

# ICMS delta cluster, Data

Stillinger-Web4 MPI x 1 Ope8 MPI x 1 Ope4 MPI x 2 Ope2 MPI x 4 Ope1 MPI x 8 OpenMP

Nodes:	Total Time:	Total Time:	Total Time:	Total Time:	Total Time:	# Nodes:
1	30.05	16.27	16.57	17.96	20.03	1
2	15.38	9.76	8.55	9.43	10.67	2
3	10.53	7.24	5.93	6.61	7.34	3
4	7.49	6.26	4.79	4.98	5.61	4
6	5.95	5.27	3.68	3.5	4.04	6
8	4.72	4.98	2.93	2.73	3.16	8
12	3.62	4.56	2.52	1.93	2.36	12
16	3.13	4.68	2.36	1.58	1.81	16
20	2.82	4.51	2.2	1.35	1.55	20
24	2.59	4.36	2.17	1.21	1.35	24
32	2.53	4.55	2.14	1.08	1.16	32

Rhodo(lj/charr4 MPI x 1 Ope8 MPI x 1 Ope4 MPI x 2 Ope2 MPI x 4 Ope1 MPI x 8 OpenMP

Nodes:	Total Time:	Total Time:	Total Time:	Total Time:	Total Time:	# Nodes:
1	14.34	9.52	10.25	14.58	22.67	1
2	7.93	6.23	5.92	8.14	12.5	2
3	5.54	5.48	4.24	5.62	8.28	3
4	4.57	5.28	3.61	4.28	6.47	4
6	3.66	4.35	3	3.25	4.62	6
8	3.25	4.42	2.82	2.5	3.54	8
12	2.58	4.77	2.28	2.11	2.76	12
16	2.41	5.24	2.17	1.85	2.1	16
20	2.47	6.31	2.28	1.56	1.82	20
24	2.43	5.86	2.26	1.4	1.56	24
32	2.56	6.61	2.47	1.27	1.34	32

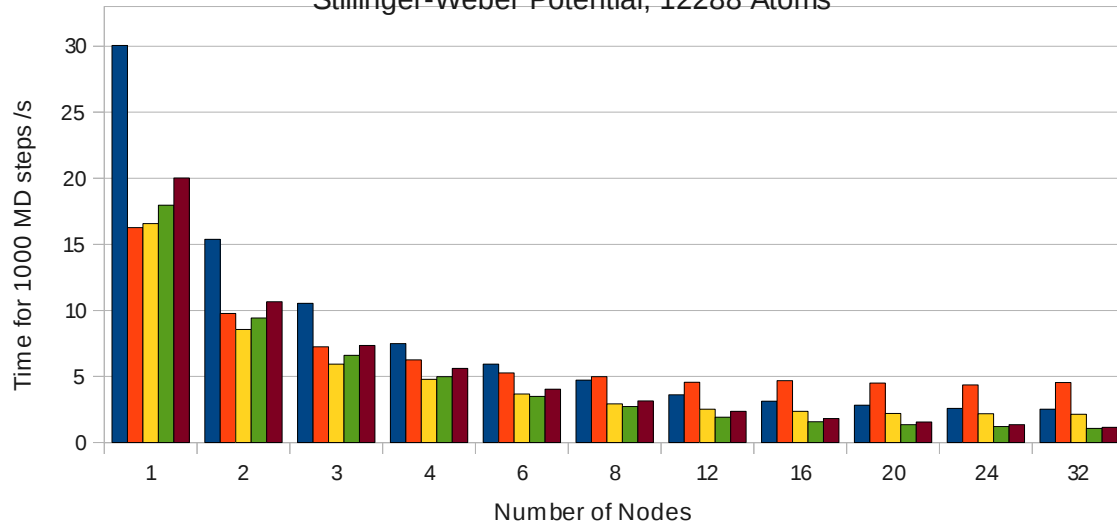
# ICMS delta cluster, Data

1CPU referenc	119.21 Factor:	14.9			
4 MPI x 1 Ope	8 MPI x 1 Ope	4 MPI x 2 Ope	2 MPI x 4 Ope	1 MPI x 8 OpenMP	hybrid ratio
50%	92%	90%	83%	74%	0.98
48%	76%	87%	79%	70%	1.14
47%	69%	84%	75%	68%	1.22
50%	60%	78%	75%	66%	1.31
42%	47%	68%	71%	61%	1.5
39%	37%	64%	68%	59%	1.73
34%	27%	49%	64%	53%	1.98
30%	20%	39%	59%	51%	2.08
26%	17%	34%	55%	48%	2.08
24%	14%	29%	51%	46%	2.14
18%	10%	22%	43%	40%	2.35

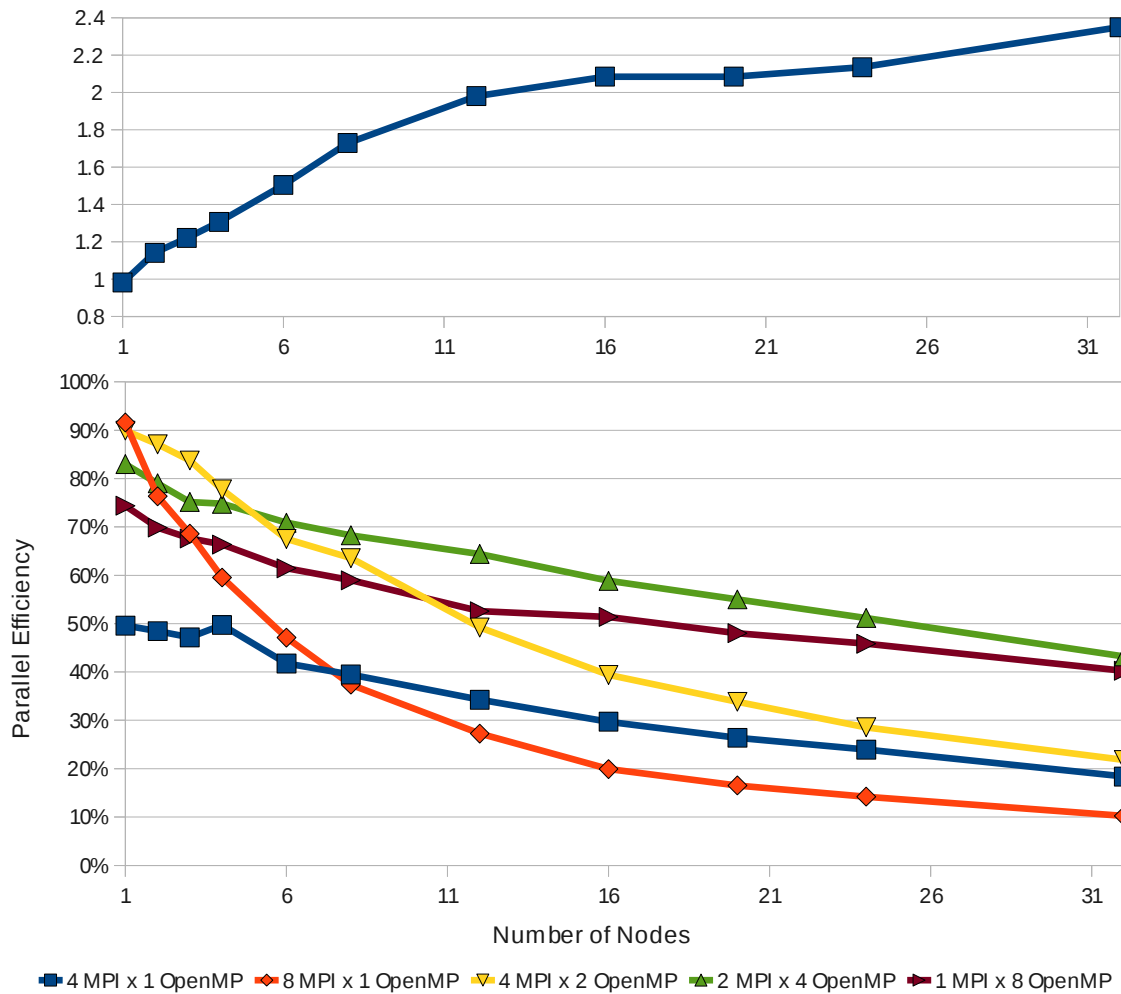
1CPU referenc	56 Factor:	7			
4 MPI x 1 Ope	8 MPI x 1 Ope	4 MPI x 2 Ope	2 MPI x 4 Ope	1 MPI x 8 OpenMP	hybrid ratio
49%	74%	68%	48%	31%	0.93
44%	56%	59%	43%	28%	1.05
42%	43%	55%	42%	28%	1.29
38%	33%	48%	41%	27%	1.27
32%	27%	39%	36%	25%	1.22
27%	20%	31%	35%	25%	1.3
23%	12%	26%	28%	21%	1.22
18%	8%	20%	24%	21%	1.3
14%	6%	15%	22%	19%	1.58
12%	5%	13%	21%	19%	1.74
9%	3%	9%	17%	16%	2.02

## 2x Intel Xeon 2.66Ghz (Harpertown) w/ DDR Infiniband

Stillinger-Weber Potential, 12288 Atoms

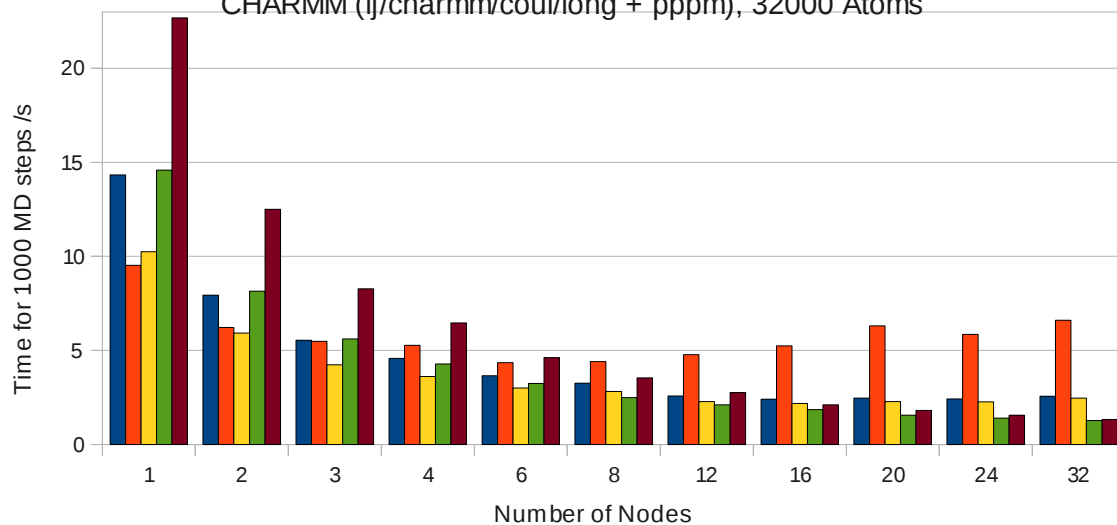


### Hybrid OpenMP/MPI to plain MPI ratio



## 2x Intel Xeon 2.66Ghz (Harpertown) w/ DDR Infiniband

CHARMM (lj/charmm/coul/long + ppm), 32000 Atoms



## Hybrid OpenMP/MPI to plain MPI ratio

