Semichem

AMPAC 9 *vs.* MOPAC 2007

PERFORMANCE SUMMARY

- ***SCF Convergence***
  - AMPAC is much faster than MOPAC (1.5 – 2.2 times)
  - The speed advantage increases with larger molecules
  - AMPAC has an advanced package of SCF convergers and is more robust

- ***Geometry Optimization***
  - AMPAC more than 3 times faster than MOPAC for congeneric structures
  - AMPAC 25 times faster than MOPAC on a polypeptide chain (MW=173)

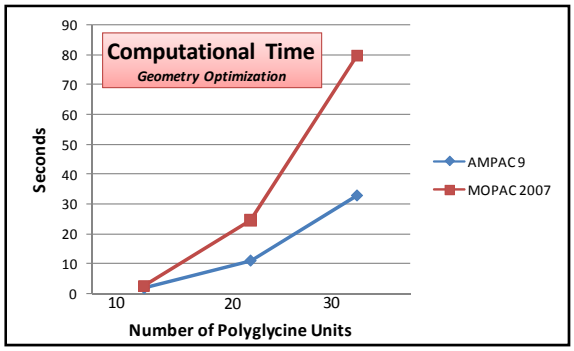
- ***Vibrational Frequencies***
  - AMPAC is 2-3 times faster on increasingly large polyglycine chains
  - AMPAC's LFORCE computes initial values 30 times faster than MOPAC

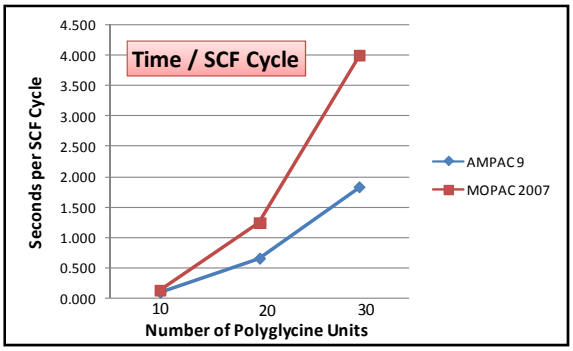
- ***TS Gradient Minimization and TS Location***
  - AMPAC averages 1.4 times faster than MOPAC on TS minimization
  - AMPAC's CHN averages 30 times faster than MOPAC's SADDLE

- ***Configuration Interaction***
  - AMPAC is much more capable than MOPAC
  - AMPAC runs over 100 times faster on average for single-point energies
  - AMPAC runs over 500 times faster on average for optimizations

Overall Computational Speed[1]

For single point energy calculations, AMPAC and MOPAC took about the same number of SCF cycles, but for each cycle MOPAC jobs were considerably slower. This speed disparity increased with system size. For example, in the case of linear polyglycine chains, MOPAC is 40% slower for 10 units, 120% for 20 units, and 140% for 28 units.





SCF Robustness and Speed

AMPAC has a quadratically convergent SCF (qcscf) algorithm in addition to its regular SCF solver. This method is automatically invoked to handle very difficult cases. MOPAC lacks this important feature. The effect of this is evident for a single point energy calculation (just 1 SCF cycle) on a truncated (9, 0) nanotube. AMPAC converged in 21 regular and 6 qcscf steps in 17 seconds. MOPAC, required 91 cycles and only converged after 27 seconds.

Geometry Optimization[2,3] Efficiency

For geometry optimizations of polygycine chains (4-24 units long) in α-helical configurations, MOPAC required 3 or more times as many geometry cycles and 3 or more times the CPU time as AMPAC. For all cases, MOPAC required twice as many SCF calculations as did AMPAC. Taken together, these results show that AMPAC SCF produces better wavefunctions at each step and AMPAC geometry optimization is more efficient and robust that MOPAC's by a considerable margin.

Additionally, two biological molecules (130 and 173 atoms respectively) were optimized as well (see Table 1). The structures of these molecules are not regular like the polyglycines and offered a different challenge. As before, AMPAC was much faster than MOPAC at this calculation, and struggled to converge to a low-gradient structure. AMPAC's advanced search methods focused each geometry optimization step for this difficult case, and the results are apparent.

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[1] All calculations were performed on the same dual Pentium III system running Windows XP Pro.

[2] All calculations use default optimization algorithm (TRUSTE for AMPAC, EF for MOPAC), with GNORM=1.0.

[3] All geometry optimizations began at the same geometry.

Table 1. Geometry Optimization Comparison[4]

System	Atoms	AMPAC 9			MOPAC 2007			Mopac2007 / AMPAC 9		
		Time	SCF	#Opt	Time	SCF	# Opt	Time	SCF	# Opt
Polyglycine α-helices	31	4	372	30	12	607	105	3.0	2.0	3.5
	115	199	664	58	637	1,071	169	3.2	2.0	2.9
	171	1,476	1,372	126	5,318	2,131	373	3.6	2.3	3.0
Antifungal Agent	130	149	540	48	545	848	125	3.7	2.3	2.6
Poly Peptide	173	35	37	3	867	392	82	25.1	2.4	27.3

Vibrational Frequency Calculations[5]

Calculation of vibrational frequencies is a key step in most computational investigations, as optimized geometries must be characterized as minima or transition states. MOPAC does offer the capability to take advantage of molecule symmetry in this computation, whereas AMPAC does not, but the practical cases where this is important are few. Returning to our previous example of polyglycine α-helices, AMPAC's superiority is evident (see Table 2), with AMPAC being 2-3 times faster than MOPAC. AMPAC's speed advantage increases with the size of system

Table 2. Vibrational Frequency Calculation Comparison

System	Atoms	AMPAC 9 Time	AMPAC 9 LFORCE Time	MOPAC 2007 Time	MOPAC2007 / AMPAC9	
					Normal	LFORCE
Polyglycine α-helices	31	11.2	5	26	2.3	4.9
	115	1,368	223	3,091	2.2	13.8
	171	5,889	592	19,476	3.3	32.9

AMPAC also has the efficient and very useful LFORCE method, which only explicitly computes the first few vibrational frequencies (all that are needed for stationary point characterization). LFORCE runs about 10 times faster than AMPAC's normal frequency method, but 30 times faster than a regular MOPAC calculation.

Also, AMPAC and MOPAC were both used to compute frequencies for the S_N1 transition state for the reaction of the methyl cation with trifluoromethane. For tests with symmetry both on and off, MOPAC incorrectly identified two negative vibrational frequencies, where

[4] All times in seconds; "SCF" and "# Opt" are the number of cycles.

[5] At fixed geometry with no optimization.

AMPAC correctly identified the single transition vector.

Transition State Gradient Minimization

In this comparison, approximate transition states were optimized by gradient minimization for eleven representative reactions.[6] AMPAC was an average of 1.4 times faster than MOPAC. MOPAC was only slightly faster in two cases.

Transition State Location Methods

AMPAC and MOPAC both feature methods locate likely transition states given the structures of reactants and products. AMPAC's CHN ("chain") was an average of 30 times faster than MOPAC's SADDLE methods on the same eleven reactions[6] used above. Also, MOPAC failed to locate a transition state in two cases and could not properly characterize the TS in another.

Configuration Interaction (CI)

The configuration interaction capability in AMPAC is both more capable and far faster than in MOPAC. On three example systems,[7] single-point energy calculations were an average of 110 times faster when using AMPAC! On geometry optimizations using CI, the speed difference is to AMPAC's advantage by almost 500 times!

Appendix

Example Reactions

Amide Neutral Hydrolysis
C_2H_2 + CO
Diels-Alder Condensation
Ethene Dimerization 1 (UHF)
Keto-enol Interconversion
Keto-enol Interconversion of Acetylacetone
Keto-enol Interconversion-Water Catalyzed
S_N2
Syn Elimination Reaction
Urethane Polymerization
Urethane Polymerization - Amine Catalyzed

Example CI Systems

Caffiene, (LUMO-3 and HOMO+3)
Dioxine derivative, (LUMO-3 and HOMO+3)
Porphyrin Ring with Mg, (LUMO-1 and HOMO+1)

[6] See Appendix.
[7] See Appendix.