

Starting input file:

$N_x \times N_y \times N_z . f2 . m0$

Generic files:

genericunv2.sh

genericwv2.sh

genericgsv2.sh

genericrcv2.sh

genericqv2.sh

`step0_v2.pl`

• `parallelize_v2.pl`

• `starterun_v2.pl`

Generates shell scripts:

$N_x \times N_y \times N_z . f2 . m0 . un . sh$

$N_x \times N_y \times N_z . f2 . m0 . w . sh$

$N_x \times N_y \times N_z . f2 . m0 - q_{flip} q_x q_y q_z . gs . sh$

$N_x \times N_y \times N_z . f2 . m0 - q_{flip} q_x q_y q_z . rc . sh$

$N_x \times N_y \times N_z . f2 . m0 - q_{flip} q_x q_y q_z . q . sh$

Generates files containing list of q-values:

$N_x \times N_y \times N_z . f2 . m0 . qscanx$

$N_x \times N_y \times N_z . f2 . m0 . qscany$

$N_x \times N_y \times N_z . f2 . m0 . qscanz$

Generates input files for specific q-values with mode 1 and unimode 1:

$N_x \times N_y \times N_z . f2 . m0 - q_{flip} q_x q_y q_z$

Submits the job

$N_x \times N_y \times N_z . f2 . m0 . un . sh$

Job output:

$N_x \times N_y \times N_z . f2 . m0 . un . bz2$