



Materials Digital Library Pathway

August 2007

MatDL Pathway is building an information infrastructure to support materials science (MS) education, research, and interactions between the two as well as to disseminate resources generated by government-funded MS collaborations. The long-term target community of MatDL Pathway is materials undergraduate and graduate students, educators, and researchers. MatDL Pathway provides stewardship for content and services needed across the MS community and contributes to a high quality educational experience for our targeted audience by offering:

1. Tools to describe, manage, exchange, archive, and disseminate data among national and international government-funded materials teams and centers, such as the Soft Matter Wiki.
2. Workspace for open access development of modeling and simulation tools, such as MatForge.
3. Services and content for virtual labs in large undergraduate introductory science courses.
4. Workspace for collaborative development of core undergraduate MS teaching materials, such as the Teaching Archive.

Since MatDL Pathway was initiated on October 1, 2005, significant progress has been made toward achieving stated goals. Presently, we have installed Fedora 2.1.1 with the Fez 1.3 interface. We are using this installation as our main repository and were first harvested as a Fedora repository in May 2007. We also provide collaborative tools, such as the Soft Matter Wiki and MatForge. The Soft Matter Wiki (http://matdl.org/matdlwiki/index.php/softmatter:Overview_of_Contents) is a publicly accessible, expert-community-driven site for scientific communication and dissemination within the sub-domain of soft matter. This site has been integrated into several undergraduate and graduate classes at the University of Michigan. MatForge (<http://matforge.org>), a Subversion/TRAC workspace for open access development of modeling and simulation codes, began hosting projects September 1, 2005 starting with the FiPy project administered by MSEL/NIST code developers. FiPy is a research code for solving partial differential equations and is useful for modeling a range of materials behavior. It has been used as an educational tool and, with extensions to streamline its usability, has good potential for more widespread use in education. Several additional research code projects with possible teaching applications have also joined MatForge: 1) Carnegie Mellon University Computational Materials Science - A collection of projects with special emphasis on digital microstructure generation, evolution, and analysis; 2) Department of Energy. Computational Materials Science Network Cooperative Research Team. Dynamics and Cohesion of Materials Interfaces and Confined Phases under Stress. This project brings together over 25 researchers from academia and national labs, supported through the Department of Energy 'Computational Materials Science Network'. 3) University of Michigan. Lab for Computational Nanoscience and Soft Matter Simulation. A library for writing molecular simulations, data analysis codes, visualization tools, and for interfacing with other simulation packages. 4) Powell Research Group. A collection of open source software tools developed at MIT.

MatDL has also made progress with virtual labs and collaborative development of teaching resources. MatDL and Carnegie Mellon University were awarded a CCLI grant to extend their work on virtual labs in large undergraduate introductory science courses. The workspace for collaborative development of core undergraduate MS teaching materials has been

established for the Transport Phenomena collection (<http://teaching.matdl.org>) with approximately 100 teaching resources.

We are nearing the completion of our work with NSDL CI at Columbia to install and implement Shibboleth 1.2 so that we can participate in community-sign-on across the NSDL projects as well as the NSDL data repository. MatDL continues to make maintaining good communication among its PIs, staff, and students a priority, holding project meetings in Arlington (September 2006) and Ann Arbor (May 2007).

Outreach Activities:

Several MatDL PIs (Bartolo and Glotzer) were among the 30 invited people who presented and participated at the NSF sponsored workshop on Cyberinfrastructure in Materials Research held at NSF in August 2006. MatDL contributed and was highlighted in the subsequently released workshop report, 'From Cyberinfrastructure to Cyberdiscovery in Materials Science'.

In cooperation with NSF and NSDL, MatDL Pathway hosted a workshop at NSF for a group of Materials Research Science & Engineering Centers (MRSECs) on September 26, 2006 to identify key issues and opportunities in the enhancement and integration of materials research and education. To help focus the discussion, workshop scope was limited to the materials sub-area of Soft Materials. Workshop participants included: 1) Directors of four Materials Research Science and Engineering Centers (MRSECs) with two representatives from each Center to speak about education, research, and shared facilities from: Cornell Center for Materials Research, MIT Center for Materials Science & Engineering, Northwestern Materials Research Center, and Princeton Center for Complex Materials; 2) PIs/CoPIs from NSDL Core Integration (NSDL CI) and 3) PIs/CoPIs from Materials Digital Library Pathway (MatDL) to talk about their missions and goals; and 4) Program Officers from NSF Division of Materials Research and Division of Undergraduate Education. The full workshop report is available at the NSF DMR site (<http://www.nsf.gov/mps/dmr/reports.jsp>). Presentations and other workshop documents are available at the MatDL site (http://matdl.org/2006_workshop.html). MatDL and the participating MRSECs have taken first steps in working together. Laura Bartolo, PI of MatDL, visited the MRSECs at Cornell, MIT, Northwestern, and Princeton to meet with the MRSEC Directors, REU students, researchers, Education Coordinators, and Shared Facilities Directors. Approximately 25 students participating in the REU programs of these MRSECs have received accounts and training on how to use MatDL's Soft Matter Wiki to support their research activities as well as communicate their research results. With approval of the MRSECs, the papers and presentations of high caliber will be made available on MatDL. Discussions are underway with the Shared Facilities Directors to facilitate collaboration and communication through a planned Instrumentation Wiki.

Over the past year, MatDL has given presentations at several MS conferences including: The Computational Materials Science Network Annual Meeting; Minerals, Metals, & Materials (TMS) Annual meeting, and; Materials Science & Technology Conference (MS&T). Additionally, a spotlight article about collaborative work being conducted by MatDL and TMS was published on Materials Technology @ TMS Education Community: Front Page (<http://materialstechnology.tms.org/TECarticle.asp?articleID=905>). MatDL PI (Bartolo) is one of the Co-Chairs of the Symposium *W, Materials Education for 2020*, at the Fall 2007 Materials Research Society. As part of the symposium, MatDL will partner with the Journal of Materials Education (JME, a fee-based, print publication) to make selected symposium papers available freely in electronic format on MatDL with links to JME. MatDL has also presented at a number of other conferences including: American Association for the Advancement of Science (AAAS) Annual Meeting; Conference on Open Repositories; International CODATA Conference; American Society for Information Science and Technology (ASIS&T); Conference on Dublin Core and Metadata Applications, and; Joint Conference on Digital Libraries (JCDL).