Supporting Information

Article title: "Optimal stomatal behavior is better represented by penalizing dynamic and stochastic risk, not hydraulic damage"

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The following Supporting Information is available for this article:

- Fig. S1. Illustration of wavelet analysis of sunflecks.
- Fig. S2. Distributions of sunfleck strength vs canopy structure.
- Fig. S3. Measures of sunfleck strength vs minimum leaf water potential.
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- Fig. S5. Physiological kinetics for square-wave sunfleck.
- Fig. S6. Optimal ψ_{50risk} vs canopy structure.
- Fig. S7. Sample physiological dynamics during a single sunfleck.
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Figure S1. Illustration of wavelet analysis of sunflecks (details given in Methods S2). The product of each leaf's PPFD timecourse (a,b) and a wavelet representing an archetypal sunfleck (c,d) is computed (e,f), and the integral of the product ("power") is computed (h; shaded red areas in e,f). This is repeated with the wavelet centered at different times (h; e.g., at ~09:45 in a,c,e, and at ~10:15 in b,d,f), and the maximum power over the day is identified (purple symbol in h). This procedure is repeated for wavelengths of different durations (with the resulting power normalized by wavelet duration to give "intensity") (i), and the duration with maximum intensity is identified (green symbol in i). This is the "peak sunfleck" (in the example here, the peak sunfleck is ~75 min long and centered at ~10:15).



Figure S2. Distribution of peak sunfleck duration (a), intensity or power (b) and composite strength (c), computed by wavelet analysis, for four canopy types (HO: homogeneous, HE: heterogeneous; S: spherical leaf angle distribution, P: planophile leaf angle distribution, E: erectophile leaf angle distribution).



Figure S3. The influence of sunfleck features on daily minimum leaf water potential in simulated leaves exposed to periodic sunflecks of fixed duration (d, min) and intensity (power, p). Neither duration nor power by themselves predicts minimum ψ_{leaf} well; their product (bottom left) predicts ψ_{leaf} but with poor sensitivity. Because the effect of sunfleck duration saturates at around 30 min, differences in duration above that value have little predictive power. Capping d at 30 min (min{d,30}), multiplying it by power, and computing the logarithm of the result (bottom right) produces a measure of sunfleck intensity that predicts minimum ψ_{leaf} , and hence hydraulic risk, well.



Figure S4. The rate constant for photosynthetic induction (α_V) has negligible influence on the economic landscape of short-term hydraulic risk. (a) The stomatal strategy (as gauged by the parameter ψ_{50risk}) that maximizes aggregated carbon gain (**A**, mean daily carbon gain across all 10,000 simulated leaf patches) is unaffected by α_V ; the point of maximum **A** in each curve is shown with a black symbol. Dashed lines in (a) represent aggregated carbon gain from simulations in which hydraulic risk was omitted by setting ψ_{50leaf} and ψ_{50stem} to -100 MPa. (b) The relationship between stomatal strategy and the aggregated carbon cost of short-term hydraulic risk (C_{risk} , the decrease in **A** caused by hydraulic risk; i.e., the difference between dashed and solid lines in (a)) is also negligibly affected by α_V .



Figure S5. Illustration of the effect of kinetic parameters (α_p , the rate constant for active stomatal responses; and SWC, the leaf water content at saturation, which controls the time scale for effects of water loss on water potential) on kinetics of key physiological variables (a,b: stomatal conductance; c,d: leaf water potential; e,f: leaf temperature). At the time indicated by vertical dashed lines, PPFD was increased from 100 to 1600 µmol m⁻² s⁻¹.



Figure S6. Optimal ψ_{50risk} (defined here as the value that maximizes aggregated carbon gain over time and across leaf patches) for cohorts of leaf patches differing in mean PPFD (colors), and its relationship to peak sunfleck strength computed by wavelet analysis, is different in canopies with different leaf angle distributions (LADs). In (b-d), the results for the homogeneous canopy with spherical LAD are shown in the background, for reference, using shaded symbols connected by dashed lines.



Figure S7. A close-up view of the dynamics of factors driving changes in leaf physiology, including an increase in the percentage loss of leaf hydraulic conductivity, during a long sunfleck (between 9 and 11 am in the leaf shown in Fig **Error! Reference source not found.**b,d,f,h). (a) Leaf-to-air evaporative gradient (Δw), photosynthetic capacity (V_{m25}), transpiration rate (*E*) and percentage loss of leaf hydraulic conductivity (PLC) (the values shown for V_{m25} and *E* are divided by 4 and multiplied by 5, respectively, to enable display on a common y-axis). (b) Components of stomatal hydromechanics: guard cell turgor pressure (P_g), GC osmotic pressure (π_g), epidermal turgor pressure (P_e), and the quantity $P_g - mP_e$, to which stomatal conductance is proportional (m = 2 is the epidermal mechanical advantage). (c) Stem and leaf water potentials. (d) Stomatal conductance and its target value.







Figure S9. Results of parameter sensitivity analysis for plant-related parameters. Each parameter (symbol given above each panel; symbols are defined in Table **Error! Reference source not found.** of the main text) was set to 75, 99, 100, 101 or 125% of its default value, simulations were performed for 500 leaves at each value, and mean daily net assimilation rate (*A*) was calculated. Lines are 2nd order polynomial fits, colored by sensitivity coefficient (the slope of a linear regression of {mean daily *A* as a fraction of its default value} vs. {parameter value as a fraction of its default value}); sensitivity coefficients are also given in Fig S11.



Figure S10. As Fig S9, but for mean minimum daily leaf water potential ($\psi_{\text{leaf,min}}$); symbols are defined in Table **Error! Reference source not found.** of the main text.



(% change in variable per 1 % change in parameter)

Figure S11. Sensitivity coefficients (percent change in a variable resulting from a 1% change in a parameter) for the variables mean daily net assimilation rate (A, blue bars) and mean daily minimum leaf water potential ($\psi_{\text{leaf,min}}$, red bars) from the sensitivity analysis shown in Figs S9 and S10. Symbols are defined in Table **Error! Reference source not found.** of the main text.



Figure S12. Results of parameter sensitivity analysis for environmental parameters. As Figs S9 and S10, but for environmental parameters.



Figure S13. Effect of variation in the mechanical advantage of the epidermis (m) on mean daily net CO₂ assimilation rate (A) and mean daily minimum leaf water potential ($\psi_{\text{leaf,min}}$) for the same 500 leaves used for the parameter sensitivity analyses shown in Figs S9-S12.



Figure S14. Hydraulic penalty functions reported by Eller et al. (2020) for different plant functional types (PFTs, indicated by colors; BDT = broadleaf deciduous tree, BET-Te = broadleaf evergreen temperate tree, BET-Tr = broadleaf evergreen tropical tree, DSh = deciduous shrubs, ESh = evergreen shrubs, NDT = needleleaf deciduous tree, NET = needleleaf evergreen tree). *Solid lines*: penalty functions based on measured hydraulic vulnerability curve parameters gathered from the literature by Eller et al. (2020); *dashed lines*: penalty functions based on parameters calibrated to produce the best fit between observed gross primary productivity (GPP) and GPP predicted by JULES-SOX (the Joint UK Land Environment Simulator-stomatal optimization based on xylem hydraulics). JULES-SOX employs the hydraulic penalty model for stomatal conductance created by Eller et al. (2020). In most cases, the best-fit penalty functions differ greatly from the hydraulics-based penalty functions.

Methods S1. Photosynthesis model

We calculated net CO₂ assimilation rate (A) using the FvCB model (Farquhar *et al.*, 1980), assuming that photosynthesis can be limited either by RuBP carboxylation ($A = A_V$) or by RuBP regeneration ($A = A_J$):

$$A_V = V_m \frac{c_i - \Gamma^*}{c_i + K_c \left(1 + \frac{K_o}{O}\right)} - R_d \text{ , Eqn S1 and}$$
$$A_J = J \frac{c_i - \Gamma^*}{c_i + 2\Gamma^*} - R_d \text{ , Eqn S2}$$

where V_m is carboxylation capacity (maximum RuBP carboxylation rate), J is potential electron transport rate, c_i is intercellular CO₂ mole fraction, Γ_* is photorespiratory CO₂ compensation point, K_c is the Michaelis constant for RuBP carboxylation, K_o is the Michaelis constant for RuBP oxygenation, O is the oxygen mole fraction (0.21), and R_d is the rate of non-photorespiratory CO₂ release in the light. J is computed as the hyperbolic minimum of the maximum potential electron transport rate (J_m) and the product of effective quantum yield of electrons (ϕ) and incident PPFD (i):

$$\theta_I J^2 - J(J_m + \phi i) + J_m \phi i = 0$$
, Eqn S3

where $\theta_{\rm I}$ is a dimensionless convexity parameter ≤ 1 and ϕ is given by $\phi = 0.5 \cdot \alpha \cdot \phi_{\rm PSIImax}$, where $\phi_{\rm PSIImax}$ is the maximum quantum yield of photosystem II and α is leaf absorptance to photosynthetically active radiation (0.9). Intercellular CO₂ mole fraction is determined by the balance between CO₂ demand by the mesophyll (Eqns S1 and S2) and diffusional supply through the stomata:

$$A = \frac{g_{sw}g_{bw}}{1.6g_{bw} + 1.37g_{sw}} (c_a - c_i) , \quad \text{Eqn S4}$$

where c_a is ambient CO₂ mole fraction, and g_{sw} and g_{bw} are stomatal and boundary layer conductances to water vapor, respectively. Combining Eqn S4 with either Eqn S1 or S2 produces a quadratic expression for c_i , whose solution for c_i can be applied to Eqn S1 or S2 to determine A_V or A_J , respectively. Assimilation rate is usually calculated as the simple minimum of A_V and A_J ; because that produces discontinuities in A, which can preclude unambiguous identification of optima, we smoothed the transition between A_V and A_J by computing A as the hyperbolic minimum of A_V and A_J with the dimensionless parameter θ_A to 0.999:

$$\theta_A A^2 - A (A_V + A_J) + A_V A_J = 0 . \quad \text{Eqn S5}$$

We assumed that R_d is proportional to V_m at 25 °C (V_{m25}) by a factor 0.0089 (de Pury & Farquhar, 1997), and that J_m at 25 °C is also proportional to V_{m25} , by a factor 2.1 (Wullschleger 1991). We used temperature responses given by Bernacchi et al (2001, 2003) to predict temperature responses for V_m , J_m , Γ_* , K', $\phi_{PSIImax}$, θ_I and R_d :

$$V_m = V_{m25} \cdot \exp\left(26.35 - \frac{65.33}{R_{gas}T_{leafK}}\right), \quad \text{Eqn S6}$$

$$J_m = 2.1 \cdot V_{m25} \cdot \exp\left(17.7 - \frac{43.9}{R_{gas}T_{leafK}}\right), \quad \text{Eqn S7}$$

$$\Gamma_* = \exp\left(19.02 - \frac{37.83}{R_{gas}T_{leafK}}\right), \quad \text{Eqn S8}$$

$$K_c = \exp\left(38.05 - \frac{79.43}{R_{gas}T_{leafK}}\right), \quad \text{Eqn S9}$$

$$K_o = \exp\left(20.3 - \frac{36.38}{R_{gas}T_{leafK}}\right), \quad \text{Eqn S10}$$

$$\phi_{PSIImax} = 0.352 + 0.022T_L - 0.00034T_{leaf}^2, \quad \text{Eqn S11}$$

$$\theta_J = 0.76 + 0.018T_L - 0.00037T_{leaf}^2, \quad \text{Eqn S12} \quad \text{and}$$

$$R_d = 0.0089V_{m25} \cdot \exp\left(18.72 - \frac{46.39}{R_{gas}T_{leafK}}\right), \quad \text{Eqn S13}$$

where T_{leaf} and T_{leafK} are leaf temperature in degrees C and kelvins, respectively, R_{gas} is the gas constant (0.00831446).

Methods S2. Quantifying sunfleck properties by wavelet analysis

We hypothesized that canopy structure (leaf angle distribution) may influence hydraulic risk via the distribution of sunfleck intensity and length. We quantified the latter distribution by wavelet analysis, using an antisymmetric Haar wavelet (Fig S1, Eqn S14) as an archetypal sunfleck. This wavelet is zero everywhere except for a finite span of width w, where it has the value +1, and two flanking spans, each of width w/2, where it has the value -1:

$$f[t, w, c] = \begin{cases} 1 & t \in [c - w/2, c + w/2) \\ -1 & if \quad t \in [c - w, c - w/2) \text{ or } t \in [c + w/2, c + w) \\ 0 & else \end{cases}$$
 Eqn S14

where t is time and c is the value of t corresponding to the center of the wavelet. The inner product of this wavelet and a PPFD timecourse (the sum of their products at each point in time), normalized by the inner product of the wavelet with itself (simply w for Eqn S14), is a measure of the similarity (s) between the PPFD timecourse and the wavelet:

$$s[w,c,L] = \frac{1}{w} \cdot \sum_{t=c-w}^{c+w-\delta t} f[t,w,c] \cdot i_L[t] \quad . \quad \text{Eqn S15}$$

where $i_{L}[t]$ is the PPFD timecourse simulated for leaf L and ∂t (in the upper limit of summation) is the discrete timestep of the PPFD timecourse (10 seconds in this study). s will be large if w and c are chosen such that the wavelet is centered over a large sunfleck of duration approximately w (e.g., Fig S1b,d,f), whereas S will be small if the values of w or c differ substantially from the actual duration or time-center of the sunfleck, respectively (Fig S1a,c,e). For each leaf's PPFD timecourse, we computed s for each possible value of c (in effect "sliding" the wavelet along the PPFD timecourse) and recorded the maximum resulting value of s for that leaf L and value of w ($s_{max}[w,L]$) (Fig S1h,i). A large value of $s_{max}[w,L]$ indicates the occurrence of a strong sunfleck with duration $\approx w$ in leaf L. Repeating this procedure for many values of w and then plotting s_{max} vs w and locating the peak (Fig S1i) thus identifies the "strongest" sunfleck event for a given leaf, along with measures of its duration (w) and strength (s_{max}). We repeated this procedure to identify the duration and strength of the peak sunfleck for each of 10,000 leaves in each of four canopies (listed in Table **Error! Reference source not found.** in the main text).

Methods S3. Parameter estimation

 $\underline{\alpha}_{\pi}$. We used the mean rate constants for stomatal opening and closing in response to light in wheat reported by Vialet-Chabrand and Lawson (2019) (191.9 and 387.9 min, respectively), and estimated α_{π} for opening and closing as the inverses of these values (0.0052 and 0.0026 min⁻¹, respectively).

<u> α_v </u>. We used the range of within-genotype medians for the time for 95% of induction of photosynthetic capacity (t_{95}) in response to saturating light in wheat reported by Salter et al (2020) (5.2 to 9.5 min); noting that, by definition, $t_{95} = \tau \ln(1/(1-0.95)) \approx 2.996 \cdot \tau$ and $\alpha = 1/\tau$, where τ is the rate constant for photosynthetic induction, we computed the range of median α_v as $0.0053 - 0.0096 \text{ s}^{-1}$, and used the mean of these two values for α_v when photosynthetic capacity was increasing (0.0075 s^{-1}). Following Taylor and Long (2017) and Salter et al. (2019), we assumed the rate of de-induction (decline of photosynthetic capacity after a decrease in light) was 3/5 of the upwards value, giving $\alpha_v = 0.0045 \text{ s}^{-1}$ when photosynthetic capacity was decreasing.

<u> g_{bw} </u>. The two-side (whole leaf) boundary layer conductance for a leaf of characteristic dimension d (m) and wind speed v (m s⁻¹) can be estimated as g_{bh} /[mol m⁻² s⁻¹] = 0.267 · ({d /m}/{v /m})^{0.5}. In the Helios simulations used for this study, individual leaves were squares 5 cm on a side. We assumed a moderate wind speed of 5 m s⁻¹, thus giving g_{bh} = 2.67 mol m⁻² s⁻¹.

<u> χ , K_{lea125max} and K_{stem25max}</u>. These three parameters determine the mutual scaling among stomatal and hydraulic conductances and photosynthetic capacity. We estimated them by assuming that these parameters collectively produce a value of intercellular CO₂ mole fraction equal to 0.7 times the ambient value of 400 µmol mol⁻¹ (Wong *et al.*, 1979) under typical mid-day conditions. For mid-day conditions of $\psi_{\text{leaf}} = -1$ MPa and $\Delta w = 0.01$ mol mol⁻¹, and assuming soil water potential = 0, the ratio $g_{\text{sw}}/K_{\text{plant}} = 100$ MPa (because $\psi_{\text{leaf}} \approx 0 - g_{\text{sw}} \cdot \Delta w/K_{\text{plant}}$). For carboxylation capacity = 100 µmol m⁻² s⁻¹, and assuming photorespiratory CO₂ compensation point = 40 µmol mol⁻¹, effective Michaelis constant for RuBP carboxylation of 740 µmol mol⁻¹, and non-photorespiratory CO₂ release rate equal to 1% of carboxylation capacity, the net assimilation rate for $c_i = 280$ µmol mol⁻¹ is A = 22.53 µmol m⁻² s⁻¹ and hence $g_{\text{sc}} = 0.1877$ mol m⁻² s⁻¹ (because $c_i \approx c_a - A/g_{\text{sc}}$). This in turn implies $g_{\text{sw}} = 0.3$ mol m⁻² s⁻¹ (1.6· g_{sc}). Thus $K_{\text{plant}} = 0.003$ mol m⁻² s⁻¹ MPa⁻¹. We assumed that plant hydraulic resistance was equally divided between the leaf and stem compartments, thus $K_{\text{leaf25max}} = K_{\text{stem25max}} = 0.006$ mol m⁻² s⁻¹. More generally we assumed these values scaled in proportion to the value of carboxylation capacity at 25 °C among leaves.

To estimate χ given $g_{sw} = 0.3 \text{ mol m}^{-2} \text{ s}^{-1}$ and $\psi_{\text{leaf}} = -1 \text{ MPa}$, we combined our estimates for osmotic pressure at full turgor ($\pi_0 = 1.9 \text{ MPa}$) and relative water content at turgor loss ($R_{\text{tlp}} = 0.925$), and used the relationship given in the main text between ψ_{leaf} , π_0 and R_{tlp} (Eqn **Error! Reference source not found.**) to calculate a leaf relative water content of 0.96 and a turgor pressure of 0.97 MPa. Assuming further that $g_{sw} = \chi \cdot \alpha \cdot P$ as implied by the stomatal model of Buckley et al. (2003), where α is the guard cell hydroactive advantage (a dimensionless number that increases with irradiance and is generally between 0 and 10), and adopting an intermediate value of $\alpha = 5$, this implies $\chi = 0.062 \text{ mol m}^{-2} \text{ s}^{-1} \text{ MPa}^{-1}$.

<u> π_0 </u>. The cross-species mean of osmotic pressure at turgor loss point in Bartlett et al (2016) was 2.22 MPa; converting this to osmotic pressure at full turgor using the relationship given by Bartlett et al. (2012a) gives $\pi_0 = 1.9$ MPa.

 ψ_{50stem} and ψ_{50leaf} . We adopted $\psi_{50stem} = -3.3$ MPa from Eller et al. (2018). To estimate ψ_{50leaf} , we computed the ratio (0.62) of mean ψ_{50leaf} to mean ψ_{50stem} from Bartlett et al. (2016) to give $\psi_{50leaf} = -2.0$ MPa. These values are similar to those reported by Bartlett et al. (2016) (-2.9 and -1.9 MPa, respectively).

LMA. We used the mean value across environments from Bartlett et al. (2012b), 140 g m⁻².

<u> $n_{\text{leaf,max}}$ </u>. We used the mean leaf water thickness across 15 species examined by John et al. (2013) and used in the MOFLO model (Buckley *et al.*, 2015, 2017), 218 µm, which is equivalent to 12 mol m⁻².

<u>*n*stem,max</u></u>. We estimated this parameter assuming $n_{\text{stem,max}} = taper \cdot f_{\text{lumen}} \cdot [SA/LA]/V_w$, where *taper* is the effective tapering coefficient (0.38, Buckley & Roberts, 2006), f_{lumen} is lumen area fraction, SA/LA is sapwood to leaf area ratio, and V_w is the molar volume of water. Noting as well that $K_{\text{stem25max}} = K_{xa} \cdot [LA/SA]/I_{\text{stem}}$, where K_{xa} is xylem area conductivity and I_{stem} is stem length, it follows that $n_{\text{stem,max}} = K_{\text{stem25max}} \cdot I^2_{\text{stem}} \cdot taper \cdot f_{\text{lumen}}/(V_w \cdot K_{xa})$. We assumed $I_{\text{stem}} = 10$ m and estimated f_{lumen} and K_{xa} (0.207 and 107 mol m⁻² s⁻¹ [MPa m⁻¹]⁻¹, respectively) from data given by Hacke et al. (2006). This gives $n_{\text{stem,max}} = 25$ mol m⁻²_{leaf}.

<u> K_{mv} </u>. We estimated this parameter by fitting the hyperbolic function in which K_{mv} is applied (V'_{m25} = {fully induced V_{m25} }·PPFD/(PPFD + K_{mv})) to measurements of % induction of RuBP carboxylation capacity vs PPFD reported by Brooks and Portis (1988), giving K_{mv} = 97 µmol m⁻² s⁻¹.

<u> e_{stem} </u>. We estimated stem elastance (the sensitivity of water potential to relative water content; inverse of capacitance) by interpolating a regression of measurements of stem elastance and ψ_{50stem} reported by Scholz et al (2011) to our ψ_{50stem} value of -3.3 MPa, giving $e_{stem} = 10$ MPa.

<u>m</u>. The mechanical advantage of the epidermis has previously been estimated to be between around 1.5 and 2.5 (e.g., Glinka, 1971; Meidner & Bannister, 1979). We adopted a value of 2, following Buckley et al. (2003).

<u>**R**ttp</u>. We used the average value across environments as reported by Bartlett et al. (2012b), $R_{ttp} = 0.925$.

 ξ . We adopted the value used by Eller et al. (2018), ξ = 5.3.

Methods S4. Parameter sensitivity analysis

We assessed the sensitivity of simulation outcomes to the numerical values of sixteen plant parameters (α_v [for V_{m25} both increasing and decreasing], α_k , g_{bw} , χ , e_{stem} , g_{min} , $K_{leaf25max}$, $K_{stem25max}$, K_{vm} , LMA, $n_{stem,max}$, ψ_{50stem} , π_o , R_{tlp} , ξ) and five environmental parameters (c_a , w_{air} , $t_{Tairmax}$, T_{airmax} , T_{airmin}) by performing diurnal simulations for each of 500 randomly selected leaves, at each of five values for each parameter: 75%, 99%, 100%, 101%, and 125% of the default values given in Table **Error! Reference source not found.**. We computed marginal sensitivity coefficients (% change in dependent variable for a 1% change in parameter value) for both mean daily net photosynthesis (A) and mean daily minimum leaf water potential ($\psi_{leaf,min}$), averaged over the 500 leaves, using the slopes of linear regressions of (A or $\psi_{leaf,min}$) vs (parameter value) for the three central values of each parameter (99%, 100% and 101% of the default values). Results are presented in Figs S9-S12.

For two additional parameters (the mechanical advantage of the epidermis [m] and soil water potential $[\psi_{soil}]$), we performed broader sensitivity analyses. For m, we used values of m between 0 and 4 (dimensionless); results are presented in Fig S13. For ψ_{soil} , we used values between 0 and -1.8 MPa. Results are presented in Fig **Error! Reference source not found.**

For two of the remaining plant parameters in Table **Error! Reference source not found.** ($n_{\text{leaf,max}}$ and α_{π}), sensitivity analyses were performed as a primary analysis in the main text (Fig **Error! Reference source not found.**). We did not modify ψ_{50leaf} across simulations.

Methods S5. Modeling canopy radiation dynamics with Helios

The Helios 3D, leaf-resolving radiation transfer model (v1.2.8; Bailey, 2018, 2019) was used to simulate the dynamics of absorbed photosynthetic photon flux density (PPFD) and longwave sky view factor for a large number of leaves within model plant canopy geometries with varying structure. The model uses an efficient reverse ray-tracing approach for both shortwave and longwave radiation transfer that enhances statistical sampling for small or complex geometric elements. The simulated canopies consisted of square leaf elements of size 0.05 x 0.05 m² with random position and orientation. Although Helios allows for representation of realistic leaf shape and curvature, this simplified leaf geometry was chosen to avoid introducing an additional variable. The canopies consisted of about 25,000 leaves, each of which were sub-divided into a uniform grid of 5 x 5 sub-leaf elements on which average radiation fluxes were calculated. Because of the high sub-leaf-scale heterogeneity in PPFD, it is important to resolve below the leaf scale in 3D models to avoid averaging out important features of PPFD timeseries as well as to avoid potentially large errors in whole-canopy fluxes (Bailey & Kent, 2021).

Two different types of canopy geometries were simulated in this study: a quasi-homogeneous canopy in which leaf positions were sampled from a uniform distribution within a rectangular canopy volume, and a heterogeneous canopy consisting of spherical crowns of radius 0.5 m filled with spatially homogeneous vegetation (i.e., no sub-crown-scale clumping) and uniform spacing of 1.5 m. In each case, the canopy was 1 m tall, had a horizontal extent of 5 x 5 m² (with laterally periodic radiation boundary conditions), and had a canopy-averaged LAI of 2.5. This meant that the leaf area density for the homogeneous canopy was 2.5 m⁻¹ and was 10.7 m⁻¹ within the spherical crowns. For the homogeneous canopy geometry, leaf angles were sampled according to a spherical distribution (i.e., isotropic). The leaf angle distribution for the homogeneous canopies followed one of three canonical distributions introduced by de Wit (1965): spherical, planophile (biased toward horizontal leaves), and erectophile (biased toward vertical leaves).

The direct component of solar radiation was assumed to be collimated (i.e., beams remain parallel, no penumbra), with the diurnal flux in the photosynthetically active band calculated using the REST2 model of Gueymard (2008). Diffuse solar radiation was assumed to be isotropic, with the diffuse fraction also calculated using REST2 assuming clear-sky conditions. Ambient longwave radiation was also assumed to be isotropic, with its magnitude set to a value of 1.0 in order to calculate the sky view factor for each leaf element. The ray-tracing simulations utilized 250 rays/element for direct solar flux calculations, and 1000 rays/element for diffuse flux calculations. For simplicity, leaves and the ground were assumed to be black in the photosynthetically active band. Sun angles were calculated using the solar position plug-in of Helios based on a latitude of 38.5°N and Julian day of year of 150. Radiation calculations were performed at 0.1 Hz for each of the 625,000 sub-leaf elements in the canopy over a diurnal cycle. Of these elements, 10,000 were randomly selected and their total PPFD timeseries and (static) sky view factors were output to file and used to drive the physiological simulations.

Methods S6. Julia simulation code

Julia code used to simulate physiological dynamics, and associated dependencies (parameter files and sample input PPFD traces from Helios), are included as a separate ZIP file (julia_code_and_dependencies.zip).

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