

Climate and Environmental Sciences Division

BERAC update

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Office of Biological and Environmental Research

Outline

- CESD updated strategic plan
 - The packaging of CESD programs
 - The role of the CMDV program
- Administrative
- Highlights facilities and new science

Planning process

A few definitions

- Climate is the multi-decadal average of statistical distributions of weather, both regionally and globally, that considers the dominant modes of natural variability
- Earth system combines weather, climate, oceans, land use, hydrology, ecology, geomorphology, infrastructures, etc., as they interact over multiple space and time scales
- Predictability is the degree to which projections can be made for systems that are inherently complex and chaotic

Guiding Principles for the new Strategic Plan

- "Earth system" predictability combines science with uncertainty quantification
- Difficult to solve on 5-10 year time horizon
- Requires DOE user facilities (ARM, EMSL, LCFs, etc.) to advance the science
- Efficiently combines modeling research with field experiment
- Exploits BERAC and community workshop outputs
- Allows DOE to exert significant leadership, yet include multiple collaborating agencies

Stakeholders – science pull

- DOE future blackouts, pipeline security, infrastructure risk, ...
- Private sector resilient infrastructures and lifetime risks and costs; reinsurance
- Other agencies component of political, economic, financial forecasting

Strategic Planning Update – preview of the next five years

<u>Vision</u>: Improve a systems level understanding and predictability of the earth system in support of DOE's mission, through integrative theory, modeling, and experiment, over a variety of spatial and temporal scales.

<u>Scope</u>: Integration of atmospheric, oceanic, terrestrial, ecological, hydrological, and human components, and inclusion of system level uncertainty quantification

High level Grand Challenges

- System forcers drivers of the coupled Earth-energy-human system
- High latitude process feedbacks and interdependencies with the global system
- Biogeochemistry biogeochemical processes and cycles across multiple scales
- Integrated water cycle scale aware and response to short and long-term perturbations
- Data-model integration: interconnected capabilities and facilities that support the integration and management of models, experiments, and data across a hierarchy of scales and complexity

Land & Ocean Temperature Departure from Average Jan–Dec 2016 (with respect to a 1981–2010 base period)

Data Source: GHCN-M version 3.3.0 & ERSST version 4.0.0



Land & Ocean Temperature Departure from Average Jan 2017 (with respect to a 1981–2010 base period)

Data Source: GHCN-M version 3.3.0 & ERSST version 4.0.0



Temperature Departure from Average NCEP GFS $0.25^{\circ}x0.25^{\circ}$



-54	-36	-18	0	18	36	54	
-30	-20	-10	0	10	20	30	
		Temperature Anomaly (°F/°C)					CFSR 1979-2000 Baseline
	World + 0.77 °C	Nort	Northern Hemisphere + 1.34 °C		Arctic + 4.28 °C		
	Tropics + 0.45 °C	Sout	Southern Hemisphere + 0.18 °C		Antarctic + 0.27 °C		

System level Earth System Science and Predictability



System level Earth System Science and Predictability



Climate Model Development and Validation (CMDV)

Goals of CMDV

- model architecture restructuring for ultra-high resolution models
- new software engineering, computational upgrades
- scale-aware physics
- enhanced efforts to assess and validate model results based on ARM and TES data

Five lab-led projects that started in FY 2016

- ACME-software modernization project (SNL lead)
- Land-liaisons to improve software and science modeling integration of NGEE-tropics, NGEE-Arctic and ACME (LBNL lead)
- Mesoscale convective systems (SGP) (PNNL lead)
- Cumulus cloud processes (SGP) (LBNL lead)
- Regionally refined validation of ACME in 3 contrasting regimes (SGP, ENA, TWP) – (LLNL lead)



Shallow Cu at SGP CF, red dots represent locations of reconstructed cloud points





Workshops set the stage for future CESD priorities

Date: 2017	Date	Venue
Sept 7-9, 2016	Terrestrial Aquatic Interface workshop	Rockville
Sept 12-14, 2016	AXCICCS (computational requirements for climate modeling) workshop	Rockville
January 4-6, 2017	Energy-Water Nexus Workshop	Bethesda
April 24, 2017	Cyberinfrastructure workshop	Bolger
June, 2017	Climate Modeling Summit	TBD
June 19-22, 2017	CESM Annual Workshop	Breckenridge
July 25-Aug 4, 2017	Energy Modeling Forum (IA/IAV week)	Snowmass

Management Update: solicitations

Funds	Program lead	Issued	Proposals	Panel	Selected
FY17	SCIDAC (ESM, ASCR)	Nov 9, 2016		May 3-4, 2017	
FY17	ASR	Aug 19, 2016	74	Feb 7-9, 2017	
FY17	DATA	White papers Dec 21, 2016	4	March 20-21, 2017	
FY17	SBR	Dec 23, 2016	60+22	April 15-17, 2017	
FY17	RGCM	pending			

Management updates: Major reviews in 2016-2017

Lab	Program	Туре	Review date	Outcome
PNNL	ASR	SFA	Feb 27-28, 2017	Approved
BNL	ASR	SFA	April 4-5, 2017	
PNNL	ARM	Facility	April 10-12	
PNNL	SBR	SFA	April 27-28, 2017	
SLAC	SBR	SFA	May 18, 2017	
LLNL	ESGF	Project	June 8-9, 2017	
UCAR	RGCM	СА	September 2017	
PNNL	EMSL	Facility	Nov 29-30, 2017	

Management updates - PI meetings: 2015-2016

Title	Program(s)	Location	Date in 2016/2017
NGEE Tropics annual PI	TES	Smithsonian	Sept 7-8, 2016
RGCM PI	RGCM	Rockville	Nov 29-Dec 1, 2016
ESGF annual meeting	Data	Wash DC	Dec 6-9, 2016
ESS PI meeting	TES, SBR, EMSL	Bolger	April 25-26, 2017
NACP PI meeting (w/other agencies)	TES	Bethesda	March 27-30, 2017
ARM/ASR Facility PI meeting	ARM, ASR	Tysons	March 13-17, 2017
ACME PI meeting	ESM	Bolger	June 5-7, 2017
CMDV PI meeting	ESM, ASR, ARM	Bolger	June 8-9, 2017

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Science Highlights – Story line focus on frontier system science

Supporting infrastructure and capabilities

- EMSL opportunities
- ACME v1 status

• Polar

- Ice sheet dynamics in Greenland
- Antarctica sea ice and natural variability
- Carbon fluxes over permafrost polygons
- Storms
 - Midwest storms in the US
 - Tropical cyclones and ocean teleconnections
- Clouds and aerosols
 - Amazon convection data from ARM
 - Aerosol science
- Subsurface
 - Hydrology
 - BGC and environmental genomics

EMSL – science and industry



Advancing discovery and mechanistic understanding of <u>molecular- to meso-scale</u> biological, chemical and physical processes and interfaces to enable predictive understanding.

EMSL provides access to <u>premier instruments</u> for experimental research, <u>high performance</u> <u>computing (HPC)</u> capabilities and a variety of <u>software codes</u> for a range of modeling studies.

Proposal Opportunities

- Science Theme call for FY2018 Projects 132 proposals received.
- FICUS (Facilities Integrating Collaborations for User Science Call for FY2018 Projects – 57 Letters of Intent received. Significant increase!

Scientific Leadership

- New Exascale Challenge Project *NWChemEx* (6 DOE labs + VA Tech)
- Workshop Reports:
 - iPASS Multi-scale Plant Modeling Dec 2016
 - Computation and Modeling of Solvent-Mediated Processes

Outreach and User Activities

- 2017 User Meeting + Multi-omics for Microbiomes Conference Aug 1-3, 2017.
- Future issues of the Molecular Bond online: <u>https://www.emsl.pnl.gov/emslweb/molecular-bond</u>



ACME - updates



Version 1 (v1) release planned for Dec 2017

- Low resolution (100 km) coupled "water-cycle" version nearing completion. It has new: ocean with prognostic SLR, ice sheet and 72-level atmosphere (all can have variable-mesh), new land BGC (with P); dams, irrigation
- In 2018: High resolution (25 km) v1 water cycle experiments, Biogeochemical simulations, Dynamic ice-ocean simulations
- Review of Phase 2 in spring 2018

V1 examples of computational performance

- Edison: 12 SYPD (100km coupled)
- Cori KNL: 6 SYPD (100km coupled), 3 SYPD (25 km atmosphere-only)
- Titan: 1.4 SYPD (25km)
- Mira: 0.33 SYPD (25km)

ECP-ACME (ASCR-Exascale Computing Project) project focus is ACME-SP-CAM on GPU's, with cloud-resolution in each grid-box



Gleckler Metrics: R5-H comparable to CAM5 and better than 50% of CMIP models



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Greenland subglacial drainage evolution regulated by weakly connected regions of the bed

Background

Surface meltwater draining to the bed of the Greenland Ice Sheet each summer causes ice flow changes that cannot be explained by the prevailing theory of channelizing subglacial drainage.

Objective

Determine if changes in weakly connected, swampy areas of the bed explain why the ice sheet slows down in late summer and winter?

Approach and results

- Develop a model for weakly-connected drainage that includes distributed and channelized flow.
- Simulate a field site in Greenland and compare model with and without weakly-connected drainage to measurements.
- Results show that the weakly connected drainage component is necessary to reproduce the observations.





Swampy backwaters of the subglacial drainage system slowly drain water toward efficient channels, lowering system-wide water pressure and slowing the ice sheet.

Impact

The existing conceptual model for subglacial drainage must be expanded to include weakly-connected drainage. Slow draining of swampy subglacial backwaters regulates the ice flow response to summer lubrication of the bed. These areas may control how the ice sheet responds to future changes in melt.

Reference: Hoffman, M. J., L. C. Andrews, S. A. Price, G. A. Catania, T. A. Neumann, M. P. Luethi, J. Gulley, C. Ryser, R. L. Hawley, and B. F. Morriss (2016), Greenland subglacial drainage evolution regulated by weakly-connected regions of the bed, *Nat. Commun., In Press.*

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Naturally occurring decadal climate variability is responsible for recent expansion of Antarctic sea ice extent

Objective

Explain why observed Antarctic sea-ice extent has accelerated since the late 1990s, but the average of all climate models shows a decline.



- Analyze observations to determine if a deepening of the Amundsen Sea Low in the southeast Pacific produced northward winds that expand sea ice extent
- Analyze climate model simulations and observations to determine if Antarctic sea ice expansion is related to the IPO
- Perform model experiments to dynamically explain negative IPO to deeper Amundsen Sea Low and greater sea ice extent





Top: observed expanding Antarctic sea ice concentrations (blue shading) since the 2000 IPO transition to negative are connected to an anomalously deeper Amundsen Sea Low ("L")

Bottom: an idealized climate model with negative precipitation and convective heating anomalies in the eastern equatorial Pacific, where IPO SST anomalies have been negative since 2000, makes a direct connection between negative IPO, deeper Amundsen Sea Low (blue shading and white "L"), northward surface wind anomalies, and expanding Antarctic sea ice

Results

Expanded Antarctic sea ice can mostly be explained by sea surface temperature and ppt anomalies from the naturally-occurring IPO in the equatorial eastern Pacific, and earth system models can simulate these processes.

Meehl, G.A., J.M. Arblaster, C. Bitz, C.T.Y. Chung, and H. Teng, 2016: Antarctic sea ice expansion between 2000-2014 driven by tropical Pacific decadal climate variability. *Nature Geoscience*, DOI: 10.1038/NGEO2751.

Large CO₂ and CH₄ Emissions from Polygonal Tundra During **Spring Thaw in Northern Alaska**



Objective

uptake and added 6% to CH₄ summer fluxes

Determine physical and biogeochemical processes governing permafrost ecology, carbon budgets, and thaw

Observations and Analysis

- LBNL scientists measured a large pulse of carbon gases released from the frozen Arctic tundra when soils started to thaw in early June 2014. The researchers show that the pulse was the result of a delayed mechanism, in which gases produced in fall were trapped in the frozen soils and released in spring.
- Findings suggest that the Arctic may be even less of a carbon sink than previously thought.
- A multi-institution team linked hydrology, biogeochemistry, and geophysics to uncover the pivotal roles of warmer fall weather and of spring rain-on-snow events, implying these pulses may be more frequent in the future.

The pre-thaw carbon flux pulse, measured by eddy correlation, offsets 46% of CO₂ summer

Laboratory experiment links pulse emissions to a delayed microbial production mechanism

A similar pulse was measured 5 km away, suggesting that this could be commonplace

The type of rain-on-snow event that triggered the pulse is gradually becoming more

Pulse

Raz Yaseef, N., M. Torn, Y. Wu, D. Billesbach, A. Liljedahl, T. Kneafsey, V. Romanovsky, D. Cook, and S. Wullschleger (2016), Large CO₂ and CH₄ emissions from polygonal tundra during spring thaw in northern Alaska, Geophys. Res. Lett., 43, doi:10.1002/2016GL071220.





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Results

ARTH & VIRONMENTAL





More Frequent, Intense, and Long-lived Storms Dominate Springtime Trend in Central U.S. Rainfall

Objective

 Determine the causes of the observed increase in extreme rainfall in the central US over the past several decades and the connections to climate change

Approach

- Develop and train an automated algorithm informed by satellite data to identify mesoscale convective systems (MCSs), the largest type of convective storm, based on precipitation data alone
- Develop an MCS database for the past 36 years using an observed high-resolution precipitation dataset
- Examine long-term trends in extreme MCS rainfall frequency, intensity, and connection to changes in large-scale circulation associated with climate change

More frequent intense and long-lived Mesoscale Convective Systems



Surface warming over the Rockies increased the pressure gradient across the central US, strengthening the southerly lowlevel jet and associated moisture transport, favoring more frequent intense and long-lived MCSs.

Impact

- Determined that the increases in MCS frequency and intensity dominate the observed increasing trend in springtime total and extreme rainfall in the central USA
- Linked MCS changes to large-scale circulation changes consistent with a warmer climate
- Provided an observational foundation for future research to improve understanding and modeling of MCSs and their response to warming

Feng Z, LR Leung, S Hagos, RA Houze, CD Burleyson and K Balaguru. 2016. "More Frequent Intense and Long-lived Storms Dominate the Springtime Trend in Central US Rainfall." *Nature Communications* 7, 13429. DOI: 10.1038/ncomms13429

A Teleconnection Between Atlantic Sea Surface Temperature and Eastern and Central North Pacific Tropical Cyclones



(top) Boxplots of seasonal East Pacific tropical cyclone activity from observations and climate model experiments forced by climatological SST and common SST patterns, including the Atlantic Meridional Mode (AMM) and El Niño (bottom).

Objective

To seek an explanation for the interannual variability of Tropical Cyclones in the Pacific Ocean

Approach

- Statistically analyze temperature anomalies in both the Pacific and Atlantic oceans, and relate the anomalies to Tropical Cyclone climatologies in different parts of the Pacific.
- Conduct modeling experiments to explore the dynamics to explain the statistical relationships.

Results

- Tropical cyclone activity was quantified using accumulated cyclone energy (ACE), which accounts for storm number, frequency, and duration.
- Atlantic sea surface temperature (SST) patterns remotely influence East Pacific tropical cyclone activity.
- Seasonal to centennial East Pacific tropical cyclone prediction can be improved using skillful predictions of Atlantic SST and El Niño. Active East Pacific hurricane seasons tend to occur with anomalously cool northern tropical Atlantic SST and El Niño.
- We confirmed that the results are robust by analyzing observations and large-ensemble, high-resolution earth system model simulations.

Citation: Patricola, C. M., R. Saravanan, and P. Chang (2016), A Teleconnection Between Atlantic Sea Surface Temperature and Eastern and Central North Pacific Tropical Cyclones. Geophysical Research Letters, DOI: 10.1002/2016GL071965







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First Climatology of Vertical Velocity in Amazonian Clouds

Motivation

- Current GCMs do not represent deep convection over the Amazon well
- Observations of vertical velocity are needed to constrain and improve GCM parameterizations of deep convection

Approach

- 2 years of ARM radar wind profiler (RWP) data during GOAmazon are used to develop statistics on vertical velocities in Amazonian convection
- Data are averaged over 1 or 3 hours to correspond to model grid cells of 20 km or 60 km resolution
- Convective vertical velocity is related to corresponding environmental conditions



Frequency of vertical velocity by altitude for all clouds (left) and those with tops above 12 km (right).

Impact

- Study provides the first climatology of vertical motion of Amazon clouds
- Stronger vertical velocity profile behaviors are seen under higher convective available potential energy (CAPE) and lower low-level moisture conditions
- Wet season regimes have higher domain-average mass flux profiles, attributed to more frequent convection that offsets weaker average convective cell vertical velocities

Reference: Giangrande SE, T Toto, MP Jensen, M Bartholomew, Z Feng, A Protat, C Williams, C Schumacher, and L Machado. 2016. "Convective cloud vertical velocity and mass-flux characteristics from radar wind profiler observations during GoAmazon2014/5." Journal of Geophysical Research: Atmospheres, 121(21), 10.1002/2016jd025303.

Phase diagrams for amorphous nanoscale organic aerosol

Motivation

- High particle viscosity affects particle uptake of vapors, pollutant lifetime against oxidation or evaporation, and particle-cloud-climate interactions.
- Observations of particle viscosity transitions are needed to develop, constrain, and improve the representation of aerosol phase in large scale models.

Approach

- Develop novel quantitative viscosity measurement method for submicron aerosols.
- Measure the temperature and RH onset of dimer coalescence to characterize the glass-to-liquid phase transition for particles.
- Develop and constrain simple physical chemistry models of the phase-state diagram for organic aerosol.
- For sucrose test aerosols, observed excellent agreement with macroscopic measurements.



Amorphous phase diagram of 100 nm sucrose aerosol

Impact

- Defines a measurement and modeling framework for well-constrained aerosol phase diagrams suitable for atmospheric models.
- Extends viscosity measurements into the semisolid regime to sub-200 nm particles. Approach can be applied to complex secondary organic aerosols.

Reference: Rothfuss, N. E and M. D. Petters. 2016a. "Coalescence-based assessment of aerosol phase state using dimers prepared through a dual-differential mobility analyzer technique" Aerosol Sci. Technol. 12, 1294-1305, doi:10.1080/02786826.2016.1221050 ; 2016b. "Characterization of the temperature and humidity-dependent phase diagram of amorphous nanoscale organic aerosol" Phys. Chem. Chem. Phys. 19, 6532-6545, doi:10.1039/c6cp08593h

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Reconciling Observations and Global Models of Terrestrial Water Fluxes



Traditional Land Surface Models



Integrated Hydrologic Models

Traditional land surface models simplify the system by solving it as a set of discrete columns without lateral groundwater flow while integrated hydrologic models connect three dimensional flow in the subsurface with processes at the land surface.

R. M. Maxwell, L. E. Condon, "Connections Between Groundwater Flow and Transpiration Partitioning." Science 353, 377-380 (2016). DOI: 10.1126/science.aaf7891



Objective

Determine importance of plant water use to regional hydrology

Scientific Achievement

A new modeling study using High Performance Computers (HPC) shows that lateral groundwater flow, not included in previous approaches, may be the missing link to predicting how plant water use influences the integrated water system.

Significance and Impact

Understanding freshwater flows at continental scales will enable scientists to better predict hydrologic response and manage water resources. The relative importance of plant transpiration remains one of the largest uncertainties in balancing water at these scales.

- The total flux of water and transpiration partitioning are connected to water table depth
- Including lateral groundwater flow in the model increases transpiration partitioning from 47±13% to 62±12%.



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New Model Integrates Biogeochemistry and Multi-Omic Sequence Data

Challenge

• Develop a model that integrates geochemical and multi-omic sequence information (DNA, RNA, protein) to explain key microbial metabolic processes in a marine ecosystem.

Approach and Results

- A team of scientists used EMSL's -omics capabilities to develop an integrated model of metagenomic, metatranscriptomic, and metaproteomic sequence data, and geochemical data.
- The new model reproduced measured biogeochemical reaction rates as well as DNA, mRNA, and protein concentration profiles at the ecosystem scale.
- Simulations also predicted the role of ubiquitous microorganisms in mediating carbon, nitrogen, and sulfur cycling.

Significance and Impact

• The findings could lead to better-informed predictions about the influence of microbial metabolic networks on future patterns of global elemental cycling.



Researchers developed a biogeochemical model that integrates data to explain key metabolic processes in oxygenstarved waters of the Saanich Inlet, British Columbia.

Participants:

The University of British Columbia, the University of Minnesota, the Canadian Institute for Advanced Research, and the Max Planck Institute for Marine Microbiology

Reference: S. Louca, A.K. Hawley, S. Katsev, M. Torres-Beltran, M.P. Bhatia, S. Kheirandish, C.C. Michiels, D. Capelle, G. Lavik, M. Doebeli, S.A. Crowe, S.J. Hallam. 2016. "Integrating biogeochemistry with multiomic sequence information in a model oxygen minimum zone." *PNAS*. [DOI: 10.1073/pnas.1602897113]

EMSL: Fundamental Science for Industry



Developing integrated metabolic flux analysis approaches for systems and synthetic biology Microscopically detailed catalyst modelling to enhance NOx reduction and engine efficiency

JM 🛠

Johnson Matthey



Achieved 3 times faster NWChem code performance for Intel Many Integrated Core (MIC) Architecturebased parallel systems



Developing subsurface predictive models for contaminant and colloid transport, non-aqueous phase liquid dissolution, and sequestration of CO₂



Chemical imaging of Niobium thin films to help develop a new class of semiconductor memory devices HALLIBURTON

Developing smallvolume (10-100 picoliters) sample delivery and detection system for NMR analysis of biological, environmental and energy applications









(NanoSynthons LLC)



PEPSICO







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