full trajectory in file
T_md = md_num_steps*md_time_step

| block 0 | block 1 | block 2 | block 3 | block 4 |
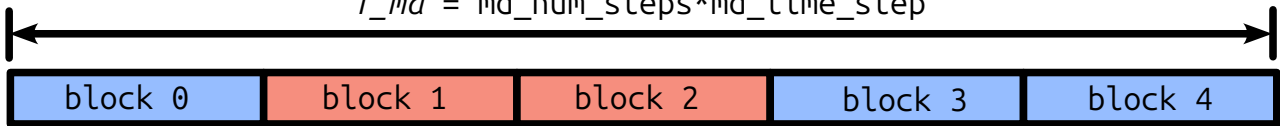
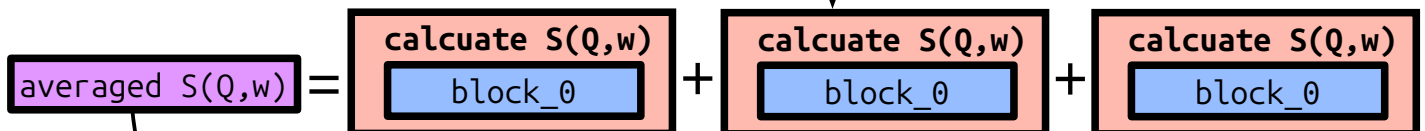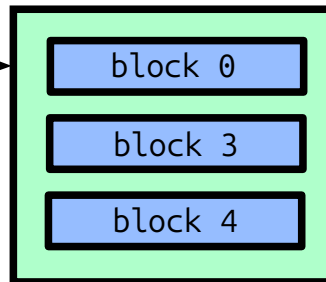**split trajectory into "blocks"**
num_trajectory_blocks = 5
trajectory_blocks = [0,3,4]
num_block_steps = md_num_steps/num_trajectory_blocks
T_block = num_block_steps*md_time_step

| block 0 |
| block 3 |
| block 4 |

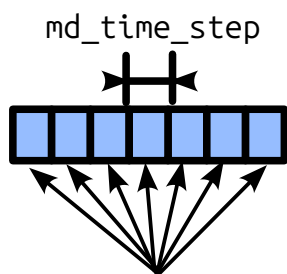| averaged S(Q,w) | = | **calcuate S(Q,w)**
block_0 | + | **calcuate S(Q,w)**
block_0 | + | **calcuate S(Q,w)**
block_0 |

average S(Q,w) over the chosen blocks
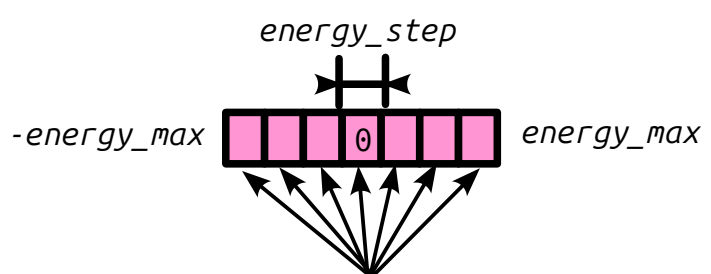sqw_avg = array([num_Qpts,num_frequencies])
for block in trajectory_blocks:
    sqw_avg = sqw_avg + calculate_sqw_on_block(block_ind)
sqw_avg = sqw_avg / num_trajectory_blocks

write averaged
S(Q,w) to file

md_time_step

num_block_steps

block_n time grid

energy_step

-*energy_max*   *energy_max*

num_energy

energy grid

energy grid
energy_max = h / (2 * md_time_step)
    = 4.135 [meV*ps] / (2 * md_time_step [ps])
num_energy = num_block_steps
energy_step = 2 * *energy_max* / *num_energy*
    = 4.135 * num_trajectory_blocks / (md_time_step * md_num_steps)