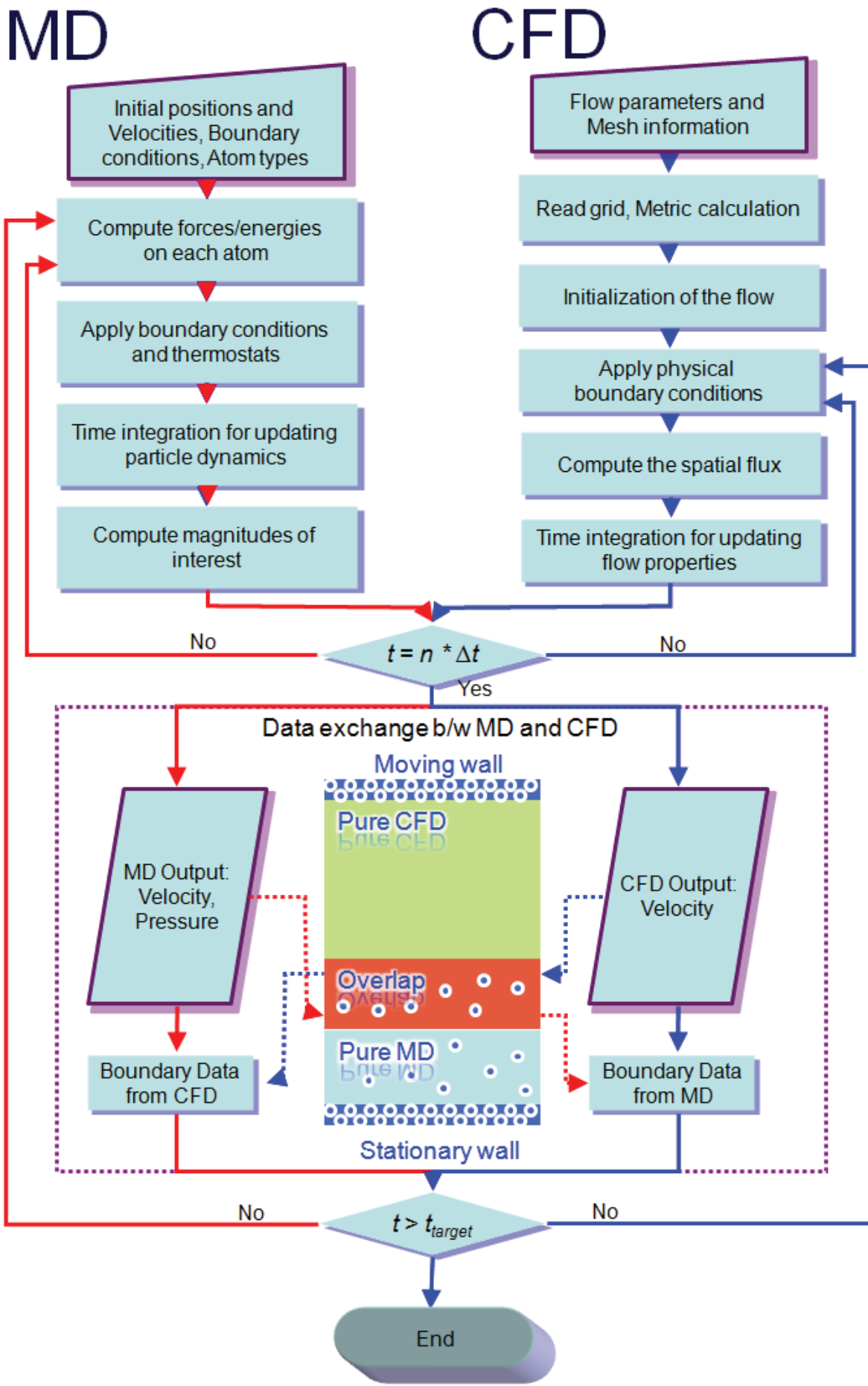
MD
CFD
Initial positions and Velocities, Boundary conditions, Atom types
Compute forces/energies on each atom
Apply boundary conditions and thermostats
Time integration for updating particle dynamics
Compute magnitudes of interest
Flow parameters and Mesh information
Read grid, Metric calculation
Initialization of the flow
Apply physical boundary conditions
Compute the spatial flux
Time integration for updating flow properties
No
$t = n * \Delta t$
No
Yes
Data exchange b/w MD and CFD
Moving wall
Pure CFD
MD Output: Velocity, Pressure
CFD Output: Velocity
Overlap
Pure MD
Boundary Data from CFD
Boundary Data from MD
Stationary wall
No
$t > t_{target}$
No
End