

Appendix A

In an attempt to verify that we get the same results with SimBit as with other simulation software, we repeated the simulations of Zeng and Corcoran (2015, their Figure 1) with SimBit, SLiM (Haller & Messer, 2017) and Nemo (Guillaume & Rougemont, 2006).

Figure A1 shows the CPU time for the simulations which results are displayed on the right graph. The left graph serves as a justification for the need of writing a new software.

Figure A2 shows mean and 95% confidence interval for F_{ST} . The colors represent simulations from different software as well as different methods to compute F_{ST} . The top and bottom red lines the neutral expectation computed from $\frac{1}{1+4Nm\frac{d}{d-1}}$ and $\frac{1}{1+4Nm(\frac{d}{d-1})^2}$, respectively (Charlesworth, 1998), where d is the number of demes.

Figure A2 is split in two halves, separated by a thin black vertical line. The left half corresponds to the same conditions simulated by Zeng and Corcoran (2015). The genome consists of 13,000 loci. In the “neutral” treatment, all mutations are neutral, while in the “purifying selection” treatment, all mutations have a deleterious selection coefficient of $s=0.01$ in the heterozygote state; there are hence no neutral loci in the “purifying selection” treatment. All sites are completely linked and the mutation rate per site is 2×10^{-6} . The simulation starts with a single patch of 1000 individuals that after 10,000 generations split into two patches of 5000 individuals each with a very low migration rate of 5×10^{-5} . Simulations last for 80,000 generations after the split. The black lines are the results from Zeng and Corcoran (2015) measured from their figure 1. F_{ST} is computed from allelic states for SimBit, SLiM and Nemo. F_{ST} is also computed from the coalescent tree from SLiM simulations.

Note that the Zeng and Corcoran (2015) neutral result is obtained from their analytical expectation (hence the perfect match with the top red line), while the result with selection is obtained from simulation and by computing F_{ST} from coalescent times. All three software packages (SimBit, SLiM and Nemo) seem to indicate that Zeng and Corcoran (2015) have used the wrong neutral expectation. For simulations of the loci under selection, all software agree that computing F_{ST} from allelic states show that loci under selection have lower F_{ST} than the neutral expectation. Computing F_{ST} from the coalescent tree, however, leads BGS to increase F_{ST} relative to the case without BGS, in this case with no recombination over a large genomic region and low migration. Zeng and Corcoran (2015) computed F_{ST} from the coalescent tree, hence the match between “SLiM coalescence” (in red) and the black line for the treatment with selection.

Note that computing F_{ST} from a coalescent tree is only feasible in theoretical settings (or in rare cases where we have access to a complete pedigree). In empirical studies, F_{ST} is always computed from allelic states.

On the right side of Figure A2, we show the results of further simulations. The goal here was to investigate the origin for the discrepancy between the coalescence and allelic state definitions of F_{ST} . We ran the same simulations but with twice as many loci, with the additional loci all being selectively neutral. In the treatment with selection, selected and neutral sites alternate. Again, all sites are completely linked. Because these simulations are longer, we only performed them in SimBit.

As expected, for the neutral treatment the mean F_{ST} is similar to the mean F_{ST} from runs with half as many loci. For the treatment with alternation of selected and neutral sites, we computed F_{ST} on neutral sites only, on selected sites only and on all sites. The selected loci show a very low F_{ST} as in the previous simulations. However, the neutral loci show a high F_{ST} that is statistically indistinguishable from F_{ST} computed from coalescence trees. F_{ST} for all loci is very similar to F_{ST} with for the neutral sites only, because the selected sites are associated with a much lower heterozygosity and are therefore down-weighted in the averaging (as per Weir and Cockerham 1984).

Tool	CPU time [hours]
Nemo	~16.5
SLiM	~8.8
SimBit	~1.2

Figure 1 is a dot plot showing the fixation probability (F_{ST}) for different software packages across four scenarios. The y-axis represents F_{ST} from 0.0 to 0.8. The x-axis categories are: 13k loci - neutral, 13k loci - negative selection, 26k loci - neutral, and 26k loci - neg. selected & neutral. The legend identifies six software packages: Nemo (green), SLiM by state (blue), SLiM coalescence (light blue), SimBit both sel. & neutral loci (orange), SimBit neutral loci (yellow), and SimBit sel. loci (red). Horizontal lines indicate theoretical values: 0.5 for neutral and 0.25 for negative selection. A vertical line separates the 13k and 26k loci groups.

Scenario	Nemo	SLiM by state	SLiM coalescence	SimBit both sel. & neutral loci	SimBit neutral loci	SimBit sel. loci
13k loci - neutral	~0.25	~0.30	~0.35	~0.35	~0.25	-
13k loci - negative selection	~0.05	~0.02	~0.65	-	-	-
26k loci - neutral	-	-	-	-	~0.35	-
26k loci - neg. selected & neutral	-	-	-	~0.70	~0.70	~0.05