Community Data-Model Integration Infrastructure (CD-MII)

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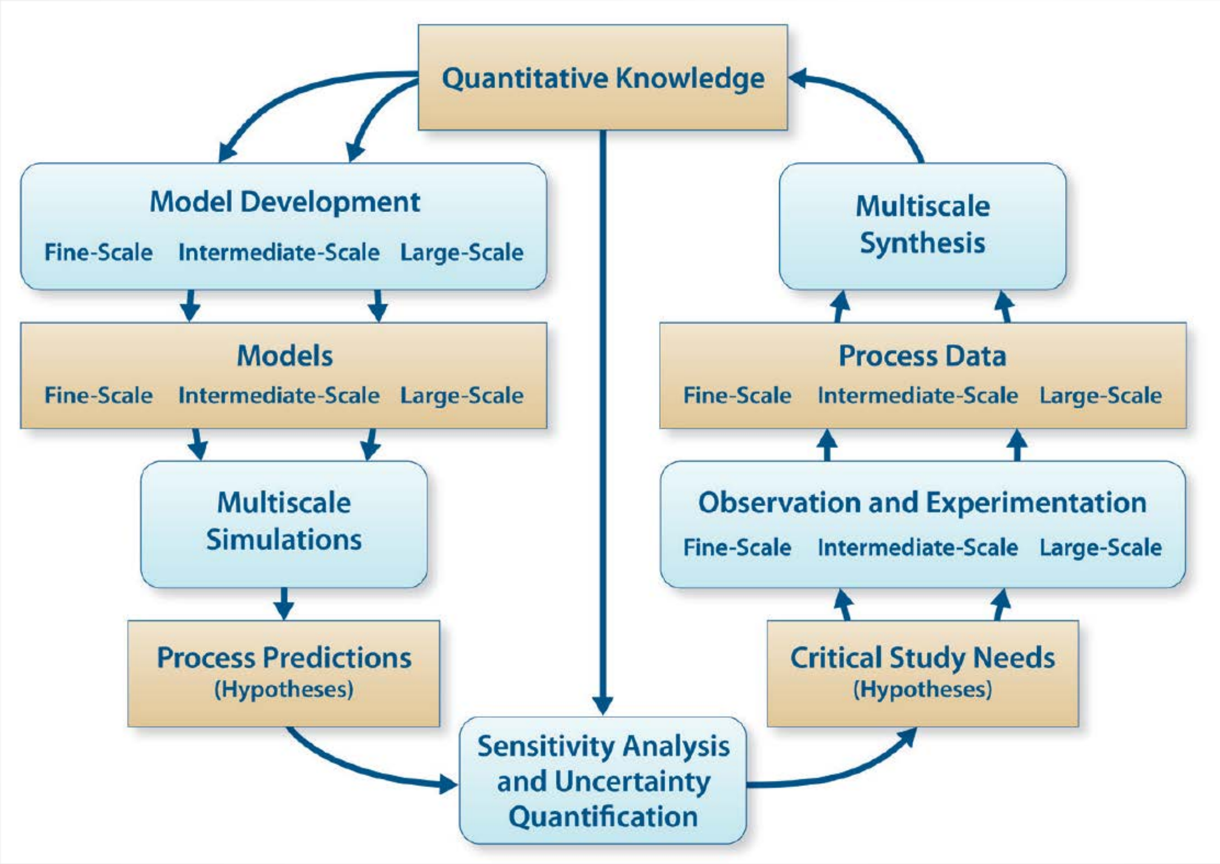
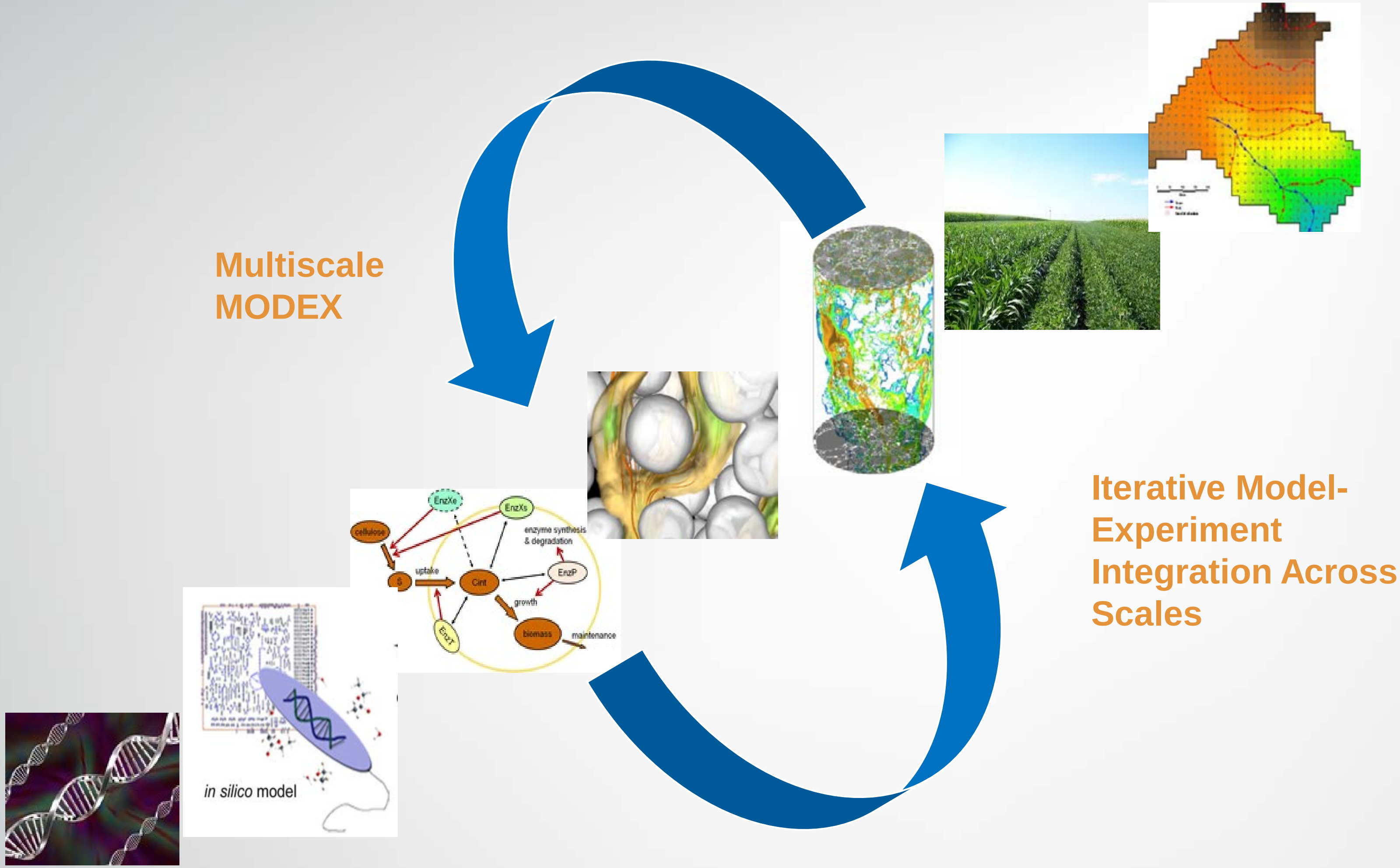
The Objective: An extensible community-based framework for data-model integration (ModEx)

Challenges:

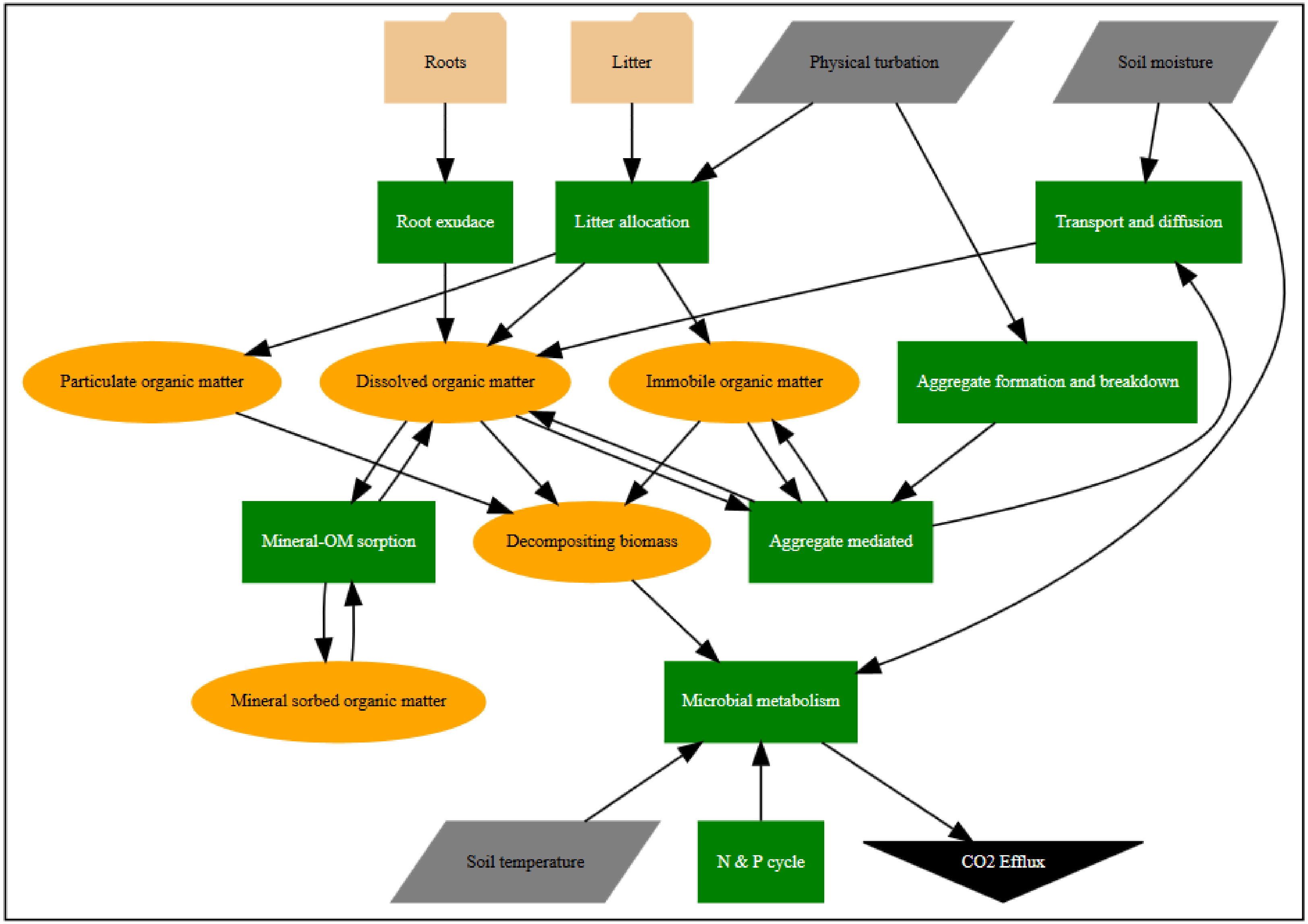
- Individual models require significant expertise
- Model couplings are mostly ad hoc and one-off (not extensible or generalizable)
- Data for model formulation and validation are lacking or inaccessible



Vision

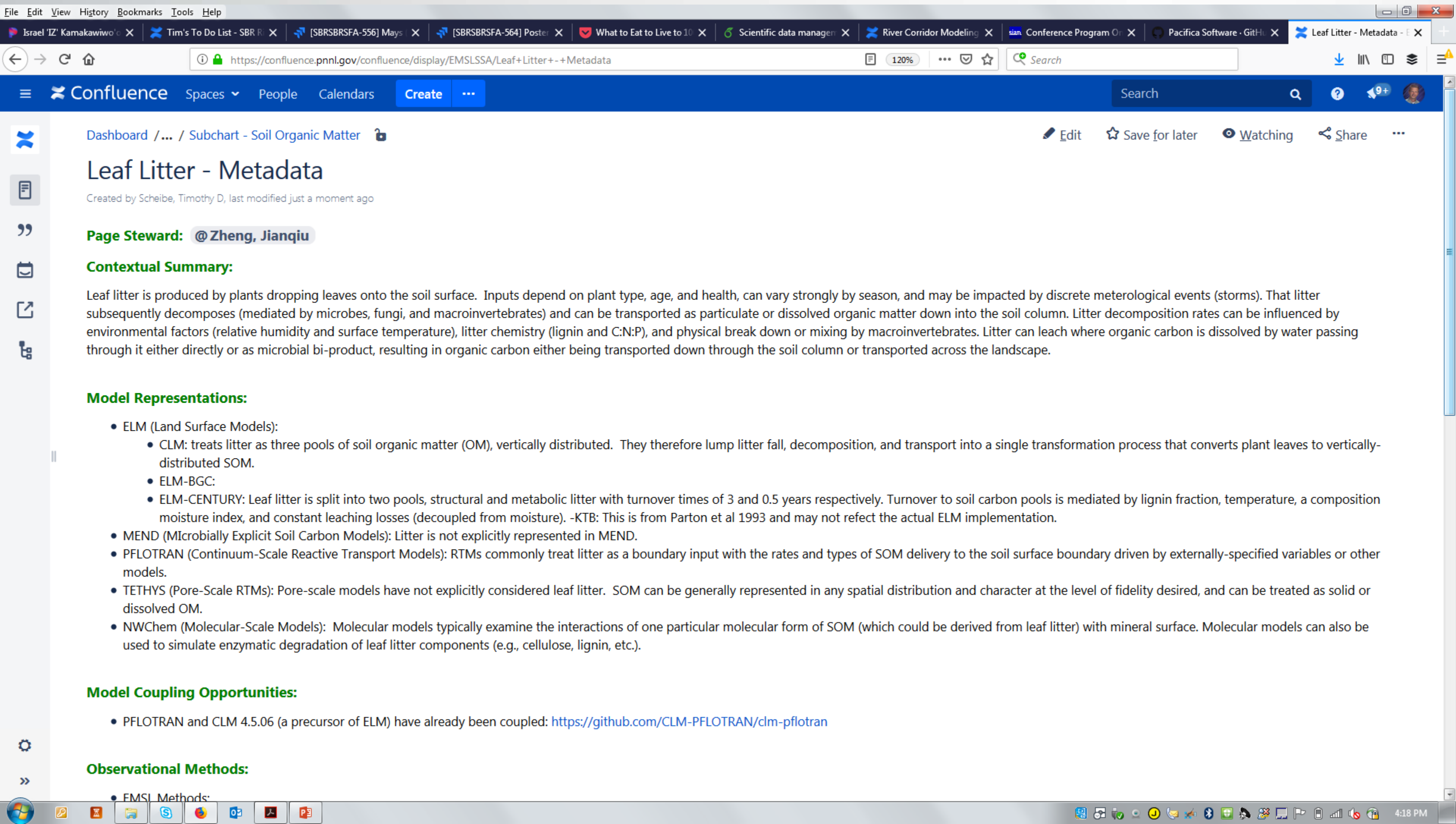

Multiscale MODEX
Iterative Model-Experiment Integration Across Scales
in silico model
cellulose
EnzXe
EnzXs
enzyme synthesis & degradation
uptake
Cint
EnzP
growth
biomass
maintenance
EnzT
S

1. Build a Conceptual Model



2. Identify a Suite of Community Codes and Potential Interconnections

- Metadata pages



Dashboard / ... / Subchart - Soil Organic Matter

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Leaf Litter - Metadata

Created by Scheibe, Timothy D, last modified just a moment ago

Page Steward: @Zheng, Jianqiu

Contextual Summary:

Leaf litter is produced by plants dropping leaves onto the soil surface. Inputs depend on plant type, age, and health, can vary strongly by season, and may be impacted by discrete meterological events (storms). That litter subsequently decomposes (mediated by microbes, fungi, and macroinvertebrates) and can be transported as particulate or dissolved organic matter down into the soil column. Litter decomposition rates can be influenced by environmental factors (relative humidity and surface temperature), litter chemistry (lignin and C:N:P), and physical break down or mixing by macroinvertebrates. Litter can leach where organic carbon is dissolved by water passing through it either directly or as microbial bi-product, resulting in organic carbon either being transported down through the soil column or transported across the landscape.

Model Representations:

- ELM (Land Surface Models):
  - CLM: treats litter as three pools of soil organic matter (OM), vertically distributed. They therefore lump litter fall, decomposition, and transport into a single transformation process that converts plant leaves to vertically-distributed SOM.
  - ELM-BGC:
  - ELM-CENTURY: Leaf litter is split into two pools, structural and metabolic litter with turnover times of 3 and 0.5 years respectively. Turnover to soil carbon pools is mediated by lignin fraction, temperature, a composition moisture index, and constant leaching losses (decoupled from moisture). -KTB: This is from Parton et al 1993 and may not refect the actual ELM implementation.
- MEND (MIcrobially Explicit Soil Carbon Models): Litter is not explicitly represented in MEND.
- PFLOTRAN (Continuum-Scale Reactive Transport Models): RTMs commonly treat litter as a boundary input with the rates and types of SOM delivery to the soil surface boundary driven by externally-specified variables or other models.
- TETHYS (Pore-Scale RTMs): Pore-scale models have not explicitly considered leaf litter. SOM can be generally represented in any spatial distribution and character at the level of fidelity desired, and can be treated as solid or dissolved OM.
- NWChem (Molecular-Scale Models): Molecular models typically examine the interactions of one particular molecular form of SOM (which could be derived from leaf litter) with mineral surface. Molecular models can also be used to simulate enzymatic degradation of leaf litter components (e.g., cellulose, lignin, etc.).

Model Coupling Opportunities:

- PFLOTRAN and CLM 4.5.06 (a precursor of ELM) have already been coupled: https://github.com/CLM-PFLOTRAN/clm-pflotran

Observational Methods:

- EMSL Methods:

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Observational Methods:

- EMSL Methods:
  - Confirmation/determination of plant-derived source using Stable Isotope Probing
  - Characterization of organic compounds in litter using Mass Spectrometry
  - C:N:P ratio using Elemental Analyzer
- Other DOE User Facilities:
  - JGI
  - Synchrotrons
  - ARM
- Other Methods:
  - Vertical profiling of soil organic matter
  - Direct field measurement of litter accumulation over time (e.g., periodic collection and dry massing of dead leaves and other detritus over time, litterbag experiments)

Knowledge or Data Gaps:

- What is the effect of wind on the spatial distribution of litter accumulation at the surface in different types of plant assemblages?
- How do macrofauna impact leaf litter amount, composition, and degradation?
- Separation of vegetation into litter quality pools across vegetation types.
- The process controls on leaching.

Key Literature:

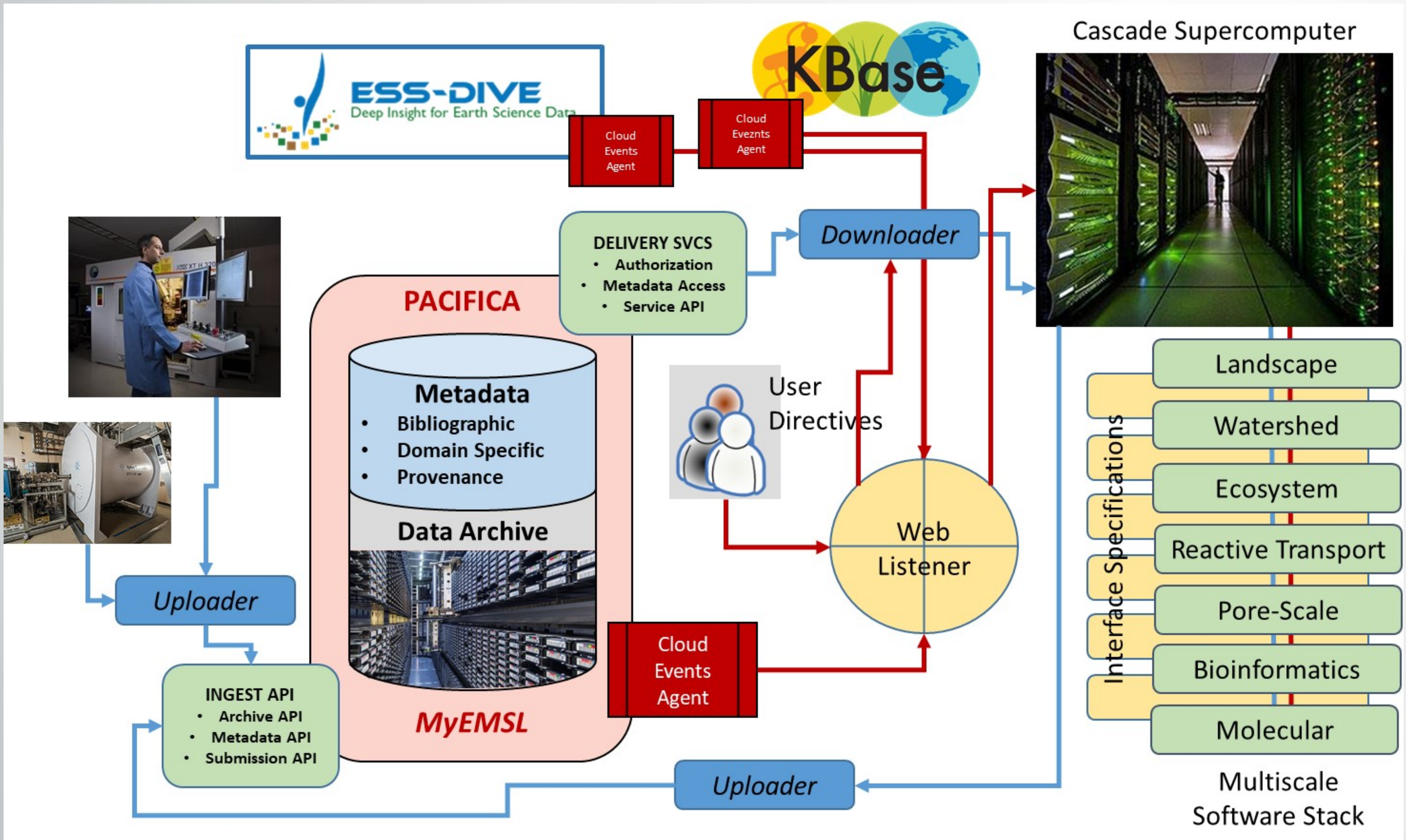
Parton, W. J., Scurlock, J. M. O., Ojima, D. S., Gilmanov, T. G., Scholes, R. J., Schimel, D. S., Kirchner, T., Menaut, J., Seastedt, T., Garcia Moya, E., Kamnalrut, A. and Kinyamario, J. I.: Observations and modeling of biomass and soil organic matter dynamics for the grassland biome worldwide, Global Biogeochem. Cycles, 7, 785–809, doi:10.1029/93GB02042, 1993.

Wang, G., Jagadamma, S., Mayes, M. A., Schadt, C. W., Megan Steinweg, J., Gu, L. and Post, W. M.: Microbial dormancy improves development and experimental validation of ecosystem model, ISME J., 9(1), 226–237, doi:10.1038/ismej.2014.120, 2015.

Nunes, F. P. and Q. S. Garcia (2015) "Adequacy assessment of mathematical models in the dynamics of litter decomposition in a tropical forest Mosaic Atlantic, in southeastern Brazil," Braz. J. Biol., 75(2): 268-272, doi: 010.1590/1519-6984.08413.

3. Construct an Extensible Framework for Multiscale Data-Model Integration

- Application of “orchestration” tools to scientific workflow
- “Event-Driven” approach



4. Implement at a Scientific User Facility for Community Use

EMSL

The event-driven orchestration methods have been implemented within Pacifica software in MyEMSL (EMSL data repository)
https://github.com/pacifica/
https://github.com/pacifica/pacifica-dispatcher

Cyberinfrastructure WGs:

- Review and revise proposed interface specifications
- Test implementations
- Propose use cases

PFLOTRAN

WRF-Hydro®

OpenFOAM

NWCHEM

EMSL

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