2015-08-10 Plants in Silico Project Planning Meeting Notes

Date

Aug 10, 2015

Attendees

- David LeBauer
- Amy Marshall-Colon
- Diwakar Shukla
- Stuti Shrivastava
- Balaji Selvam
- Kenton McHenry
- Lengyue Chen
- Unknown User (mfelarca)
- Unknown User (mfreemon)

Goals

- Initial discussions to determine what the initial steps are that need to be taken to move the projects as a whole forward.

Transcribed Notes

Plants in Silico - Multi-scale modeling.

- Need to allow models to talk to each other. This will allow higher resolution and accuracy into the overall modeling.
- Different levels of models are (generally)
    - Molecule
    - Cell
    - System
    - Ecosystem
- Primary objectives
    1. Localize heterongeneous models
    2. Provide data sharing, storage, and management
    3. Import tools for model integration - Investigate and re-use existing tools where possible
    4. Create a web interface for access and visualization - Should be intuitive to use, especially for those unfamiliar with the models
- The seed funding is to be used to determine how and where to go with these things. Proof of principle type of situation.
- Immediate users to be targetted
    - Marshall-Colon Group
    - Shukla Group
    - Long/LeBauer Group - Phenomic? Information -> Observation, modelling, prediction
- After a brief BrownDog overview by Kenton, discussions on models as extractors within DAP?
- Available integration points?
    - What types of services could be used or needed?
    - Other types of functionality? Data management? Curation/publication?
- What is needed from the NCSA end?
    1. Level of compute resources needed
        a. Hardware
        b. Data size
            i. This is going to be dependent on the model?
    2. Need to understand the issues with different timescales that the models operate on
        a. When can things be dynamically coupled and when is that not practical or possible?
    3. Prioritize the the need for NDS to allow for easy reproducibility/access to existing data so research can be more easily referenced/re-used instead of re-created.
    4. Need to define the functional requirements. This is the layer between the high-level roadmap and the low-level implementation details.
        a. What is the data that is to be converted
        b. What is to be built into the datasets
        c. What is to be shared
        d. What services are needed and potentially wanted in the future
        e. What further analysis would users potentially need or want to perform
    5. Try to get early engagement between the application engineers and the scientists in order to facilitate integration and feedback.

Action Items

- [ ] The scientists are going back to hash out some more of the high-level roadmap details, and then will integrate with Unknown User (mfelarca) as they hit a point where discussions can move on to functional requirement definition.