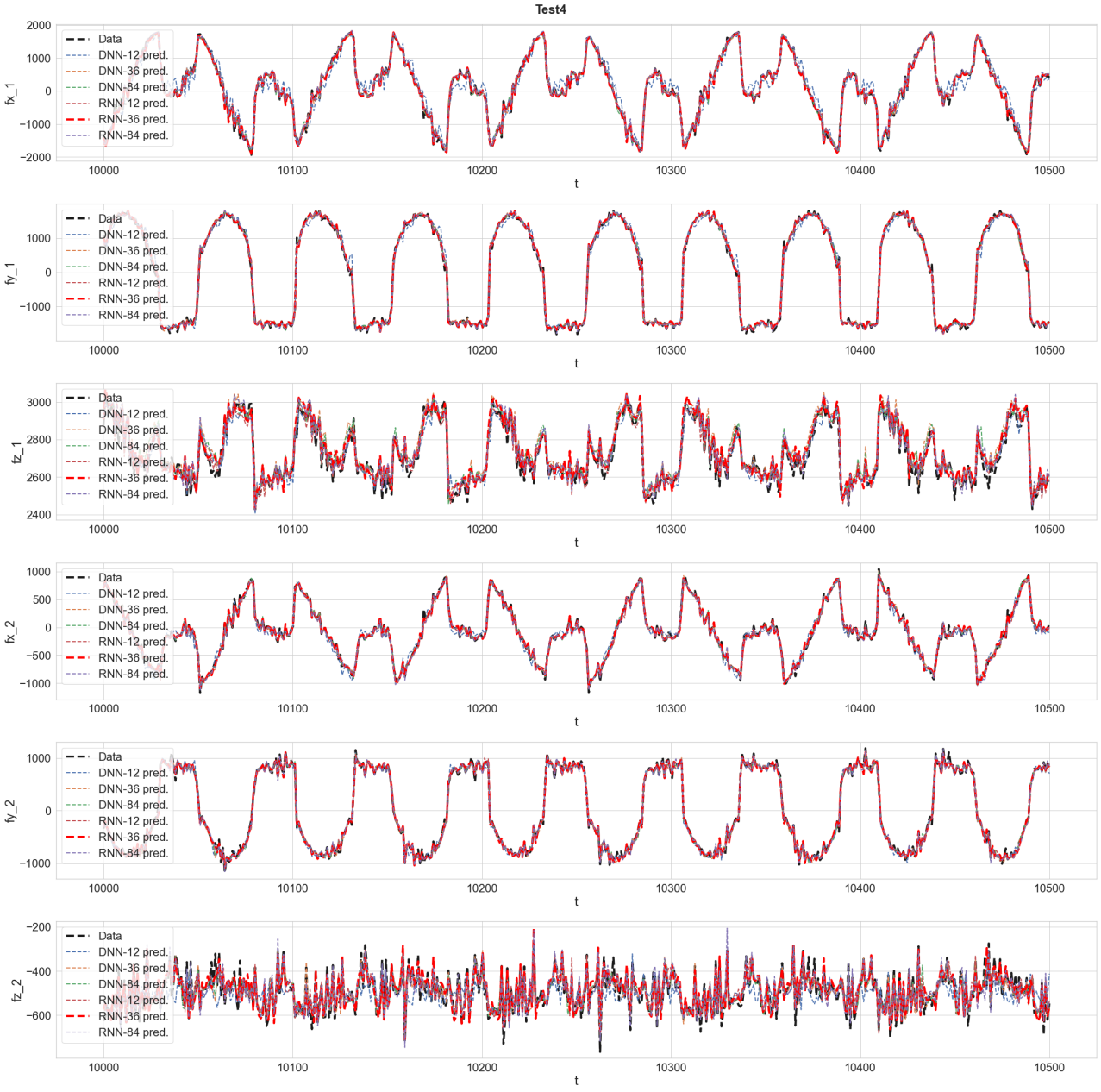

Test2
Data
DNN-12 pred.
DNN-36 pred.
DNN-84 pred.
RNN-12 pred.
RNN-36 pred.
RNN-84 pred.
fx_1
fy_1
fz_1
fx_2
fy_2
fz_2
t



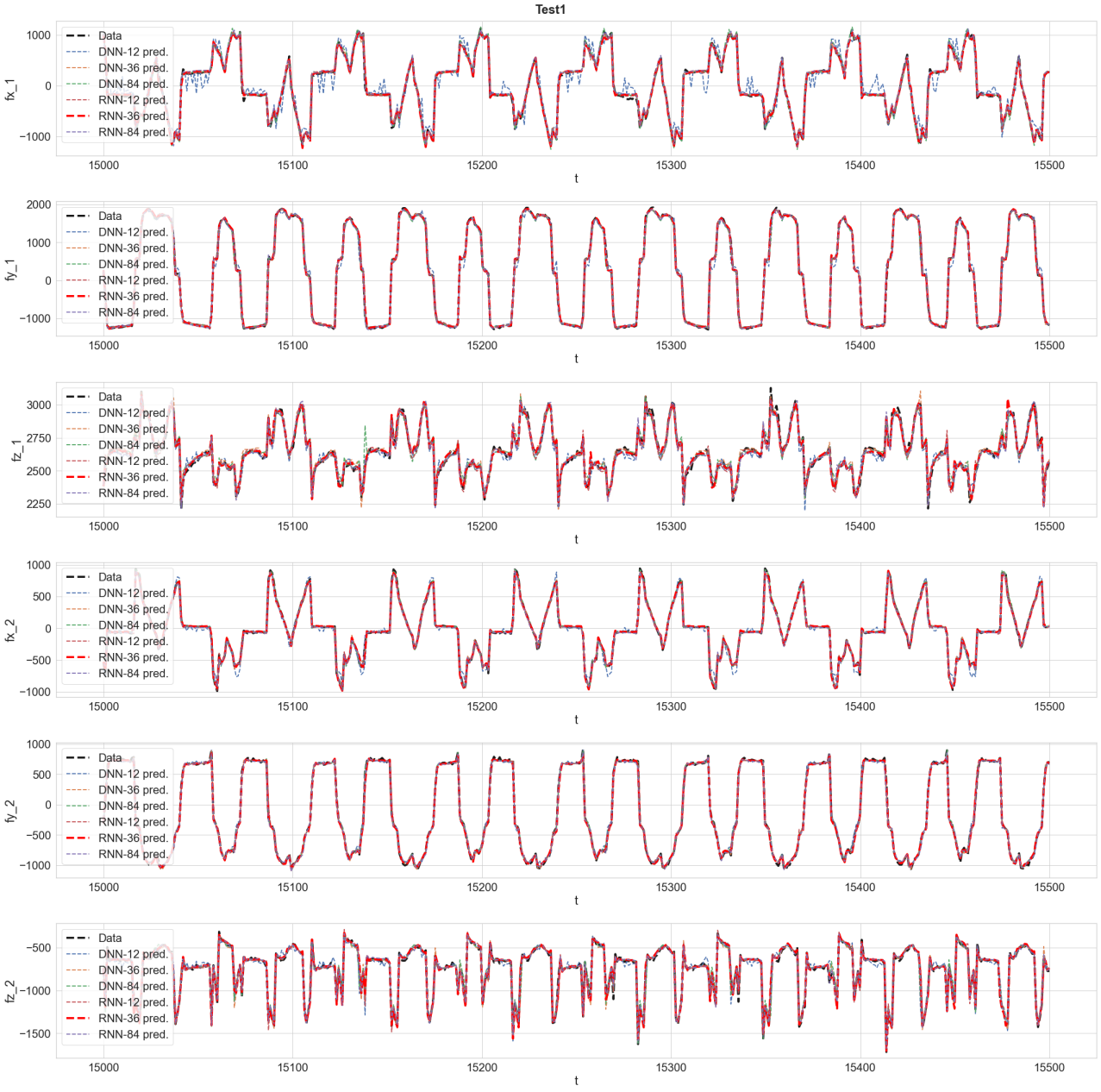
In [95]:
```
plot_timeseries(tmin=10000, tmax=10500)
```

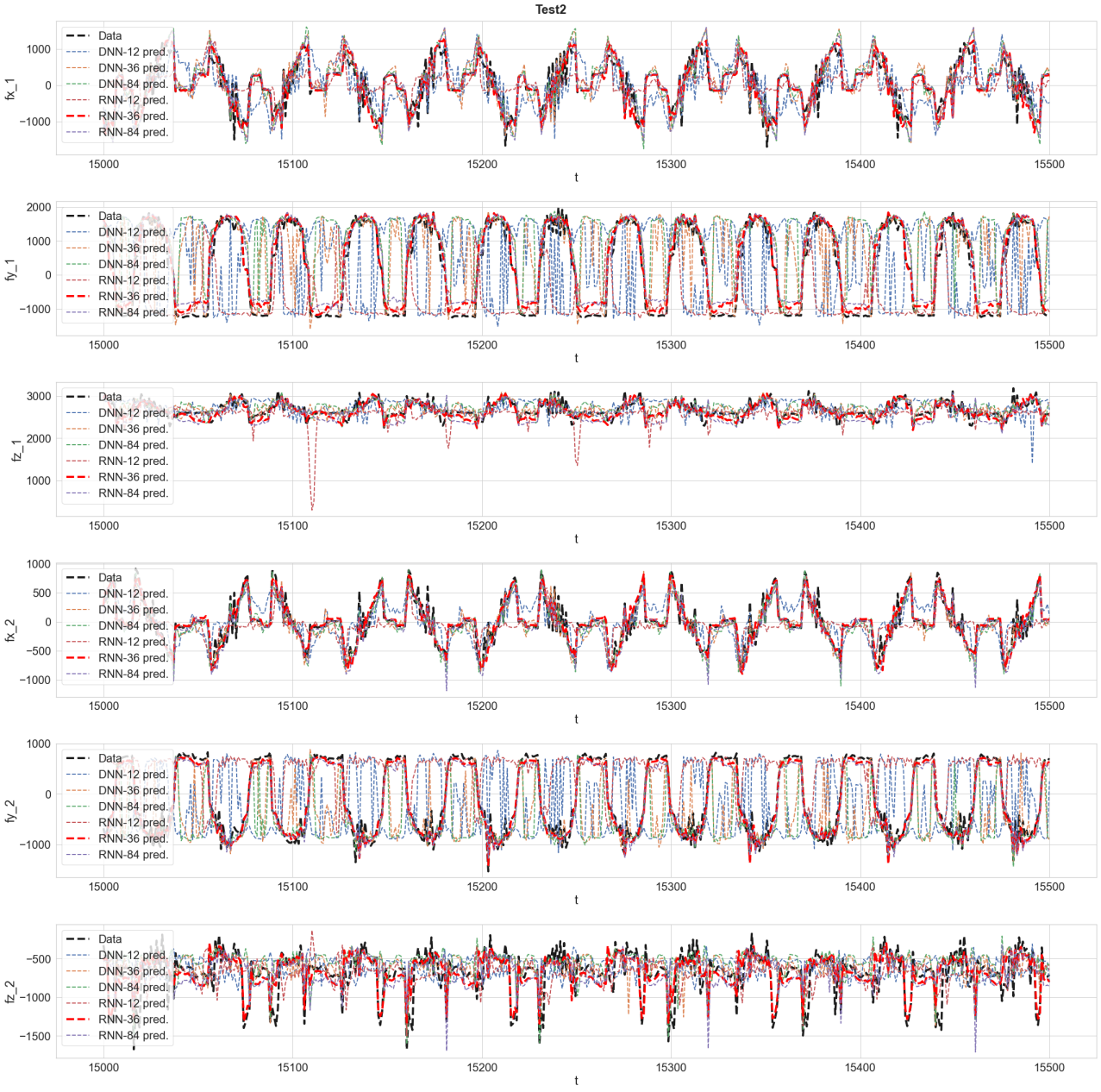

Test1
fx_1
fy_1
fz_1
fx_2
fy_2
fz_2
t
Data
DNN-12 pred.
DNN-36 pred.
DNN-84 pred.
RNN-12 pred.
RNN-36 pred.
RNN-84 pred.

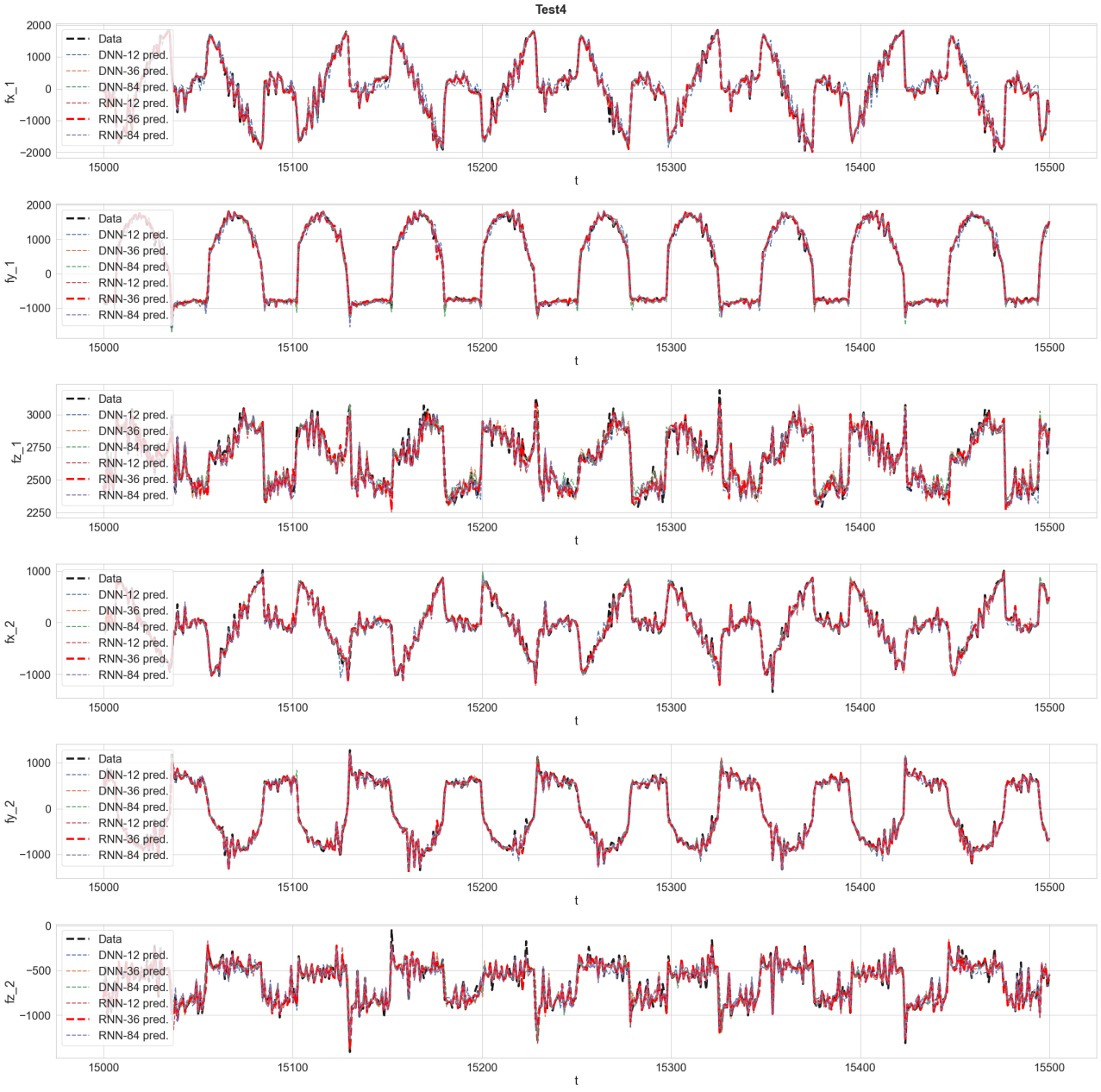

Test2
Data
DNN-12 pred.
DNN-36 pred.
DNN-84 pred.
RNN-12 pred.
RNN-36 pred.
RNN-84 pred.
fx_1
fy_1
fz_1
fx_2
fy_2
fz_2
t
10000
10100
10200
10300
10400
10500



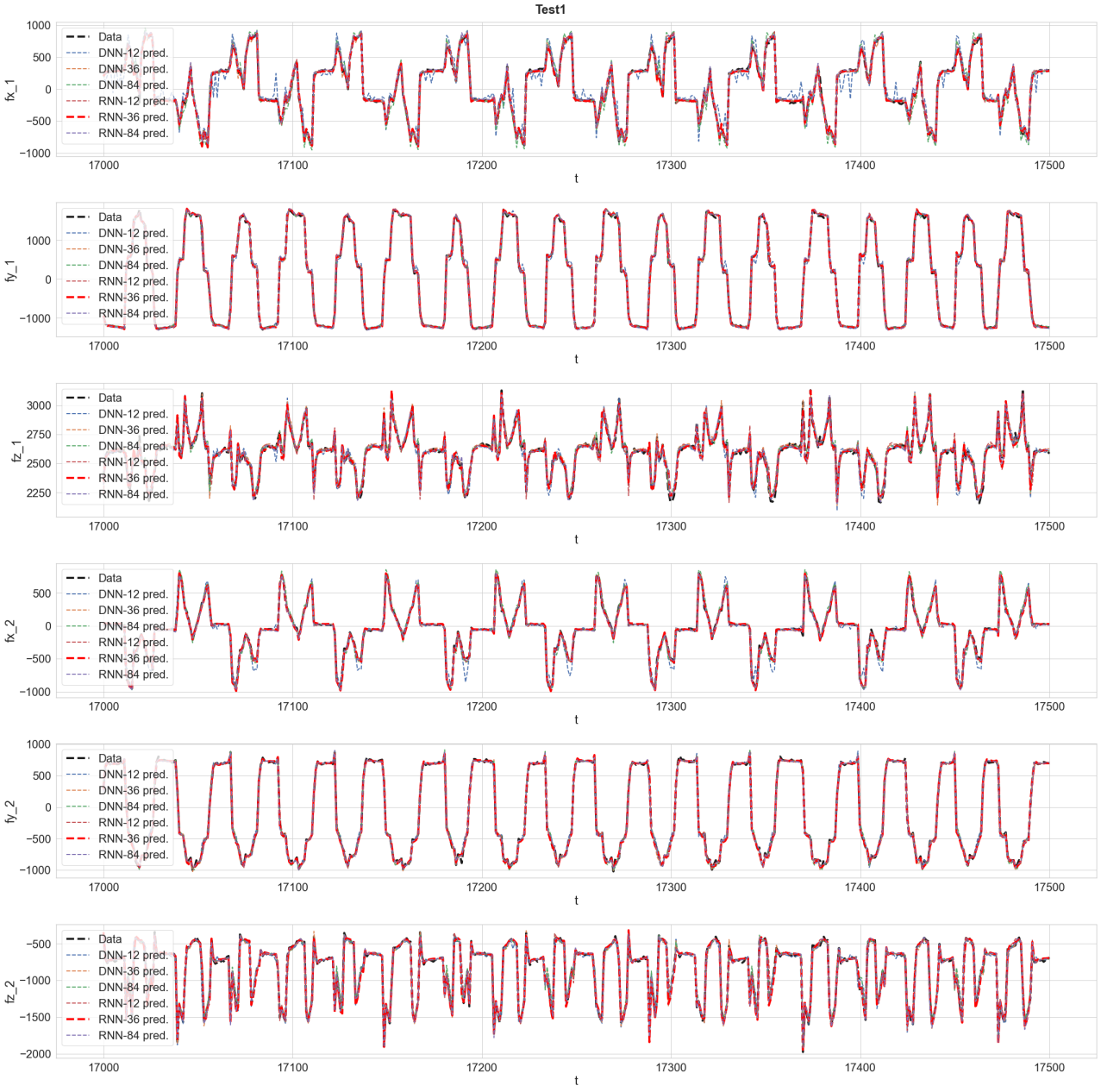
In [96]:
```
plot_timeseries(tmin=15000, tmax=15500)
```

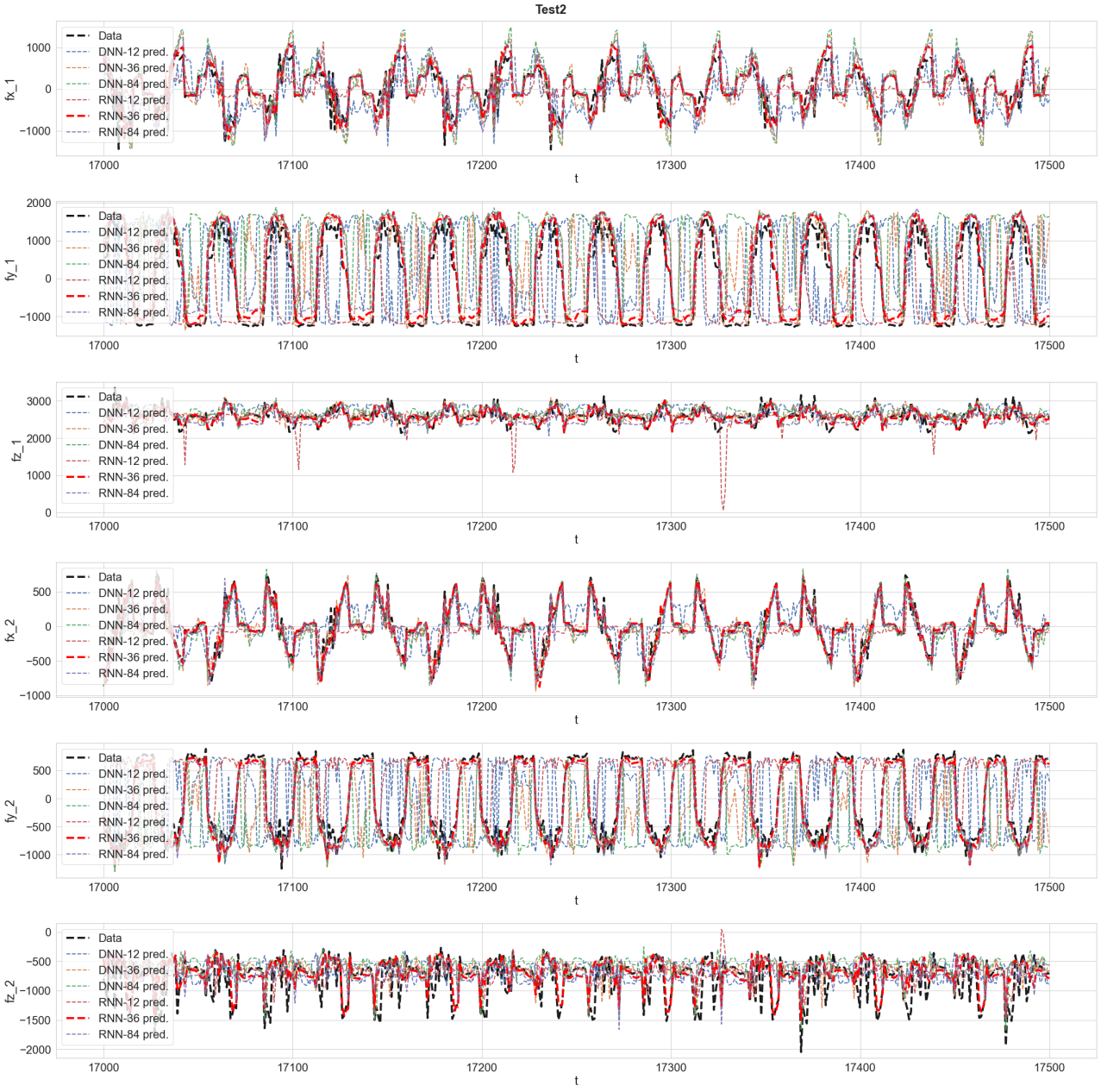

Test1
fx_1
fy_1
fz_1
fx_2
fy_2
fz_2
t
Data
DNN-12 pred.
DNN-36 pred.
DNN-84 pred.
RNN-12 pred.
RNN-36 pred.
RNN-84 pred.

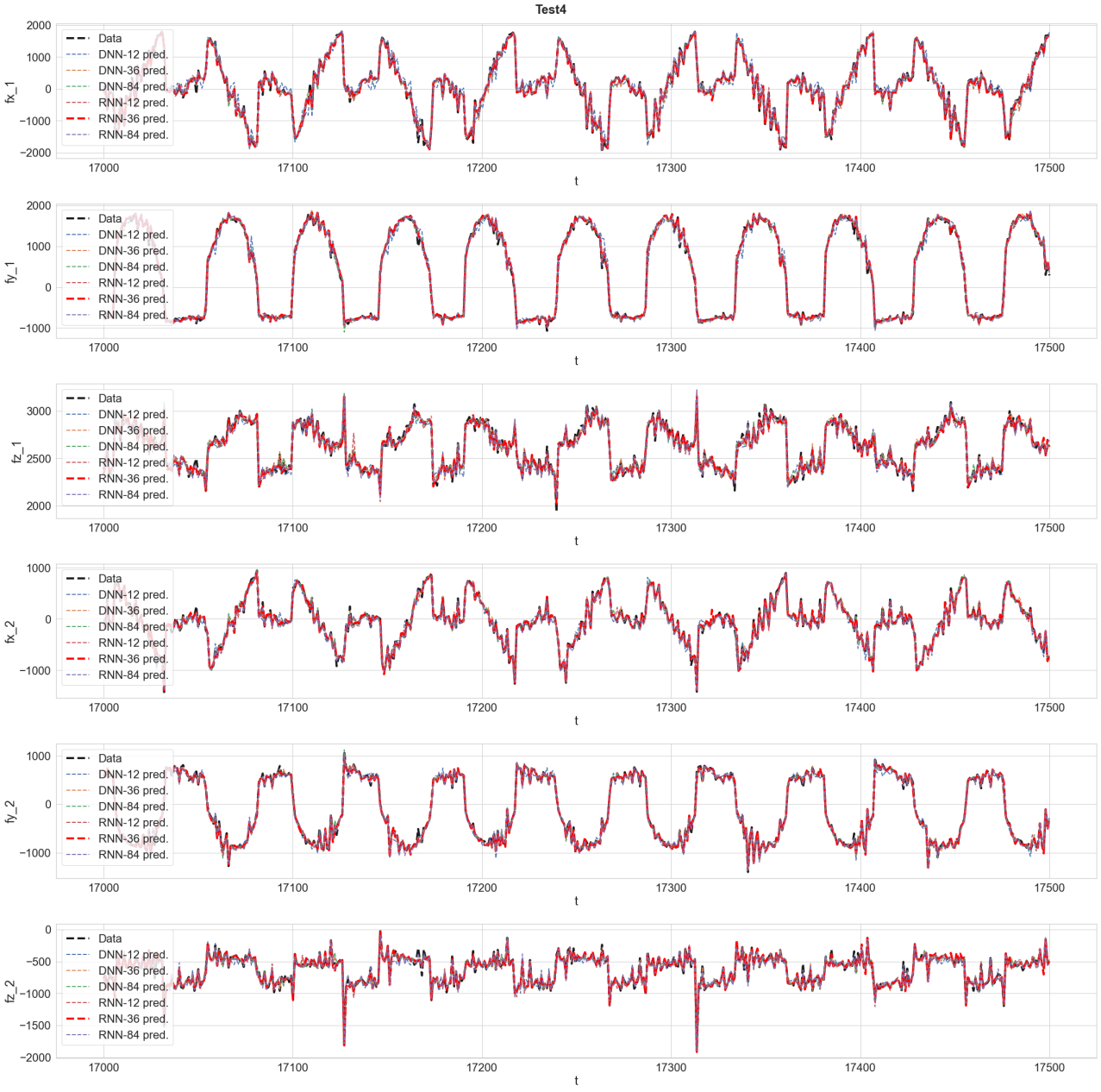

Test2
Data
DNN-12 pred.
DNN-36 pred.
DNN-84 pred.
RNN-12 pred.
RNN-36 pred.
RNN-84 pred.
fx_1
fy_1
fz_1
fx_2
fy_2
fz_2
t
15000
15100
15200
15300
15400
15500



In [97]:
```
plot_timeseries(tmin=17000, tmax=17500)
```

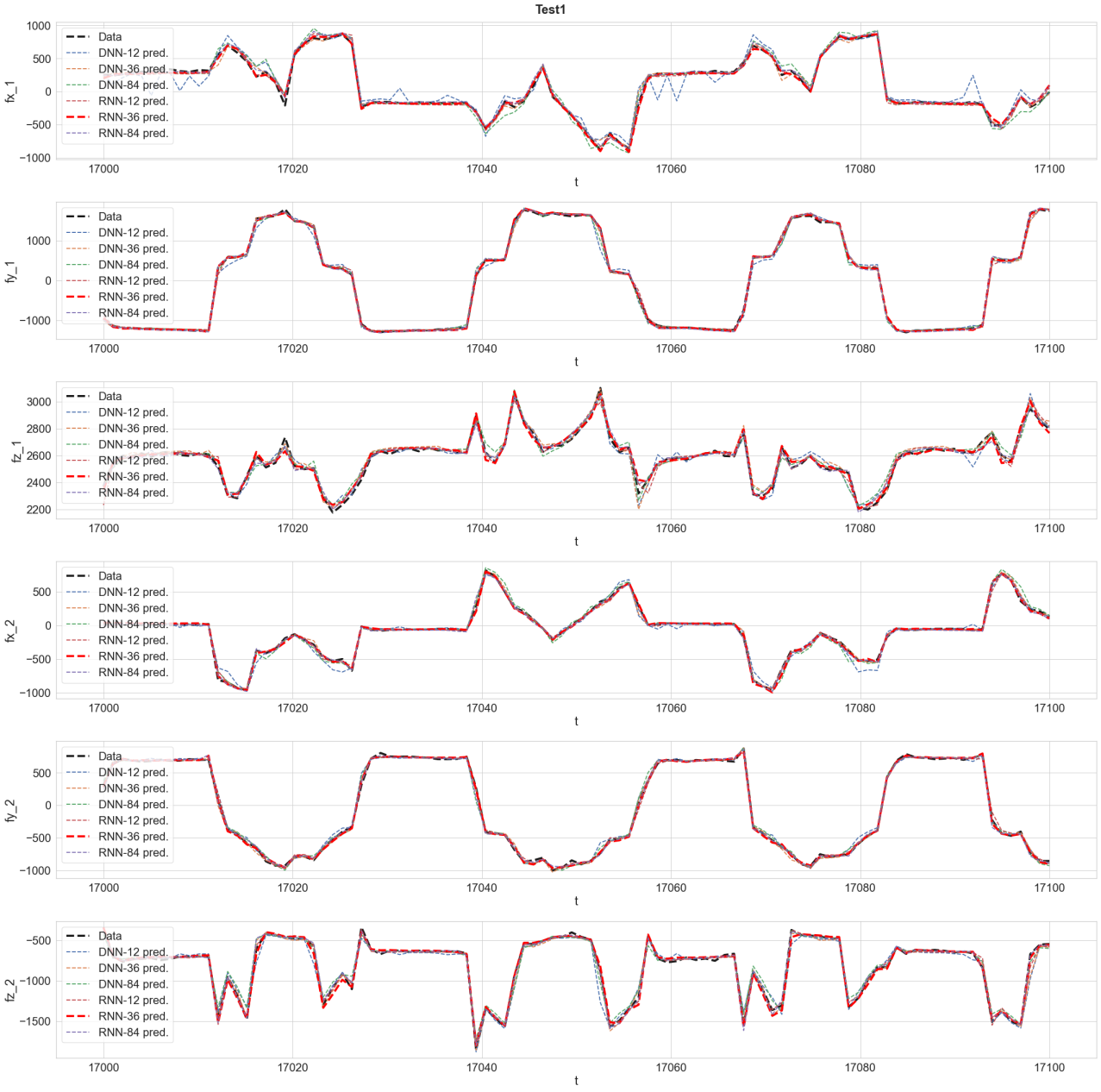

Test1
fx_1
fy_1
fz_1
fx_2
fy_2
fz_2
t
Data
DNN-12 pred.
DNN-36 pred.
DNN-84 pred.
RNN-12 pred.
RNN-36 pred.
RNN-84 pred.

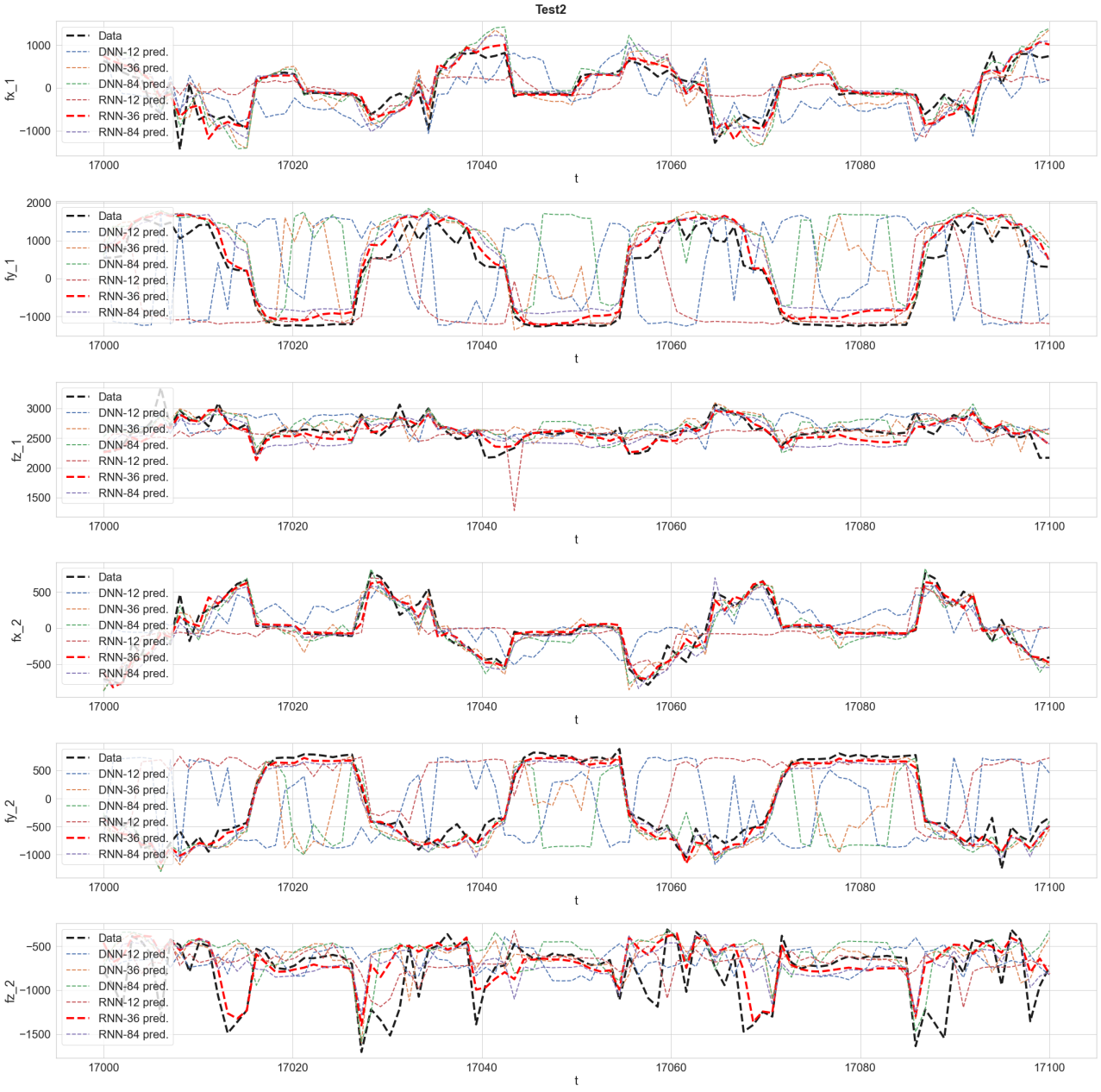

Test2
Data
DNN-12 pred.
DNN-36 pred.
DNN-84 pred.
RNN-12 pred.
RNN-36 pred.
RNN-84 pred.
fx_1
fy_1
fz_1
fx_2
fy_2
fz_2
t
17000
17100
17200
17300
17400
17500

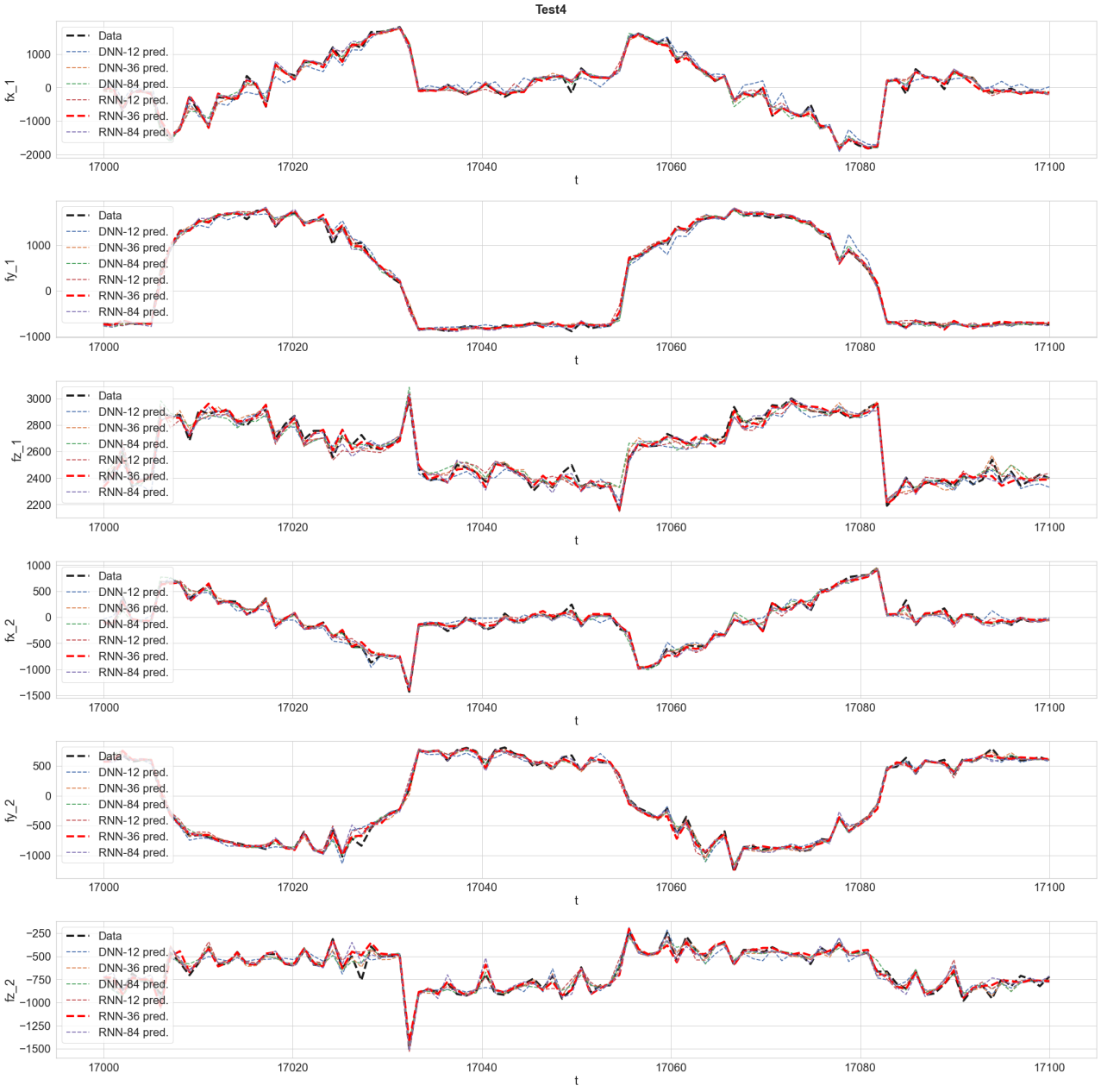


In [98]:

```
plot_timeseries(tmin=17000, tmax=17100)
```


Test1
Data
DNN-12 pred.
DNN-36 pred.
DNN-84 pred.
RNN-12 pred.
RNN-36 pred.
RNN-84 pred.
fx_1
fy_1
fz_1
fx_2
fy_2
fz_2
t
17000
17020
17040
17060
17080
17100

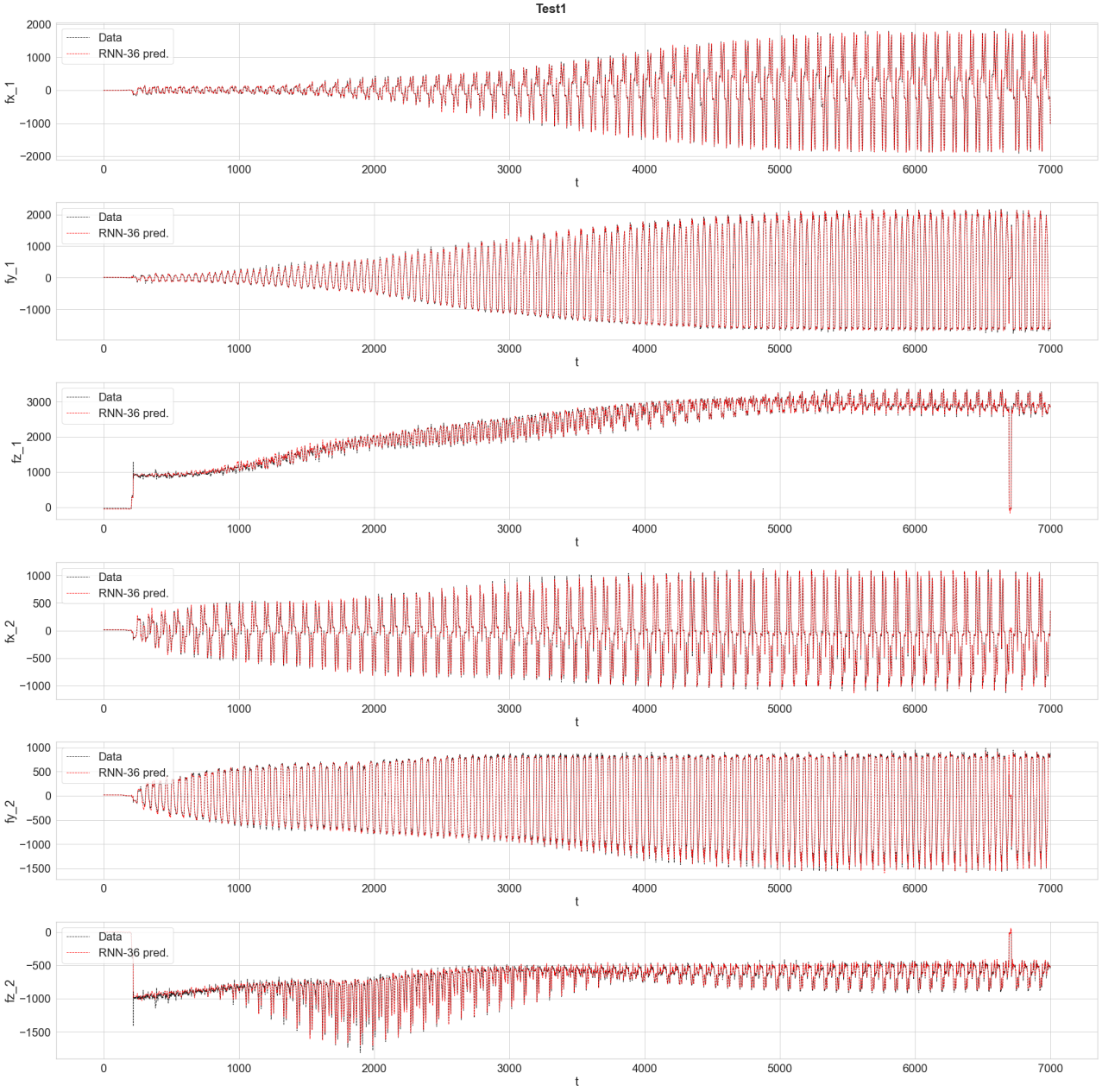

Test2
fx_1
fy_1
fz_1
fx_2
fy_2
fz_2
t
Data
DNN-12 pred.
DNN-36 pred.
DNN-84 pred.
RNN-12 pred.
RNN-36 pred.
RNN-84 pred.
17000
17020
17040
17060
17080
17100

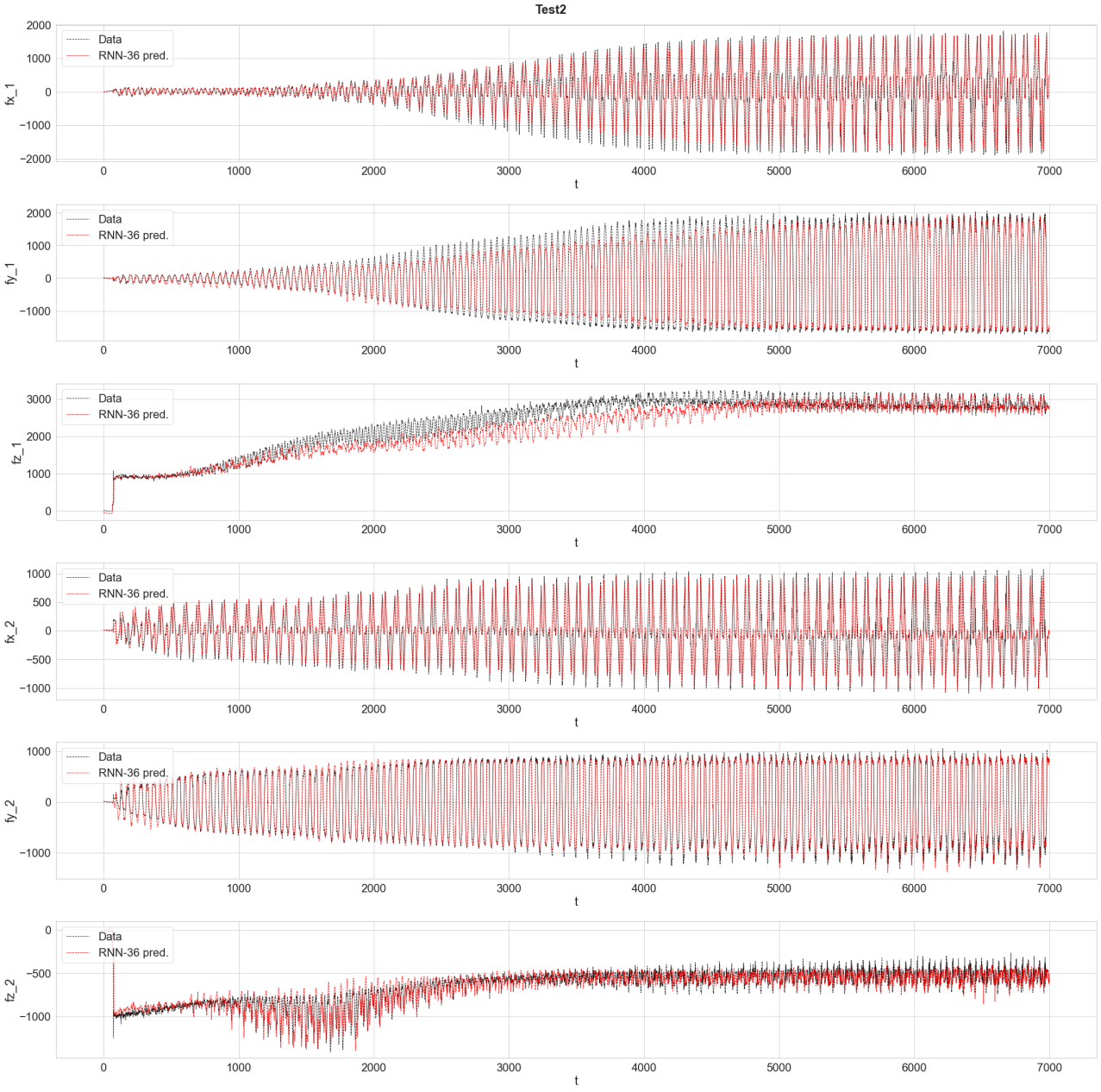


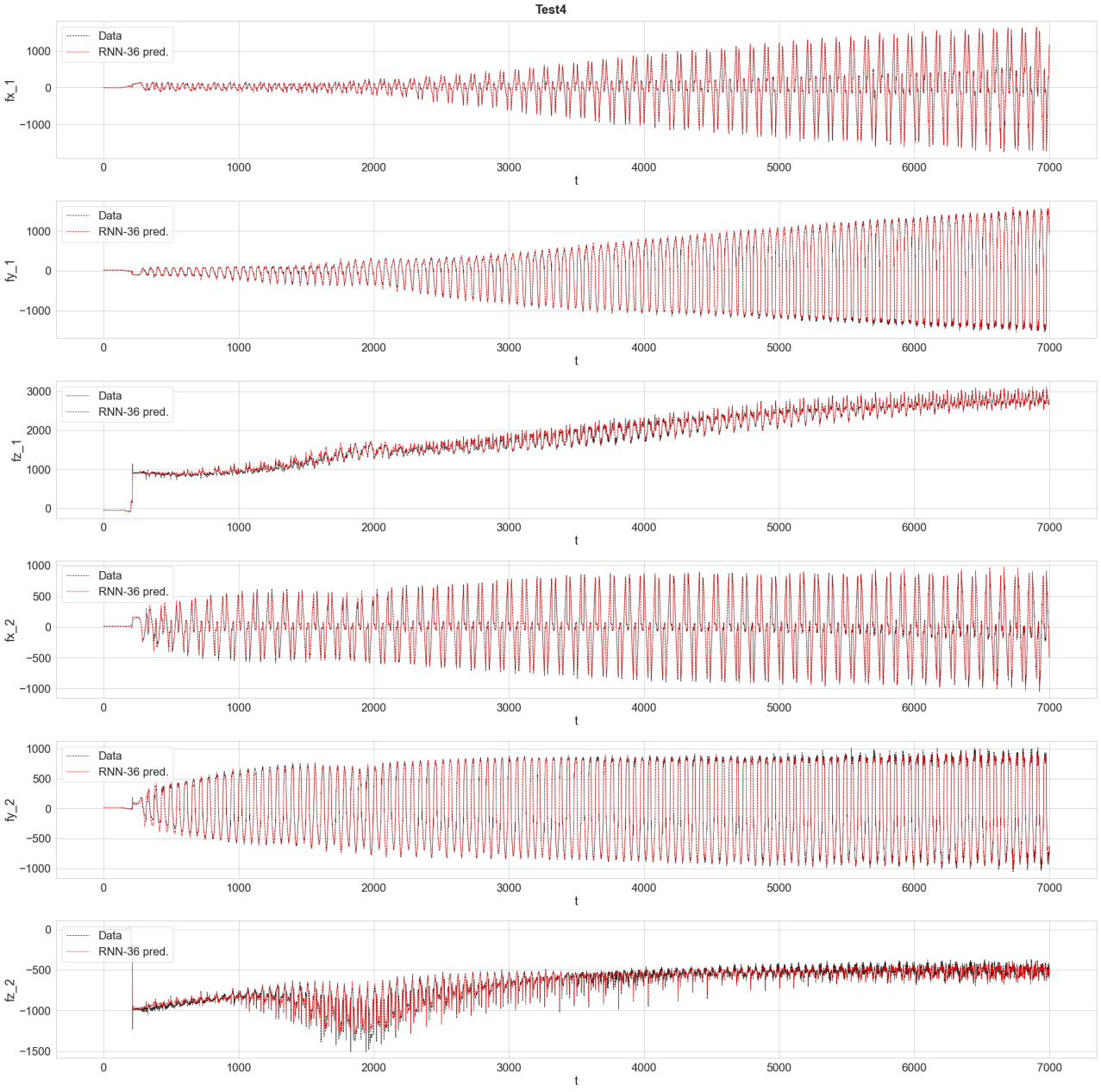
In [99]:

```
# plot large range for best model
tmin = 0
tmax = 7000
t = np.linspace(tmin, tmax, tmax-tmin)
sns.set(font_scale = 2)
sns.color_palette()
sns.set_style("whitegrid")
linewidth=1
for filename in dataset_filenames:

    fig = plt.figure(figsize=(30,30))
    fig.suptitle(filename, weight='bold').set_fontsize('24')
    for i in range(6):
        ax = fig.add_subplot(6, 1, i+1)
        ax.plot(t, tests_12[filename]['Y'].T[i][tmin+n_steps-1:tmax+n_steps-1],
        #ax.plot(t, tests_12[filename]['Y_pred'].T[i][tmin+n_steps-1:tmax+n_step
        #ax.plot(t, tests_36[filename]['Y_pred'].T[i][tmin+n_steps-1:tmax+n_step
        #ax.plot(t, tests_84[filename]['Y_pred'].T[i][tmin+n_steps-1:tmax+n_step
        #ax.plot(t, tests_12[filename]['Y_seq_pred'].T[i][tmin:tmax], label='RNN
```

```
        ax.plot(t, tests_36[filename]['Y_seq_pred'].T[i][tmin:tmax], label='RNN-
        #ax.plot(t, tests_84[filename]['Y_seq_pred'].T[i][tmin:tmax], label='RNN
        ax.set_xlabel('t')
        ax.set_ylabel(outputs[i])
        ax.legend(loc=2)
    plt.tight_layout()
    plt.savefig(output_dir/'{}_timeseries_t{}to{}.pdf'.format(filename, tmin, tm
```




Test2
Data
RNN-36 pred.
fx_1
fy_1
fz_1
fx_2
fy_2
fz_2
t



6. Summary and prospects

Six neural networks (three DNNs and three RNNs) were trained to predict tool-tip forces from input positions and angles (and their higher-order derivatives). The models were trained on 70% of the combined Test1 and Test4 datasets. Test2 was left out of the training entirely to evaluate the performance of the models on unseen runs of the robots.

The RNN models clearly outperformed the DNN models. This is especially clear from looking at the predicted tool-tip forces as a function of time for the Test2 dataset (unseen during training) above.

Adding the first-order (velocity) and second-order (acceleration) derivatives of the positions and angles as additional input features reduced the loss and significantly improved performance. Adding up to 6th order derivatives seemed helpful in some earlier DNN models (with fewer layers) that I trained (not shown in this notebook). However, the performance

comparisons between DNN-84 and DNN-36 in this notebook indicate that the impact is marginal.

Although the RNN did a decent job, all models struggled in generalizing to Test2. A more comprehensive hyperparameter optimization could be done to improve the performance. Adding training data from more runs with robots would probably help a lot.

You would probably want to further optimize and tailor the model to the application. A deeper (and recurrent) model will likely perform better if the goal is to achieve optimal accuracy. However, if the goal is to run fast inference on resource-constrained hardware, you'd want to optimize a smaller model that is *good enough* for the job.