

Molecules to Organisms Working Group Second Meeting Agenda

Sunday, April 17, 2016

Working group members arrive.

Monday, April 18, 2016

8:00 – 9:00 Breakfast

9:00 – 9:30 Introductions – Terry Mathews and Angie Peace were not at the last meeting.

9:30-10:30 Cheryl will give a presentation that will recap the last meeting, the status of book chapter, and assign what has to be finished. She will also introduce what has been worked on since last meeting – Daphnia experiment, $KE(c) + KE(o) \rightarrow DEB$, $KE(m) \rightarrow DEB$

10:30-10:45 Break

10:45-11:30 Roger will talk about the planned Daphnia Experiment, design and modeling

11:30-12:15 Natalia gives an overview of the data she anticipates collecting in the “ideal world” – the type and the structure of molecular data.

12:15 – 13:15 Lunch (with discussions)

13:15-14:00 Philip gives an overview of his explorations into how to scale molecular processes to DEB

14:00-14:45 Erik and Dina talk about their approaches on how to link vitellogenesis to DEB (Irv and Karen may need to be ready to discuss the types of data they have available to model)

14:45-15:00 Break

15:00-16:00 Open Discussion of the main projects from the morning and break into groups along those projects.

16:00-17:00 Work/write in small groups, come up with objectives, identify data gaps, suggest methods for filling them, draft a work plan.

17:30 NIMBioS reception and group photo

Tuesday, April 19, 2016

8:00–9:00 Breakfast

9:00-9:45 Discuss progress from yesterday

9:45 – 12:00 Continue to work in groups to tackle objectives, identify data gaps, suggest methods for filling them, draft a workplan.

12:00 – 13:00 Lunch

13:00 – 17:00 Work in small groups or individually to make progress on tasks identified at the end of the morning's session.

17:00 Reconvene to discuss progress

Wednesday, April 20, 2016

8:00 – 9:00 Breakfast

9:00 – 9:30 Cheryl will give a brief presentation showing a road map of the potential collaborations and projects involved with this working group. She will ask for progress on writing assignments here.

9:30-10:15 Roger will discuss the Organisms-Ecosystems DEB attempts with trout and associated issues.

10:15-10:30 Break

10:30-noon Split back into groups to continue progress.

12:00 – 18:00 Box lunch and hiking in Great Smoky Mountains National Park - good opportunity to discuss broader collaborations and questions that come up in individual group.

Thursday, April 21, 2016

8:00 – 9:00 Breakfast

9:00 – 12:00 Report back on questions/tasks assigned the previous afternoon. Work in small groups or individually on model analyses, data gathering, and/or writing.

12:00 – 13:00 Lunch

13:00 – 14:00 Final session; assess progress achieved; develop plan for completing Meeting 2 Objectives; agree on next steps to be taken and deadlines to prepare for Meeting 3.

14:30 – working group member depart.

Reminder of Our First Two Objectives:

Objective 1 (October 2015): *Develop, and translate into mathematical terms, a conceptual model for each of the two case study species (Daphnia, rainbow trout) that focuses on the molecular to organism linkage.*

We will focus on sublethal effects of contaminants, and the first step will be to compile the data sources for our case studies, review the modeling tools and identify key processes that will allow for molecular and toxicokinetic data to be incorporated into DEB. We will decide on which contaminants, specific modes of action, and modeling platforms to use. We will address how molecular data, as it is measured and modeled currently within the AOP framework, can translate to behavior, reproduction, growth and reserve processes relevant to DEBs. We anticipate that this exercise will direct some ongoing studies with Daphnids at ORNL that will provide relevant data. After we compile all the available and the “wish-list” data, we will construct a conceptual model, and explore how each of the different types of quantitative tools can contribute or be modified to create linkages between molecular responses and DEBs, with restrictions and limitations highlighted for both case study species which will be shared with the sister group. We anticipate that this conceptual model and review of the modeling tools will be written into 2 or more book chapters for a book titled “A Systems Biology Approach for Advancing Adverse Outcome Pathways for Risk Assessment”, edited by Natalia Garcia-Reyero and Cheryl Murphy with publication date of February 2016.

Objective 2 (May 2016): *Refine conceptual model and mathematical implementations, conduct preliminary tests of model predictions, identify data gaps and further refine models.*

Portions of the conceptual model will be assigned to different teams of participants to refine mathematical and simulation models prior to the meeting. At the meeting and beyond, modeling efforts will be assembled, evaluated, refined and validated with existing data sets. Identified data gaps can inform activities at ORNL which can feed back to further refine model sets. We anticipate products from this objective will be prepared, submitted to scientific journals and will also be presented at national and international meetings.

Things to be completed by the end of the meeting: SETAC abstracts, next meeting date, slides for Valery’s and Cheryl’s talks this summer.