full trajectory in file T_md = md_num_steps*md_time_step block 0 block 1 block 2 block 4 block 3 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 calcuate S(Q,w) calcuate S(Q,w) calcuate S(Q,w) averaged S(Q,w) block 0 block 0 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