In [1]:

```python
import numpy as np
import matplotlib.pyplot as plt
import os
import sys
import pandas as pd
from mpltools import annotation
##from matplotlib import rc
#rc('font', **{'family': 'serif', 'serif': ['Computer Modern']})
#rc('text', usetex=True)
```

In [2]:

```python
# Import the .txt-file generated by 'autotest.sh'
txtname = "tree_test.txt"
data = np.loadtxt(txtname)
data.shape
```

Out[2]: (24, 7)

In [3]:

```python
# Map boolean input of quadrupoles to strings.
def convert(x):
    if x == 0:
        return "Mono"
    else:
        return "Quad"
```

In [4]:

```python
N      = "N"
theta  = "$\\theta_c$"
quad   = "Multipole expansion"
tree   = "Tree code t(s)"
dirsum = "Direct t(s)"
relerr = "Relative error"
intact = "Avg interactions"

data_ls = []
for i in range(len(data)):
    data_ls.append({
        N:      int(data[i,0]),           # Number of particles
        theta:  data[i,1],                # Opening angle threshold
        quad:   convert(int(data[i,2])),  # Using quadrupoles (bool)
        tree:   data[i,3],                # Execution time tree code (sec)
        dirsum: data[i,4],                # Execution time direct summation (sec)
        relerr: data[i,5],                # Mean relative force error
        intact: data[i,6]                 # Mean number of particle-node interactions
    })
df = pd.DataFrame(data_ls) # Create dataframe

# Retain an unaltered copy of the dataframe.
df_copy = df.copy()
df_copy
```

Out[4]:

	N	θ_c	Multipole expansion	Tree code t(s)	Direct t(s)	Relative error	Avg interactions
0	5000	0.2	Mono	0.604802	1.78396	0.000279	1735.480
1	5000	0.2	Quad	1.066630	1.77675	0.000022	1735.480
2	5000	0.4	Mono	0.163367	1.77674	0.002177	501.845
3	5000	0.4	Quad	0.297304	1.77734	0.000384	501.845
4	5000	0.8	Mono	0.034382	1.78090	0.014926	109.968
5	5000	0.8	Quad	0.064255	1.78542	0.006886	109.968
6	10000	0.2	Mono	2.109320	7.51979	0.000245	2403.890
7	10000	0.2	Quad	3.418570	8.09434	0.000020	2403.890
8	10000	0.4	Mono	0.485566	8.28296	0.001814	621.909
9	10000	0.4	Quad	0.951817	8.40635	0.000332	621.909
10	10000	0.8	Mono	0.094773	8.13719	0.012776	127.757
11	10000	0.8	Quad	0.184383	8.12671	0.006108	127.757
12	20000	0.2	Mono	5.444850	31.64360	0.000225	3120.220
13	20000	0.2	Quad	9.589140	31.52720	0.000019	3120.220
14	20000	0.4	Mono	1.129170	29.20930	0.001527	737.402
15	20000	0.4	Quad	1.927480	29.28240	0.000294	737.402
16	20000	0.8	Mono	0.225642	30.22290	0.010606	144.197
17	20000	0.8	Quad	0.420236	29.02400	0.005340	144.197
18	40000	0.2	Mono	16.810400	116.58500	0.000195	3976.430
19	40000	0.2	Quad	25.686300	117.13400	0.000016	3976.430
20	40000	0.4	Mono	3.272910	117.49900	0.001299	866.969
21	40000	0.4	Quad	4.933170	119.81100	0.000248	866.969
22	40000	0.8	Mono	0.587553	117.86300	0.008915	161.829
23	40000	0.8	Quad	0.888337	118.21700	0.004823	161.829

In [5]:

```python
# Group by N, theta and quadrupole moment
df = df.groupby([N, theta, quad]).first().unstack()
df
```

Out[5]:

		Tree code t(s)		Direct t(s)		Relative error		Avg interactions	
	Multipole expansion	**Mono**	**Quad**	**Mono**	**Quad**	**Mono**	**Quad**	**Mono**	**Quad**
N	θ_c								
5000	**0.2**	0.604802	1.066630	1.78396	1.77675	0.000279	0.000022	1735.480	1735.480
	0.4	0.163367	0.297304	1.77674	1.77734	0.002177	0.000384	501.845	501.845
	0.8	0.034382	0.064255	1.78090	1.78542	0.014926	0.006886	109.968	109.968
10000	**0.2**	2.109320	3.418570	7.51979	8.09434	0.000245	0.000020	2403.890	2403.890
	0.4	0.485566	0.951817	8.28296	8.40635	0.001814	0.000332	621.909	621.909
	0.8	0.094773	0.184383	8.13719	8.12671	0.012776	0.006108	127.757	127.757
20000	**0.2**	5.444850	9.589140	31.64360	31.52720	0.000225	0.000019	3120.220	3120.220
	0.4	1.129170	1.927480	29.20930	29.28240	0.001527	0.000294	737.402	737.402
	0.8	0.225642	0.420236	30.22290	29.02400	0.010606	0.005340	144.197	144.197
40000	**0.2**	16.810400	25.686300	116.58500	117.13400	0.000195	0.000016	3976.430	3976.430
	0.4	3.272910	4.933170	117.49900	119.81100	0.001299	0.000248	866.969	866.969
	0.8	0.587553	0.888337	117.86300	118.21700	0.008915	0.004823	161.829	161.829

Need to fix the direct summation column, misleading to have 'Mono' and 'Quad' labels there. We also calculate the mean execution time of the direct summation method as the average of the two elements at each row.

In [6]:

```python
# Calculate the mean of direct summation columns, insert back into the dataframe.
df[('Direct t(s)','-')] = df.iloc[:,2:4].mean(axis=1)

# Drop the two old direct summation columns.
df = df.drop(df.columns[2:4], axis=1)

# Rearange order of columns, such that the direct summation (avg)
# column retakes its old position.
col_list = list(df.columns)
col_list.insert(2,col_list[-1])
col_list.pop(-1)
df = df[col_list]
```

In [7]:

```python
# Specify formatting of floating point numbers for each column.
format_1 = "{0:.3f}".format # Timings, tree code and direct summation
format_2 = "{0:.2e}".format # Relative errors
format_3 = "{0:.1f}".format # Average interactions
df[list(df.columns)[0:3]]= df[list(df.columns)[0:3]].applymap(format_1)
df[list(df.columns)[3:5]]= df[list(df.columns)[3:5]].applymap(format_2)
df[list(df.columns)[5:]] = df[list(df.columns)[5:]].applymap(format_3)
df
```

Out[7]:

		Tree code t(s)		Direct t(s)	Relative error		Avg interactions	
	Multipole expansion	**Mono**	**Quad**	**-**	**Mono**	**Quad**	**Mono**	**Quad**
N	θ_c							
5000	**0.2**	0.605	1.067	1.780	2.79e-04	2.21e-05	1735.5	1735.5
	0.4	0.163	0.297	1.777	2.18e-03	3.84e-04	501.8	501.8
	0.8	0.034	0.064	1.783	1.49e-02	6.89e-03	110.0	110.0
10000	**0.2**	2.109	3.419	7.807	2.45e-04	2.01e-05	2403.9	2403.9
	0.4	0.486	0.952	8.345	1.81e-03	3.32e-04	621.9	621.9
	0.8	0.095	0.184	8.132	1.28e-02	6.11e-03	127.8	127.8
20000	**0.2**	5.445	9.589	31.585	2.25e-04	1.90e-05	3120.2	3120.2
	0.4	1.129	1.927	29.246	1.53e-03	2.94e-04	737.4	737.4
	0.8	0.226	0.420	29.623	1.06e-02	5.34e-03	144.2	144.2
40000	**0.2**	16.810	25.686	116.859	1.95e-04	1.59e-05	3976.4	3976.4
	0.4	3.273	4.933	118.655	1.30e-03	2.48e-04	867.0	867.0
	0.8	0.588	0.888	118.040	8.91e-03	4.82e-03	161.8	161.8

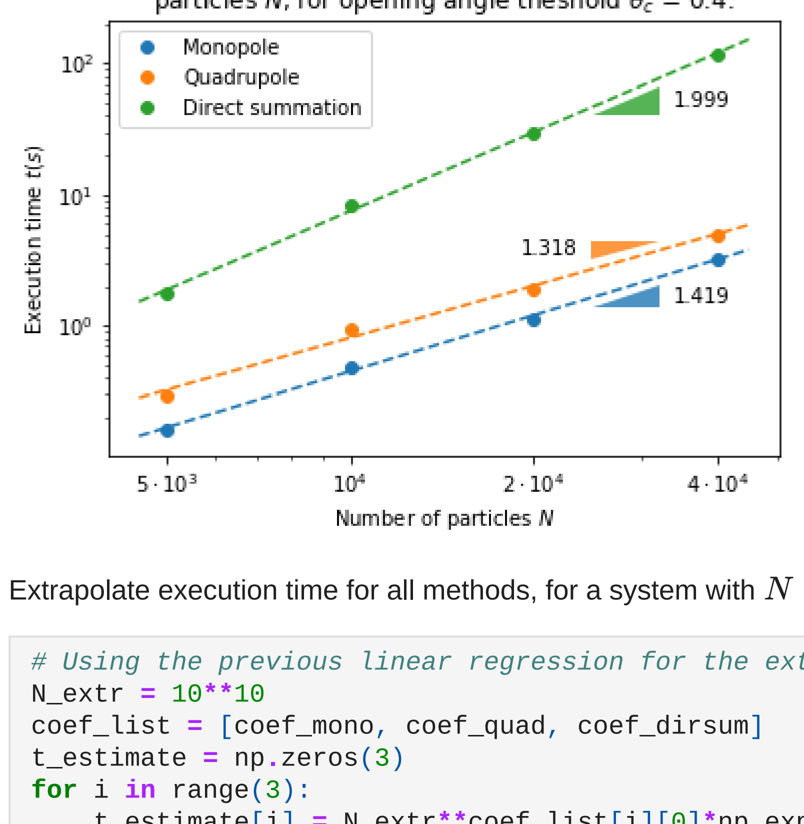
In [8]:

```python
# Export table to latex
print(df.to_latex())
```

```
\begin{tabular}{lllllllll}
\toprule
      & {} & \multicolumn{2}{l}{Tree code t(s)} & Direct t(s) & \multicolumn{2}{l}{Relative error} & \multic
olumn{2}{l}{Avg interactions} \\
      & Multipole expansion &           Mono &    Quad &           - &           Mono &      Quad &
    Mono &    Quad \\
N & \$\textbackslash theta\_c\$ &                &         &             &                &           &
          &         \\
\midrule
5000  & 0.2 &          0.605 &   1.067 &       1.780 &       2.79e-04 &  2.21e-05 &           1735.5 &  173
5.5 \\
      & 0.4 &          0.163 &   0.297 &       1.777 &       2.18e-03 &  3.84e-04 &            501.8 &   50
1.8 \\
      & 0.8 &          0.034 &   0.064 &       1.783 &       1.49e-02 &  6.89e-03 &            110.0 &   11
0.0 \\
10000 & 0.2 &          2.109 &   3.419 &       7.807 &       2.45e-04 &  2.01e-05 &           2403.9 &  240
3.9 \\
      & 0.4 &          0.486 &   0.952 &       8.345 &       1.81e-03 &  3.32e-04 &            621.9 &   62
1.9 \\
      & 0.8 &          0.095 &   0.184 &       8.132 &       1.28e-02 &  6.11e-03 &            127.8 &   12
7.8 \\
20000 & 0.2 &          5.445 &   9.589 &      31.585 &       2.25e-04 &  1.90e-05 &           3120.2 &  312
0.2 \\
      & 0.4 &          1.129 &   1.927 &      29.246 &       1.53e-03 &  2.94e-04 &            737.4 &   73
7.4 \\
      & 0.8 &          0.226 &   0.420 &      29.623 &       1.06e-02 &  5.34e-03 &            144.2 &   14
4.2 \\
40000 & 0.2 &         16.810 &  25.686 &     116.859 &       1.95e-04 &  1.59e-05 &           3976.4 &  397
6.4 \\
      & 0.4 &          3.273 &   4.933 &     118.655 &       1.30e-03 &  2.48e-04 &            867.0 &   86
7.0 \\
      & 0.8 &          0.588 &   0.888 &     118.040 &       8.91e-03 &  4.82e-03 &            161.8 &   16
1.8 \\
\bottomrule
\end{tabular}
```

In [9]:

```python
# Mask specific threshold
mask_theta = df_copy[theta] == 0.4

# Mask mono-/quadrupoles
mask_mono = df_copy[quad] == 'Mono'
mask_quad = mask_mono == False

# Extract timing vectors.
df_copy[mask_theta & mask_mono]
N_vec       = df_copy[mask_theta & mask_mono][N].to_numpy()
t_tree_mono = df_copy[mask_theta & mask_mono][tree].to_numpy()
t_dirsum_m  = df_copy[mask_theta & mask_mono][dirsum].to_numpy()

t_tree_quad = df_copy[mask_theta & mask_quad][tree].to_numpy()
t_dirsum_q  = df_copy[mask_theta & mask_quad][dirsum].to_numpy()

# Get average of direct summation vectors.
t_dirsum = (t_dirsum_m + t_dirsum_q)/2


# Simple linear regression in loglog.
coef_mono   = np.polyfit(np.log(N_vec), np.log(t_tree_mono), 1)
coef_quad   = np.polyfit(np.log(N_vec), np.log(t_tree_quad), 1)
coef_dirsum = np.polyfit(np.log(N_vec), np.log(t_dirsum), 1)

N_lin = np.linspace(4500, 45000)

# Positions of slope markers
mono_slope_pos   = (25000, 1.4)
quad_slope_pos   = (32000, 4.5)
dirsum_slope_pos = (25000, 40)

# Plotting
#----------------------------------------------------------------------
plt.figure()

# Obtained data points
plt.loglog(N_vec, t_tree_mono, 'o', label='Monopole')
plt.loglog(N_vec, t_tree_quad, 'o', label='Quadrupole')
plt.loglog(N_vec, t_dirsum, 'o', label='Direct summation')

# Linear regressions
plt.loglog(N_lin, N_lin**coef_mono[0]*np.exp(coef_mono[1]),'--', color='tab:blue')
plt.loglog(N_lin, N_lin**coef_quad[0]*np.exp(coef_quad[1]),'--', color='tab:orange')
plt.loglog(N_lin, N_lin**coef_dirsum[0]*np.exp(coef_dirsum[1]),'--', color='tab:green')

# Slope indicators
annotation.slope_marker(mono_slope_pos, np.around(coef_mono[0], 3),
                        poly_kwargs={'facecolor': 'tab:blue', 'alpha': 0.8})
annotation.slope_marker(quad_slope_pos, np.around(coef_quad[0], 3), invert=True,
                        poly_kwargs={'facecolor': 'tab:orange', 'alpha': 0.8})
annotation.slope_marker(dirsum_slope_pos, np.around(coef_dirsum[0], 3),
                        poly_kwargs={'facecolor': 'tab:green', 'alpha': 0.8})

# Plot settings
plt.ylabel('Execution time $t(s)$')
plt.xlabel('Number of particles $N$')
plt.title('Execution time $t(s)$ as a function of number of \nparticles $N$, for opening angle theshold $\\t
plt.legend()

# Manual xticks
x_list = ['$\\mathdefault{5 \cdot 10^{3}}$', '$\\mathdefault{10^{4}}$',
          '$\\mathdefault{2 \cdot 10^{4}}$', '$\\mathdefault{4 \cdot 10^{4}}$']
plt.xticks(N_vec, x_list)

# Save figure
plt.savefig('loglog_TofN.pdf')
```



Extrapolate execution time for all methods, for a system with $N = 10^{10}$ particles.

In [10]:

```python
# Using the previous linear regression for the extrapolation.
N_extr = 10**10
coef_list = [coef_mono, coef_quad, coef_dirsum]
t_estimate = np.zeros(3)
for i in range(3):
    t_estimate[i] = N_extr**coef_list[i][0]*np.exp(coef_list[i][1])

# Print results
print(f'Tree code, monopoles:   Est. time for N = {N_extr:.2e}, t = {t_estimate[0]:.2} sec or {t_estimate[0]
print(f'Tree code, quadrupoles: Est. time for N = {N_extr:.2e}, t = {t_estimate[1]:.2} sec or {t_estimate[1]
print(f'Direct summation:       Est. time for N = {N_extr:.2e}, t = {t_estimate[2]:.2} sec or {t_estimate[2]
```

```
Tree code, monopoles:   Est. time for N = 1.00e+10, t = 1.5e+08 sec or 4.7 years.
Tree code, quadrupoles: Est. time for N = 1.00e+10, t = 6.5e+07 sec or 2.1 years.
Direct summation:       Est. time for N = 1.00e+10, t = 7.5e+12 sec or 2.4e+05 years.
```