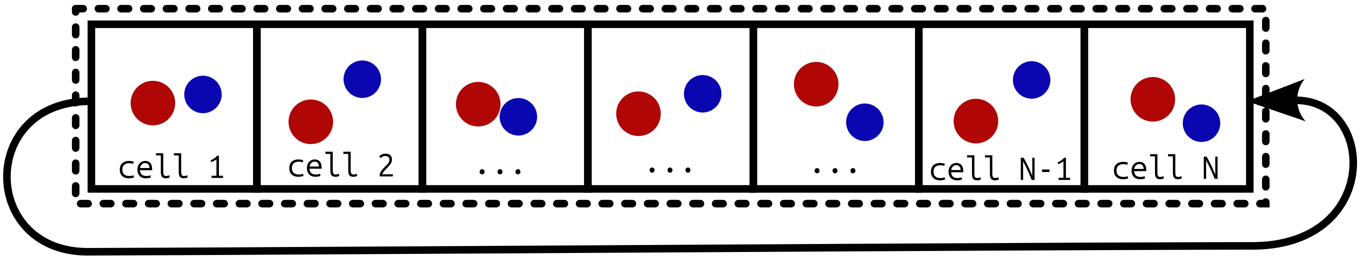
simulation box = N unitcells



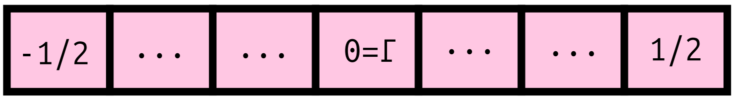
periodic boundary conditions

Q = G+q are the neutron momentum transfer vectors

G ➔ miller indices = Bragg peaks (all integers are allowed)

q ➔ reduced wave vector in 1st BZ (q in (-0.5,0.5])

allowed values of q are in the grid



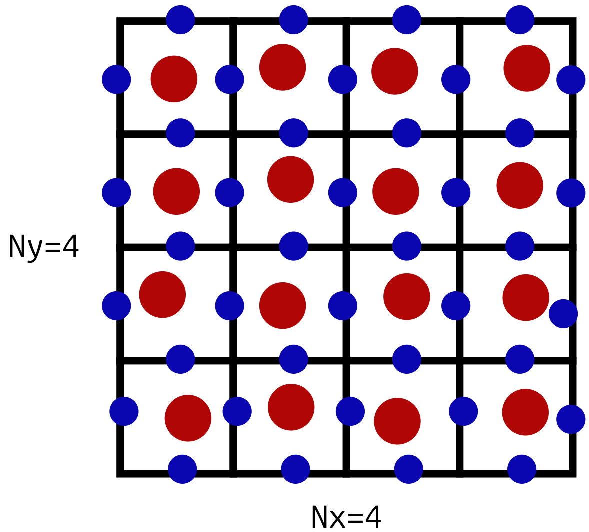
dq = 1 / num_unitcells

E.g. if you want to calculate S(**Q**,w) spanning a whole BZ from G_x to G_x+1 etc (including edges) you should pick

Q = G+q

$$\mathbf{q} = \left(\frac{n_x}{N_x},\frac{n_y}{N_y}\right)$$

simulation box = Nx * Ny unitcells



$(\frac{0}{4},\frac{4}{4})$	$(\frac{1}{4},\frac{4}{4})$	$(\frac{2}{4},\frac{4}{4})$	$(\frac{3}{4},\frac{4}{4})$	$(\frac{4}{4},\frac{4}{4})$
$(\frac{0}{4},\frac{3}{4})$	$(\frac{1}{4},\frac{3}{4})$	$(\frac{2}{4},\frac{3}{4})$	$(\frac{3}{4},\frac{3}{4})$	$(\frac{4}{4},\frac{3}{4})$
$(\frac{0}{4},\frac{2}{4})$	$(\frac{1}{4},\frac{2}{4})$	$(\frac{2}{4},\frac{2}{4})$	$(\frac{3}{4},\frac{2}{4})$	$(\frac{4}{4},\frac{2}{4})$
$(\frac{0}{4},\frac{1}{4})$	$(\frac{1}{4},\frac{1}{4})$	$(\frac{2}{4},\frac{1}{4})$	$(\frac{3}{4},\frac{1}{4})$	$(\frac{4}{4},\frac{1}{4})$
$(\frac{0}{4},\frac{0}{4})$	$(\frac{1}{4},\frac{0}{4})$	$(\frac{2}{4},\frac{0}{4})$	$(\frac{3}{4},\frac{0}{4})$	$(\frac{4}{4},\frac{0}{4})$

Q_mesh_H = $[G_x, G_x+1, N_x+1]$

Q_mesh_K = $[G_y, G_y+1, N_y+1]$