

## Comparison of accuracy and speed between phangorn and other phylogenetic packages

For the comparison of phangorn with other phylogenetic programs we used 50 nucleotide data sets (S2) and 50 amino acid data sets (S3). These data sets were previously used in a comparison of several versions of PhyML with RaxML and taken from phyml website (<http://www.atgc-montpellier.fr/phyml/benchmarks>) and come originally from treebase (<http://www.treebase.org>). The analysis was performed using the following programs:

- Paup4.0b10 (<http://paup.csit.fsu.edu/>)
- phyml 3.0 (<http://www.atgc-montpellier.fr/phyml>)
- phylip 3.69 (<http://evolution.genetics.washington.edu/phylip.html>)
- phangorn 1.2-0 (<http://cran.r-project.org/web/packages/phangorn/index.html>).

All simulations have been performed on a Toshiba notebook with Intel(R) Pentium(R) Dual CPU T3400 @ 2.16GHz.

### Maximum likelihood analysis

The accuracy and speed of the maximum likelihood algorithm in phangorn were compared with those in PhyML. To obtain comparable likelihood values for the two programs we optimized, for the trees estimated with phangorn, the edge length and parameters in PhyML again. However the topology of the trees was kept fixed.

We analyzed 50 nucleotide data sets using GTR +  $\Gamma(4)$  model and Nearest Neighbor Interchange (NNI) rearrangements. Both programs have a similar search strategy. The accuracy of both programs was therefore about equal - 24 times the (log-)likelihood for phangorn was higher 23 times lower than for PhyML. However phangorn was in generally faster (table 1).

We obtained similar results for the 50 protein data sets. We optimized each data set with WAG +  $\Gamma(4)$  model and NNI rearrangements. Again the accuracy was very similar, the trees from phangorn achieved 15 times higher, 13 times lower and about 22 times an log-likelihood that is about equal to PhyML (table 2).

### Maximum parsimony analysis

We made two separate analyses to compare speed and accuracy of maximum parsimony between phangorn and Paup\* and between phangorn and phylip. In phylogenetic analyses there is always a trade-off between accuracy and time, we adjusted therefore some of the standard parameters to limit the time of the simulation. For the parsimony analysis with Paup\* we used the command hsearch with the option nbest=1. The parsimony analysis with the phylip program dnaps used the default values except for the parameter V (Number of trees to save), which was reduced to 10 (from 10000). For both analyses the phangorn function pratchet using the default values and the random seed was

set 1 before each run.

The results of the comparison between phangorn and Paup\* are shown in table 3. Trees estimated with Paup\* contained in most cases a lower p-score (28 times lower, 10 times higher) and the computing time is up to 100 times faster in Paup\*.

In the phylib function dnapars gaps "-" are coded as a fifth base. There is the possibility to recode gaps "-" as unknown states "?" to make the analysis compatible with Paup\*. I have to thank Prof. Felsenstein for pointing out these differences to me. In phangorn one can easily define to user-defined character states, so we performed the same coding for gaps as in dnapars. In most cases trees obtained from phylib have a lower p-score (25 versus 12), but the runtime is higher than with phangorn.

## Summary

The phangorn will likely produce reasonable trees for up to about 100 taxa. For higher number of taxa more sophisticated tree rearrangements (SPR, TBR) would be necessary to find good topologies. This restriction is noticeable in the comparison of the parsimony scores as phylib or Paup\* have the more sophisticated algorithms. However phangorn is capable of coping with a high number of sites, restricted mainly by the memory.

All the scripts and trees generated during these study can be obtained on request from the author.

Data set	Maximum likelihood - DNA			
	phangorn		phyML	
	log-likelihood	time	log-likelihood	time
nucleic_M2564_142x1130_2006.phy	-20435.79	1 m 53 s	-20445.45	18 m 39 s
nucleic_M2565_51x1951_2006.phy	-14657.68	29 s	-14659.42	3 m 56 s
nucleic_M2566_73x918_2006.phy	-12011.73	46 s	-12000.74	6 m 20 s
nucleic_M2567_64x1044_2006.phy	-6790.84	23 s	-6790.68	2 m 3 s
nucleic_M2572_191x990_2006.phy	-3505.22	39 s	-3505.21	1 m 39 s
nucleic_M2587_117x1910_2006.phy	-16445.61	4 m 15 s	-16135.63	21 m 36 s
nucleic_M2588_68x1196_2006.phy	-12012.42	1 m 52 s	-12011.10	8 m 31 s
nucleic_M2599_66x1137_2006.phy	-2163.06	5 s	-2162.58	14 s
nucleic_M2600_69x814_2006.phy	-1752.90	5 s	-1755.93	11 s
nucleic_M2606_110x1206_2006.phy	-26860.34	1 m 46 s	-26860.91	12 m 46 s
nucleic_M2623_139x1044_2006.phy	-46073.80	6 m 26 s	-45981.42	20 m 2 s
nucleic_M2627_54x1915_2006.phy	-35136.54	1 m 20 s	-35136.55	14 m 31 s
nucleic_M2655_50x872_2006.phy	-6516.99	17 s	-6516.99	2 m 7 s
nucleic_M2661_66x1027_2006.phy	-9130.70	26 s	-9130.12	2 m 51 s
nucleic_M2662_60x1348_2006.phy	-12344.62	48 s	-12346.63	4 m 42 s
nucleic_M2675_51x1537_2006.phy	-7878.35	21 s	-7879.82	2 m 20 s
nucleic_M2696_50x1472_2006.phy	-6165.37	21 s	-6169.76	1 m 25 s
nucleic_M2702_54x886_2006.phy	-5387.25	20 s	-5384.91	2 m 4 s
nucleic_M2707_115x1677_2006.phy	-9765.34	3 m 11 s	-9783.05	15 m 0 s
nucleic_M2708_78x1107_2006.phy	-6547.12	52 s	-6537.09	5 m 6 s
nucleic_M2711_123x1181_2006.phy	-10651.89	1 m 30 s	-10665.85	7 m 28 s
nucleic_M2716_79x1252_2006.phy	-3372.43	36 s	-3362.93	2 m 12 s
nucleic_M2733_60x1207_2006.phy	-10920.00	43 s	-10919.17	4 m 30 s
nucleic_M2738_53x1538_2006.phy	-13903.14	49 s	-13903.14	8 m 9 s
nucleic_M2752_106x1292_2006.phy	-7871.28	36 s	-7870.17	2 m 32 s
nucleic_M2764_57x803_2006.phy	-10150.01	36 s	-10150.01	3 m 21 s
nucleic_M2770_86x1628_2006.phy	-5814.35	42 s	-5822.55	2 m 15 s
nucleic_M2771_52x1896_2006.phy	-13981.66	34 s	-13983.47	6 m 17 s
nucleic_M2772_77x900_2006.phy	-7194.07	54 s	-7197.32	4 m 0 s
nucleic_M2786_104x1051_2006.phy	-15657.01	1 m 16 s	-15667.87	8 m 18 s
nucleic_M2792_166x812_2006.phy	-10593.95	2 m 18 s	-10566.66	7 m 26 s
nucleic_M2826_60x1398_2006.phy	-14342.13	38 s	-14352.24	4 m 9 s
nucleic_M2845_68x1715_2006.phy	-11375.41	37 s	-11360.22	3 m 34 s
nucleic_M2856_61x970_2006.phy	-25037.08	49 s	-25032.81	7 m 58 s
nucleic_M2862_54x1011_2006.phy	-16196.69	44 s	-16199.25	6 m 42 s
nucleic_M2879_70x800_2006.phy	-5789.28	49 s	-5788.49	2 m 28 s
nucleic_M2901_56x1802_2006.phy	-7839.45	1 m 1 s	-7867.90	3 m 56 s
nucleic_M2902_51x908_2006.phy	-7593.51	27 s	-7589.85	2 m 7 s
nucleic_M2913_81x897_2006.phy	-2433.31	37 s	-2435.08	1 m 53 s
nucleic_M2916_143x897_2006.phy	-3491.37	1 m 9 s	-3491.26	5 m 38 s
nucleic_M2921_54x966_2006.phy	-6443.45	18 s	-6438.54	2 m 2 s
nucleic_M2922_77x1101_2006.phy	-3044.21	18 s	-3036.46	1 m 3 s
nucleic_M2928_81x1651_2006.phy	-6688.41	41 s	-6688.42	2 m 17 s
nucleic_M2932_68x1712_2006.phy	-14923.29	1 m 17 s	-14923.65	16 m 51 s
nucleic_M2933_99x1634_2006.phy	-7628.64	1 m 27 s	-7647.42	10 m 4 s
nucleic_M2944_80x1495_2006.phy	-8985.80	29 s	-9011.54	3 m 38 s
nucleic_M2945_62x1271_2006.phy	-34980.46	1 m 30 s	-34987.79	9 m 8 s
nucleic_M2946_110x1003_2006.phy	-17018.87	1 m 37 s	-17006.52	16 m 17 s
nucleic_M2974_56x827_2006.phy	-5383.47	16 s	-5382.99	1 m 41 s
nucleic_M2975_93x982_2006.phy	-12304.88	1 m 24 s	-12302.69	6 m 45 s

Table 1: Comparison of (log-)likelihood and speed for the analysis of a GTR +  $\Gamma(4)$  model on 50 nucleotide data sets between phangorn and phymml

Data set	Maximum likelihood - AA			
	phangorn		phyML	
	log-likelihood	time	log-likelihood	time
proteic_M1372_23x394_2003.phy	-4474.49	17 s	-4474.49	58 s
proteic_M1373_23x392_2003.phy	-3535.88	16 s	-3539.49	37 s
proteic_M1375_23x530_2003.phy	-7769.71	23 s	-7789.80	1 m 39 s
proteic_M1376_36x484_2003.phy	-11531.09	39 s	-11531.23	3 m 17 s
proteic_M1377_19x1566_2003.phy	-17597.22	1 m 16 s	-17576.09	3 m 51 s
proteic_M1378_18x1561_2003.phy	-16060.74	55 s	-16045.65	3 m 2 s
proteic_M1379_9x1557_2003.phy	-11634.54	9 s	-11634.54	38 s
proteic_M1380_9x1558_2003.phy	-12023.40	11 s	-12023.40	36 s
proteic_M1381_9x1557_2003.phy	-12099.21	9 s	-12099.21	34 s
proteic_M1382_9x1560_2003.phy	-12335.18	12 s	-12335.18	37 s
proteic_M1383_11x1561_2003.phy	-13724.27	16 s	-13730.12	58 s
proteic_M1384_11x391_2003.phy	-2884.86	3 s	-2882.79	12 s
proteic_M1385_11x530_2003.phy	-5615.96	5 s	-5609.47	25 s
proteic_M1392_57x430_2003.phy	-8178.97	2 m 30 s	-8174.61	4 m 29 s
proteic_M1487_52x981_2003.phy	-16320.68	3 m 49 s	-16291.04	7 m 36 s
proteic_M1499_22x513_2003.phy	-12471.64	11 s	-12471.64	1 m 39 s
proteic_M1503_23x479_2003.phy	-9851.03	22 s	-9851.03	1 m 41 s
proteic_M1504_37x547_2003.phy	-12585.53	29 s	-12585.53	3 m 46 s
proteic_M1508_22x431_2003.phy	-3155.15	9 s	-3155.09	40 s
proteic_M1601_36x340_2003.phy	-6918.85	47 s	-6921.32	2 m 1 s
proteic_M1768_31x228_2004.phy	-1052.53	6 s	-1052.53	14 s
proteic_M1812_34x176_2004.phy	-5420.53	16 s	-5420.53	57 s
proteic_M1882_8x705_2004.phy	-6191.99	7 s	-6191.99	1 m 5 s
proteic_M1989_18x173_2004.phy	-3179.90	10 s	-3179.90	28 s
proteic_M1990_35x153_2004.phy	-1454.33	13 s	-1454.26	55 s
proteic_M1991_32x129_2004.phy	-2393.89	21 s	-2394.11	47 s
proteic_M1992_46x68_2004.phy	-2922.82	19 s	-2921.40	48 s
proteic_M1993_28x93_2004.phy	-2007.73	13 s	-2005.49	25 s
proteic_M2302_24x365_2005.phy	-4204.53	13 s	-4204.52	43 s
proteic_M2304_31x429_2005.phy	-5506.04	20 s	-5506.04	1 m 17 s
proteic_M2344_7x232_2005.phy	-1583.46	1 s	-1583.46	6 s
proteic_M2345_7x232_2005.phy	-1583.46	1 s	-1583.46	6 s
proteic_M2363_38x251_2004.phy	-11713.42	1 m 34 s	-11723.22	4 m 40 s
proteic_M2382_28x162_2005.phy	-2707.96	28 s	-2712.46	43 s
proteic_M2476_30x719_2005.phy	-24548.58	42 s	-24548.59	4 m 3 s
proteic_M2477_39x888_2005.phy	-21163.44	52 s	-21163.44	4 m 48 s
proteic_M2478_30x276_2005.phy	-8725.38	32 s	-8725.38	1 m 29 s
proteic_M2479_30x627_2005.phy	-18059.96	35 s	-18059.96	3 m 50 s
proteic_M2480_40x430_2005.phy	-23899.13	1 m 2 s	-23871.28	3 m 15 s
proteic_M2512_14x717_2006.phy	-20099.72	23 s	-20102.12	5 m 44 s
proteic_M2558_27x1060_2005.phy	-37185.91	2 m 23 s	-37186.25	12 m 20 s
proteic_M2624_139x348_2006.phy	-13086.63	11 m 34 s	-13142.76	56 m 47 s
proteic_M2636_20x1275_2006.phy	-19066.77	50 s	-19066.77	2 m 13 s
proteic_M2637_19x380_2006.phy	-1604.55	4 s	-1606.52	26 s
proteic_M2638_18x378_2006.phy	-1691.49	2 s	-1693.32	13 s
proteic_M2639_19x331_2006.phy	-5745.68	10 s	-5743.37	48 s
proteic_M2640_18x243_2006.phy	-2510.77	3 s	-2510.77	23 s
proteic_M2641_18x326_2006.phy	-5153.58	10 s	-5153.58	48 s
proteic_M2899_25x444_2006.phy	-9961.38	29 s	-9960.55	1 m 44 s
proteic_M2954_5x1006_2006.phy	-3241.74	< 1 s	-3241.74	3 s

Table 2: Comparison of (log-)likelihood and speed for the analysis of a GTR +  $\Gamma(4)$  model on 50 protein data sets between phangorn and PhyML

Data set	Maximum Parsimony - DNA			
	phangorn		Paup	
	p-score	time (sec.)	p-score	time (sec.)
nucleic_M2564_142x1130_2006.phy	4021	19.92	4006	0.61
nucleic_M2565_51x1951_2006.phy	2390	5.18	2392	0.05
nucleic_M2566_73x918_2006.phy	2300	6.49	2301	0.16
nucleic_M2567_64x1044_2006.phy	955	4.24	956	0.05
nucleic_M2572_191x990_2006.phy	367	6.96	367	0.23
nucleic_M2587_117x1910_2006.phy	2544	16.38	2398	0.59
nucleic_M2588_68x1196_2006.phy	2683	6.33	2669	0.16
nucleic_M2599_66x1137_2006.phy	80	1.64	80	0.02
nucleic_M2600_69x814_2006.phy	88	1.71	88	0.03
nucleic_M2606_110x1206_2006.phy	5768	14.32	5769	0.28
nucleic_M2623_139x1044_2006.phy	11905	31.65	11665	1.87
nucleic_M2627_54x1915_2006.phy	8231	8.82	8231	0.16
nucleic_M2655_50x872_2006.phy	1104	3.03	1103	0.03
nucleic_M2661_66x1027_2006.phy	1835	5.3	1829	0.08
nucleic_M2662_60x1348_2006.phy	2204	6.86	2192	0.08
nucleic_M2675_51x1537_2006.phy	1194	3.62	1189	0.02
nucleic_M2696_50x1472_2006.phy	696	3.28	687	0.01
nucleic_M2702_54x886_2006.phy	846	3.15	846	0.06
nucleic_M2707_115x1677_2006.phy	1788	10.34	1762	0.37
nucleic_M2708_78x1107_2006.phy	1250	5.7	1235	0.13
nucleic_M2711_123x1181_2006.phy	1983	12.2	1983	0.23
nucleic_M2716_79x1252_2006.phy	358	2.64	333	0.17
nucleic_M2733_60x1207_2006.phy	1931	5.99	1935	0.05
nucleic_M2738_53x1538_2006.phy	2596	4.7	2596	0.08
nucleic_M2752_106x1292_2006.phy	1002	5.09	1003	0.09
nucleic_M2764_57x803_2006.phy	1936	4.66	1936	0.09
nucleic_M2770_86x1628_2006.phy	512	5.96	508	0.06
nucleic_M2771_52x1896_2006.phy	2299	6.67	2299	0.08
nucleic_M2772_77x900_2006.phy	1206	8.03	1204	0.13
nucleic_M2786_104x1051_2006.phy	3189	10.85	3190	0.27
nucleic_M2792_166x812_2006.phy	1880	16.32	1879	0.36
nucleic_M2826_60x1398_2006.phy	2538	6.27	2531	0.09
nucleic_M2845_68x1715_2006.phy	1588	6.65	1588	0.08
nucleic_M2856_61x970_2006.phy	6298	7.96	6304	0.09
nucleic_M2862_54x1011_2006.phy	3932	5.07	3938	0.05
nucleic_M2879_70x800_2006.phy	875	4.04	875	0.05
nucleic_M2901_56x1802_2006.phy	925	4.35	907	0.08
nucleic_M2902_51x908_2006.phy	1341	4.6	1340	0.05
nucleic_M2913_81x897_2006.phy	218	2.37	211	0.14
nucleic_M2916_143x897_2006.phy	351	5.99	341	0.48
nucleic_M2921_54x966_2006.phy	1004	4.03	1003	0.03
nucleic_M2922_77x1101_2006.phy	282	2.34	280	0.01
nucleic_M2928_81x1651_2006.phy	882	4.87	882	0.05
nucleic_M2932_68x1712_2006.phy	3186	8.68	3175	0.25
nucleic_M2933_99x1634_2006.phy	1096	8.48	1087	0.20
nucleic_M2944_80x1495_2006.phy	1237	6.02	1235	0.06
nucleic_M2945_62x1271_2006.phy	9252	10.5	9253	0.20
nucleic_M2946_110x1003_2006.phy	3461	13.09	3457	0.58
nucleic_M2974_56x827_2006.phy	864	3.1	862	0.03
nucleic_M2975_93x982_2006.phy	2345	11.3	2333	0.22

Table 3: Comparison of parsimony scores and speed between phangorn and Paup\* on 50 nucleotide data sets

Data set	Maximum Parsimony - DNA			
	phangorn		phylip	
	p-score	time (sec.)	p-score	time (sec.)
nucleic_M2564_142x1130_2006.phy	4573	21.05	4558	420.36
nucleic_M2565_51x1951_2006.phy	2835	6.58	2835	10.97
nucleic_M2566_73x918_2006.phy	2661	6.66	2664	52.88
nucleic_M2567_64x1044_2006.phy	994	4.52	994	24.82
nucleic_M2572_191x990_2006.phy	710	7.43	710	22.2
nucleic_M2587_117x1910_2006.phy	7552	19.92	7496	348.88
nucleic_M2588_68x1196_2006.phy	3042	7.02	2967	46.23
nucleic_M2599_66x1137_2006.phy	391	1.8	391	3.1
nucleic_M2600_69x814_2006.phy	96	1.62	96	2.42
nucleic_M2606_110x1206_2006.phy	5768	15.7	5768	205.22
nucleic_M2623_139x1044_2006.phy	16911	26.38	16941	239.45
nucleic_M2627_54x1915_2006.phy	8795	9.04	8795	36.51
nucleic_M2655_50x872_2006.phy	1256	3.41	1256	4.76
nucleic_M2661_66x1027_2006.phy	2418	5.91	2418	10.77
nucleic_M2662_60x1348_2006.phy	2612	6.11	2596	16.3
nucleic_M2675_51x1537_2006.phy	1735	3.86	1737	12.16
nucleic_M2696_50x1472_2006.phy	1991	3.49	1994	24.73
nucleic_M2702_54x886_2006.phy	1061	4.26	1060	16.53
nucleic_M2707_115x1677_2006.phy	4047	12.7	4020	196.26
nucleic_M2708_78x1107_2006.phy	2747	7.86	2751	59.11
nucleic_M2711_123x1181_2006.phy	3672	13.54	3681	178.15
nucleic_M2716_79x1252_2006.phy	2145	4.25	2131	16.63
nucleic_M2733_60x1207_2006.phy	1931	6.27	1933	29.93
nucleic_M2738_53x1538_2006.phy	3034	5.1	3034	16.08
nucleic_M2752_106x1292_2006.phy	1141	5.91	1141	64.13
nucleic_M2764_57x803_2006.phy	4077	6.52	4066	13.24
nucleic_M2770_86x1628_2006.phy	2227	5.33	2219	56.83
nucleic_M2771_52x1896_2006.phy	3960	5.74	3921	21.32
nucleic_M2772_77x900_2006.phy	3528	7.24	3525	37.71
nucleic_M2786_104x1051_2006.phy	6410	10.88	6409	185.02
nucleic_M2792_166x812_2006.phy	2573	17.52	2554	248.46
nucleic_M2826_60x1398_2006.phy	2538	6.59	2530	49.5
nucleic_M2845_68x1715_2006.phy	2102	7.64	2089	59.55
nucleic_M2856_61x970_2006.phy	6622	7.39	6623	12.28
nucleic_M2862_54x1011_2006.phy	3932	5.29	3937	20.03
nucleic_M2879_70x800_2006.phy	1861	4.57	1845	24.6
nucleic_M2901_56x1802_2006.phy	925	4.59	908	34.55
nucleic_M2902_51x908_2006.phy	1341	4.84	1336	16.44
nucleic_M2913_81x897_2006.phy	332	2.45	325	10.41
nucleic_M2916_143x897_2006.phy	493	5.79	486	49.96
nucleic_M2921_54x966_2006.phy	1548	4.45	1548	18.49
nucleic_M2922_77x1101_2006.phy	587	2.65	584	6.68
nucleic_M2928_81x1651_2006.phy	889	5.12	889	15.97
nucleic_M2932_68x1712_2006.phy	8632	8.77	8588	66.01
nucleic_M2933_99x1634_2006.phy	3932	8.28	3888	75.61
nucleic_M2944_80x1495_2006.phy	1788	6.95	1784	59.19
nucleic_M2945_62x1271_2006.phy	10252	8.8	10243	23.43
nucleic_M2946_110x1003_2006.phy	4082	14.41	4085	148.76
nucleic_M2974_56x827_2006.phy	1653	3.88	1654	9.66
nucleic_M2975_93x982_2006.phy	6725	11.17	6686	67.55

Table 4: Comparison of parsimony scores and speed between phangorn and phylic on 50 nucleotide data sets