Question 4: Profiling

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The `simple_md.c` program was compiled with no optimisations and timed five times with the C-Shell `time` command, the timings were:

```
68.515u 0.178s 1:08.83 99.7%    0+0k 0+3io 0pf+0w
69.940u 0.151s 1:10.18 99.8%    0+0k 0+4io 0pf+0w
68.186u 0.105s 1:08.34 99.9%    0+0k 0+5io 0pf+0w
69.129u 0.156s 1:09.39 99.8%    0+0k 0+4io 0pf+0w
64.415u 0.023s 1:04.44 99.9%    0+0k 0+3io 0pf+0w
```

and the results were:

```
PE     KE     Error
49854482.9581703916192054748 5  0.0000000000000000000  0.00000000000000000000
49854482.9581703916192054748 5  0.0024367223627876507 2  0.00000000004887664439
```

The same was done with compiler optimisations on:

```
12.341u 0.013s 0:12.36 99.9%    0+0k 0+1io 0pf+0w
12.396u 0.012s 0:12.41 99.9%    0+0k 0+4io 0pf+0w
11.978u 0.008s 0:11.99 99.8%    0+0k 0+1io 0pf+0w
12.038u 0.006s 0:12.04 99.9%    0+0k 0+4io 0pf+0w
12.068u 0.007s 0:12.08 99.8%    0+0k 0+1io 0pf+0w
PE     KE     Error
49854482.9581703916192054748 5  0.0000000000000000000  0.00000000000000000000
49854482.9581703916192054748 5  0.0024367223627876507 2  0.00000000004887664439
```

The optimised version runs in about a sixth of the time and often uses fewer blocks of IO. Both versions of the program have almost complete CPU utilisation so the speed-ups are due to optimisations in the code (rather than other a smaller load on the CPU).