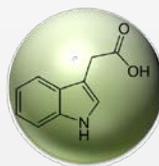




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Integrated Plant-Atmosphere- Soil Systems (iPASS) Initiative

December 2016

C Jansson



$$Y_{ijk} = \alpha_i + \beta_j + \gamma_{ij} + e_{ijk}$$

U.S. DEPARTMENT OF
ENERGY

Prepared for the U.S. Department of Energy
under Contract DE-AC05-76RL01830

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Pacific Northwest National Laboratory
Richland, Washington 99352

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The iPASS Initiative

Christer Jansson, Initiative Lead; Nancy Hess, Deputy Initiative Lead

1.0 The iPASS Initiative

The integrated Plant-Atmosphere-Soil Systems (iPASS) Initiative is a Pacific Northwest National Laboratory (PNNL) Laboratory-Directed Research and Development (LDRD) project aimed at deciphering fundamental principles that govern the plant ecosystem, from plant genotype through multiple scales to ecosystem traits and responses. The project consists of four highly integrated focus areas. The hallmark of iPASS is to approach the plant ecosystem as an interactome of plants, microbes, the atmosphere and the soil (Fig. 1). Funding is \$10M over four years. The project started in May 2016.

1.1 Goal

The overarching goal of iPASS is to *define first-principles that govern flow and transformations of carbon, nitrogen and water through the integrated plant-atmosphere-soil system* (Fig. 2). A particular focus is on *how the plant genotype influences ecosystem carbon cycling*. This goal supports the US Department of Energy (DOE) Office of Science's Office of Biological and Environmental Research (BER) mission in exploring frontiers of genome-enabled biology, e.g., *develop predictive understanding of the plant phenome* (1), *linking molecular properties and phenomics across time and length scales* (2), as well as PNNL's Scientific Vision to understand, predict, and control the behavior of complex adaptive systems.

The iPASS goal also aligns with the 2016 National Science Foundation (NSF) report on Big Ideas for Future Investment, which declared *the universally recognized biggest gap in our biological knowledge is our inability to predict the phenotype of a cell or organism from what we know about the genome and environment* (3). In iPASS we address the genotype-to-phenotype challenge in the context of terrestrial carbon cycling by examining of model plant ecosystems under highly controlled environmental conditions.

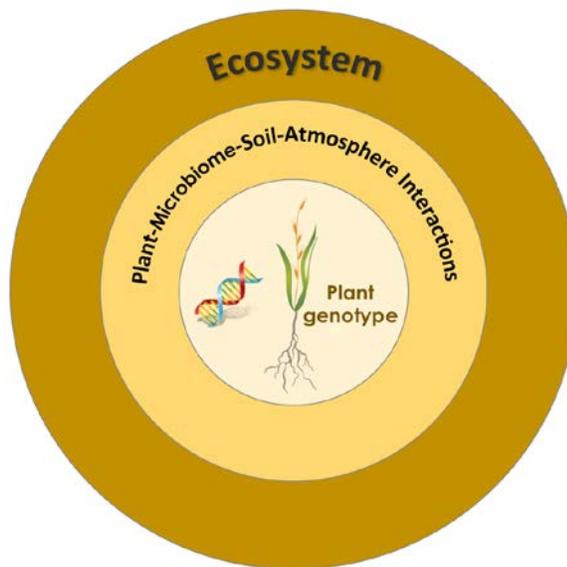


Figure 1. Information in the plant genome propagates through plant-microbiome-soil-atmosphere interactions to inform emergent traits and responses at the ecosystem level.

1.2 Questions and Hypotheses

Two recurring and related questions that infiltrate the iPASS Initiative are:

- *How does the plant genotype inform traits and responses at the ecosystem level?*
- *How do interactions between biotic and abiotic factors and environmental conditions shape emergent properties of the integrated plant ecosystem?*

We have formulated main hypotheses that guide the iPASS Initiative:

- *Ecosystem traits and responses can be predicted from the plant genotype.*
- *Information in the plant genome propagates through plant-microbiome-soil-atmosphere interactions to inform emergent properties at the ecosystem level.*

Linked to these main hypotheses are sub-level postulations, such as:

- Allocation of carbon to above- and below-ground biomass can be predicted from the plant genotype.
- Increase in soil carbon storage is mainly limited by the incorporation of recent photosynthate into soil and less by the decomposition of existing soil carbon.
- The plant genotype determines exudate chemistry and rhizosphere community composition.
- Emission of plant volatile organic compounds (VOC) in response to drought and other stressors will vary between genotypes.

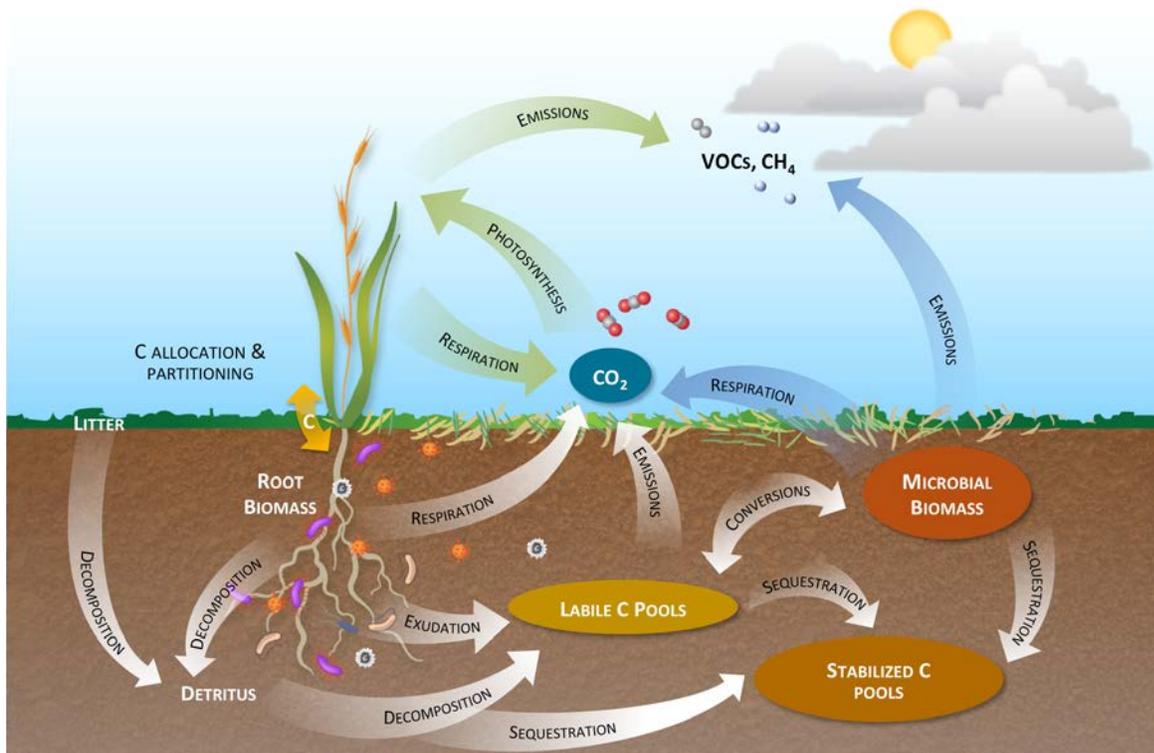


Figure 2. Carbon (C) flow and transformations in the plant ecosystem. Carbon enters the soil as root exudates or via decomposition of root or aboveground biomass. In the soil, C exists in root or microbial biomass, as bioavailable labile organic C, or in more stabilized C pools. Carbon exits the soil as direct emissions, or via root or microbial respiration, with microbial-mediated soil respiration being the major source of CO₂ from terrestrial ecosystems. Carbon is also lost from the ecosystem as VOCs and methane (CH₄).

1.3 Approach

We use designed, highly controlled experimental ecosystems based on the genomics model grass *Brachypodium distachyon*, (*Brachypodium*) to enable quantitative prediction of ecosystem traits and responses as a function of plant genotype and environmental variables (Fig. 3). *Brachypodium* offers a suite of advantages as a model system (4-6), including 1) small (270 Mbp) diploid genome; 2) large collections of natural accessions, recombinant inbred lines and mutants, 3) complete genome sequence information for >50 accessions; high genotypic diversity for bioenergy traits such

as biomass accumulation, root system architecture (RSA), and drought tolerance; 4) small stature (10-15 cm); 5) short life cycle (6-9 weeks); 6) established protocols for transgenic and genome editing approaches. The purpose of using a model system is to derive information and

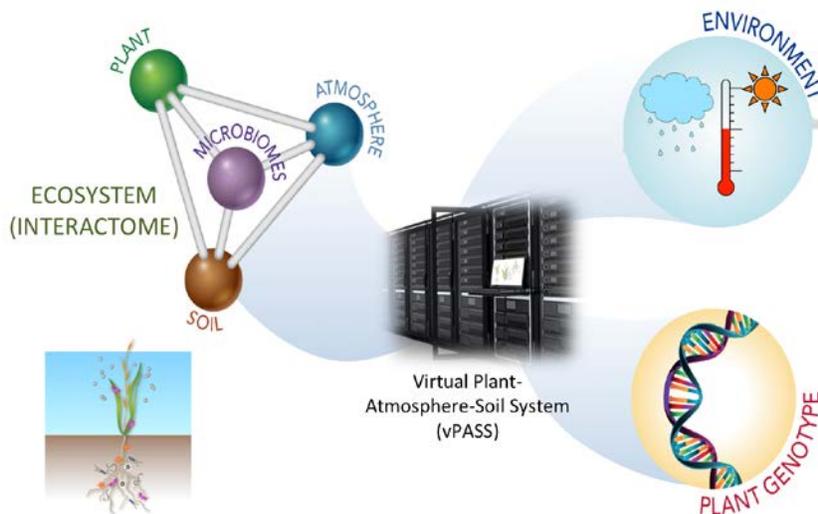


Figure 4. Building a virtual plant ecosystem. The iPASS Initiative will develop a computational model of virtual Plant-Atmosphere-Soil Systems, with predictive linkages between plant genotype, environment and the plant-microbe-atmosphere-soil integrated system.

genomic and environmental variables inform predictions of traits and responses at different scales, from molecules to plant to ecosystem (Fig. 4). The vPASS model is built along three parallel paths:

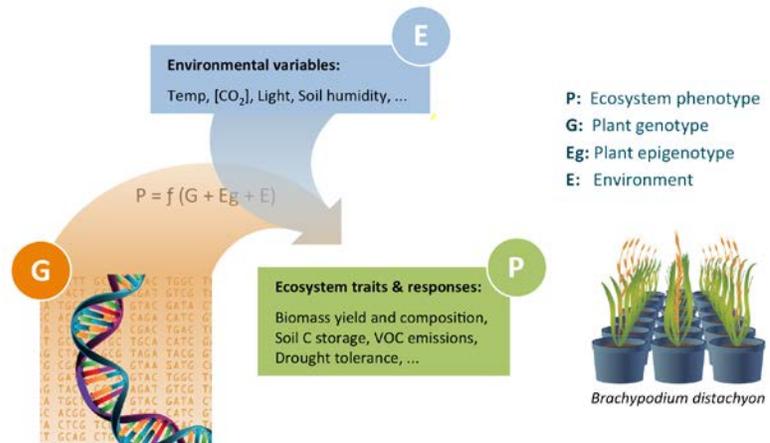


Figure 3. Different genotypic accessions of *B. distachyon* are exposed to drought and/or enhanced CO₂ levels, and the phenotypic responses are followed at different scales.

knowledge that would otherwise be difficult to obtain, and that can subsequently be tested on and applied to non-model plants and plant ecosystem (see also Section 1.5).

Research is directed along four focus areas, Computational Modeling, Plant Biology and Microbiomics, Atmospheric Processes, and Soil Biogeochemistry.

Computational Modeling. A key deliverable of iPASS is a virtual plant ecosystem – a virtual Plant-Atmosphere-Soil System (vPASS) - a predictive computational model describing how

- vPASS1: An empirically based statistical model of system phenomic response based on iPASS experimental data. This is a correlative model linking plant genotypic information and environmental variables to plant phenotype and ecosystem traits and responses.
- vPASS2: A process-based model of a single plant coupled to soil and atmospheric processes, and linked to genomics controls through vPASS1. This model aims to explain how interactions between biotic and abiotic factors and environmental conditions shape emergent properties of the plant and the integrated plant ecosystem.
- vPASS3: A community software and data management framework that will facilitate linkages between the single-plant model (vPASS2) and models of complex systems (e.g., ecosystems and watersheds).

Biological processes span several scales in space, from the single molecules to organisms and ecosystems (Fig. 5). A holistic understanding of biological systems therefore requires multiscale models that capture the relevant properties on all these scales and the complex interactions between different organization levels in those systems. For example, plants respond to

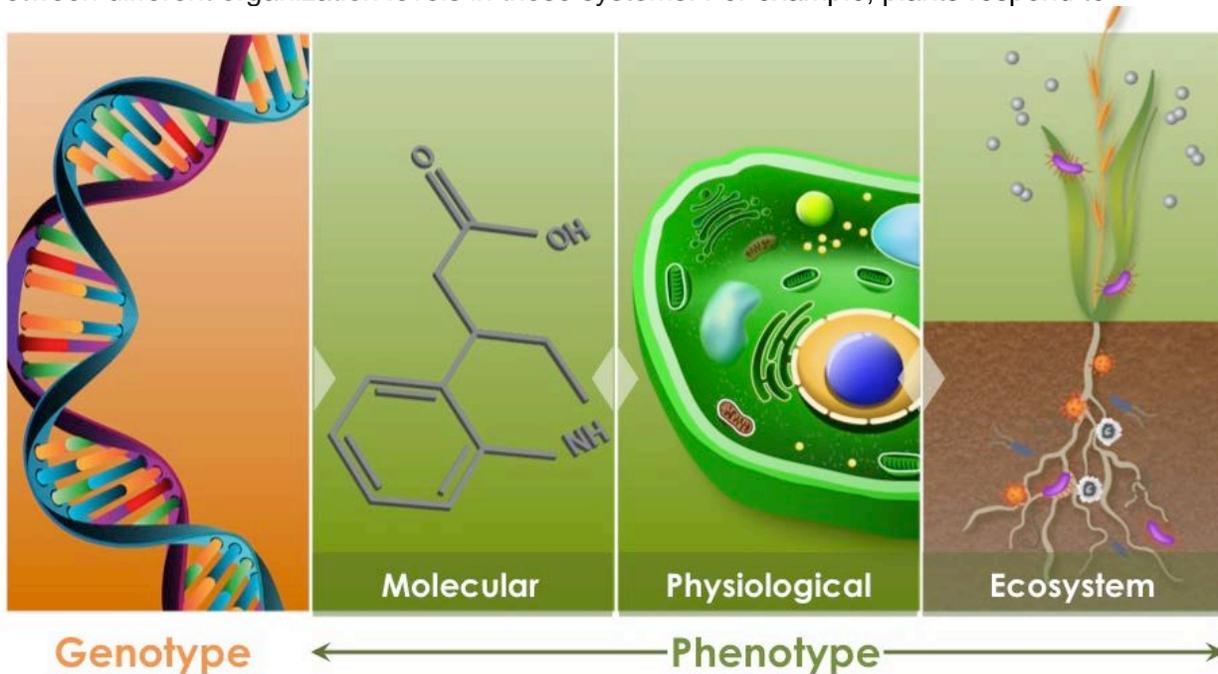


Figure 5. Plant multiscale modeling. Information in the plant genome is translated to phenotypic information across different scales or levels. Information between the different phenotypic levels can flow in both directions.

environmental change by triggering biochemical and developmental networks across multiple scales. Multiscale models that link genetic input to the whole-plant scale and beyond will therefore improve biological understanding and trait prediction.

Multiscale modeling also is required to obtain mechanistic understanding for how the genotype interacts with the environment to shape the phenotype of a biological system such as a plant, and for how genotypic information is translated to trait and responses across levels from molecules to organisms to ecosystems.

A multiscale approach is necessary in constructing the vPASS1 and vPASS2 models in order to obtain mechanistic understanding of observed plant phenotypes and ecosystem properties. As is indicated in Fig. 5 by double arrows, both upward and downward causation of properties occur between different phenotypic scales or levels. Thus just as traits and responses at the

whole-plant or ecosystem scales are informed by molecular properties, phenotypic traits at the molecular scale can be informed by properties at higher scales.

Plant Biology and Microbiomics. The physiological basis of biomass maintenance under biotic stress such as drought or increasing levels of atmospheric CO₂ or other greenhouse gases remains poorly understood, due both to numerous genetic and physiological mechanisms that plants can use to respond to these conditions and the complexity of the stress itself. A key to understanding plant responses is to link phenotypic traits at organismal and ecosystem

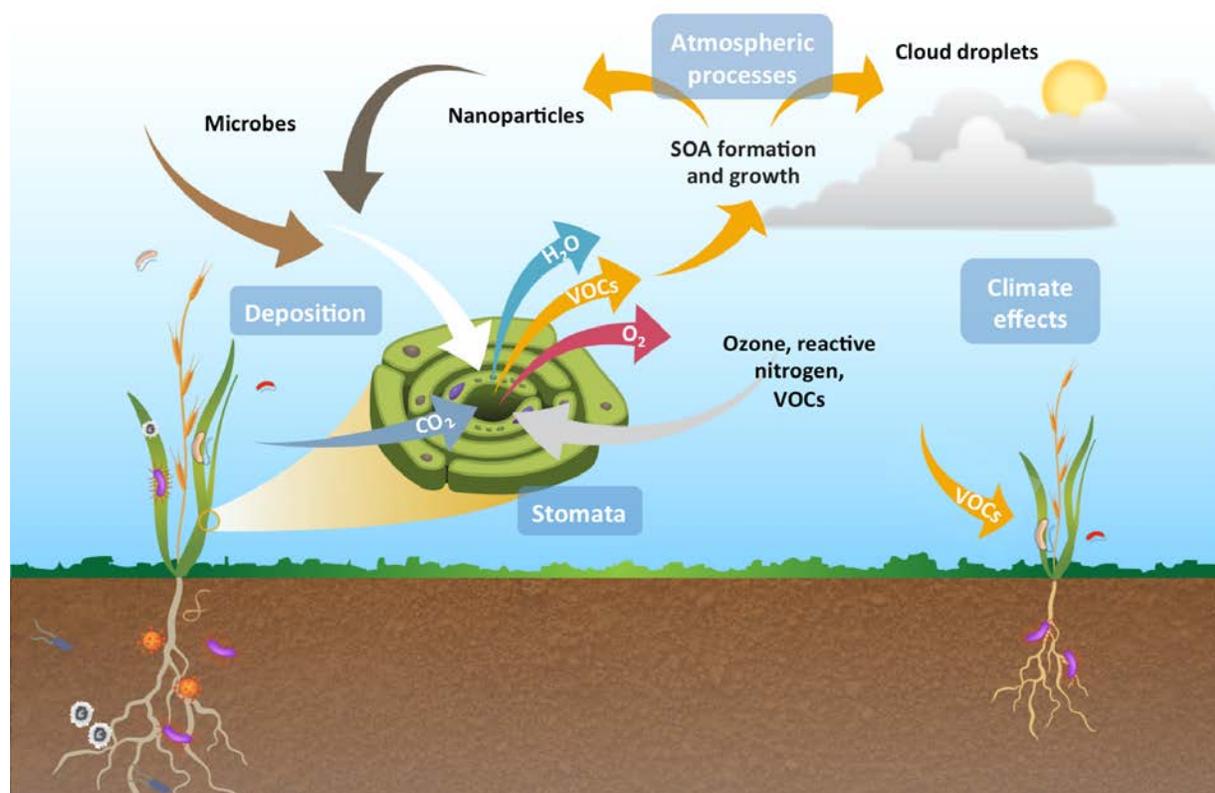


Figure 6. Plants emit a great diversity of biogenic VOCs; e.g., terpenes, fatty acid derivatives, alcohols and alkanes. VOCs are a vital element of a plant's phenotype and are a central character in plant ecosystem as signaling molecules, e.g., in pollination, and in response to biotic or abiotic stress. Many VOCs are constitutively expressed by plants but emissions typically increase dramatically upon exposure to abiotic or biotic stresses such as drought or pathogens. The role(s) of VOCs in constitutive or stress-induced emissions are not clear. Intriguingly, VOCs emitted as stress signals from one plant can be perceived by a neighboring plant not yet under stress, triggering an anticipatory stress response. The emissions of VOCs are the major source of secondary organic aerosols (SOAs) in the atmosphere, which, in turn, affect climate and air quality.

scales to molecular-scale phenotypes under a variety of conditions. To obtain sophisticated understanding of CO₂ uptake and source-sink communications as central components of ecosystem carbon cycling, this focus area will develop methods for advanced and automated physiological characterization of a wide variety of plant phenotypes, develop an advanced plant based metabolomics library for the characterization of plant metabolites and augment, and apply advanced omics measurements to the characterization of *Brachypodium* genotypes. Data collection and analysis will be geared toward integration into the models described in the Computational Modeling Focus Area.

Atmospheric Processes. Plants and associated microbiota emit a diverse array of VOCs and particles into the atmosphere and actively remove other constituents from the air and thus control distributions of atmospheric organics including secondary organic aerosol (SOA) (Fig. 6). One of the greatest challenges with respect to predicting regional climate change on decadal time scales is developing a quantitative understanding of plant VOC and particle uptake and emission and their interactions with anthropogenic pollution to produce SOA. The greatest uncertainty in climate model simulations is the effects of aerosols on radiative forcing, hence the need to better understand the factors responsible for their production. Conceptually, the potential linkages and feedbacks among climate, plant-atmosphere VOC fluxes, and aerosol formation are clear. Yet there are major gaps in understanding the mechanisms controlling these processes and the fundamental molecular-scale properties of VOC and SOA, as well as how to link this molecular-scale knowledge to the mesoscale characteristics and behavior of such atmospheric components. Incorporating a molecular-scale understanding of the production of SOA from plant VOC emissions could significantly reduce uncertainties in predictive climate simulations and advance, potentially in a transformative way, the representation of biosphere-atmosphere feedback couplings. This focus area will address questions related to plant-aerosol interactions.

Soil Biogeochemistry. Predictive understanding of dynamic processes that impact the exchange of C between soil and atmosphere is largely missing and results in large uncertainties in model predictions of future atmospheric CO₂ concentrations. Information will be collected at the molecular to soil pore-scale to develop and inform the high-resolution model of the hydrologic and biogeochemical processes in soil and rhizosphere that impact belowground carbon allocation and dynamics and plant growth (Fig. 2). Soil processes and properties that are likely to be affected by plant activities are soil chemical properties and the rhizospheric microbial community. The scope includes composition, deposition, and function of root exudates and other soil organic matter and the chemical exchange of SOM between soil, plant, and microbes; and the fate, storage of photosynthate-derived soil organic carbon, and potential emission of plant or microbially respired soil organic carbon as CO₂.

1.4 Scientific Outcomes

The iPASS Initiative will build expertise and novel capabilities in molecular plant phenotyping, multiscale plant modeling, root phenotyping and modeling, and plant genotype-to-phenotype mapping. A major outcome is vPASS, a computational mechanistic plant ecosystem model at the molecular-to-ecosystem scale in which perturbations at one scale are prognostic for alterations at other scales. The iPASS Initiative will also result in conceptual ideas and drivers to support the development of capabilities for integrative studies of designed or imported plant ecosystems under simulated and controlled environmental conditions (EcoSimulator Facility).

1.5 From Model System to Translational Applications

The iPASS Initiative is based on fundamental research aimed at providing the knowledge base for studying plant ecosystems as an integrated unit comprising interactions between plants, microbes, soil and atmosphere. This understanding, together with developed capabilities and technologies, will be applied to more complex plant systems, such as energy sorghum plantations and native grasslands.

1.6 The iPASS Team

The iPASS team is presented in Fig. 7.



Figure 7. The iPASS team and focus areas. Within the iPASS Initiative, specific projects are solicited as open calls and selected by the iPASS management. Key Staff shown represents PIs for awarded FY 2017 projects.

2.0 Current iPASS Projects

The following eight 3-year iPASS projects are ongoing, or scheduled for start in FY 2017.

1. **GoBrachy.** Develop trait associations network models for carbon allocation in *Brachypodium* under different environmental conditions.
2. **vPASS 1.0: Quantifying signatures of phenomic expression of a *Brachypodium* ecosystem as a function of genomic and environmental variables.** Develop empirical models of traits and responses in the *Brachypodium* ecosystem as a function of controlled environmental conditions and plant genotypic variations.
3. **vPASS 2.0: Mechanistic process components of a virtual plant simulator.** Develop a novel prognostic vPASS model that integrates a comprehensively detailed mechanistic single plant model with microbial, atmospheric, and soil system processes in its immediate environment.
4. **PhenoAccess: Physiological phenotyping of *Brachypodium* accessions.** Develop capabilities for high-throughput image-based plant phenotyping as a screening tool for selecting specimens for molecular phenotyping. PhenoAccess also includes the subproject **PhenoGrass**, which aims at physiological characterization of C₃ and C₄ model grasses (*Brachypodium* and *Setaria*, respectively) under elevated CO₂ levels.

5. **Molecular phenotyping of *Brachypodium* to Provide Metabolic and Functional Linkages to the Plant-Atmosphere-Soil-Systems (iPASS) Model.** Develop the fundamental molecular characterization necessary to build a model that ultimately links phenotypic measurements to the atmospheric processes and soil biogeochemistry associated with *Brachypodium* during its lifecycle and under conditions of drought stress and increased atmospheric CO₂ concentrations.
6. **Response of *Brachypodium* associated microbiomes to drought and/or elevated CO₂ illuminated by biogeochemical and molecular measurements.** Combine both biogeochemical profiling and molecular profiling approaches to compare the phyllosphere and rhizosphere of drought tolerant and drought resistant *Brachypodium* variants grown under current and elevated CO₂ conditions.
7. **VOC emissions from the plant, soil, microbial ecosystem and their climate implications.** Study VOC emissions of plant/soil/microbial ecosystem and how these emissions depend on plant genotype, phenotype, and response to climate change-related stress, and how the atmospheric transformation of these VOCs form SOAs.
8. **Hydraulics of the *Brachypodium*-root-soil system under variable environmental conditions.** Generate the fundamental root and hydraulic data needed for the soil biogeochemistry module of vPASS2 and to compare the experimental data with vPASS2.0 results and alternative (empirical and continuum) models.

3.0 Contact Info

[Christer Jansson](#), [Nancy Hess](#) (Science)

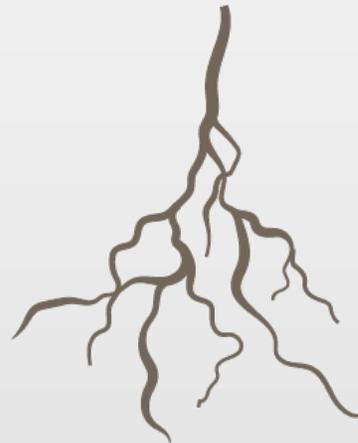
[Mary McGown](#) (Administration)

Website (to be activated in January 2017)

[Internal website](#) (requires login)

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