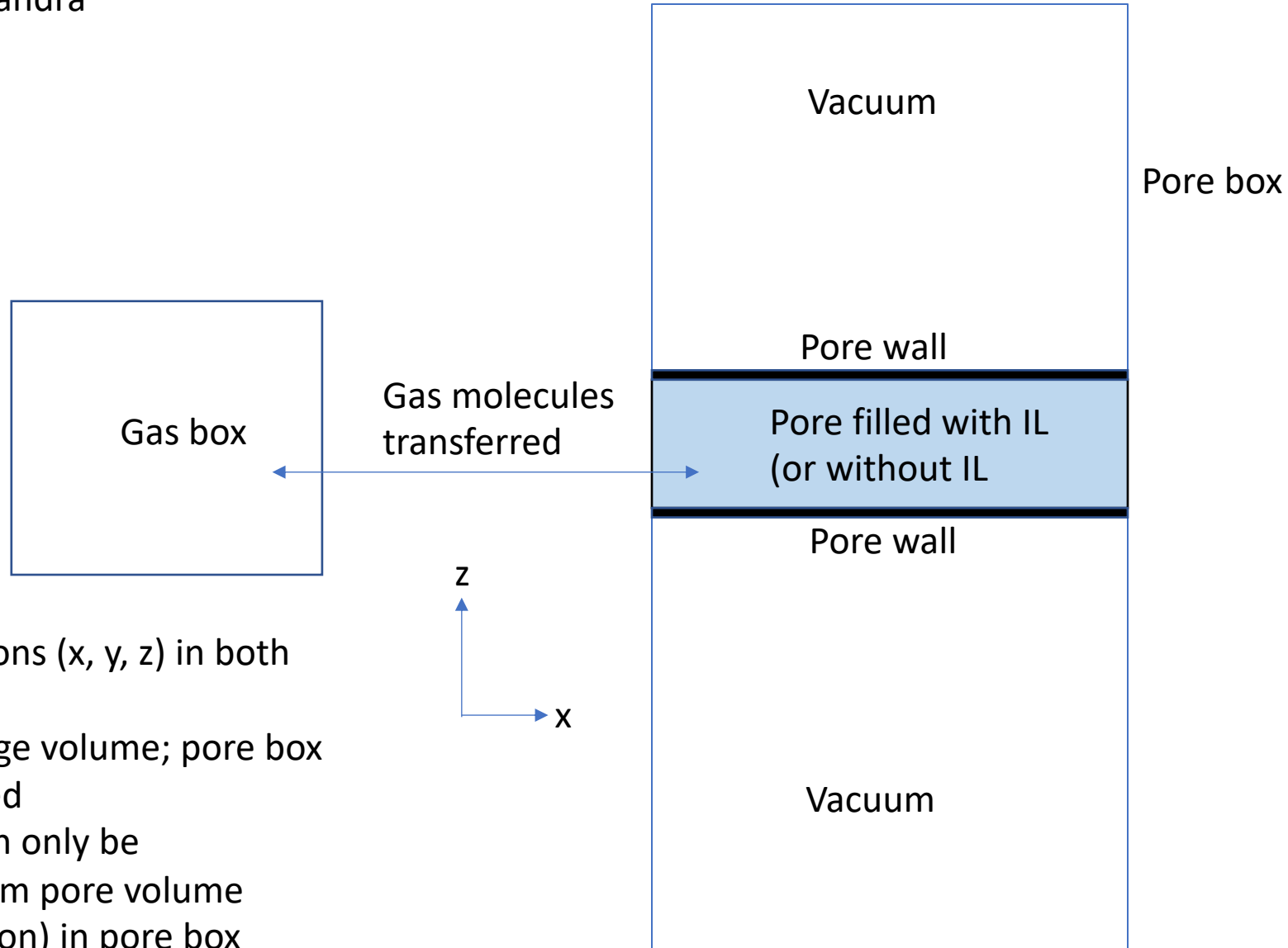
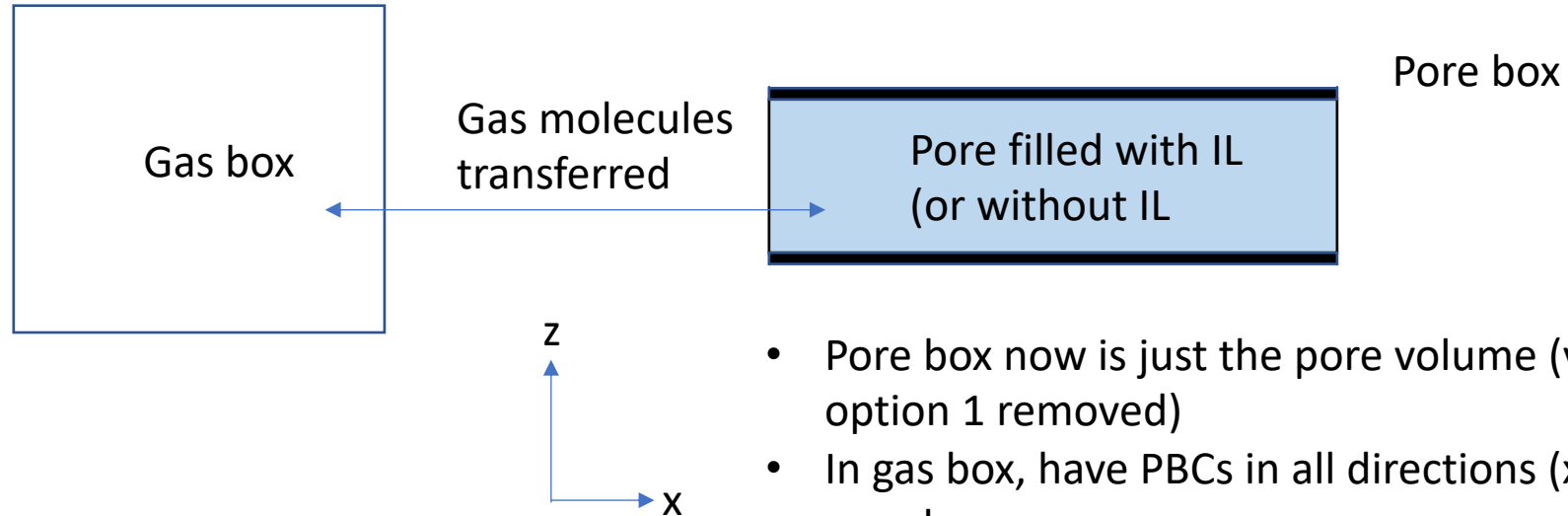


GEMC setup in Cassandra Option 1



- PBCs in all directions (x, y, z) in both boxes
- Gas box can change volume; pore box keeps volume fixed
- Gas molecules can only be transferred to/from pore volume (blue-shaded region) in pore box
 - Can we do this in Cassandra?

GEMC setup in Cassandra Option 2



- Pore box now is just the pore volume (vacuum regions from option 1 removed)
- In gas box, have PBCs in all directions (x, y, z) and volume can change
- In pore box, have PBCs only in x and y (not in z); volume is fixed
 - Can we do this in Cassandra?
- Gas molecules transferred between the two boxes