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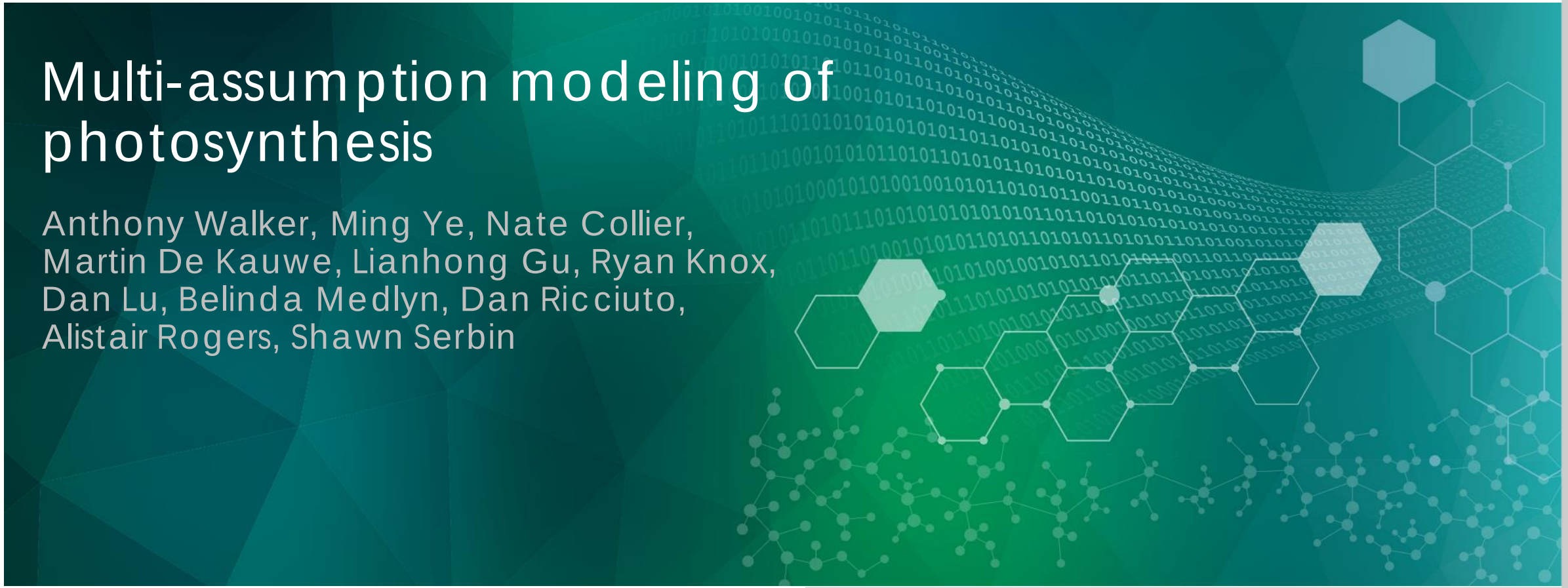
Multi-assumption modeling of photosynthesis

Anthony Walker, Ming Ye, Nate Collier, Martin De Kauwe, Lianhong Gu, Ryan Knox, Dan Lu, Belinda Medlyn, Dan Ricciuto, Alistair Rogers, Shawn Serbin



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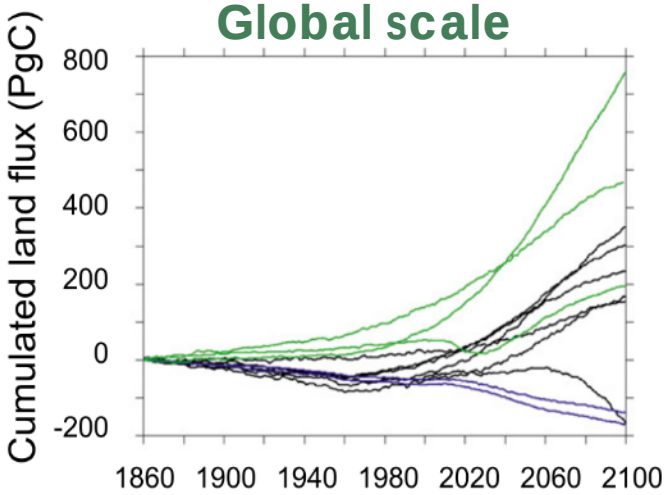
Identifying (structural) causes of model variability - Assumption Centered Modelling

PERSPECTIVE
PUBLISHED ONLINE: 21 MAY 2015 | DOI: 10.1038/NCLIMATE2621
nature climate change

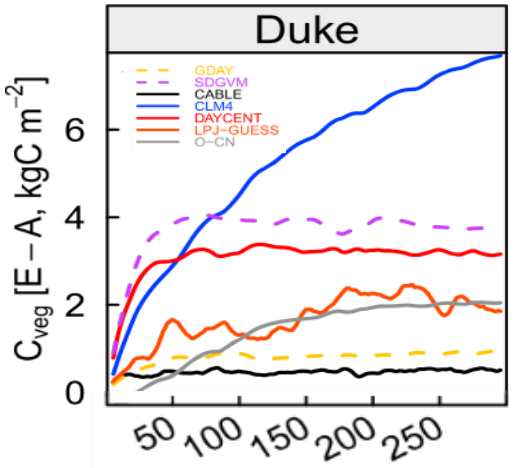
Using ecosystem experiments to improve vegetation models

Belinda E. Medlyn[1,2*], Sönke Zaehle[3], Martin G. De Kauwe[1], Anthony P. Walker[4], Michael C. Dietze[5], Paul J. Hanson[4], Thomas Hickler[6], Atul K. Jain[7], Yiqi Luo[8], William Parton[9], I. Colin Prentice[1,10], Peter E. Thornton[4], Shusen Wang[11], Ying-Ping Wang[12], Ensheng Weng[13], Colleen M. Iversen[4], Heather R. McCarthy[8], Jeffrey M. Warren[4], Ram Oren[14,15] and Richard J. Norby[4]

Global scale

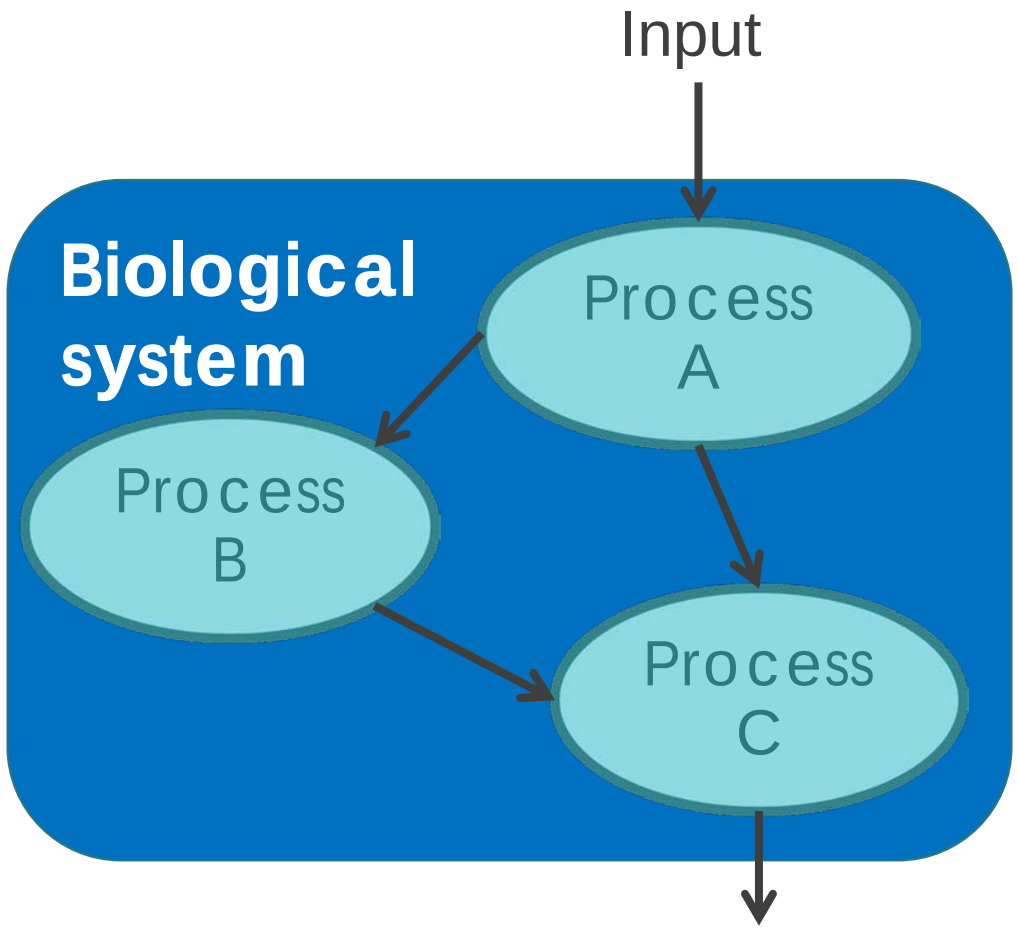


Forest stand scale



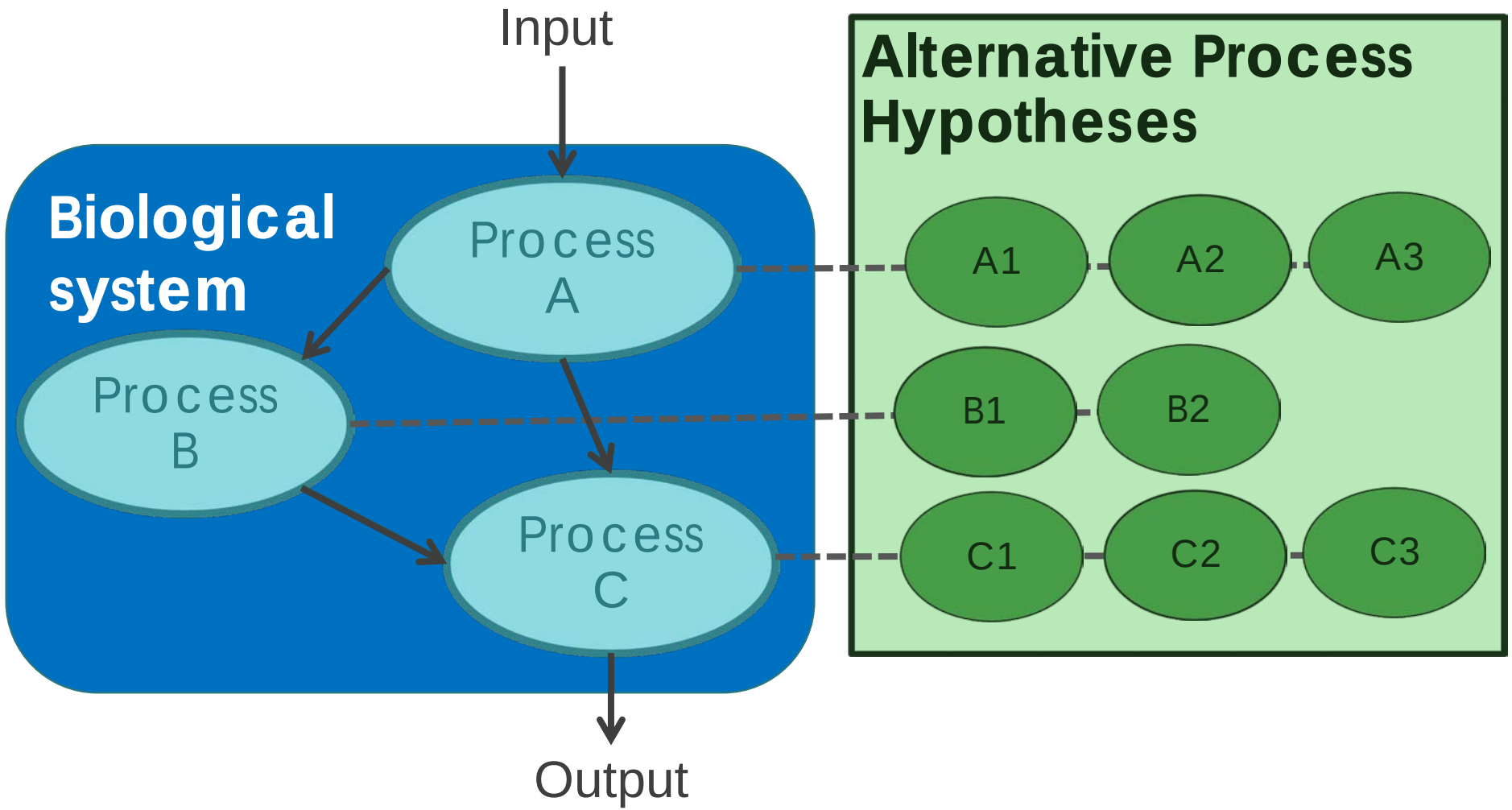
Years after step-change in CO_2

Systems are composed of multiple processes

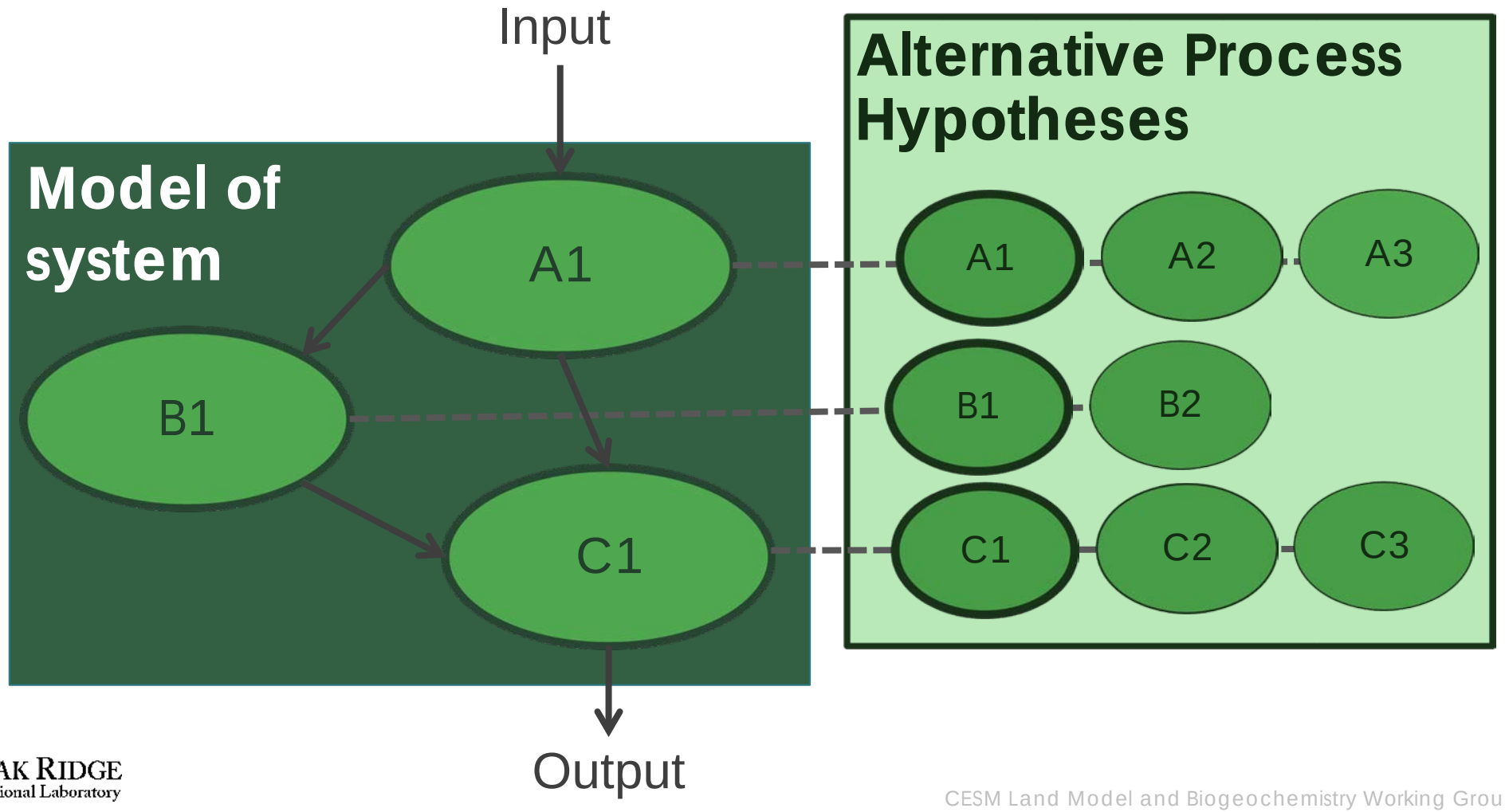


Systems are composed of multiple processes

Competing hypotheses can exist for each process



Systems are composed of multiple processes
Competing hypotheses can exist for each process
Resulting in multiple possible models of the system



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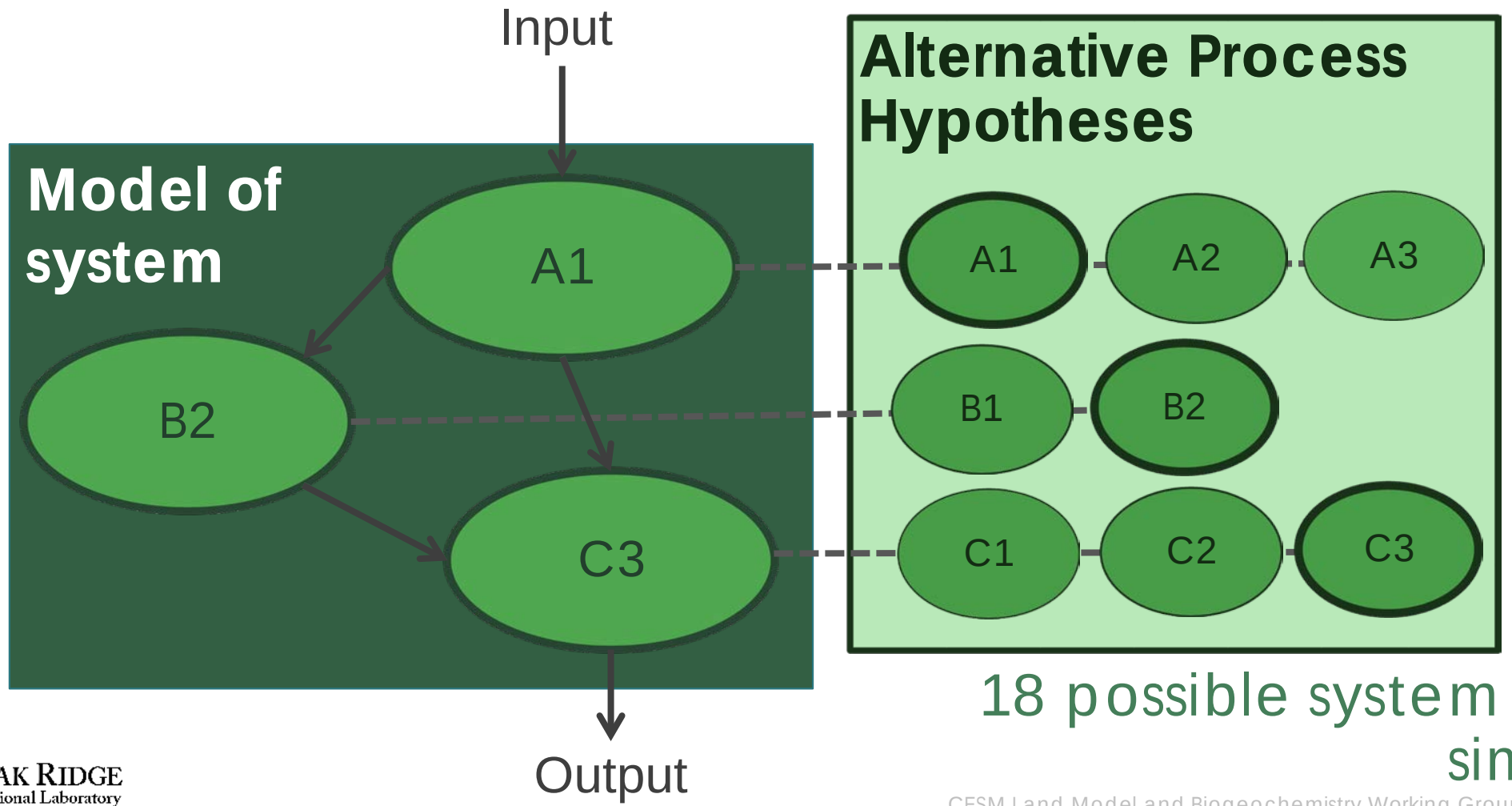


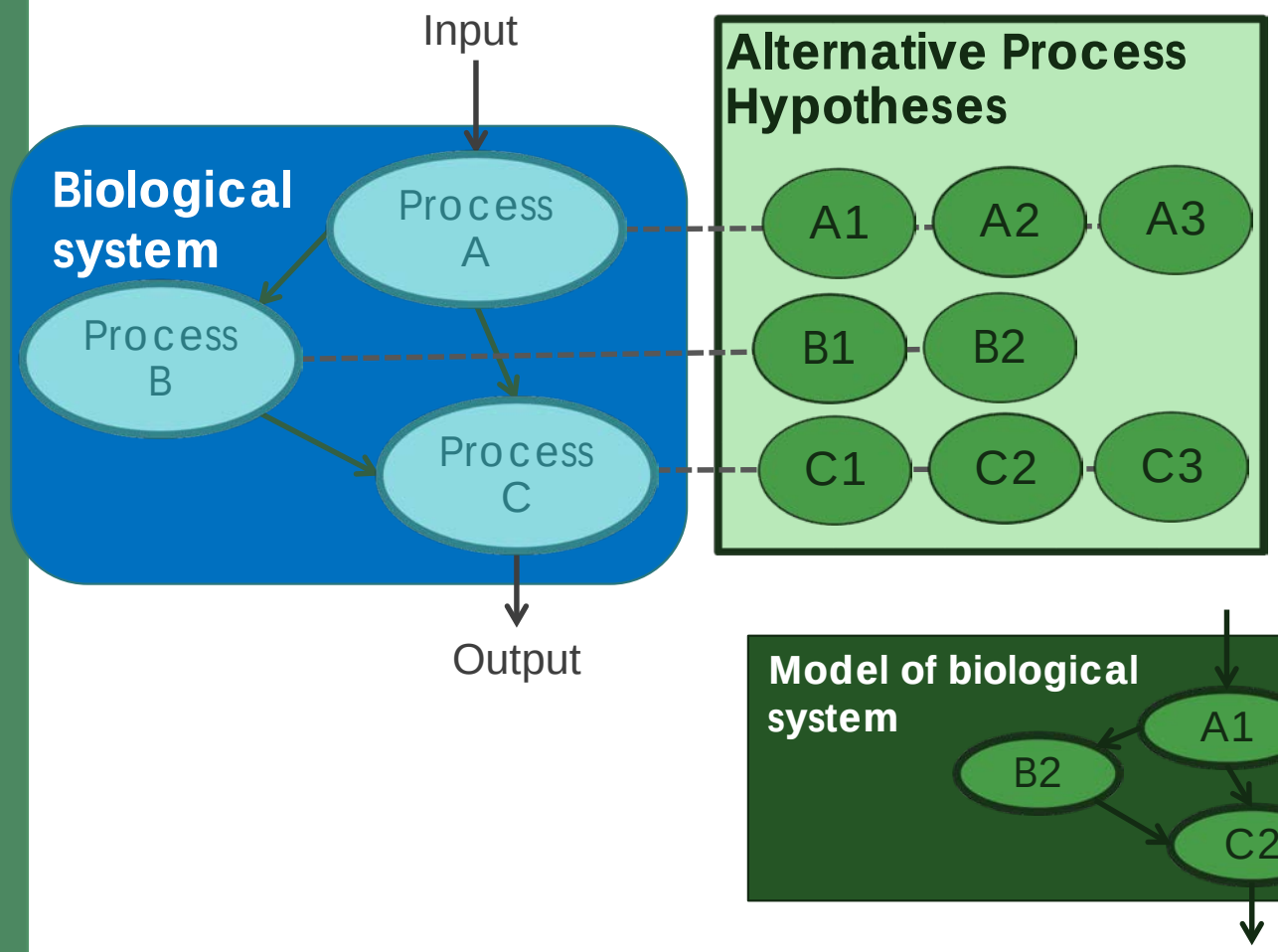
18 possible system models in this simple example

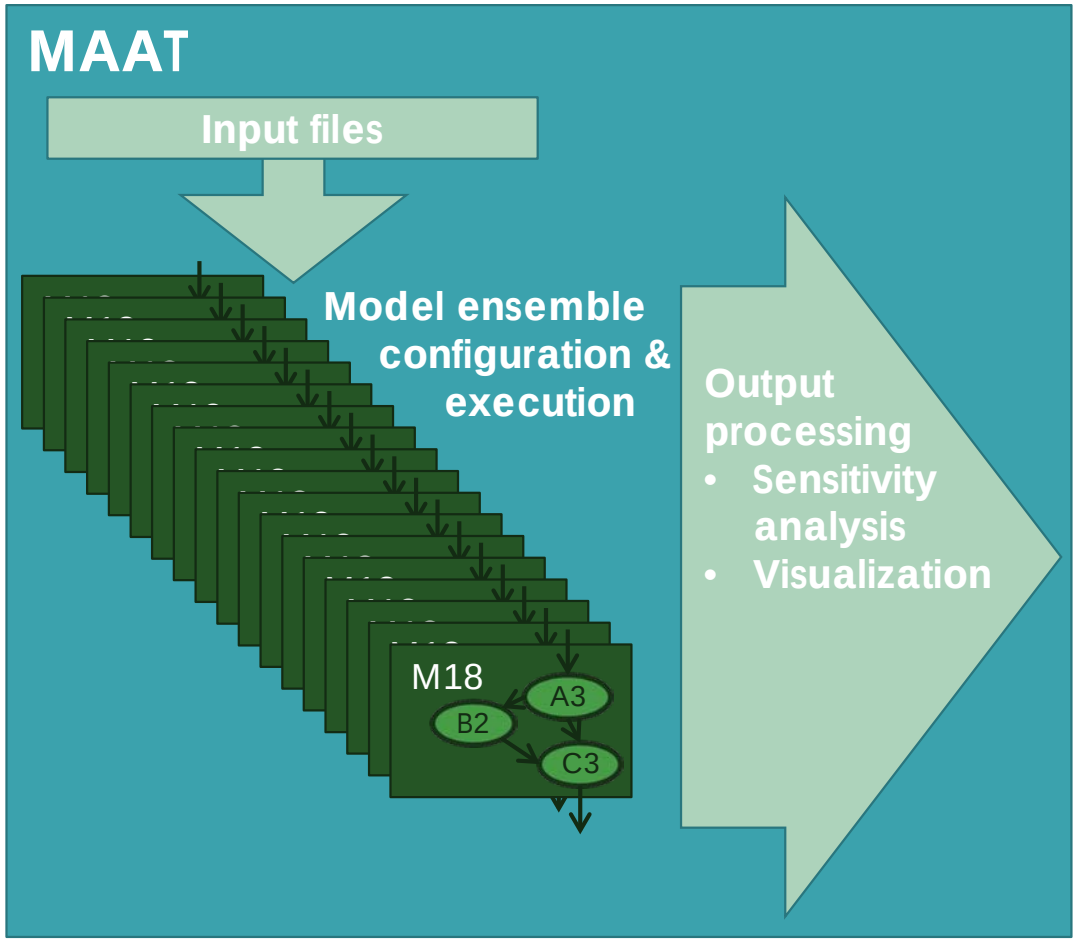
Multi-Assumption Architecture & Testbed (MAAT)

- A multi-assumption/multi-hypothesis software framework developed to allow on-the-fly system model configuration during runtime with:
  - alternative process assumptions/hypotheses,
  - parameters (traits),
  - boundary conditions
- Designed to generate large ensembles of possible models
- Framework is general and not system specific
- Encodes a novel algorithm for process-level global sensitivity analysis (Dai, *et al.* 2017 *WRR*) and global parameter sensitivity analysis (Saltelli *et al.*, 2010)

https://github.com/walkeranthonyp/MAAT
Walker et al. (2018) GMD

Multi-assumption / multi-hypothesis modeling





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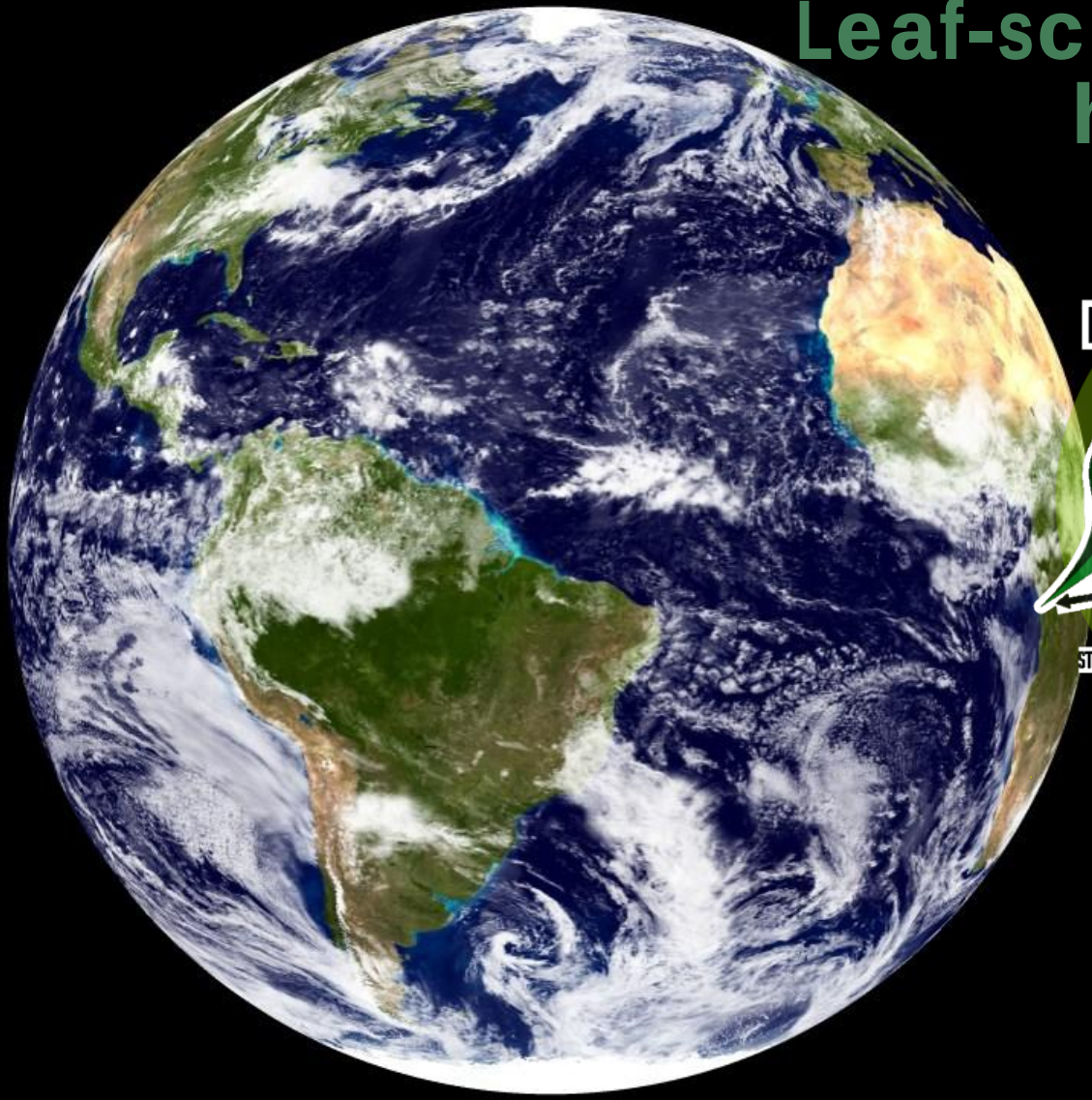
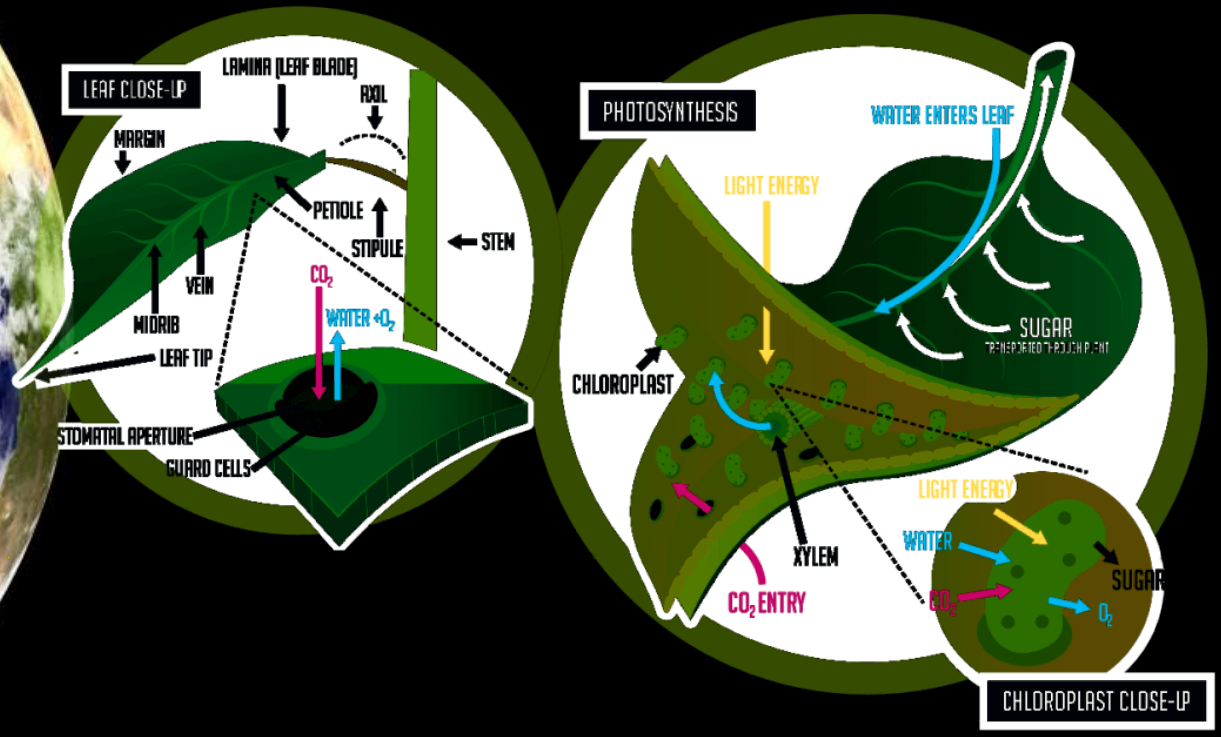
Leaf-scale photosynthesis models are the heart of Earth-System Land Models

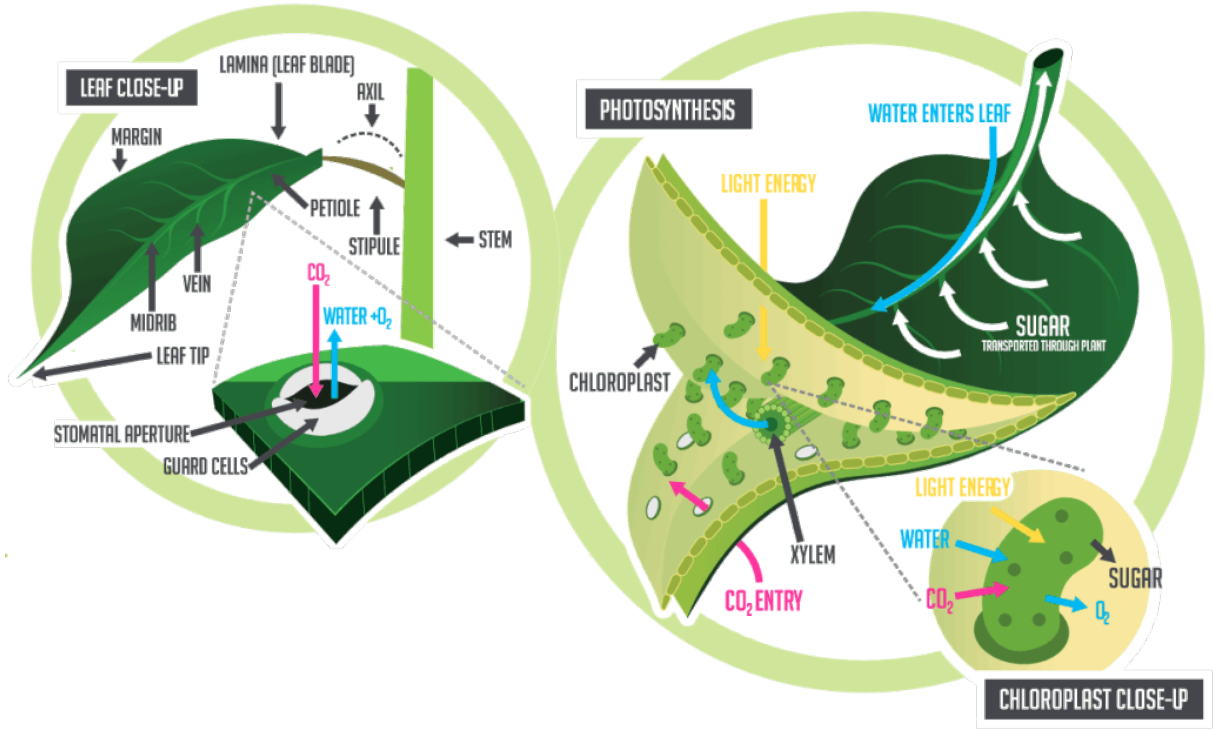




... to allow mechanistic simulation of physiological responses to increasing atmospheric CO_2

Multi-assumption leaf photosynthesis model

- MAAT contains a leaf-scale photosynthesis model
- Can mimic FATES, CLM(4.0 & 4.5), LM3, JULES, BETHY, + others … or can create and run all possible model combinations



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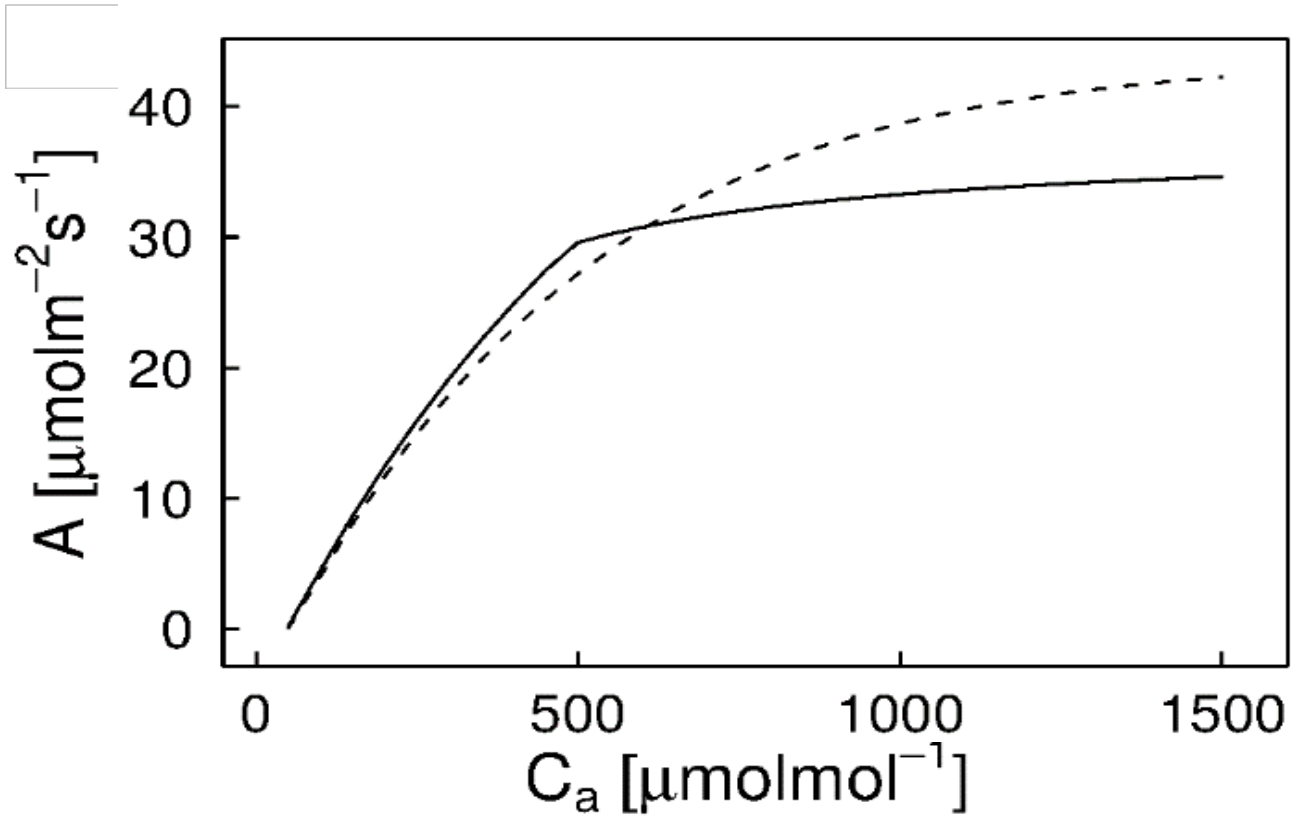
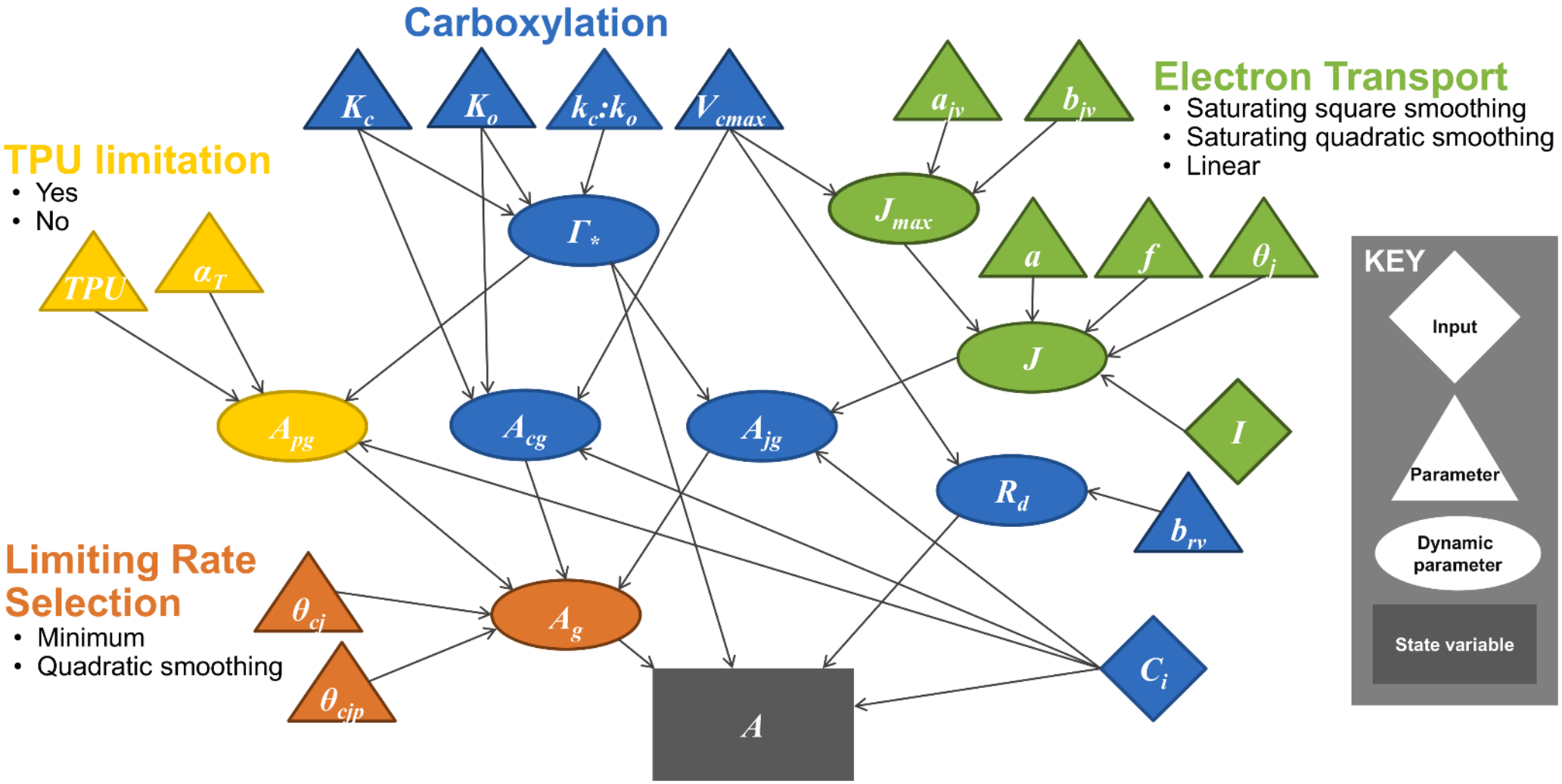
Farquhar or Collatz?
Two main flavors of photosynthesis model



Sensitivity analysis to compare Farquhar and Collatz

- Of leaf carbon assimilation and its response to atmospheric CO_2
- Four processes: electron transport (3 representations), carboxylation (1 representation), limiting rate selection (2 representations), and TPU limitation (2 representations)
- 12 system models
- 14 parameters across processes: common lit values +- 10%, uniform distribution
- Atmospheric CO_2 of 280, 400, 600 ppm and PAR 200, 500, 1000 μmol m^{-2} s^{-1}
- Stomatal conductance based on Medlyn et al. (2011) fixed g_0 and g_1
- 25 °C i.e. no temperature scaling
- Process SA 100M member ensemble, ~2hrs on 32 processors
- Parameter SA 86.4M member ensemble, ~2hrs on 32 processors

Farquhar enzyme kinetic model of C3 photosynthesis



Walker et al. (in prep)

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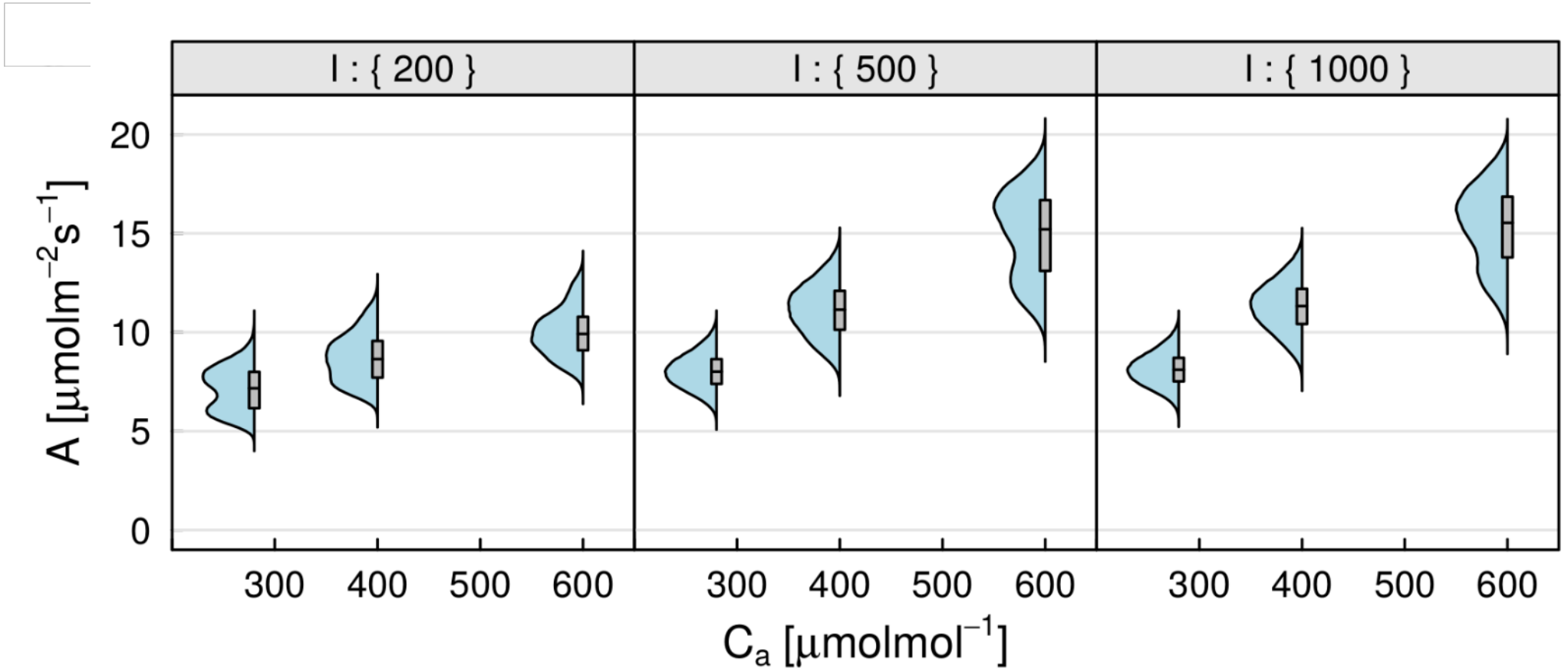
Parameter values

V_{cmax}	Maximum RuBisCO carboxylation rate	**45-55**	μmol CO_2 m^{-2} s^{-1}
K_c	Micaelis-Menten constant of RuBisCO for CO_2	**36.5-44.5**	Pa
K_o	Micaelis-Menten constant of RuBisCO for O_2	**25.0-30.6**	kPa
k_o:k_c	Ratio of RuBisCO turnover numbers for O_2 and CO_2	**0.19-0.23**	-
a_{jv}	Intercept $J_{max}$to V_{cmax} relationship	**26.2-36.0**	μmol q m^{-2} s^{-1}
b_{jv}	Slope $J_{max}$to V_{cmax} relationship	**1.48-1.80**	mol q mol^{-1} CO_2
a	Leaf absorbtance of visible solar radiation	**0.72-0.88**	-
f	Fraction of absorbed light not absorbed by photrosystems	**0.207-0.253**	-
θ_j	Electron transport smoothing	**0.81-0.99**	-
θ_{cj}	Assimilation rate smoothing 1	**0.81-0.99**	-
θ_{cjp}	Assimilation rate smoothing 2	**0.81-0.99**	-
TPU	Triose phosphate utilisation	**0.150 – 0.184 V_{cmax}**	μmol P m^{-2} s^{-1}
α_{tpu}	Fraction of phosphate exported from chloroplast not returned	**0.45-0.55**	-
R_d	Dark respiration	**0.150 – 0.184 V_{cmax}**	μmol CO_2 m^{-2} s^{-1}

Variability in carbon assimilation



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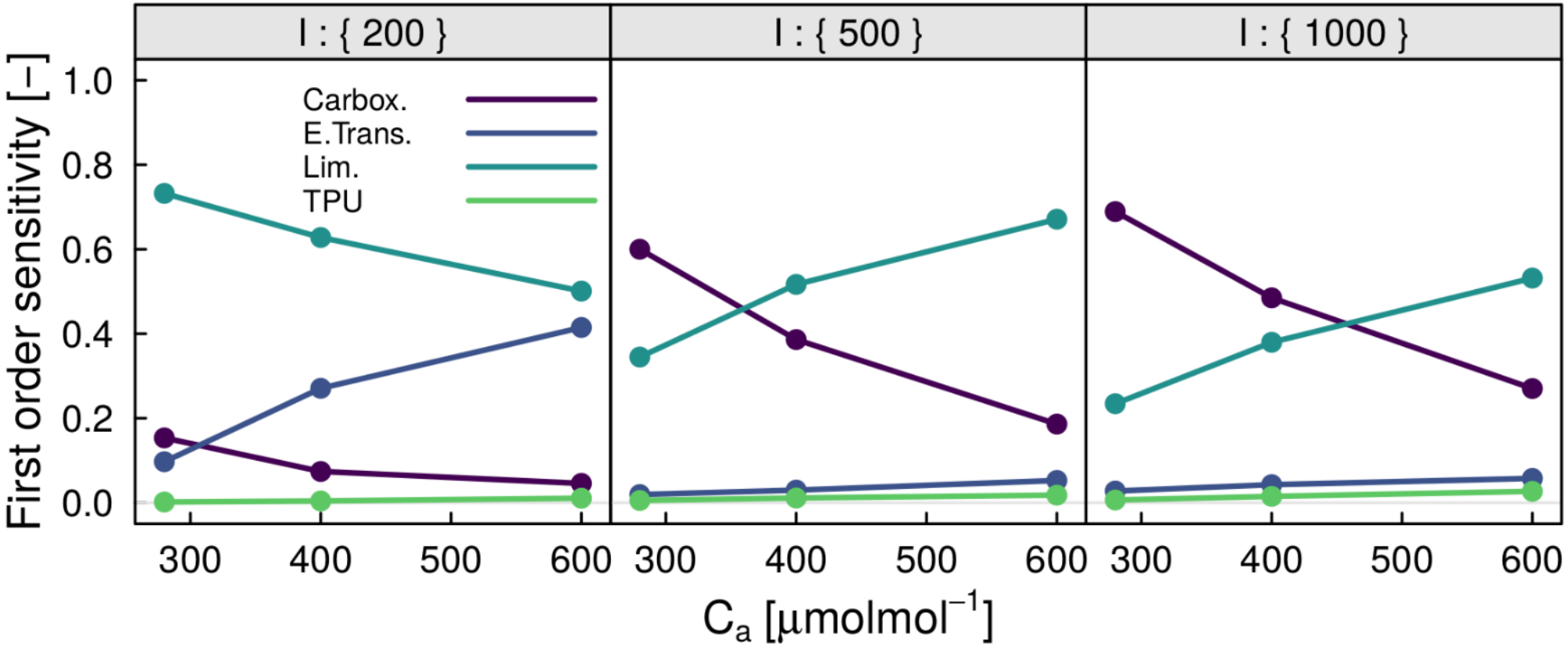
Assimilation sensitivity to processes



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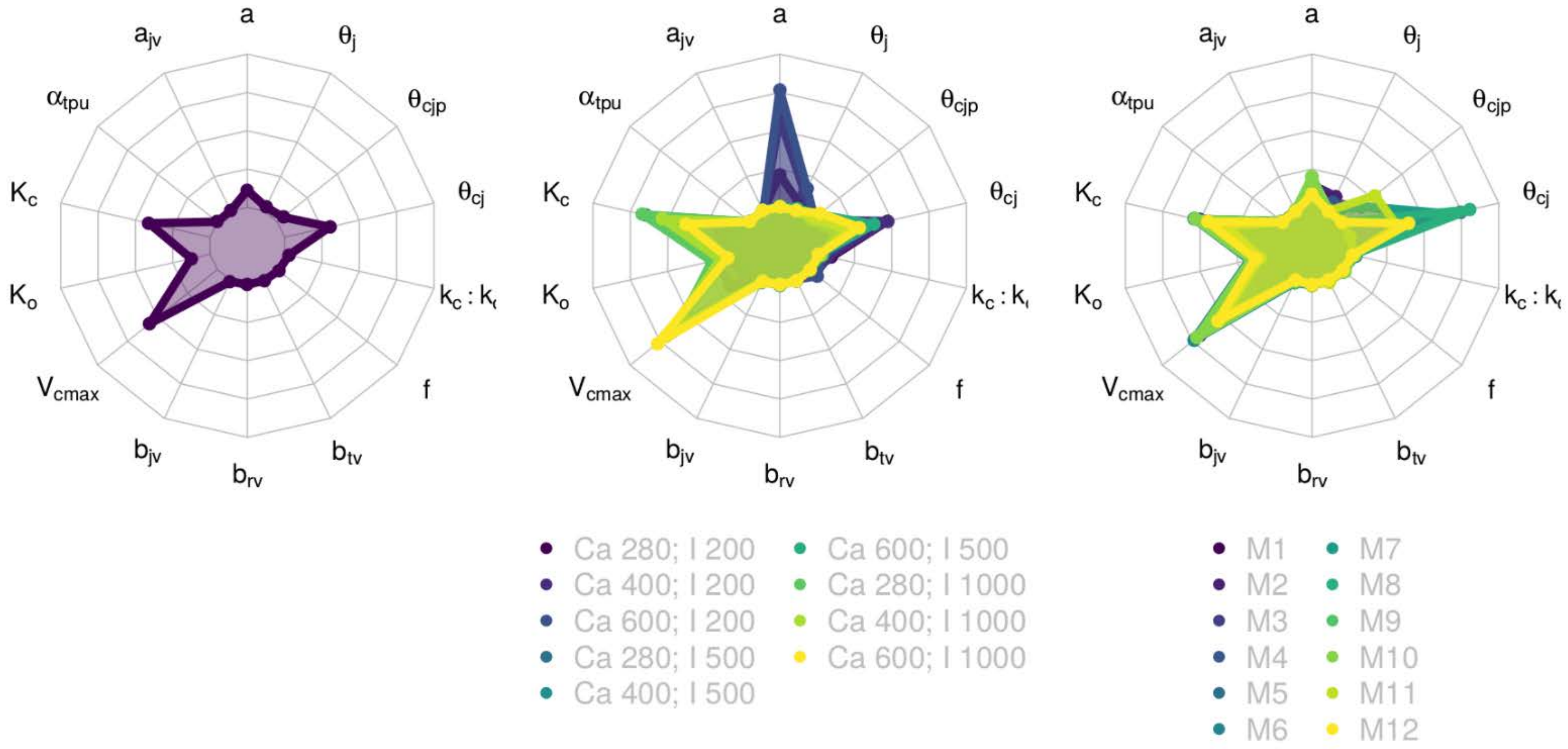
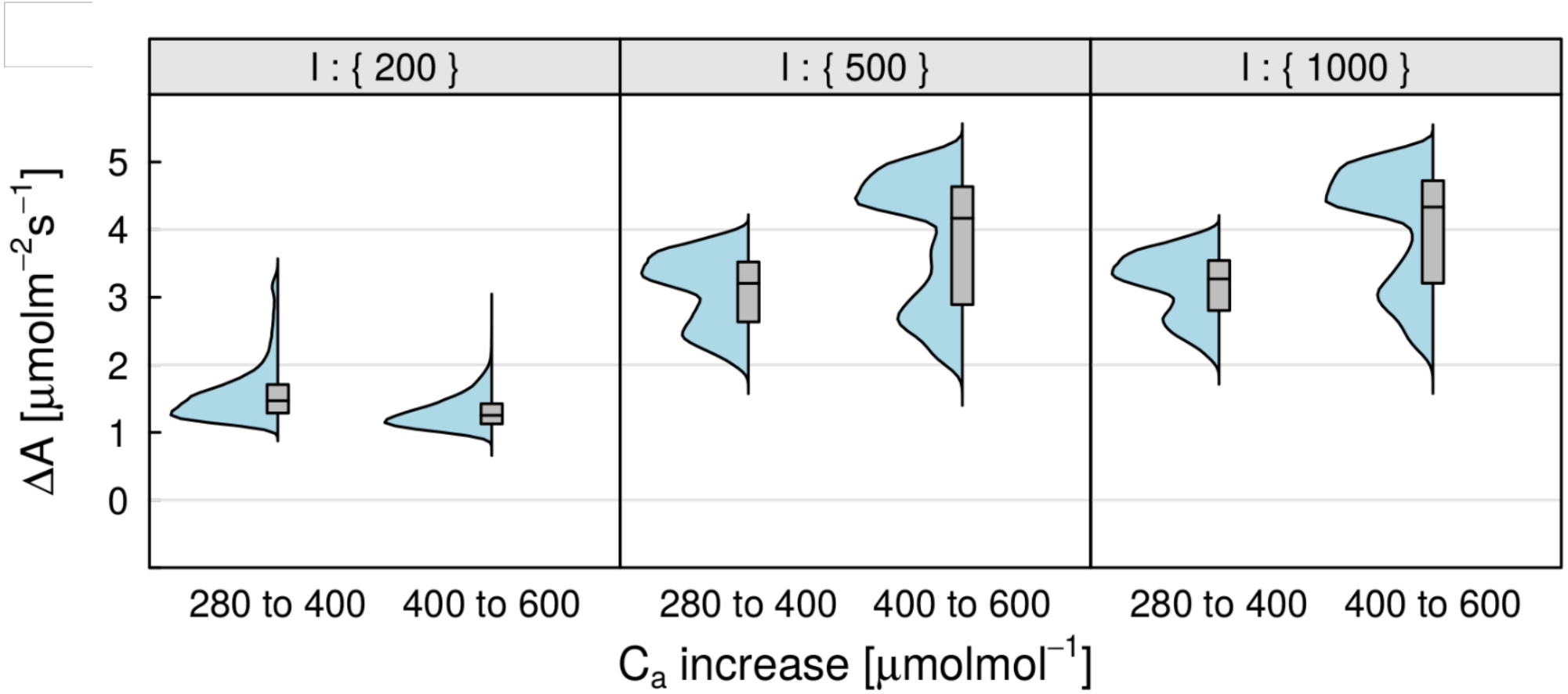
Assimilation sensitivity to parameters



Variability in assimilation response to CO_2 increase



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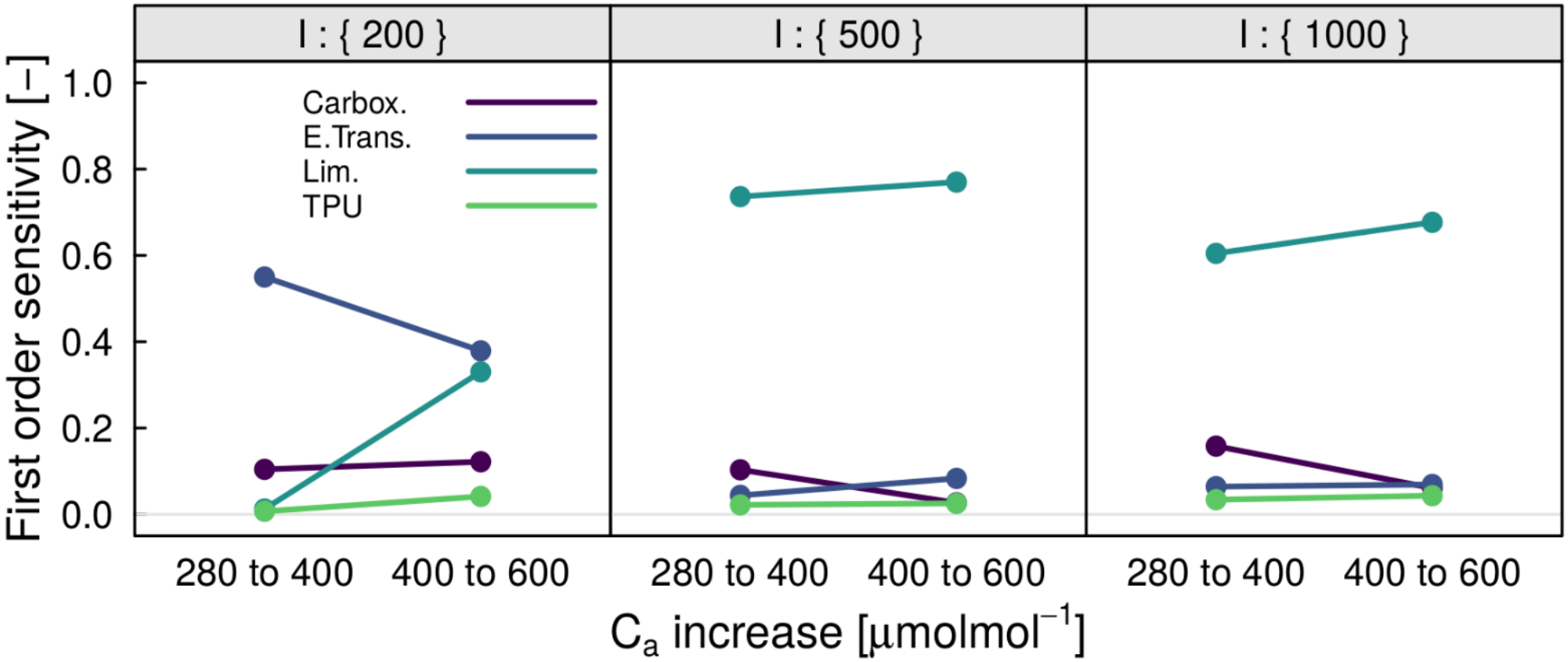
Assimilation response sensitivity to processes



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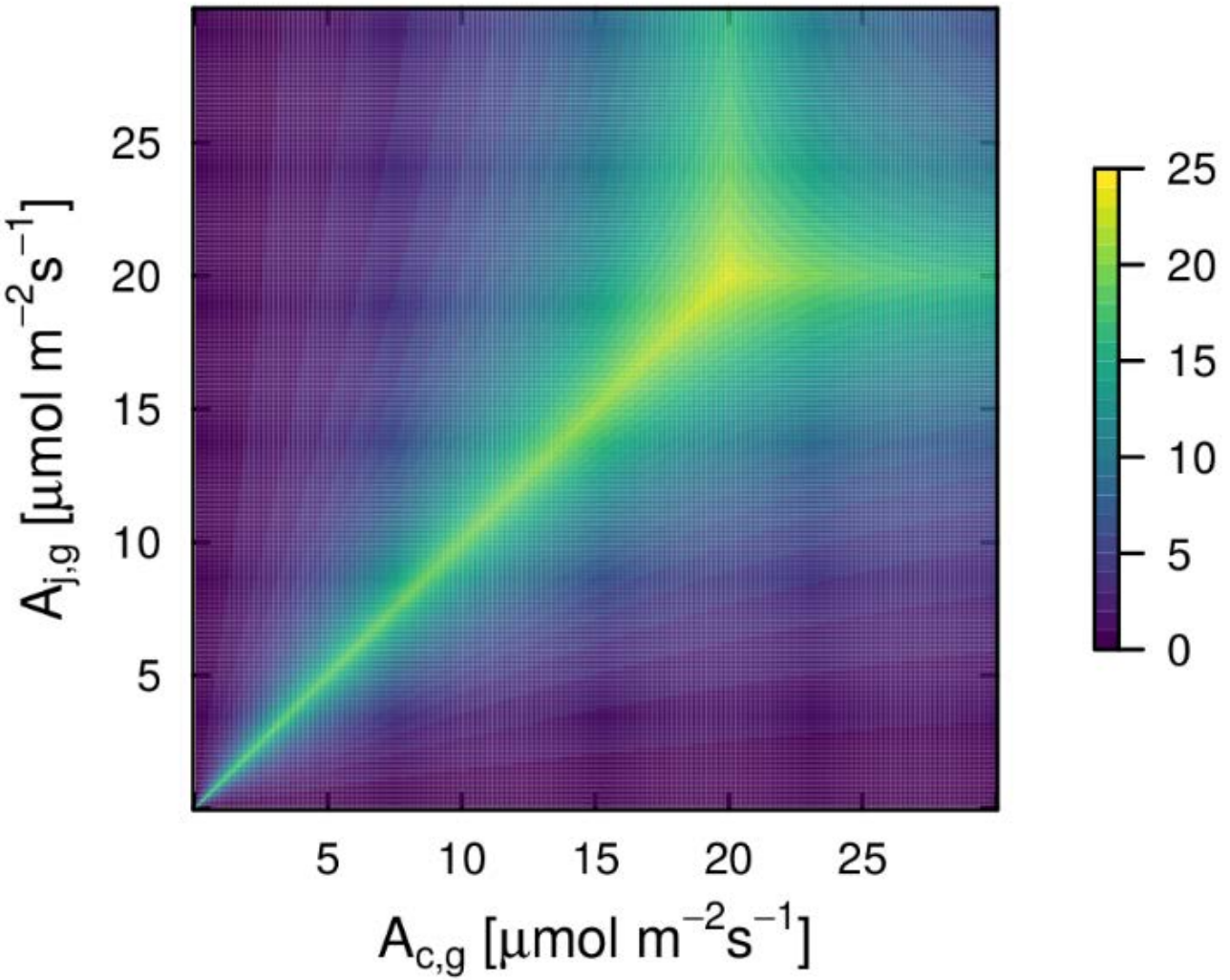
Gross assimilation reduction with smoothed vs. minimum limiting rate selection



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Summary

- Competing hypotheses are a key component of model variability / predictive uncertainty.
- Even for a relatively well-understood model of photosynthesis, multi-hypothesis methods have revealed substantial variability and surprising sensitivities.
  - i.e. sensitivity to the non-mechanistic process of limiting rate selection (under the conditions of the SA, environment, parameter values, ± 10 %).
- Limiting rate selection?
- With tools like MAAT (and others) the influence of competing hypotheses can be approached in a less *ad hoc* way.
- Allow rapid detailed investigation: e.g. faster photosynthesis solve.

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Thank you.

Terrestrial Ecosystem Science SFA

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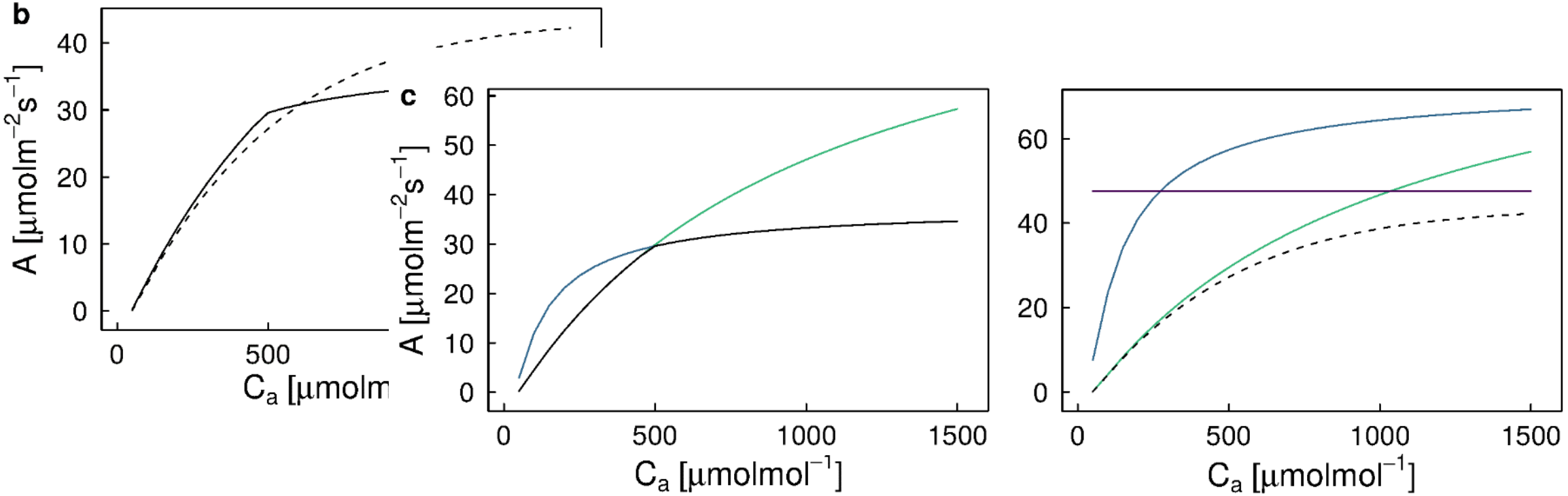
github.com/walkeranthonyp/MAAT

Farquhar or Collatz?
Two main flavors of photosynthesis model



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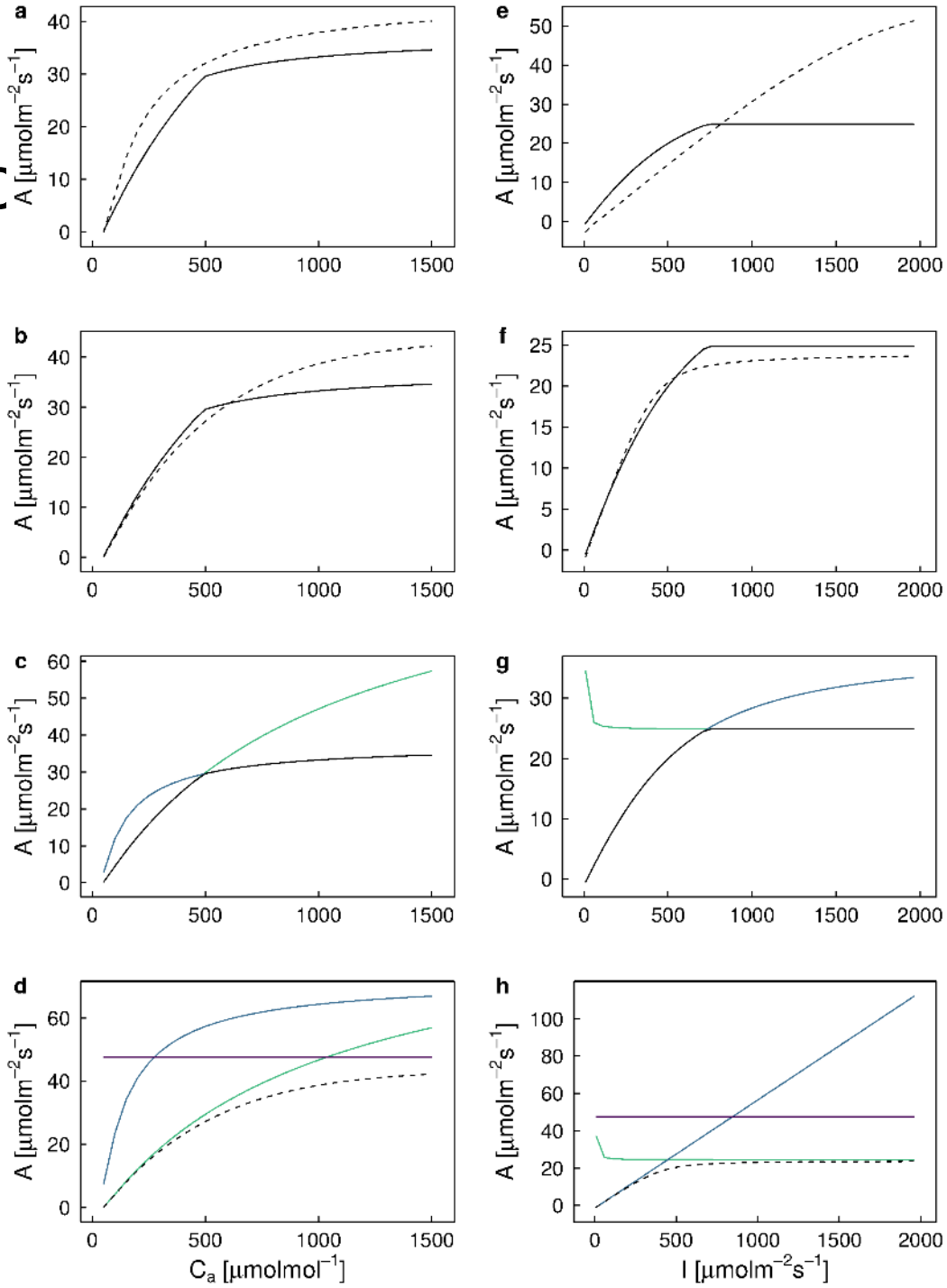

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Faster photosynthesis solve

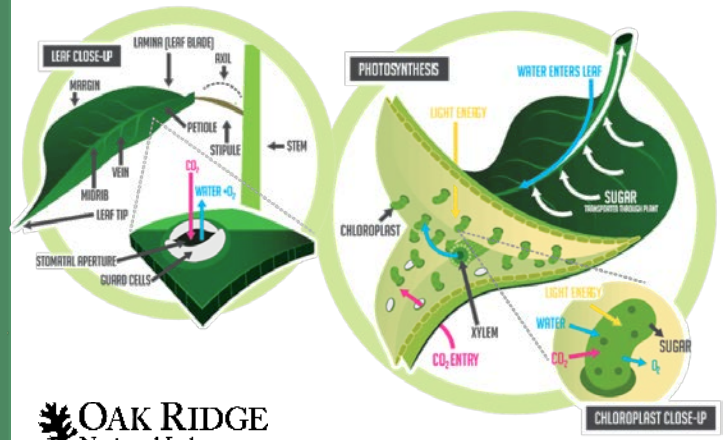
Leaf-scale photosynthesis models can be costly to solve & are solved many times at each timestep

Canopy scaling requires multiple leaf solves:

10 FATES
2 CLM
LAI SDGVM

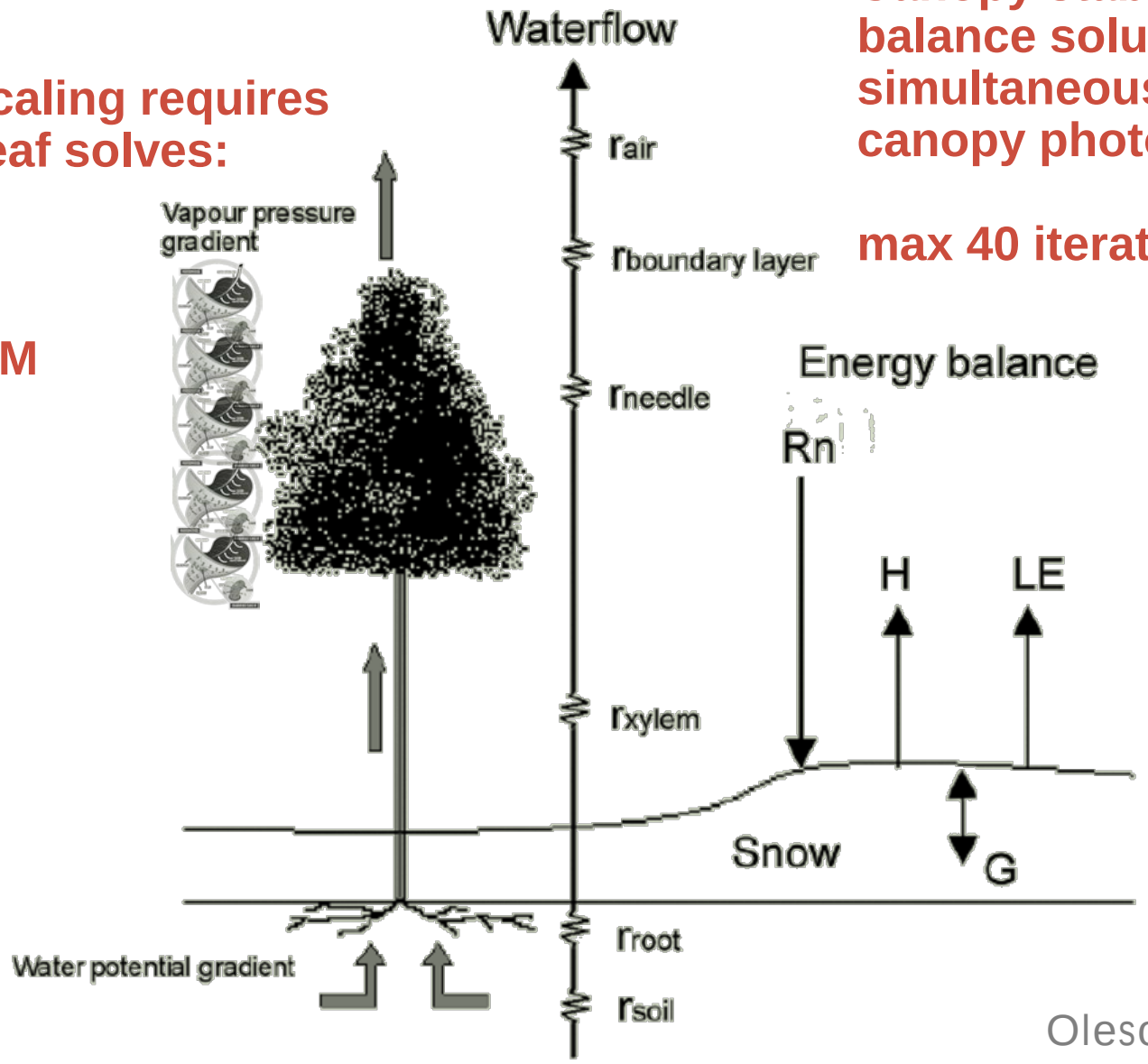
Leaf A numerical solution:

max 5 iterations FATES
max 40 iterations CLM



Canopy stability/energy balance solution requires simultaneous solve of canopy photosynthesis:

max 40 iterations in CLM



Oleson et al., 2013

A maximum of 2000 leaf photosynthesis calculations (400 solves) per timestep

Time spent in CLM5 on canopy stability solve

- Prescribed vegetation mode (CLM5SP) - 26%
- Prognostic biogeochemistry (CLM5BGC-crop) - 8%
- Prognostic BGC with isotopes (CLM5BGC-crop-iso) - 4%

D. Lawrence, pers. comm.

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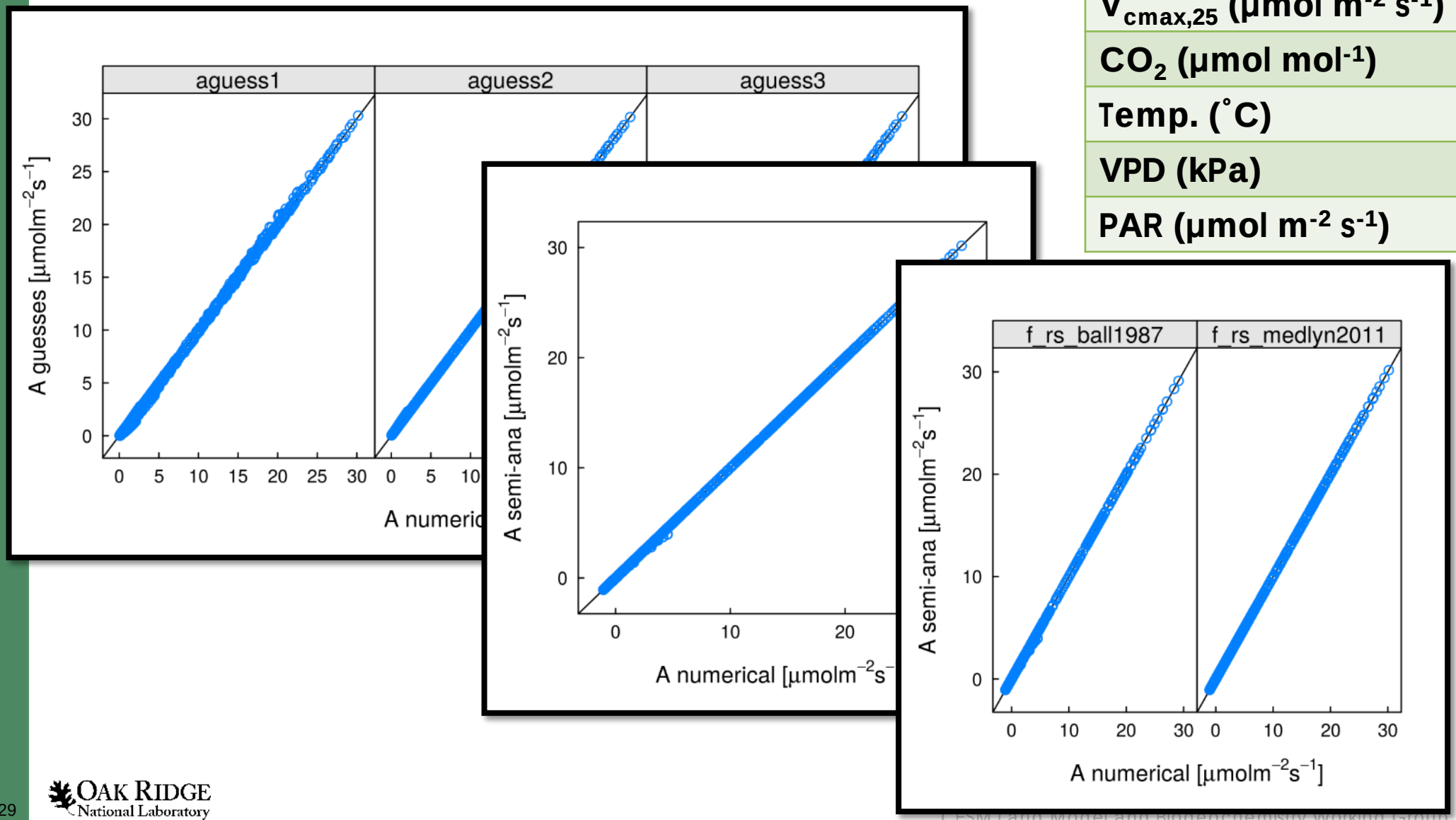
D. Lawrence, pers. comm.

Semi-Analytical Method: Educated guess, guaranteed span

g_s function	Medlyn, Ball
Lim. Rate selection	Farquhar, Collatz
$V_{cmax,25}$ (µmol m^{-2} s^{-1})	10 to 100 by 10
CO_2 (µmol mol^{-1})	50, 400, 1000
Temp. (˚C)	2, 25, 40
VPD (kPa)	0.1, 1, 3
PAR (µmol m^{-2} s^{-1})	10, 500, 1000

9720 combinations



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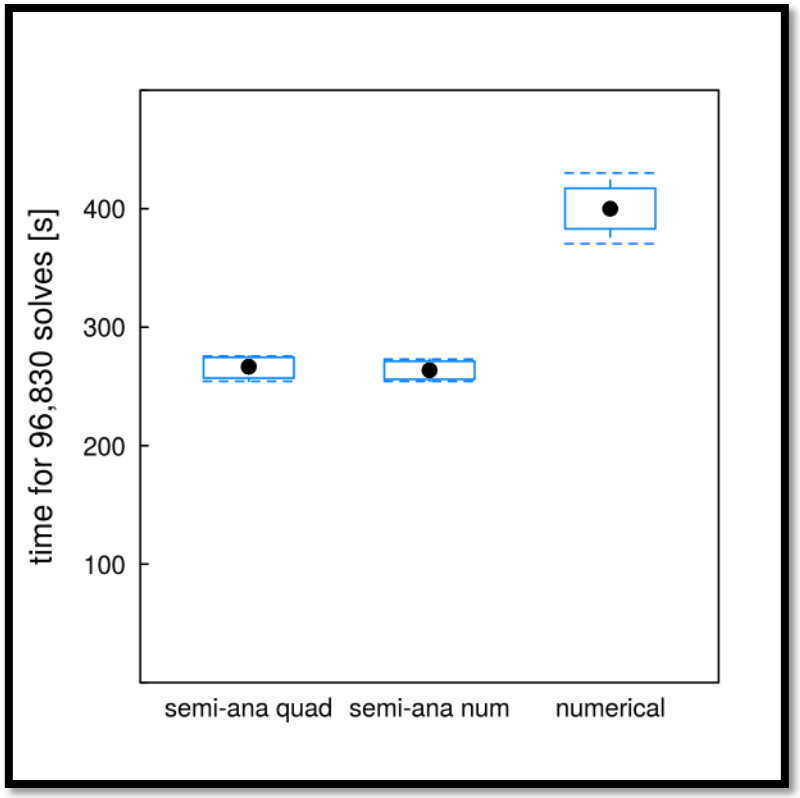
Speed improvement over numerical solve

MAAT ~34 % decrease in leaf solve runtime



FATES / CLM ~? %

Summary

- Developed a method (EGGS) to solve leaf photosynthesis semi-analytically
- Accurate (>99.9 % cases), 34 % speed increase in solves
- Need to fine tune algorithm when initial guess < 0
- Final algorithm development in MAAT, translate to FATES & test