**Predictability and feedbacks of the ocean-soil-plant-atmosphere water cycle: deep learning water conductance in Earth System Model**

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## Focal Area(s)

This white paper responds to Focal Area 2. We seek to build predictive models of leaf and surface conductance of water by implementing deep learning (DL) data assimilation techniques. These new models would then be implemented in existing Land Surface Models (LSMs) and Earth System models (ESMs), generating novel water cycle feedbacks. In doing so, we would improve predictability of expected changes in land precipitation, soil moisture, and vegetation dynamics in the long-term, and the role of land cover on the impacts and feedbacks of extreme weather events in the short-term.

## Science Challenge

Improve the predictability and understanding of feedbacks and/or emergent properties that arise from the (ocean)-soil-plant-atmosphere water cycle continuum.

## Rationale

ESM predictions of the variations in land precipitation, soil moisture, and its impacts on vegetation dynamics are highly uncertain. This contrasts with predictions of factors that are more predictable such as increasing atmospheric $CO_2$, temperature, water demand (vapor pressure deficit), and sea level rise (IPCC, 2014). Because of these uncertainties in the water cycle, there is no consensus in ESMs as to whether future Earth will be browner (e.g., more deserts, savannas) or greener (e.g., more, or denser forests), where water will be, and whether water can be managed in a sustainable manner.

While substantial amounts of data are being collected at different spatial scales and at different time resolutions, we are not interrogating the data in a manner that enable us to discern unidentified emergent properties or identify scalable non-linear variables. For instance, the annual growth of atmospheric $CO_2$ concentrations is highly correlated ($r^2 = 0.72$) with terrestrial water storage (Humphrey et al., 2018). The causal relationships behind this correlation are not known and they emerge from interactions between the land and the atmosphere that are not yet understood. Other potential emergent properties of the land-atmosphere interactions in the water cycle include, for example, the role of vegetation driving ocean moisture far inland via the biotic pump mechanism (Pearce, 2020), or the effect of reduced soil moisture in drylands on convective initiation to enhance moisture transport into these drylands (Zhou et al., 2021). To implement these large scale feedbacks between soil moisture, land precipitation and vegetation in modeling, the use of ESMs in necessary, as offline studies uses predefined meteorological inputs (e.g., soil moisture, precipitation, temperature), and therefore turn off feedbacks (Berg & Sheffield, 2018).


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The mechanisms regulating leaf and surface conductance, which are key drivers of the water cycle at the land-atmosphere interface and potentially involved in all these emergent mechanisms, are not fully understood. Soil moisture and atmospheric water demand exerts a strong feedback on stomatal behavior, which in turn influences carbon assimilation in the short-term, and plant community composition in the long-term. In addition, frequency and intensity of extreme weather events are also a strong determinant of this feedback as plants adapt to survive extreme weather events by limiting their response to optimal conditions. Therefore, plants may saturate their response to water availability earlier than predicted. Importantly, while stomatal conductance is a critical process in climate models, future stomatal/surface conductance is largely uncertain, particularly given that it decreases with increasing temperature and atmospheric water demand or as atmospheric $CO_2$ rises.

Current models are either purely empirical (Ball et al., 1987) or based on optimal stomatal conductance by the plant, maximizing carbon gain while minimizing water loss (Medlyn et al., 2011). Though these models provide valuable estimates of stomatal conductance, multiple instances of non-conforming stomatal responses have been observed that are not captured by most current models. For example, unexpectedly high transpiration at night are widespread in terrestrial ecosystems and across multiple plant functional types (Caird et al., 2007; Dawson et al., 2007). Natural oscillations in environmental drivers (e.g. oscillations in light levels driven by predictable cloud cover) can interact with oscillatory tendencies in stomata guard cell biochemistry to produce higher, lower, or even chaotic stomatal opening compared with the expected response (Cardon et al., 1994). Additionally, transpiration can remain notably higher than predicted during drought in diverse seasonally-dry ecosystems (Fu et al., 2018; Neumann & Cardon, 2012), supported by hydraulic redistribution of water from deep to shallow soil through plant root systems at night. Furthermore, leaf and surface conductance can be uncoupled under certain boundary layer conditions (Berkelhammer et al., 2020).

Because of the large amount of data already at hand on vegetation conductance (from FLUXNET and other programs) some of these seemingly anomalous stomatal responses could become predictable as new data assimilation approaches, machine learning, and improved feature detection in data streams come online (for example by constructing DL dynamic assimilation models). In turn, applying new vegetation conductance responses could have substantial impact on (ocean-)soil-plant-atmosphere water cycle feedbacks at different temporal scales and under different atmospheric conditions that could help capture emergent mechanisms.

## Narrative

Next generation ESMs will be hybrid (Reichstein et al., 2019) and modular (Fisher & Koven, 2020), combining DL and mechanistic approaches, and allowing easier comparisons between ESMs, as well as understanding the impact of specific modules on simulations.

The first step is to create a dynamic module of DL models designed for data assimilation of surface and stomatal conductance, using a ModEx approach (dynamic: enabling generation of new models as new data become available, and new DL algorithms are developed). The DL models would be trained and tested using many databases (e.g., FACE sites, FLUXNET, Sapfluxet, and leaf level gas exchanges).

DL, the branch of machine learning that utilizes neural networks with multiple node/hidden layers, has proven to be a key factor towards the development of data-driven models, as opposed to traditional knowledge-driven models, making DL our choice for data assimilation. As an example, generative adversary networks have been used to emulate ESMs, showing their capacity of capturing and modelling complex interactions (Puchko et al., 2020). The potential of DL greatly scales with the size of the dataset, which gives a real value to the hybrid approach presented here. Given the amount of data currently available and its likely increase in the next decade with the arrival of new advanced technologies, the integration of machine learning algorithms can help build adaptable and evolutive models. Although the intrinsic quality of the DL 'black-box' has been a real brake to its adoption in scientific modelling, recent projects funded towards eXplainable AI (Gunning, 2017) are aiming at reversing this trend.

Beyond simple emulation, the simulation of a process at a lower spatial scale such as stomatal conductance with DL can benefit from these new approaches. The use of variational auto-encoders, a specific neural network that combines an encoder (reduction of dimensionalities of a dataset) and a decoder (generation of the output from reduced dimensionalities), can help understand the regulation factors involved in such mechanisms. Finally, recent studies on ‘saliency maps’ (Yamamoto, 2019) have shown the promises of novel methods where neural networks can be distilled to recover mathematical equations. Those formalisms could in turn be used to enhance process-based models for a better predictability (Bonan et al., 2011).

The second step is to implement the developed DL leaf conductance module in an ESM, instead of the Medlyn or Ball-Berry models, and use the developed DL surface conductance to constrain the ESM. The final step is to analyze the ESM output to understand how conductance generates emergent feedbacks at various scales between soil moisture, land precipitation and vegetation.

Communication and collaboration between empiricists and modelers in land surface models (LSM) need to be improved. A possible avenue is to go toward the use of a common modern programming language that is fast and dynamic. On top of engaging young scientists, empiricists and modelers could share their code more easily, and working with DL and visualization libraries would be more straightforward (Perkel, 2019; Schneider et al., 2017). Furthermore, modular LSM would allow empiricists to create their package for a module, hosted online (e.g. GitHub), which could be directly used by any LSM and ESM. Community cyberinfrastructure development (such as web platforms for visualization of data and ESM outputs, or online code repositories) will be key to building a new era of data-model integration, and empiricist-modeler collaboration, in order to have accessible, scalable, transparent tools that integrate the expertise of the whole community (Fer et al., 2021). In this future world of larger collaborations in open-source science, it will be important to adapt our metrics of contribution to research beyond authorship (Casari et al., 2021).

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## Suggested Partners/Experts (Optional)

Note that the authors have not contacted the suggested potential partners below.

- Belinda Medlyn, Western Sydney University, is the author of the widely used optimal stomatal conductance model, and PhD co-supervisor of the lead author of this whitepaper.
- The climate modelling alliance (https://clima.caltech.edu/, https://github.com/CliMA/ClimateMachine.jl), are working on building a new ESM using AI and new technologies (written in Julia).
- Markus Reichstein, who called wrote a perspective manuscript on hybrid models and included conductance as an example (in the references)
- Alexis Berg & Justin Sheffield, who wrote a manuscript about the importance of ESMs simulations to predict future soil drought and plant water stress (in the references)
- Joe Berry, author of the widely used Ball-Berry empirical model of stomatal conductance, is the PhD supervisor of Zoe Cardon, and supervisor of Miquel Gonzalez-Meler postdoc.

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