Supplement material of

Assimilating ESA-CCI Land Surface Temperature into the ORCHIDEE Land Surface Model: Insights from a multi-site study across Europe

Table S1. DA experiments performed and ORCHIDEE variables optimized.

| Experiment name	Selected observational constraint
LST13	LST at 13:00 local time (12:00 UTC)
Tmin	Minimum daily LST over 3-hourly interval
Tmax	Maximum daily LST over 3-hourly interval
Ampl	Daily amplitude LST over 3-hourly interval
slope13	Temporal gradient between 10:00 and 13:00 LT
slope19	Temporal gradient between 16:00 and 19:00 LT
LST13+slope13	LST13 + slope13
LST13+slope19	LST13 + slope19
LST13+slope13+slope19	LST13 + slope13 + slope19
LST13+slope13+slope19+Ampl	LST13+slope13+slope19+Ampl
LST13+slope13+slope19+Ampl+Tmax	LST13+slope13+slope19+Ampl+Tmax
3h-LST	3-hourly LST series
3h-LST+Tmin	3h-LST + Tmin
3h-LST+Tmax	3h-LST + Tmax
3h-LST+Ampl	3h-LST + Ampl
3h-LST+Ampl+Tmax	3h-LST + Ampl + Tmax
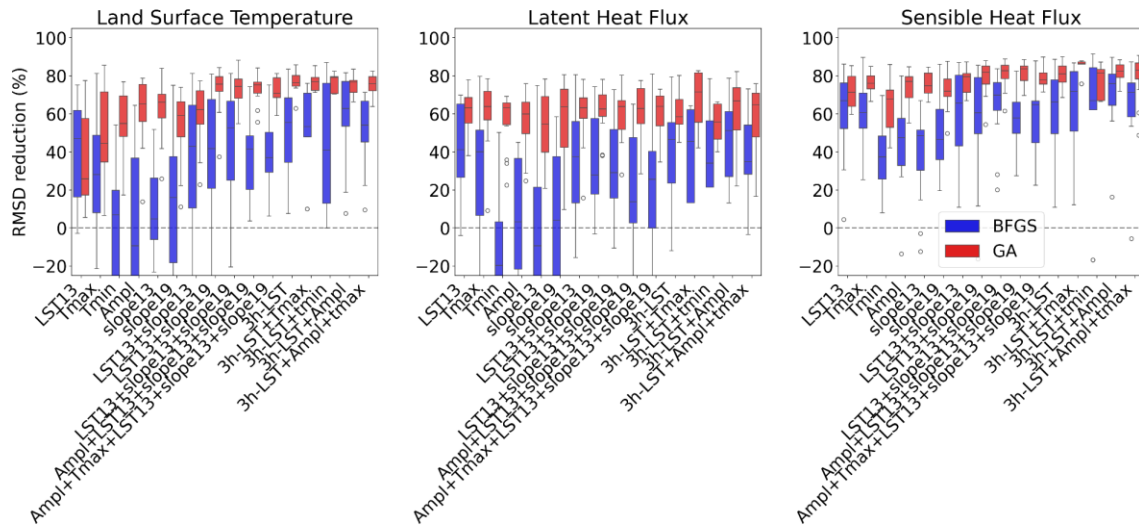
Figure S1. Boxplots obtained within 16 optimization tests with random first-guess parameter values for each DA experiment over the selected site in Spain (ES-Abr) comparing the performances between the gradient-based (in blue) and genetic (in red) methods in terms of model–data RMSD reduction (%) obtained for 30-min LST, LE and H. The x-axis indicates the DA experiment assimilating different observational constraints detailed in Table S1.
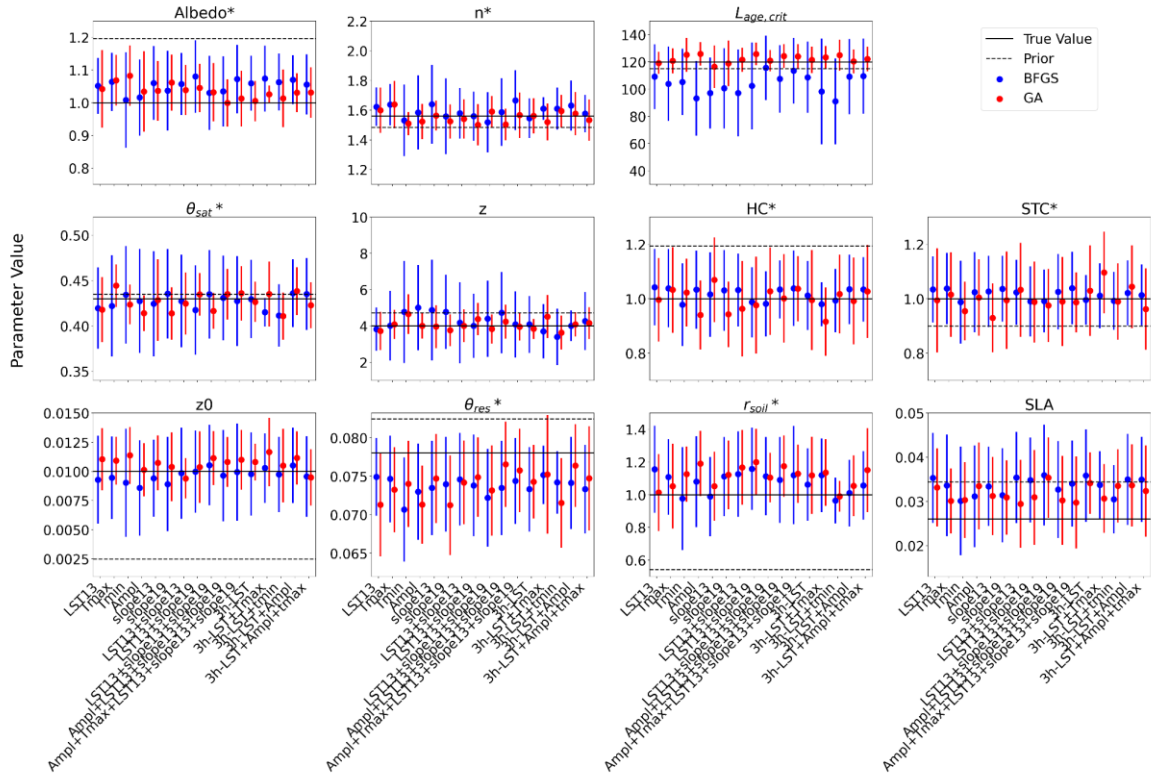
Figure S2. Parameter estimates for each DA experiment over the selected site in Spain (ES-Abr) comparing the 11 optimized parameters between the gradient-based (in blue) and genetic (in red) methods. Parameter estimates are represented by the mean and standard deviation across 16 optimization tests with random first-guess parameter values. The x-axis indicates the experiment assimilating 3-hourly LST pseudo-observations and the derived characteristics of the diurnal cycle. The 'true' parameter (default ORCHIDEE value) and prior values (defined randomly) are represented by the solid and dashed horizontal lines, respectively.
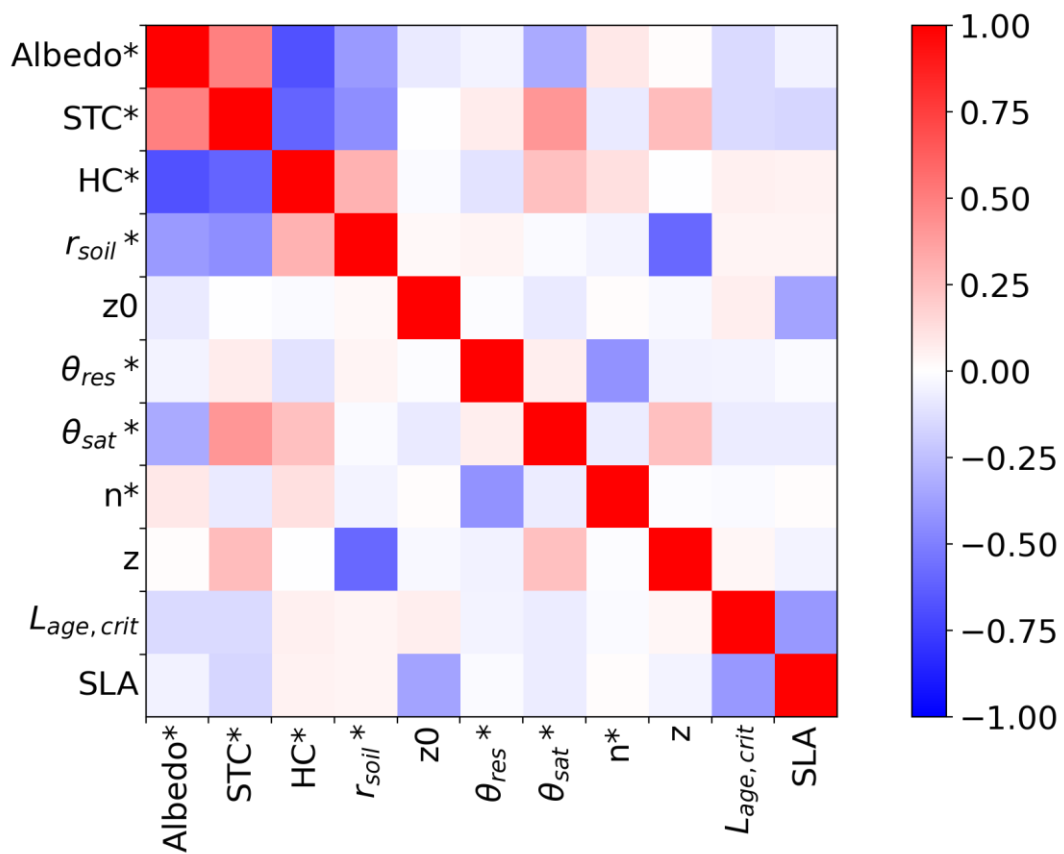
Figure S3. Covariance matrix of posterior parameter estimates assimilating the full 3-hourly LST series alone (3h-LST DA experiment) over the selected site in Spain (ES-Abr).
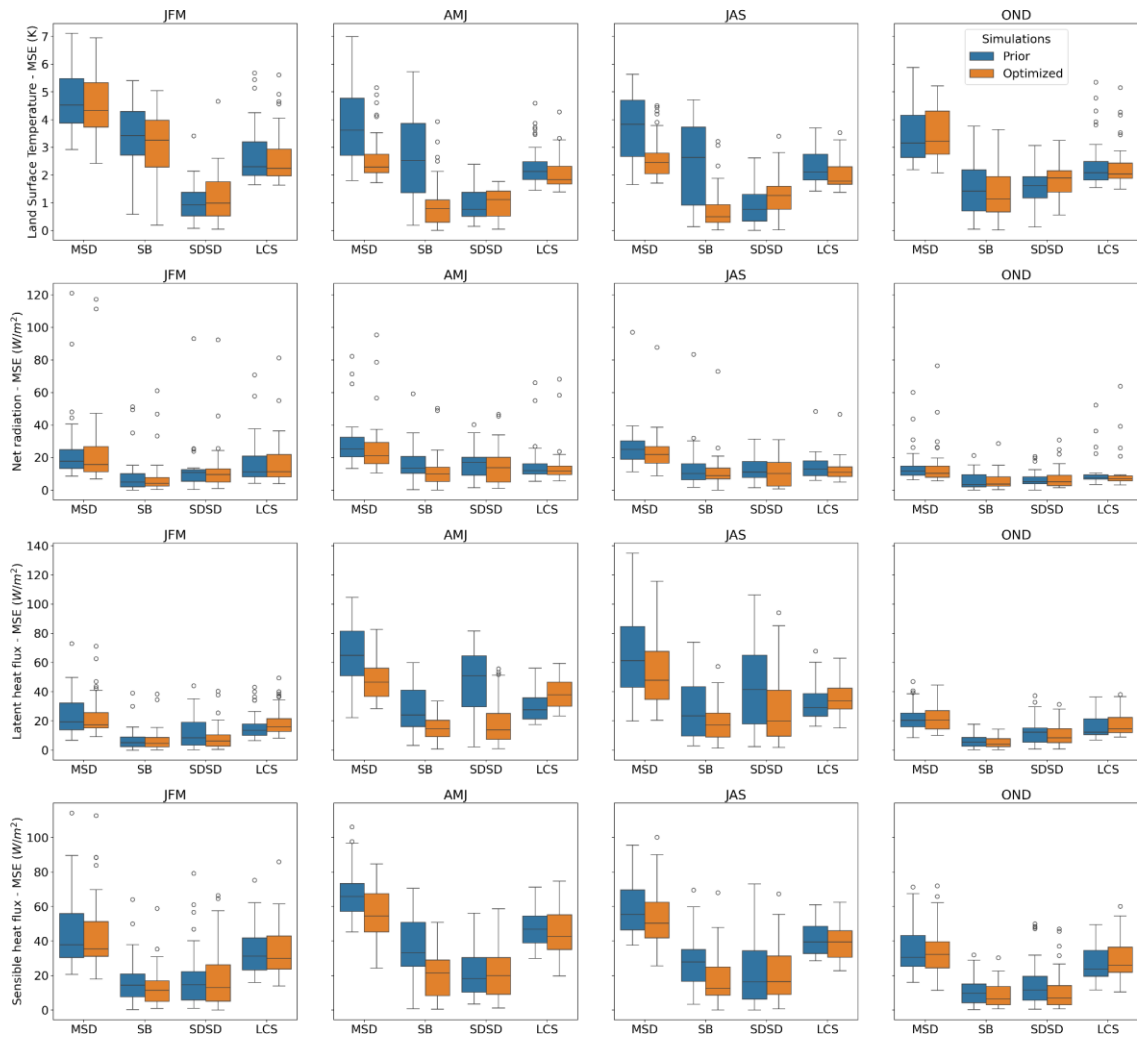
Figure S4. Boxplots showing the decomposition of MSE per season in terms of bias (SB), difference of standard deviations (SDSD) and lack of correlation (LCS) between the model and observations for half-hourly LST, Rn, LE and H across sites in 2018.