

Supplemental for The Calibrated Rapid Assimilation and Forecasting Technique (CRAFT) for Earth system and ecological modeling using machine learning and Bayesian estimation

Geoscientific model development

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Table S1: The FATES-HYDRO parameters tested from Xu et al., 2022. Not that Organ=All denote four tissues being parameterized (Leaf, Stem, Transfer Roots, Absorbing Roots), Organ=Whole Tree denotes a single parameter, and other combination is the number of organs listed.

Parameter (abbreviation)	Organ	Unit	Range
Saturated Water Content	All	cm ³ cm ⁻³	Leaf: Beta (9.69, 6.20) Stem, TRoot, ARoot Beta (22.98, 5.29)
Osmotic potential at full turgor	All	MPa	Leaf: G [9.8,6.26], Stem, TRoot, ARoot: LN [0.32,0.39]
Bulk elastic modulus	All	MPa	Leaf: G (4.07, 4.12) Stem, TRoot and ARoot: G [3.57, 3.84]
Residual water fraction	All	unitless	Leaf: B [2.14,4.10] Stem, TRoot and ARoot: B [2.71, 4.53]
Fraction of water in capillary reserve	All	unitless	U [0.1, 0.7]
Water potential at 50% loss of conductivity	Stem and Roots	MPa	Stem, TRoot and ARoot: G [2.07, 1.18]
Vulnerability curve shape	Stem and Roots	unitless	Stem, TRoot and ARoot: LN [0.82, 0.66].
Xylem conductivity per unit sapwood area	Whole plant	kg m ⁻¹ s ⁻¹ MPa ⁻¹	G [1.41,2.37]
Xylem taper exponent for sapwood	Whole plant	unitless	U (0.08, 0.5)
Leaf area to sapwood area ratio	Whole plant	unitless	LN (-0.48, 0.77)
specific root length	Whole plant	m g ⁻¹	G [1.70,35.31]
absorbing root radius	Whole plant	mm	LN [1.91,0.79]
fraction of total tree resistance that is aboveground (rfrac_stem)	Whole plant	Unitless	U [0.1,0.7]
root-soil interface conductivity per unit surface area (Kr1)	Whole plant	kg m ⁻¹ s ⁻¹ MPa ⁻¹	G [1.41,2.37]
maximum root water loss rate (Kr2)	Whole plant	kg m ⁻¹ s ⁻¹ MPa ⁻¹	LN [-6.80, 0.92]
Specific leaf area at top of canopy (SLA)	Whole plant	m ² gC ⁻¹	U [0.003-0.046]

maximum carboxylation rate of Rub. at 25C, canopy top (Vcmax25)	Whole plant	$\mu\text{mol CO}_2$ $\text{m}^{-2}\text{s}^{-1}$	U [30,100]
mean density of woody tissue in plant (wood_density)	Whole plant	g cm^{-3}	U [0.2,0.8]
stomatal slope parameter, as per Ball-Berry (ball_berry_slope)	Whole plant	unitless	U [4,16]

Table S2: All Shapley importance values from FATES-HYDRO variables for FATES GPP outputs

FATES Hydro Parameter	Shapley Importance Value
sla_top	0.434526
Vcmax25	0.299593
ball_berry_slope	0.110143
month	0.023381
p_taper	0.023181
p50_gs	0.01836
kmax_node_stem	0.01596
year	0.010746
rootpara_b	0.005681
latosa	0.004968
p50_node_stem	0.003127
thetas_node_aroot	0.002472
epsil_node_stem	0.002451
rs2	0.002414
srl	0.002369
bbopt_c3	0.002351
pitlp_node_leaf	0.002144
pitlp_node_aroot	0.002104
rsurf2	0.002071
rsurf1	0.002044
p50_node_troot	0.001902
epsil_node_aroot	0.001837
resid_node_leaf	0.001825
avuln_node_stem	0.001691
avuln_node_troot	0.001526
rfrac_stem	0.001523
resid_node_stem	0.001492
resid_node_troot	0.001445
epsil_node_leaf	0.001443
thetas_node_troot	0.001414
resid_node_aroot	0.001282
thetas_node_stem	0.001214
fcap_node_stem	0.001171
pitlp_node_troot	0.001135
thetas_node_leaf	0.001132
avuln_node_aroot	0.001092
pitlp_node_stem	0.001051
rootshoot	0.001043
wood_den	0.00094
p50_node_aroot	0.000889
fcap_node_troot	0.000783
rootpara_a	0.000782
epsil_node_troot	0.000689
hf_flg_threshold	0.000613

Table S3: All Shapley importance values from FATES-HYDRO variables for QRUNOFF outputs

FATES Hydro Parameter	Shapley Importance Value
month	0.469669
year	0.312945
p_taper	0.081732
kmax_node_stem	0.025466
latosa	0.016723
rfrac_stem	0.016288
sla_top	0.01174
rs2	0.011399
ball_berry_slope	0.006156
srl	0.004753
rootshoot	0.003068
Vcmax25	0.002774
rootpara_a	0.001497
pitlp_node_leaf	0.001315
bbopt_c3	0.001259
thetas_node_aroot	0.001256
thetas_node_stem	0.001247
wood_den	0.001236
fcap_node_troot	0.001232
hf_flg_threshold	0.001196
resid_node_troot	0.001193
epsil_node_aroot	0.001181
resid_node_stem	0.001174
fcap_node_stem	0.001166
avuln_node_aroot	0.00116
avuln_node_stem	0.001159
pitlp_node_stem	0.001153
avuln_node_troot	0.001148
p50_node_aroot	0.00114
pitlp_node_aroot	0.001138
rsurf1	0.001135
epsil_node_stem	0.001132
p50_node_stem	0.001124
rsurf2	0.001121
thetas_node_leaf	0.001121
resid_node_aroot	0.001118
p50_gs	0.00111
resid_node_leaf	0.001109
rootpara_b	0.001108
p50_node_troot	0.001101
pitlp_node_troot	0.00108
epsil_node_leaf	0.001079
thetas_node_troot	0.001056
epsil_node_troot	0.001043

Table S4: All Shapley importance values from FATES-HYDRO variables for H2OSOI1 outputs

FATES Hydro Parameter	Shapley Importance Value
month	0.629393
year	0.124244
sla_top	0.107962
p_taper	0.043007
kmax_node_stem	0.01805
latosa	0.014695
rfrac_stem	0.012816
rs2	0.006271
srl	0.003294
ball_berry_slope	0.002075
rootshoot	0.001897
Vcmax25	0.001824
resid_node_stem	0.001386
pitlp_node_troot	0.001378
thetas_node_troot	0.001315
wood_den	0.001277
rsurf1	0.001273
pitlp_node_aroot	0.001269
thetas_node_aroot	0.001207
epsil_node_aroot	0.001155
p50_node_aroot	0.001135
fcap_node_troot	0.001129
p50_gs	0.001112
resid_node_troot	0.001112
hf_flg_threshold	0.00111
p50_node_stem	0.0011
avuln_node_aroot	0.001096
thetas_node_stem	0.001087
pitlp_node_stem	0.001071
fcap_node_stem	0.00105
resid_node_aroot	0.001032
avuln_node_stem	0.001019
epsil_node_stem	0.000993
thetas_node_leaf	0.000991
bbopt_c3	0.000959
avuln_node_troot	0.000959
epsil_node_leaf	0.000951
p50_node_troot	0.000943
rootpara_b	0.000939
rootpara_a	0.000922
rsurf2	0.000904
resid_node_leaf	0.000887
pitlp_node_leaf	0.000868
epsil_node_troot	0.000842

Table S5: All Shapley importance values from FATES-HYDRO variables for minimum Leaf water potential outputs

FATES Hydro Parameter	Shapley Importance Value
p50_node_aroot	0.22339
rs2	0.116195
p_taper	0.106388
latosa	0.04018
ball_berry_slope	0.044518
kmax_node_stem	0.03638
srl	0.035862
rfrac_stem	0.035598
rootshoot	0.034182
bbopt_c3	0.032491
rootpara_b	0.024127
epsil_node_stem	0.021028
p50_gs	0.018077
Vcmax25	0.014486
epsil_node_leaf	0.012171
avuln_node_troot	0.012003
hf_flg_threshold	0.010228
pitlp_node_troot	0.009912
resid_node_stem	0.009548
thetas_node_troot	0.009415
fcap_node_stem	0.009292
fcap_node_troot	0.00865
Year	0.007823
epsil_node_troot	0.007607
avuln_node_stem	0.007301
wood_den	0.007291
thetas_node_stem	0.007035

avuln_node_aroot	0.00691
rsurf2	0.006693
resid_node_troot	0.006564
p50_node_aroot	0.006551
resid_node_leaf	0.006396
p50_node_stem	0.005806
DOY	0.00579
pitlp_node_leaf	0.005694
rsurf1	0.005643
rootpara_a	0.005626
pitlp_node_aroot	0.00508
resid_node_aroot	0.004869
sla_top	0.003606
pitlp_node_stem	0.003549
thetas_node_leaf	0.00348
thetas_node_aroot	0.003397
epsil_node_aroot	0.00317

Table S6: All Shapley importance values from FATES-HYDRO variables for evapotranspiration potential outputs.

FATES Hydro Parameter	Shapley Importance Value
ball_berry_slope	0.400983
month	0.311402
Vcmax25	0.078631
year	0.065808
sla_top	0.052088
p_taper	0.01383
p50_gs	0.011702
bbopt_c3	0.011176
kmax_node_stem	0.007943
latosa	0.003436
p50_node_troot	0.003296
rs2	0.002629
wood_den	0.002088
p50_node_stem	0.001868
rfrac_stem	0.001767
pitlp_node_leaf	0.001657
rootpara_b	0.001592
resid_node_aroot	0.00141
fcap_node_troot	0.00137
thetas_node_stem	0.001347
rootshoot	0.001282
epsil_node_stem	0.001234
resid_node_leaf	0.001225
p50_node_aroot	0.001217
hf_flg_threshold	0.001137
fcap_node_stem	0.001129

thetas_node_leaf	0.001113
avuln_node_stem	0.001093
pitlp_node_stem	0.001058
epsil_node_aroot	0.001053
rootpara_a	0.001023
srl	0.00101
rsurf1	0.000955
pitlp_node_troot	0.000939
resid_node_stem	0.000909
avuln_node_aroot	0.000889
rsurf2	0.000881
avuln_node_troot	0.00088
pitlp_node_aroot	0.000866
thetas_node_aroot	0.000866
thetas_node_troot	0.00083
epsil_node_troot	0.00082
epsil_node_leaf	0.000812
resid_node_troot	0.000755

Table S7: Comparison of the derivative relationship for change in input and out variables of FATES, and an emulator for all variables selected for the wet season

Output Variable	Input Variable	p-value	Significance
Wet Season GPP	p_taper	1	NA
Wet Season GPP	ball berry slope	1	NA
Wet Season GPP	Vcmax25	1	NA
Wet Season GPP	sla_top	1	NA
Wet Season GPP	P50_node_Aroot	1	NA
Wet Season GPP	rs2	1	NA
Wet Season GPP	year	0.82	NA
Wet Season GPP	month	1	NA
Wet Season ET	p_taper	1	NA
Wet Season ET	ball berry slope	1	NA
Wet Season ET	Vcmax25	1	NA
Wet Season ET	sla_top	1	NA
Wet Season ET	P50_node_Aroot	1	NA
Wet Season ET	rs2	0.91	NA
Wet Season ET	year	0.97	NA
Wet Season ET	month	1	NA
Wet Season RO	p_taper	1	NA
Wet Season RO	ball berry slope	0.37	NA
Wet Season RO	Vcmax25	1	NA
Wet Season RO	sla_top	1	NA
Wet Season RO	P50_node_Aroot	0.16	NA
Wet Season RO	rs2	0.99	NA
Wet Season RO	year	1	NA
Wet Season RO	month	1	NA
Wet Season H2O Soil 1	p_taper	1	NA
Wet Season H2O Soil 1	ball berry slope	0.05	<0.05
Wet Season H2O Soil 1	Vcmax25	0.97	NA
Wet Season H2O Soil 1	sla_top	1.0	NA
Wet Season H2O Soil 1	P50_node_Aroot	0.15	NA
Wet Season H2O Soil 1	rs2	0.58	NA
Wet Season H2O Soil 1	year	0.47	NA
Wet Season H2O Soil 1	month	1	NA
Wet Season LWP_max	p_taper	1	NA
Wet Season LWP_max	ball berry slope	1	NA
Wet Season LWP_max	Vcmax25	1	NA
Wet Season LWP_max	sla_top	0.04	<0.05
Wet Season LWP_max	P50_node_Aroot	1	NA
Wet Season LWP_max	rs2	1	NA
Wet Season LWP_max	year	1	NA

Wet Season LWP_max	month	1	NA
Wet Season LWP_min	p_taper	1	NA
Wet Season LWP_min	ball berry slope	0.82	NA
Wet Season LWP_min	Vcmax25	1	NA
Wet Season LWP_min	sla_top	1	NA
Wet Season LWP_min	P50_node_Aroot	0.21	NA
Wet Season LWP_min	rs2	1	NA
Wet Season LWP_min	year	0.08	NA
Wet Season LWP_min	month	1	NA

Table S8: Comparison of the derivative relationship for change in input and out variables of FATES, and an emulator for all variables selected for the dry season

Output Var	Input Variable	p-value	Significance
Dry Season GPP	p_taper	1	NA
Dry Season GPP	ball berry slope	1	NA
Dry Season GPP	Vcmax25	1	NA
Dry Season GPP	sla_top	1	NA
Dry Season GPP	P50_node_Aroot	1	NA
Dry Season GPP	rs2	1	NA
Dry Season GPP	year	0.58	NA
Dry Season GPP	month	1	NA
Dry Season ET	p_taper	1	NA
Dry Season ET	ball berry slope	1	NA
Dry Season ET	Vcmax25	1	NA
Dry Season ET	sla_top	1	NA
Dry Season ET	P50_node_Aroot	1	NA
Dry Season ET	rs2	0.70	NA
Dry Season ET	year	0.02	< 0.05
Dry Season ET	month	1	NA
Dry Season RO	p_taper	1	NA
Dry Season RO	ball berry slope	0.58	NA
Dry Season RO	Vcmax25	0.99	NA
Dry Season RO	sla_top	1.0	NA
Dry Season RO	P50_node_Aroot	0.02	< 0.05
Dry Season RO	rs2	1	NA
Dry Season RO	year	1	NA
Dry Season RO	month	1	NA
Dry Season H20 Soil 1	p_taper	1	NA
Dry Season H20 Soil 1	ball berry slope	0.99	NA
Dry Season H20 Soil 1	Vcmax25	0.10	NA
Dry Season H20 Soil 1	sla_top	1.0	NA
Dry Season H20 Soil 1	P50_node_Aroot	0.58	NA
Dry Season H20 Soil 1	rs2	0.01	<0.05
Dry Season H20 Soil 1	year	0.99	NA
Dry Season H20 Soil 1	month	0.99	NA
Dry Season LWP_max	p_taper	1	NA
Dry Season LWP_max	ball berry slope	1	NA
Dry Season LWP_max	Vcmax25	1	NA
Dry Season LWP_max	sla_top	1	NA
Dry Season LWP_max	P50_node_Aroot	1	NA
Dry Season LWP_max	rs2	1	NA
Dry Season LWP_max	year	1	NA
Dry Season LWP_max	month	1	NA
Dry Season LWP_min	p_taper	1	NA

Dry Season LWP_min	ball berry slope	1	NA
Dry Season LWP_min	Vcmax25	1	NA
Dry Season LWP_min	sla_top	1	NA
Dry Season LWP_min	P50_node_Aroot	0.82	NA
Dry Season LWP_min	rs2	1	NA
Dry Season LWP_min	year	1	NA
Dry Season LWP_min	month	0.91	NA