Biositemaps Status and Plans

March 1, 2013 Stanford Biositemaps Team

Summary

This document describes the current state of the Biositemaps software and outlines possible future work. The Biositemaps Web site is up and the software is now running at Stanford. The central Biositemaps file repository is now hosted at Stanford as well. There is no longer any danger that the Biositemaps system might go down and become permanently unrecoverable.

We have identified a number of changes to the Biositemaps system that we need to make to improve its usability in the short term. In addition, we have begun exploring both what it would mean and what it would take to merge the Biositemaps and eagle-i systems. We have developed a concrete vision and proposal for integrating the two architectures into a single seamless system.

Completed Work

Biositemaps Software Redeployment

The Biositemaps software is now up and running on Stanford servers. This software includes the Biositemaps file creation and editing system, the Biositemaps Registry, and the Biositemaps Resource Discovery System (RDS) search tool. We also have moved the software to a source code control system at Stanford (https://bmir-gforge.stanford.edu/) and we have recompiled and redeployed this software. The software code base is complicated and consists of roughly 110,000 lines of code in a number of different modules. We have created an automated monitoring system for the production Biositemaps software that will notify us in real time if the software should become unavailable for any reason. This system makes calls to Biositemaps every few minutes and verifies that the system is still responsive. We list the complete set of Biositemaps components and their current disposition in Appendix 1.

The **biositemaps.org** domain name now points to the instance of the Biositemaps software at Stanford. The University of Pittsburgh instance of Biositemaps is still running, but this instance is now a backup. The **biositemaps.ncbcs.org** domain is now redirected to the canonical **biositemaps.org** domain.

Biositemaps Evaluation and Fixes

We have fixed a serious bug in the RDS system, wherein a user could not filter resource search results by resource type. The system now supports searching by resource type. The system now retrieves the available resource types from the latest version of the Biomedical Resource Ontology (BRO) in the NCBO BioPortal.

We have also identified the following usability issues in the RDS software:

- Filtering is very slow when one combines free text search with resource types
- Filtering does not update the matching resource numbers in parentheses

- The "Resource Type" facet shows only the top three levels of BRO. There is no way to directly filter for more specific resource types
- The display of multi-line items in the facet browsers (at the left hand side of RDS) is very confusing. The display should use the standard "hanging indentation" style typically seen for multi-line items in lists. This change would cause the first line to stand out to the left and allow for easier scanning.

In addition to evaluating the RDS UI, we also evaluated the code and documentation for all the Biositemaps software components. The Biositemaps API is well documented and well crafted. The RDS, on the other hand, is poorly documented and does not appear to be well written. As an example, both the RDS system and the older Biositemaps search system use the same underlying search API. Nevertheless, the RDS search is notably slower than that of the older system. While we can make incremental improvements to the RDS system, fixing all of the problems would require a substantial amount of rework and would require significant development resources.

Biositemaps and eagle-i Investigation

One possibility that we explored in our previous report on Biositemaps is the possibility of using some or all of the eagle-i infrastructure for creating and browsing Biositemaps content. The eagle-i search tool is both more user-friendly and works much better than the current Biositemaps RDS. As part of our work, we have downloaded and rebuilt the eagle-i software system and now have it running internally on a Stanford development system. eagle-i is a large system comprising more than 255,000 lines of code. We have made preliminary exploration of the source code and we believe that we have identified the places in the code where adapters could be placed to allow import and export of Biositemaps files.

We have continued thinking about how to bridge the "impedance mismatch" between the eagle-i ontology and the BRO. In order to better define the scope of the problem, we have made a list of all BRO terms that appear in any Biositemaps file. The BRO contains 485 terms but we have found that only 233 appear in any current file. Thus, it may be possible to simplify the mapping between the two systems. It may be possible to replace the "potential" problem of aligning 485 terms from BRO to eagle-i with instead the "actual problem" of mapping 233 terms. We list the terms used in Biositemaps files in Appendix 2.

The Biositemap information model also needs to be aligned with the eagle-i data model. These information models describe the properties that may appear on a resource. We reviewed an early alignment made by members of the Biositemaps and eagle-i teams from three years ago. While much of this work is still valid, additional alignment will be needed since both systems have evolved since the previous work was done.

Possible Future Work

Biositemaps Software Improvements

One path forward is simply to fix the RDS usability problems. Some of these issues such as the multi-line display are straightforward to address. Others, such as improving search performance, will take more time. A more detailed exploration of the application, and perhaps some feedback from users, may result in us adding items to this list.

Biositemaps and eagle-i Integration

To evaluate the possibility of leveraging the eagle-i infrastructure for Biositemaps, we have downloaded, installed, and explored the eagle-i software. We have identified likely spots in the code that may require modification for Biositemaps compatibility. However, we would need to meet with the eagle-i software authors at Harvard to review our conclusions, brainstorm alternatives, and arrive at an implementation plan and schedule if we are to pursue the possibility of building on the eagle-i code base. We have delayed holding this meeting because of the uncertainty related to the funding of this effort. To be productive, this meeting should take place when there is clear agreement on organizational responsibilities moving forward. Our understanding is that no group has current explicit plans or funding for additional eagle-i software development. Thus we assume that any necessary software changes may need to be carried out at Stanford with guidance from the team at Harvard.

Our vision is a system in which eagle-i can import existing Biositemaps resource files and allow a user to modify them in the eagle-i editor. The files will then be available to the eagle-i search system in the same way that native eagle-i resources are. In addition to being able to import Biositemaps resource files, the system should be able to export a Biositemaps file for a given set of resources. The user can then place this file on a Web site (as occurs with the Biositemaps files today) and register this location with the biositemap registry. Such a system would provide a seamless, two-way integration of the Biositemaps and eagle-i systems. It would retain the distributed nature of the biositemaps system while allowing biositemaps users to take advantage of the eagle-i authoring and search interfaces.

In order to implement this vision, it is necessary to develop a two-way mapping between the Biomedical Resource Ontology (BRO) and the eagle-i research resource ontology (ERO). These ontologies have been developed independently over several years and, as one would expect, there are notable differences between them. In some cases there is a direct one-to-one mapping between BRO terms and eagle-i terms, sometimes with the same name, sometimes with synonyms for the same concept. For example, the term *software* is identical in both ontologies. The term *funding resource* in BRO is very close to the term *funding organization* in the eagle-i ontology. In other cases, BRO contains terms that are not in eagle-i, often because BRO contains a more granular model for some areas. For example, the term *software* has an entire hierarchy of dozens of classes underneath, distinguishing among many types of software. In each case, it is necessary to evaluate whether the BRO distinction is important to maintain. If so, then a corresponding concept can be added to the eagle-i ontology. If the BRO distinction is not important, then it is possible to map the BRO term to a higher-level concept in the eagle-i ontology.

Appendix 1: Biositemaps Components and Source Code

System Components

The Biositemaps software system consists of the following components:

- biositemap.org homepage
- Biositemaps editor and browser (for creating and editing Biositemaps files)
- Biositemaps Registry (for registering the location of each biositemap file)
- public file server hosting Biositemap files for others
- basic Biositemaps search interface
- Biositemaps Resource Discovery System (RDS) search tool
- Biositemaps Web services

Source Code

The Biositemaps source code is organized into the following repositories and modules.

- The original Biositemaps project is available at <u>https://bmir-gforge.stanford.edu/gf/project/Biositemaps/</u> and contains the following modules:
 - **BiositemapAPI** a simple API for handling individual biositemap files (including creation, modification, querying, and saving)
 - BiositemapEditor code for Biositemap Editor and Biositemap Browser using GWT
 - BiositemapWebServices
 - BioPortal-ResourceGenerator
- The Biositemaps Reference Implementation is available at: <u>https://bmir-gforge.stanford.edu/gf/project/Biositemaps_ref/</u> and contains the following modules:
 - api Biositemaps search api and command line tools
 - **cgi** Perl script for the Biositemaps registry
 - editor
 - search basic Biositemaps search tool
- The RDS (previously called CIRWP) is available at <u>https://bmir-gforge.stanford.edu/gf/project/cirwp_project/</u> and contains the following modules:
 - SparqlConnection
 - cirwp_rdfloader
 - cirwp_utils
 - **cirwp_webservice** Web service that uses the Biositemaps search API to provide information (also to RDS) about the content of all the registered biositemaps
 - cirwp_webui RDS user interface

Appendix 2: BRO to eagle-i Mapping Discussion

The 233 terms listed below are from the Biomedical Resource Ontology and have been used in at least one of the existing Biositemaps files. In order to move Biositemaps files into eagle-i, a mapping must exist from each of these concepts into a concept in eagle-i resource ontology (ERO). The BRO contains 485 classes, but the remaining classes are not used in any existing Biositemaps resource. Thus, it may not be essential to map all these remaining classes into their eagle-i equivalents (if any). The classes marked with "(M)" are identical to ERO classes with the same name, and mappings between these concepts already exist in BioPortal.

BRO:Aggregate Human Data BRO:Algorithm (M) BRO:Animal_Models_Facility **BRO:**Application Programming Interface BRO:Assessment_Material_Resource BRO:Atlas_Generation BRO:Backup_Archives_and_Disaster_Recovery BRO:Biobank_Facility BRO:Biomaterial_Manufacture BRO:Biomaterial_Supply_Resource BRO:Biomedical_Supply_Resource BRO:Biosafety_Level_Facility BRO:CT_Scanner (M) BRO:Calculation of Solvent Accessible Area BRO:Calendar_Schedule_and_Resource_Management BRO:Cardiovascular_Model BRO:Cell_Biology_Facility BRO:Cell_Culture_Facility BRO:Cell Model BRO:Certificate_Program BRO:Clinical Care Data BRO:Clinical Data BRO:Clinical Research Data BRO:Clinical Trial Data BRO:Communication_Interface BRO:Communication_and_Collaborative_Work **BRO:Computational Geometry BRO:Computational Model** BRO:Computational_Service **BRO:Contact Modeling** BRO:Continuum Method Simulation **BRO:Controllers** BRO:Cortical_Modeling BRO:Data Acquisition Software BRO:Data_Analysis_Software BRO:Data Annotation **BRO:Data Computation Service** BRO:Data_Exploration BRO:Data_Mining_and_Inference BRO:Data_Processing_Software BRO:Data Repository BRO:Data_Resource BRO:Data_Service BRO:Data Storage (M) BRO:Data_Storage_Repository BRO:Data_Storage_Service (M) BRO:Data_Transfer_and_Communication BRO:Data_Transforms BRO:Data_Visualization (M) BRO:Database (M) BRO:Database_Software BRO:Delimited_Table BRO:Dissemination_Vehicle

BRO:Metabolomics Facility BRO:Microarray_Scanner BRO:Microscope (M) BRO:Microscopy_Facility BRO:Model_Fitting_Algorithm BRO:Modeling_and_Simulation BRO:Modular_Component BRO:Molecular_Biology_Facility BRO:Molecular_Dynamics BRO:Molecular_Force_Field_Calculator BRO:Molecular_Interaction BRO:Molecular_Model BRO:Molecular_Modeling_and_Classification BRO:Molecular_Trajectory_Data BRO:Molecular_Visualization BRO:Molecular_and_Cellular_Data BRO:Monte_Carlo_Simulation BRO:Multibody_Dynamics **BRO:NMR** Facility BRO:Narrative_Resource **BRO:Natural Language Processing** BRO:Network_Characterization BRO:Network Interaction Model BRO:Network Model BRO:Network_and_Communication BRO:Neuromuscular_Model BRO:Next Generation Sequencer (M) BRO:Numerical Calculation of Electrostatic Potential BRO:Numerical_Integrator BRO:Numerical_Method **BRO:Numerical Model BRO:Ontology** BRO:Ontology_Development_and_Management **BRO:Ontology Visualization** BRO:Optimizer BRO:Outreach Program **BRO:PCR** Facility BRO:PCR_Instrument (M) BRO:PET_Scanner (M) BRO:Paper BRO:Pathology Laboratory Screening BRO:Pattern_Inference_Algorithm BRO:Pattern_Recognition BRO:Pattern and Motif Inference BRO:People_Resource BRO:Pharmacokinetics_Pharmacodynamics_Expertise BRO:Phenotypic_Measurement BRO:Phlebotomy_Facility BRO:Physico-Chemical_Model BRO:Physiology_Facility BRO:Physioloigcal_Model BRO:Pipeline_Manager **BRO:Portal**

BRO:Document Retrieval BRO:Dynamic_Model **BRO:Education** BRO:Electron Microscope (M) BRO:Experimental_Measurement BRO:Exploratory_Data_Analysis **BRO:Fabrication Facility** BRO:Facility Core BRO:Faraday_Cage (M) BRO:Feature_Analysis BRO:Federal_Funding_Resource BRO:Finite_Element_Model BRO:Flow_Cytometry_Cell_Sorting_Facility BRO:Fourier_Transform BRO:Funding_Resource BRO:Gene_Expression BRO:Genomic_Phenotypic_Analysis BRO:Genomics_Facility BRO:Grant_Preparation_Expertise BRO:Graph_Analysis BRO:Graph Viewer BRO:Graph_Viewers BRO:Graphical_Integration BRO:Grid_Computing (M) BRO:Homology_Modeling BRO:Human_Studies_Compliance_Resource BRO:Image (M) BRO:Image_Algorithm BRO:Image_Processing **BRO:Imaging** BRO:Imaging_Facility BRO:Immune_Monitoring_Facility BRO:Immunohistochemistry_Facility BRO:Individual Human Data **BRO:Industry Partnership Expertise** BRO:Inference_From_Data BRO:Information_Resource BRO:Information Retrieval BRO:Instrument (M) **BRO:Instrument Manufacture** BRO:Integration_and_Interoperability_Tool BRO:Interaction_Modeling BRO:Interaction_Network **BRO:Interactive Network Analysis** BRO:Interactive_Tool BRO:Interactive_Web-Based_Tool BRO: Journal Article (M) BRO:Knowledge Environment BRO:Knowledge_Extraction BRO:Knowledge_Mining_and_Capturing BRO:Knowledgebase BRO:Laboratory_Supply_Resource BRO:Light Microscope BRO:Linear Algebra Tool BRO:MRI_Scanner BRO:Manifold_Viewers **BRO:Mass Spectra Identification** BRO:Mass_Spectrometer (M) BRO:Material_Resource BRO:Material Service **BRO:**Mechanical Simulation BRO:Medical_Device (M) BRO:Mesh_Model BRO:Metabolism_Facility

BRO:Prediction of Side-Chain Conformations BRO:Processing_Pipeline BRO:Protein-Protein Interaction **BRO:Protein Expression** BRO:Protein_Interaction_Modeling BRO:Protein_Model **BRO:Proteomics Facility BRO:Protocol Development Expertise** BRO:Psychometrics_Expertise **BRO:Publication** BRO:RNA Model BRO:Radioisotopes_Facility BRO:Reagent_Manufacture BRO:Reagent_Resource **BRO:Registration** BRO:Regulatory_Compliance_Resource BRO:Regulatory_Policy_Resource BRO:Regulatory_Signaling_Network_Reconstruction BRO:Relational_Database BRO:Research_Animals_Facility **BRO:Resource** BRO:Robotic_Arrayer BRO:Searching_Sorting_and_Indexing **BRO:Segmentation** BRO:Seminar_Series BRO:Sequence_Annotation BRO:Sequence_Similarity_Searching BRO:Sequence_Visualization BRO:Service_Resource BRO:Shape_Analysis BRO:Signal_Processing BRO:Signaling_Network_Reconstruction BRO:Software (M) BRO:Software Development Tool **BRO:Software** Distribution BRO:Software_Documentation BRO:Source Code **BRO:Standalone** Application BRO:Statistical Algorithm **BRO:Statistical Analysis BRO:Statistical Package** BRO:Structural_Model BRO:Structure-Based_Protein_Classification **BRO:Structured Data** BRO:Structured_Knowledge_Resource **BRO:Support BRO:Technical Support** BRO:Three D Image BRO:Three_Dimensional_Data BRO:Time_Series_Analysis **BRO:Tissue Organ Facility BRO:Toolkit** BRO:Toxicology_Expertise BRO:Training Resource BRO:Training_Service (M) BRO:Two_D_Image BRO:Visualization (M) BRO:Wavelet_Transform BRO:Web_Service **BRO:Website** BRO:X-Ray_Crystallography_Facility BRO:XML_Data BRO:XML_Database