

GROMACS - Bug #2564

Result Summary Different For Jobs With Different Numbers of Nodes

07/05/2018 02:39 PM - Dan Whitehouse

Status: New	
Priority: Normal	
Assignee:	
Category:	
Target version:	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 2016.3	

Description

I've been running some benchmarks using MPI and I have noticed that when the jobs complete the summary is displayed in a different way depending on how many nodes I use.

For a two node job:

```
Time:      Core t (s)   Wall t (s)   (%)
          151386.697   3153.890    4800.0
          52:33
          (ns/day)    (hour/ns)
Performance: 0.044         546.867
Finished mdrun on rank 0 Thu Jun 7 15:12:51 2018
```

And for a 256 node job:

```
Time:      Core t (s)   Wall t (s)   (%)
          960396.768   156.315    614400.0
          (ns/day)    (hour/ns)
Performance: 0.885         27.104
Finished mdrun on rank 0 Wed Nov 15 06:26:15 2017
```

What is the significance of the "52:33" which is displayed for the 2 node job and not the 256 node job?