## Applying Computational Efficient Schemes for Biogeochemistry ACES4BGC

Philip Cameron-Smith

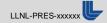
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Don Lucas

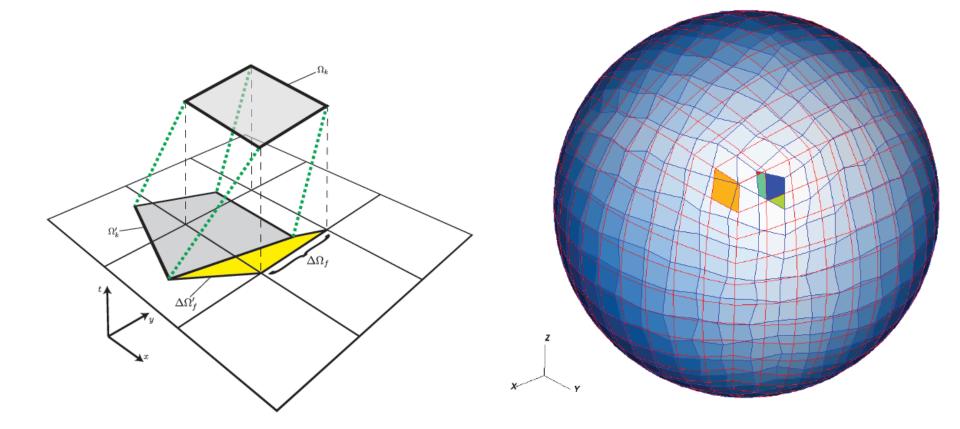
ACES4BGC team

www.aces4bgc.org

Lawrence Livermore National Laboratory

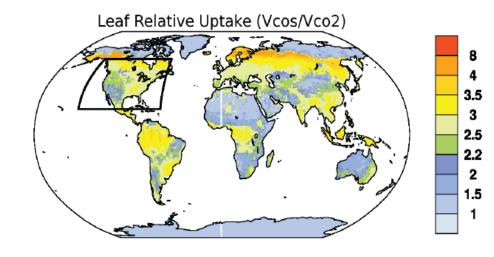


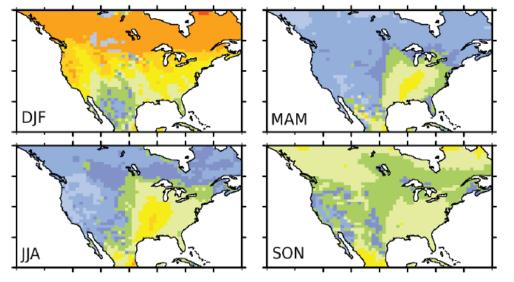
# Implementing efficient advection algorithm for thousands of tracers



Incremental remapping using the FASTMath MOAB technology for unstructured, variable resolution grids.

### **Focus on Earth System Modeling**





- Aerosol schemes (SECT & MAM),
- Emissions of biogenic VOCs, Uptake of COS (to constrain photosynthesis),
  - Biogeochemical interactions between atmosphere, land, and ocean,
  - UQ to constrain process parameters and feedbacks,
  - Performance engineering for DOE supercomputers.

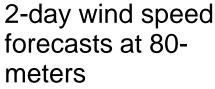
Leaf relative uptake of COS uptake in CLM (Fu et al., in prep.).

#### **ACES4BGC Team**

Name	Lab	Science Team	Торіс
Pavel B. Bochev	SNL	Atmosphere	Advection
Philip J. Cameron-Smith <sup>†</sup>	LLNL	Atmosphere	Atm. BGC
Richard C. Easter, Jr.	PNNL	Atmosphere	Aerosols
Scott M. Elliott <sup>†</sup>	LANL	Ocean	Ocean BGC
Forrest M. Hoffman <sup>†</sup>	ORNL	Land	Land BGC
Xiaohong Liu	PNNL	Atmosphere	Aerosols
Robert B. Lowrie	LANL	Ocean	Advection
Donald D. Lucas	LLNL	Atmosphere	UQ
Richard T. Mills	ORNL	Comp. Tools & Perf.	Performance
Timothy J. Tautges <sup>‡</sup>	ANL	Comp. Tools & Perf.	Mesh Tools
Mark A. Taylor	SNL	Atmosphere	Advection
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Patrick H. Worley <sup>†‡</sup>	ORNL	Comp. Tools & Perf.	Performance

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#### UQ for wind energy show source of uncertainty



Ensemble spread from 11 parameters

PDF

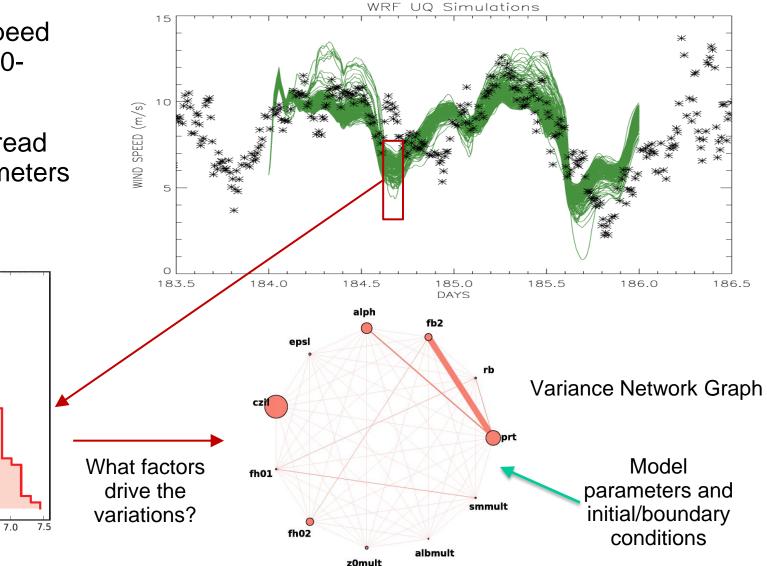
5.0

4.5

5.5

6.0

Wind Speed (m/s)



6.5

## **LLNL Chem-Aerosol Activities**

- Sectional aerosol scheme (SECT) queued for trunk.
- Coupled super-fast mechanism to MAM for CAM5.
- Connect atmospheric chemistry to biogenic emissions.
- Implement OCS and CO<sup>18</sup>O tracers.
- Revitalize tracer test-suite in CAM with <sup>222</sup>Rn/<sup>210</sup>Pb and SF<sub>6</sub>
- Tracer conservation algorithms for MOAB.

## **UQ** Activities

- Quantify sensitivities and uncertainties of atmospheric chemistry and biosphere-atmosphere interactions (O<sub>3</sub>, NO<sub>x</sub>, VOCs, SOA formation)
- Challenged by the "Curse of Dimensionality" Brute force sampling ~ M<sup>N</sup> for M levels and N sources of uncertainty (about 10<sup>100</sup>, a *googol*, for MOZART chemistry)
- Use computational and statistical methods to overcome the "Curse"
  - Single column ensembles with CAM5Chem
  - Latin hypercube sampling and machine learning based feature selection to reduce the dimensionality
- Apply UQ framework to calibrate/validate model chemistry with observations (targeting GOAMAZON)