MatDL: Making Connections between MSE Education and Research

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Massachusetts Institute of Technology — Colorado, University of Colorado at Boulder — Kent State University

Transport Archive and Course Composer

Transport Phenomena Archive

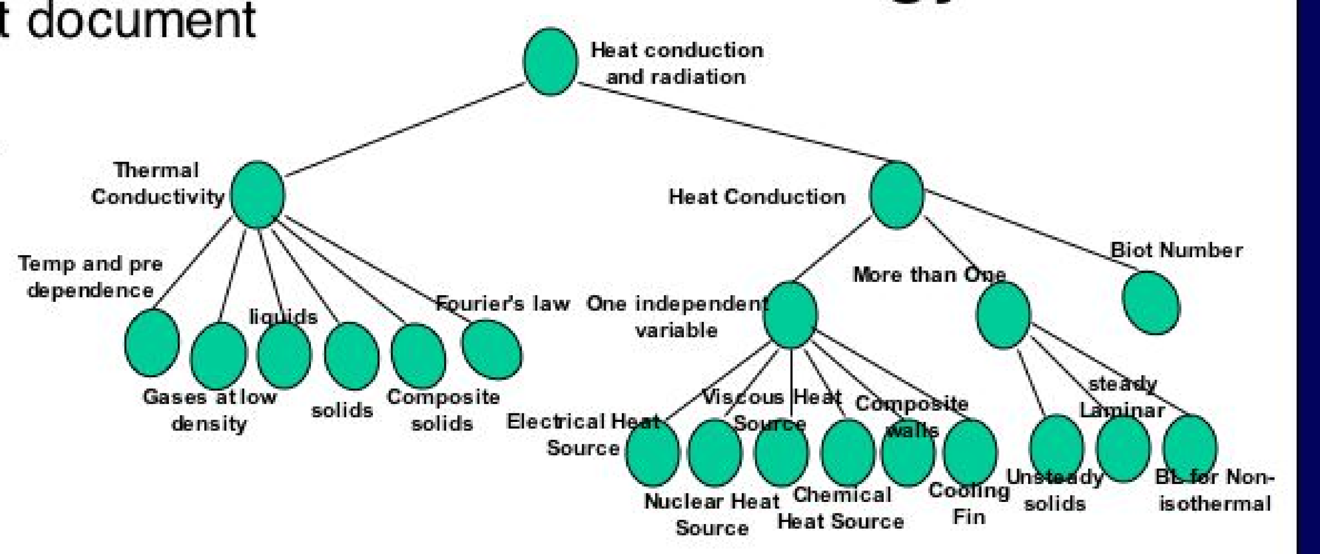
- Initiated by MIT
- Includes teaching resources:
  - ➢Problems/exercises
  - ➢Handouts & courseware
- Allows modifications & additions
- International editorial board
- Metis workflow technology (CU) for review process
- Initial content for testing course composer

Course Composer

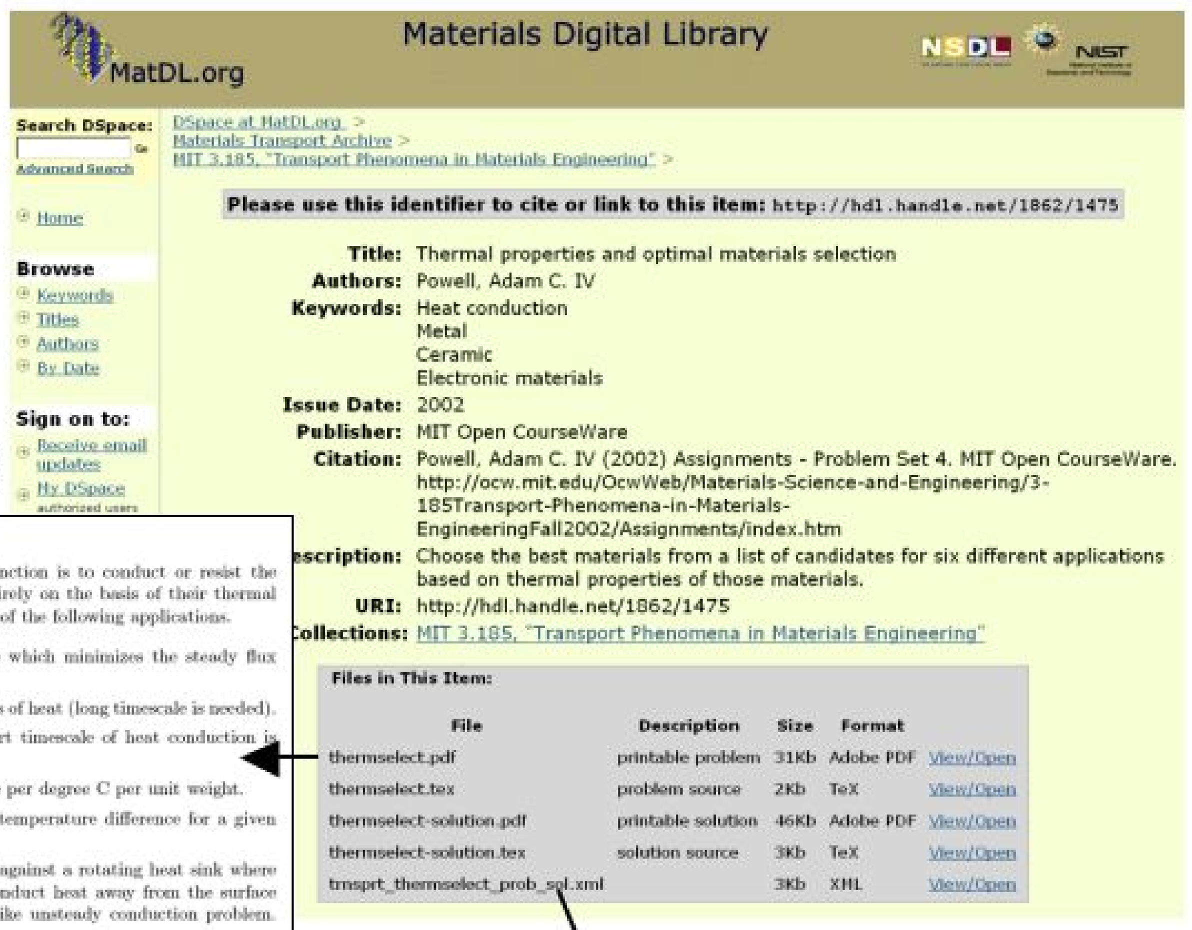
- Enables flexible reuse
- Content selection:
  - ➢ LOM metadata
  - ➢ Graphical ontology
- Content adaptation:
  - ➢ Transcode
  - ➢ Compose
  - ➢ Output document

Student developers:
- Thong Chanchaem (KSU)
- Sandeep Kumar Davu (KSU)
- Yongbin Ma (KSU)

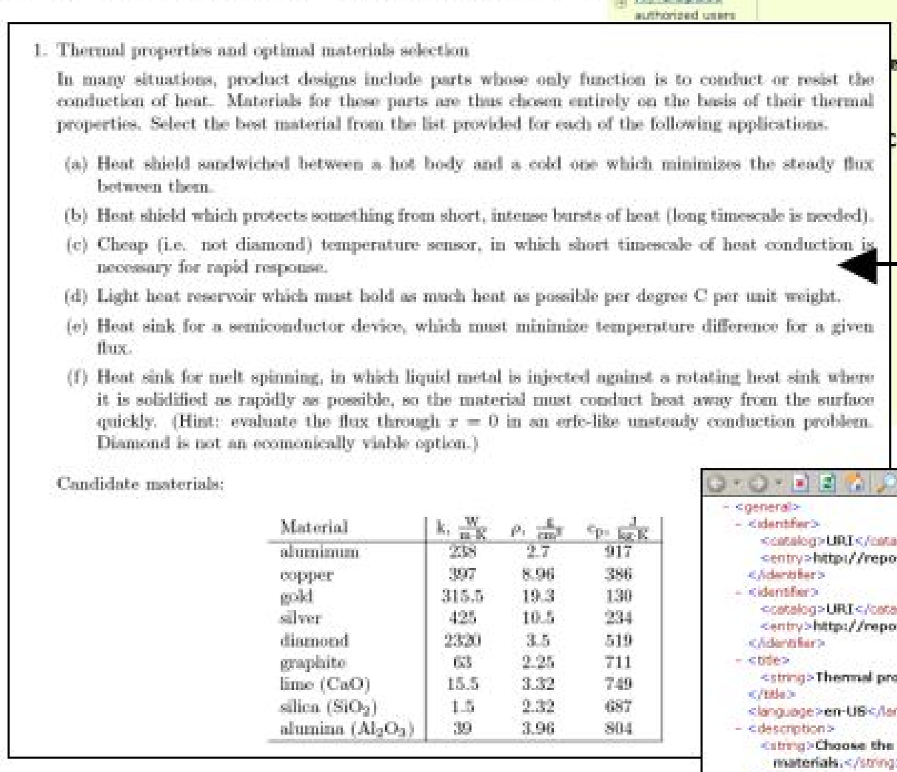
Partial Ontology



Transport Resource Viewed in MatDL



Problem/Exercise



1. Thermal properties and optimal materials selection

In many situations, product designs include parts whose only function is to conduct or resist the conduction of heat. Materials for these parts are thus chosen entirely on the basis of their thermal properties. Select the best material from the list provided for each of the following applications.

(a) Heat shield sandwiched between a hot body and a cold one which minimizes the steady flux between them.

(b) Heat shield which protects something from short, intense bursts of heat (long timescale is needed).

(c) Cheap (i.e. not diamond) temperature sensor, in which short timescale of heat conduction is necessary for rapid response.

(d) Light heat reservoir which must hold as much heat as possible per degree C per unit weight.

(e) Heat sink for a semiconductor device, which must minimize temperature difference for a given flux.

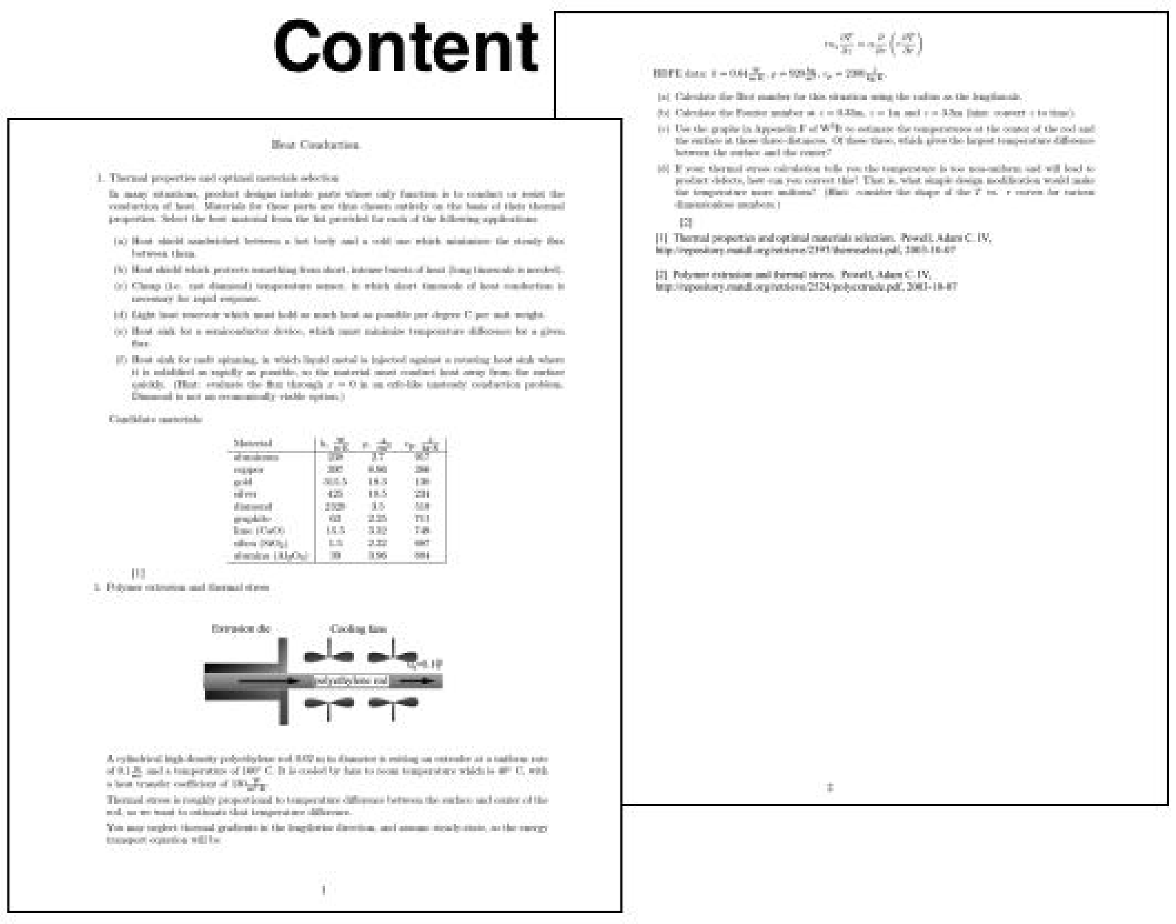
(f) Heat sink for melt spinning, in which liquid metal is injected against a rotating heat sink where it is solidified as rapidly as possible, so the material must conduct heat away from the surface quickly. (Hint: evaluate the flux through $x = 0$ in an erfc-like unsteady conduction problem. Diamond is not an economically viable option.)

Candidate materials:

Material	$k, \frac{W}{m \cdot K}$	$\rho, \frac{g}{cm^3}$	$c_p, \frac{J}{kg \cdot K}$
aluminum	238	2.7	917
copper	397	8.96	386
gold	315.5	19.3	130
silver	425	10.5	234
diamond	2320	3.5	519
graphite	63	2.25	711
lime (CaO)	15.5	3.32	749
silica (SiO_2)	1.5	2.32	687
alumina (Al_2O_3)	39	3.96	804

LOM Metadata

Assembled Content



Kent State University — Massachusetts Institute of Technology

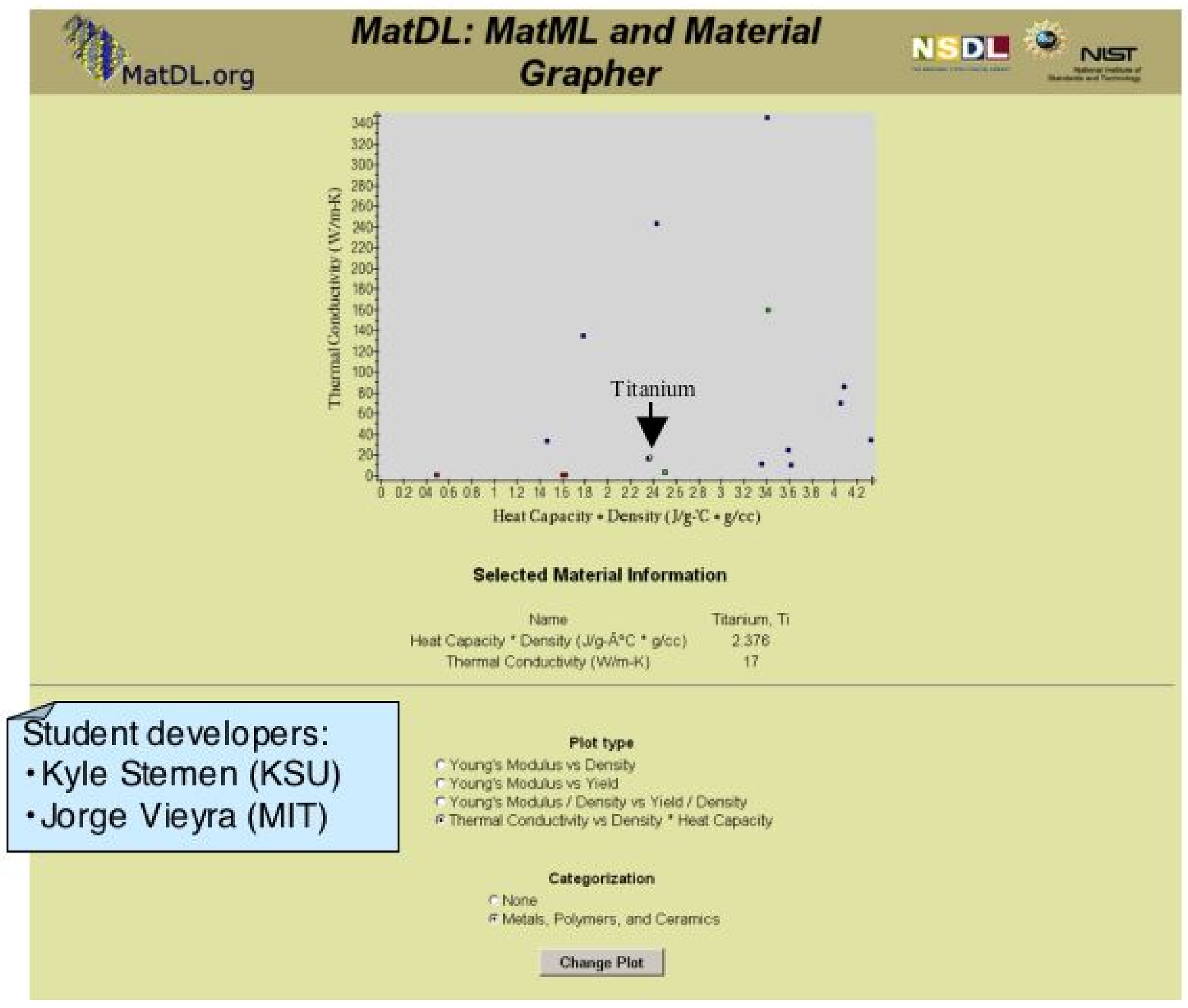
MatML and Material Grapher

Materials Markup Language (MatML) is an XML-based language for exchange of materials property data

Currently:
- Few available MatML example resources
- Few examples using MatML with applications

Goal:
- Provide complete example in educational context
  - ➢Tagging materials property data with MatML
  - ➢Parsing MatML
  - ➢Using data in software application
- "Real" data for realistic learning experience

MatML Example: Selected Properties of Ti



Student developers:
- Kyle Stemen (KSU)
- Jorge Vieyra (MIT)

Materials Property Sheet

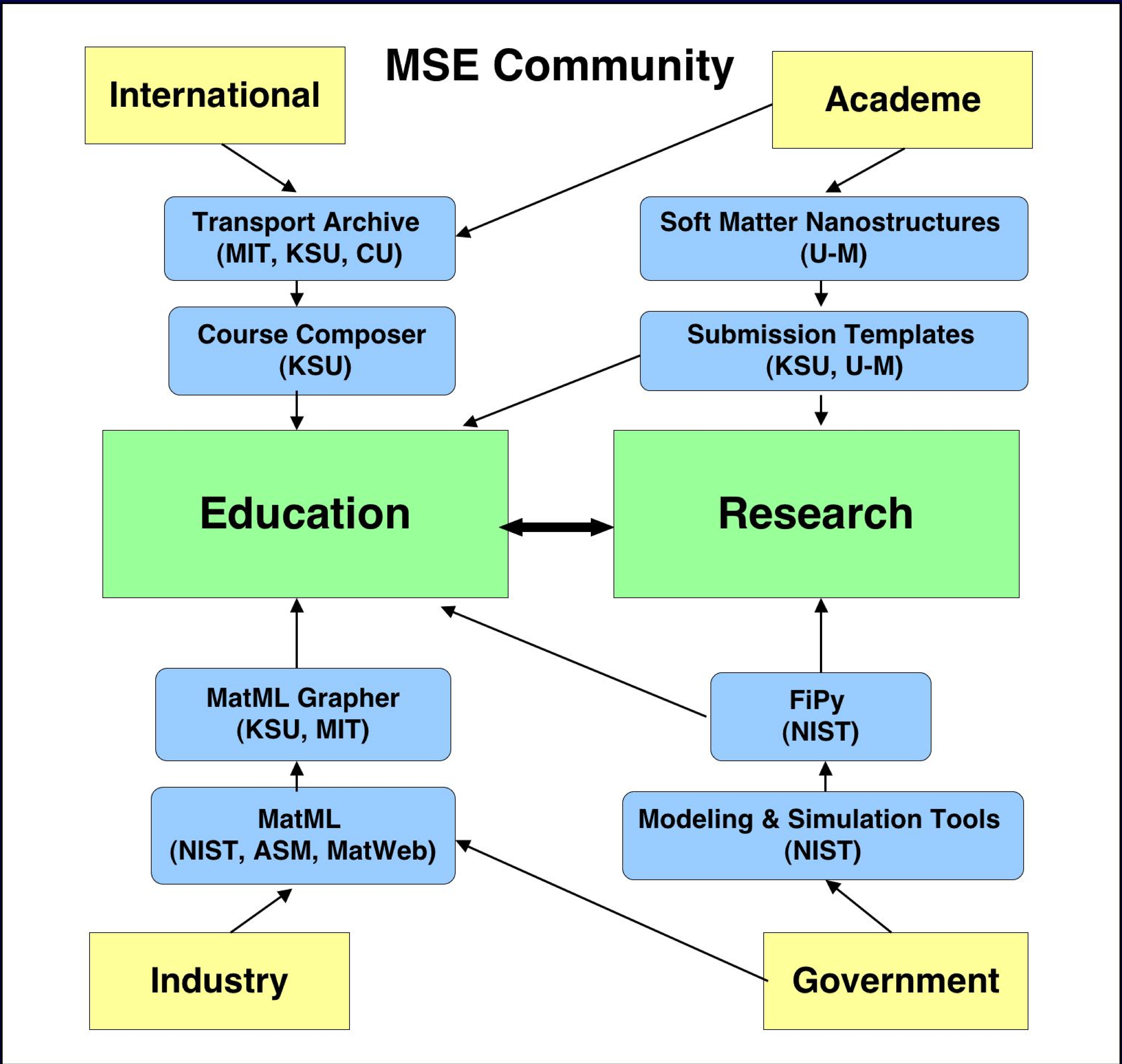
*reproduced with permission

Materials Digital Library

MatDL.org

Abstract

A primary goal of the Materials Digital Library (MatDL) is to bring materials science research and education closer together. MatDL is beginning to realize that goal by serving as an intersection for content, tools, and use among academe, government, industry, and the international community. MatDL is collaboratively developing a course composition tool (KSU), a submission tool (KSU and U-M), and a materials property grapher (KSU and MIT). An international editorial board is being assembled to review new contributions of teaching materials to the MatDL Transport Phenomena Archive using Metis workflow technology developed at CU. Archive resources, described with DC and LOM metadata, serve as initial content for testing the course composition tool which enables flexible reuse based on user selection criteria and dynamic topic weighting. The submission tool has been integrated into the regular workflow of U-M students and researchers generating nanostructure images. It prompts users for domain-specific information, automatically generating and attaching keywords and editable descriptions. MatML is an extensible markup language for exchanging materials information developed by materials data experts in industry, government, standards organizations, and professional societies. The web-based MatML grapher allows students to compare selected materials properties across approximately 80 MatML-tagged materials. The MatML grapher adds value in this educational context by allowing students to utilize real property data to make optimal material selection decisions. MatDL is also making available to interested students and researchers Python codes (FiPy) developed at NIST that use the finite volume method to solve partial differential equations and generate images.



KENT STATE UNIVERSITY

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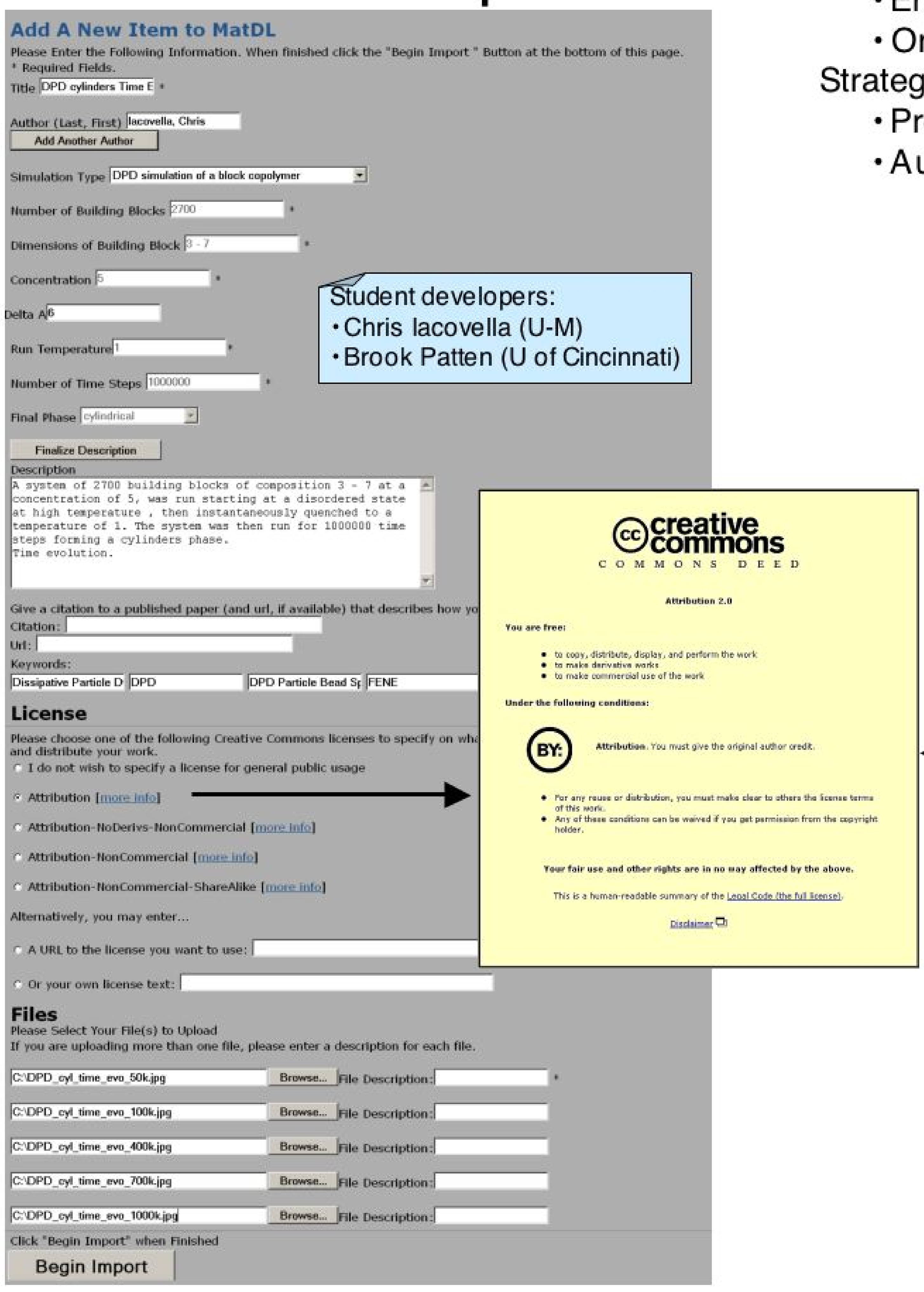
Submission Tool for Soft Matter Nanostructures

Submission Template

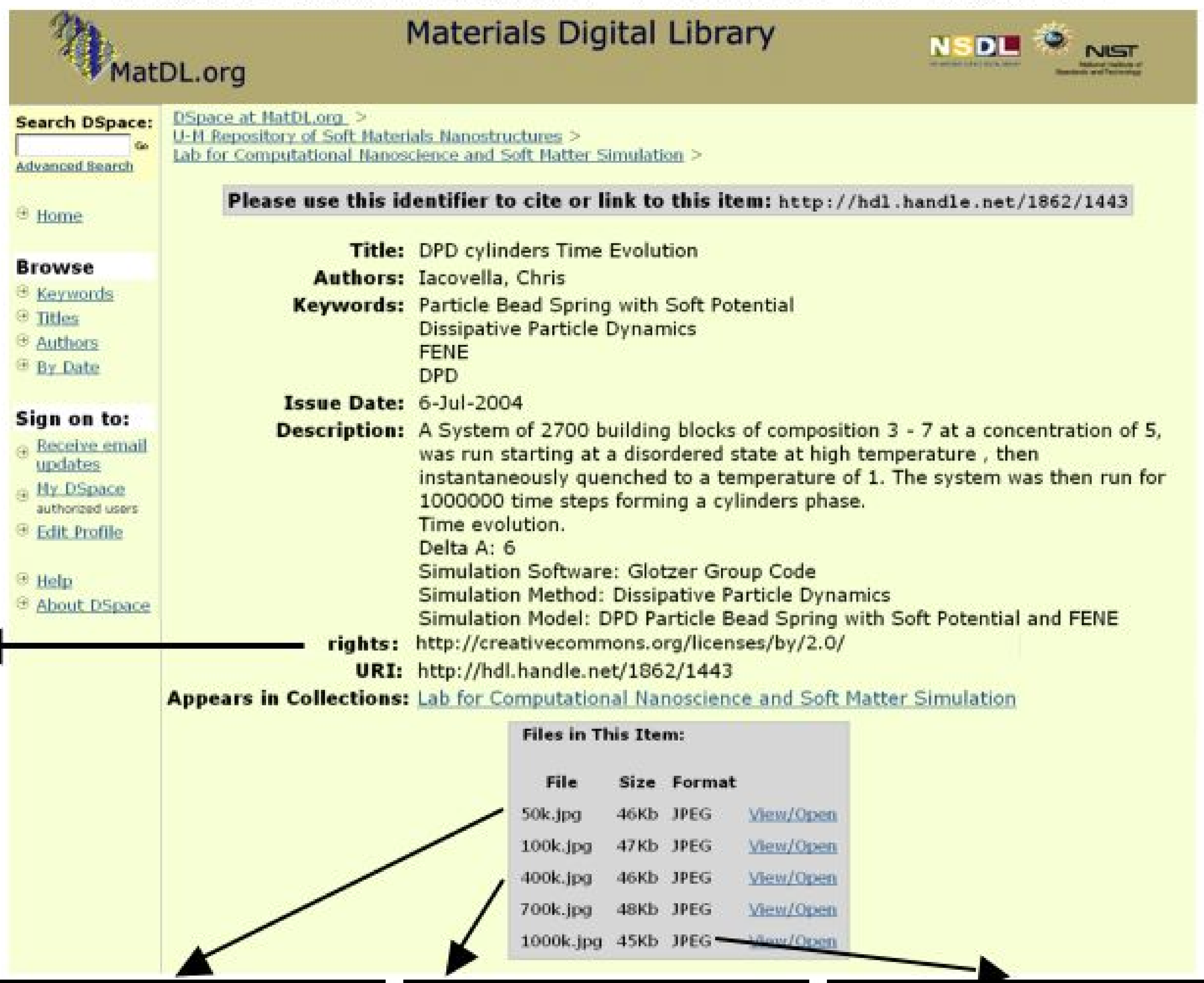


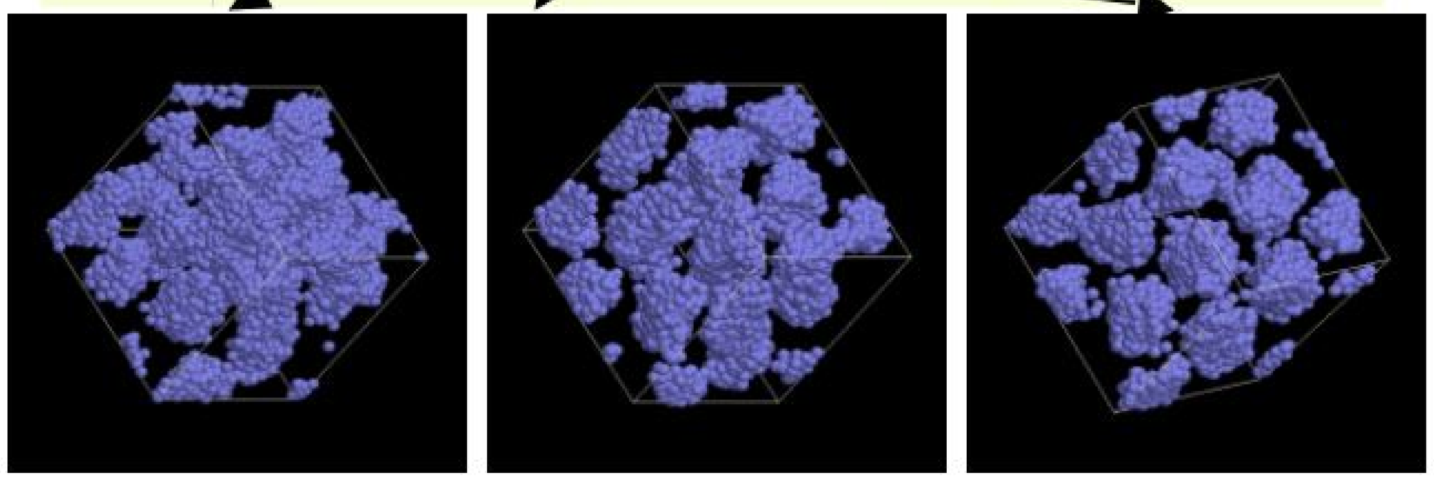
Student developers:
- Chris Iacovella (U-M)
- Brook Patten (U of Cincinnati)

Goal:
- Ensure adequate level of detail & consistency
- Organize results for intelligent access and storage

Strategy:
- Provide drop-down selections & specific prompts
- Automatically generate keywords & description from responses

Final Submission Viewed in MatDL





NIST National Institute of Standards and Technology

Modeling and Simulation Tools

Materials Science and Engineering Laboratory/National Institute of Standards and Technology

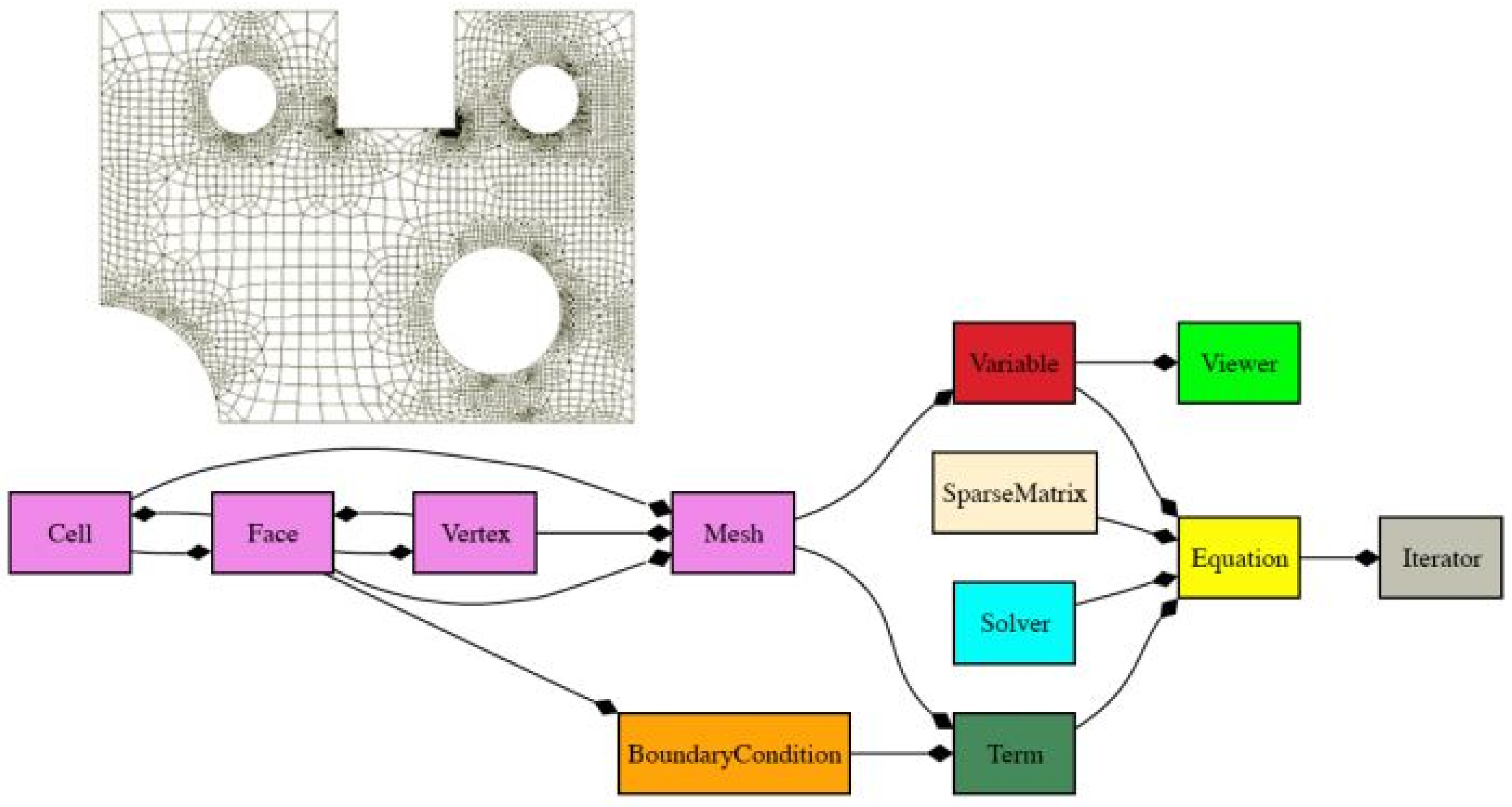
A Finite Volume PDE Solver Using Python (FiPy)

Jonathan E. Guyer, Daniel Wheeler & James A. Warren
Metallurgy Division

FiPy Overview

- Finite Volume code for solving coupled sets of PDEs
- Code currently addresses Phase Field models
- Code will be freely available
- Large archive of test problems
- User controls program flow

FiPy Design - Objects



Finite Volume Method

- Solve a general PDE on a given domain for a field ϕ
- Integrate PDE over arbitrary control volumes
- Evaluate PDE over polyhedral control volumes
- Obtain a large coupled set of linear equations in ϕ

$$\begin{pmatrix} a_{11} & a_{12} & & \\ a_{21} & a_{22} & \ddots & \\ & \ddots & \ddots & \ddots \\ & & \ddots & a_{nn} \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

Example Problem - Grain Impingement Governing Equations

- Phase field variable
  - $0 \le \phi \le 1$

$$\underbrace{Q(\phi, \nabla\theta)\frac{\partial \phi}{\partial t}}_{\text{transient}} = \underbrace{\alpha^2 \nabla^2 \phi}_{\text{diffusion}} - \underbrace{\frac{\partial f}{\partial \phi} - \frac{\partial g}{\partial \phi} s |\nabla \phi| - \frac{\partial h}{\partial \phi}\frac{\epsilon^2}{2}|\nabla \phi|^2}_{\text{source}}$$

- Orientation variable
  - $-\pi \le \theta \le \pi$

$$\underbrace{P(\phi, \nabla\theta)\frac{\partial \theta}{\partial t}}_{\text{transient}} = \underbrace{\nabla \cdot \left[h\epsilon^2 \nabla\theta + gs\frac{\nabla\theta}{|\nabla\theta|} \right]}_{\text{diffusion}}$$

R. Koybayashi, W. C. Carter, and J. A. Warren