```
seed = -1
treefile = MyTree.tre
Imapfile = MyImap.txt
species&tree = 3  A  B  C
                  2  1  0
((A #0.05, B) :0.005 #0.001, C #0.05) :0.01 #0.01;
loci&length = 1000000 50
migration = 1
            C A 1.0
```

Fig. S1: BPP control file (`MCcoal-ABC-mscm.ctl`) for simulating 10^6 gene trees under the MSC-M model of Fig. 10. The species tree is specified using the Newick notation, with numbers after colon ':' indicating node ages (τ) while those after '#' are population sizes (θ). Note that species C is needed in the specification of the tree and migration rate, but no sequences are sampled from C when gene trees are simulated. The sequence length is unused since no sequence data are simulated. Run BPP with the command

```
bpp --simulate MCcoal-ABC-mscm.ctl
```

```
Number of species in starting delimitation:  5
(X, ((A, B), (C, D)));

*** Iteration 1 ***

Estimated tau and theta parameters:
        theta                   tau
X       0.0100 (0.0097, 0.0103)
A       0.0111 (0.0095, 0.0126)
B       0.0242 (0.0193, 0.0294)
C       0.0262 (0.0209, 0.0318)
D       0.0106 (0.0093, 0.0120)
XABCD   0.0330 (0.0321, 0.0340) 0.0106 (0.0104, 0.0108)
ABCD    0.0442 (0.0434, 0.0450) 0.0005 (0.0005, 0.0006)
AB      0.0068 (0.0041, 0.0095) 0.0004 (0.0003, 0.0004)
CD      0.0059 (0.0037, 0.0084) 0.0004 (0.0004, 0.0005)

Proposal results:
Node pair        gdi 1   gdi 2   merge accepted?
'A', 'B'         0.068   0.032    True
'C', 'D'         0.031   0.075    True

Number of species after iteration 1:  3
(X, (AB, CD));

*** Iteration 2 ***

Estimated tau and theta parameters:
        theta                   tau
X       0.0100 (0.0097, 0.0103)
AB      0.0203 (0.0190, 0.0216)
CD      0.0204 (0.0191, 0.0217)
XABCD   0.0331 (0.0322, 0.0340) 0.0106 (0.0104, 0.0108)
ABCD    0.0433 (0.0425, 0.0441) 0.0006 (0.0005, 0.0006)

Proposal results:
Node pair        gdi 1   gdi 2   merge accepted?
'AB', 'CD'       0.054   0.054   True

Number of species after iteration 2:  2
(X, ABCD);

*** Iteration 3 ***

Estimated tau and theta parameters:
        theta                   tau
X       0.0100 (0.0097, 0.0103)
ABCD    0.0434 (0.0427, 0.0440)
XABCD   0.0331 (0.0321, 0.0340) 0.0106 (0.0104, 0.0108)


Proposal results:
Node pair        gdi 1   gdi 2   merge accepted?
'X', 'ABCD'      0.879   0.388    False

Number of species after iteration 3:  2
(X, ABCD);

Final delimitation reached.
```

Fig. S2: Screen output from running the hierarchical merge algorithm to analyze the simulated dataset of Fig. 4.

```
# Note that species are renamed as follows:
# gir_ang = giraffa+angolensis
# tip_tho = tippelskirchi+thornicrofti
# cam_rot_ant = camelopardalis+rothschildi+antiquorum
# per = peralta
# ret = reticulata

# output
output_directory = res_giraffe_merge

# input files
Imapfile = Imap_Giraffe.txt
seqfile = MSA_Giraffe.txt

# guide tree
guide_tree = ((gir_ang, tip_tho), ((cam_rot_ant, per), ret));

# migration events and priors
migration = {
   ret <-> tip_tho,
   ret <-> cam_rot_ant,
}
migprior = 0.1 10

# hierarchical algorithm settings
mode = merge
gdi_threshold = <=0.3, <=1.0

# BPP MCMC settings
threads = 8
burnin = 50000
nsample = 200000
```

Fig. S3: HHSD control file for the merge algorithm in analysis of the giraffe data. The control file for the split algorithm is the same except for the hierarchical-algorithm settings: `mode = split` and `gdi_threshold = >0.7`. The results are in Fig. 13c&d.

```
# Note species are renamed as follows:
# Po = polyzona
# Ab = abnorma
# Mi = micropholis
# An = annulata
# Ge = gentilis
# Tr = triangulum
# El = elapsoides

# output
output_directory = res_milksnake_merge

# input files
Imapfile = Imap_Lampropeltis.txt
seqfile = MSA_Lampropeltis.txt

# guide tree
guide_tree = (((Mi, (Po, Ab)), (An, (Ge, Tr))), El);

# migration events and priors
migration = {
   Po <-> Ab,
   Po <-> An,
   An <-> Ge,
   Ge <-> Tr,
   Ge <-> El,
   Tr <-> El,
}
migprior = 0.1 10

# hierarchical algorithm settings
mode = merge
gdi_threshold = <=0.3, <=1.0

# BPP MCMC settings
threads = 8
burnin = 50000
nsample = 200000
```

Fig. S4: HHSD control file for the merge analysis of the milksnakes data. The control file for the split algorithm is the same except for the hierarchical-algorithm settings: `mode = split` and `gdi_threshold = >0.7`. The results are in Fig. 14c&d.

```
# output
output_directory = # will be set from the command line

# input files
Imapfile = # will be set from the command line
seqfile = trigentalt.txt

# guide tree
guide_tree = ((Ge, Tr), Al);

# migration events and priors
migration = { Ge <-> Tr }
migprior = 0.1 10


# hierarchical algorithm settings
mode = merge
gdi_threshold = <0.3

# BPP MCMC settings
threads = 8
burnin = 200000
nsample = 500000
```

Fig. S5: HHSD control file for the analysis of the milksnake data under the five delimitation hypotheses with arbitrary East-West divide of *gentilis* and *triangulum* samples (Fig. 14e). The `Imapfile` and `output_directory` parameters are left empty, as they will be provided at the command line (Fig. S6), to ensure that they correspond to the delimitation hypotheses being tested. *L. alterna* (Al) is used as an outgroup, following Chambers and Hillis (2020).

```
hhsd --cfile cf_milksnake_EW.txt --cfpor \
Imapfile = 1alt.Imap.txt, output_directory = res_EW_1

hhsd --cfile cf_milksnake_EW.txt --cfpor \
Imapfile = 2alt.Imap.txt, output_directory = res_EW_2

hhsd --cfile cf_milksnake_EW.txt --cfpor \
Imapfile = 3alt.Imap.txt, output_directory = res_EW_3

hhsd --cfile cf_milksnake_EW.txt --cfpor \
Imapfile = 4alt.Imap.txt, output_directory = res_EW_4

hhsd --cfile cf_milksnake_EW.txt --cfpor \
Imapfile = 5alt.Imap.txt, output_directory = res_EW_5
```

Fig. S6: Shell script used to iterate through the five East-West delimitation hypotheses for the milksnakes (Fig. 14e). The `-cfpor` (control file parameter override) flag is used to override parameters of the control file via the command-line interface, setting the Imap file to match the delimitation hypothesis, and specifying the output directory for each analysis.

```
# Note species are renamed:
# PEL = pelastes
# OZK = ozark
# MEG = megalotis
# LIT = ouachita
# SOL = solis
# AQU = aquilensis

# output
output_directory = res_sunfish_merge

# input files
Imapfile = Imap_Sunfish.txt
seqfile = MSA_Sunfish.txt
phase = 1 # alignment is phased

# guide tree
guide_tree = (((((PEL, OZK), MEG), LIT), SOL), AQU);

# migration
migration = {
   MEG -> PEL,
   MEG -> SOL,
   MEG -> OZK
}
migprior = 0.1 10

# hierarchical algorithm settings
mode = merge
gdi_threshold = <=0.3, <=1.0

# BPP MCMC settings
threads = 12
burnin = 50000
nsample = 200000
```

Fig. S7: HHSD control file for the merge analysis of the sunfish data (Fig. 15). The control file for the split algorithm is the same except for the hierarchical-algorithm settings: `mode = split` and `gdi_threshold = >0.7`.

Table S1: Rate matrix for Markov chain describing transitions between states in multispecies coalescent with migration model with two populations (A and B) and three sequences (a_1, a_2, and b).

	AAA	AAB	ABA	ABB	BAA	BAB	BBA	BBB	$A_{a_1}A$	$A_{a_2}A$	A_bA	$B_{a_1}B$	$B_{a_2}B$	B_bB	$A_{a_1}B$	$A_{a_2}B$	A_bB	AB_{a_1}	AB_{a_2}	AB_b	$A\|B$
AAA	·	ϖ_{BA}	ϖ_{BA}		ϖ_{BA}				c_A	c_A	c_A										
AAB	ϖ_{AB}	·		ϖ_{BA}		ϖ_{BA}														c_A	
ABA	ϖ_{AB}		·	ϖ_{BA}			ϖ_{BA}												c_A		
ABB		ϖ_{AB}	ϖ_{AB}	·				ϖ_{BA}							c_B						
BAA	ϖ_{AB}				·	ϖ_{BA}	ϖ_{BA}											c_A			
BAB		ϖ_{AB}			ϖ_{AB}	·		ϖ_{BA}								c_B					
BBA			ϖ_{AB}		ϖ_{AB}		·	ϖ_{BA}									c_B				
BBB				ϖ_{AB}		ϖ_{AB}	ϖ_{AB}	·				c_B	c_B	c_B							
$A_{a_1}A$									·						ϖ_{BA}			ϖ_{BA}			c_A
$A_{a_2}A$										·						ϖ_{BA}			ϖ_{BA}		c_A
A_bA											·						ϖ_{BA}			ϖ_{BA}	c_A
$B_{a_1}B$												·			ϖ_{AB}			ϖ_{AB}			c_B
$B_{a_2}B$													·			ϖ_{AB}			ϖ_{AB}		c_B
B_bB														·			ϖ_{AB}			ϖ_{AB}	c_B
$A_{a_1}B$									ϖ_{AB}			ϖ_{BA}			·						
$A_{a_2}B$										ϖ_{AB}			ϖ_{BA}			·					
A_bB											ϖ_{AB}			ϖ_{BA}			·				
AB_{a_1}									ϖ_{AB}			ϖ_{BA}						·			
AB_{a_2}										ϖ_{AB}			ϖ_{BA}						·		
AB_b											ϖ_{AB}			ϖ_{BA}						·	
$A\|B$																					·

Note.— $\varpi_{AB} = 4M_{AB}/\theta_B = m_{AB}/\mu$ and $\varpi_{BA} = 4M_{BA}/\theta_A = m_{BA}/\mu$ are mutation-scaled migration rates, and $c_A = 2/\theta_A$ and $c_B = 2/\theta_B$ are the coalescent rates, when one time unit is the expected time to accumulate one mutation per site. The state of the chain is given by the population IDs (A or B) and sequence IDs (a_1, a_2, b). For example the initial state $A_{a_1}A_{a_2}B_b$ means that the three sequences a_1, a_2, and b are in populations A, A, and B, respectively. States with three sequences are abbreviated, with the three sequences assumed to be in the order a_1, a_2, b so that the sequence IDs are suppressed. Thus $A_{a_1}A_{a_2}B_b$ is 'AAB'. State $A_{a_1a_2}B_b$ means that two sequences remain in the sample, with the ancestor of sequences a_1 and a_2 is in population A while sequence b is in population B. This is abbreviated 'AB_b', with the sequence ID 'a_1a_2' suppressed. '$A|B$' is an absorbing state in which only one sequence remains in the sample, in either A or B, after two coalescent events have occurred. From Leaché *et al.* (2019).

Table S2: Hierarchical merge algorithm under the MSC model applied to data simulated under the model of Fig. 4a

Pair	gdi_A (aab data)	gdi_B (abb data)	Decision
Using the cutoff: $gdi < 0.2$			
Iteration 1: merging A-B into AB, C-D into CD			
A-B	0.067	0.033	**accepted**
C-D	0.031	0.075	**accepted**
Iteration 2: merging AB-CD into $ABCD$			
AB-CD	0.054	0.054	**accepted**
Iteration 3: merging X-$ABCD$ into $XABCD$			
X-$ABCD$	0.879	0.388	rejected
Final model:	two species: X, $ABCD$		
Using the cutoff: $gdi < 0.7$			
Iteration 1: same as above			
Iteration 2: same as above			
Iteration 3: merging X-$ABCD$ into $XABCD$			
Final model:	one species: $XABCD$		

Note.— The guide tree, $(((A, B), (C, D)), X)$, is inferred under the MSC model with no gene flow (Fig. 4b). Under MSC model with no gene flow, gdi_J and gdi_K are equivalent (equation 2). A merge (between sister lineages) is accepted if either gdi_A or gdi_B is less than the cutoff, with multiple merges allowed in each iteration.

Table S3: Hierarchical merge algorithm under the MSC-M model allowing the merge of non-sister lineages applied to data simulated under the model of Fig. 4a

	gdi_J			gdi_K		
Pair	aab	abb	Decision	aab	abb	Decision
Using cutoff: $gdi < 0.2$						
Iteration 1: merge of nonsister lineages A and B is accepted						
X-A	0.876	0.433	rejected	0.861	0.428	rejected
A-B	0.078	0.028	**accepted**	0.322	0.284	rejected
A-C	0.126	0.075	rejected	0.399	0.365	rejected
B-C	0.052	0.052	rejected	0.351	0.350	rejected
A-D	0.153	0.159	rejected	0.434	0.439	rejected
B-D	0.082	0.138	rejected	0.387	0.424	rejected
C-D	0.031	0.090	rejected	0.354	0.392	rejected
Iteration 2: merge of nonsister lineages C and D is accepted						
X-AB	0.874	0.402	rejected			
AB-C	0.060	0.066	rejected			
AB-D	0.088	0.148	rejected			
C-D	0.031	0.088	**accepted**			
Iteration 3: merge of nonsister lineages AB and CD is accepted						
X-AB	0.877	0.388	rejected			
AB-CD	0.073	0.070	**accepted**			
Iteration 4: merge of sister lineages X and $ABCD$ is rejected						
X-$ABCD$	0.879	0.388	rejected			
Final model:	two species: X, $ABCD$			five species: X, A, B, C, D		
Using cutoff: $gdi < 0.7$						
Iteration 1: merge of sister lineages X and A is accepted						
X-A	0.876	0.433	**accepted**	0.861	0.428	**accepted**
A-B	0.078	0.028	rejected	0.322	0.284	rejected
A-C	0.126	0.075	rejected	0.399	0.365	rejected
B-C	0.052	0.052	rejected	0.351	0.350	rejected
A-D	0.153	0.159	rejected	0.434	0.439	rejected
B-D	0.082	0.138	rejected	0.387	0.424	rejected
C-D	0.031	0.090	rejected	0.354	0.392	rejected
Iteration 2: merge of sister lineages XA and B is accepted						
XA-B	0.132	0.237	**accepted**	0.357	0.433	**accepted**
XA-C	0.150	0.214	rejected	0.405	0.450	rejected
B-C	0.085	0.039	rejected	0.375	0.344	rejected
XA-D	0.159	0.270	rejected	0.438	0.512	rejected
B-D	0.121	0.127	rejected	0.413	0.417	rejected
C-D	0.030	0.081	rejected	0.353	0.386	rejected
Iteration 3: merge of sister lineages XAB and C is accepted						
XAB-C	0.048	0.142	**accepted**	0.292	0.362	**accepted**
XAB-D	0.064	0.214	rejected	0.374	0.475	rejected
C-D	0.036	0.093	rejected	0.356	0.394	rejected
Iteration 4: merge of sister lineages $XABC$ and D is accepted						
$XABC$-D	0.024	0.169	**accepted**	0.317	0.418	**accepted**
Final model:	one species: $XABCD$			one species: $XABCD$		

Note.— gdi values are calculated under the MSC-M model by simulating gene trees using posterior means of parameters (which are very similar to the posterior means of gdi as the dataset is large). The MSC-M model of Fig. 4a is used as the guide tree (initial delimitation).