

Supplementary Materials

Supplementary Figures and Tables

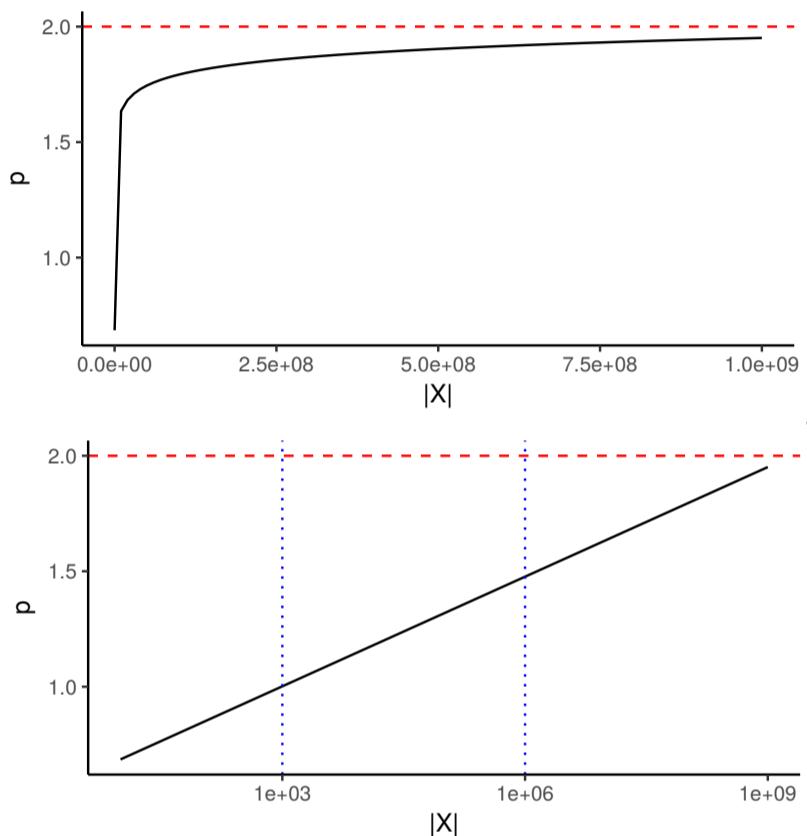


Figure S1. Required p for $|X|$ for $\epsilon = 10^{-10}$ shown in normal (top) and log (bottom) scales. On the right, the range of values of $|X|$ seen in practice is shown as dotted vertical lines.

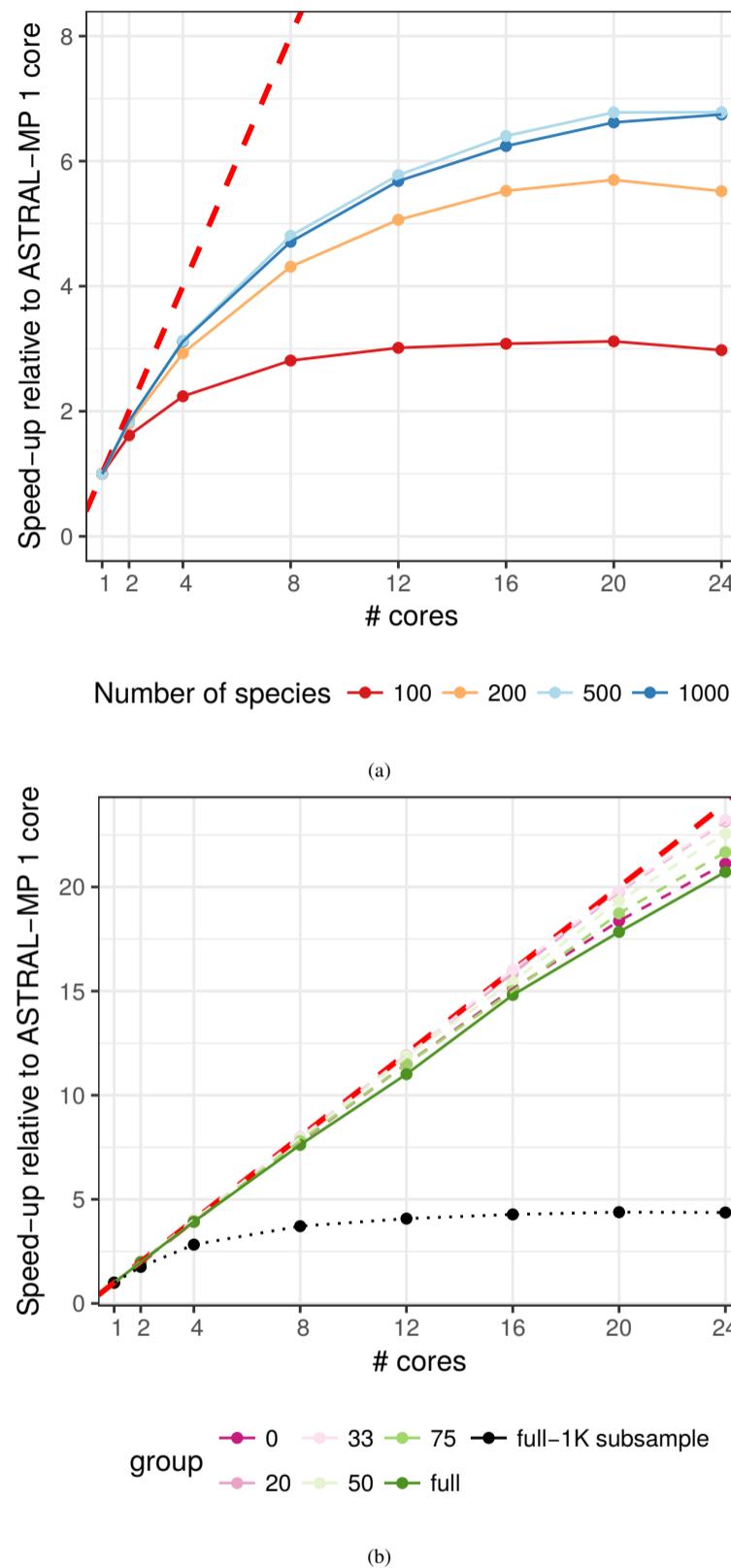


Figure S2. Speedups of ASTRAL-MP with CPU parallelization. The speedup is computed with respect to ASTRAL-MP run with 1 core and each dot shows the average speedups over all replicates. **(a)** The SV datasets with 100, 200, 500, and 1000 species (10 replicates each). **(b)** The avian dataset with contraction levels respectively set to full, 0%, 20%, 33%, 50%, and 75% (1 replicate each). The “full-1K subsample” corresponds to datasets (10 replicates) with random samples of 10^3 gene trees with no contraction.

	24 core no GPU	24 core 4 GPU
ASTRAL topology: % cases identical	88.9	91.1
minimum	$-4.57 \cdot 10^{-4}$	$-2.07 \cdot 10^{-4}$
Increase in the quartet score (ASTRAL-MP – ASTRAL-III)	mean	$-9.99 \cdot 10^{-6}$
median	0	0
maximum	$2.70 \cdot 10^{-4}$	$-2.66 \cdot 10^{-4}$

Table S1. **Verification of output of ASTRAL-MP against the output of ASTRAL-III.** In $\approx 90\%$ of cases, the two versions produce identical results. In the remaining cases, the quartet score is sometimes increased or decreased by a small margin due to stochastic nature of the composition of set X . We show the difference in quartet score, calculated by subtracting the normalized score of ASTRAL-III from the normalized score of ASTRAL-MP. The results include both the SV datasets and the avian datasets (only full datasets, without subsampling).

datasets	ASTRAL-III			ASTRAL-MP 1 core			ASTRAL-MP same number of cores		
	1	6	24	1	6	24	1	6	24
SV, 100	4.70	6.73	6.68	1.79	2.68	2.64	1.79	1.04	0.880
SV, 200	7.38	14.5	17.6	2.16	4.27	5.18	2.16	1.21	0.935
SV, 500	6.98	15.7	20.9	2.15	4.86	6.48	2.15	1.01	0.956
SV, 1000	6.97	15.5	20.9	2.13	4.65	6.25	2.13	1.25	0.927
Avian, 0	42.2	77.5	116	10.4	19.0	28.4	10.4	3.25	1.35
Avian, 20	42.5	56.9	100	14.6	19.5	34.3	14.6	3.26	1.48
Avian, 33	35.9	49.3	89.8	13.8	19.0	34.6	13.8	3.16	1.49
Avian, 50	28.9	41.1	78.0	11.8	16.8	32.0	11.8	2.85	1.41
Avian, 75	20.0	30.8	60.6	9.03	13.9	27.3	9.02	2.34	1.26
Avian, full	50.3	83.7	113	11.4	19.0	25.7	11.4	3.29	1.24

Table S2. **Full scaling results.** Runtimes of ASTRAL-MP with 1 CPU core + 1 GPU, 6 CPU cores + 1 GPU, and 24 CPU cores + 1 GPU in comparison with ASTRAL-III, ASTRAL-MP with 1 CPU core no GPU, and ASTRAL-MP with the same number of cores no GPU on various datasets.

Supplementary Algorithms

Algorithm S1 - Weight calculation. Input is a set of gene trees \mathcal{G} and a tripartition $X|Y|Z$. Each part (e.g., X) is a bitset indexed by the species; thus, $X[u]$ is 1 if leaf u is in X and otherwise is 0. G_3 gives the set of all permutations of $\{1, 2, 3\}$.

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function WEIGHT( $\mathcal{G}, X|Y|Z$ )
     $w \leftarrow 0$ 
    for  $g \in \mathcal{G}$  do
         $S \leftarrow$  empty stack
        for  $u \in postOrder(g)$  do
            if  $u$  is a leaf then
                 $(x, y, z) \leftarrow (X[u], Y[u], Z[u])$ 
            else
                 $(\mathbf{C}_{11}, \mathbf{C}_{12}, \mathbf{C}_{13}) \leftarrow$  pull from  $S$ 
                 $(\mathbf{C}_{21}, \mathbf{C}_{22}, \mathbf{C}_{23}) \leftarrow$  pull from  $S$ 
                 $(x, y, z) \leftarrow (\mathbf{C}_{11} + \mathbf{C}_{21}, \mathbf{C}_{12} + \mathbf{C}_{22}, \mathbf{C}_{13} + \mathbf{C}_{23})$ 
                 $(\mathbf{C}_{31}, \mathbf{C}_{32}, \mathbf{C}_{33}) \leftarrow (|X| - x, |Y| - y, |Z| - z)$ 
                 $w \leftarrow w + \frac{1}{2} \sum_{(a,b,c) \in G_3} \mathbf{C}_{1a}\mathbf{C}_{2b}\mathbf{C}_{3c}(\mathbf{C}_{1a} + \mathbf{C}_{2b} + \mathbf{C}_{3c} - 3)$ 
            push  $(x, y, z)$  to  $S$ 

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