Parallel Molecular Dynamics: FAQ

Q. Why define vector process ID?

A. Vector process ID (`vid[3]`) is used only to find the ranks (`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 */
  nn[ku] = k1[0]*vproc[1]*vproc[2]+k1[1]*vproc[2]+k1[2];
  /* 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()`:
```c
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];
```

Parallel Molecular Dynamics: FAQ

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

Mapping: $\overbrace{(x,p)}^{t} \rightarrow \overbrace{(x',p')}^{t+\Delta t}$

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

In Euler algorithm:

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