

# PRAFOR - updating hydrological balance

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## 1 Updating the FR 3PG model with improved hydrological sub-models

A key limitation in the original 3PG model when considering drought, is its relatively simplistic approach to soil hydrology. This has implications for accurate simulation of ecophysiological processes in tree plantations, e.g. under-estimation of evapotranspiration. Therefore, productivity outputs from simulations during drought periods are potentially erroneous.

To overcome these limitations, a new set of hydrological balance equations were proposed and validated by Almedia and Sands (2016). These expand the original 3PG hydrology by including finer-scale processes to drive soil water content through evaporation, drainage and re-charge of the rooting zone from surrounding soil.

To build on the FR 3PGN model, which includes additional soil respiration and decomposition functions described by Xenakis et al., we have incorporated the hydrological sub-models from Almedia and Sands as described below.

## 1.1 Hydrological balance equation

The hydrological balance in the 3PG model specifies changes to the soil water content SWC  $\Theta$  (mm) within a discrete time period ( $\delta t$ ).

$$\Theta(t + \delta t) = \Theta(t) + R - I_R - E_C - E_S - q_D - q_R \quad (1)$$

Where:

$R$  = Rainfall (mm)

$I_R$  = The rainfall intercepted by the canopy (mm)

$E_C$  = Canopy transpiration (mm)

$E_S$  = Evaporation from the soil (mm)

$q_R$  = Surface run-off (mm)

## 1.2 Soil water content and available soil water

Considering the hydrological balance equation for  $\Theta(t + \delta t)$  (eq. 1). if the soil profile is  $z$  (mm) deep the volumetric soil water content SWC  $\theta$  ( $m^3 m^{-3}$ ) can be considered  $\Theta/z$ .

The relative plant available soil water (ASW) within this soil profile ( $\theta_r$ ) is then the ratio of the current plant ASW to the maximum ASW:

$$\theta_r = \frac{\theta - \theta_{wp}}{\theta_{fc} - \theta_{wp}} \quad (2)$$

Where  $\theta_{fc}$  and  $\theta_{wp}$  are the volumetric SWC of the soil profile at field capacity and wilting point respectively.

The value of  $\theta_r$  is bounded between 0-1 and drives tree growth and decomposition in the soil by modifying the soil water growth modifier ( $f_\theta$ ).

$$f_\theta = \frac{1 - (1 - \theta_r)^{n_\theta}}{1 + (1 - 2c_\theta^{n_\theta})[(1 - \theta_r)/c_\theta]^{n_\theta}} \quad (3)$$

Where  $c_\theta$  and  $n_\theta$  are texture dependant soil parameters.

Almedia and Sands (2016) describes two zones in the soil profile, the root zone ( $z_r$ ) and non-root zone ( $z_{nr}$ ). The size of the root zone can be derived from the allocation of biomass to the roots,  $z_r = \min[\sigma_{zR} W_r 0.1, z_{rx}]$ , where  $W_r$  is the root biomass,  $\sigma_{zR}$  is a modifier for the volume of soil explored per kg of root biomass,  $z_{rx}$  is a maximum rooting depth and 0.1 is a conversion factor from tons per hectare to kilograms per square meter.

The rooting zone is in principle contact with the external environment and its SWC  $\Theta_{rz}(t)$  is derived as in eq. 1. Additionally, we consider that recharge occurs from the non-rooting zone along the water pressure gradient, dependent on the SWC of the rooting and non-rooting zones at the beginning of the time-step ( $\Theta_{rz0}$  and  $\Theta_{nr0}$  respectively) and the volume of the root-zone ( $V_{rz}$ ) and non-root ( $V_{nr}$ ).

$$\Theta_{rz}(t) = \frac{\Theta_{rz0}V_{nr} - \Theta_{nr0}V_{rz}}{V_{rz} + V_{nr}}e^{-t/t_{s0}} + \frac{V_{rz}}{V_{rz} + V_{nr}}(\Theta_{rz0} + \Theta_{nr0}) \quad (4)$$

Where  $t_{s0}$  is the time constant for water movement based on the conductivity of the soil  $K_S$  and assuming both zones have a shared area  $A(m^2)$ :

$$t_{s0} = \frac{V_{rz}V_{nr}}{K_SA(V_{rz} + V_{nr})} \quad (5)$$

### 1.3 Soil evaporation

Soil evaporation rate ( $E_S$ ) is split into two phases, following a model by Ritchie (1972). In phase 1, an upper layer of soil is assumed to act as a barrier to further evaporation below the surface, forming a protective layer as it dries. Therefore, evaporation occurs at a maximum potential rate ( $e_0$ ) directly after a wetting event, until a threshold value ( $E_{S1}$ ) is reached and the upper layer has dried out. Subsequently in phase 2, evaporation rate slows hyperbolically at a rate based on soil texture ( $E_{S2}$ ) (Figure 2).

If the duration of phase 1 is  $t_{S1} = E_{S1}/e_0$  the value of  $E_S(t)$  can be considered:

$$E_S(t) = \begin{cases} e_0 t & t \leq t_{S1} \\ E_{S1} + E_{S2}(\sqrt{1 + 2(e_0/E_{S2})(t - t_{S1})} - 1) & t > t_{S1} \end{cases} \quad (6)$$

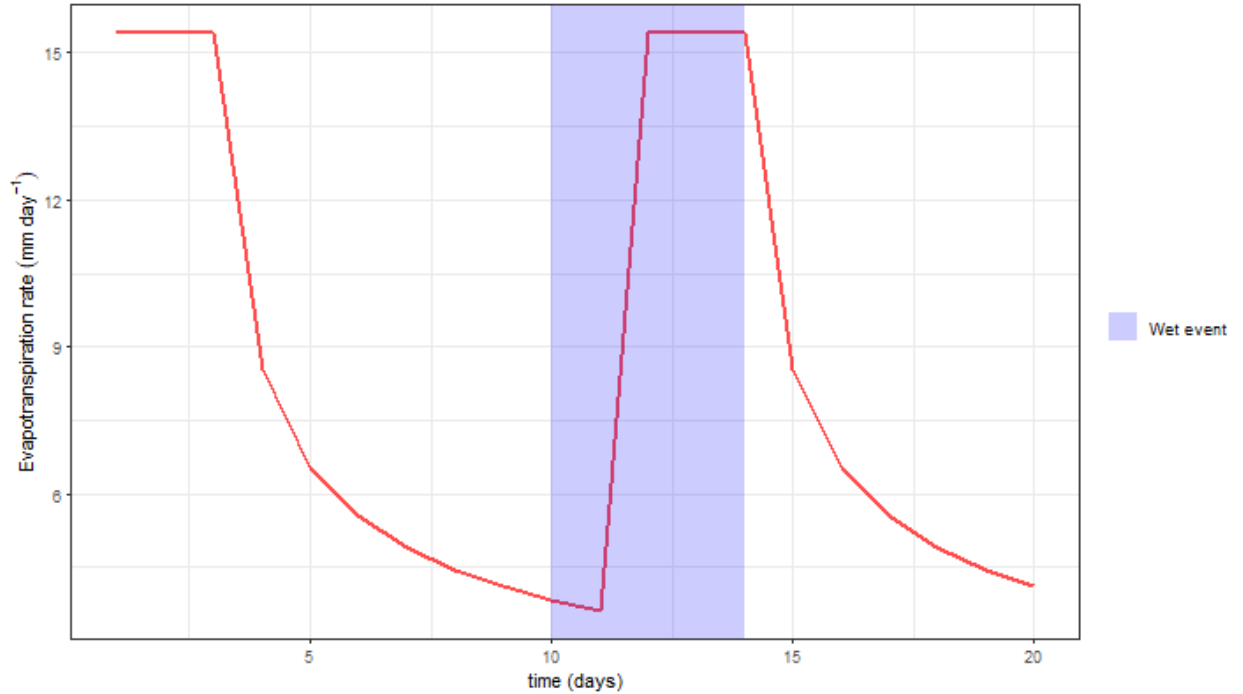


Figure 2. Soil evaporation rate  $E_S$  (mm) is shown over time. The blue shaded areas represent wetting events, after such an event,  $E_S$  occurs at the maximum potential rate  $e_0$  (mm day<sup>-1</sup>) until a threshold cumulative value  $E_{S1}$  (mm) is reached.  $E_S$  then declines hyperbolically at a rate based on soil texture  $E_{S2}$  until another wetting event occurs, which reduces the cumulative  $E_S$  by the volume of water input in mm. For clarity, this

figure assumes the cumulative value  $E_S$  has reached zero before the next wetting event

The maximum potential evaporation rate ( $e_0$ ) is calculated using a Penman-Monteith equation driven by solar radiation reaching the soil and the vapor pressure deficit (VPD) above the soil. Aerodynamic boundary layer conductance  $g_{as}$  is lower than at the canopy at approximately  $0.01g_{ac}$ , and soil surface conductance  $g_{Ac}$  in place of canopy conductance is considered infinite (Almeida and Sands 2016). Solar radiation reaching the soil ( $\varphi_{sr}$ ) is a factor of the amount of radiation absorbed by the canopy  $\varphi_{na}$ . Where, following Beers law, which estimates the amount of radiation absorbed by a material,  $\varphi_{na} = a + b\varphi_i$ , where  $a$  and  $b$  have values for sitka plantations of -90 and 0.8 respectively (F. Minunno et al. 2010).  $\varphi_i$  is driven by the daily insolation  $Q(MJm^{-2}day^{-1})$  over the day length ( $h$ ), the leaf area index ( $L$ ) and the extinction coefficient for absorption of photosynthetic active radiation (PAR) by the canopy ( $k$ ) (Figure 3), thus:

$$\varphi_i = 10^6 \frac{Q}{h} (1 - e^{(-kL)}) \quad (7)$$

and

$$\varphi_{sr} = 10^6 \frac{Q}{h} - \varphi_{na}. \quad (8)$$

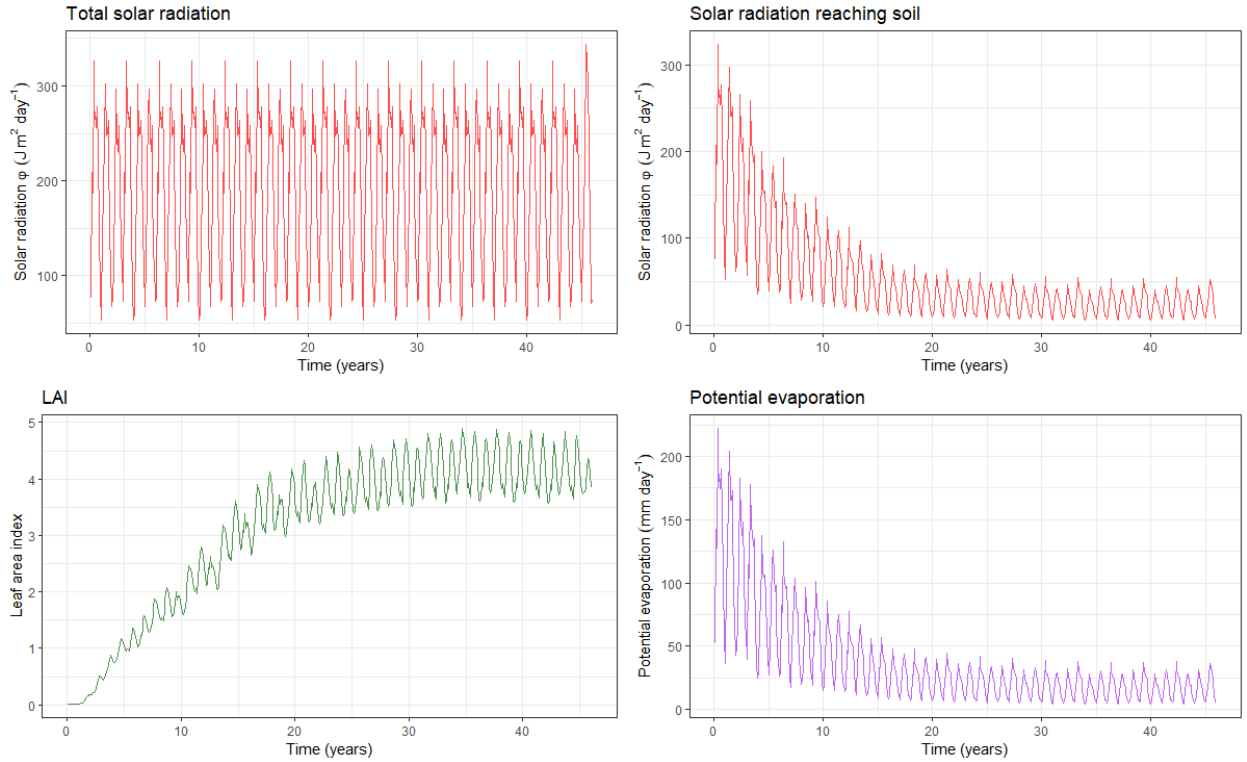


Figure 3. Total solar radiation occurring in weekly time-steps over Harwood forest plantation, and the solar radiation reaching the soil reduced by canopy absorption. As the trees grow over time, canopy size increases reducing the amount of solar radiation that is able to reach the soil.

To calculate the volume of water evaporated during a time-step, we take the cumulative value at the beginning of the time-step and consider this  $E_{S0}$ , by re-arranging the equation for  $E_S(t)$  for  $t$  we can get a corresponding value of  $t_0$ :

$$t_0 = (-2E_{S0}E_{S1}) + (E_{S0}^2) + (2E_{S0}) + (E_{S1}^2) - (2E_{S1}) + 1 + (2e0E_{S2}t_{s1} - (E_{S2}^2)) \quad (9)$$

Thus, the soil evaporation during the time-step can be derived as:

$$E_S(t_0 + \delta t) - E_{S0} \quad (10)$$

## 1.4 drainage and run-off

Rainfall replenishes the volumetric water content  $\theta$  of the soil profile, until it reaches a saturation point ( $\theta_{sat}$ ), and excess is considered to be surface run-off. Further, if the value of  $\theta$  exceeds the field capacity of the soil  $\theta_{fc}$ , any excess is available for drainage. Here, assuming that replenishment through rainfall and irrigation occurs in the rooting zone of the soil, drainage is the movement of water from the rooting zone, to the non-rooting zone and subsequently out of the system. Drainage is considered to occur proportional to the volume of excess water, with a rate determined by the constant  $k_{drain}(day^{-1})$ , a texture dependent soil parameter. Considering this, drainage over  $t$  days from the root-zone to non-root zone, and non-root zone out of the system is:

$$q_{Drz}(t) = (\Theta_0 - V_{rz}\theta_{fc})(1 - e^{-k_{drain}t}) \quad (11)$$

$$q_{Dnr}(t) = (\Theta_0 - V_{nr}\theta_{fc})(1 - e^{-k_{drain}t}) \quad (12)$$

Where  $\Theta_0$  is the initial SWC of the soil profile,  $V_{rz}$  and  $V_{nr}$  are the volume of the rooting and non-rooting soil profiles respectively.

## 2 Abridged outline of hydrology sub-models in FR 3PG

A schematic of the updated hydrological sub-models is shown in figure 4. The incorporation of the submodels specifically into the current FR implementation of the 3PG is described below. For clarity, only the updated hydrological sub-models are explained in detail.

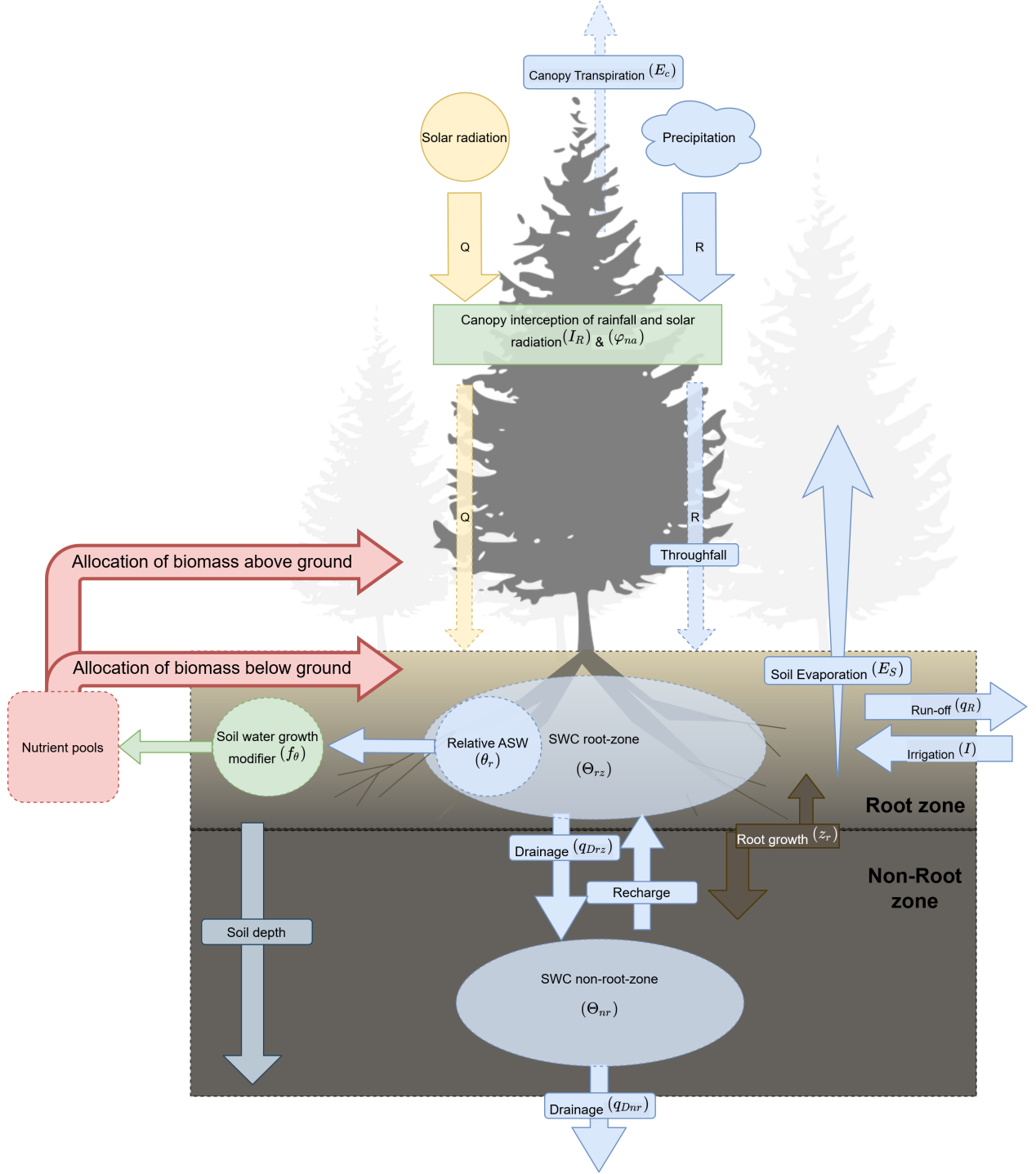


Figure 4. Schematic diagram of the hydrological balance submodel based on Almedia and Sands (2016).

The FR 3PG model runs in discrete time-steps ( $\delta t$ ), during each time-step, states of the trees/stand (e.g. biomass) are updated based on the states at the end of the previous time-step, parameter values and calculated modifiers.

⇒ **Start of time-step in FR 3PG model**

⇒ Estimate solar radiation and interception

⇒ Calculate modifiers

⇒ Estimate productivity

⇒ **Update soil water content (SWC) for rooting zone**

- Refer to section 1.2 for full details.
- Estimate current depth of rooting zone  $z_r$  (m) from root biomass ( $W_r$ ) at the end of previous time-step and parameter  $\sigma_{zR}$  which dictates the volume of soil explored by 1kg of root biomass

$$z_r = \min[\sigma_{zR} W_r 0.1, z_{nR}]$$

(0.1 is a conversion from tons per hectare to kg per square meter)

- Calculate SWC of the rooting zone  $\Theta_{rz}$  for the end of the time-step, but before the addition of rainfall and irrigation. As described by Almedia and Sands (2016) SWC at the end of the time-step can be derived using the SWC of the rooting zone and non-rooting zone at the start of the time-step ( $\Theta_{rz0}, \Theta_{nr0}$ ), the size of the root-zone ( $V_{rz}$ ) and non-root ( $V_{nr}$ ), the length of the time-step in days ( $\delta t$ ) and soil water conductivity ( $K_s$ ) (see eq. 4).
- Volumetric SWC  $\theta_{rz}$  is then calculated as  $\Theta_{rz}/(z_r * 1000)$ , ( $z_r$  is multiplied by 1000 to get value in mm)
- Using eq. 2 and the values derived for the rooting zone, calculate the relative available soil water in the rooting zone  $\theta_r$

$$\theta_r = \frac{\theta_{rz} - \theta_{wp}}{\theta_{fc} - \theta_{wp}}$$

Where  $\theta_{fc}$  and  $\theta_{wp}$  are the volumetric SWC's of the soil profile at field capacity and wilting point respectively. The value of  $\theta_r$  is bounded between 0-1 and drives tree growth and decomposition in the soil by modifying the soil water growth modifier ( $f_\theta$ ).

⇒ **Calculate the volume of water evaporation from soil during the time-step**

- Refer to section 1.3 for full details.
- Calculate the potential rate of evaporation ( $e_0$ ) using the Penman-Monteith equation, where aerodynamic boundary layer conductance is lower than at the canopy, and surface conductance is considered infinite. Radiation reaching the ground during the time-step is reduced by canopy cover based on leaf area index (LAI) and canopy absorption.
- Using soil property parameters, the length of time-step ( $\delta t$ ) and the potential evaporation rate ( $e_0$ ), calculate the amount of moisture lost during the time-step in two stages:
  1. Surface evaporation occurs at the potential evaporation rate ( $e_0$ ) until a cumulative threshold value ( $E_{S1}$ ) is reached, suggesting that the surface layer has dried out
  2. As water deeper in the soil profile becomes less accessible to solar radiation, evaporation rate declines from the potential value hyperbolically, dependent on soil texture parameters. Cumulative evaporation is stored, minus throughfall and irrigation.

⇒ **Calculate any excess soil water and drainage from water input, water output, current SWC,  $\theta_{sat}$  and  $\theta_{fc}$**

⇒ **Update SWC for non-rooting zone**

- Size of non-rooting zone is a set maximum value minus the size of the rooting zone
- The SWC of the non-rooting zone is replenished via drainage from the rooting zone ( $q_{Drz}$ ) assuming rainfall and irrigation are initially captured in the rooting zone, and diminished by drainage out of the system ( $q_{Dnr}$ ). Drainage is dependent on the soil texture parameter  $K_{drain}$  and the volume of the soil zones.

⇒ **Add weekly rainfall and irrigation, minus evaporation, transpiration and excess water to the root zone SWC**

- Allocate biomass based on available water and nutrients
- Estimate mortality
- Update soil nutrients and decomposition

- Predict useful state variables e.g. LAI
- End of time step, repeat.

### 3 Calibration

#### 3.1 Data

Data for calibration and validation of the modified 3-PGN model, came from 51 experimental plots of Scots pine, receiving different silvicultural treatments, and were part of the UK Forestry Commission permanent sample plot (PSP) data base. Validation of the model simulations has been recently applied to new data from the Harwood forest site, which has monthly recording of fluxes between 2015 and 2018.

Model runs on monthly, weekly or daily time-steps where data is available.

#### 3.2 Sensitivity analysis

To identify the influence of each new parameter in the hydrological sub-models on calibration, we conducted a sensitivity analysis. We used the Morris method, which for each parameter outputs a metric for the influence on the model output and the degree of interaction with other parameters/non-linearity (Morris 1991).

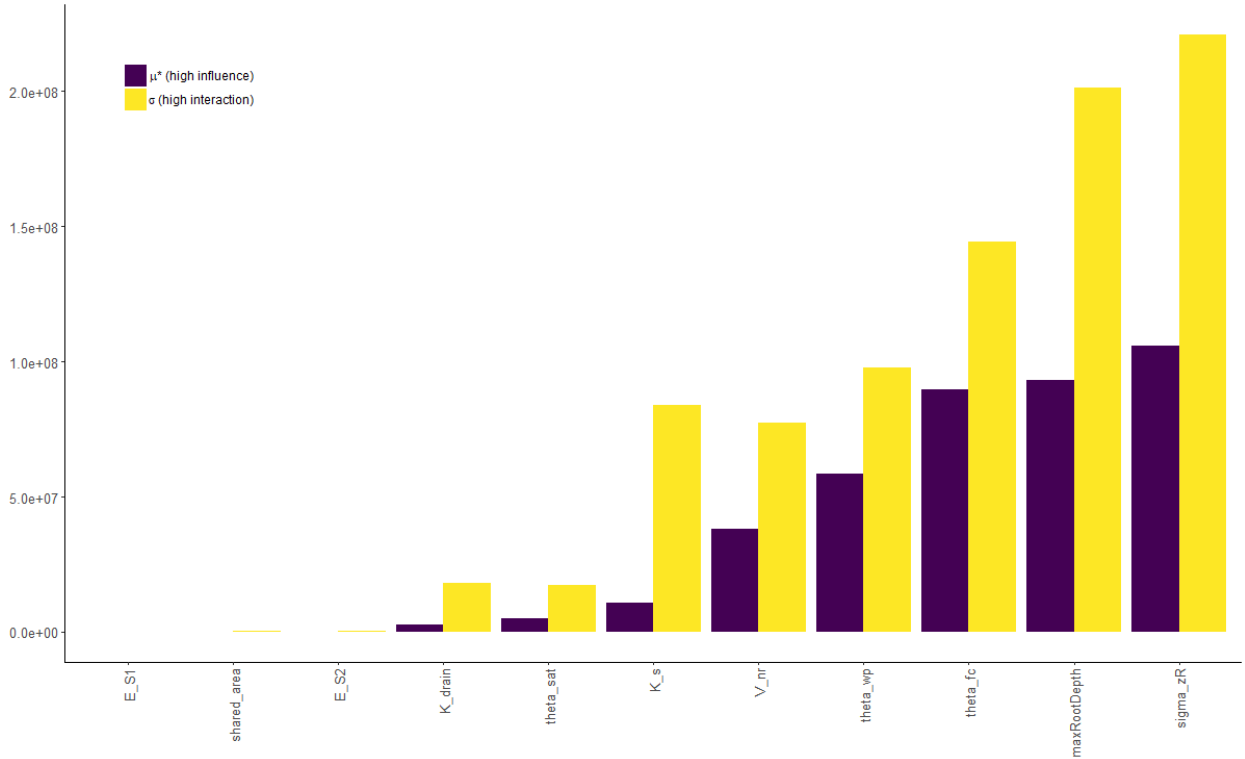


Figure 5 Morris sensitivity analysis conducted on parameters for new hydrological sub-models. Values show the degree of influence for each parameter on the model output ( $\mu^*$ ), and the level of interaction/non-linearity ( $\sigma$ )



### 3.3 Likelihood function

Calibration of the model followed similar methods to previous publications including Minunno et al (2010) and Xenakis et al. (2020) (unpublished) using likelihood based MCMC algorithms. Here we defined the likelihood function based around a normal distribution, where for the data  $y$  with mean  $\mu$  and S.D.  $\sigma$ , a vector of parameters  $\theta$  and simulated value  $x$ ,

$$p(y(\mu, \sigma)|x, \theta) = \frac{1}{\sqrt{(2\pi)}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \quad (13)$$

Thus for observed data  $y_{1:t}$  the full likelihood value can be considered:

$$\mathcal{L}(\theta|y_{1:t}) = \prod_{n=1}^t p(y_n|x_n, \theta) \quad (14)$$

### 3.4 Priors

parameter	low	high
wiltPoint	0.080	0.14
fieldCap	0.200	0.35
satPoint	0.300	0.60
K_s	0.001	10.00
V_nr	3.000	5.00
sigma_zR	0.200	0.90
E_S1	1.000	100.00
E_S2	0.500	20.00
shared_area	2.000	6.00
maxRootDepth	2.000	4.00
K_drain	0.100	0.50

### 3.5 MCMC algorithm

We used a Differential-Evolution MCMC (Braak and Vrugt 2008) in the BayesianTools R package (Hartig, Minunno, and Paul 2018), which utilises a genetic algorithm for chains to learn from each-other as they progress, in addition to a snooker updater. We run the MCMC algorithm for 2 million iterations over 7 chains and a burn-in period of 10%.

MCMC outputs are shown in appendices for calibration with monthly, weekly and daily time-steps.

## 4 Spatial analysis

As part of the PRAFOR project we aim to apply the calibrated FR 3PG model to spatial climatic and environmental data.

As proof of principle, we have developed a framework to apply the model to 1km or 5km grid-square longitudinal climatic data from CEDA (figure 5). This outputs the “potential” productivity of each grid-square which can then subsequently be plotted as a map (figure 6).

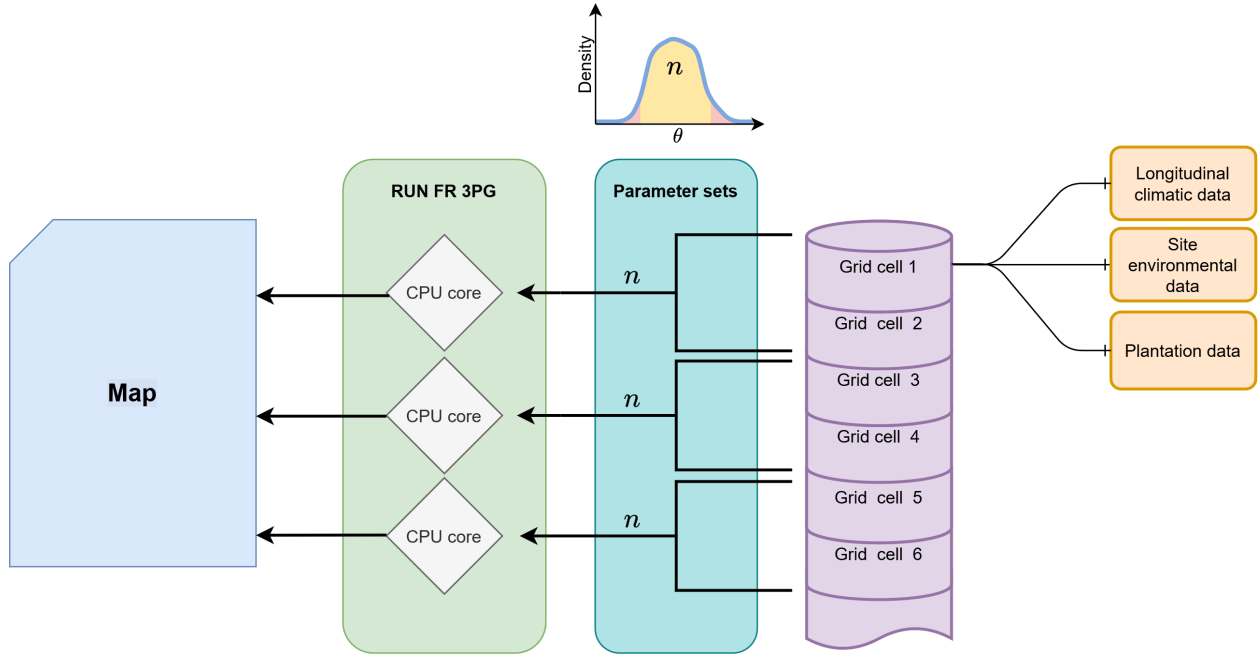


Figure 6 Schematic of spatial modelling framework, here showing how the data from six grid cells is processed in parallel accross multiple cpu cores. For each grid cell, the FR 3PG model is also run for  $n$  parameter sets sampled from the posterior of the MCMC calibration, enabling the calculation of an average and 95% CI range for the output. The output (e.g. biomass) is then plotted as a map using the georeferenced locations associated with each cell.

For each grid-square we run the FR3PG model with multiple parameter sets sampled from the posterior distribution. of the MCMC calibration. From this we take an average value and 95% credible intervals as a measure of uncertainty

The framework is flexible in that it allows us to attach any additional grid-referenced data to a corresponding grid square, e.g. soil type, current land use etc. Further, replacing grid squares with polygons for individual forests would be relatively trivial. Computationally, running the model for this number of locations and parameter sets is intensive (e.g. for 500 parameter sets and 100,000 grid squares would be 50 million runs of the model), however the framework is developed for parallel computation, and is highly scaleable, with each grid square able to be run on a seperate core. Utilising the batch computing facilities of JASMIN, it should be possible to undertake runs for the entire UK in relatively short periods.

### Spatial analysis of FR3PGN model - Scotland

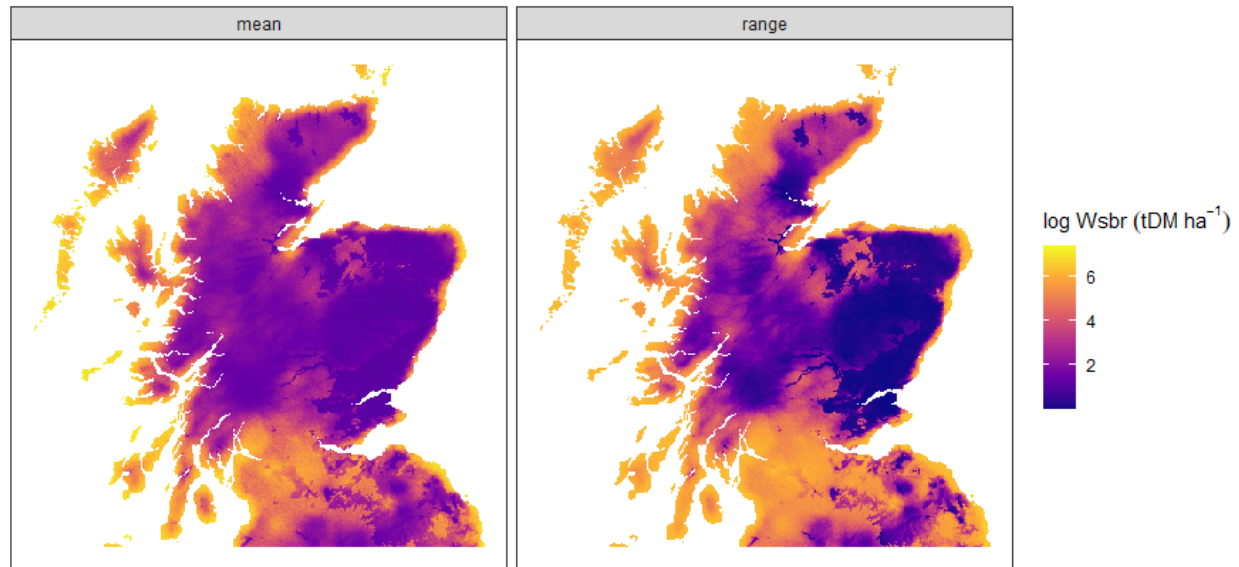


Figure 7 Example spatial analysis conducted using FR 3PG model with updated hydrological sub-models for 1km grid cells of climatic data taken from CEDA for part of Scotland. Note: Mean values are likely inaccurate and ranges are quite high as model has yet to be properly calibrated with hydrological sub-models

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