

December 2016

iPASS

Multiscale Plant Modeling Workshop Report



Prepared for the U.S. Department of Energy's Office of Biological
and Environmental Research under Contract DE-AC05-76RL01830

Pacific Northwest National Laboratory
Richland, Washington 99352

About the cover



According to the National Science Foundation's (NSF) 2016 report, "10 Big Ideas for Future NSF Investment" (1), *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.*

This genome-to-phenome challenge entails understanding how information in the genome is translated to phenotypic expression at the molecular scale, and how the molecular interactions inform emergent traits and responses at subsequently larger scales, eventually resulting in the organismal phenotype, and, to varying degrees, properties at even larger scales such as ecosystems.

The figure on the cover illustrates the genome-to-phenome pathway for a plant (the annual grass *Brachypodium distachyon*). As is indicated by double arrows, phenotypic information can flow in both directions; for example, phenotypic traits at the molecular scale can be informed by properties at higher scales. In the figure, the plant is depicted with associated rhizospheric and phyllosperic microbiomes and is shown emitting volatile organic compounds.

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C Jansson

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Acronyms and Abbreviations

BER	Office of Biological and Environmental Research at the Department of Energy
BioCro	Plant growth model
DIRT	Digital Imaging of Root Traits – a root imaging model
DOE	Department of Energy
EMSL	Environmental Molecular Sciences Laboratory
iPASS	integrated Plant-Atmosphere-Soil Systems
KBase	The Department of Energy Systems Biology Knowledgebase
MPM	Multiscale Plant Modeling
PlantGro	Plant growth model
PNNL	Pacific Northwest National Laboratory
SimRoot	a root imaging model
vPASS	virtual Plant-Atmosphere-Soil Systems
XCT	X-ray Computed Tomography

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1.0 Introduction

On August 25–26, 2016, EMSL, the Environmental Molecular Sciences Laboratory, hosted a workshop on the Pacific Northwest National Laboratory (PNNL) campus in Richland, Washington, through the integrated Plant-Atmosphere-Soil Systems (iPASS) Laboratory-Directed Research and Development Initiative. Twelve internationally leading scientists from Europe, Canada, and the U.S. were invited to the workshop together with the iPASS team and additional staff at PNNL. The purposes of the workshop were to inform the iPASS effort on state-of-the-art multiscale plant modeling (MPM) research and to explore how best to integrate MPM in the iPASS initiative. As an add-on to the MPM Workshop, EMSL through iPASS also organized a Roots Mini Symposium at PNNL from October 4–6, 2016 to specifically discuss root phenotyping and modeling.

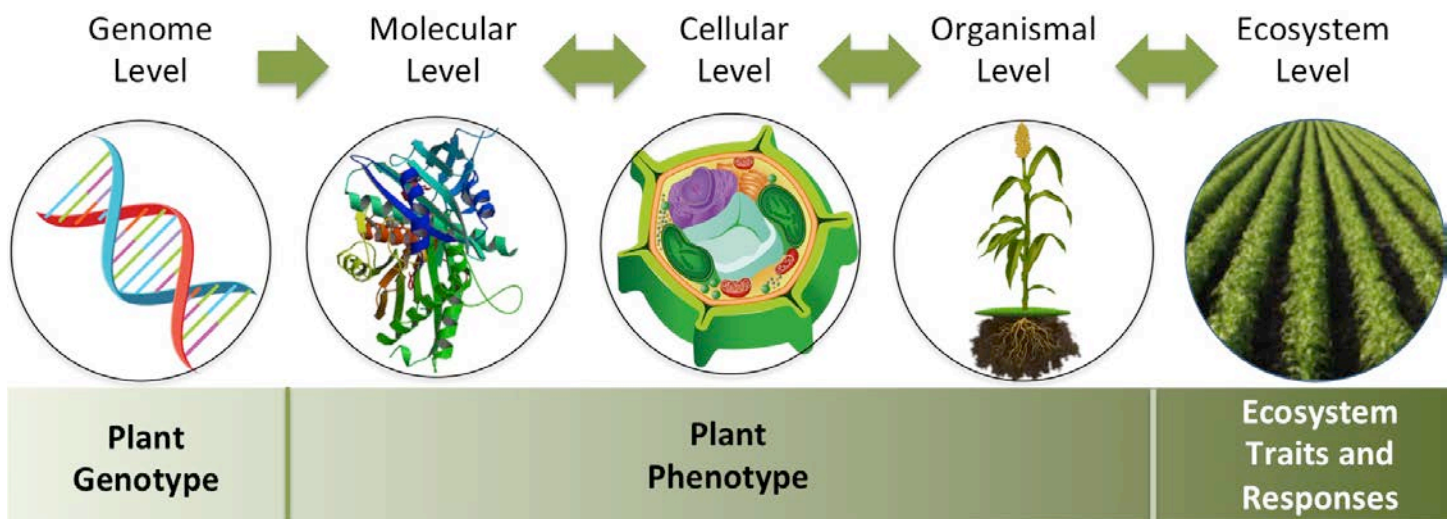


Figure 1.1. Plant Multiscale Modeling. Information in the plant genome is translated to phenotypic information across different scales or levels. Information between the different phenotypic levels can flow in both directions.

Biological processes span several spatial scales, from single molecules to organisms and ecosystems. A holistic understanding of biological systems requires multiscale models that capture relevant properties on all these scales and complex interactions between different organization levels in those systems. For example, plants respond to 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 of how the genotype interacts with the environment to shape the phenotype of a biological system such as a plant, and how genotypic information is translated to traits and responses across levels from molecules to organisms to ecosystems.

A key deliverable of iPASS is a virtual plant ecosystem – a virtual Plant-Atmosphere-Soil System (vPASS) – a predictive computational model describing how genomic and environmental variables inform predictions of traits and responses at different scales, from molecules to plant to ecosystem (Figure 1.1). The vPASS model (Figure 1.2) is built along three parallel paths:

1.0 Introduction

- 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).

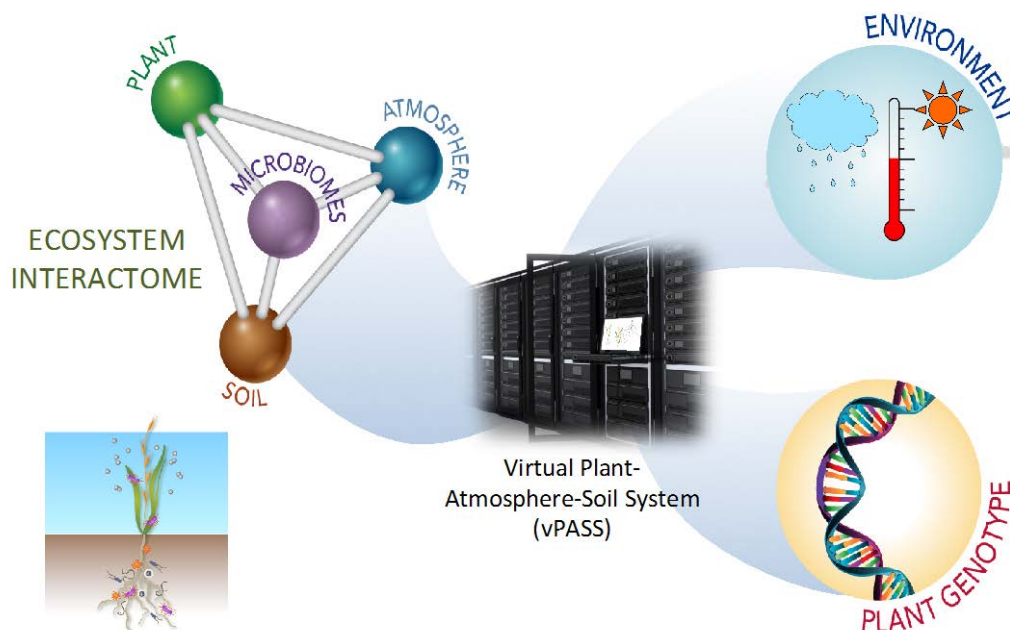


Figure 1.2. Computational Modeling in iPASS. The vPASS models are built to describe how information in the plant genome propagates through plant-microbiome-soil-atmosphere interactions to influence emergent traits and responses at the ecosystem level, and how these interactions are impacted by environmental variables.

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 indicated in Figure 1.1 by double arrows, both upward and downward causation of properties occurs between different phenotypic scales or levels. Thus just as 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.

2.0 Workshop Summary

2.1 EMSL Science and Capabilities

The August 25 and 26 morning sessions were used to brief external participants on EMSL as an Office of Science Office of Biological and Environmental Research (BER) user facility and research institution. On the morning of August 25, Christer Jansson gave an overview of EMSL. This was followed by a discussion about EMSL where Nancy Hess, Christer Jansson, and other EMSL staff answered questions about the role EMSL has in the scientific community. On the morning of August 26, Mark Bowden led a tour of EMSL with participation from science theme and capability leads and their teams at different stations.

2.2 The iPASS Initiative

The August 25 morning sessions also included an overview of the iPASS Initiative. Christer Jansson presented the goals, approach, and deliverables of iPASS, and Steve Yabusaki gave a more detailed description of the Computational Modeling focus area. In the ensuing discussion, Christer Jansson, Nancy Hess, Tim Scheibe, Steve Yabusaki, Ruby Leung, Mary Lipton, Amir Ahkami, and Xingyuan Chen answered questions about iPASS in the context of PNNL and BER missions, and its role for programmatic research projects in climate change and bioenergy.

2.3 Workshop Presentations

2.3.1 Whole-Plant Modeling

Several presenters described different approaches to whole-plant, multiscale modeling, from a structural and/or functional perspective.

Steve Long (Professor), Department of Crop Sciences & Plant Biology, University of Illinois at Urbana-Champaign – Crops *in silico*: What & Why Now? Long discussed the Crops *in Silico* project (2), an integrative and multiscale modeling platform that combines modeling efforts toward the generation of virtual crops, which is open and accessible to the entire plant biology community. He stressed that the Crops *in Silico* project has to be a community effort without single-institution ownership, and compared it to the existing Virtual Rat project and the Astrophysics community. Steve also mentioned the PlantGro model, which is a whole-plant model that scales from the leaf to the canopy level. This model also includes a separate root and soil model and a phenology model. These models can be coupled and solved iteratively to obtain a whole plant and even stand of plants representation. The inputs for this model include climate variables such as precipitation, humidity, CO₂, and temperature, while the outputs include energy and mass fluxes for canopy transpiration, C flux, and yield; and plant properties such as leaf area index and canopy height.

Yin Hoon Chew (Postdoctoral Researcher), Icahn School of Medicine, Mount Sinai, New York – Linking Genotype to Phenotype through Multiscale Models. Chew presented her work on *Arabidopsis thaliana* whole-plant modeling at different spatio-temporal scales, and modular approach to combine existing models. Their *Arabidopsis* model (3) has been validated and deposited in the Plant Systems-Biology Modeling (PlaSMo) database.

Mikolaj Cieslak (Senior Research Associate), Department of Computer Sciences, University of Calgary, Canada – Plant Modeling with L-Systems. Cieslak described the L-System or Lindenmayer System for generating architectural models of plant structures such as canopies and roots to simulate optimal functionalities like light penetration and nutrient uptake.

2.0 Workshop Summary

Christophe Pradal (Staff Researcher), The VirtualPlant Initiative, INRIA, Montpellier, France – Multiscale Plant Modeling & Phenotyping using Scientific Workflow in OpenAlea. Pradal presented the VirtualPlant Initiative and its objective of modeling plant morphogenesis from genes to phenotypes. The VirtualPlant Initiative uses OpenAlea, which is an open-source project primarily aimed at the plant research community, with a particular focus on Plant Architecture Modeling at different scales.

Chris Meyers (Professor), Department of Physics, Cornell University – Multiscale Modeling of Plant Metabolism across Space & Time. Meyers described genome-to-phenome modeling of plant metabolism with focus on photosynthesis and source-sink transition in C₃ and C₄ plants, and presented a metabolic reconstruction of maize. He mentioned and compared existing photosynthesis models that are either biochemical, kinetic, or constraint-based in nature.

Roeland Merks (Professor), the Mathematical Institute, University of Leiden, The Netherlands – Multiscale, Cell-based Modeling of Plant Development & Microbial Communities. Merks' presentation covered multiscale modeling of biological developmental processes, including blood vessel growth and plant growth. He described cell-based models and simulation methods for plant tissues in *Arabidopsis thaliana*, and how tissue structure feeds back on cell behavior and gene expression, exemplified by auxin transport and stomatal models. Special emphasis was on symplastic tissue mechanics employing the Metropolis algorithm.

Jörg Schwender (Senior Staff Scientist), Biology Department, Brookhaven National Laboratory – Charting Plant Metabolism: Quantitative Analysis of Metabolic Flux in Plants. Schwender discussed work on ¹³C metabolic flux analysis and metabolic modeling in plants, particularly oil seed crops. He described models of growth and storage metabolism and regulation of carbon partitioning, e.g., lipid-starch tradeoff, during seed development in *Brassica napus* (rapeseed). A related topic was on genotypic variation in *B. napus* seed composition.

Michael Knoblauch (Professor), Department of Plant Biology, Washington State University – Phloem Transport & Unloading: Key Elements in Assimilate Allocation. Knoblauch described how long-distance transport of photosynthate in sieve tubes of the phloem, and unloading of photosynthate to roots is regulated. He provided strong support for the Münch hypothesis, which describes a mechanism of osmotically generated pressure differentials that are supposed to drive the movement of sugars and other solutes in the phloem.

Pankaj Jaiswal (Professor), Department of Plant Pathology, Oregon State University – Plant Reactome. Jaiswal gave a presentation on the Plant Reactome, a NSF-funded free, open-source, curated and peer reviewed pathway database. The goal of Plant Reactome is to provide intuitive bioinformatics tools for the visualization, interpretation and analysis of pathway knowledge to support basic research, genome analysis, modeling, systems biology and education. It contains tools for omics data analysis and visualization, as well as cross-species pathway comparisons. Currently, Plant Reactome provides orthology-based pathway projections for 62 plant species.

2.3.2 Root Modeling

In addition to aspects of root modeling covered as part of whole-plant modeling, three workshop presentations offered a specific focus on root modeling and plant-soil interactions.

Alexander Bucksch (Principal Investigator), School of Biology, Georgia Institute of Technology – DIRT: Digital Imaging of Root Traits in the Field. Bucksch described his Digital Imaging of Root Traits (DIRT) (4): a high-throughput computing and collaboration platform for field-based root phenomics. DIRT is an open-source, online platform that enables researchers to store images of plant roots, measure dicot and monocot root traits under field conditions, and share data and results within collaborative teams and the broader community.

Jonathan Lynch (Professor), Department of Plant Science, Penn State – Modeling Phenotypes and Phenotypes for Soil Resource Capture. Lynch described his root model SimRoot (5). SimRoot is an architectural root model that simulates growth of a root system over time in a 3D virtual space. In SimRoot, growth is predefined; an infinite number of root classes can be defined, each with its own growth and branching pattern. Currently input files for maize and bean are available.

Tiina Roose (Professor), School of Engineering Sciences, University of Southampton, UK – Multiscale Modeling of Plant-Soil Interactions. Roose presented capabilities at the University of Southampton in X-ray Computed Tomography (XCT) imaging, and her mathematical approach to pore-scale reconstruction and modeling, upscaling, and rhizosphere modeling (6).

2.3.3 Multiscale Plant Modeling and KBase

To learn how iPASS and the multiscale plant modeling effort can best interact with the DOE Systems Biology Knowledgebase (KBase) we included a tutorial during the workshop on the *Annotate Plant Coding Sequences with Metabolic Functions* method that is part of the KBase Narrative Interphase.

Sam Seaver (Assistant Computational Scientist; Head of the Plant Modeling Group at KBase), Argonne National Laboratory – Plant Workflows in Persistent KBase Narratives. Seaver guided us through the concept of *Narrative* in KBase as an interactive “publication” that includes analysis steps, data, commentary and visualization. In this context, he described PlantSEED, a NSF-funded collaboration between Argonne National Lab and University of Florida.

3.0 Workshop Outcomes and Future Directions

The workshop demonstrated a wide spectrum of MPM approaches and plant systems (Figure 3.1). The workshop presentations and discussions were highly informative suggesting the way forward for MPM in iPASS. Tim Scheibe, Steve Yabusaki and others on the iPASS modeling team engaged participants in several follow-up discussions, resulting in specific collaborations and other initiatives.

- We have received and are utilizing Yin Hoon Chew's code, and we are working with her to implement the whole-plant *Arabidopsis* model (3) she presented for the *Brachypodium*-based model in iPASS.
- We have received codes for Steve Long's BioCro (7, 8) and PlantGro models. Discussions are ongoing with Venkat Srinivasan, a postdoctoral researcher in Steve Long's group, and with Xinguang Zhu, a former postdoctoral researcher in Long's group and now an established researcher at the Chinese Academy of Sciences (CAS) and the Max Planck (MPG) Partner Institute in Shanghai, to utilize BioCro and PlantGro 3D, the "whole" plant model from Steve Long's group that will supersede BioCro. As part of this effort, Yilling Fang from the iPASS modeling team visited Zhu at his CAS-MPG institute in late September, and Yillin subsequently arranged for Zhu to visit PNNL in late November. Our strategy is for iPASS modeling to become a participant for the Plants *in Silico* movement.

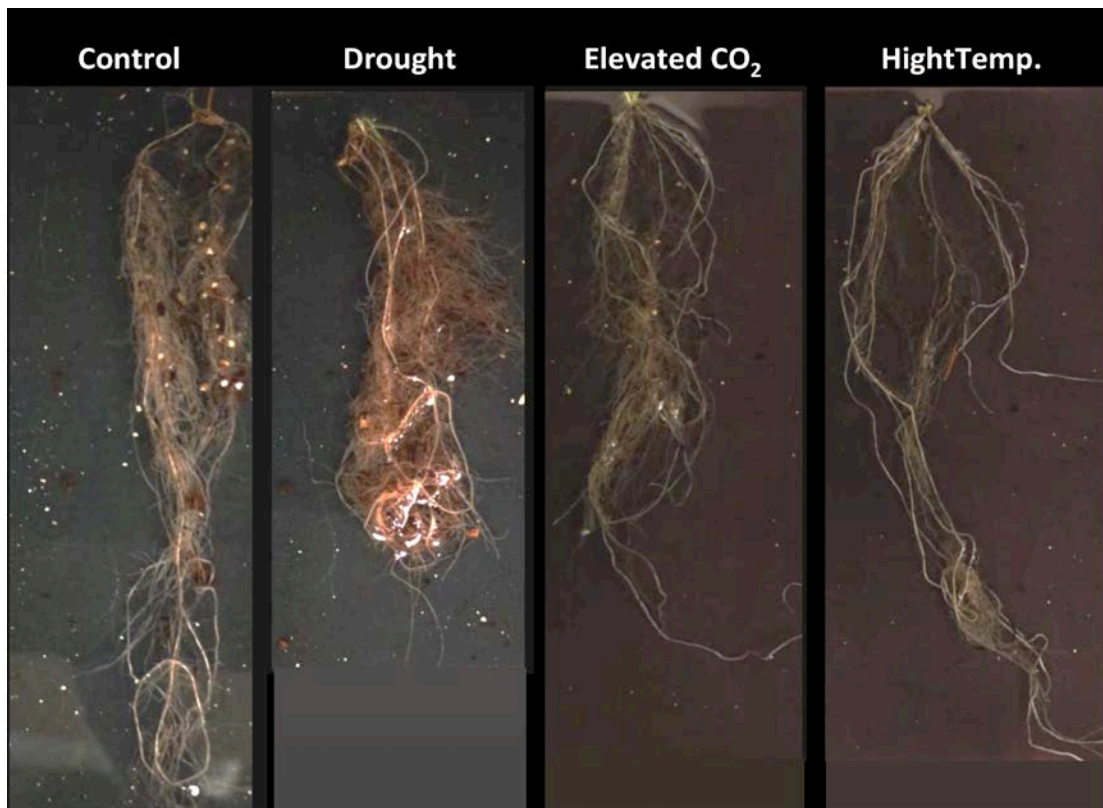


Figure 3.1. *Brachypodium* Root Images . One of the examined *B. distachyon* genotypes grown under different environmental conditions in the EMSL phytotron. Photo: Pubudu Handakumbura.

- We received access to SimRoot (5) and are currently testing it with the help of Jonathan Lynch and Johannes Postma, a former postdoctoral researcher of Lynch's who is now a researcher at the Plant Sciences Institute, Forschungszentrum Jülich, Germany.

3.0 Workshop Outcomes and Future Directions

- We have received Tiina Roose's code for root modeling (6) and are collaborating with her on improving EMSL's XCT capabilities for visualizing *Brachypodium* roots (Figure 3.2). As part of this collaboration, Nancy Hess facilitated a visit by Tamas Varga from EMSL to the Roose Southampton Lab in mid-November. Due to their fine structure, imaging of *Brachy-podium* roots with XCT at EMSL has been a challenge. The joint effort with Tiina Roose's lab holds great promise to significantly improve *Brachypodium* root phenotyping and modeling in iPASS. In discussions following the workshop, Tiina Roose expressed an interest in doing a sabbatical at PNNL and this opportunity was reinforced in connection with Varga's site visit.
- We are discussing the option of sending root images of *Brachypodium* genotypes to Alexander Bucksch's lab for digitalization and characterization.
- We have initiated discussions with Sam Seaver for how best to make use of KBase in iPASS.
- Several of the invited participants expressed a strong interest in utilizing the EMSL capabilities and engaging in collaborative efforts in future user proposals.



Figure 3.2. EMSL Scientist and iPASS Co-PI at the XCT Instrument

4.0 Root Mini Symposium

As an extension of the MPM Workshop, and keeping with the initiated discussions and activities in root phenotyping and modeling resulting from the workshop, EMSL organized an iPASS Root Mini Symposium on October 4–6. Professor Philip Benfey from Duke University, NC, and Principal Investigator Christopher Topp from Donald Danforth Plant Science Center, MO, were invited to give presentations and interact with scientists at EMSL and PNNL. The mini symposium included presentations by Benfey and Topp, a tour of EMSL led by Nancy Washton, small-group meetings with Christer Jansson, Nancy Hess, Tim Johnson, Mart Oostrom, Lili Paša-Tolić, Kim Hixon, Amir Ahkami, Pubudu Handakumbura, Steve Yabusaki, and Yillin Fang, and a round-table discussion on root phenotyping and modeling.

The Root Mini Symposium and ensuing discussions integrated seamlessly with initiatives resulting from the MPM Workshop. Specifically, Amir Ahkami is communicating with Benfey and Topp in developing a gel-based *Brachypodium* root phenotyping platform to complement the XCT measurements, and Mart Oostrom is traveling to both the Benfey Lab and Danforth Plant Science Center to exchange information on advanced root-soil sampling design.

Appendix A

References

Appendix A – References

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Appendix B

Workshop & Symposium Agendas

Appendix B – Workshop & Symposium Agendas

iPASS Multiscale Plant Modeling Workshop EMSL Board Room August 25 – 26, 2016

AGENDA

Thursday, August 25, 2016	
Time	Topic/Participant(s)
7:30 a.m.	Badging; Morning refreshments
8:00 a.m.	Welcome and Introductions – Christer Jansson
8:15 a.m.	EMSL overview & iPASS Initiative Vision and Plan – Christer Jansson
8:45 a.m.	Questions & Discussions
8:55 a.m.	iPASS Computational Modeling –Steve Yabusaki,
9:30 a.m.	Questions & Discussions
9:40 a.m.	Pankaj Jaiswal, Oregon State University – “Plant Reactome: A portal for plant pathways and comparative analysis”
10:10 a.m.	Questions & Discussions
10:20 a.m.	Break
10:30 a.m.	Jonathan Lynch, Penn State (via Skype) – “Roots for the 10B: modeling phenes and phenotypes for soil resource capture”
11:00 a.m.	Questions & Discussions
11:10 a.m.	Alexander Bucksch, University of Georgia, Athens – “DIRT: Computational root phenotyping in the field”
11:40 a.m.	Questions & Discussions
11:50 a.m.	Working Lunch, iPASS Computational Modeling, cont. discussion
12:50 p.m.	Break
1:00 p.m.	Roeland Merks, Mathematical Institute (MI), Leiden University, Leiden - “Multiscale, cell-based modeling of plant development and of microbial communities”

Appendix B – Workshop & Symposium Agendas

1:30 p.m.	Questions/Discussions
1:40 p.m.	Jörg Schwender, Brookhaven National Lab – “Charting plant metabolism: Quantitative analysis of metabolic flux in plants”
2:10 p.m.	Questions/Discussions
2:20 p.m.	Michael Knoblauch, Washington State University – “Phloem transport and unloading: Key elements in assimilate allocation”
2:50 p.m.	Questions/Discussions
3:00 p.m.	Steve Long, University of Illinois at Urbana-Champaign (via Skype) – “Modeling photosynthesis from metabolism to plant production”
3:30 p.m.	Questions/Discussions
3:40 p.m.	Yin Hoon Chew, Mount Sinai School of Medicine – “Linking Genotype to Phenotype through Multiscale Models”
4:10 p.m.	Questions/Discussions
4:20 p.m.	Mik Cieslak, University of Calgary, Canada – “Plant Modeling with L-systems”
4:50 p.m.	Questions/Discussions
5:00 p.m.	Adjourn
6:00 p.m.	Reception Dinner (by invitation only), Dr. Bill’s
Friday, August 26, 2016	
Time	Topic/Participant(s)
7:30 a.m.	Morning refreshments
8:00 a.m.	EMSL Tour (external participants)
9:00 a.m.	Tiina Roose, University of Southampton, UK – “Multiscale image based modeling of plant-soil interaction”
9:30 a.m.	Questions/Discussions
9:40 a.m.	Sam Seaver, Argonne National Lab – “Plant Workflows in persistent KBase Narratives”
10:10 a.m.	Questions/Discussions
10:20 a.m.	Christophe Pradal, INRIA France – “Multi-scale plant modeling and phenotyping with Scientific Workflows in OpenAlea”

10:50 a.m.	Questions/Discussions
11:00 a.m.	Chris Myers, Cornell University – “Multiscale modeling of plant metabolism across space and time”
11:30 a.m.	Questions/Discussions
11:40 a.m.	Wrap up – Christer Jansson
12:00 p.m.	Adjourn

iPASS Roots Mini Symposium
EMSL Board Room
October 4–6, 2016

AGENDA

Tuesday, October 4, 2016	
Time	Topic/Participant(s)
10: p.m.	Chris Topp: Arrive at PNNL; Check in at The Guest House at PNNL
Wednesday, October 5, 2016	
Time	Topic/Participant(s)
8:00 a.m.	Topp Badging; Breakfast – Christer Jansson
9:00 a.m.	Christer Jansson
9:30 a.m.	Nancy Hess
10:00 a.m.	Steve Yabusaki, Yilin Fang
10:30 a.m.	Tim Johnson, Mart Oostrom
11:00 a.m.	Lili Paša-Tolić, Kim Hixson
11:30 a.m.	Lunch – Christer Jansson
1:45 p.m.	Philip Benfey Check in at the Guest House at PNNL; badging
2:00 p.m.	iPASS Presentation – Christer Jansson, Nancy Hess,

Appendix B – Workshop & Symposium Agendas

3:00 p.m.	EMSL Tour – Nancy Washton
4:30 p.m.	Root Phenotyping & Modeling discussion – Christer Jansson, Nancy Hess, Tim Scheibe, Steve Yabusaki, Yilin Fang, Xingyuan Chen, Tim Johnson, Mart Oostrom, Amir Ahkami
5:30 p.m.	Dinner (TBD)
Thursday, August 6, 2016	
Time	Topic/Participant(s)
8:00 a.m.	Breakfast – Amir Ahkami, Pubudu Handakumbura
9:00 a.m.	Benfey Seminar – EMSL Boardroom
10:00 a.m.	Topp Seminar – EMSL Boardroom
11:00 a.m.	Questions/Discussions – EMSL Boardroom
12:00 p.m.	Departure

Appendix C

Workshop & Symposium Attendees

Appendix C – Workshop & Symposium Attendees

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