Q. Why define vector process ID?

A. Vector process ID ($\text{vid}[3]$) is used only to find the ranks ($\text{nn}[6]$) of the six neighbor processes during the initialization of the run, in function set_topology()

```c
/* Integer vectors to specify the six neighbor ranks */
int iv[6][3] = { {-1,0,0},{1,0,0},{0,-1,0},{0,1,0},{0,0,-1},{0,0,1} };
int ku,a,k1[3];

/* Set up neighbor tables, nn & sv */
for (ku=0; ku<6; ku++) {
    /* Vector index of neighbor ku (with wrap-around condition) */
    for (a=0; a<3; a++)
        k1[a] = (vid[a]+iv[ku][a]+vproc[a])%vproc[a];
    /* Scalar neighbor ID, nn */
    /* Shift vector, sv */
    for (a=0; a<3; a++) sv[ku][a] = al[a]*iv[ku][a];
}

/* Set up the node parity table, myparity */
for (a=0; a<3; a++) {
    if (vproc[a] == 1)
        myparity[a] = 2;
    else if (vid[a]%2 == 0)
        myparity[a] = 0;
    else
        myparity[a] = 1;
}

Serial process ID

In main():

    MPI_Comm_rank(MPI_COMM_WORLD, &sid);
    vid[0] = sid/(vproc[1]*vproc[2]);
    vid[1] = (sid/vproc[2])%vproc[1];
    vid[2] = sid%vproc[2];
```
Q. Why accelerate the velocity for half time-step in the velocity Verlet algorithm, instead of full time-step as in Euler algorithm?

A. By doing so, a conservation law called Liouville’s theorem (or phase-space volume conservation) is satisfied exactly by velocity Verlet (but not Euler) algorithm; this in turn leads to superior long-term stability of the trajectory in the former, reflected, e.g., in better energy conservation.

See slides 25-28 in [http://cacs.usc.edu/education/phys516/02MD-slide.pdf](http://cacs.usc.edu/education/phys516/02MD-slide.pdf)

Mapping: \(\left(\frac{t}{x,p}\right) \rightarrow \left(\frac{t+\Delta t}{x',p'}\right)\)

Liouville’s theorem: \(\frac{\partial (x',p')}{\partial (x,p)} = 1\)

In Euler algorithm:

\(\tilde{v}_i(t + \Delta) \leftarrow \tilde{v}_i(t) + \tilde{a}_i(t)\Delta\)