Gaussian process regression-based Bayesian optimisation (G-BO) of model parameters – a WRF model case study of southeast Australia heat extremes

*P. Jyoteeshkumar Reddy[1, *], Sandeep Chinta[2], Harish Baki[3], Richard Matear[1], John Taylor[4, 5]*

[1] Commonwealth Scientific and Industrial Research Organisation Environment, Hobart, TAS, Australia

[2] Center for Global Change Science, Massachusetts Institute of Technology, Cambridge, MA, USA

[3] Faculty of Civil Engineering and Geosciences, TU Delft, Delft, The Netherlands

[4] Commonwealth Scientific and Industrial Research Organisation Data61, Canberra, ACT, Australia

[5] Australian National University, Canberra, ACT, Australia

[*] Corresponding author: P. Jyoteeshkumar Reddy (jyoteesh.papari@csiro.au)

Supplementary material

Contents

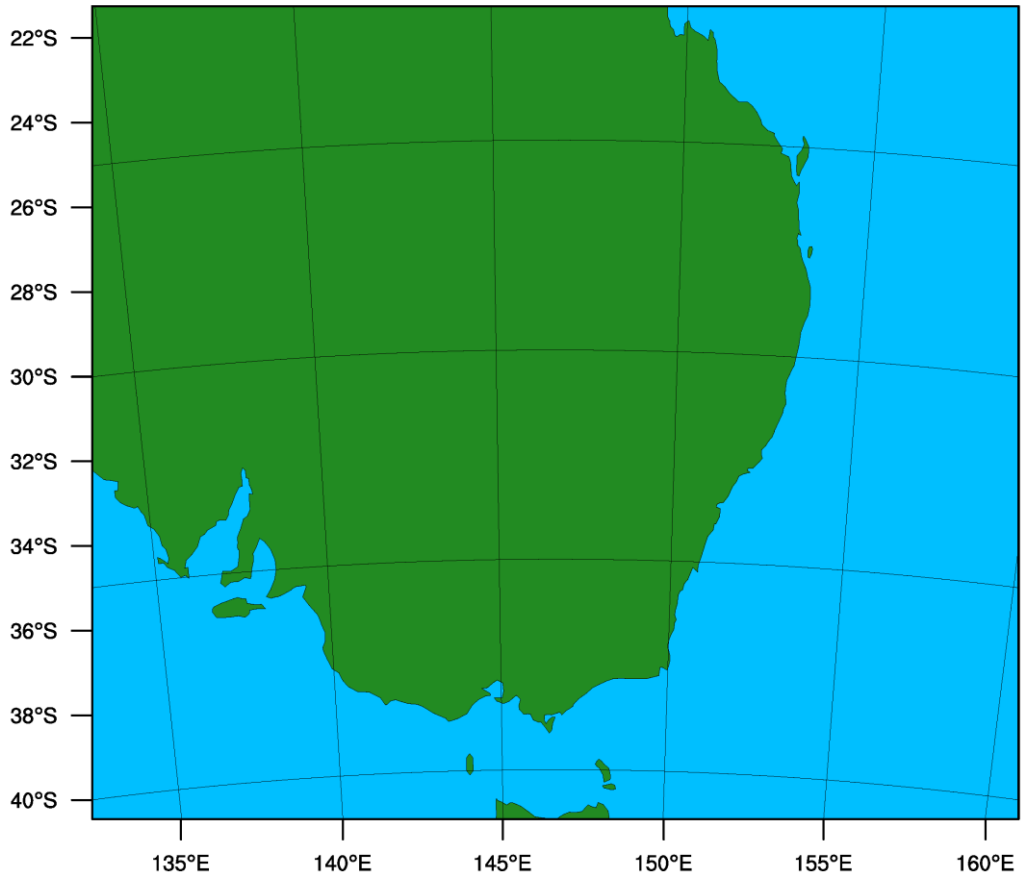

Fig. S1 *Domain considered for the WRF model simulation.*

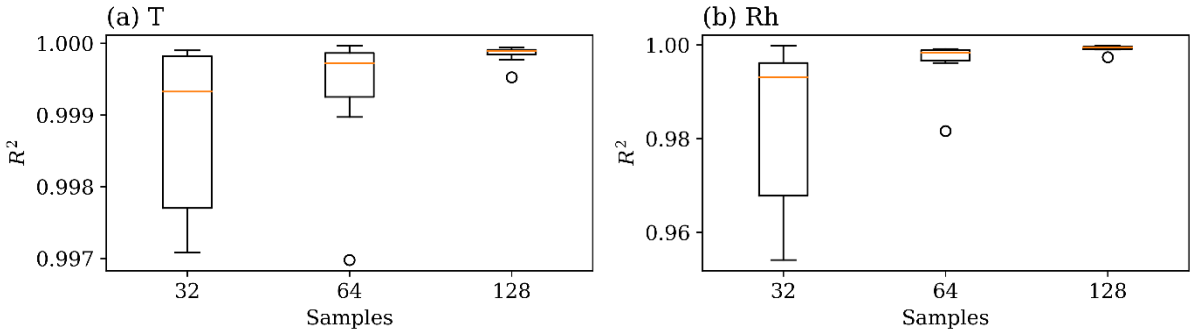

Fig. S2 *Boxplots of goodness of fit (R^2) values of K-fold cross-validation (K=8) of the GPR surrogate model trained with different sample sizes of 32, 64, and 128 for hourly temperature (T) (a) and relative humidity (Rh) (b) of the combined data of both considered events (2009 and 2019). Box represents the lower and upper ends of the interquartile (25^{th} - 75^{th}) range. The whiskers extend to 1.5 times the respective interquartile range. The lines inside the boxes indicate the median and the empty circles are the outliers.*

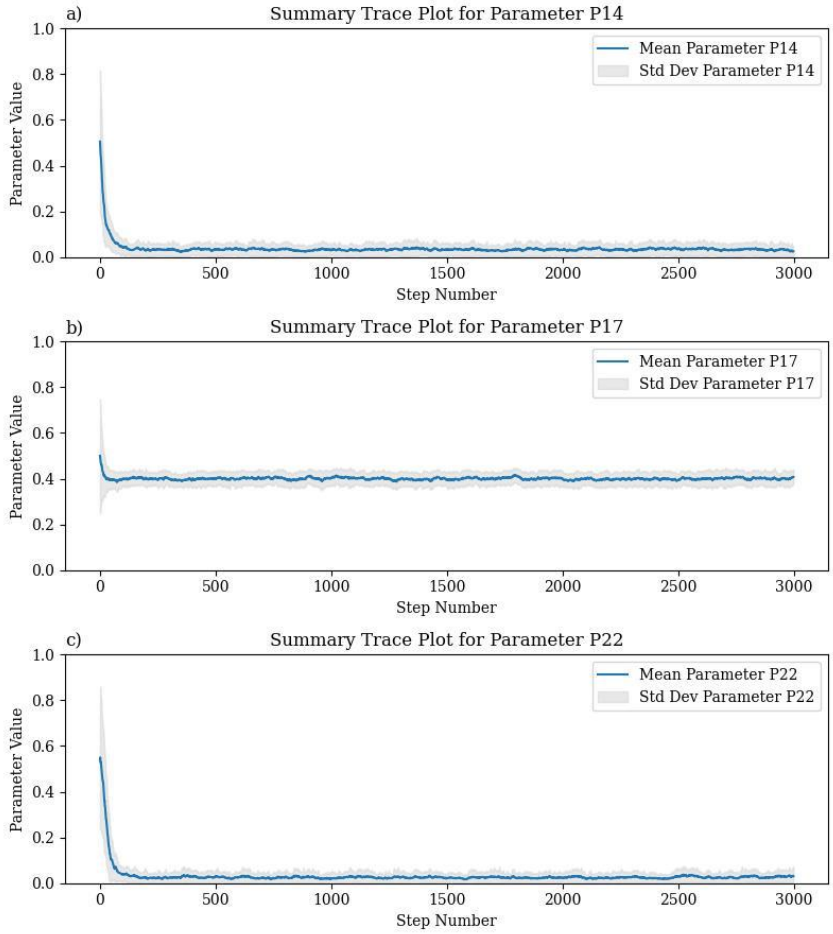

Fig. S3 *Convergence trace plots of 50 Markov Chain Monte Carlo (MCMC) sampling chains for the three parameters: a) P14, b) P17, and c) P22. The chains are run for 3000 steps to ensure convergence, while the first 1000 steps are discarded as burn-in. The shaded area represents standard deviations of the 50 chains while the blue line represents the means of the chains.*

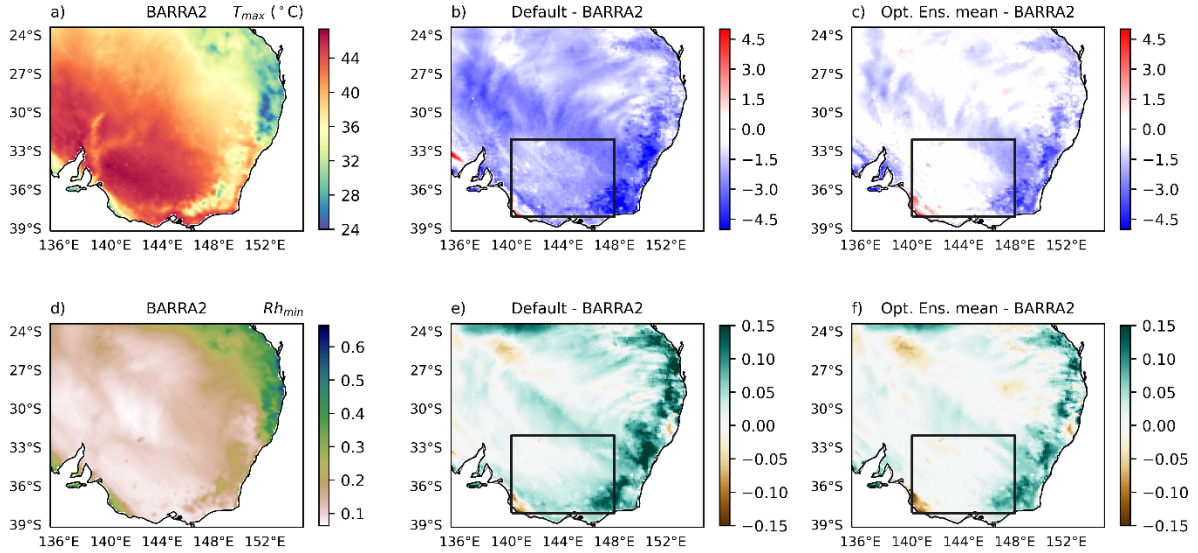

Fig. S4 *Spatial plot of daily maximum temperature (T_{max}; °C) (a) and daily minimum relative humidity (Rh_{min}) (d) during the extremely hot day of the 2009 event (i.e., 07th Feb 2009) using the BARRA2 data. Comparison of the WRF default parameters run (default) and optimised ensemble mean (of randomly drawn ten parameter combinations from the optimal posterior distribution of both T and Rh combined) parameters run (Opt. Ens. mean) with respect to BARRA2 data for the considered meteorological variables. The mean bias of T_{max} (b-c) and Rh_{min} (e-f) between default and Opt. Ens. mean runs with respect to BARRA2. The black box represents the extremely hot region with temperature greater than approximately 42 °C.*

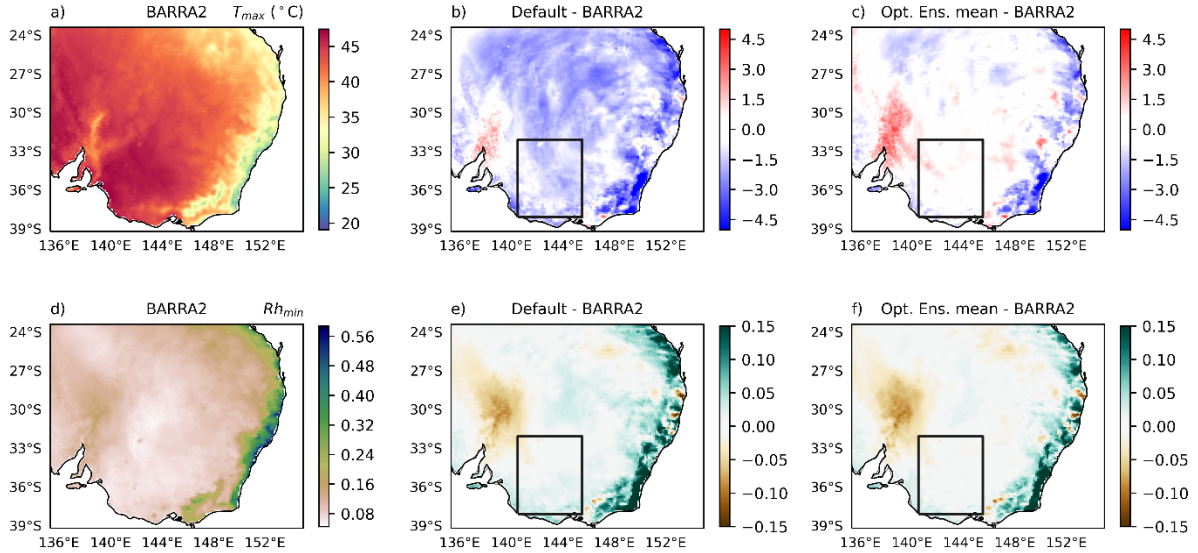

Fig. S5 *Spatial plot of daily maximum temperature (T_{max}; °C) (a) and daily minimum relative humidity (Rh_{min}) (d) during the extremely hot day of the 2019 event (i.e., 20th Dec 2019) using the BARRA2 data. Comparison of the WRF default parameters run (default) and optimised ensemble mean (of randomly drawn ten parameter combinations from the optimal posterior distribution of both T and Rh combined) parameters run (Opt. Ens. mean) with respect to BARRA2 data for the considered meteorological variables. The mean bias of T_{max} (b-c) and Rh_{min} (e-f) between default and Opt. Ens.*

mean runs with respect to BARRA2. The black box represents the extremely hot region with temperature greater than approximately 42 °C.

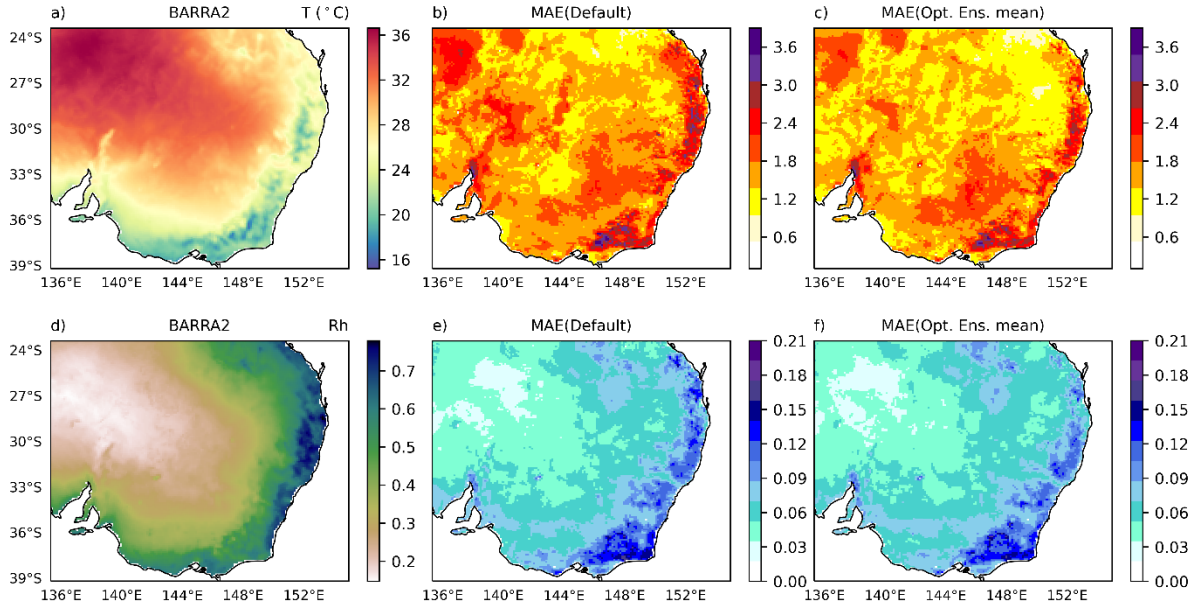

Fig. S6 *Spatial plot of average daily maximum temperature (T_{max}; °C) (a) and daily minimum relative humidity (Rh_{min}) (d) during all days of 2013 event using the BARRA2 data. MAE of the WRF default parameters run (default) and optimised ensemble mean (of randomly drawn 10 parameter combinations from the optimal posterior distribution of both T and Rh combined) parameters run (Opt. Ens. mean) with respect to BARRA2 data for the considered meteorological variables. The MAE of T (b-c) and Rh (e-f) for default and Opt. Ens. mean runs with respect to BARRA2.*

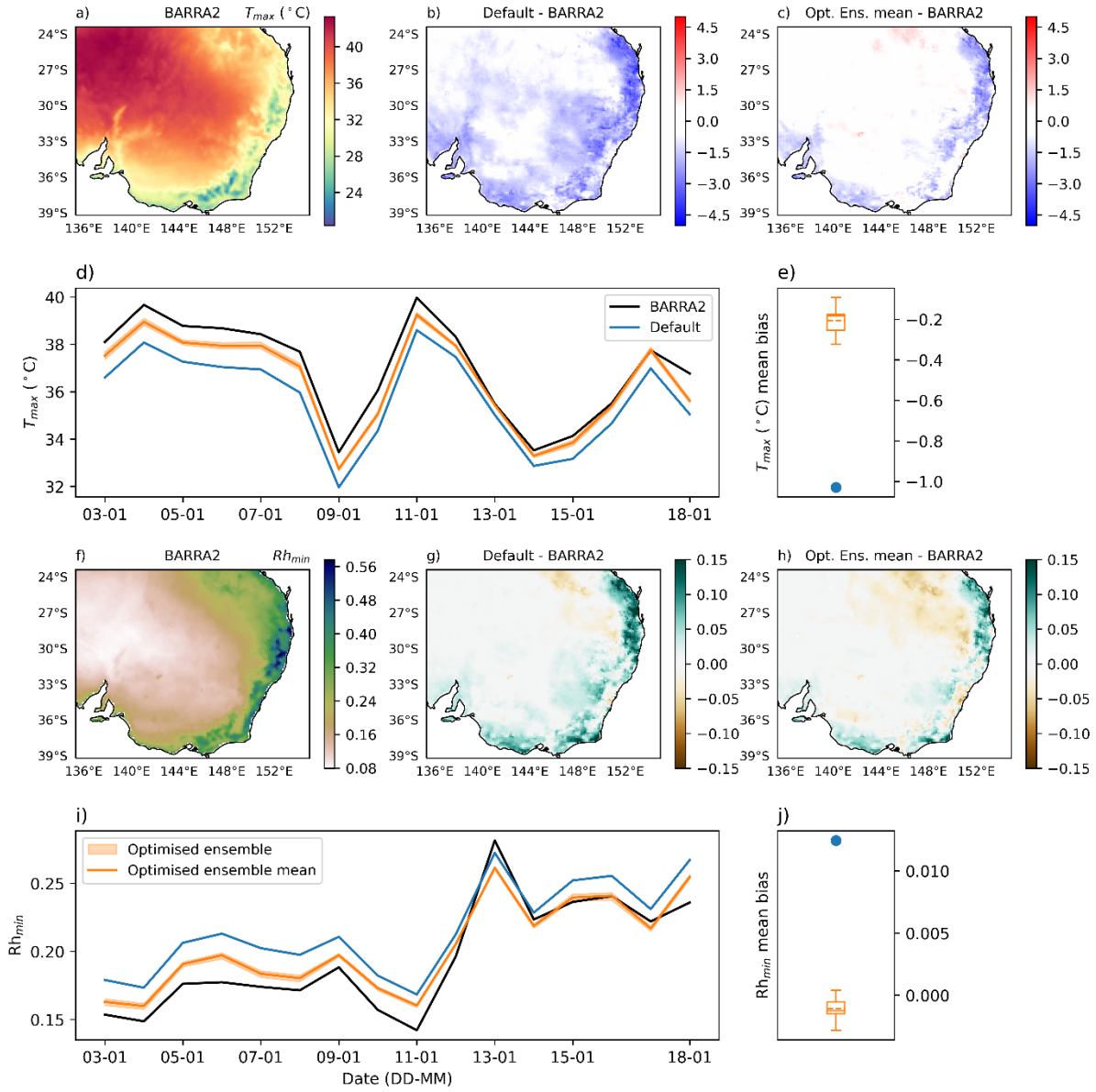

Fig. S7 *Spatial plot of average daily maximum temperature (T_{max}; °C) (a) and daily minimum relative humidity (Rh_{min}) (f) during all days of 2013 event using the BARRA2 data. Comparison of the WRF default parameters run (default) and optimised ensemble mean (Opt. Ens. mean) (of randomly drawn ten parameter combinations from the optimal posterior distribution of both T and Rh combined) with respect to BARRA2 data for the considered meteorological variables. The mean bias of T_{max} (b-c) and Rh_{min} (g-h) between default and Opt. Ens. mean runs with respect to BARRA2. Domain average temporal comparison of daily maximum temperature (T_{max}; °C) (d), and daily minimum relative humidity (Rh_{min}) (i) of BARRA2 (black line), default (blue line), optimised ensemble (orange shading), and optimised ensemble mean (orange line) during all days of 2009 and 2019 events (events are separated with dotted vertical lines). Box plots of domain average bias of optimised ensemble with respect to BARRA2 and the default domain average bias value is shown as a blue dot (T_{max}(e) and Rh_{min}(j)).*

Table S1. *Description of three sensitive parameters, their respective default values and range.*

Sensitive parameter	Description	Default	Range
P14	Scattering tuning parameter (m^2 kg^{-1})	1×10^{-5}	0.5×10^{-5} – 2.0×10^{-5}
P17	Multiplier for the saturated soil water content	1.0	0.5 – 2.0
P22	Profile shape exponent for calculating the momentum diffusivity coefficient	2.0	1.0 - 3.0

Table S2. *The 10 randomly sampled parameter sets (of sensitive parameters) from the G-BO calibrated posterior distribution.*

Calibrated ensemble parameter sets	P14 (Default: 1×10^{-5})	P17 (Default: 1.0)	P22 (Default: 2.0)
1	0.504×10^{-5}	1.131	1.064
2	0.508×10^{-5}	1.185	1.018
3	0.570×10^{-5}	1.039	1.049
4	0.508×10^{-5}	1.086	1.047
5	0.603×10^{-5}	1.045	1.054
6	0.529×10^{-5}	1.095	1.001
7	0.542×10^{-5}	1.166	1.145
8	0.527×10^{-5}	1.110	1.079
9	0.573×10^{-5}	1.107	1.000
10	0.551×10^{-5}	1.035	1.011