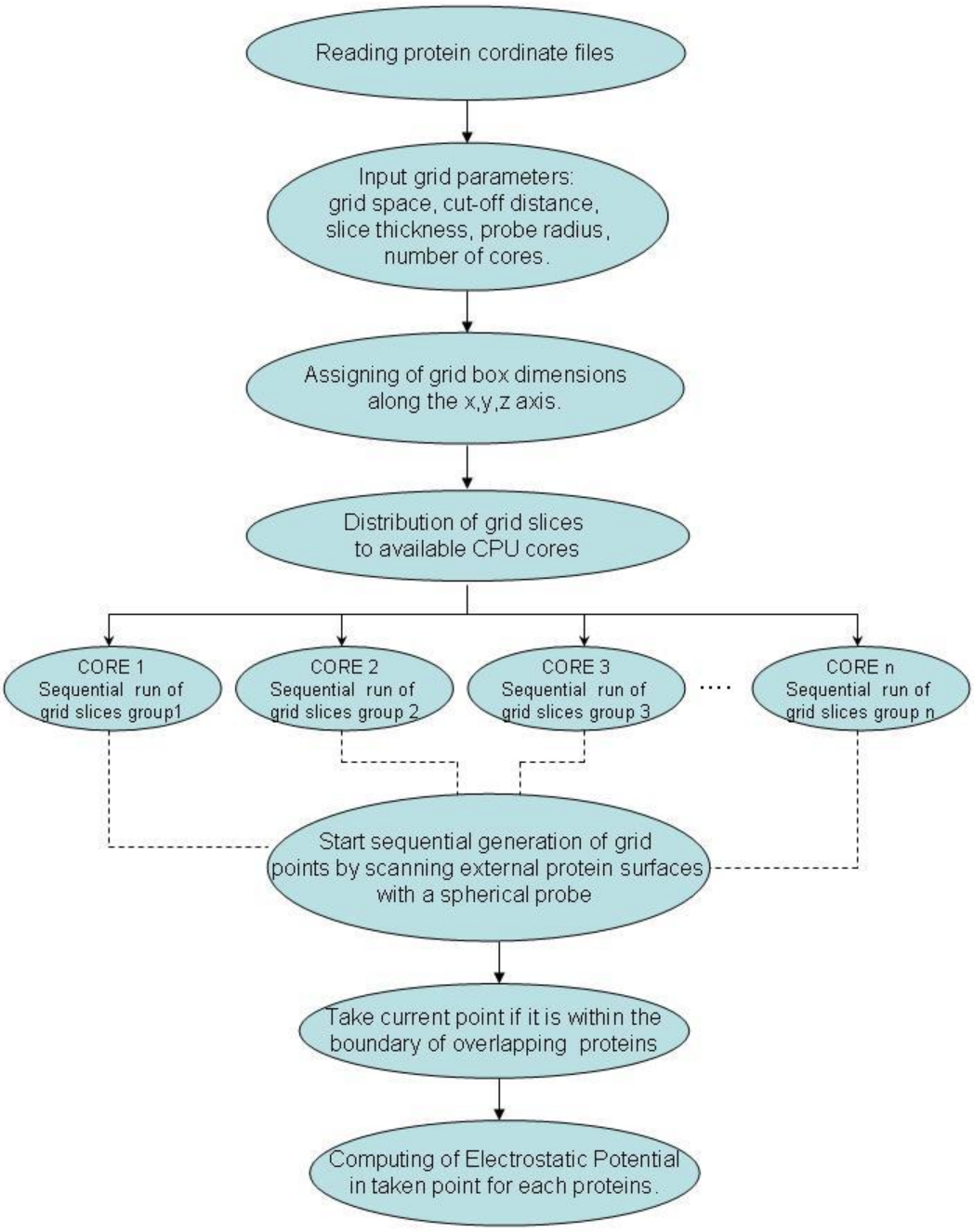
Reading protein cordinate files
Input grid parameters:
grid space, cut-off distance,
slice thickness, probe radius,
number of cores.
Assigning of grid box dimensions
along the x,y,z axis.
Distribution of grid slices
to available CPU cores
CORE 1
Sequential run of
grid slices group1
CORE 2
Sequential run of
grid slices group 2
CORE 3
Sequential run of
grid slices group 3
....
CORE n
Sequential run of
grid slices group n
Start sequential generation of grid
points by scanning external protein surfaces
with a spherical probe
Take current point if it is within the
boundary of overlapping proteins
Computing of Electrostatic Potential
in taken point for each proteins.