Cell Behavior Ontology and Standards for Multicellular Model Specification Workshop

Background: Building a functional simulation of tissue, organ or even an entire organism requires an unprecedented effort to fuse techniques derived from biology, chemistry, physics, computer science and information science. Developing models that can be explored using a range of different simulation techniques requires a common language capable of describing heterogeneous features and behaviors at various length-scales ranging from molecule to organism. While languages exist for some necessary subareas (e.g. cell physiology and molecular dynamics, systems biology), many researchers still use ad-hoc formats and vocabulary to describe cell-based multi-cell models (e.g. Cellular Potts Models, Center Models, FEM). The creation of the Cell Behavior Ontology is an essential first step in providing a universally agreed upon means to describe cell behaviors and consequently (in the longer term) achieve a standardization level similar to the one which the Systems Biology community has managed to achieve with SBML, CellML and Systems Biology Ontology. Just as applications conforming to SBML or CellML can share models encoded in the two standards, so applications conforming to the CBO derived standards (like proposed CBMSL) will achieve similar capacity for model sharing.

From a practical point of view, ontologies are logical structures that provide a formal description of (scientific) concepts. An ontology is simply a hierarchy of terms with agreed meanings and sets of subterms and modifiers which can apply to each term. Ontologies are unglamorous and tedious to develop, but also crucial for the development of software applications in their subject areas. In some cases an ontology has revolutionized a scientific discipline. For example, in genomics, ontologies like the Gene Ontology (*GO*) allow the hundreds of programs which process genetic-sequence information to communicate with each other seamlessly—the output of any program serving as the input for another.

Scientific Impact: The Cell Behavior Ontology is an enabling technology that will permit standardized annotation of experimental data ranging from developmental biology experiments to clinical pathology data. Multi-scale modeling in which linking across scales is important will be the strongest benefactor of the successful deployment of the CBO. Linking CBO and CBMSL with existing standards for model description at the molecular level (SBML, Cell ML) will create an integrated suite of standards capable of describing in great detail a much broader range of biological systems than is currently possible. The successful linking of the Systems Biology standards with those derived from CBO will allow us to describe in a unified fashion models in which cell behaviors are parameterized based on the state of the internal metabolic network thus creating truly multi scale model which, for example, would allow one to study the effects of how perturbations taking place at molecular level affect patterning at the tissue level. While such models do exist currently, they are usually hard coded and

therefore nearly impossible to share with a broad community ranging from modelers to clinicians.

Workshop Format: The general format of the workshop will follow the successful convention of past CBO workshops. The first part of the workshop (Day 1) will consist of a series of talks and discussions that will focus on the current state of the CBO development and Cell Behavior Model Specification Language, progress on a number of current multi-scale multi-cell model simulation packages as well as an overview of the tasks to be accomplished during the 3rd workshop. **To attract a possibly large group of genuinely interested participants we will reserve enough time slots for scientists willing to present their modeling methodologies/platforms along with a list of problems they run into when they attempt to share/validate/curate their models.** A proposed list of speakers and topics is given below under "Proposed Workshop Agenda". **Please note that this is not a final agenda and if you are interested in contributing your talk please contact us as soon as possible.**

The second part of the workshop (Day 2) will consist of two parallel sessions (which can be held in the same room if necessary) where participants will actually work on improving current version of the CBO (separate tasks will be assigned to the two groups of scientists) and draft a White Paper summarizing progress made on the CBO and Cell Behavior Model Specification Language. The workshop will conclude with a summary talk delivered by James Glazier.

Deliverables: We aim to

- produce a third version of the CBO draft White Paper summarizing recent progress in CBO and reviewing existing multi-cell modeling frameworks;
- prepare an initial specification of the Cell Behavior Model Specification Language (CBMSL) and discuss possible development strategies;
- engage a larger community of researchers to actively participate in the CBO efforts. In particular, we would like to form closer collaborations with researchers from systems biology community who have experience in setting/maintaining model description standards.

Fees and Logistics: There is a registration fee of $125 ($100 if you register for the ISCB 2010 conference) which will cover lunches, refreshments and workshop materials. We expect to provide (pending final funding) limited travel funds for speakers (up to $300 to cover local expenses) and waive registration fee. Participation in the ICSB conference is not required to attend the CBO workshop. However we strongly encourage you consider attending.

Registration and Contact Information: To register for the workshop please send an e-mail to Dr. Maciej Swat (mswat@indiana.edu) by June 15th 2010. Should you have any questions regarding the workshop please feel free to contact any member of the organizing committee (Dr. James A. Glazier (glazier@indiana.edu), Dr. Nick Monk (nick.monk@nottingham.ac.uk), Dr. Maciej Swat (mswat@indiana.edu)).

We would very much appreciate a quick indication of your level of interest by April 15th so we can begin to make up our program. For convenience, you may

reply to our e-mail adding (will attend/will not attend/may attend) to the subject heading.
Lodging and local information: For information about hotels, and any other issues regarding your stay in Edinburgh please contact Fiona Clark fclark1@inf.ed.ac.uk

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Proposed Workshop Agenda:
James Glazier: "Cell Behavior Ontology – current status and roadmap"
Herbert Sauro - "Lessons from the SBML and SBO communities"
Dan Cook – "Reusing patterns from Ontology of Physics for Biology "
Allyson Lister – "Overview of relevant existing ontologies"
Nick Monk – "Defining standards for the description of multi-cell, multi-scale models"
Michael Galdzicki – "Challenges in the Cell Behavior Ontology"
Trish Whetzel – "Protégé, GO, and CBO"
Nadine Peryeras – "Experimentalist's approach to modeling standards"
Peter Hunter – "FieldML and the Physiome Project"
Christophe Godin – "OpenALEA — Modelling Plant Architecture"
David Gavaghan – "CHASTE — Multiscale Simulation of Physiology"
Maciej Swat – "Towards Virtual Tissues – multi-scale modeling using CompuCell3D "