

## 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:

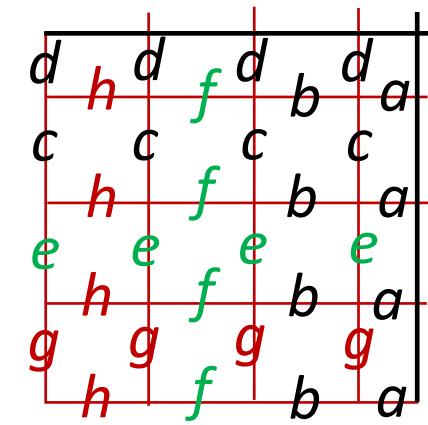
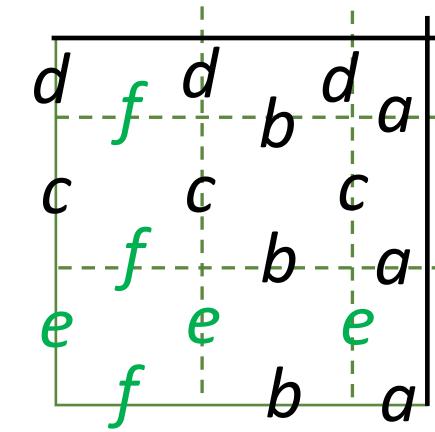
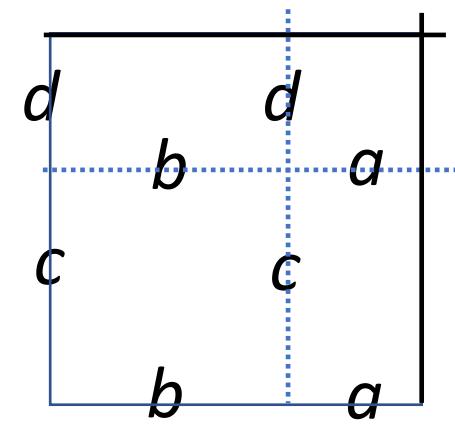
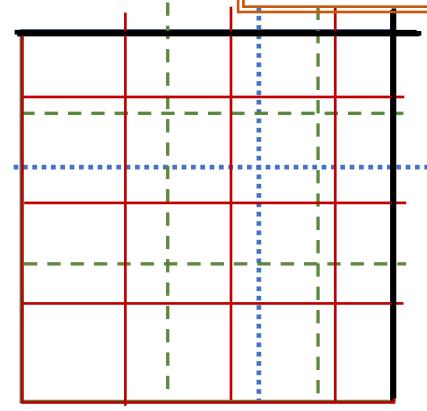
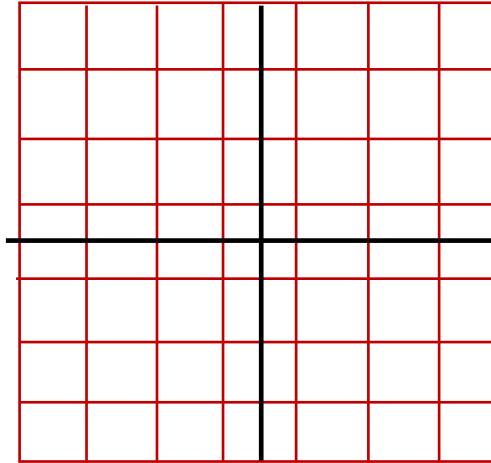
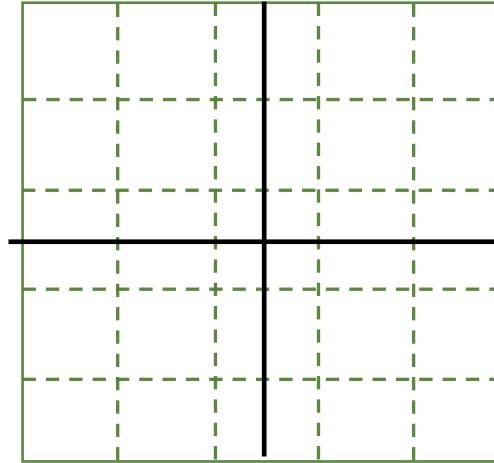
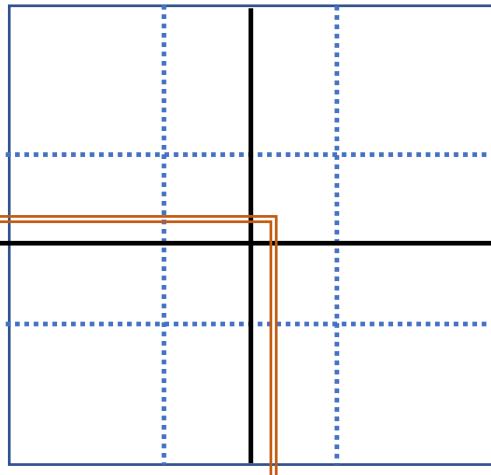
- 1- Train the model with  $3\times 3$ ,  $5\times 5$  and  $7\times 7$  patterns and get acceptable predictions, the observations include:
  - different pieces (9, 25, 49)
  - different angles (4 – 8 different angles)
    - all the angles are fixed from (5, 10, 15, 20, 25),
    - randomly chosen from the list
  - different length ratios (0.5, 0.75, 1, 1.25, 1.5, 1.75, 2)
- 2- Make a grid of possible length ratios and angles 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, .... )

## Questions:

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

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

Let's look  
at  $\frac{1}{4}$  of the  
panels

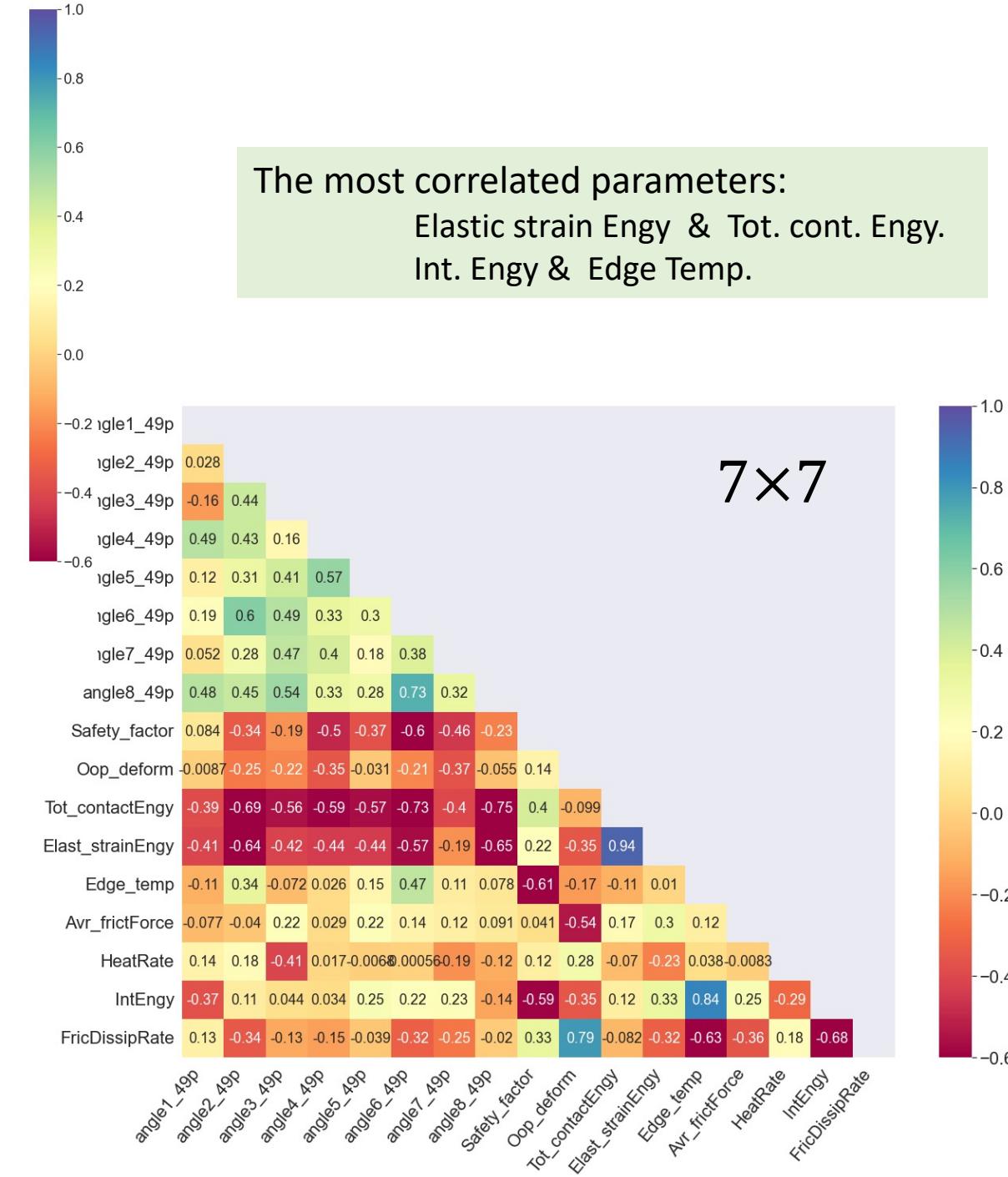
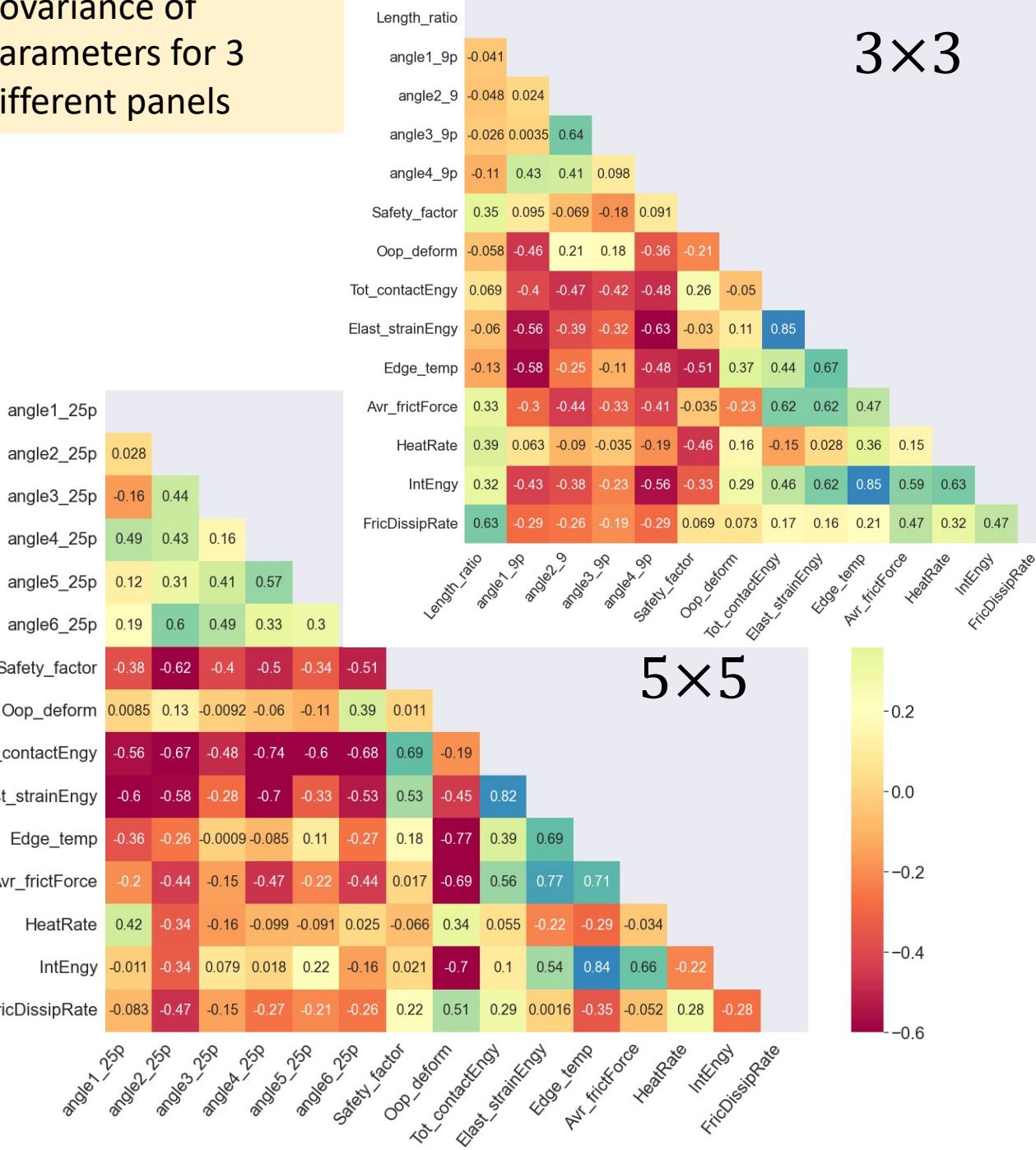


pieces	angle1_9p	angle2_9	angle3_9p	angle4_9p	angle1_25p	angle2_25p	angle3_25p	angle4_25p	angle5_25p	angle6_25p	angle1_49p	angle2_49p	angle3_49p
49.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	10.0	10.0	10.0
9.0	5.0	5.0	5.0	5.0	5.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
25.0	0.0	0.0	0.0	0.0	0.0	15.0	15.0	15.0	15.0	15.0	0.0	0.0	0.0

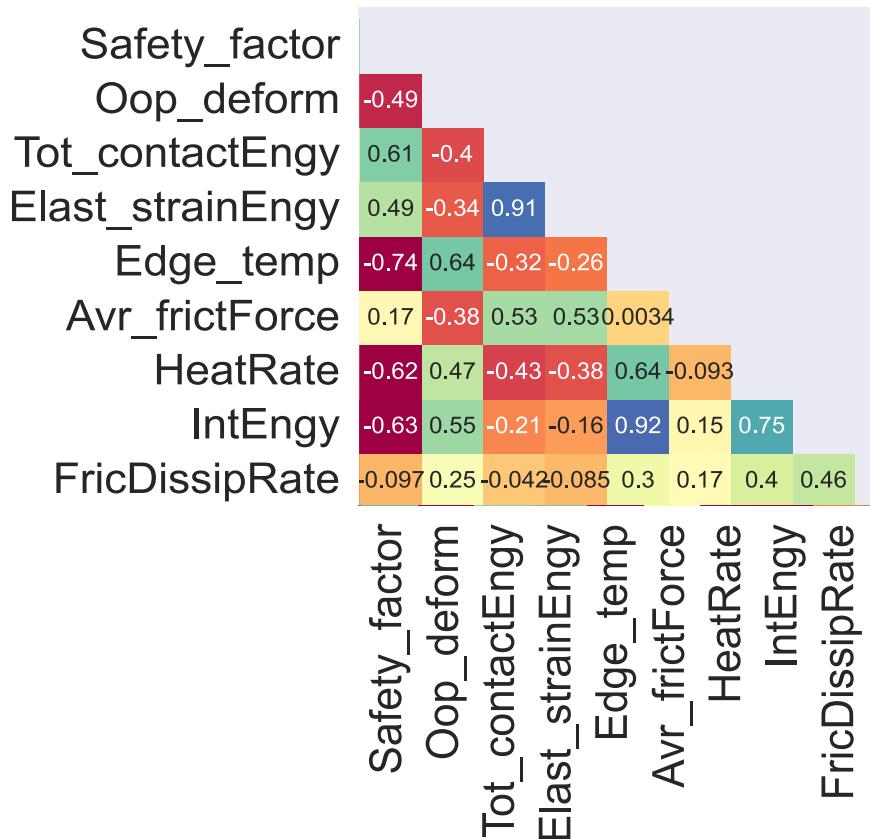
## Exploratory analysis

- 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

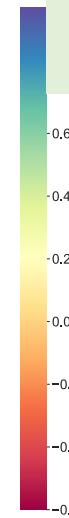


## Correlations for all the panels



The most correlated parameters:

Elastic strain Engy & Tot. cont. Engy.  
Int. Engy & Edge Temp.

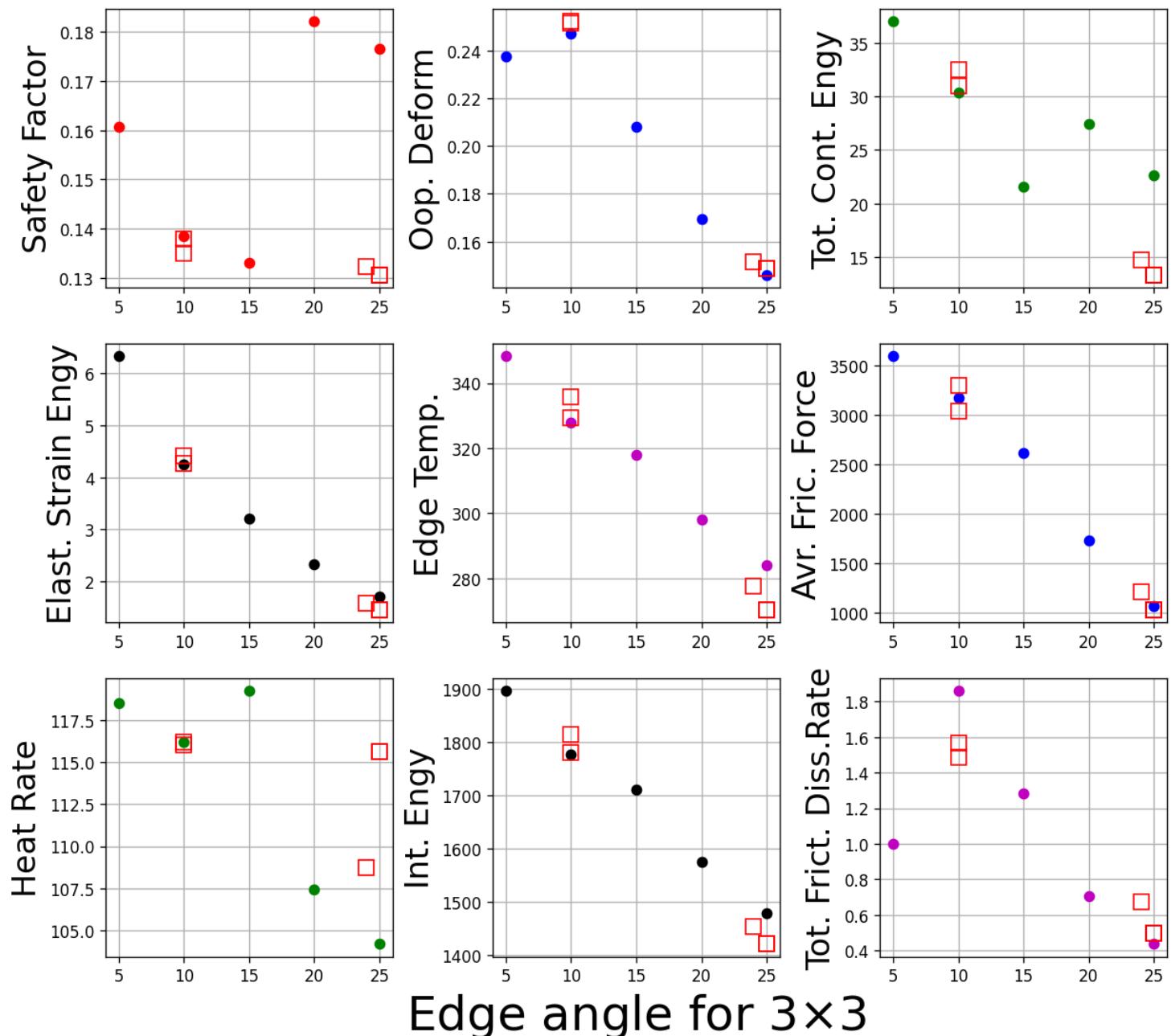


Repeating some runs to check parameter fluctuations

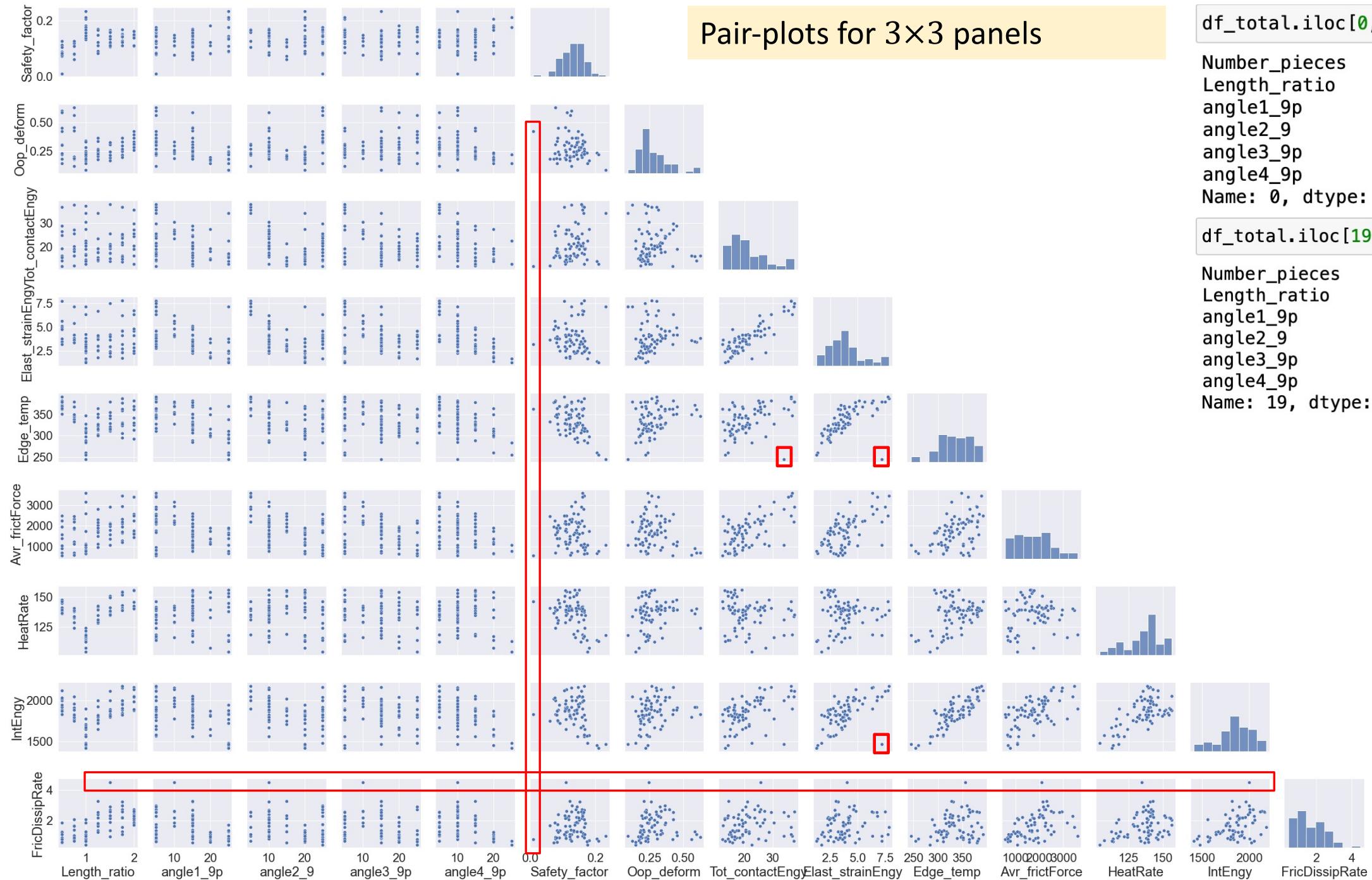
Repeated runs are shown with squares.

Correlated parameters from pairplots:

Elastic strain Engy & Tot. cont. Engy.  
Int. Engy & Edge Temp.



## Pair-plots for 3x3 panels



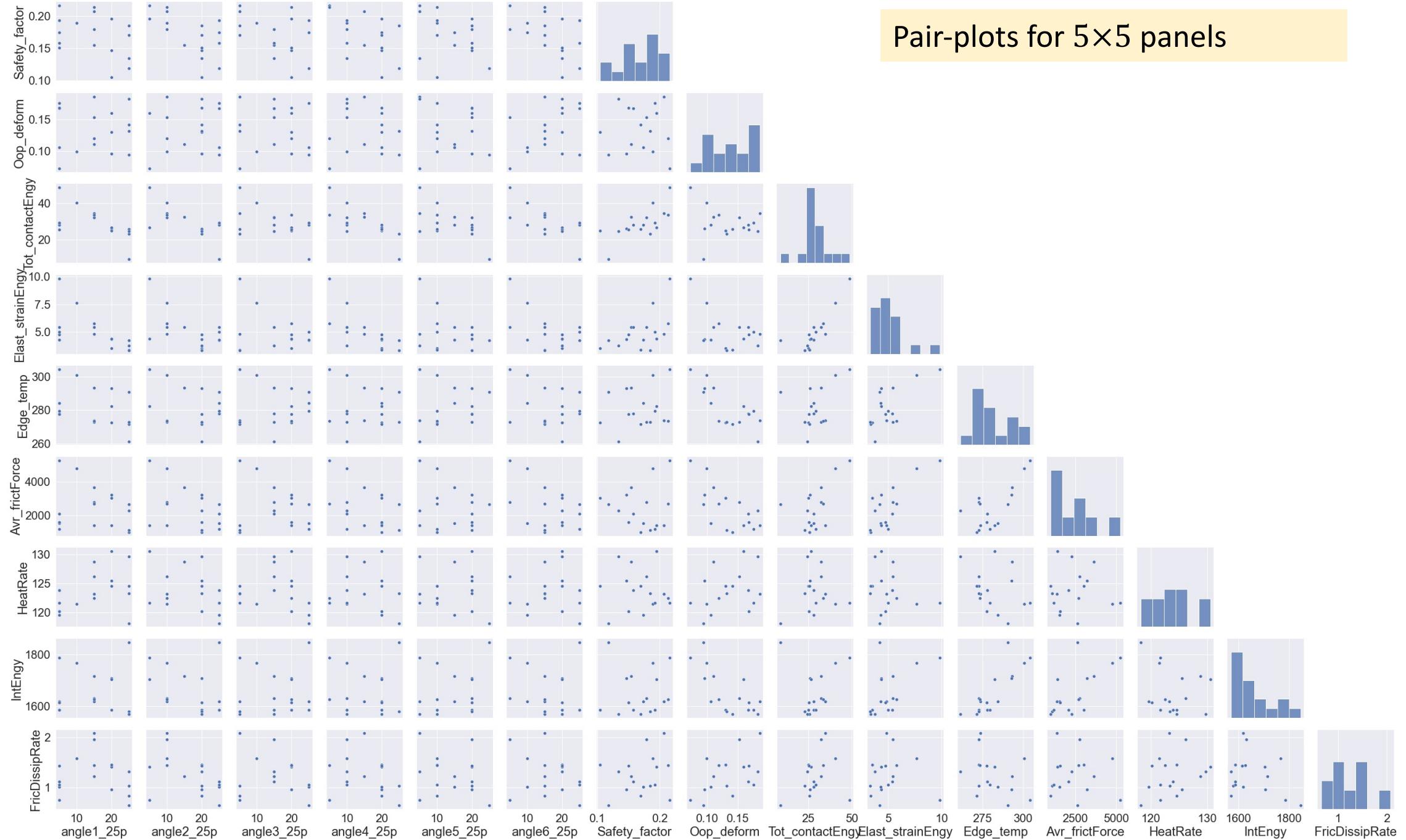
df\_total.iloc[0,:6]

```
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
```

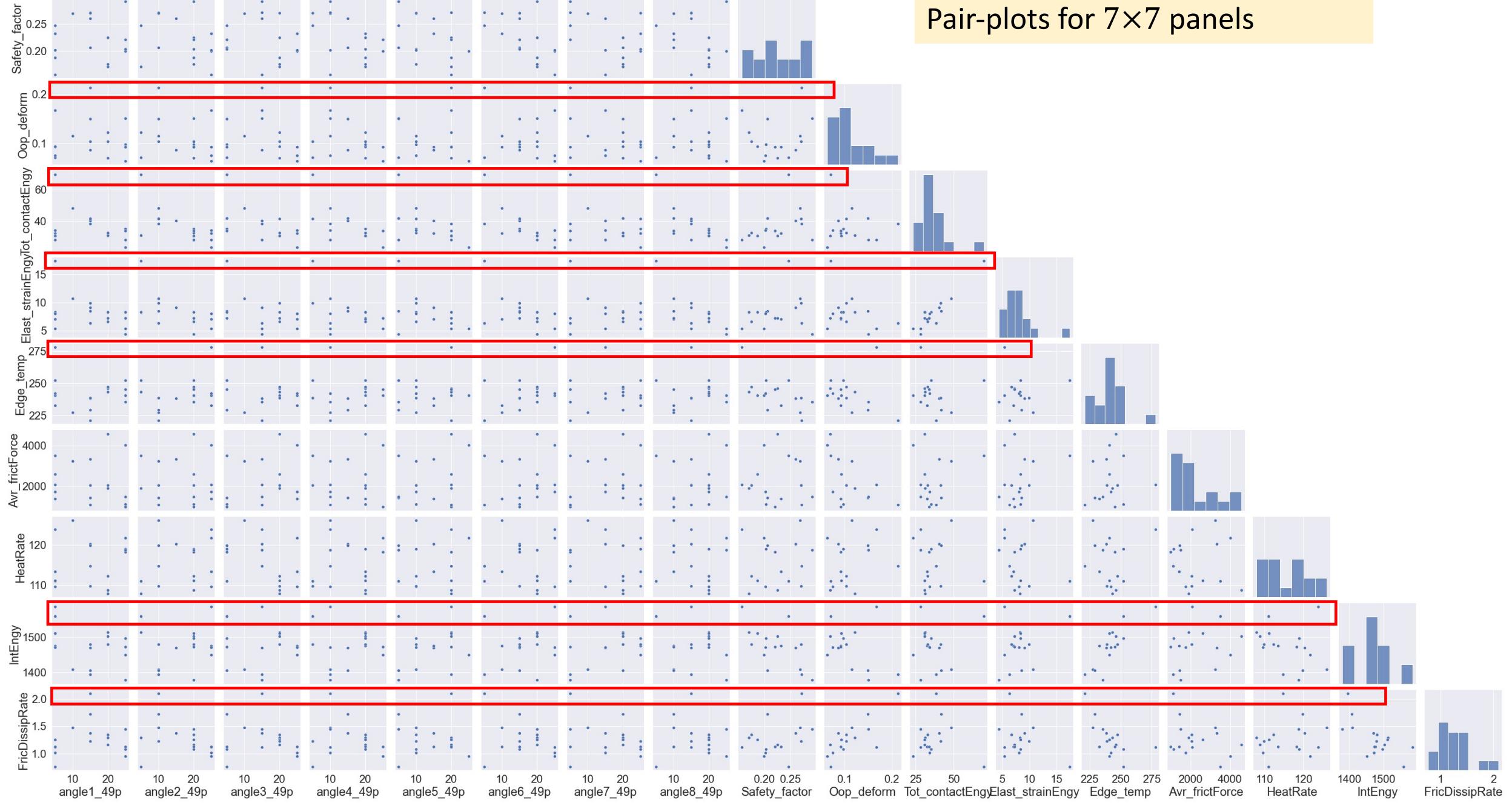
df\_total.iloc[19,:6]

```
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
```

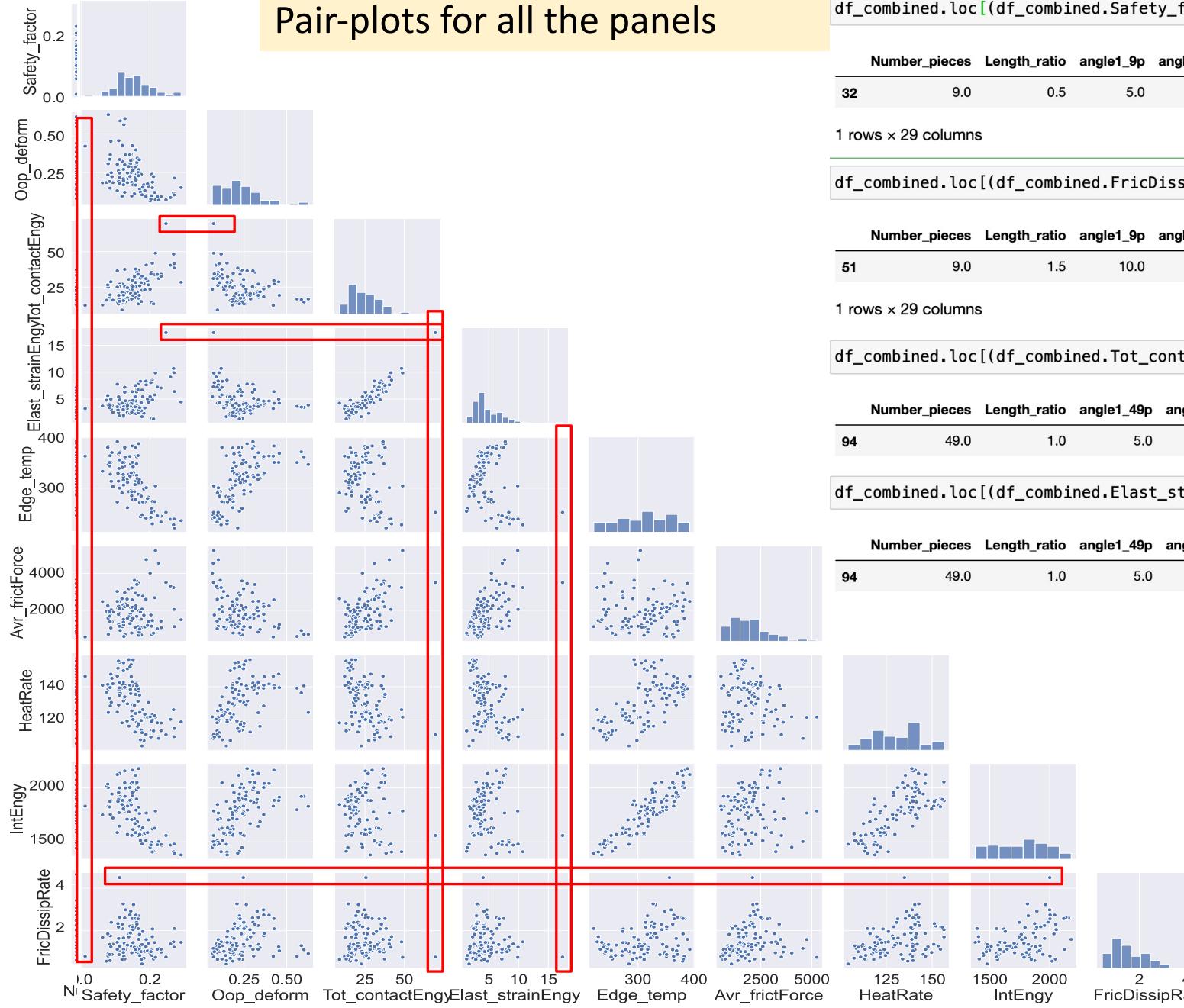
## Pair-plots for 5×5 panels



## Pair-plots for 7x7 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 x 29 columns

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

51 9.0 1.5 10.0 10.0 10.0 10.0 0.0 0.0 0.0 0.0 0.0 ...

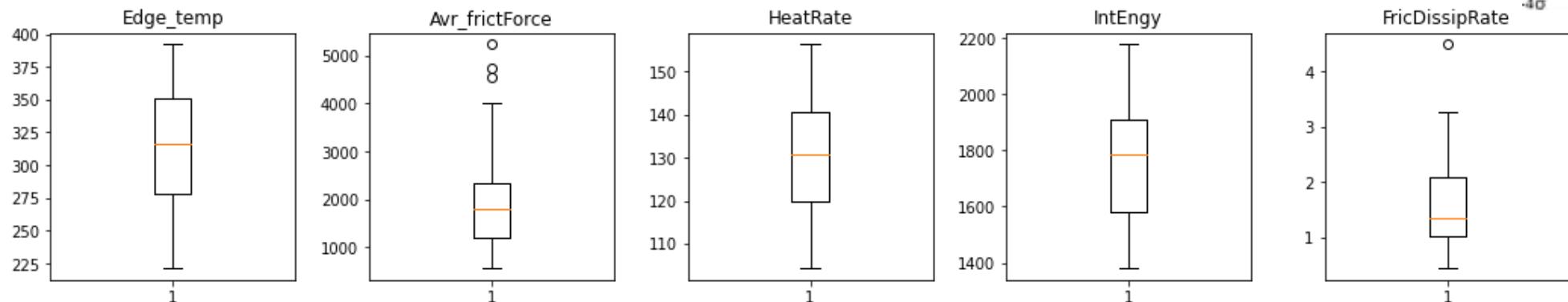
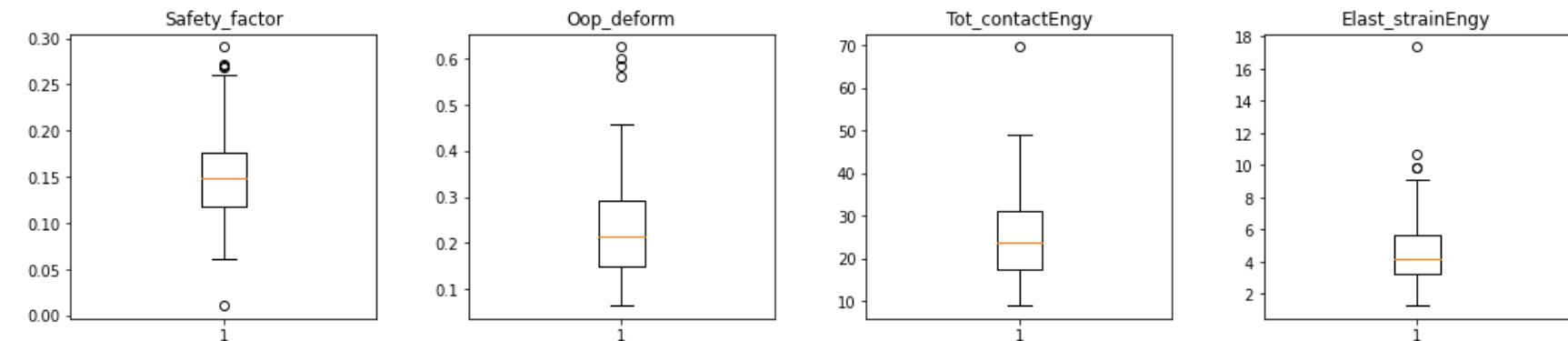
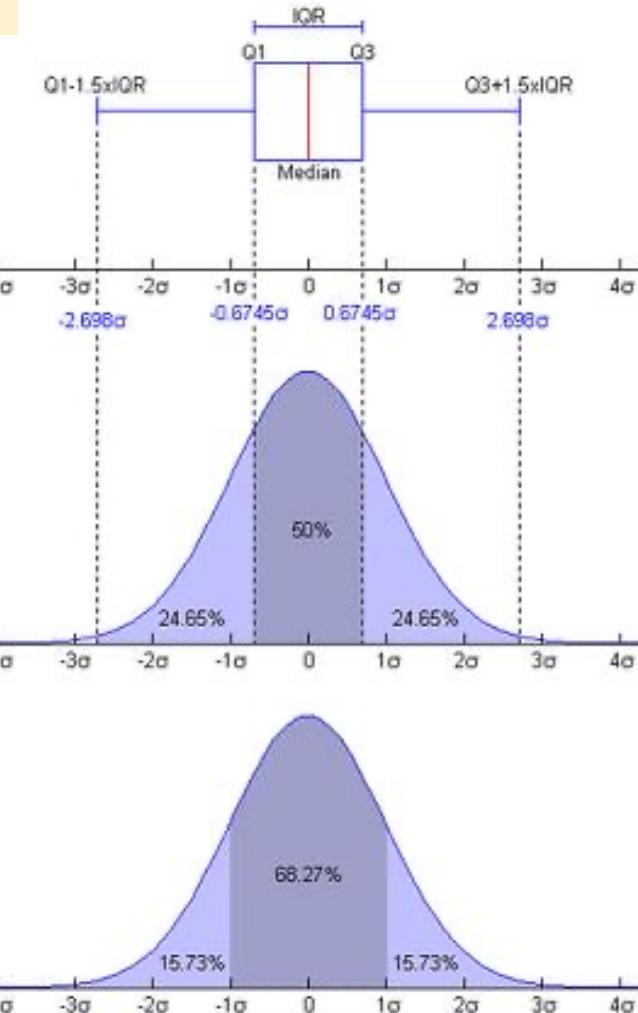
1 rows x 29 columns

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

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

## 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

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

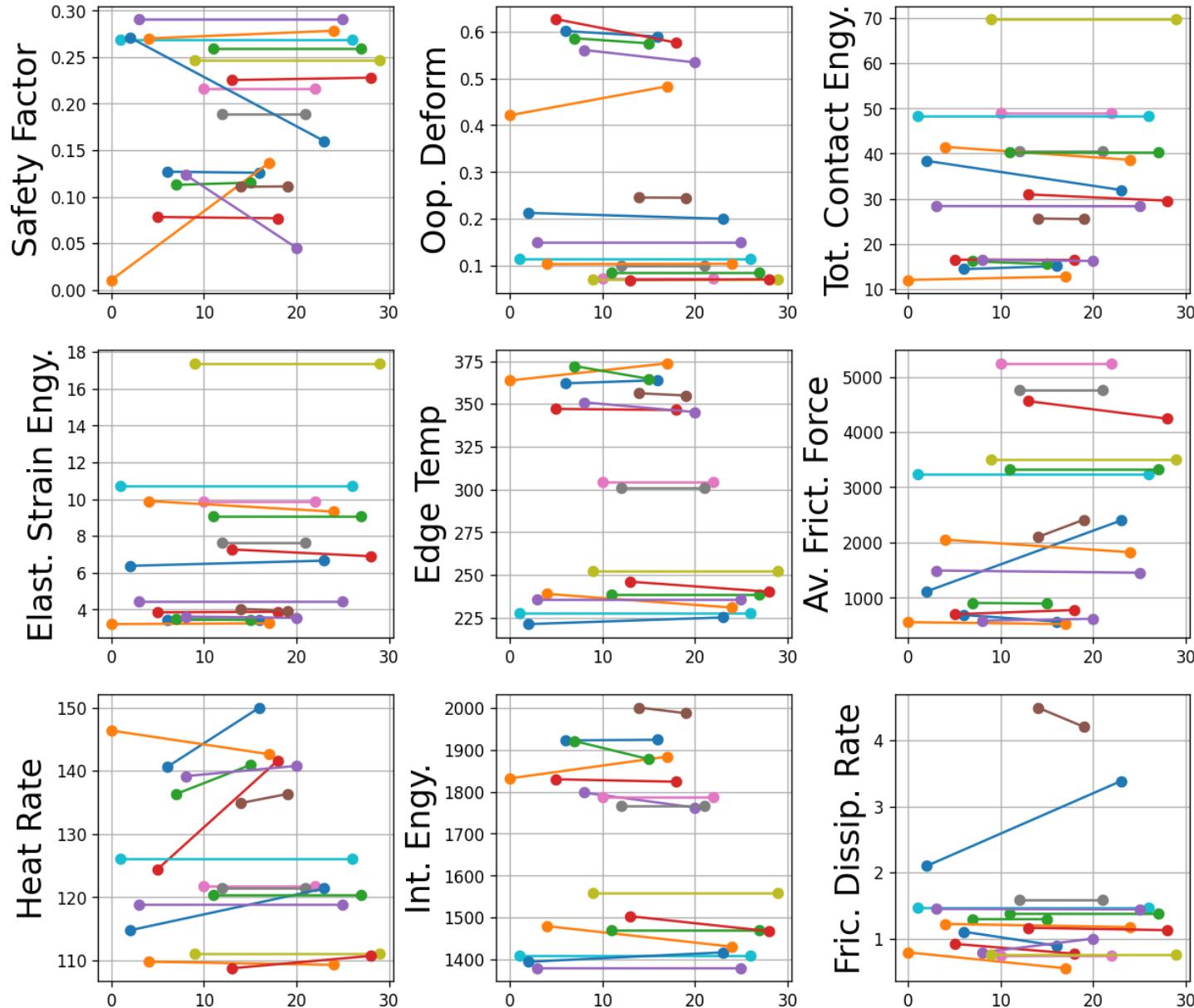
    # finding the 3rd quartile
    q3 = np.quantile(arr, 0.75)
    med = np.median(arr)

    # finding the iqr region
    iqr = q3-q1

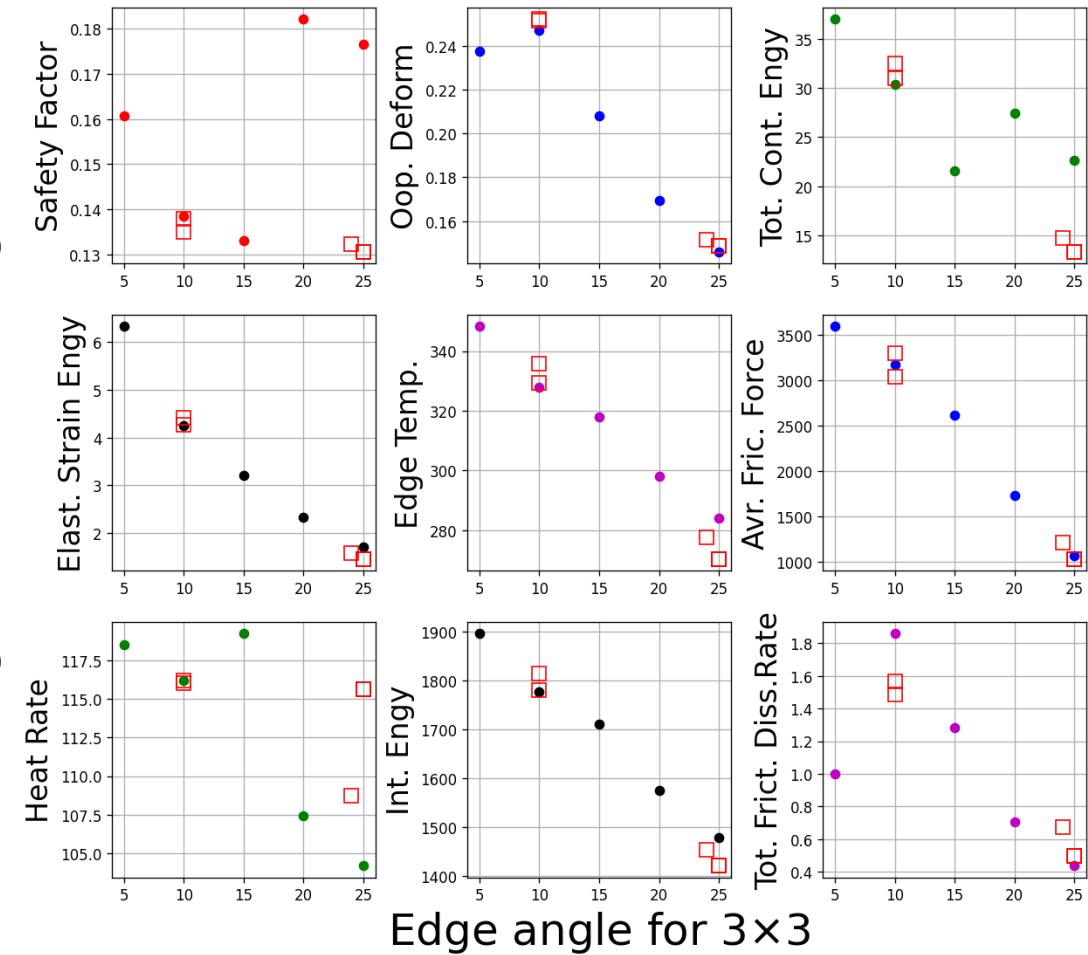
    # finding upper and lower whiskers
    upper_bound = q3+(1.5*iqr)
    lower_bound = q1-(1.5*iqr)
    return df_combined.loc[(arr > upper_bound) | (arr < lower_bound)]
```

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

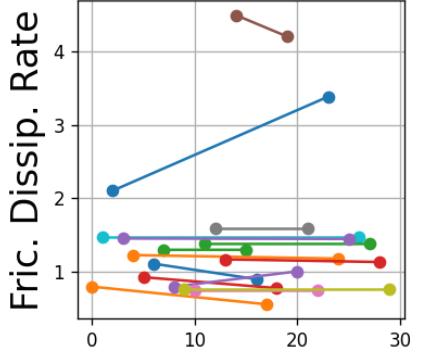
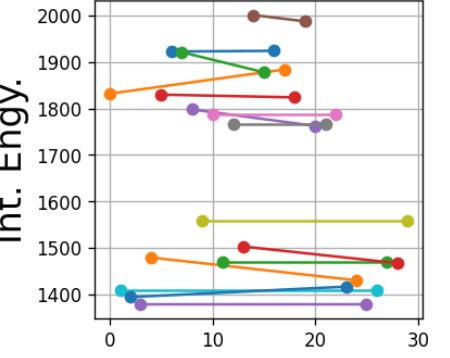
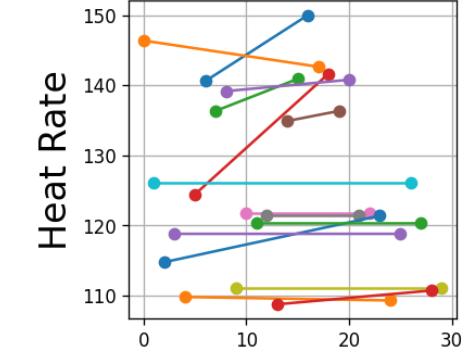
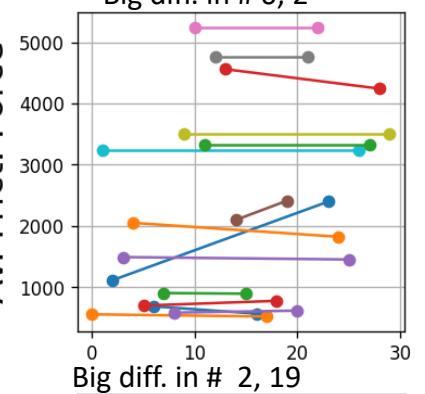
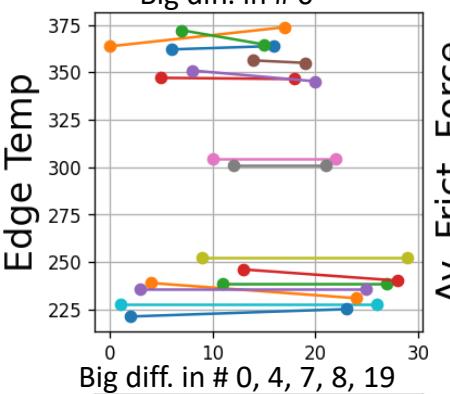
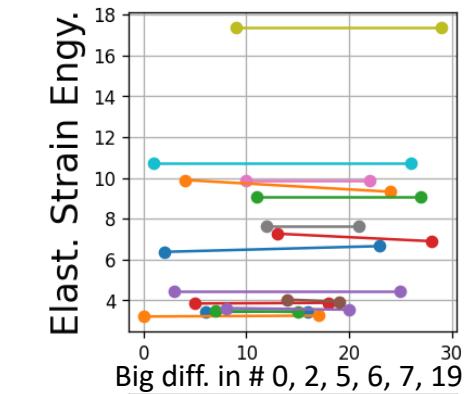
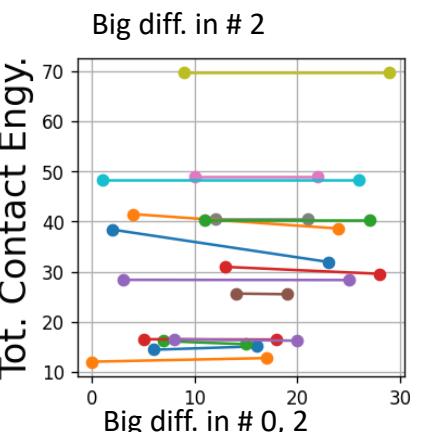
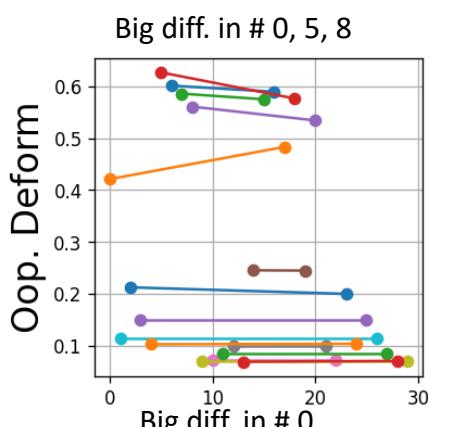
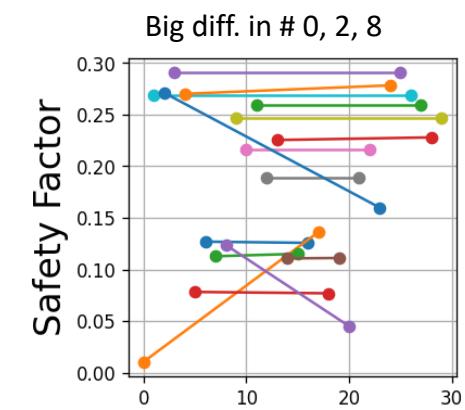
## Repeating 15 cases of all the designs



## Repeating 3 cases of all the designs



Edge angle for 3x3



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[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[2,:2], df\_tot

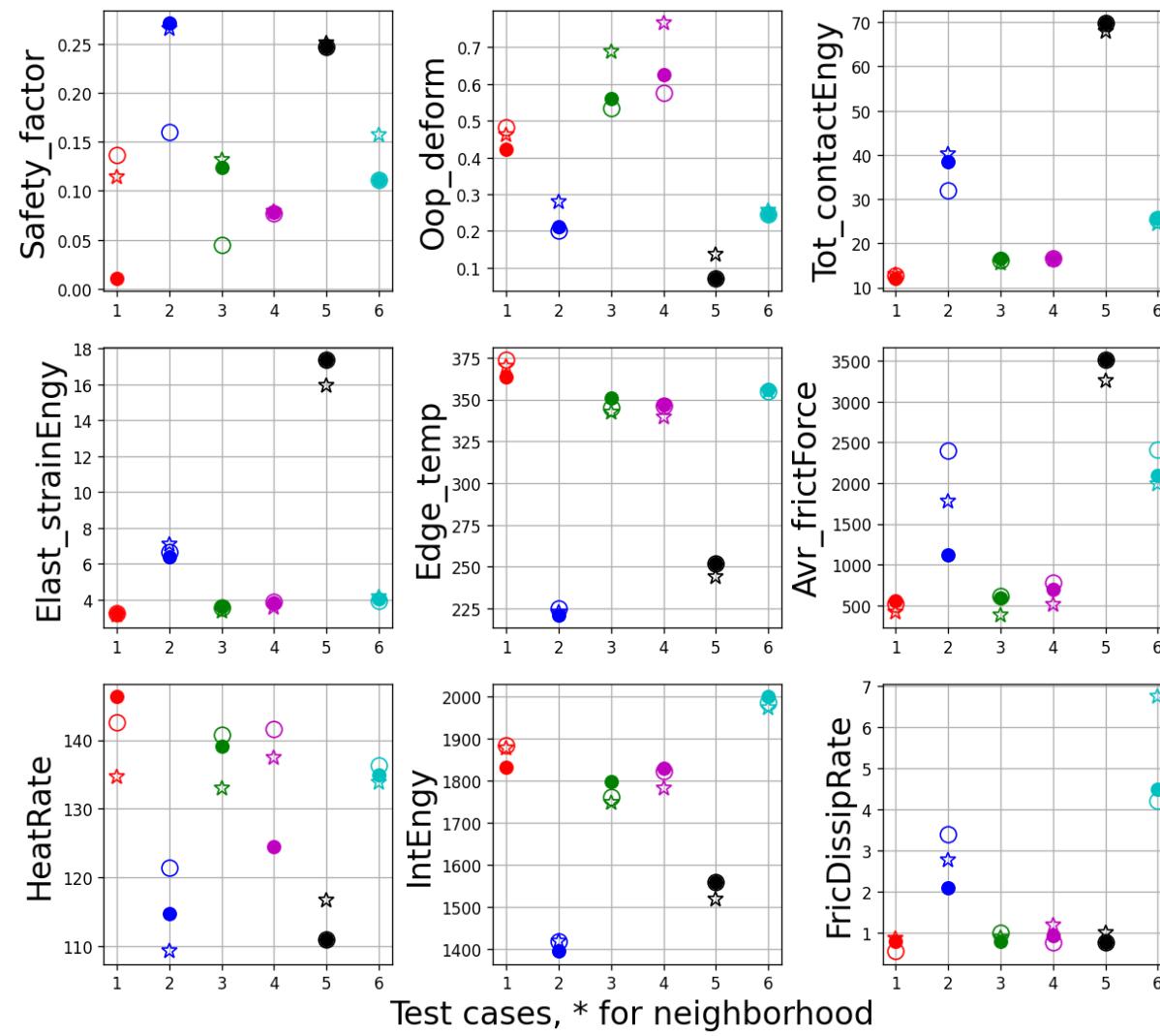
Number_pieces	49.0
Length_ratio	1.0
Name: 2, dtype: float64,	
angle1_49p	15.0
angle2_49p	10.0
angle3_49p	15.0
angle4_49p	10.0
angle5_49p	20.0
angle6_49p	5.0
angle7_49p	5.0
angle8_49p	15.0
Name: 19, dtype: float64	

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	

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	

## Repeated runs and at neighborhood:



	Number_pieces	Length_ratio	angle1_9p	angle2_9p	angle3_9p	angle4_9p	angle1_49p	angle2_49p	angle3_49p	angle4_49p	angle5_49p	angle7_49p	angle8_49p
<b>0</b>	49	1.00	0	0	0	0	14	9	14	9	19	4	14
<b>1</b>	49	1.00	0	0	0	0	6	6	6	6	6	6	6
<b>2</b>	9	1.40	10	10	10	10	0	0	0	0	0	0	0
<b>3</b>	9	0.45	5	25	25	10	0	0	0	0	0	0	0
<b>4</b>	9	0.75	4	24	24	9	0	0	0	0	0	0	0
<b>5</b>	9	0.75	4	24	14	9	0	0	0	0	0	0	0

### Just for 3by 3 panels (74 data points)

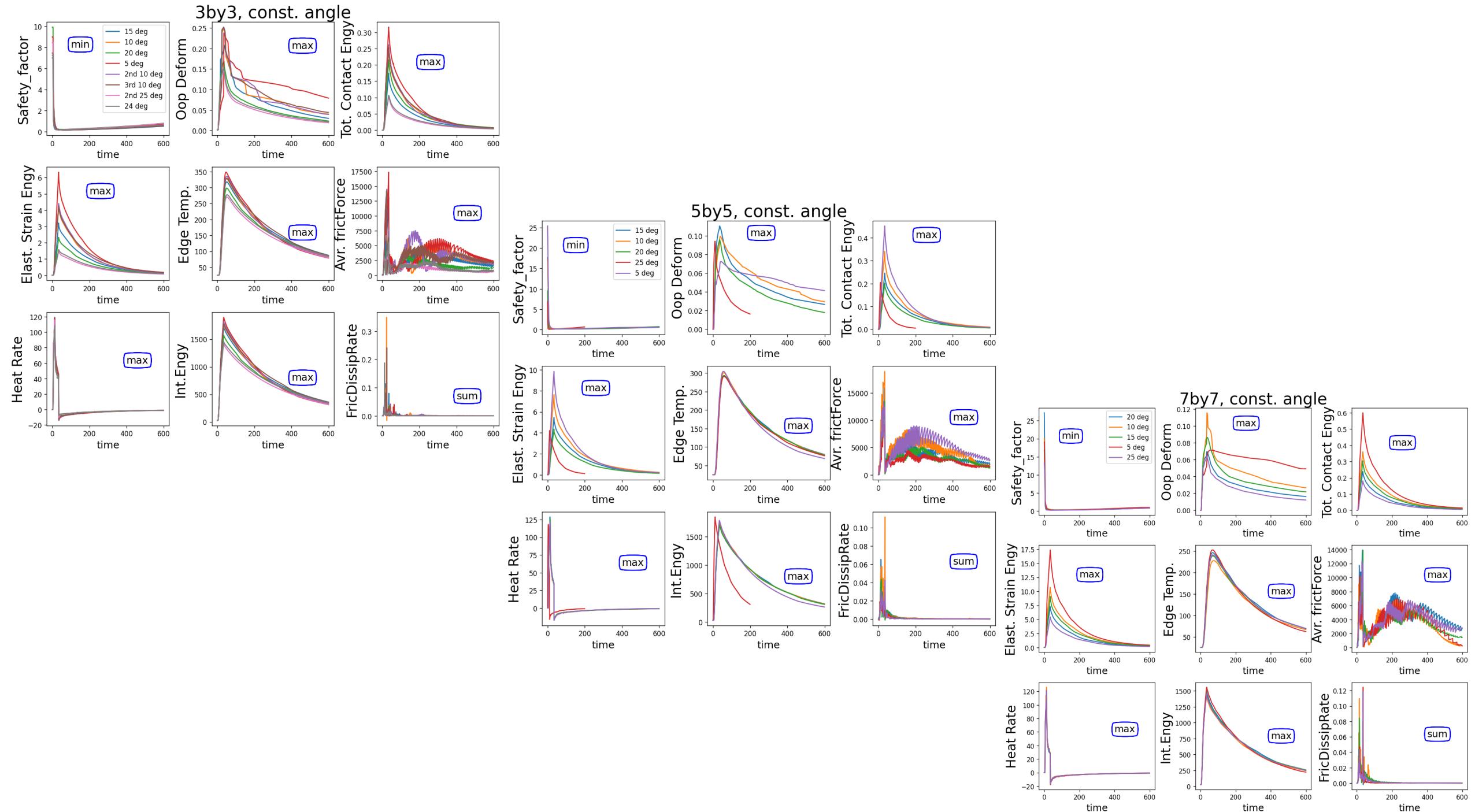
Bootstrap R2 (%)	Safety_factor	Oop deform	Tot. Contact Engy	Elast. Strain Engy	Edge Temp	Avr. Fric. Force	Heat Rate	Int. Engy	Fric. Diss. Rate
LR	-10	2	22	44	26	13	-2	25	43
2 <sup>nd</sup> Poly	-1	24	45	63	56	40	25	57	45
3 <sup>rd</sup> Poly	-51	-27	-10	-3	13	-31	17	26	22
XGB	44	26	36	52	65	60	81	78	60
2 <sup>nd</sup> Poly & XGB	42	36	41	30	62	56	75	76	61
3 <sup>rd</sup> Poly & XGB	52	32	37	62	63	56	76	77	62
Gauss. Process Reg.	-1	52	61	68	55	67	35	56	58

For all panels (114 data points), 18 angles

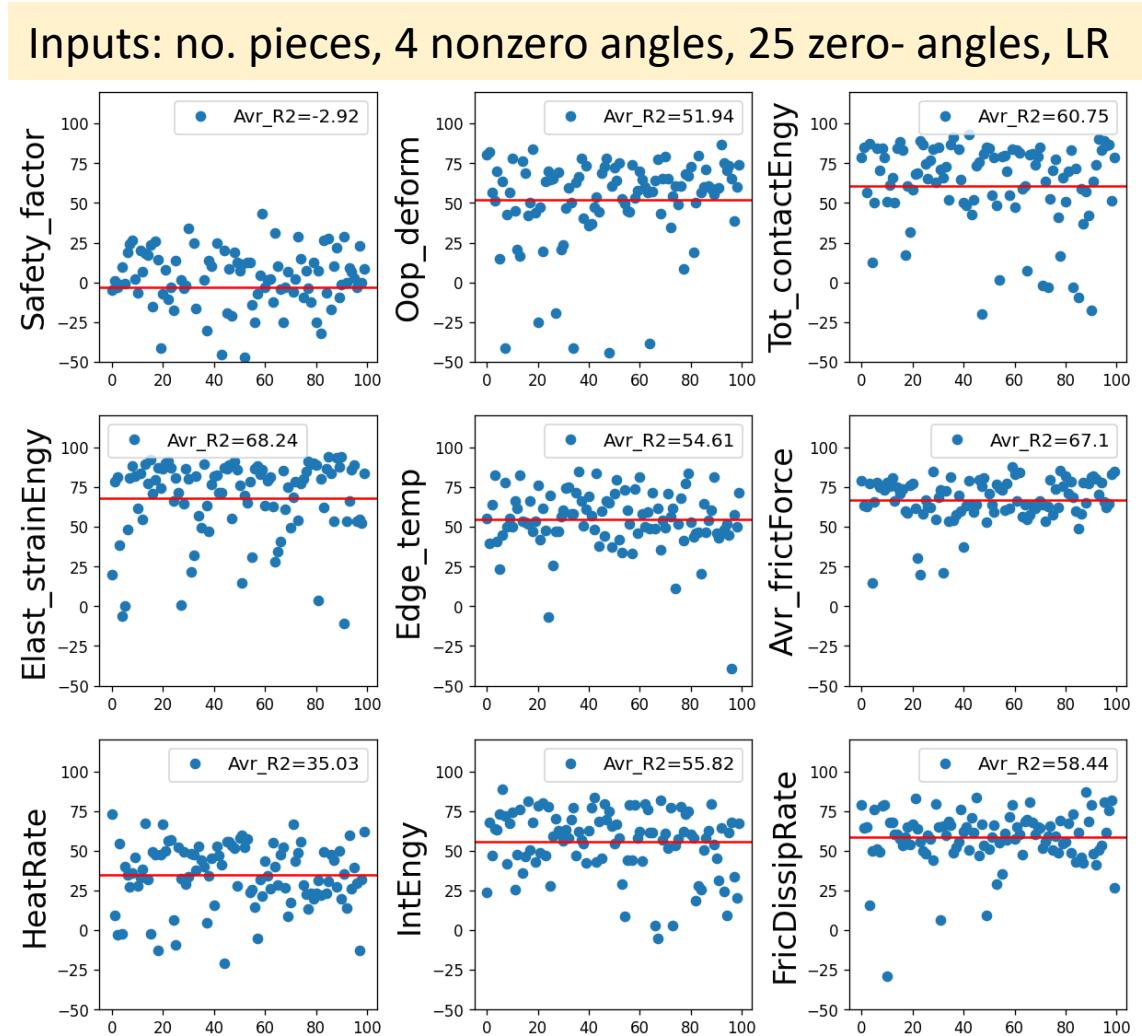
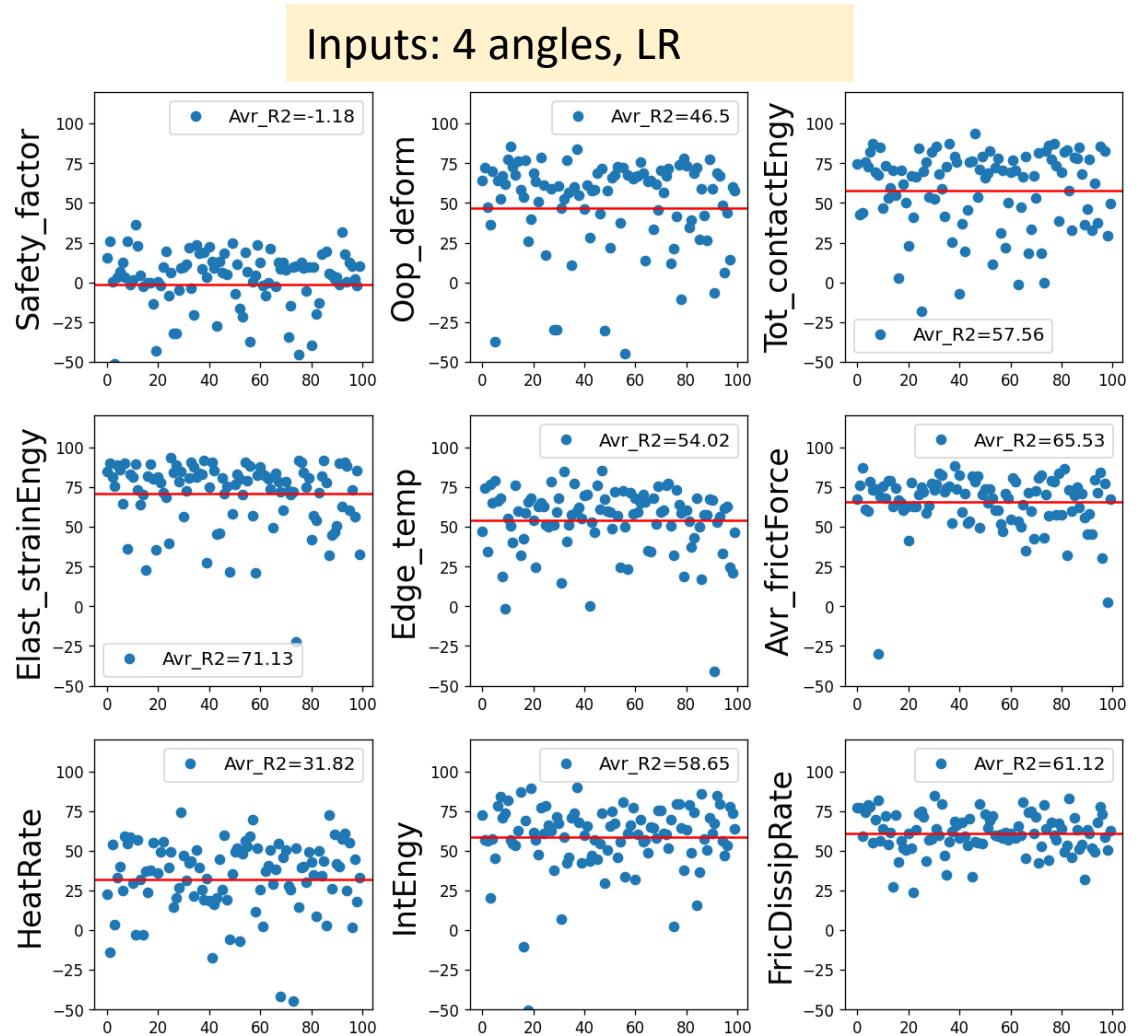
Bootstrap R2 (%)	Safety_f actor	Oop deform	Tot. Contact Engy	Elast. Strain Engy	Edge Temp	Avr. Fric. Force	Heat Rate	Int. Engy	Fric. Diss. Rate
LR	-10	-10	-10	-10	45	-10	-12	24	-10
2 <sup>nd</sup> Poly	-2	-2	-8	-1	-4	-1	-8	-5	-1
3 <sup>rd</sup> Poly	-1	-6	-3	-8	-2	-5	-8	-7	-8
XGB	55	58	58	58	82	-24	87	82	54
2 <sup>nd</sup> Poly & XGB	58	55	58	63	82	-30	85	82	56
3 <sup>rd</sup> Poly & XGB	60	58	56	64	82	-22	83	82	50
Gauss. Process Reg.	54.3	63	79	76	83	59	53	80	56

After checking the output calculations, for all the simulations (135 data sets):

Bootstrap R2 (%)	Safety_f actor	Oop deform	Tot. Contact Engy	Elast. Strain Engy	Edge Temp	Avr. Fric. Force	Heat Rate	Int. Engy	Fric. Diss. Rate
LR	-10	30	12	-10	75.5	-10	-10	54	-10
2 <sup>nd</sup> Poly	-2	-2	-8	-1	-4	-1	-8	-5	-1
3 <sup>rd</sup> Poly	-1	-6	-3	-8	-2	-5	-8	-7	-8
XGB	55	76	60	50	90	55	88	82	58
2 <sup>nd</sup> Poly & XGB	56	77	62	47	88	5	86	82	61
3 <sup>rd</sup> Poly & XGB	55	69	65	51	88	56	84	82	51
NN	43	84	82	82	87	63	71	86	44
Gauss. Process Reg.	56	77	85	87	87	74	68	84	59



Gaussian Process Regression for 74 data points, 3 by 3 panels.  
Results for two different sets of 100 bootstrapped train-test splits.

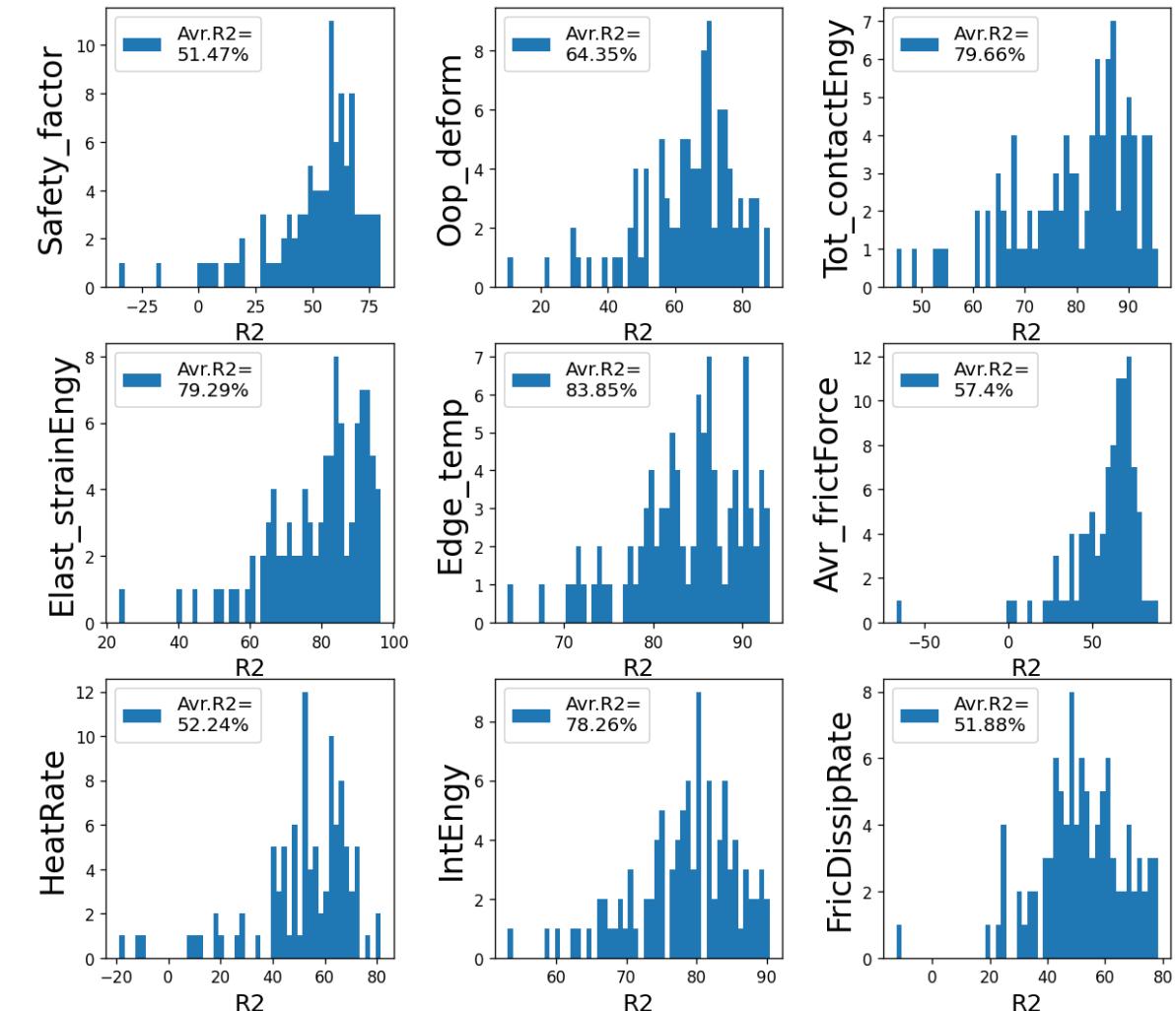
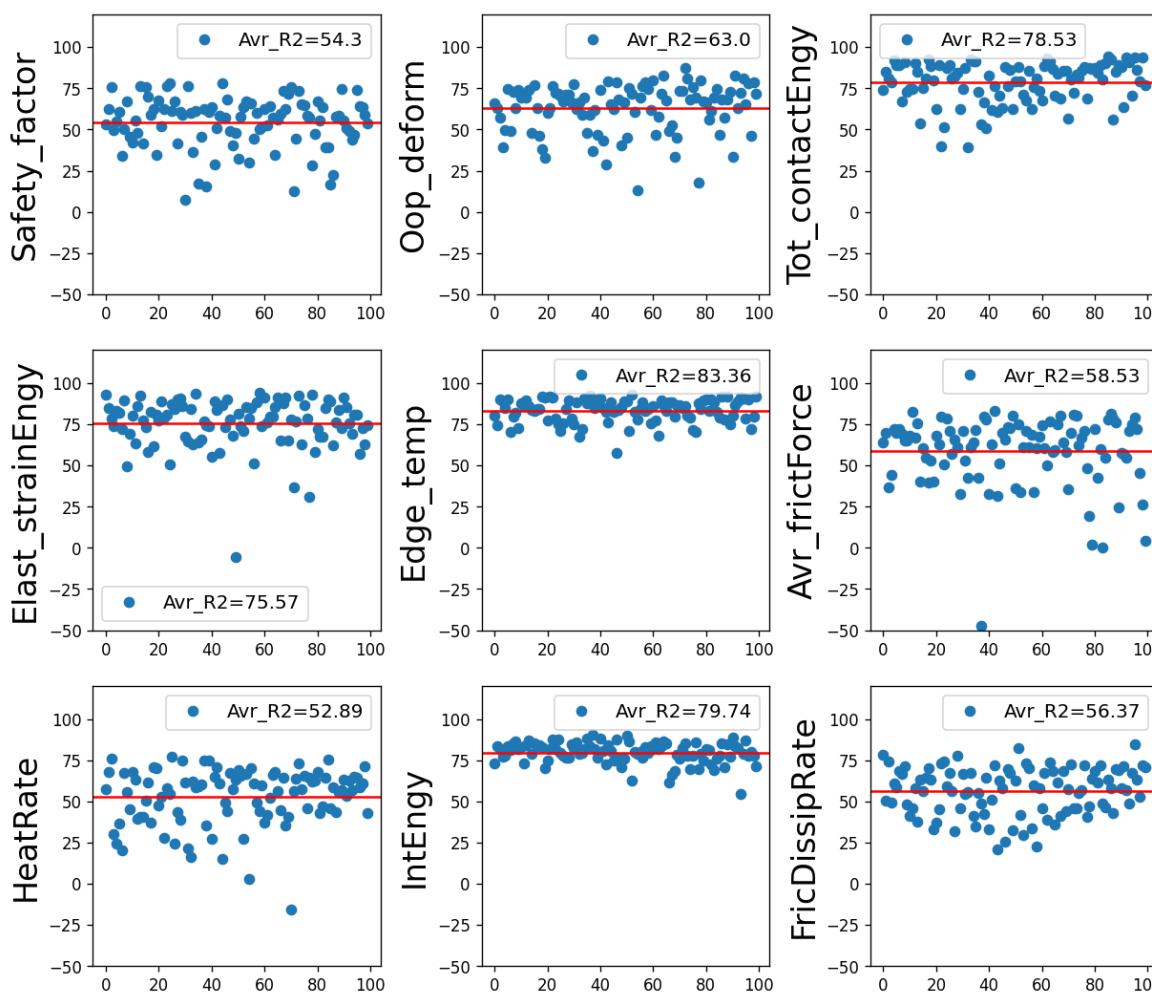


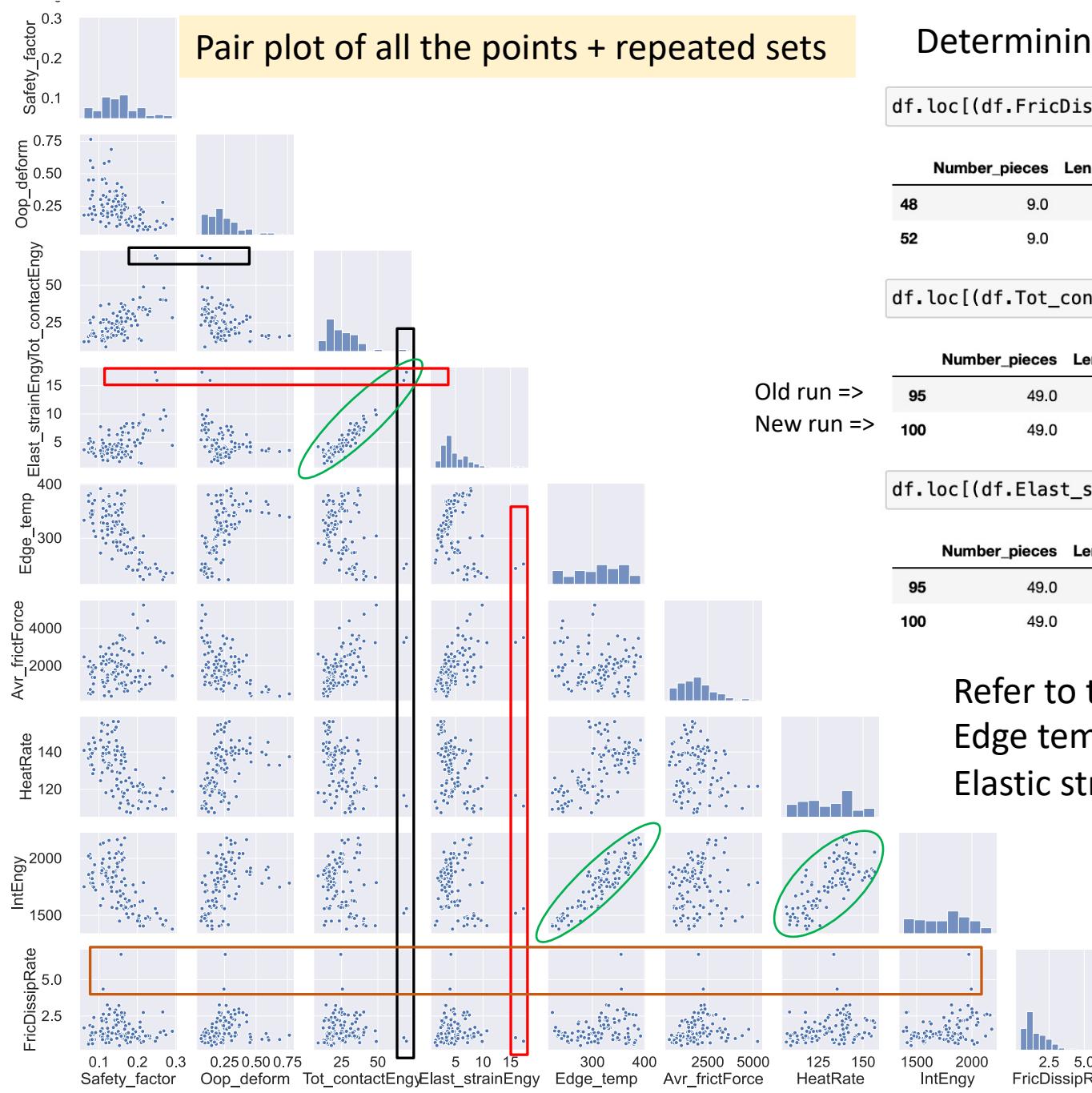
Gaussian Process Regression for all the 114 data points. Results for two different sets of 100 bootstrapped train-test splits.  
 Inputs: no. of pieces, LR, 3 sets of angles (29 angles in total),  
 nonzero angles:

3by3 panels: angle9\_1, . . . , angle9\_4

5by5 panels: angle25\_1, . . . , angle25\_6

7by7 panels: angle49\_1, . . . , angle49\_8





## Determining the outliers:

```
df.loc[(df.FricDissipRate > 4)].iloc[:, :6]
```

Number_pieces	Length_ratio	angle1_9p	angle2_9p	angle3_9p	angle4_9p
---------------	--------------	-----------	-----------	-----------	-----------

48	9.0	1.4	10.0	10.0	10.0
----	-----	-----	------	------	------

<= New run

52	9.0	1.5	10.0	10.0	10.0
----	-----	-----	------	------	------

<= Old run

```
df.loc[(df.Tot_contactEngy > 50)].drop(df.iloc[:, 2:12], axis='columns').iloc[:, :10]
```

Number_pieces	Length_ratio	angle1_49p	angle2_49p	angle3_49p	angle4_49p	angle5_49p	angle6_49p	angle7_49p	angle8_49p
---------------	--------------	------------	------------	------------	------------	------------	------------	------------	------------

95	49.0	1.0	5.0	5.0	5.0	5.0	5.0	5.0	5.0
----	------	-----	-----	-----	-----	-----	-----	-----	-----

100	49.0	1.0	6.0	6.0	6.0	6.0	6.0	6.0	6.0
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```
df.loc[(df.Elast_strainEngy > 15)].drop(df.iloc[:, 2:12], axis='columns').iloc[:, :10]
```

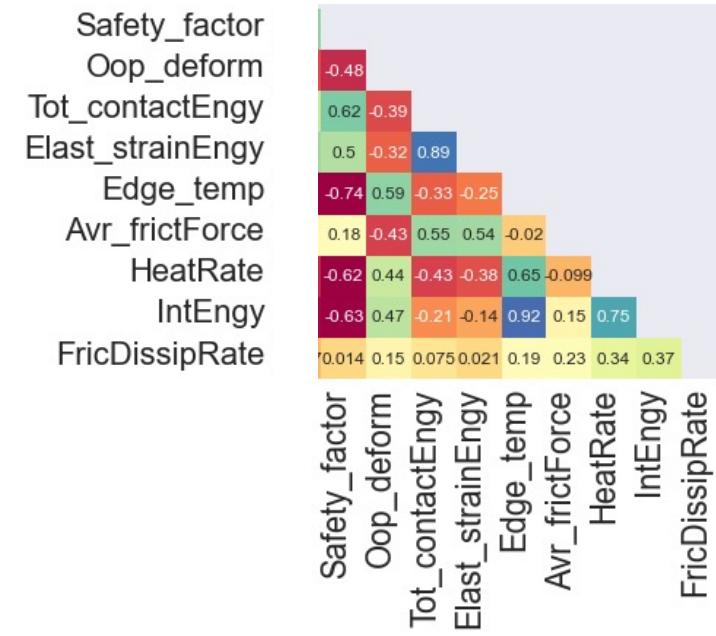
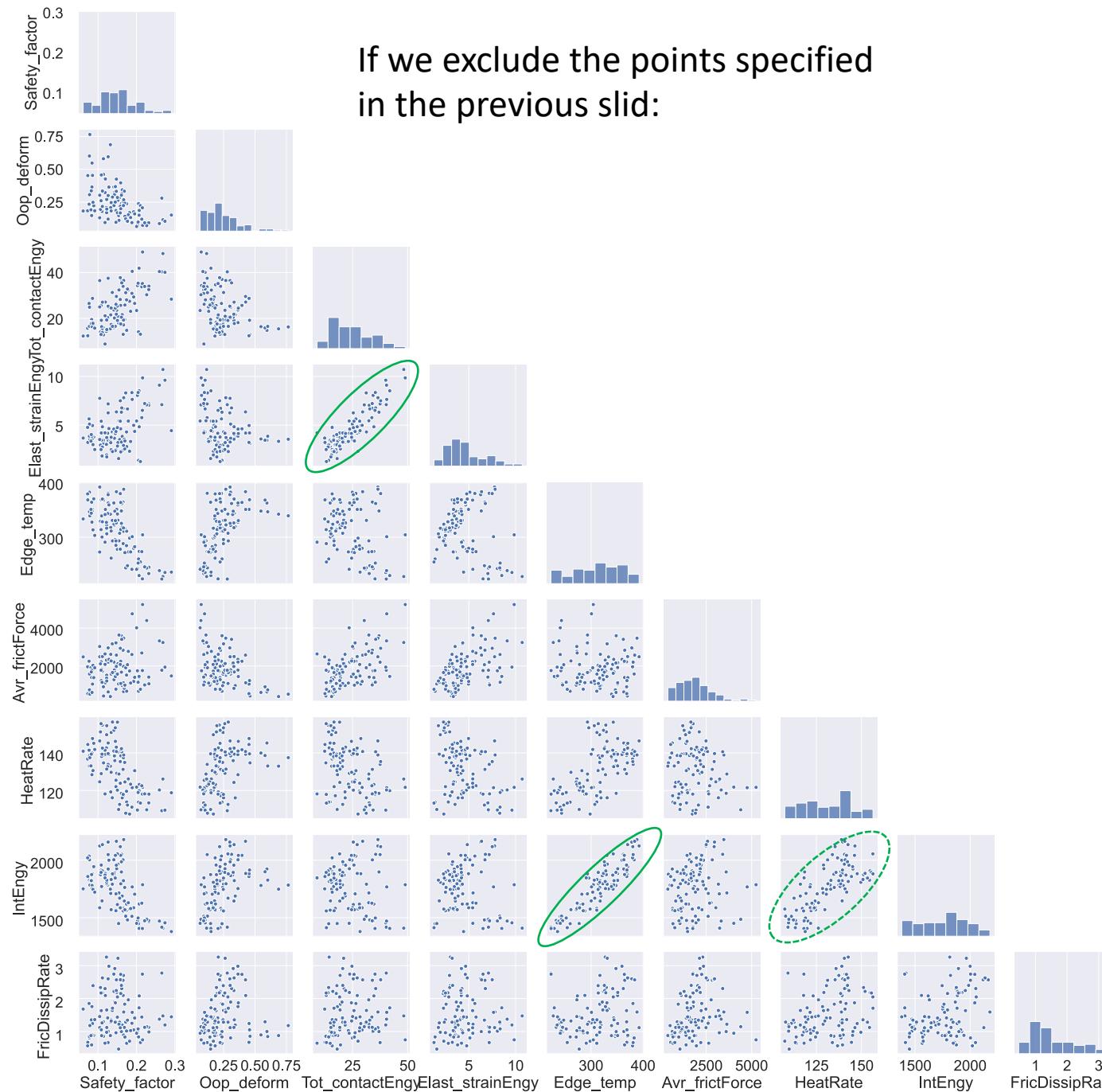
Number_pieces	Length_ratio	angle1_49p	angle2_49p	angle3_49p	angle4_49p	angle5_49p	angle6_49p	angle7_49p	angle8_49p
---------------	--------------	------------	------------	------------	------------	------------	------------	------------	------------

95	49.0	1.0	5.0	5.0	5.0	5.0	5.0	5.0	5.0
----	------	-----	-----	-----	-----	-----	-----	-----	-----

100	49.0	1.0	6.0	6.0	6.0	6.0	6.0	6.0	6.0
-----	------	-----	-----	-----	-----	-----	-----	-----	-----

Old run =>  
New run =>

Refer to the covariances, correlated out puts are:  
**Edge temp & Int Engy**  
**Elastic strain Engy & Tot. Contact Engy**



Correlated parameters with higher covariances are distinguished in the pair-plots, green lines.

We expect a kind of correlation between dissipative parameters, which are Friction dissipation rate and Average friction force. It is worth double checking the equations used for calculating these parameters.