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| **1.** | **Benchmark Results** |

The tables in this section provide CPU benchmarks for basic TINKER energy and derivative evaluations, vibrational analysis and molecular dynamics. All times are in seconds and were measured with TINKER executables dimensioned to **maxatm** of 10000 and **maxhess** of 1000000 in the source file **sizes.i**. All calculations were run twice in rapid succession on a quiet machine. The times reported for each benchmark are the results from the second run. If you have built TINKER on an alternative machine type and are able to run the benchmarks on the additional machine type, please send the results for inclusion in a future listing.

**BENCHMARK #1: Calmodulin Energy Evaluation**

The system is an isolated molecule of the 148-residue protein calmodulin with 2264 atoms using the Amber ff94 force field. All interactions are computed with no use of cutoffs. Times listed are for calculation setup followed by a single energy, energy/gradient and Hessian evaluation.

**MACHINE-OS-COMPILER TYPE MHz SETUP ENERGY GRAD HESS**

Athlon XP 2400+ (RH 8.0, Intel) 2000 0.13 0.28 0.60 2.96

Athlon XP 2400+ (RH 8.0, PGI) 2000 0.16 0.31 0.70 3.60

Athlon XP 2400+ (RH 8.0, g77 3.2) 2000 0.17 0.28 0.66 3.67

Athlon Thunderbird (RH 8.0, Intel) 1400 0.22 0.41 0.86 5.15

Athlon Thunderbird (RH 8.0, PGI) 1400 0.21 0.44 1.00 5.92

Athlon Thunderbird (RH 8.0, g77 3.2) 1400 0.19 0.40 0.94 5.81

Athlon Classic (RH 8.0, Intel) 950 0.30 0.64 1.42 7.07

Athlon Classic (RH 8.0, PGI) 950 0.30 0.69 1.65 7.96

Athlon Classic (RH 8.0, g77 3.2) 950 0.31 0.63 1.57 7.94

Compaq Evo N610c P4 (RH 8.0, Intel) 2000 0.18 0.45 0.87 3.08

Compaq Evo N610c P4 (RH 8.0, PGI) 2000 0.22 0.44 1.06 4.27

Compaq Evo N610c P4 (RH 8.0, Absoft) 2000 0.17 0.52 1.06 3.95

Compaq Evo N610c P4 (RH 8.0, g77 3.2) 2000 0.19 0.41 1.07 4.41

Compaq Evo N610c P4 (WinXP, CVF 6.6) 2000 0.16 0.38 0.98 3.54

Compaq Evo N610c P4 (WinXP, g77 3.2) 2000 0.16 0.40 1.08 4.45

Apple Power Mac G4 (OSX 10.2, Absoft) 733 0.41 2.96 5.12 17.83

Apple Power Mac G4 (OSX 10.2, g77 3.3) 733 0.37 1.98 3.79 14.48

Compaq AlphaServer DS10 (Tru64 5.0) 466 0.35 1.33 1.93 8.40

SGI IndigoII R10K (Irix 6.5, MIPS) 195 1.17 3.49 6.35 23.03

**BENCHMARK #2: Crambin Crystal Energy Evaluation**

The system is a unit cell of the 46-residue protein crambin containing 2 polypeptide chains, 2 ethanol and 178 water molecules for a total of 1360 atoms using the OPLS-UA force field. Periodic boundaries are used with particle mesh Ewald for electrostatics and a 9.0 ≈ cutoff for vdW interactions. Times listed are for calculation setup followed by a single energy, energy/ gradient and Hessian evaluation.

**MACHINE-OS-COMPILER TYPE MHz SETUP ENERGY GRAD HESS**

Athlon XP 2400+ (RH 8.0, Intel) 2000 0.12 0.12 0.21 0.66

Athlon XP 2400+ (RH 8.0, PGI) 2000 0.13 0.14 0.24 0.63

Athlon XP 2400+ (RH 8.0, g77 3.2) 2000 0.14 0.13 0.28 0.81

Athlon Thunderbird (RH 8.0, Intel) 1400 0.19 0.17 0.30 0.91

Athlon Thunderbird (RH 8.0, PGI) 1400 0.18 0.18 0.32 0.91

Athlon Thunderbird (RH 8.0, g77 3.2) 1400 0.17 0.17 0.38 1.11

Athlon Classic (RH 8.0, Intel) 950 0.26 0.25 0.47 1.46

Athlon Classic (RH 8.0, PGI) 950 0.29 0.27 0.50 1.42

Athlon Classic (RH 8.0, g77 3.2) 950 0.27 0.27 0.56 1.70

Compaq Evo N610c P4 (RH 8.0, Intel) 2000 0.15 0.14 0.27 0.64

Compaq Evo N610c P4 (RH 8.0, PGI) 2000 0.22 0.19 0.33 0.88

Compaq Evo N610c P4 (RH 8.0, Absoft) 2000 0.14 0.22 0.39 0.84

Compaq Evo N610c P4 (RH 8.0, g77 3.2) 2000 0.15 0.20 0.45 1.13

Compaq Evo N610c P4 (WinXP, CVF 6.6) 2000 0.14 0.17 0.33 0.83

Compaq Evo N610c P4 (WinXP, g77 3.2) 2000 0.12 0.22 0.52 1.16

Apple Power Mac G4 (OSX 10.2, Absoft) 733 0.32 0.58 1.09 3.11

Apple Power Mac G4 (OSX 10.2, g77 3.3) 733 0.31 0.42 0.79 2.37

Compaq AlphaServer DS10 (Tru64 5.0) 466 0.29 0.38 0.64 1.95

SGI IndigoII R10K (Irix 6.5, MIPS) 195 0.92 0.74 1.41 3.89

**BENCHMARK #3: Peptide Normal Mode Calculation**

The system is a minimum energy conformation of a 20-residue peptide containing one of each of the standard amino acids for a total of 328 atoms using the OPLS-AA force field without cutoffs. The time reported is for computation of the Hessian and calculation of the normal modes of the Hessian matrix and the vibration frequencies requiring two separate matrix diagonalization steps.

**MACHINE-OS-COMPILER TYPE MHz NORMAL MODES**

Athlon XP 2400+ (RH 8.0, Intel) 2000 22

Athlon XP 2400+ (RH 8.0, PGI) 2000 26

Athlon XP 2400+ (RH 8.0, g77 3.2) 2000 24

Athlon Thunderbird (RH 8.0, Intel) 1400 31

Athlon Thunderbird (RH 8.0, PGI) 1400 34

Athlon Thunderbird (RH 8.0, g77 3.2) 1400 33

Athlon Classic (RH 8.0, Intel) 950 46

Athlon Classic (RH 8.0, PGI) 950 51

Athlon Classic (RH 8.0, g77 3.2) 950 48

Compaq Evo N610c P4 (RH 8.0, Intel) 2000 19

Compaq Evo N610c P4 (RH 8.0, PGI) 2000 19

Compaq Evo N610c P4 (RH 8.0, Absoft) 2000 20

Compaq Evo N610c P4 (RH 8.0, g77 3.2) 2000 19

Compaq Evo N610c P4 (WinXP, CVF 6.6) 2000 19

Compaq Evo N610c P4 (WinXP, g77 3.2) 2000 20

Apple Power Mac G4 (OSX 10.2, Absoft) 733 67

Apple Power Mac G4 (OSX 10.2, g77 3.3) 733 62

Compaq AlphaServer DS10 (Tru64 5.0) 466 39

SGI IndigoII R10K (Irix 6.5, MIPS) 195 144

**BENCHMARK #4: TIP3P Water Box Molecular Dynamics**

The system consists of 216 rigid TIP3P water molecules in a 18.643 ≈ periodic box, 9.0 ≈ shifted energy switch cutoffs for nonbonded interactions. The time reported is for 1000 dynamics steps of 1.0 fs each using the modified Beeman integrator and Rattle constraints on all bond lengths.

**MACHINE-OS-COMPILER TYPE MHz DYNAMICS**

Athlon XP 2400+ (RH 8.0, Intel) 2000 37

Athlon XP 2400+ (RH 8.0, PGI) 2000 34

Athlon XP 2400+ (RH 8.0, g77 3.2) 2000 45

Athlon Thunderbird (RH 8.0, Intel) 1400 52

Athlon Thunderbird (RH 8.0, PGI) 1400 47

Athlon Thunderbird (RH 8.0, g77 3.2) 1400 63

Athlon Classic (RH 8.0, Intel) 950 77

Athlon Classic (RH 8.0, PGI) 950 71

Athlon Classic (RH 8.0, g77 3.2) 950 96

Compaq Evo N610c P4 (RH 8.0, Intel) 2000 53

Compaq Evo N610c P4 (RH 8.0, PGI) 2000 54

Compaq Evo N610c P4 (RH 8.0, Absoft) 2000 55

Compaq Evo N610c P4 (RH 8.0, g77 3.2) 2000 91

Compaq Evo N610c P4 (WinXP, CVF 6.6) 2000 63

Compaq Evo N610c P4 (WinXP, g77 3.2) 2000 94

Apple Power Mac G4 (OSX 10.2, Absoft) 733 209

Apple Power Mac G4 (OSX 10.2, g77 3.3) 733 170

Compaq AlphaServer DS10 (Tru64 5.0) 466 106

SGI IndigoII R10K (Irix 6.5, MIPS) 195 280

**BENCHMARK #5: TINKER Water Box Molecular Dynamics**

The system consists of 216 AMOEBA flexible polarizable atomic multipole water molecules in a 18.643 ≈ periodic box using regular Ewald summation for the electrostatics and a 12.0 ≈ switched cutoff for vdW interactions. The time reported is for 100 dynamics steps of 1.0 fs each using the modified Beeman integrator and 0.01 Debye rms convergence for induced dipole moments.

**MACHINE-OS-COMPILER TYPE MHz DYNAMICS**

Athlon XP 2400+ (RH 8.0, Intel) 2000 108

Athlon XP 2400+ (RH 8.0, PGI) 2000 104

Athlon XP 2400+ (RH 8.0, g77 3.2) 2000 128

Athlon Thunderbird (RH 8.0, Intel) 1400 165

Athlon Thunderbird (RH 8.0, PGI) 1400 158

Athlon Thunderbird (RH 8.0, g77 3.2) 1400 183

Athlon Classic (RH 8.0, Intel) 950 282

Athlon Classic (RH 8.0, PGI) 950 261

Athlon Classic (RH 8.0, g77 3.2) 950 307

Compaq Evo N610c P4 (RH 8.0, Intel) 2000 156

Compaq Evo N610c P4 (RH 8.0, PGI) 2000 191

Compaq Evo N610c P4 (RH 8.0, Absoft) 2000 226

Compaq Evo N610c P4 (RH 8.0, g77 3.2) 2000 243

Compaq Evo N610c P4 (WinXP, CVF 6.6) 2000 176

Compaq Evo N610c P4 (WinXP, g77 3.2) 2000 263

Apple Power Mac G4 (OSX 10.2, Absoft) 733 680

Apple Power Mac G4 (OSX 10.2, g77 3.3) 733 479

Compaq AlphaServer DS10 (Tru64 5.0) 466 358

SGI IndigoII R10K (Irix 6.5, MIPS) 195 868