

# CESD – ESS CYBERINFRASTRUCTURE WORKING GROUPS

## Annual Meeting Highlights

J. David Moulton (LANL)

ESS PI Meeting, Bolger Center, Potomac, MD  
April 30, 2019.

# Outline

## Recap and Highlights from 2018

Motivation, how we formed, our structure ...

Activities

## Annual Meeting (yesterday)

Recap of groups scope and activities

Internal DOE, external highlights on Cyberinfrastructure

Planning discussions

# ESS Cyberinfrastructure Working Groups Structure

*Following recommendations of the workshop report and feedback from 2015 AGU Town Hall the Working Groups Kickoff was in 2016*

## ***Established an Executive Committee***

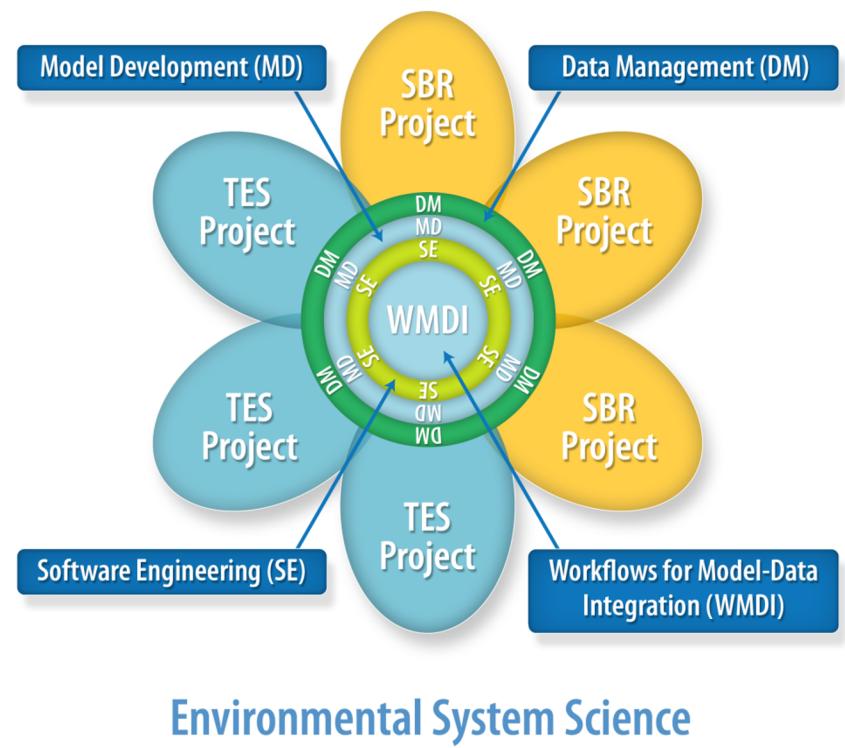
Deb Agarwal, Xingyuan Chen, Paul Hanson,  
Forrest Hoffman, David Moulton (Chair),  
Eric Pierce, Dean Williams, Roelof Versteeg,  
Stan Wullschleger

## ***Established Three Working Groups***

- ❑ Data Management
- ❑ Model-Data Integration
- ❑ Software Engineering and Interoperability

## ***Reporting on Working Group Activities***

- ❑ Informal reporting to S.C. (PMs) and E.C. (PIs)
- ❑ Annual reporting at ESS PI Meeting



# Highlights from the Working Groups

## **Model Intercomparison and Benchmarks participation**

- ❑ International Land Model Benchmarking (ILAMB) Workshop and Tools
- ❑ Soil Carbon Dynamics Working Group for data synthesis

## **Community Outreach**

- ❑ Co-Led sessions for AGU Fall Meeting 2018:
  - Computational Methods and Tools for Model-Data Integration
  - Big Data in the Geosciences: New Approaches to Storage, Sharing, and Analysis
- ❑ Breakout Sessions tonight
  - Open Watersheds: Amplifying the Impact of SBR Science
  - ILAMB Soil C Demonstration and Tutorial

# Highlights from the Working Groups

## Facilitate communication across projects

- MDI conducted a Community survey on workflows and model-data integration tools last year
- We had 30 respondents
- Suggestions for topics not covered and future activities will be incorporated for next year

### *Sample questions:*

*What software tools do you prefer for data analysis?*

*What software tools do you use or prefer for workflow management, provenance tracking and archiving?*



# Working Groups Annual Meeting

Annual Meeting to be held on:

**Monday preceding the ESS PI Meeting**

58 participants, 7 BER representatives

A quick recap of recent activities

Community oriented projects:

- ❑ ESS DIVE
- ❑ IDEAS-Watersheds
- ❑ ILAMB/IOMB, RUBISCO Soil Carbon Dynamics Working Group

Cyberinfrastructure activities

- ❑ Within DOE, and external to DOE

Brainstorming for the future ...



# DOE Flash Talks

## Cyberinfrastructure in practice, progress and needs:

Danielle Christianson - Ameriflux processing pipelines

Chris Henry - KBase connectivity with ESS Cyberinfrastructure

Kjierstan Fagnan - National Microbiome Data Collaborative/JGI

Dave Millard - MyEMSL

collaborations with ESS-DIVE, KBase

Ethan Coon and Dipankar Dwivedi -

ExaSheds

Ben Sulman - NGE Arctic -

E3SM/PFLOTRAN Liaison talk

Roelof Versteeg - Phase 1 SBIR

John Tourtellot - Kitware Phase 1 SBIR.

Informal discussion (pop ups) included Joanna Martin from OSTI.



# External Flash Talks

## Cyberinfrastructure in practice, progress and needs:

Dwayne Young - EPA Internet of Water

Tim Kern - USGS

Peter Arbuckle - USDA

Lejo Flores - CUAHSI

Matt Jones - DataONE



NMDC Vision expresses common theme:

*Empower the research community* to harness  
microbiome data exploration and discovery *through*  
*a collaborative integrative data science ecosystem.*

# Looking Ahead

Explore adjustments to structure to help make us more effective during the rest of the year

Identify leads for small groups attacking ``hot topics''

Plan and hold a **workshop** on needs for model data

- ❑ Traceability of simulations (model input and model output)
- ❑ Include stages of data preparation (raw to product)

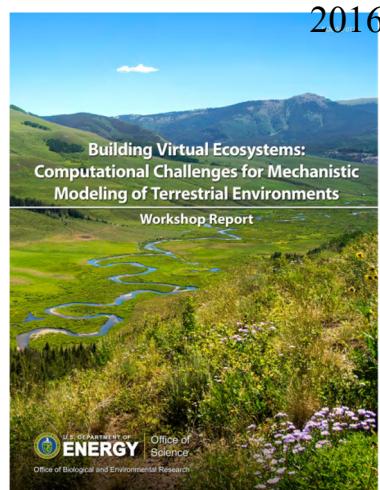
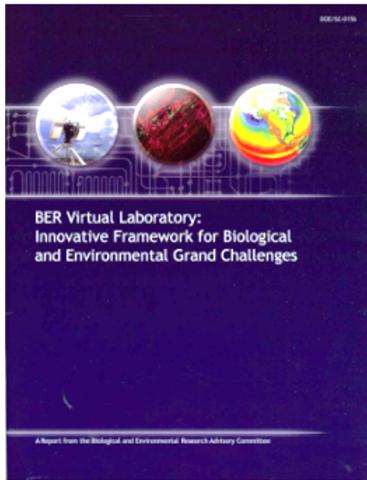
Work closely with community oriented projects:

- ❑ ESS-DIVE, IDEAS-Watersheds, RUBISCO, WHONDRS, etc.

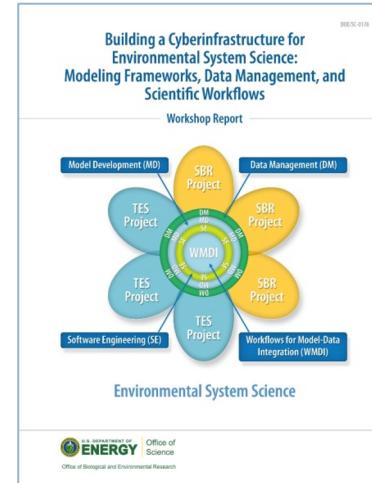
Continue community outreach

# Building Community Cyberinfrastructure ...

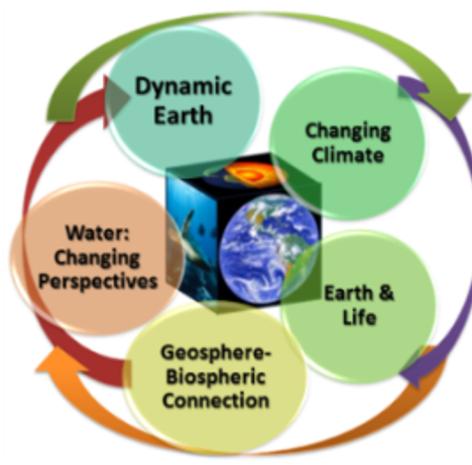
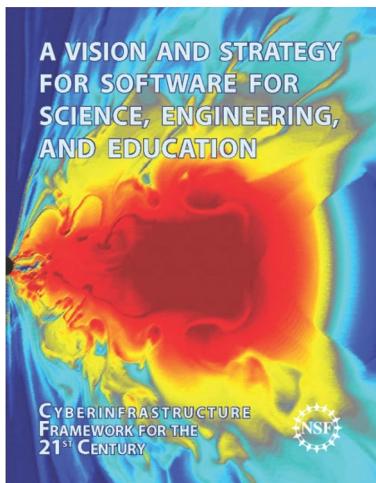
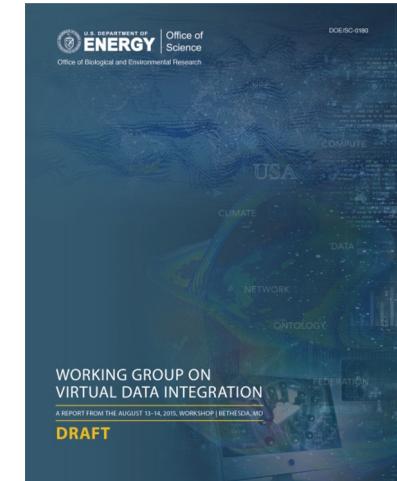
2013



2014



2015



# ESS Executive Committee Workshop on Data Infrastructure

**Workshop:** August 29-30, 2016; Germantown, MD  
**Organizers:** Jay Hnilo (CESD) and David Moulton (LANL, EC – Chair)  
**Participants:** 10 participants representing Executive Committee, 7 DOE PMs

## Motivation:

*"the innovation most needed is a framework that allows seamless integration of multiscale observations, experiments, theory, and process understanding into predictive models for knowledge discovery"* (BERAC 2013)

Exponential growth in the amount, variety and complexity of scientific data

Significant fragmentation across projects and disciplines still remains

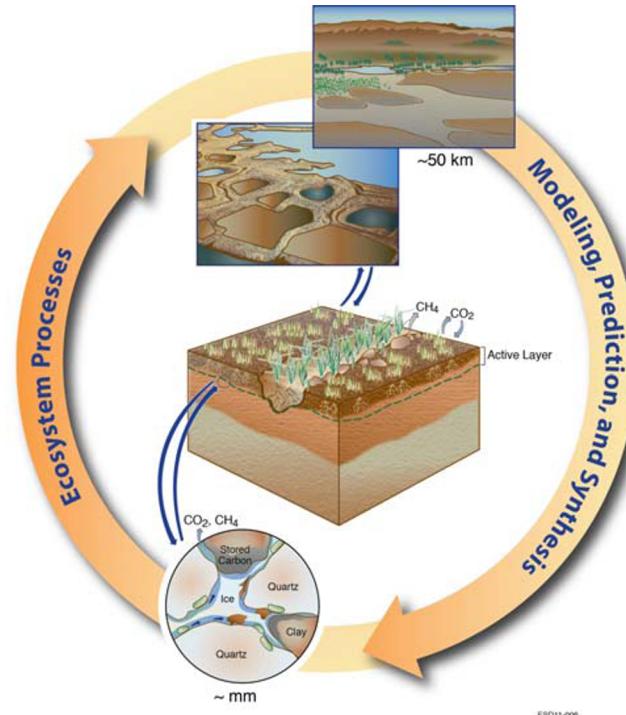
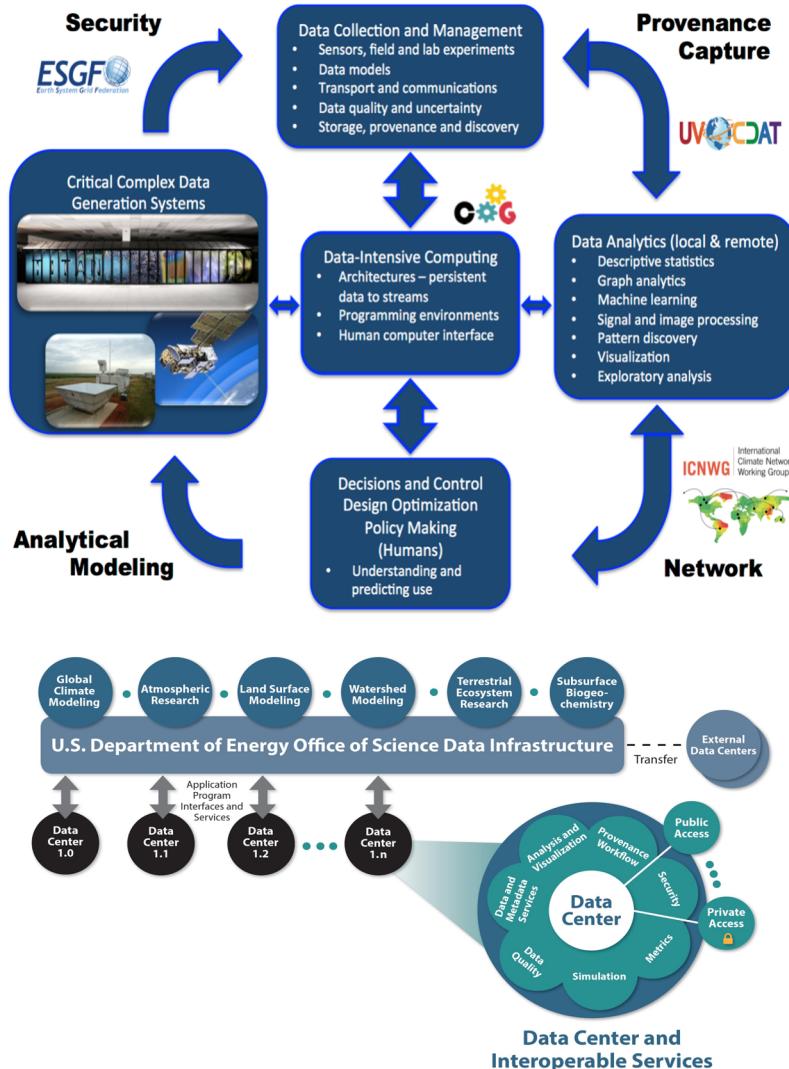
A need for a data center that would be a foundational part of a community cyberinfrastructure

[http://science.energy.gov/media/ber/pdf/workshop%20reports/Towards\\_a\\_Shared\\_ESS\\_Cyberinfrastructure.pdf](http://science.energy.gov/media/ber/pdf/workshop%20reports/Towards_a_Shared_ESS_Cyberinfrastructure.pdf)

Towards a Shared ESS Cyberinfrastructure:  
Vision and First Steps

Report from the ESS Executive Committee Workshop on Data Infrastructure  
August 29-30, 2016.  
DOE Headquarters, Germantown, MD

# ESS Community Cyberinfrastructure and the Virtual Laboratory



Reconciling ***different view points and emphasis into requirements*** for a new data center and a phased approach to community-based cyberinfrastructure development.