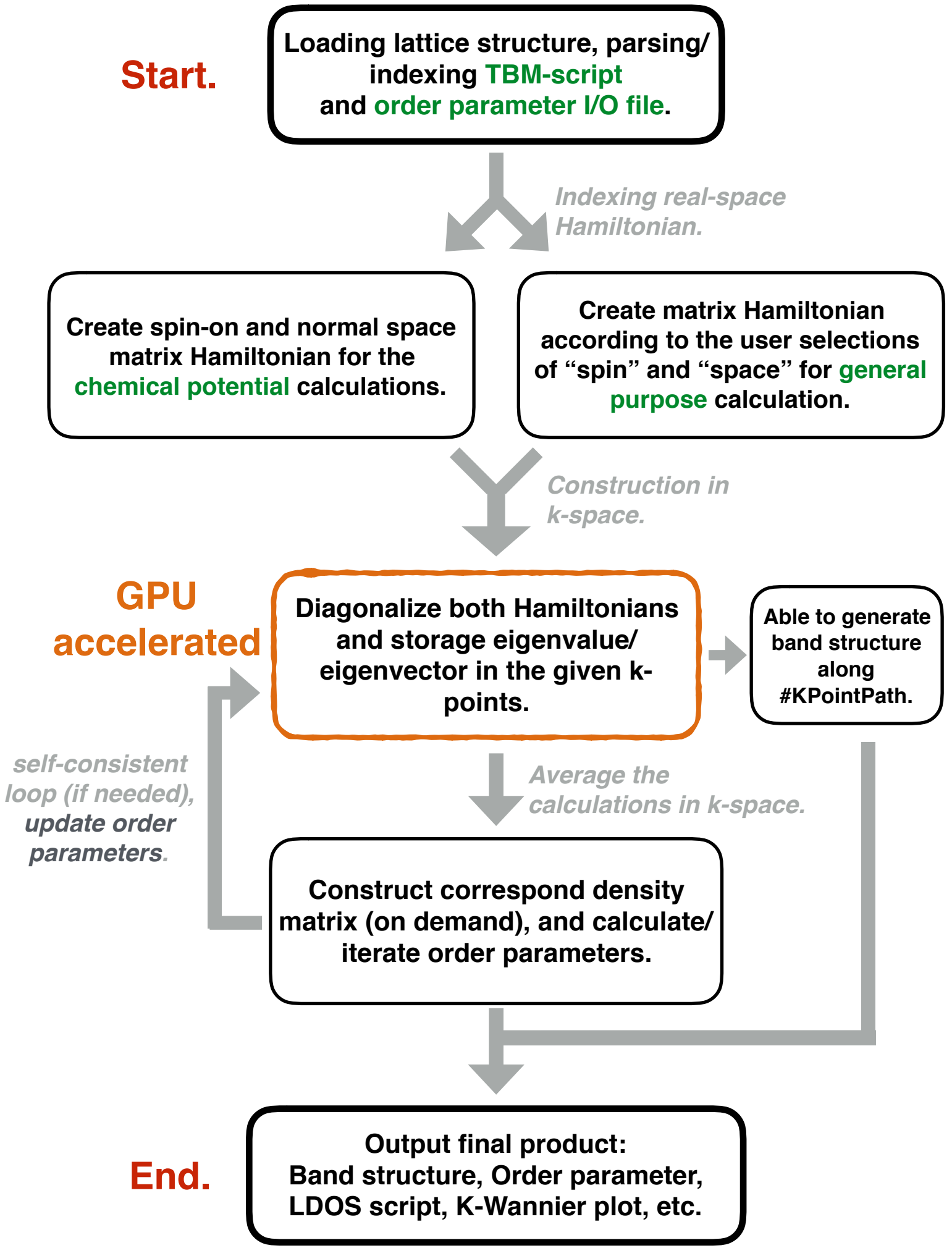
Start.
Loading lattice structure, parsing/ indexing TBM-script and order parameter I/O file.
Indexing real-space Hamiltonian.
Create spin-on and normal space matrix Hamiltonian for the chemical potential calculations.
Create matrix Hamiltonian according to the user selections of “spin” and “space” for general purpose calculation.
Construction in k-space.
GPU accelerated
Diagonalize both Hamiltonians and storage eigenvalue/ eigenvector in the given k-points.
Able to generate band structure along #KPointPath.
self-consistent loop (if needed), update order parameters.
Average the calculations in k-space.
Construct correspond density matrix (on demand), and calculate/ iterate order parameters.
End.
Output final product: Band structure, Order parameter, LDOS script, K-Wannier plot, etc.