

**full trajectory in file**  
 $T_{md} = md\_num\_steps * md\_time\_step$



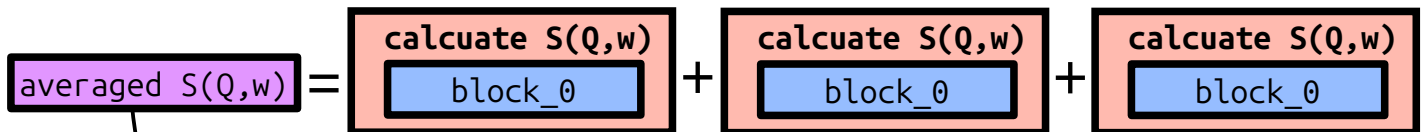
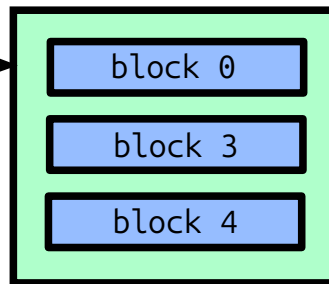
**split trajectory into "blocks"**

$num\_trajectory\_blocks = 5$

$trajectory\_blocks = [0, 3, 4]$

$num\_block\_steps = md\_num\_steps / num\_trajectory\_blocks$

$T_{block} = num\_block\_steps * md\_time\_step$



**average  $S(Q, w)$  over the chosen blocks**

$sqw\_avg = \text{array}([num\_Qpts, num\_frequencies])$

for block in trajectory\_blocks:

$sqw\_avg = sqw\_avg + \text{calculate\_sqw\_on\_block}(block\_ind)$

$sqw\_avg = sqw\_avg / num\_trajectory\_blocks$

write averaged  
 $S(Q, w)$  to file