Molecular dynamics 2015

Exercises 4 to chapter 4: `mdmorse`: solving the equations of motion
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1. (12 p) Write the subroutine **`Solve1`**, which does the predictor part of the solution of the equations of motion with the velocity Verlet-algorithm.

Add also periodic boundary condition control in the code. That is, if the variable `periodic%x` (or `periodic.x` in the C version) is set to a nonzero value, the atoms which move outside the cell in the x dimension should be correctly returned inside it, and same for y and z.

3. (8 p) Write the subroutine **`Solve2`**, which does the corrector part of the velocity Verlet solution of the equations of motion.

Return the exercises as the file `solve.f90/.c` and some output that shows that the code works (e.g. screen dump of `dpc` output).

If you solve this exercise right, and have a working solution to the exercise 3, the atoms will start moving when you run `mdmorse`. But since the force calculation is not yet implemented, the atoms will move in straight paths.

You can animate the motion on with `dpc`:

```
dpc cube 9.1 xyz erase sort 2 3 4 5 atoms.out
```

More info on `dpc` in the first lecture notes or by giving the command `dpc` without any arguments.