

---

# HydroShoot Documentation

*Release 1.0.0*

**Rami Albasha**

**Oct 23, 2021**



---

## Contents:

---

<b>1</b>	<b>Installation</b>	<b>1</b>
<b>2</b>	<b>Overview</b>	<b>3</b>
2.1	What is HydroShoot about? . . . . .	3
2.2	Why would you be interested in it? . . . . .	4
<b>3</b>	<b>Model description</b>	<b>5</b>
3.1	Ecophysiological processes . . . . .	5
3.1.1	Hydraulic structure . . . . .	5
3.1.2	Gas exchange . . . . .	7
3.1.3	Energy budget . . . . .	10
3.2	Processes interactions . . . . .	11
3.3	References . . . . .	12
<b>4</b>	<b>Usage</b>	<b>15</b>
4.1	Set the required files up . . . . .	16
4.2	Outputs . . . . .	16
4.3	Run the model . . . . .	17
<b>5</b>	<b>Indices and tables</b>	<b>19</b>



# CHAPTER 1

---

## Installation

---

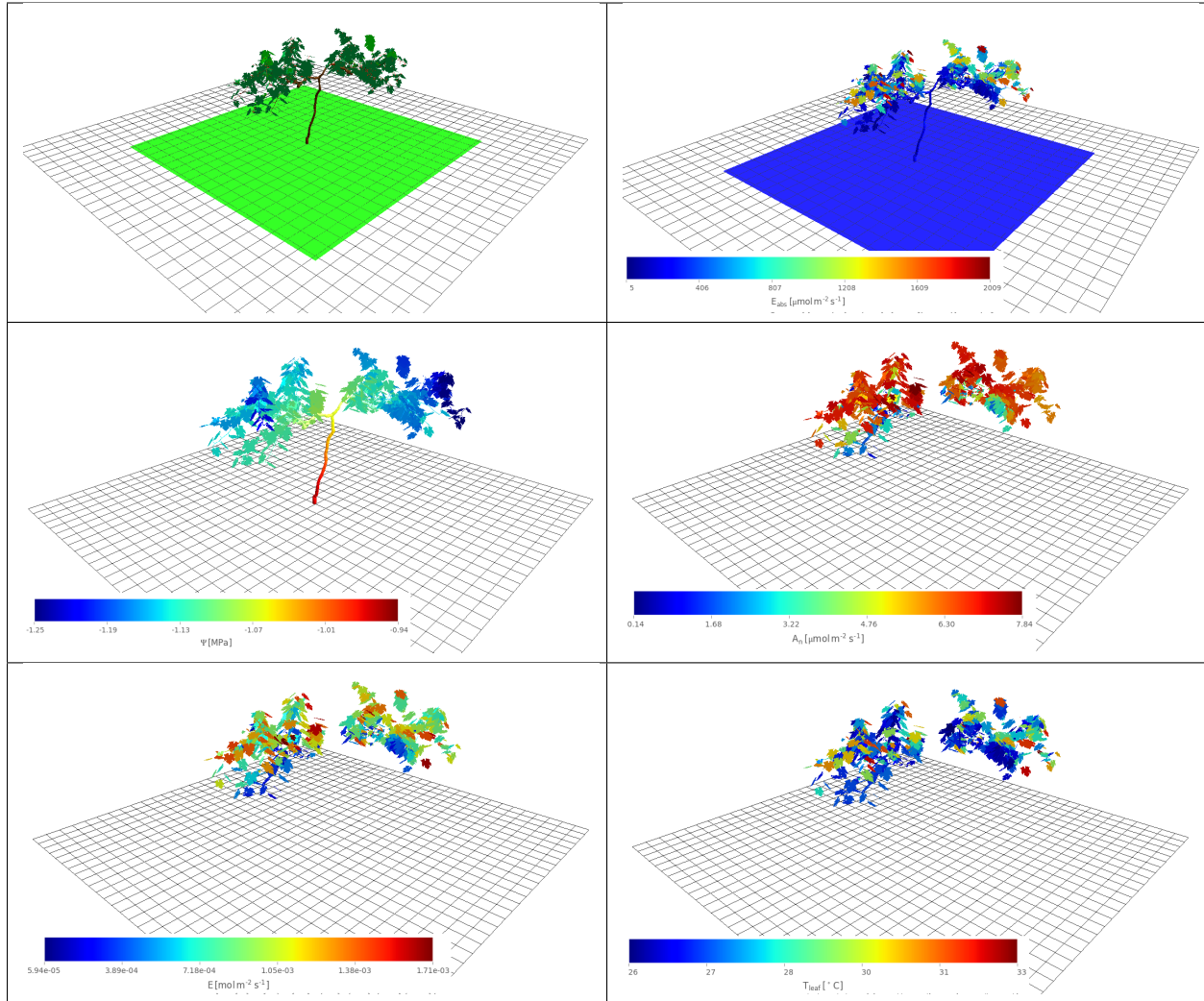
Download sources and use setup:

```
$ python setup.py install  
or  
$ python setup.py develop
```



### 2.1 What is HydroShoot about?

HydrShoot is a functional-structural plant model that simulates the interactions between shoot's hydraulic structure, gas-exchange and energy-budget, at the organ level.



**Plant shoot is static** to HydroShoot. That is the model does not simulate plant growth nor its development. Its usage would therefore be only sound only if shoot's structure can be assumed constant across a given span of time (let's say a week or so for grapevine).

## 2.2 Why would you be interested in it?

HydroShoot may be useful for example if you would like to explore:

- how leaf net carbon assimilation rate ( $A_n$ ), transpiration rate ( $E$ ), temperature ( $T$ ) and bulk water potential ( $\Psi_{\text{leaf}}$ ) interact across the canopy
- how soil water status impacts  $A_n$ ,  $E$ ,  $T$ , and  $\Psi_{\text{leaf}}$
- how the structure of the shoot impacts  $A_n$ ,  $E$ ,  $T$ , and  $\Psi_{\text{leaf}}$
- how soil water potential ( $\Psi_{\text{soil}}$ ) propagates across plant's shoot



All information in this section are taken from HydroShoot's paper (**Albasha et al., 2019** <<https://doi.org/10.1093/insilicoplants/diz007>>). Please refer to the this paper for a thorough description of model's formulae and evaluation.

### 3.1 Ecophysiological processes

#### 3.1.1 Hydraulic structure

The *hydraulic* module computes the distribution of xylem water potential across plant segments by analogy to Ohm's law (Fig. 3.1)

Water flux ( $F$ ,  $kg\ s^{-1}$ ) across the hydraulic segment of length ( $L$ ,  $m$ ) is driven by the difference of xylem pressures across this segment ( $H_u - H_l$ ,  $MPa$ ) and regulated by segment's hydraulic conductivity ( $K$ ,  $kg\ s^{-1}\ m\ MPa^{-1}$ ):

$$F = -K \cdot \frac{H_u - H_l}{L}$$

The hydraulic conductivity varies with water potential as a result of xylem cavitation under water deficit (**Tyree and Sperry, 1989**). This relationship is described in HydroShoot as:

$$K = K_{max} \cdot \frac{1}{\left(1 + \left(\frac{\Psi}{\Psi_{crit, stem}}\right)^{c_{x1}}\right)}$$

where  $K_{max}$  [ $kg\ s^{-1}\ m\ MPa^{-1}$ ] is the maximum conductivity of the segment,  $\Psi$  [ $MPa$ ] is the arithmetic mean of xylem potential of the segment,  $\Psi_{crit, stem}$  [ $MPa$ ] and  $c_{x1}$  [–] are shape parameters.

$K_{max}$  is estimated empirically as proposed by **Tyree and Zimmermann (2002)** as:

$$K_{max} = c_{x2} \cdot D^{c_{x3}}$$

where  $D$  [ $m$ ] is the average diameter of the segment, and  $c_{x2}$  and  $c_{x3}$  are shape parameters, mostly given within the ranges of [2.5, 2.8] and [2.0, 5.0], respectively.

The last two equations apply to all conducting segments (not leaves blades). Water potential of the upper extremity of the petiole is assumed equal to that of the lumped leaf water potential  $\Psi_{leaf}$  [ $MPa$ ].

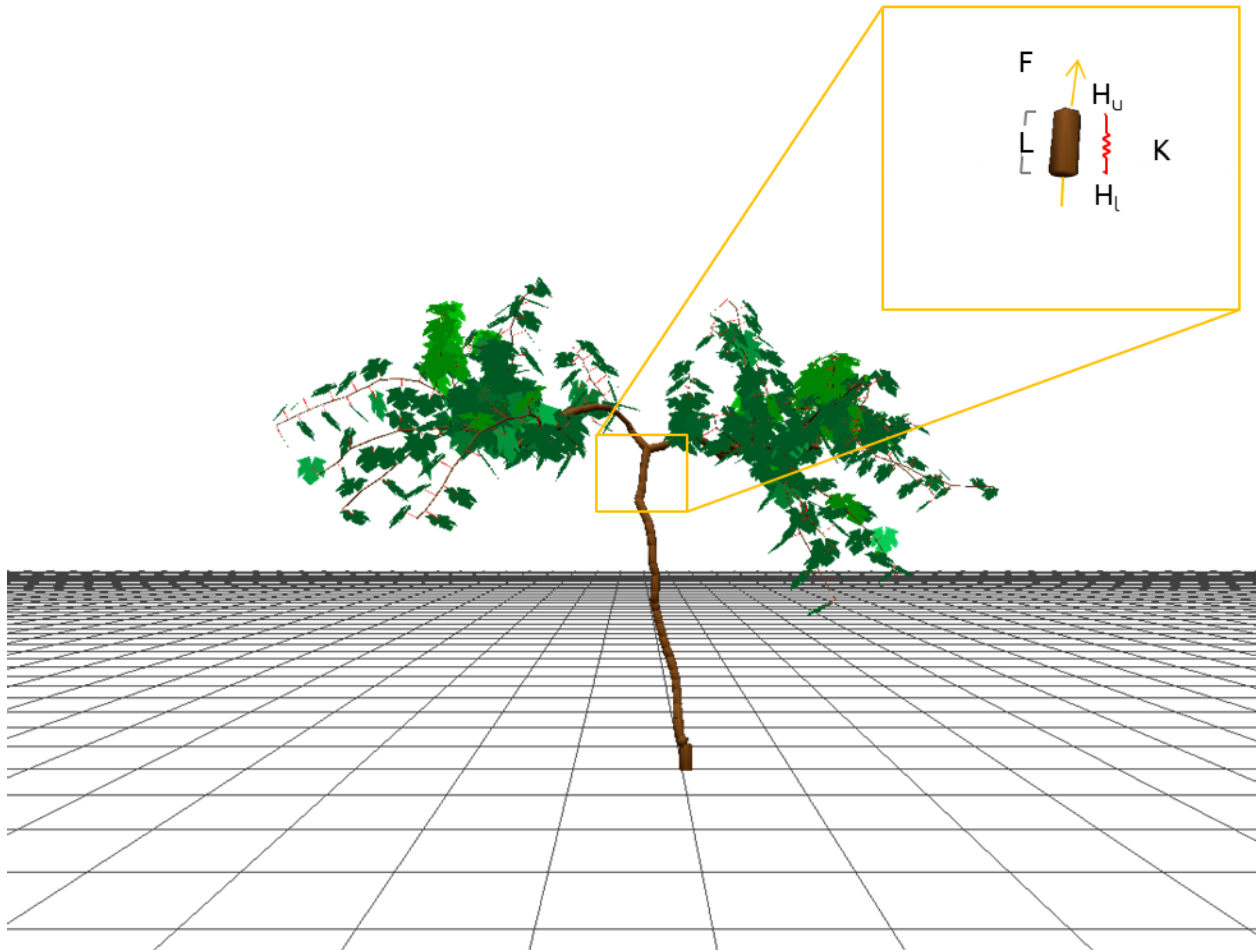
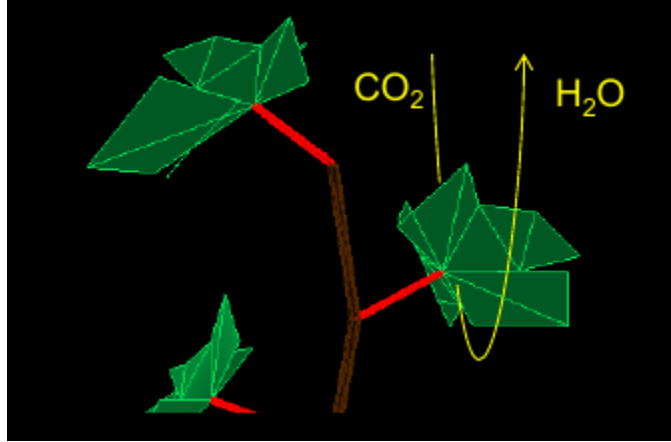


Fig. 3.1: Illustration of the variables required to calculate the hydraulic structure: water flux ( $F$ ), hydraulic conductivity ( $K$ ), water pressure at upper (downstream) and lower (upstream) extremities of the conducting element (respectively  $H_u$  and  $H_l$ ), and the length of the segment ( $L$ ).

### 3.1.2 Gas exchange



The *exchange* module computes the rates of net carbon assimilation of C3 plants ( $A_n$ ), stomatal conductance to  $CO_2$  ( $g_{s, CO_2}$ ) and water vapor ( $g_{s, H_2O}$ ), and transpiration ( $E$ ) per unit leaf surface area as a function of micrometeorological conditions and leaf water status.

$A_n$  and  $g_{s, CO_2}$  are coupled based on the analytical solution proposed by **Yin et al. (2009)** which also considers mesophyll conductance to  $CO_2$  diffusion  $g_m$ . The solution is based on the following equations (following **Evers et al. 2010** supporting information):

$$A_n = \frac{(C_c - \Gamma) \cdot x_1}{C_c + x_2} - R_d$$

$$C_c = C_i - \frac{A_n}{g_m}$$

$$g_{s, CO_2} = g_{s0, CO_2} + m_0 \cdot \frac{A_n + R_d}{C_i - \Gamma} \cdot f_w$$

$$g_{s, CO_2} = \frac{A_n}{C_a - C_i - A_n \cdot r_{tb}}$$

where  $A_n$  [ $\mu\text{mol m}^{-2} \text{s}^{-1}$ ] is net carbon assimilation rate,  $R_d$  [ $\mu\text{mol m}^{-2} \text{s}^{-1}$ ] is mitochondrial respiration in the light,  $\Gamma$  [ $\mu\text{bar}$ ] is  $CO_2$  compensation point in the absence of mitochondrial respiration,  $x_1$  [ $\mu\text{mol m}^{-2} \text{s}^{-1}$ ] and  $x_2$  [ $\mu\text{bar}$ ] are intermediate parameters,  $g_m$  [ $\mu\text{mol m}^{-2} \text{s}^{-1} \mu\text{bar}^{-1}$ ] is mesophyll conductance for  $CO_2$  diffusion,  $g_{s, CO_2}$  [ $\text{mol m}^{-2} \text{s}^{-1} \mu\text{bar}^{-1}$ ] is stomatal conductance to  $CO_2$ ,  $g_{s0, CO_2}$  [ $\text{mol m}^{-2} \text{s}^{-1} \mu\text{bar}^{-1}$ ] is the residual stomatal conductance to  $CO_2$ ,  $m_0$  [–] is a shape parameter regulating the slope between  $A_n$  and  $g_{s, CO_2}$ ,  $f_w$  [–] is a dimensionless function representing the response of stomatal conductance to soil or plant water status,  $r_{tb}$  [ $\text{m}^2 \text{s} \mu\text{bar} \mu\text{mol}^{-1}$ ] is the combined turbulence and boundary layer resistance for  $CO_2$ ,  $C_a$  [ $\mu\text{bar}$ ] is air  $CO_2$  partial pressure,  $C_i$  [ $\mu\text{bar}$ ] is intercellular  $CO_2$  partial pressure, and  $C_c$  [ $\mu\text{bar}$ ] is chloroplast  $CO_2$  partial pressure.

#### Net carbon assimilation rate per unit leaf area

$A_n$  is given as:

$$A_n = V_c \cdot \left(1 - \frac{\Gamma}{C_c}\right) - R_d$$

where  $V_c$  [ $\mu\text{mol m}^{-2} \text{s}^{-1}$ ] is carboxylation rate,  $\Gamma$  [ $\mu\text{mol}_{CO_2} \text{mol}_{CO_2}^{-1}$ ]  $CO_2$  compensation point in the absence of mitochondrial respiration,  $C_c$  [ $\mu\text{mol}_{CO_2} \text{mol}^{-1}$ ] chloroplast  $CO_2$  concentration, and  $R_d$  [ $\mu\text{mol m}^{-2} \text{s}^{-1}$ ] is mitochondrial respiration rate in the light.

$V_c$  is given as:

$$V_c = \min(W_c, W_j, W_p)$$

where  $W_c$ ,  $W_j$ , and  $W_p$  [ $\mu\text{mol m}^{-2} \text{s}^{-1}$ ] are respectively Rubisco-limited carboxylation rate, RuBP-limited carboxylation rate, and Triose phosphates-limited carboxylation rate, given as:

$$W_c = \frac{C_c \cdot V_{c, \max}}{C_c + K_c \cdot \left(1 + \frac{O}{K_o}\right)}$$

$$W_j = \frac{J}{4 + 8 \cdot \frac{C_c}{C_c}}$$

$$W_p = \frac{3 \cdot TPU}{\left(1 - \frac{C_c}{C_c}\right)}$$

where  $V_{c, \max}$  [ $\mu\text{mol m}^{-2} \text{s}^{-1}$ ] is the maximum carboxylation rate,  $J$  [ $\mu\text{mol m}^{-2} \text{s}^{-1}$ ] electron transport rate,  $TPU$  [ $\mu\text{mol m}^{-2} \text{s}^{-1}$ ] Triose phosphates transport rate,  $K_c$  [ $\mu\text{mol mol}^{-1}$ ] Michaelis-Menten constant for the carboxylase,  $K_o$  [ $\text{mmol mol}^{-1}$ ] Michaelis-Menten constant for the oxygenase, and  $O$  [ $\text{mmol mol}^{-1}$ ] oxygen concentration.

Finally,  $J$  is given as:

$$J = \frac{\alpha \cdot PPFD}{\sqrt{1 + \frac{\alpha^2 \cdot PPFD^2}{J_{\max}^2}}}$$

where  $J_{\max}$  [ $\mu\text{mol m}^{-2} \text{s}^{-1}$ ] is maximum electron transport rate, and  $PPFD$  [ $\mu\text{mol m}^{-2} \text{s}^{-1}$ ] is photosynthetic photon flux density.

The impact of leaf temperature on the photosynthesis parameters is accounted for using Arrhenius functions. For  $V_{c, \max}$ ,  $J_{\max}$ ,  $TPU$ , and  $R_d$  temperature dependency writes:

$$P = P^{25} \cdot \frac{\exp\left(c - \frac{\Delta H_a}{R \cdot T_{leaf}}\right)}{1 + \exp\left(\frac{\Delta S \cdot T_{leaf} - \Delta H_d}{R \cdot T_{leaf}}\right)}$$

where  $P$  denotes any of  $V_{c, \max}$ ,  $J_{\max}$ ,  $TPU$ , and  $R_d$  parameters,  $P^{25}$  is the value of  $P$  at  $25^\circ\text{C}$ ,  $c$   $[-]$  is a shape parameter,  $\Delta H_a$  [ $\text{kJ mol}_{CO_2}^{-1}$ ] is activation energy of the Arrhenius functions,  $\Delta H_d$  [ $\text{kJ mol}_{CO_2}^{-1}$ ] is deactivation energy of the Arrhenius functions,  $\Delta S$  [ $\text{kJ K}^{-1} \text{mol}_{CO_2}^{-1}$ ] is entropy term,  $R$  [ $\text{kJ K}^{-1} \text{mol}^{-1}$ ] is the ideal gas constant, and  $T_{leaf}$  [ $^\circ\text{C}$ ] is leaf temperature.

Finally, for  $\Gamma$ ,  $K_c$ , and  $K_o$  temperature dependency writes:

$$P = \exp\left(c - \frac{\Delta H_a}{R \cdot T_{leaf}}\right)$$

### Variable intra-canopy photosynthetic capacities

Leaf photosynthetic traits ( $V_{cmax}$ ,  $J_{max}$ ,  $TPU$  and  $R_d$ ; cf. Appendix I in **Albasha et al., 2019**) are set to vary as a function leaf nitrogen content per unit leaf surface area ( $N_a$ ,  $g_N \text{m}^{-2}$ ) following **Prieto et al. (2012)**:

$$P^{25} = S_{N_a} N_a - b_{N_a}$$

where  $P^{25}$  [ $\mu\text{mol m}^{-2} \text{s}^{-1}$ ] is the value at  $25^\circ\text{C}$  for any of the rates of  $V_{cmax}$ ,  $J_{max}$ ,  $TPU$  or  $R_d$ ,  $S_{N_a}$  [ $\mu\text{mol g}_N^{-1} \text{s}^{-1}$ ] and  $b_{N_a}$  [ $\mu\text{mol m}^{-2} \text{s}^{-1}$ ] are the slope and the intercept of the linear relationship with  $N_a$  specific to each rate.

$N_a$  is calculated as the product of nitrogen content per unit leaf dry mass ( $N_m$ ,  $g_N g_{drymatter}^{-1}$ ) and leaf dry mass per area ( $LMA$ ,  $g_{drymatter} \text{m}^{-2}$ ).  $N_m$  linearly varies with plant age, expressed as the thermal time cumulated since budburst, and  $LMA$  is determined by leaf exposure to light during the last past days (**Prieto et al., 2012**), as expressed respectively in the two following equations:

$$N_m = a_N \cdot \sum_{i=budburst}^d (\max(0, T_{air, i} - T_b)) + b_N$$

$$LMA = a_M \cdot \ln(PPFD_{10}) + b_M$$

where  $T_{air, i}$  [ $^{\circ}C$ ] is the mean temperature of the day  $i$ ,  $T_b$  [ $^{\circ}C$ ] is the base temperature (minimum required for growth), set to  $10^{\circ}C$  for grapevine and used for the calculation of thermal time since budburst,  $a_N$  [ $g_N g_{drymatter}^{-1} ^{\circ}C d^{-1}$ ] and  $b_N$  [ $g_N g_{drymatter}^{-1}$ ] are the slope and intercept of the linear relationship between  $N_m$  and accumulated thermal time since budburst,  $PPFD_{10}$  [ $mol_{photon} m^{-2} d^{-1}$ ] is the cumulative photosynthetic photon flux density irradiance intercepted by the leaf (output of the energy module) averaged over the past 10 days,  $a_M$  [ $g_{drymatter} mol_{photon}^{-1} d^{-1}$ ] and  $b_M$  [ $g_{drymatter} m^{-2}$ ] are the slope and intercept of the linear relationship between  $LMA$  and the logarithm of  $PPFD_{10}$ .

## Photoinhibition

HydroShoot is provided with an empirical photoinhibition model which assumes that combined heat and water stresses inhibit photosynthesis by reducing the electron transport rate ( $J$ ):

$$\Delta H_d = \Delta H_{d, max} - \max \left( 0, (\Delta H_{d, max} - \Delta H_{d, T}) \cdot \min \left( 1, \frac{\Psi_{leaf} - \Psi_{leaf, max}}{\Psi_{leaf, min} - \Psi_{leaf, max}} \right) \right)$$

$$\Delta H_{d, t} = \Delta H_{d, t1} - (\Delta H_{d, t1} - \Delta H_{d, t2}) \cdot \min \left( 1, \max \left( 0, \frac{T_{leaf} - T_{leaf1}}{T_{leaf2} - T_{leaf1}} \right) \right)$$

where  $\Delta H_d$  [ $kJ mol^{-1}$ ] is calculated after accounting for the joint effects of leaf water potential  $\Psi_{leaf}$   $MPa$  and temperature  $T_{leaf}$  [ $K$ ],  $\Delta H_{d, max}$  [ $kJ mol^{-1}$ ] is the value of  $\Delta H_d$  without accounting for photoinhibition,  $\Delta H_{d, T}$  [ $kJ mol^{-1}$ ] is the value of  $\Delta H_d$  after accounting for the effect of  $T_{leaf}$ ,  $\Psi_{leaf, max}$  and  $\Psi_{leaf, min}$  [ $MPa$ ] are leaf water potential values at which photoinhibition starts and reaches its maximum effect, respectively, finally,  $\Delta H_{d, T1}$  and  $\Delta H_{d, T2}$  [ $kJ mol^{-1}$ ] are empirical thresholds corresponding to leaf temperatures  $T_{leaf1}$  and  $T_{leaf2}$  which are temperatures at which photoinhibition starts and reaches its maximum effect, respectively.

## Transpiration rate per unit leaf area

The transpiration rate ( $E$ ,  $mol m^{-2} s^{-1}$ ) is calculated as:

$$E = \frac{1}{\frac{1}{g_{b, H_2O}} + \frac{1}{1.6 \cdot g_{s, CO_2}}} \left( \frac{VPD}{P_a} \right)$$

where  $P_a$  [ $kPa$ ] is the atmospheric pressure and  $g_{b, H_2O}$  [ $mol m^{-2} s^{-1}$ ] is the boundary layer conductance to water vapor derived from **Nobel (2005)** as:

$$g_{b, H_2O} = \frac{D_{H_2O} \cdot P_v}{R \cdot T_{leaf} \cdot \Delta x}$$

with

$$D_{H_2O} = D_{H_2O, 0} \cdot \frac{P_a}{P_v} \cdot \left( \frac{T_{leaf}}{273} \right)^{1.8}$$

where  $D_{H_2O}$  is the diffusion coefficient of H<sub>2</sub>O in the air at  $0^{\circ}C$  ( $2.13 \cdot 10^{-5} m^2 s^{-1}$ ),  $P_a$  [ $MPa$ ] is the ambient air pressure at  $0^{\circ}C$ ,  $P_v$  [ $MPa$ ] is water vapor partial pressure, and  $\Delta x$  [ $m$ ] is the thickness of the boundary layer defined following **Nobel (2005)** as:

$$\Delta x = 0.004 \sqrt{\frac{l}{v}}$$

where  $l$  [ $m$ ] is the mean length of the leaf in the downwind direction (set to 70% of blade length), and  $v$  [ $m s^{-1}$ ] is wind speed in the vicinity of the leaf.

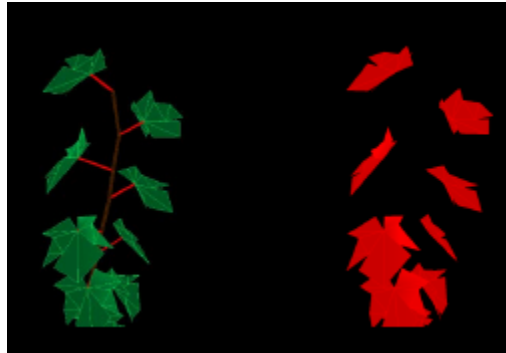
Finally, the impact of water stress on stomatal conductance (i.e. via the  $f_w$  function) is calculated using one of the following options:

$$f_w = \begin{cases} \frac{1}{1 + \left(\frac{VPD}{D_0}\right)} & (a) \\ \frac{1}{1 + \left(\frac{\Psi_{leaf}}{\Psi_{crit, leaf}}\right)^n} & (b) \\ \frac{1}{1 + \left(\frac{\Psi_{soil}}{\Psi_{crit, leaf}}\right)^n} & (c) \end{cases}$$

where  $VPD$  [kPa] is vapor pressure deficit (between the leaf and the air),  $D_0$  [kPa] shape parameter,  $\Psi_{leaf}$  [MPa] leaf bulk xylem potential,  $\Psi_{soil}$  [MPa] soil bulk water potential (assumed equal to xylem potential at the base of the shoot), and  $\Psi_{crit, leaf}$  [MPa] leaf water potential at which stomatal conductance reduces to half its maximum value.

In case the option *a* is used, stomatal conductance reduction is considered independent from the soil water status (i.e. following **Leuning, 1995**). In contrast, Both options *b* and *c* allow simulating stomatal conductance as a function either of leaf water potential (i.e. regarding shoot hydraulic structure) or soil water potential (i.e. disregarding the hydraulic structure of the shoot).

### 3.1.3 Energy budget



The *energy* module computes the temperature of individual leaves based on a detailed energy balance model (see Supporting Information S3 in **Albasha et al., 2019**).

Energy gain of each leaf comes from:

1. the absorbed shortwave;
2. thermal longwave radiation from the sky;
3. thermal longwave radiation from the sky;
4. thermal longwave radiation from the soil;
5. thermal longwave radiation from the neighbouring leaves.

Energy loss of each leaf is due to

1. thermal longwave radiation emitted by the leaf
2. latent heat due to transpiration (evaporative cooling)

Energy gain or loss may result from heat exchange between the each leaf and the surrounding air by thermal conduction-convection.

The resulting leaf-scale energy balance equation writes:

$$\begin{aligned}
 0 = & \alpha_{i, R_g} \cdot \Phi_{i, R_g} \\
 & + \epsilon_{i, leaf} \cdot \sigma \cdot (k_{i, sky} \cdot \epsilon_{sky} \cdot T_{sky}^4 + k_{i, soil} \cdot \epsilon_{soil} \cdot T_{soil}^4 + [1 - (k_{sky} + k_{soil})]) \\
 & - 2 \cdot \epsilon_{i, leaf} \cdot \sigma \cdot T_i^4 \\
 & - \lambda \cdot E_i \\
 & - 2 \cdot K_{air} \cdot \frac{T_i - T_{air}}{\Delta x_i}
 \end{aligned}$$

where  $i$  refers to leaf identifier,  $j$  refers to neighbouring leaves identifier,  $\Omega$  denotes the upper hemisphere surrounding the leaf  $i$ ,  $\alpha_{R_g}$   $[-]$  is lumped leaf absorptance in the shortwave band,  $\Phi_{R_g}$   $[W m_{leaf}^{-2}]$  flux density of shortwave global irradiance,  $\epsilon_{leaf}$   $[-]$  emissivity-absorptivity coefficients of the leaf,  $\epsilon_{sky}$   $[-]$  emissivity-absorptivity coefficients of the leaf,  $\epsilon_{soil}$   $[-]$  emissivity-absorptivity coefficients of the soil,  $\lambda$   $[W s mol^{-1}]$  is latent heat for vaporization,  $\sigma$   $[W m^{-2} K^{-4}]$  the Stefan-Boltzmann constant,  $k_{sky}$   $[-]$  form factor of the sky,  $k_{soil}$   $[-]$  form factor of the soil,  $T$   $[K]$  leaf temperature,  $T_{air}$  air temperature,  $T_{sky}$   $[K]$  sky temperature,  $T_{soil}$   $[K]$  soil temperature,  $K_{air}$   $[W m^{-1} K^{-1}]$  the thermal conductivity of air,  $E$   $[mol m_{leaf}^{-2} s^{-1}]$  transpiration flux, and  $\Delta x_i$   $[m]$  thickness of the boundary layer.

**Note:** Only the forced convective heat transfer is currently considered in HydroShoot since forced convection dominates free convection once wind speed exceeds roughly  $0.1 m s^{-1}$  (Nobel 2005). This wind speed threshold is generally exceeded during diurnal hours. However, under low wind conditions heat transfer may be underestimated.

### Sky and soil form factors: the *Pirouette Cacahuete* issue!

You may notice once you do your first run something like this:

```

GDD since budbreak = 1000 °Cd
Energy_budget: True
Hydraulic structure: True
Computing form factors...
... pirouette
... cacahuete
Soil class: Sand

```

This refers to the method used to calculate the lumped sky and soil form factors (respectively  $k_{sky}$  and  $k_{soil}$ ).

In order to reduce calculation costs,  $k_{sky}$  and  $k_{soil}$  are obtained by flip flopping the canopy:

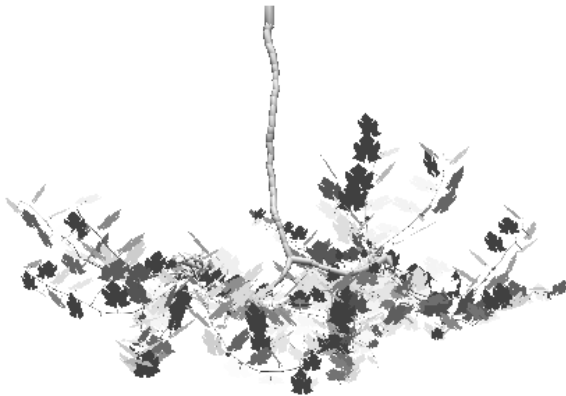
At first, the canopy is turned downwards. A unit irradiance is emitted from each sky sector and irradiance that is intercepted by a leaf  $i$  is assumed equivalent to the form factor between that leaf and the “soil”. In the second step, the canopy is turned upwards again and similarly, a unit irradiance is emitted from each sky sector. In this case, irradiance that is intercepted by a leaf  $i$  is assumed equivalent to the form factor between that leaf and the “sky”.

This method is clearly not 100% precise. It may need further improvements in the future.

## 3.2 Processes interactions

Interactions among the physiological processes occur.

Pirouette



Cacahuète



Fig. 3.2: Solving the interactions between leaf's water potential, transpiration rate and temperature !

From the one hand. Leaf water potential ( $\Psi$ ) exerts a control on stomatal conductance to water vapor ( $g_{s, H_2O}$ ) and, consequently, on transpiration flux ( $E$ ). However, the latter also determines how much water will flow through the hydraulic segments to be withdrawn from the soil, which affects the distribution of water potential across those segments (Ohm's law). Hence, we have a reciprocity between the distribution of water potential across the shoot (hydraulic structure) and transpiration fluxes from individual leaves.

From the other hand, leaf temperature ( $T$ ) determines the rate of leaf photosynthesis (Arrhenius functions) and stomatal conductance to both  $CO_2$  ( $g_{s, CO_2}$ ) and water vapor ( $g_{s, H_2O}$ ). This means that  $T$  affects also the transpiration flux  $E$  which also means that  $T$  exerts a further control on the hydraulic structure.

Putting it all together:

For a given initial temperature ( $T_0$ ) and soil water potential ( $\Psi_0$ ), a leaf can fix  $CO_2$  with a rate  $A_{n, 0}$  while having a stomatal conductance rate of  $g_{s, H_2O, 0}$ . The corresponding water flux transpired by this leaf will be  $E_0$ . Summed up across all leaves, plant transpiration will withdraw water from the soil, reducing thus soil water potential and resulting in a new  $\Psi$  value ( $\Psi_1$ ).  $\Psi_1$ , will hence impose a new stomatal conductance  $g_{s, H_2O, 1}$  and consequently a new transpiration flux  $E_1$ . Yet, this new  $E_1$  means that leaf temperature is  $T_1$ ... **REWIND!**

HydroShoot resolve this interactions iteratively until reaching steady rate values of  $A_n$ , and  $E$  ( implying steady state distribution of water potential cross the shoot). Fig. 3.3 shows how interactions between the hydraulic, energy and gas-exchange processes is handled in HydroShoot.

### 3.3 References

- Albasha R, Fournier C, Pradal C, Chelle M, Prieto J, Louarn G, Simonneau T, Lebon E. 2019.** HydroShoot: a functional-structural plant model for simulating hydraulic structure, gas and energy exchange dynamics of complex plant canopies under water deficit - application to grapevine (*Vitisvinifera* L.) in silico Plants, diz007, <https://doi.org/10.1093/insilicoplants/diz007>
- Evers J, Vos J, Yin X, Romero P, van der Putten P, Struik P. 2010.** Simulation of wheat growth and development based on organ-level photosynthesis and assimilate allocation. Journal of Experimental Botany 61: 2203–2216



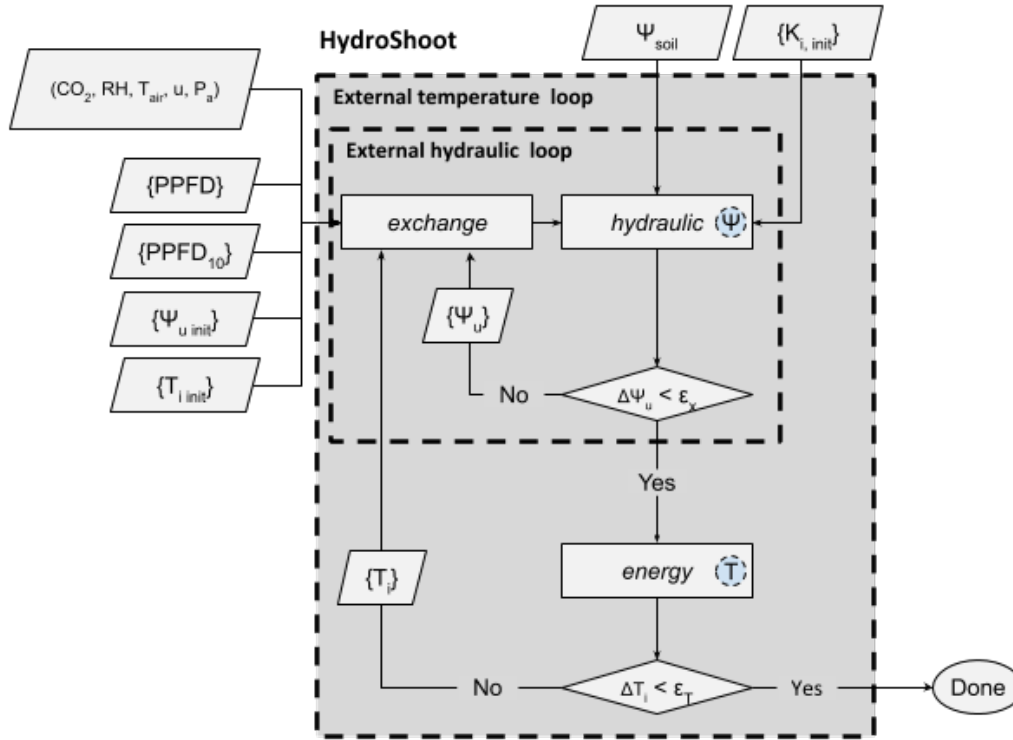


Fig. 3.3: Schematic representation of the numerical resolution of HydroShoot. Meteorological inputs that are common to all leaves are air temperature ( $T_{air}$ ,  $K$ ), air relative humidity ( $RH$ ,  $-$ ), air  $CO_2$  concentration [ $\mu mol\ mol^{-1}$ ], wind speed ( $u$ ,  $m\ s^{-1}$ ), and atmospheric pressure ( $P_a$ ,  $kPa$ ). Inputs per individual leaves are the absorbed photosynthetic photon flux density ( $PPFD$ ,  $\mu mol\ m^{-2}\ s^{-1}$ ) and  $PPFD_{10}$  the absorbed  $PPFD$  during the last 10 days.  $\Psi_u [MPa]$  is xylem water potential at the nodes between each pair of hydraulic segments.  $\Psi_{u, init} [MPa]$  is initial  $\Psi_u$ .  $\Psi_{soil} [MPa]$  is soil water potential.  $T_i [K]$  is leaf temperature.  $T_{i, init} [K]$  is initial  $T_i$ .  $K_{init} [kg\ s^{-1}\ m\ MPa^{-1}]$  is initial hydraulic conductivity of each segment.  $\epsilon_x [MPa]$  is the maximum allowable error of the estimation of xylem water potential. Finally,  $\epsilon_T [K]$  is the maximum allowable error of the estimation of leaf temperature. Circles inside module boxes indicate internal iteration loops. Symbols between curly brackets represent spatially structured variables.

- Farquhar G, von Caemmerer S, Berry J. 1980.** A biochemical model of photosynthetic CO<sub>2</sub> assimilation in leaves of C<sub>3</sub> species. *Planta* 149: 78–90.
- Leuning R. 1995.** A critical appraisal of a combined stomatal-photosynthesis model for C<sub>3</sub> plants. *Plant, Cell and Environment* 18: 339–355.
- Nobel P. 2005.** Temperature and energy budgets. In Nobel S, eds. *Physicochemical and Environmental Plant Physiology*. Elsevier Academic Press.
- Prieto J, Louarn G, Perez Peña J, Ojeda H, Simonneau T, Lebon E. 2012.** A leaf gas exchange model that accounts for intra-canopy variability by considering leaf nitrogen content and local acclimation to radiation in grapevine (*Vitis vinifera* L.) *Plant, Cell and Environment* 35: 1313–1328.
- Tyree M, Sperry J. 1989.** Vulnerability of xylem to cavitation and embolism. *Annual review of plant physiology and plant molecular biology* 40: 19–38.
- Tyree M, Zimmermann M. 2002.** Xylem structure and the ascent of sap, Springer Series in Wood Science.
- Yin X, Struik P. 2009.** C<sub>3</sub> and C<sub>4</sub> photosynthesis models: An overview from the perspective of crop modelling. *NJAS - Wageningen Journal of Life Sciences* 57: 27–38.

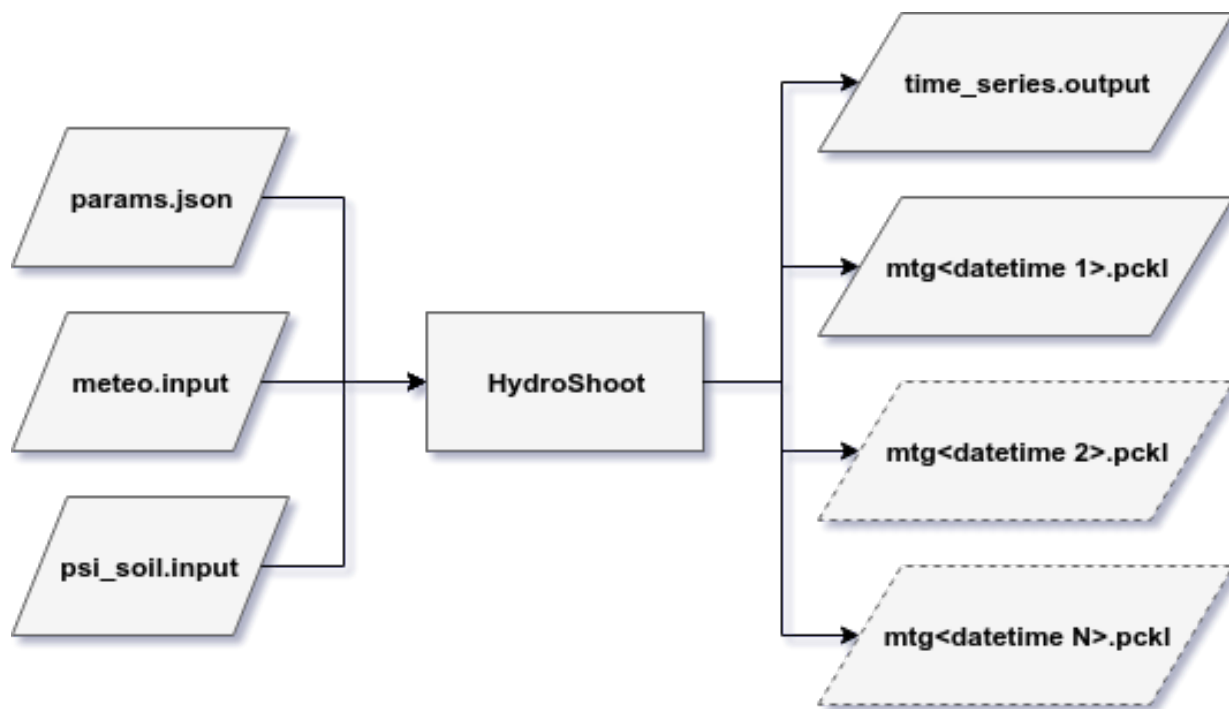


Fig. 4.1: Illustration of inputs and outputs of HydroShoot.

Three input files are required in order to run HydroShoot. The first contains all model parameters, the second meteorological data, and the third (optional) soil predawn water potential data. The model returns an undetermined number of files ( $\geq 3$ ) of two types of outputs.

## 4.1 Set the required files up

### 1. Model parameters

Almost all model parameters are setup in the **params.json** file. *params.json* is a *JavaScript Object Notation (JSON)* file that contains the following sections:

- “simulation”
- “phenology”
- “mtg\_api”
- “numerical\_resolution”
- “irradiance”
- “energy”
- “hydraulic”
- “exchange”
- “soil”

Each of the above sections refers to its homonym process. An exhaustive and thoroughly detailed description of all the parameters inside each section, their units and their expected values, are given in the *params\_schema.json* file (src/hydroshoot/). The reader is encouraged to refer to this file to know how exactly to fill up the *params.json* file.

### 2. Meteorological data (time series)

Meteorological data must be provided using a .csv file whose name must be given in the *params.json* file (“meteo” parameters). This file must contain the following columns: \* *time*: a *datetime* string having the format YYYY-MM-DD HH:MM:SS \* *Tac*: air temperature [ $^{\circ}C$ ] \* *hs*: relative humidity (%) \* *u*: wind speed [ $m\ s^{-1}$ ] \* *Rg*: solar radiation (shortwave irradiance) given even in [ $W_{global}\ m_{ground}^{-2}$ ], [ $W_{PAR}\ m_{ground}^{-2}$ ] or [ $\mu mol_{PPFD}\ m_{ground}^{-2}\ s^{-1}$ ]. The user must provide the unit of *Rg* in the *params.json* file (“E\_type” parameter).

### 3. Soil predawn water potential data (time series)

There are two ways to supply predawn soil water potential ( $\Psi_{soil}$ ) to the model:

- a. using an external file that must be named “psi\_soil.input” (the user will be able to give other names to the file in the future).
- b. using the keyword argument “psi\_soil” when calling the simulator:

```
from hydroshoot import model

model.run(g, working_directory, psi_soil=-0.5)
```

In this case, the value given in the ‘psi\_soil’ keyword overrides **all values** given in ‘psi\_soil.input’ file. HydroShoot will force soil water potential value **at each time step** to that given by the keyword ‘psi\_soil’.

## 4.2 Outputs

The first output file is a *comma-separated values* (csv) file named “time\_series.output” (only one file is returned) that contains the following time-dependent outputs:

- **time**: datetime string (YYYY-MM-DD HH:MM:SS)

- **An**: net carbon assimilation flux of the whole plant [ $\mu\text{mol s}^{-1}$ ]
- **E**: tranpiration flux of the whole plant [ $\text{g h}^{-1}$ ]
- **Rg**: absorbed shortwave irradiance by the whole plant [ $\text{W m}_{\text{ground}}^{-2}$ ]
- **Tleaf**: median leaf temperature [ $^{\circ}\text{C}$ ]

The second type of outputs is a pickle (pckl) file in which is stored mtg data **for each simulated time step**. Note that **pckl files do not contain geometry data**. Geometry is not currently stored as an output since the model expects it as an input.

## 4.3 Run the model

Let’s take the simple example provided in ‘~/example/potted\_grapevine/'. We will use for this example **architecture** and **display** modules provided with HydroShoot package (these packages may be removed in the future).

This example runs HydroShoot on a small potted grapevine canopy having two primary shoots.

Let’s build the mock-up using the digitalization data provided in “grapevine\_pot.csv” file:

```
from os import getcwd

from openalea.mtg import traversal
from openalea.plantgl.all import Scene
from hydroshoot import architecture, display, model

# Path for plant digitalization data.
g = architecture.vine_mtg('grapevine_pot.csv')

# Local Coordinates Correction
for v in traversal.iter_mtg2(g, g.root):
    n = g.node(g.Trunk(v, Scale=1)[0])
    theta = 180 if int(n.index()) < 200 else -90 if int(n.index()) < 300 else 0
    architecture.vine_orientation(g, v, theta, local_rotation=True)

# Scene rotation
for v in traversal.iter_mtg2(g, g.root):
    architecture.vine_orientation(g, v, 90., local_rotation=False)

for v in traversal.iter_mtg2(g, g.root):
    architecture.vine_phyto_modular(g, v)
    architecture.vine_mtg_properties(g, v)
    architecture.vine_mtg_geometry(g, v)
    architecture.vine_transform(g, v)
```

Display now the scene using **display** module, you should be having something like Fig. 4.2:

```
scene = display.visu(g, def_elmnt_color_dict=True, scene=Scene(),
                    view_result=True)
```

You’re now ready to run the model using the meteorological data provided in “meteo.input”, and forcing soil water potential to a fixed value of  $-0.5 \text{ MPa}$ . Ensure first that the model will run over one hour only by setting start and end dates of the simulation in the “params.json” file (“sdate”: “2012-08-01 11:00:00”, “edate”: “2012-08-01 11:00:00”).

```
model.run(g, str(getcwd()) + '/', scene, psi_soil=-0.5,
          gdd_since_budbreak=1000.)
```

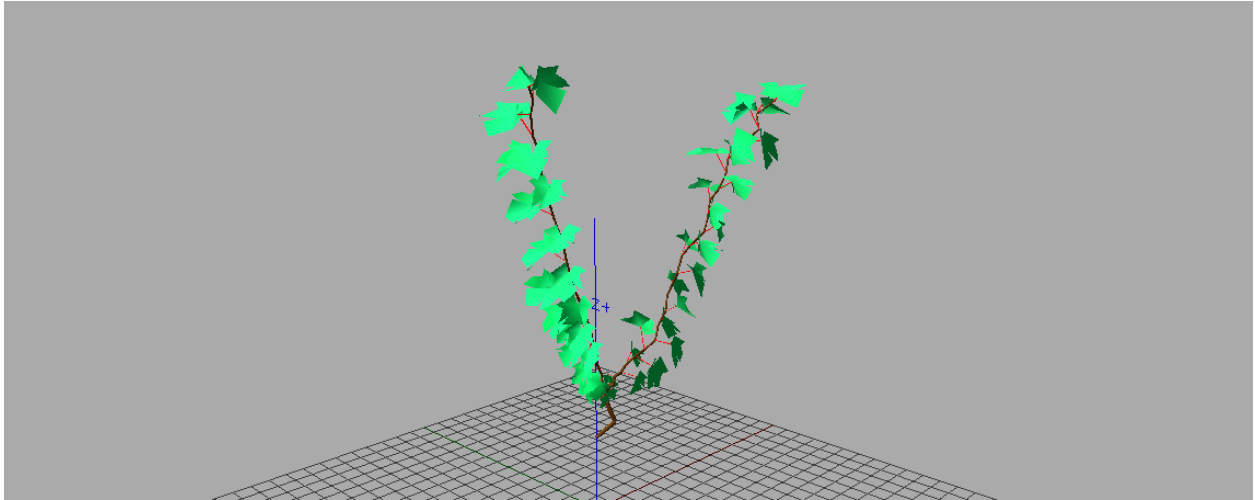


Fig. 4.2: Screen shot of the mock-up produced by the “potted\_grapevine” example.

You should now have created the ‘/output/’ folder where output files (“time\_series.ouput”, “mtg20120801110000.pckl”) are stored. “time\_series.ouput” file should contain close values to those below:

```
time;An;E;Rg;Tleaf  
2012-08-01 11:00:00;7.39720795547;183.455877322;84.8798347191;27.0144824618
```



## CHAPTER 5

---

### Indices and tables

---

- `genindex`
- `modindex`
- `search`