Finite element simulation data for 3×3, 5×5 and 7×7 divisions of the surface

Input parameter:

- Number of pieces
- Angle 1-4 (for all the cases)
- Angle 5,6 (for 5×5 and 7×7)
- Angle 7, 8 (for 7×7)
- Length ratio

Output parameter:

- Safety factor: min(safety factor)
- Max out of plane deformation
- Max total contact energy
- Max elastic strain energy
- Max average reaction force
- Max edge temp
- Max average friction force
- Max heat rate
- Max internal energy
- Total friction dissipation rate: area under the curve

Goals:

1- Train the model with 3×3, 5×5 and 7×7 patterns and get acceptable predictions, the observations include:

- different pieces (9, 25, 49)
- different angles (4 – 8 different angles)
    - all the angles are fixed from (5, 10, 15, 20, 25),
    - randomly chosen from the list
- different length ratios (0.5, 0.75, 1, 1.25, 1.5, 1.75, 2)

2- Make <u>a grid of possible length ratios and angles</u> and feed it to the trained model and get the predictions

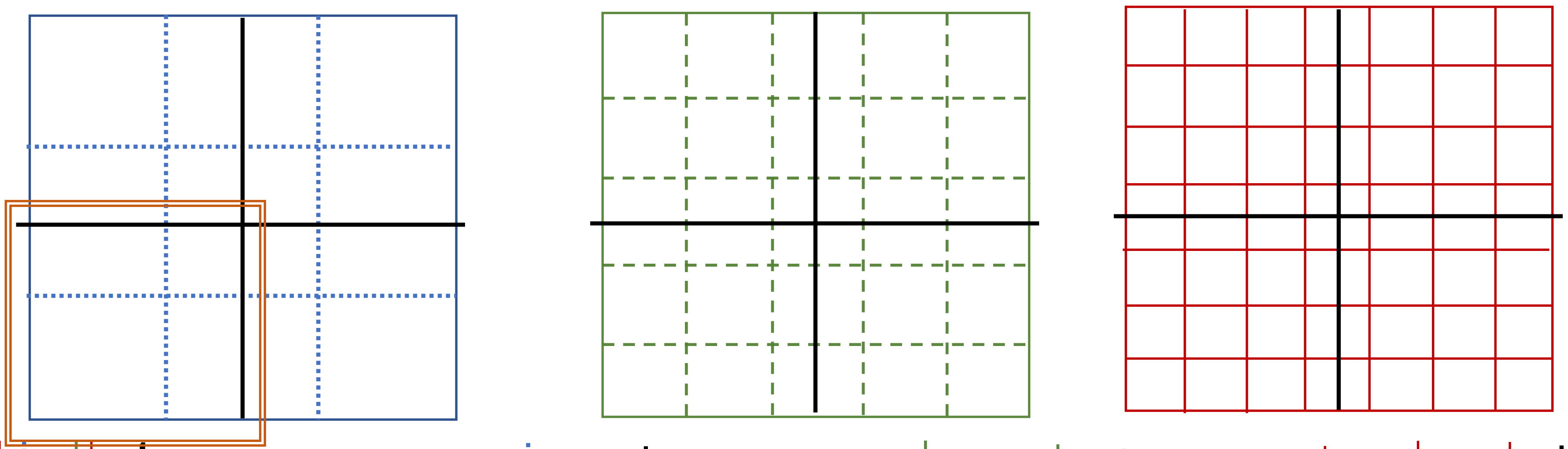
3- Filter the ceramic designs corresponding to the **desired predicted outputs** (eg. min Oop. deform., min heat rate, ….)

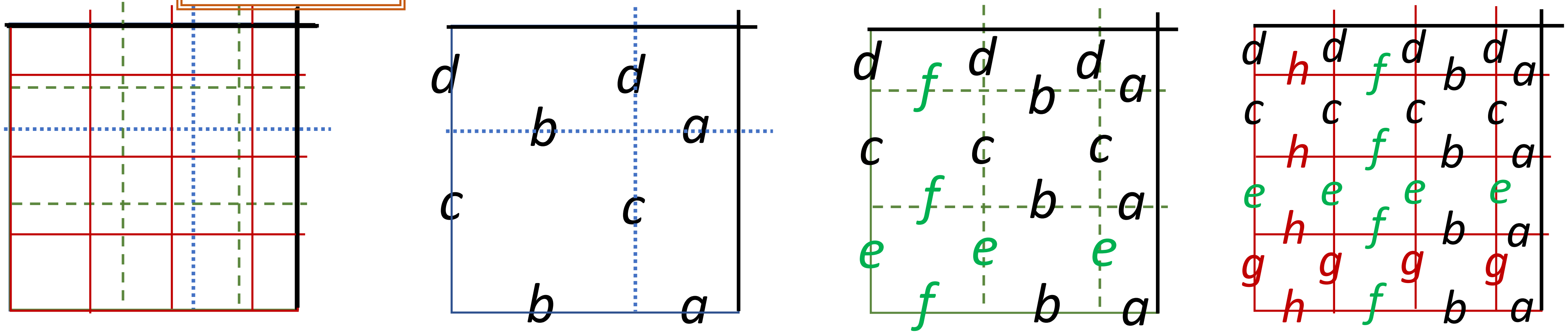
<u>Questions:</u>

- Can we mix the simulation results for 3×3, 5×5 and 7×7 patterns
- If the number of inputs for 3×3 is different from 5×5 and 7×7 patterns, they can not be used in the same data sets for ML model

Schematic of the simulated panels with 3×3, 5×5 or 7×7 small parts locked together united as single panels

Let's look at ¼ of the panels



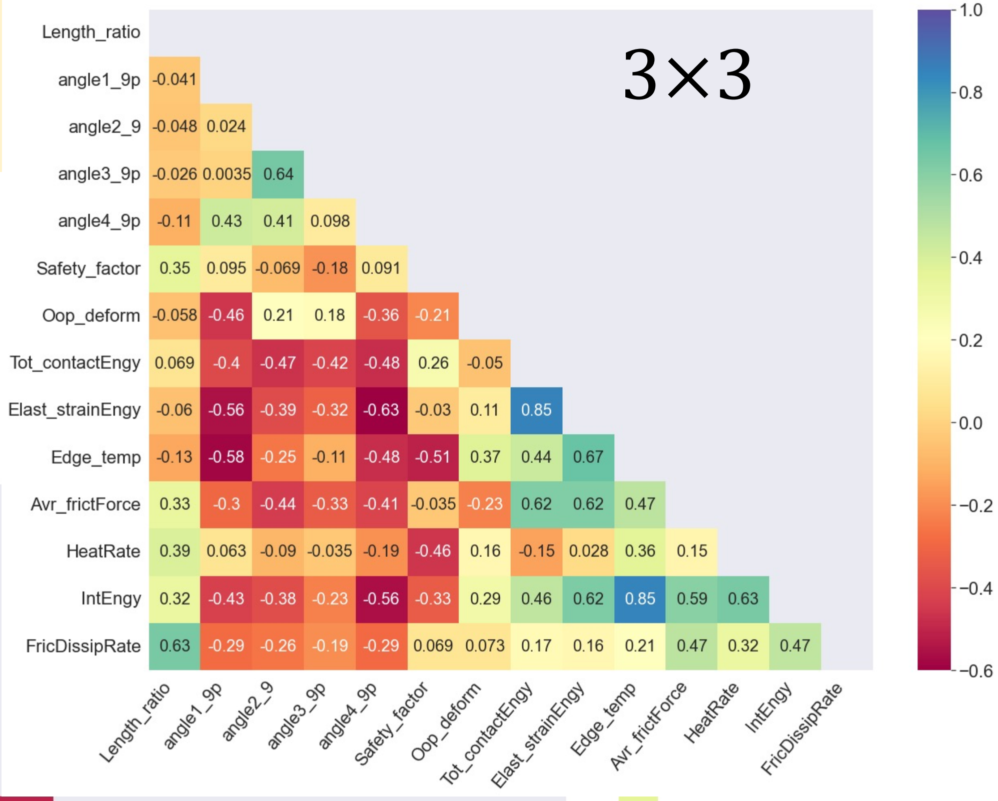


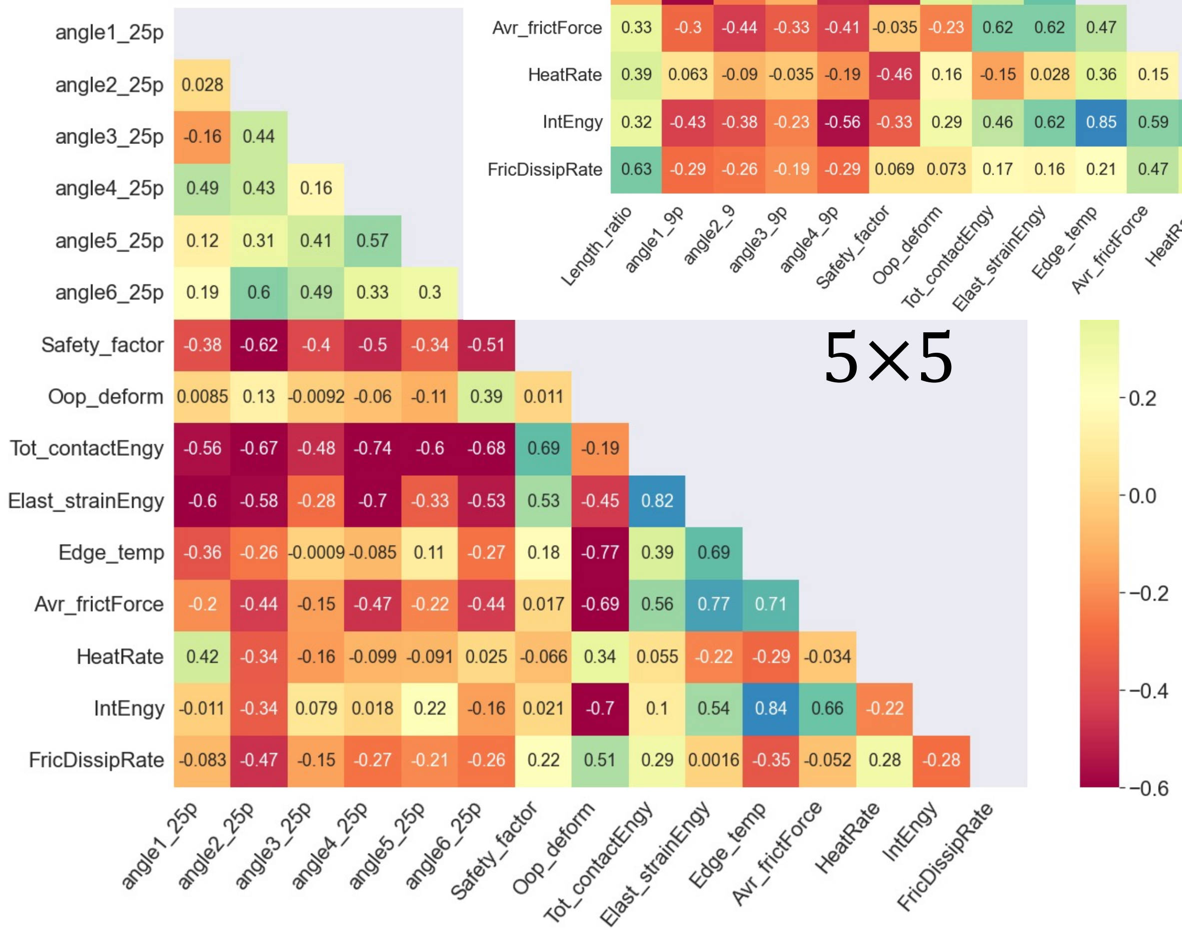
_pieces	angle1_9p	angle2_9	angle3_9p	angle4_9p	angle1_25p	angle2_25p	angle3_25p	angle4_25p	angle5_25p	angle6_25p	angle1_49p	angle2_49p	angle3_
49.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	10.0	10.0	
9.0	5.0	5.0	5.0	5.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
25.0	0.0	0.0	0.0	0.0	15.0	15.0	15.0	15.0	15.0	15.0	0.0	0.0	

Exploratory analysis

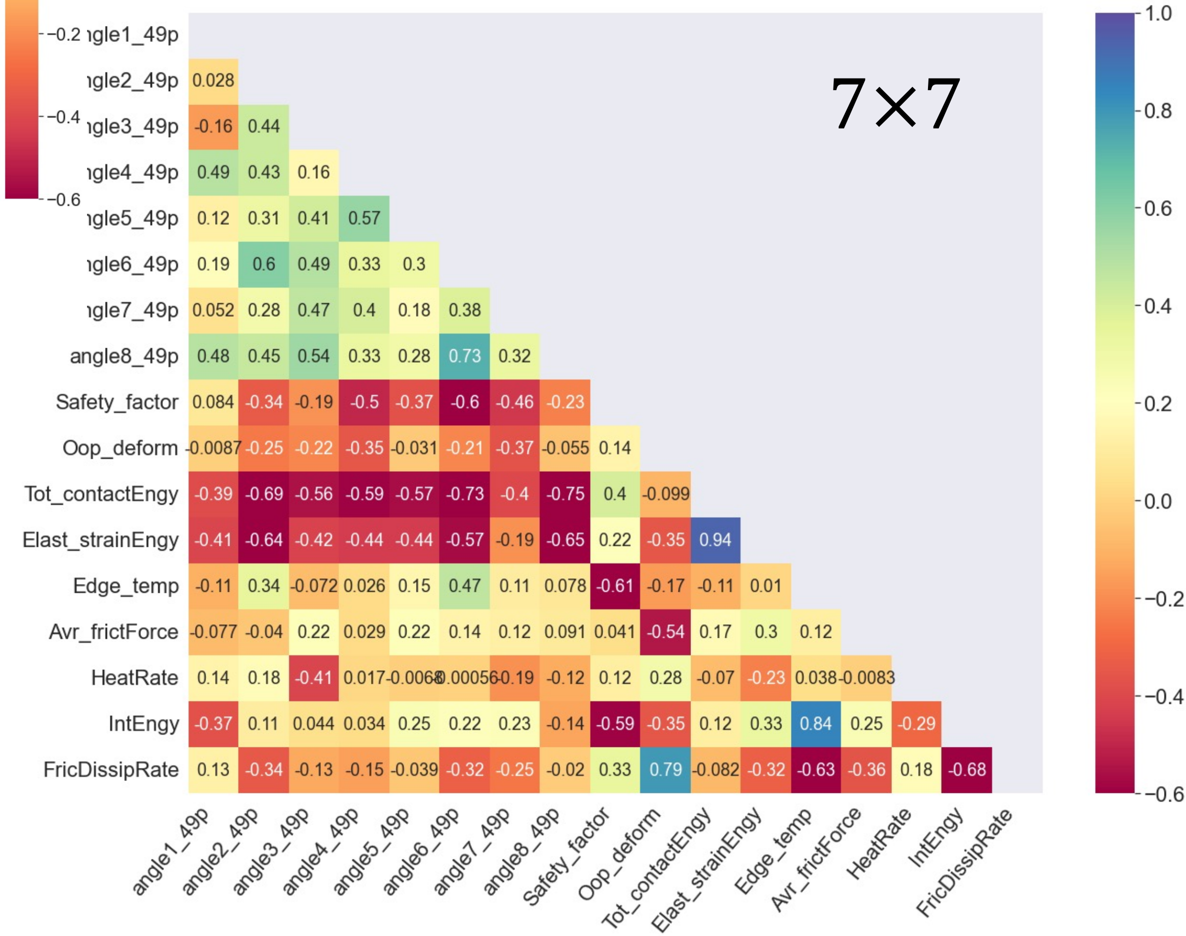
- Looking at the covariance of parameters to find the most correlated parameters for three different panel structures
- Looking at the pair-plots for three panel structures to compare the range of each parameter change
- Finding the possible outliers based on distribution of outputs and set up reruns
- Comparing the reruns with the initial runs
- Determining the output parameters for predicting via ML models

Covariance of parameters for 3 different panels

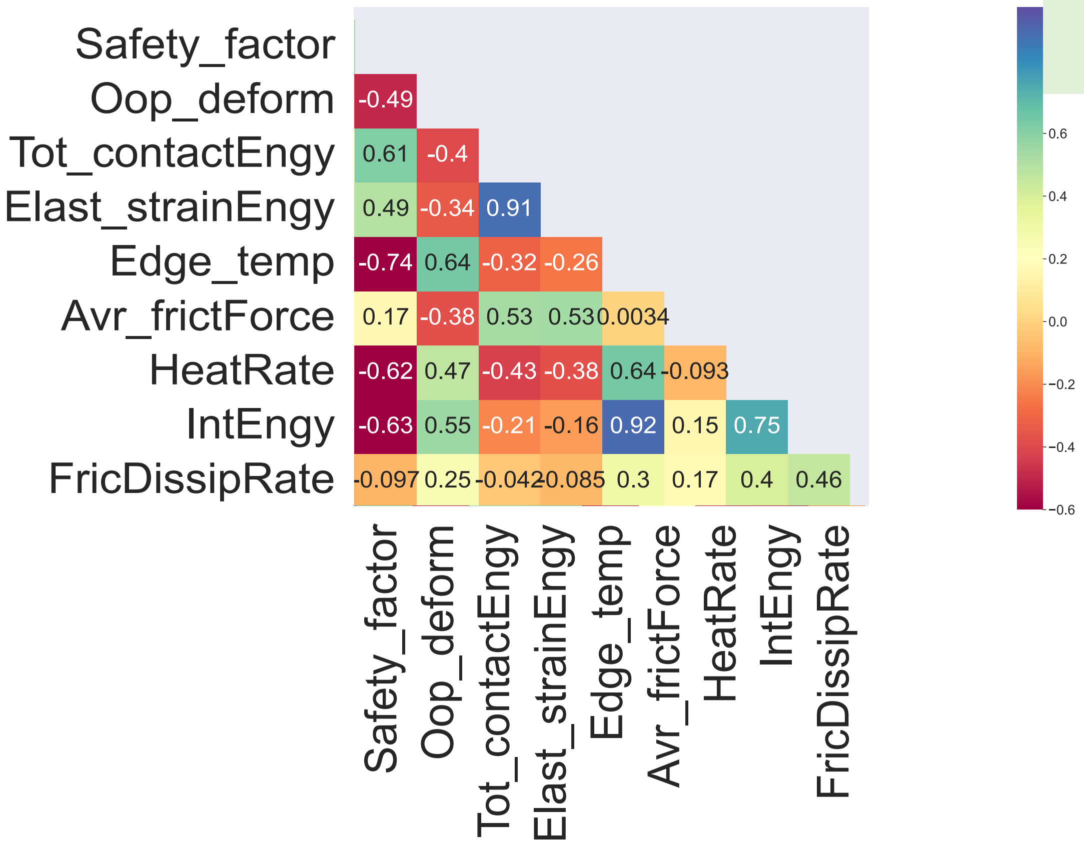




The most correlated parameters:
Elastic strain Engy & Tot. cont. Engy.
Int. Engy & Edge Temp.



Correlations for all the panels



The most correlated parameters:

Elastic strain Engy & Tot. cont. Engy.

Int. Engy & Edge Temp.

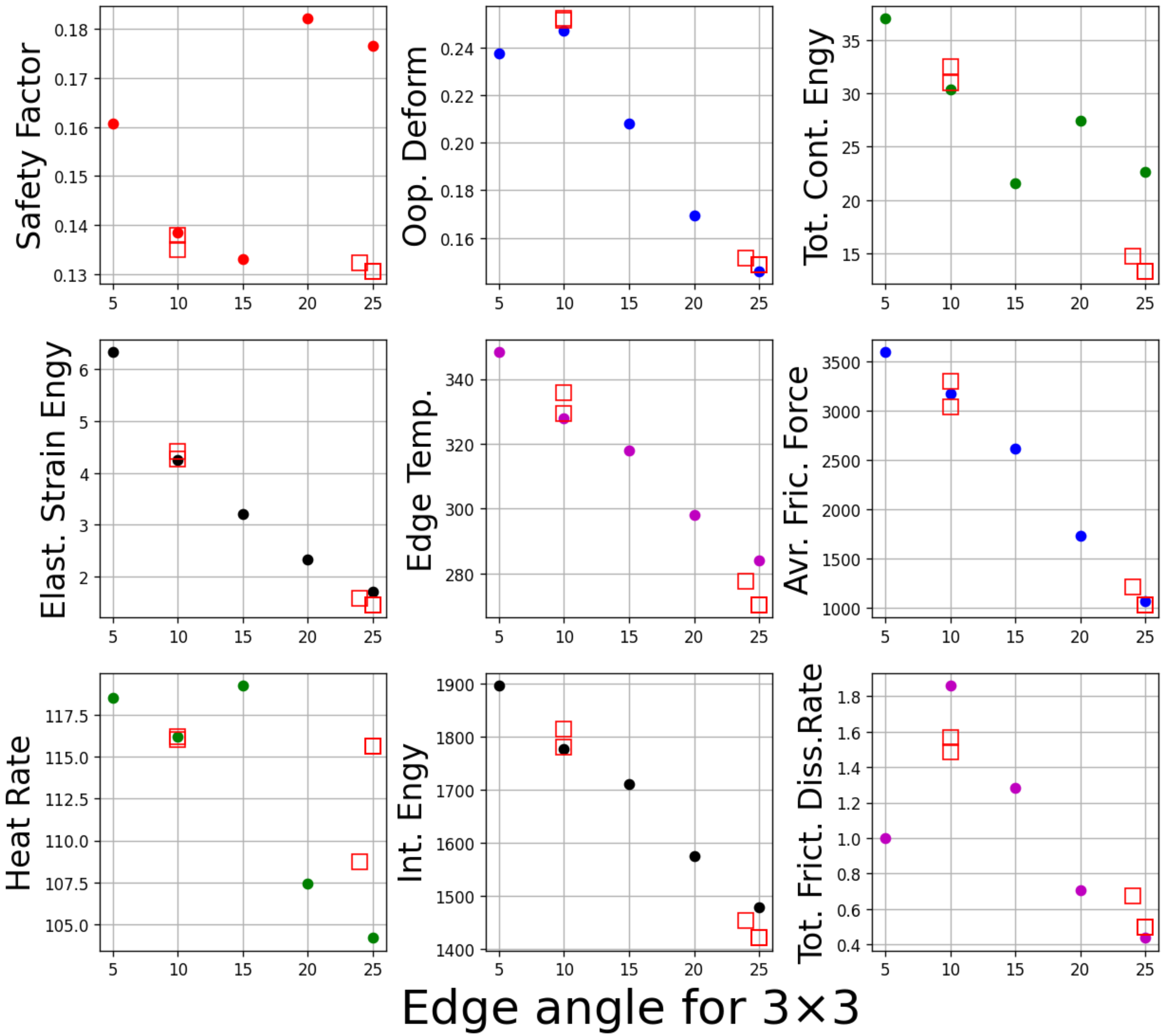
Repeating some runs to check parameter fluctuations

Repeated runs are shown with squares.

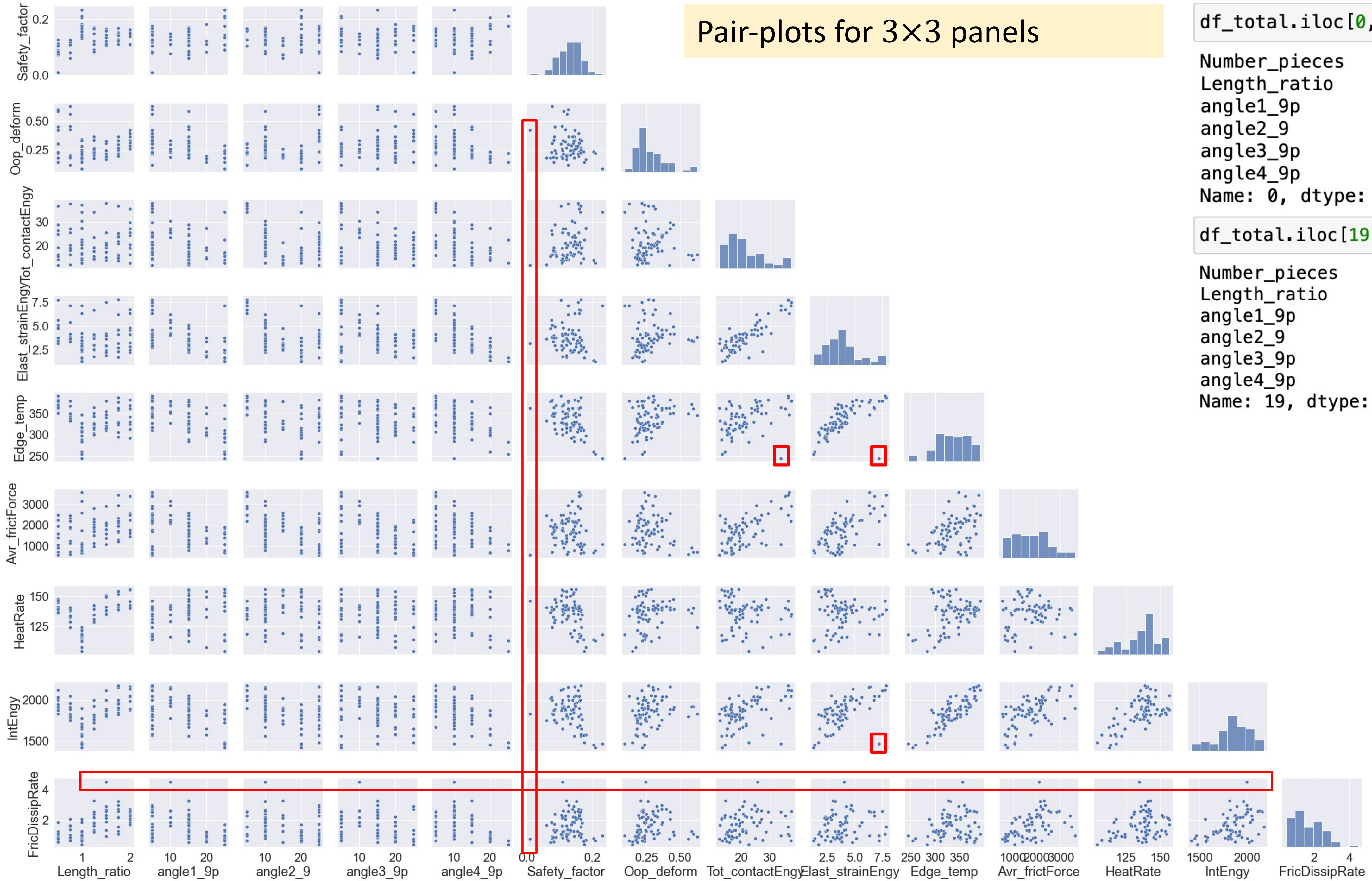
Correlated parameters from pairplots:

Elastic strain Engy & Tot. cont. Engy.

Int. Engy & Edge Temp.



Pair-plots for 3×3 panels



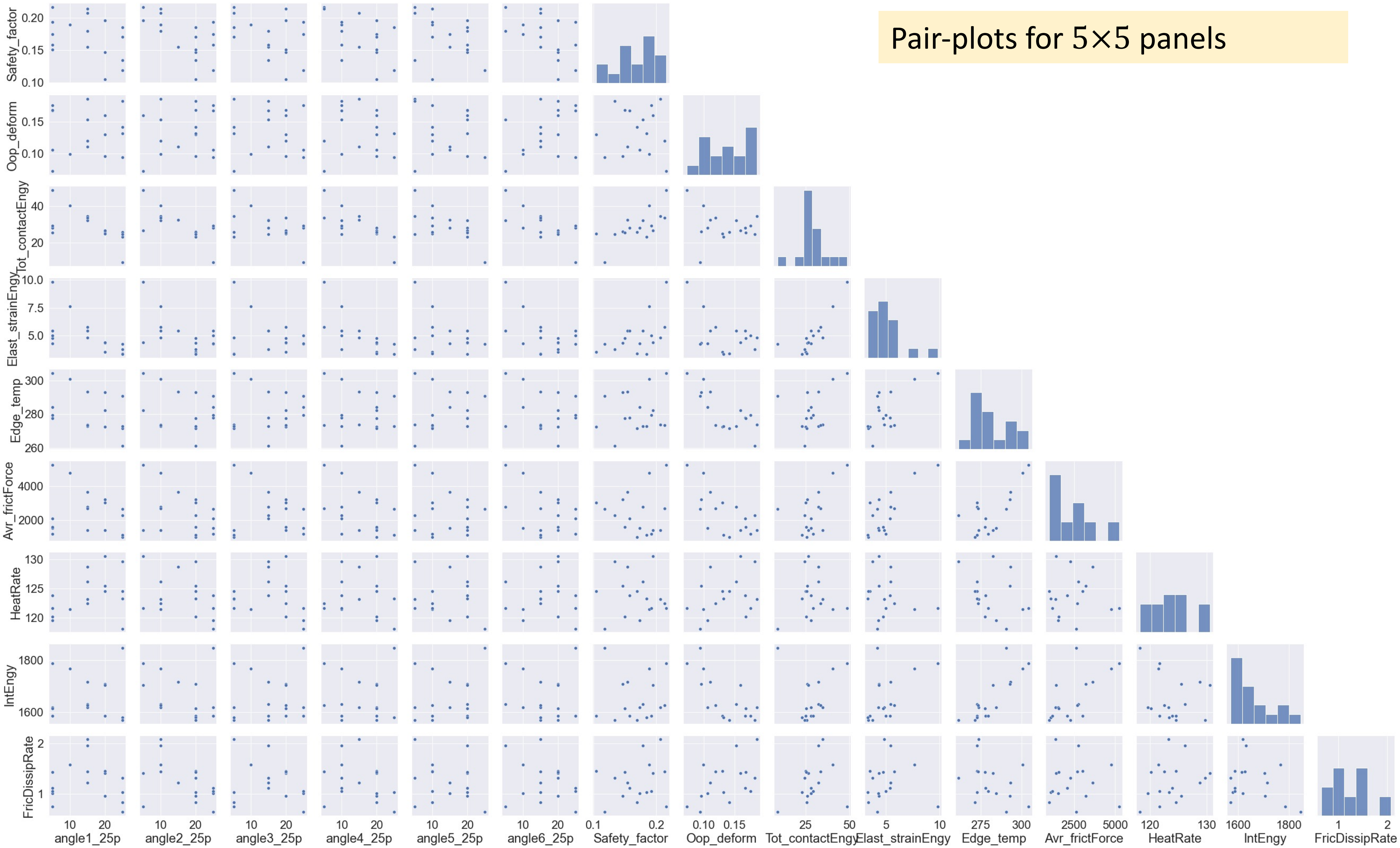

```
df_total.iloc[0,:6]
```

```
Number_pieces      9.0
Length_ratio       0.5
angle1_9p          5.0
angle2_9          25.0
angle3_9p         25.0
angle4_9p         10.0
Name: 0, dtype: float64
```

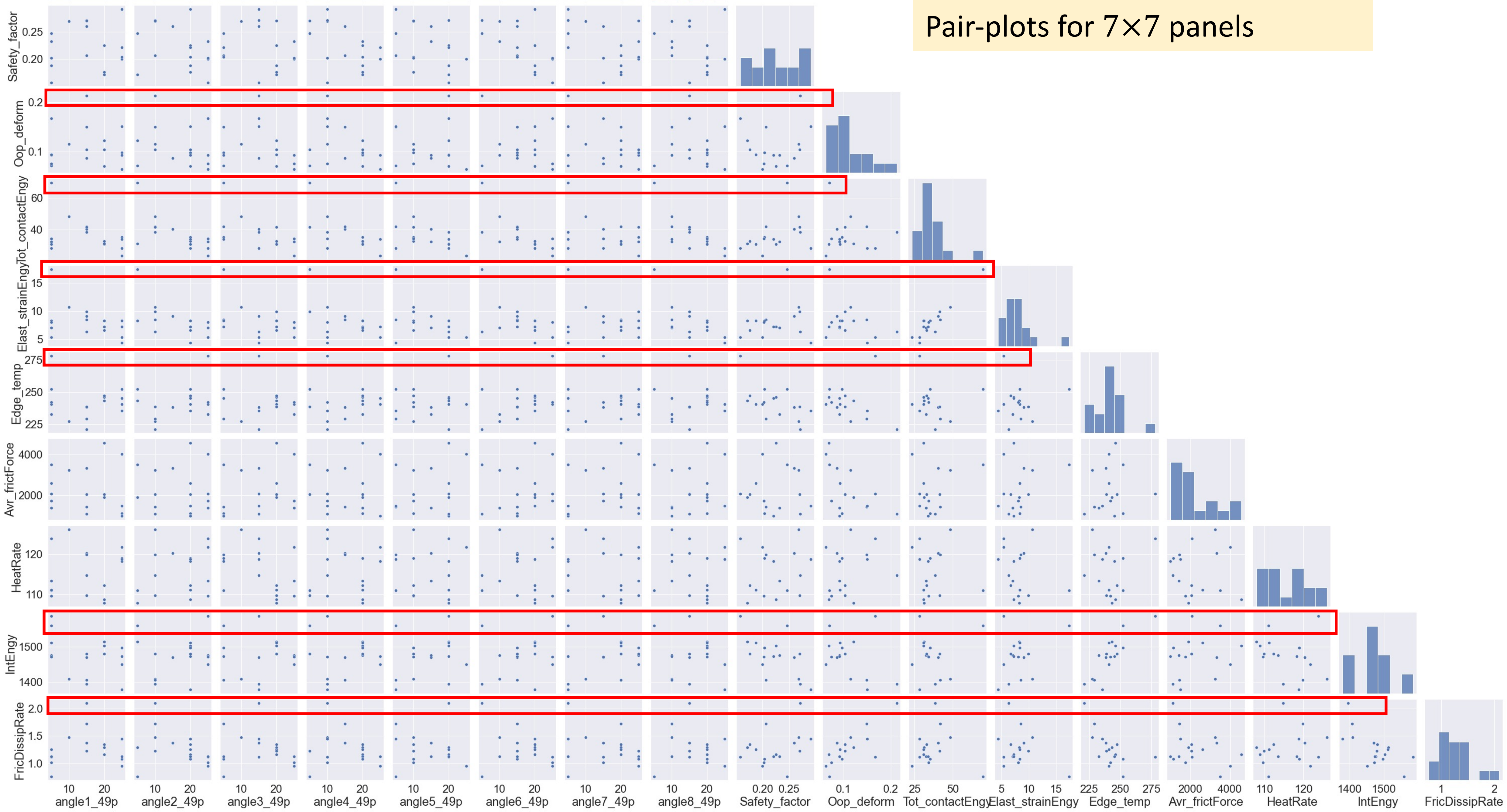
```
df_total.iloc[19,:6]
```

```
Number_pieces     9.0
Length_ratio      1.5
angle1_9p        10.0
angle2_9         10.0
angle3_9p        10.0
angle4_9p        10.0
Name: 19, dtype: float64
```

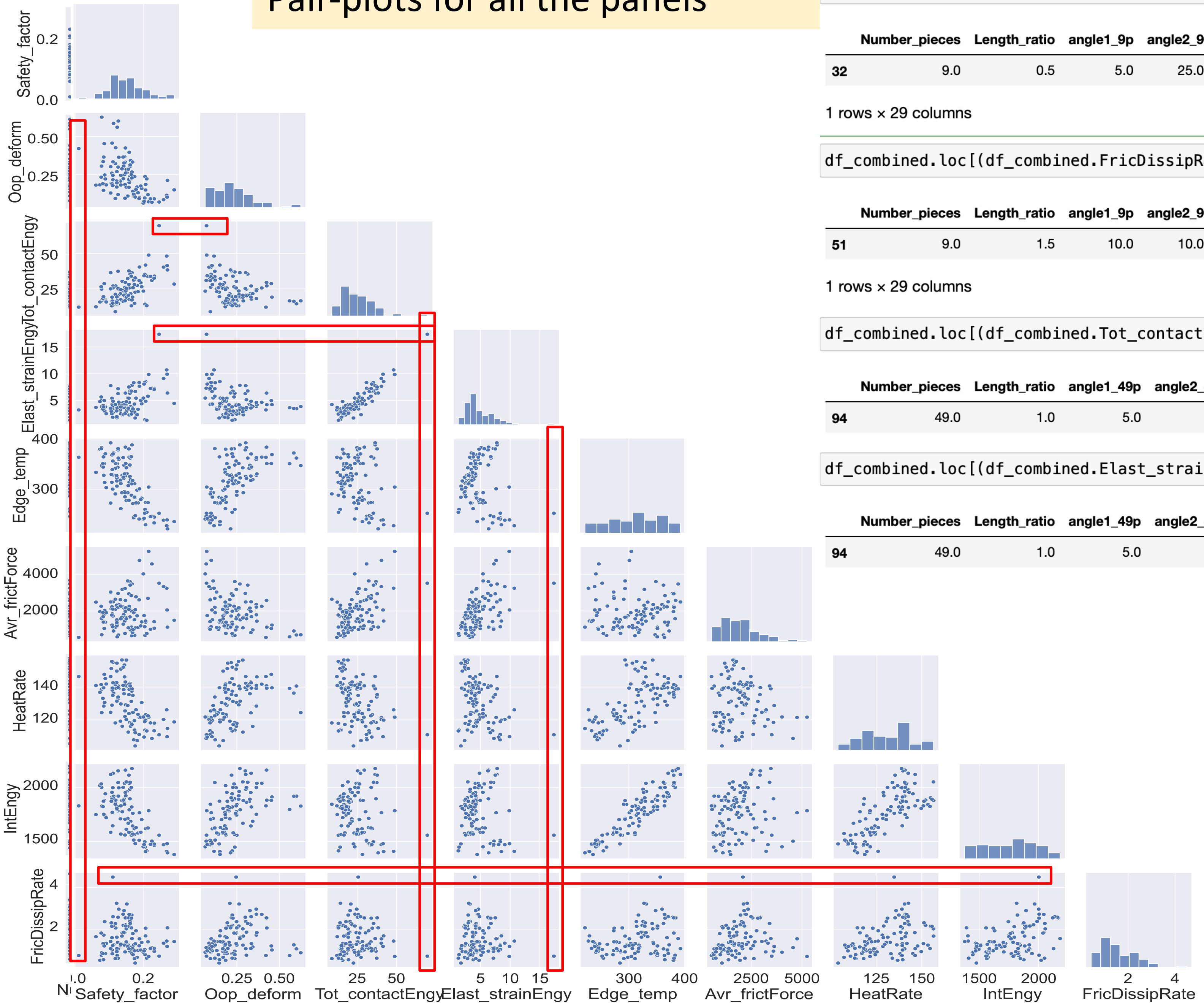
Pair-plots for 5×5 panels



Pair-plots for 7×7 panels



Pair-plots for all the panels




```
df_combined.loc[(df_combined.Safety_factor < 0.015)]
```

	Number_pieces	Length_ratio	angle1_9p	angle2_9	angle3_9p	angle4_9p	angle1_25p	angle2_25p	angle3_25p	angle4_25p	...	angle
32	9.0	0.5	5.0	25.0	25.0	10.0	0.0	0.0	0.0	0.0	...	

1 rows × 29 columns

```
df_combined.loc[(df_combined.FricDissipRate > 4)]
```

	Number_pieces	Length_ratio	angle1_9p	angle2_9	angle3_9p	angle4_9p	angle1_25p	angle2_25p	angle3_25p	angle4_25p	...	angle
51	9.0	1.5	10.0	10.0	10.0	10.0	0.0	0.0	0.0	0.0	...	

1 rows × 29 columns

```
df_combined.loc[(df_combined.Tot_contactEngy > 50)].drop(df_combined.iloc[:,2:12], axis = 'columns')
```

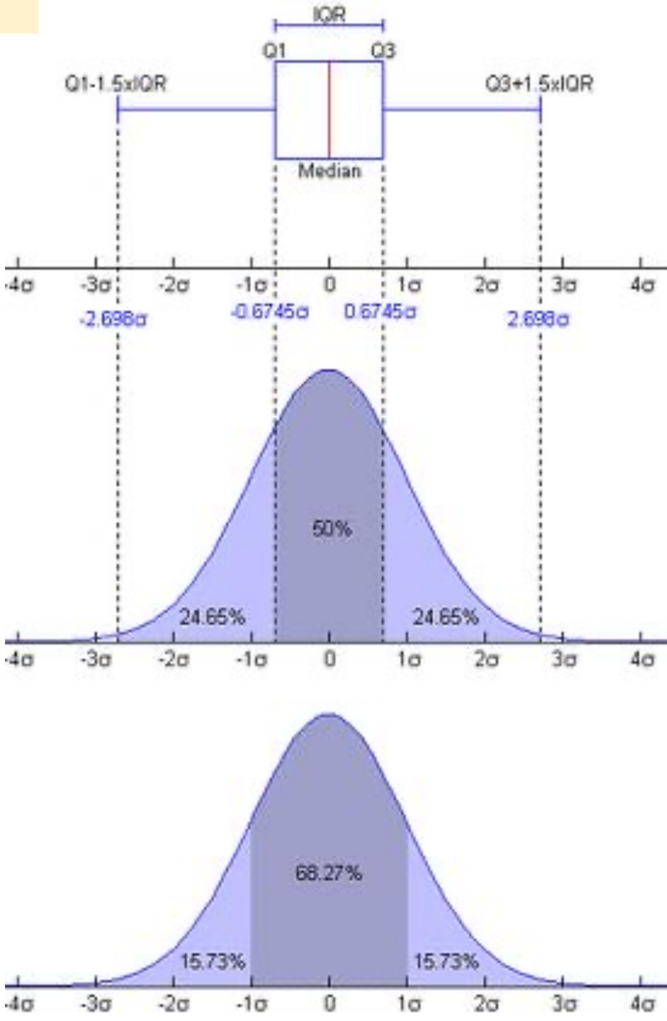
	Number_pieces	Length_ratio	angle1_49p	angle2_49p	angle3_49p	angle4_49p	angle5_49p	angle6_49p	angle7_49p	angle8_49p	Saf
94	49.0	1.0	5.0	5.0	5.0	5.0	5.0	5.0	5.0	5.0	

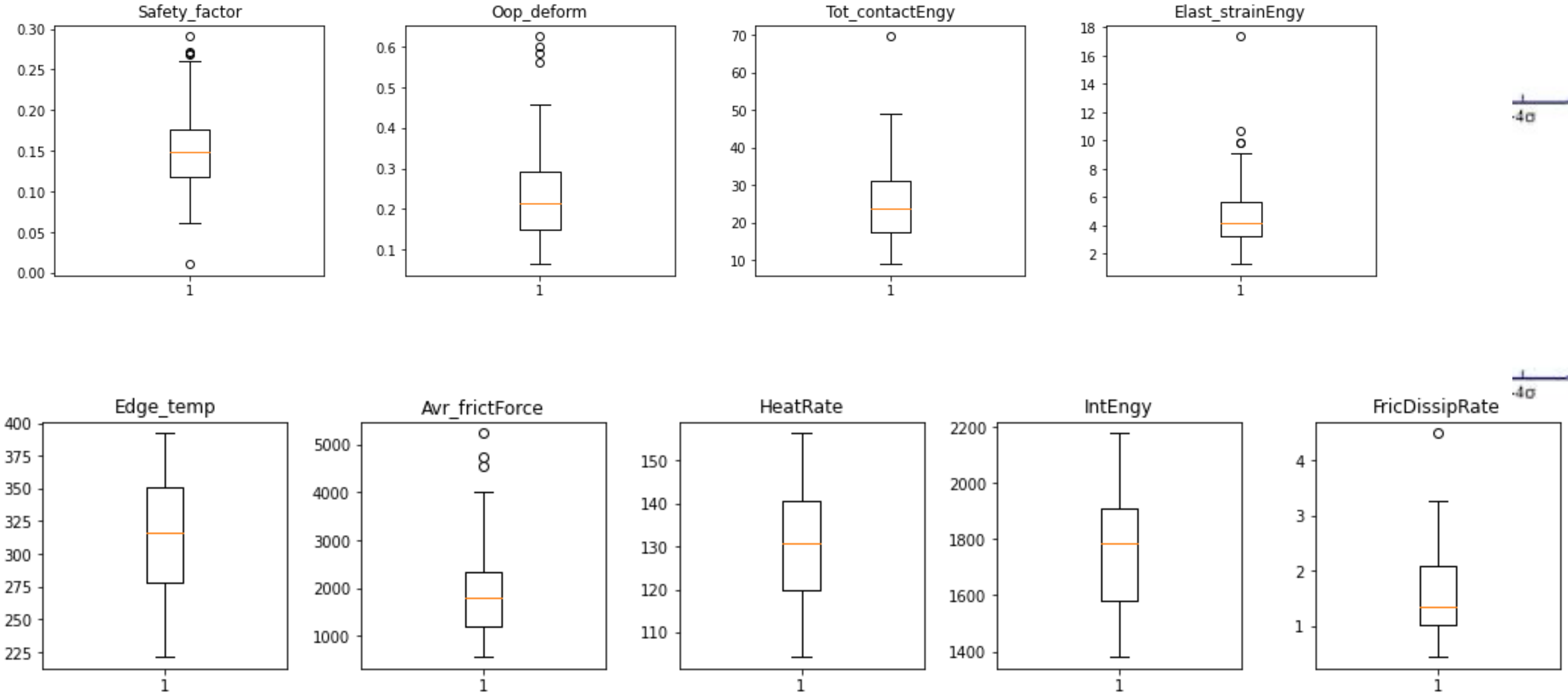
```
df_combined.loc[(df_combined.Elast_strainEngy > 15)].drop(df_combined.iloc[:,2:12], axis = 'columns')
```

	Number_pieces	Length_ratio	angle1_49p	angle2_49p	angle3_49p	angle4_49p	angle5_49p	angle6_49p	angle7_49p	angle8_49p	Saf
94	49.0	1.0	5.0	5.0	5.0	5.0	5.0	5.0	5.0	5.0	

Finding possible outliers

A box plot is a method for graphically depicting groups of numerical data through their quartiles. The box extends from the Q1 to Q3 quartile values of the data, with a line at the median (Q2). The whiskers extend from the edges of box to show the range of the data. By default, they extend no more than *1.5 * IQR (IQR = Q3 - Q1)* from the edges of the box, ending at the farthest data point within that interval. Outliers are plotted as separate dots.





Finding possible outliers and send for rerunning

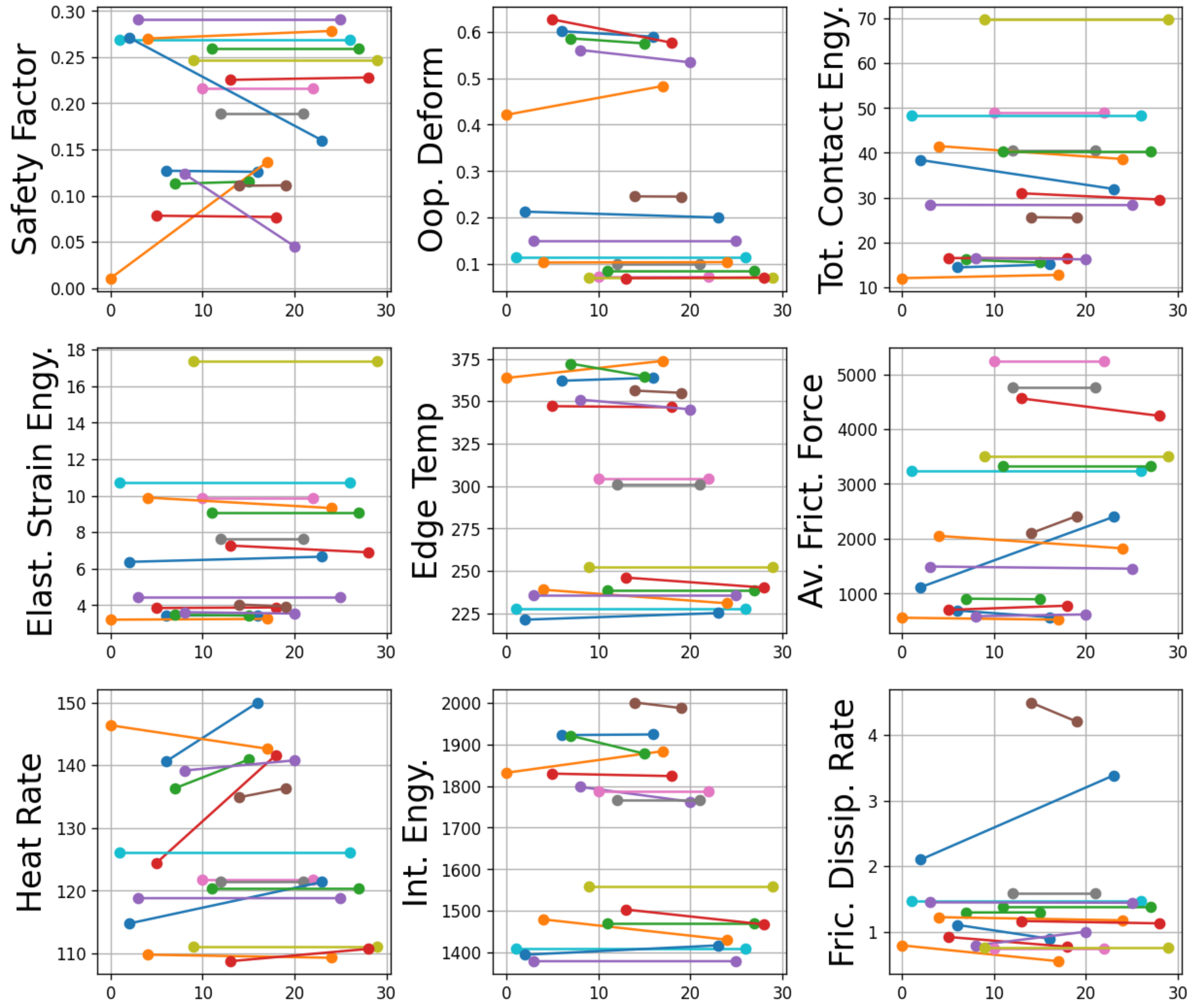
```python
def boxplot_outliers(arr):
    # finding the 1st quartile
    q1 = np.quantile(arr, 0.25)

    # finding the 3rd quartile
    q3 = np.quantile(arr, 0.75)
    med = np.median(arr)

    # finding the iqr region
    iqr = q3-q1

    # finding upper and lower whiskers
    upper_bound = q3+(1.5*iqr)
    lower_bound = q1-(1.5*iqr)
    return df_combined.loc[(arr > upper_bound) | (arr < lower_bound)]
```

Number_pieces	Length_ratio	angle1_9p	angle2_9	angle3_9p	angle4_9p
9.0	0.50	5.0	25.0	25.0	10.0
9.0	0.75	5.0	25.0	15.0	10.0
9.0	0.50	5.0	25.0	15.0	10.0
9.0	0.50	15.0	10.0	20.0	5.0
9.0	0.75	5.0	25.0	25.0	10.0
9.0	1.50	10.0	10.0	10.0	10.0

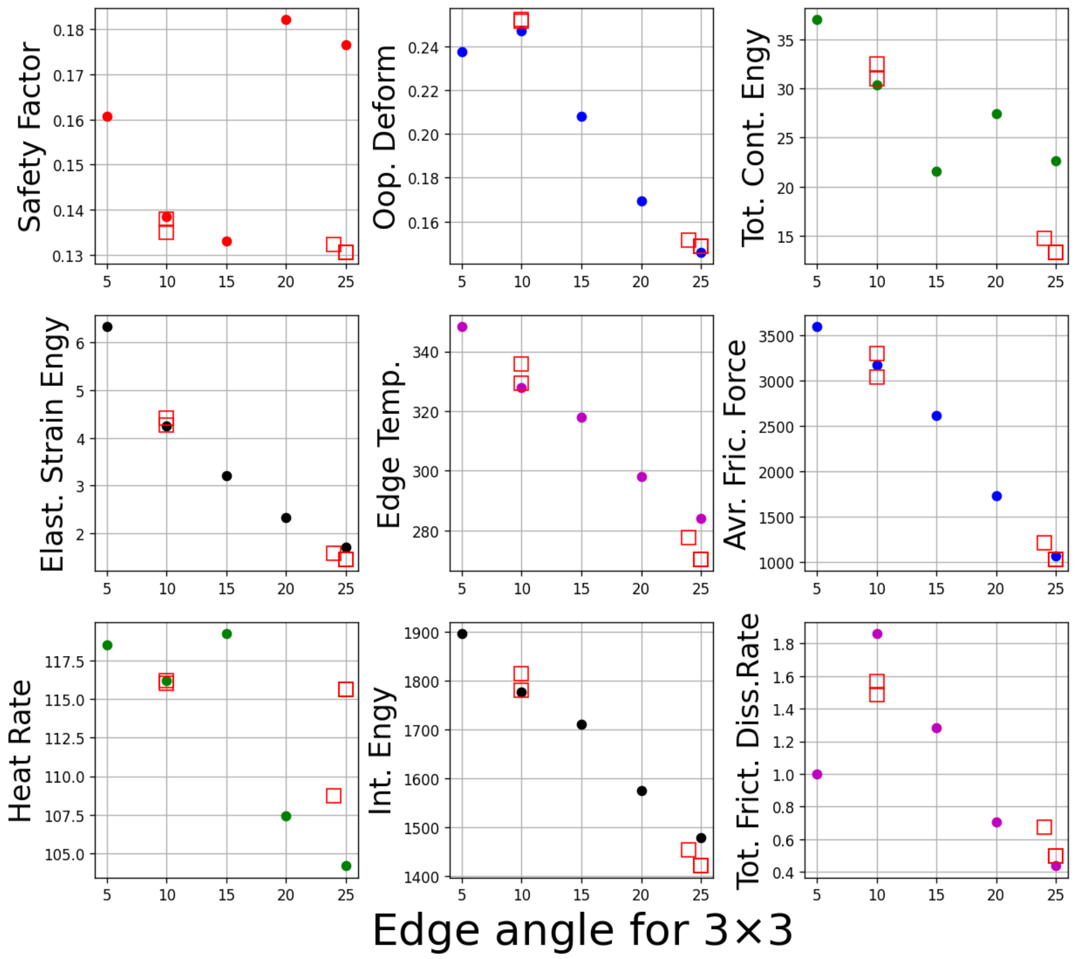
Number_pieces	Length_ratio	angle1_25p	angle2_25p	angle3_25p	angle4_25p	angle5_25p	angle6_25p
25.0	1.0	5.0	5.0	5.0	5.0	5.0	5.0
25.0	1.0	10.0	10.0	10.0	10.0	10.0	10.0

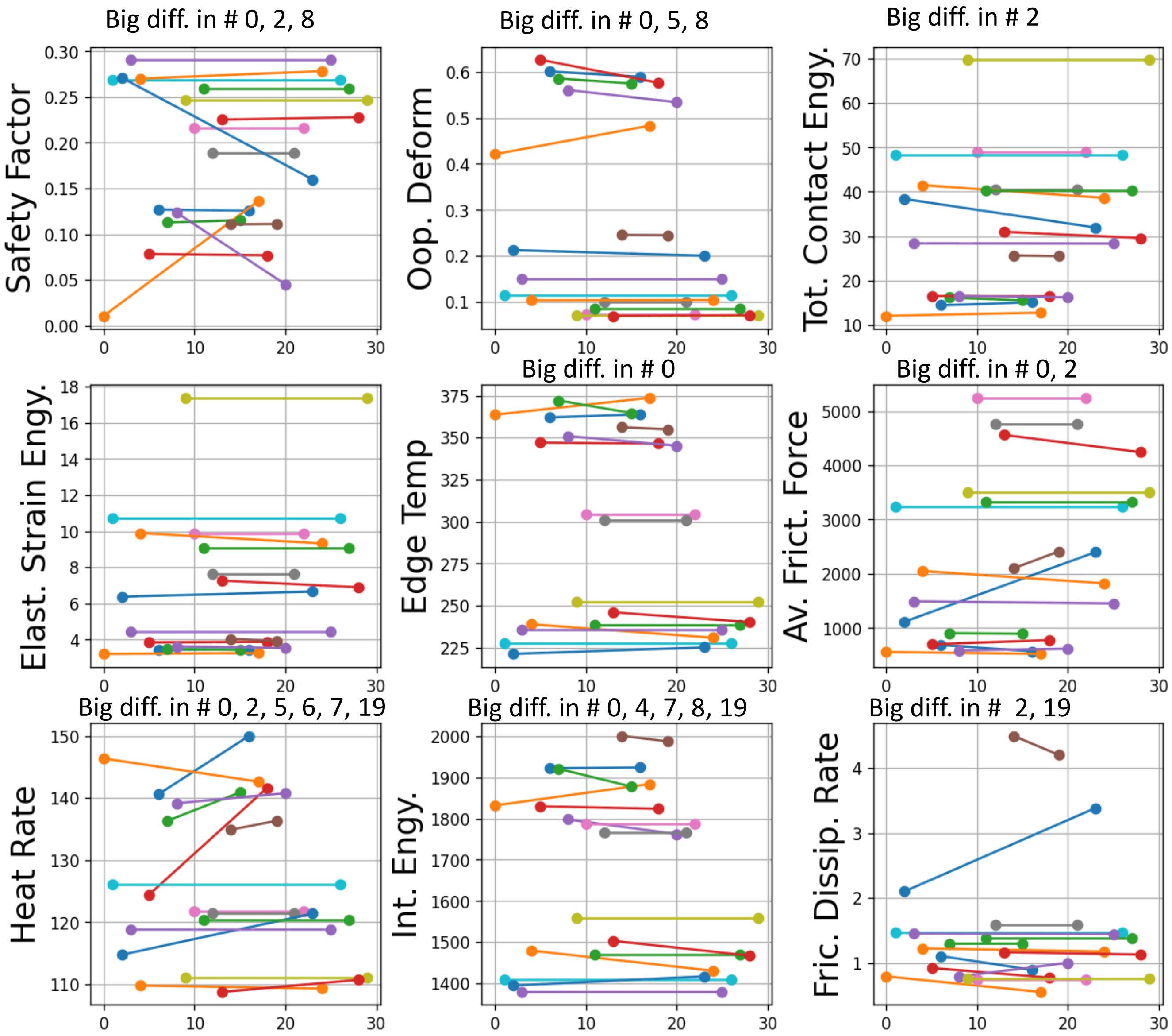
Number_pieces	Length_ratio	angle1_49p	angle2_49p	angle3_49p	angle4_49p	angle5_49p	angle6_49p	angle7_49p	angle8_49p
49.0	1.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
49.0	1.0	15.0	10.0	15.0	10.0	20.0	5.0	5.0	15.0
49.0	1.0	25.0	20.0	15.0	10.0	5.0	20.0	5.0	25.0
49.0	1.0	15.0	10.0	20.0	5.0	10.0	15.0	25.0	15.0
49.0	1.0	5.0	5.0	5.0	5.0	5.0	5.0	5.0	5.0
49.0	1.0	15.0	15.0	15.0	15.0	15.0	15.0	15.0	15.0
49.0	1.0	20.0	20.0	20.0	20.0	20.0	20.0	20.0	20.0

Repeating 15 cases of all the designs



Repeating 3 cases of all the designs






```
df_total.iloc[0,:6]
```

```
Number_pieces      9.0
Length_ratio       0.5
angle1_9p          5.0
angle2_9          25.0
angle3_9p         25.0
angle4_9p         10.0
Name: 0, dtype: float64
```

```
df_total.iloc[2,:2], df_tot
```

```
(Number_pieces     49.0
 Length_ratio       1.0
 Name: 2, dtype: float64,
 angle1_49p     15.0
 angle2_49p     10.0
 angle3_49p     15.0
 angle4_49p     10.0
 angle5_49p     20.0
 angle6_49p      5.0
 angle7_49p      5.0
 angle8_49p     15.0
 Name: 2, dtype: float64)
```

```
df_total.iloc[5,:6]
```

```
Number_pieces      9.00
Length_ratio       0.75
angle1_9p          5.00
angle2_9          25.00
angle3_9p         15.00
angle4_9p         10.00
Name: 5, dtype: float64
```

```
df_total.iloc[8,:6]
```

```
Number_pieces      9.00
Length_ratio       0.75
angle1_9p          5.00
angle2_9          25.00
angle3_9p         25.00
angle4_9p         10.00
Name: 8, dtype: float64
```

```
df_total.iloc[19,:6]
```

```
Number_pieces      9.0
Length_ratio       1.5
angle1_9p         10.0
angle2_9          10.0
angle3_9p         10.0
angle4_9p         10.0
Name: 19, dtype: float64
```

Just for 3by 3 panels (74 data points)

Bootstrap R2 (%)	Safety_factor	Oop deform	Tot. Contact Engy	Elast. Strain Engy	Edge Temp	Avr. Fric. Force	Heat Rate	Int. Engy	Fric. Diss. Rate
LR	-19	2	22	44	26	13	-2	25	43
2nd Poly	-1	24	45	63	56	40	25	57	45
3rd Poly	-51	-27	-93	-3	13	-31	17	26	22
XGB	44	26	36	52	65	60	81	78	60
2nd Poly & XGB	42	36	41	30	62	56	75	76	61
3rd Poly & XGB	52	32	37	62	63	56	76	77	62

for all panels (108 data points), 18 angles

Bootstrap R2 (%)	Safety_factor	Oop deform	Tot. Contact Engy	Elast. Strain Engy	Edge Temp	Avr. Fric. Force	Heat Rate	Int. Engy	Fric. Diss. Rate
LR	-100	-100	-100	-100	45	-100	-12	24	-100
2nd Poly	-2	-2	-8	-1	-4	-1	-8	-5	-1
3rd Poly	-1	-6	-3	-8	-2	-5	-8	-7	-8
XGB	55	58	58	58	82	-24	87	82	54
2nd Poly & XGB	58	55	58	63	82	-30	85	82	56
3rd Poly & XGB	60	58	56	64	82	-22	83	82	50

Model selection in under progress . . .