MOSCITOBENCH

Timings:

System	SMALL-SPCE	BIG-SPCE	TIP4P	Methanol	C8E6	PCH5
Linux 5-PC-Cluster *5 Duron (1400 MHz), 100MBit Ethernet, gcc-2.95.3, LAM 6.3*	0.017	0.161	-	0.029	0.089	0.145
Linux 5-PC-Cluster *5 Duron (750 MHz), 100MBit Ethernet, gcc-2.95.2, LAM 6.3*	0.019	0.213	-	0.040	0.120	0.202
Linux–PC *Athlon XP 1800+ (1533 MHz), gcc-2.95.3*	0.023	0.360	0.075	0.055	0.219	0.353
NEC Cenju-4 (5 Nodes) *5 R10000 (200 MHz)*	0.033	0.492	-	0.072	0.241	0.394
Linux–PC *Athlon (1400 MHz), gcc-2.95.3*	0.026	0.432	0.087	0.062	0.248	0.415
Linux 5-PC-Cluster *5 Celeron (433 MHz), 100MBit Ethernet, pgcc-2.95.2, mpich 1.2.0*	0.038	0.423	-	0.086	0.299	0.411
Linux–PC *Athlon (750 MHz), pgcc-2.95.2*	0.046	0.751	0.154	0.109	0.435	0.695
Linux–PC *Celeron (500 MHz), pgcc-2.95.2*	0.090	1.379	0.301	0.209	0.948	1.277
Linux–PC *Pentium II MMX (400 MHz), pgcc-2.90.29*	0.111	1.676	0.376	0.261	1.029	1.669
Linux–PC *Celeron (400 MHz), pgcc-2.90.29*	0.107	1.698	0.369	0.260	1.172	1.684
IBM RS/6000 SP (Silver) *PowerPC 604e (333 MHz), IBM xlf 5.1.1.0*	0.115	1.941	0.378	0.259	1.058	1.412
Linux–PC *Pentium II MMX (300 MHz), pgcc-2.90.29*	0.148	2.263	0.499	0.351	1.370	2.260
IBM RS/6000 SP *POWER2 (133 MHz), IBM xlf 3.2.5.0*	0.158	2.637	0.534	0.348	1.712	1.960

IBM RS/6000 Mod. 43p-140 *PowerPC 604e (233 MHz), IBM xlf 3.2.3.0*	0.181	3.159	0.594	0.411	1.674	2.272
IBM RS/6000 SP *POWER2 (120 MHz), IBM xlf 3.2.5.0*	0.190	3.084	0.644	0.440	2.069	2.278
IBM RS/6000 Mod. 43p *PowerPC 604 (133 MHz), IBM xlf 3.2.3.0*	0.326	5.486	1.064	0.718	2.734	3.845
Linux–PC *Pentium MMX (200 MHz), pgcc-2.90.29*	0.332	5.234	1.061	0.765	2.815	4.408
Linux–PC *AMD486DX4 (100 MHz), pgcc-2.90.29*	2.570	41.713	8.136	5.413	19.239	29.733
Linux–PC *486DX (40 MHz), pgcc-2.90.29*	6.138	97.098	19.772	13.196	45.860	71.972

CPU-times per simulation-step in seconds. Date: May 14, 2002

Model Systems:

SMALL-SPCE: 256 rigid SPC/E molecules at a density of $1.0\ \mathrm{g\,cm^{-3}}$ (768 interaction sites). Cutoff–radius: 8.0 Å. Smooth–PME on a $16\times16\times16$–mesh.

BIG-SPCE: 4000 rigid SPC/E molecules at a density of $1.0\ \mathrm{g\,cm^{-3}}$ (12000 interaction sites). Cutoff–radius: 8.0 Å. Smooth–PME on a $32\times32\times32$–mesh.

TIP4P: 500 rigid TIP4P molecules at a density of $1.0\ \mathrm{g\,cm^{-3}}$ (2000 interaction sites). Cutoff–radius: 8.0 Å. Smooth–PME on a $20\times20\times20$–mesh.

Methanol: 216 Methanol molecules at a pressure of 1 atm (1296 interaction sites). Cutoff–radius: 9.0 Å. Smooth–PME on a $20\times20\times20$–mesh.

C8E6: System of one flexible nonionic surfactant molecule of type C8E6 surrounded by 1315 rigid SPC/E water molecules (3999 interaction sites) at a pressure of 1 atm. Cutoff–radius: 8.0 Å. Smooth–PME on a $28\times28\times28$–mesh.

PCH5: System of 200 PCH5 molecules (6600 interaction sites), forming a liquid crystalline phase of nematic type [333 K, 1 atm]. Cutoff–radius: 9.0 Å. Smooth–PME on a $24\times60\times36$–mesh.

All simulations are performed with smooth–PME using 4'th order b–spline interpolation. A Verlet–type neighbor list is always employed (For the BIG-SPCE and PCH5 systems a linkcell algorithm is used to construct the Verlet–list).