Universal differential equations for estimating terrestrial evaporation

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1. Introduction

Terrestrial evaporation (E)

- Crucial role in modulating climate dynamics and water resources.
- Not directly observable from space, limited in-situ observations.
- Challenging to model due to variety of atmospheric drivers and environmental stressors.
- Objective: Improve E modelling by leveraging the universal differential equation framework.

Approaches to modelling evaporation

Process-based models	Hybrid models	Machine learning
LSM: CLM, HTESSEL…	GLEAM4	FLUXCOM-X
RS: JPL-PT, PM-MOD…	3SEB-FR	

2. Universal differential equations

Universal Differential Equations (UDEs) combine process-based ordinary differential equations (ODEs) with data-driven universal approximators (U), such as neural networks, enabling the integration of physical models and machine learning.

State-space model

For the vector or state variables $\boldsymbol{x}$ with inputs $\boldsymbol{u}$, outputs $\boldsymbol{y}$ and parameters $\boldsymbol{\theta}$, the general state-space model (SSM) is given by:

$$\frac{d\boldsymbol{x}}{dt} = g(\boldsymbol{x}, \boldsymbol{u}, \boldsymbol{\theta})$$
$$\boldsymbol{y} = h(\boldsymbol{x}, \boldsymbol{u}, \boldsymbol{\theta}^*)$$

Depending on the model type, g is given by:

ODE	Neural ODE	UDE
$(g_1 \circ g_2 \circ g_3)(\boldsymbol{x}, \boldsymbol{u}, \boldsymbol{\theta})$	$U(\boldsymbol{x}, \boldsymbol{u}, \boldsymbol{\theta})$	$(g_1 \circ g_2 \circ U)(\boldsymbol{x}, \boldsymbol{u}, \boldsymbol{\theta})$

with g_i a process-based submodel.

Training data-driven universal approximators

Example: $U(\boldsymbol{x}, \boldsymbol{u}, \boldsymbol{\theta}_U)$ replaces $\boldsymbol{y}_{\text{int}} = g_3(\boldsymbol{x}, \boldsymbol{u}, \boldsymbol{\theta}_3)$

- Offline training: $\min_{\boldsymbol{\theta}_U} J(U(\boldsymbol{x}, \boldsymbol{u}, \boldsymbol{\theta}_U), \boldsymbol{y}_{\text{int,obs}})$
  - (+) Easier implementation: U trained independent of SSM
  - (-) $\boldsymbol{y}_{\text{int,obs}}$ does not always exist, possibly unstable hybrid model
- Online training: $\min_{\boldsymbol{\theta}_U} J(\boldsymbol{y}, \boldsymbol{y}_{\text{obs}})$
  - (+) Directly optimise on output of interest $\boldsymbol{y}$
  - (-) Need for SSM implemented in a differentiable programming framework to efficiently calculate $\frac{\partial J}{\partial \boldsymbol{\theta}_U}$

Differentiable programming frameworks

Programming frameworks compatible with automatic differentiation (AD) and/or adjoint models:

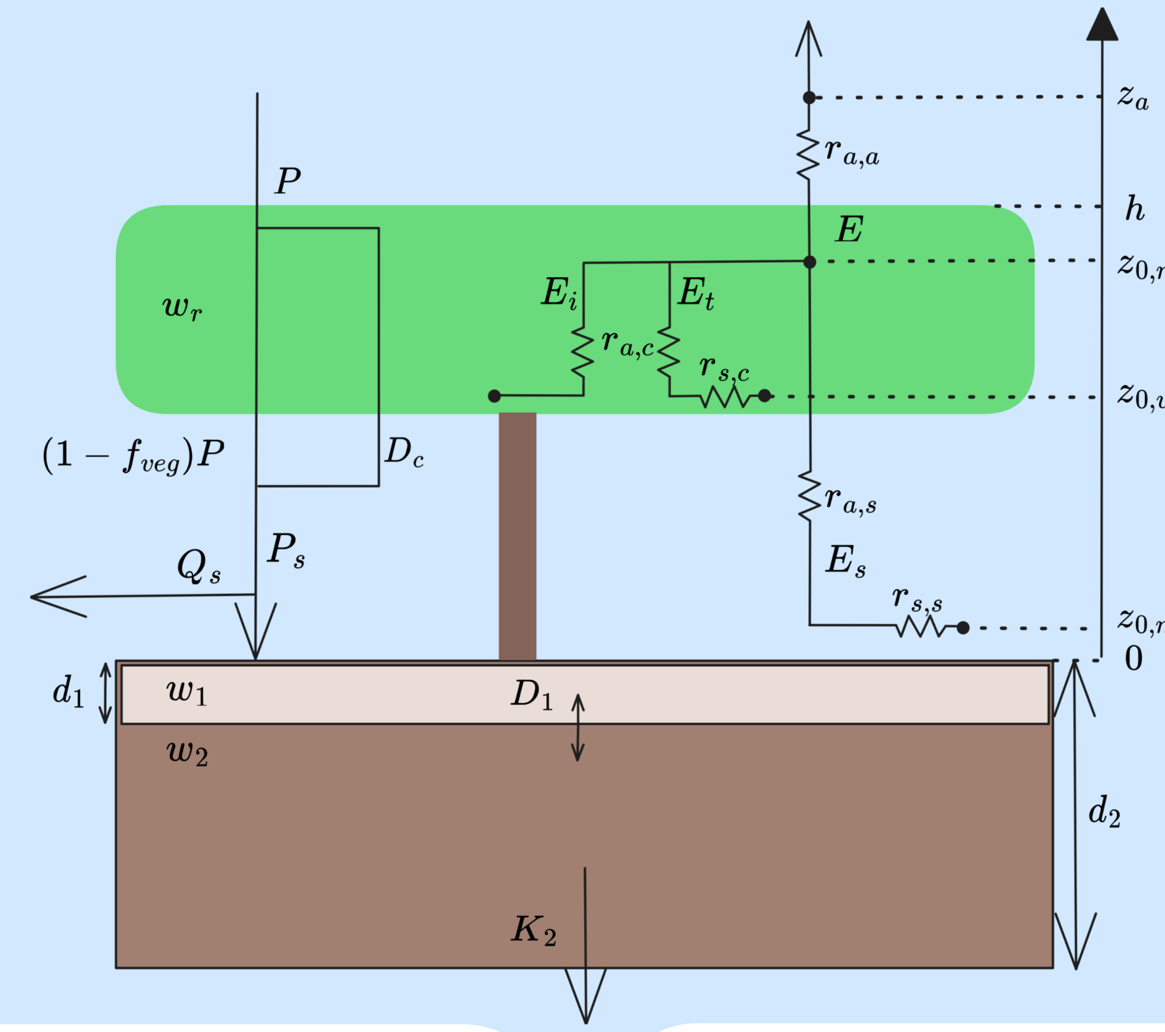
JAX · PyTorch · SciML (Framework of choice)

3. Model and method

Model description: 3SEB-FR

The three source energy balance force-restore (3SEB-FR) model aims to combine a relatively complex description of surface fluxes (3SEB) with a simpler soil moisture scheme (FR) to account for water stress limitation on E.

Subscript	Component
s	Soil
c	Canopy
a	Air



3SEB

The Shuttleworth-Wallace 2SEB model [1], which accounts for soil evaporation (λE_s) and transpiration (λE_t), is extended to explicitly include interception (λE_i). Each of the λE components is calculated using the Penman-Monteith equation (PM) with varying inputs of available energy (A) and aerodynamic/surface resistances (r_a/r_s):

$$\lambda E = \lambda E_i + \lambda E_t + \lambda E_s =$$
$$f_{wet}\lambda E_{PM}(0, r_{ac}, A_c) + (1 - f_{wet})\lambda E_{PM}(r_{sc}, r_{ac}, A_c)$$
$$+ \lambda E_{PM}(r_{ss}, r_{as}, A_s)$$

FR

The SSM is based on the ISBA-2L model [2]:

$$\frac{dw_1}{dt} = \frac{C_1}{\rho_w d_1}(P_s - Q_s - E_s) - D_1$$
$$\frac{dw_2}{dt} = \frac{1}{\rho_w d_2}(P_s - Q_s - E_s - E_t) - K_2$$
$$\frac{dw_r}{dt} = f_{veg}P - E_i - D_c$$

Following [3], a wet vegetation fraction (f_{wet}) is defined based on w_r.

Numerical ODE solution

Despite evidence that the numerical method chosen to solve the nonlinear differential equations of the hydrological SSM has a large effect on the numerical error, many hydrological models use ad hoc "sequential flux update" approaches [4]. By implementing the model in Julia, a wide variety of established numerical solvers is available via the DifferentialEquations.jl software and hence their effect on the simulation can be assessed.

Example: SSM with $\boldsymbol{x} = [x_1, x_2]^T$ and $g(\boldsymbol{x}, \boldsymbol{u}, \boldsymbol{\theta}) = g(\boldsymbol{x})$

Sequential flux updates

$$x_1(t + \Delta t) = x_1(t) + g([x_1(t), x_2(t)]^T)\Delta t$$
$$x_2(t + \Delta t) = x_2(t) + g([x_1(t + \Delta t), x_2(t)]^T)\Delta t$$
$$\Delta t = \text{fixed}$$

(-) Order of state updating matters

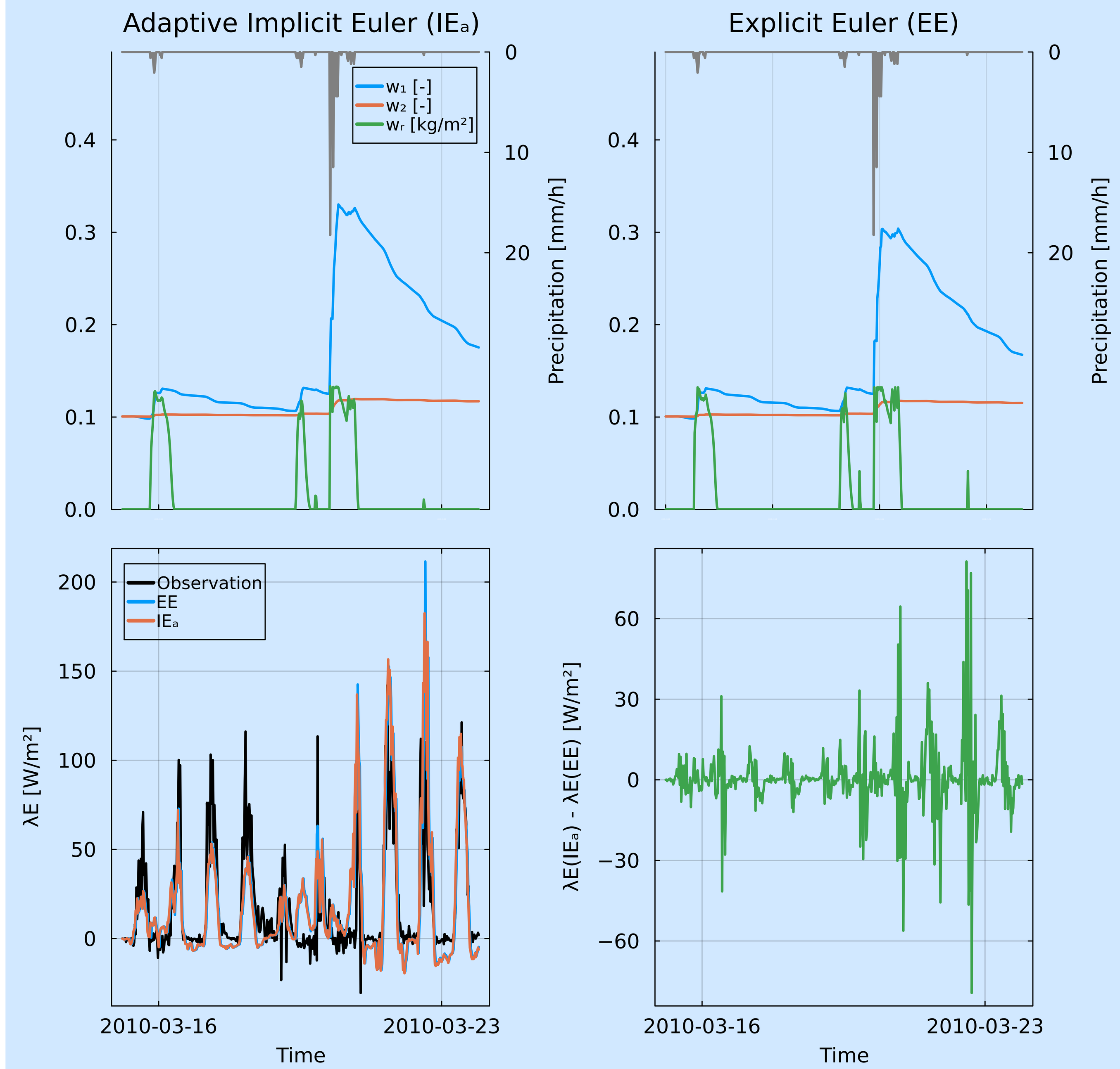
(-) No separation of conceptual model and numerical implementation
$\Rightarrow$ no distinction between conceptual and numerical error

Established numerical solvers

1) **Explicit Euler** (EE): $\boldsymbol{x}(t + \Delta t) = \boldsymbol{x}(t) + g(\boldsymbol{x}(t))\Delta t$, Δt = fixed
   - (+) Computationally cheap for large enough Δt
   - (-) Stability can require very small $\Delta t \Rightarrow$ hydrologists often apply manual corrections for states to be within physical bounds
2) **Adaptive Implicit Euler** (IE): $\boldsymbol{x}(t + \Delta t) = \boldsymbol{x}(t) + g(\boldsymbol{x}(t + \Delta t))\Delta t$, $\Delta t \neq$ fixed
   - (+) Stable method, avoids overshoots
   - (+) Computationally efficient adapting of Δt based on model stiffness to match user-defined error tolerance

4. Results

Model forcings and λE observations from the ICOS eddy covariance site BE-Bra from FluxDataKit [5] at 30' temporal resolution. Therefore, fixed-step schemes are applied with Δt =30'. The EE scheme is applied with manual state correction (cf. pane 3.).



- Difference in numerical scheme alters the simulated states and fluxes.
- Choice of forcing interpolation method affects stability of the ODE solver (not shown).

5. Future perspectives

Hybrid model development

- Leverage UDE framework to replace the empirical r_{sc} formulation by an online-trained U at the BE-Bra site.
- Extend the analysis to multiple eddy covariance sites, allowing the prediction of r_{sc} by U to be modulated based on static ecosystem characteristics.
- Benchmark the model predictions by comparing to an empirical machine learning method from [6].

Numerical considerations

- Further experiment with different numerical solvers considering numerical error, stability and computational expense.
- Explore the different options on how to calculate gradients of numerical solutions of ODEs outlined in [7] and assess how these interact with the solvers.

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https://github.com/olivierbonte/DifferentiableEvaporation