

MatDL: Making Connections between MSE Education and Research

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DUE-0333520

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)

Transport Resource Viewed in MatDL

Title: Thermal properties and optimal materials selection
Authors: Powell, Adam C. IV
Keywords: Heat conduction, Metal, Ceramic, Electronic materials
Issue Date: 2002
Publisher: MIT Open CourseWare
Citation: Powell, Adam C. IV (2002) Assignments - Problem Set 4. MIT Open CourseWare. <http://ocw.mit.edu/OcwWeb/Materials-Science-and-Engineering/3-185Transport-Phenomena-in-Materials-EngineeringFall2002/Assignments/index.htm>
URI: <http://hdl.handle.net/1862/1475>
Collections: MIT 3.185, "Transport Phenomena in Materials Engineering"

File	Description	Size	Format
thermselect.pdf	printable problem	31Kb	Adobe PDF
thermselect.tex	problem source	2Kb	TeX
thermselect-solution.pdf	printable solution	46Kb	Adobe PDF
thermselect-solution.tex	solution source	3Kb	TeX
transport_thermselect_prob_sol.xml		3Kb	XHL

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.

- Heat shield sandwiched between a hot body and a cold one which minimizes the steady flux between them.
- Heat shield which protects something from short, intense bursts of heat (long timescale is needed).
- Cheap (i.e. not diamond) temperature sensor, in which short timescale of heat conduction is necessary for rapid response.
- Light heat reservoir which must hold as much heat as possible per degree C per unit weight.
- Heat sink for a semiconductor device, which must minimize temperature difference for a given flux.
- 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 $r = 0$ in an air-like unsteady conduction problem. Diamond is not an economically viable option.)

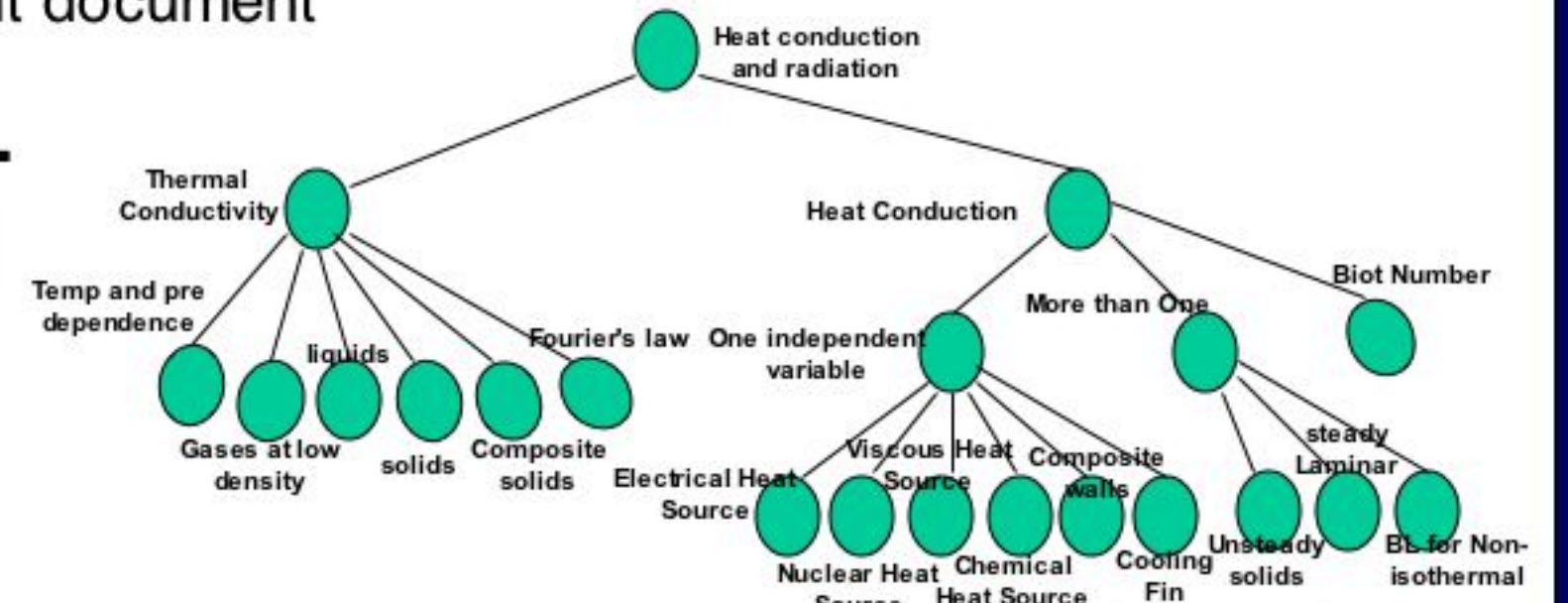
Candidate materials:

Material	k, W/mK	ρ , kg/m ³	c_p , J/kgK
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	65	2.25	711
lime (CaO)	15.5	3.32	749
silica (SiO ₂)	1.5	2.32	687
alumina (Al ₂ O ₃)	39	3.96	804

LOM Metadata

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<rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:dc="http://purl.org/dc/terms/"
    xmlns:matdl="http://repository.matdl.org/retrieve/2399/thermselect.pdf/"
    xmlns:matdl2="http://repository.matdl.org/retrieve/2399/thermselect-solution.pdf/"
    >
  <matdl:ThermalPropertiesAndOptimalMaterialsSelection/ >
    <dc:title>Thermal properties and optimal materials selection</dc:title>
    <dc:creator>Powell, Adam C. IV</dc:creator>
    <dc:subject>Heat conduction; Metal; Ceramic; Electronic materials</dc:subject>
    <dc:issued>2002</dc:issued>
    <dc:publisher>MIT Open CourseWare</dc:publisher>
    <dc:citation>Powell, Adam C. IV (2002) Assignments - Problem Set 4. MIT Open CourseWare. http://ocw.mit.edu/OcwWeb/Materials-Science-and-Engineering/3-185Transport-Phenomena-in-Materials-EngineeringFall2002/Assignments/index.htm</dc:citation>
    <dc:uri>http://hdl.handle.net/1862/1475</dc:uri>
    <dc:collection>MIT 3.185, "Transport Phenomena in Materials Engineering"</dc:collection>
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    <dc:source>thermselect.tex</dc:source>
  </matdl:ThermalPropertiesAndOptimalMaterialsSelection/thermselect.pdf/>
  <matdl:ThermalPropertiesAndOptimalMaterialsSelection/thermselect-solution.pdf/>
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    <dc:source>thermselect-solution.tex</dc:source>
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  <matdl:ThermalPropertiesAndOptimalMaterialsSelection/transport_thermselect_prob_sol.xml/>
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  </matdl:ThermalPropertiesAndOptimalMaterialsSelection/transport_thermselect_prob_sol.xml/>
</rdf:RDF>
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Partial Ontology



Assembled Content

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:

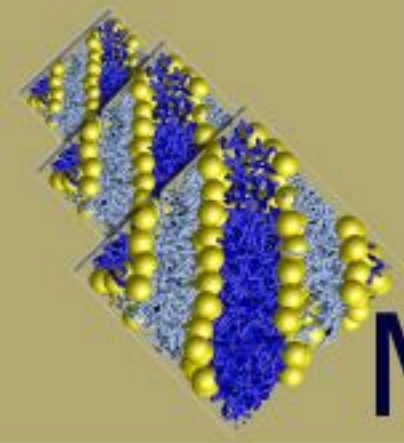
- Provide complete example in educational context
 - Tagging materials property data with MatML
 - Parsing MatML
 - Using data in software application
- "Real" data for realistic learning experience

MatML Example: Selected Properties of Ti

```
<?xml version="1.0" encoding="UTF-8"?>
<matml:Doc xmlns:matml="http://www.matweb.com/research/Specialized/Objects/matml"
    xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:dc="http://purl.org/dc/terms/"
    xmlns:matweb="http://www.matweb.com/research/Specialized/Objects/matml"
    >
  <matml:Material
    <dc:title>Titanium, Ti</dc:title>
    <dc:source>[source]</dc:source>
    <matml:PropertyData
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  </matml:Material>
</matml:Doc>
```

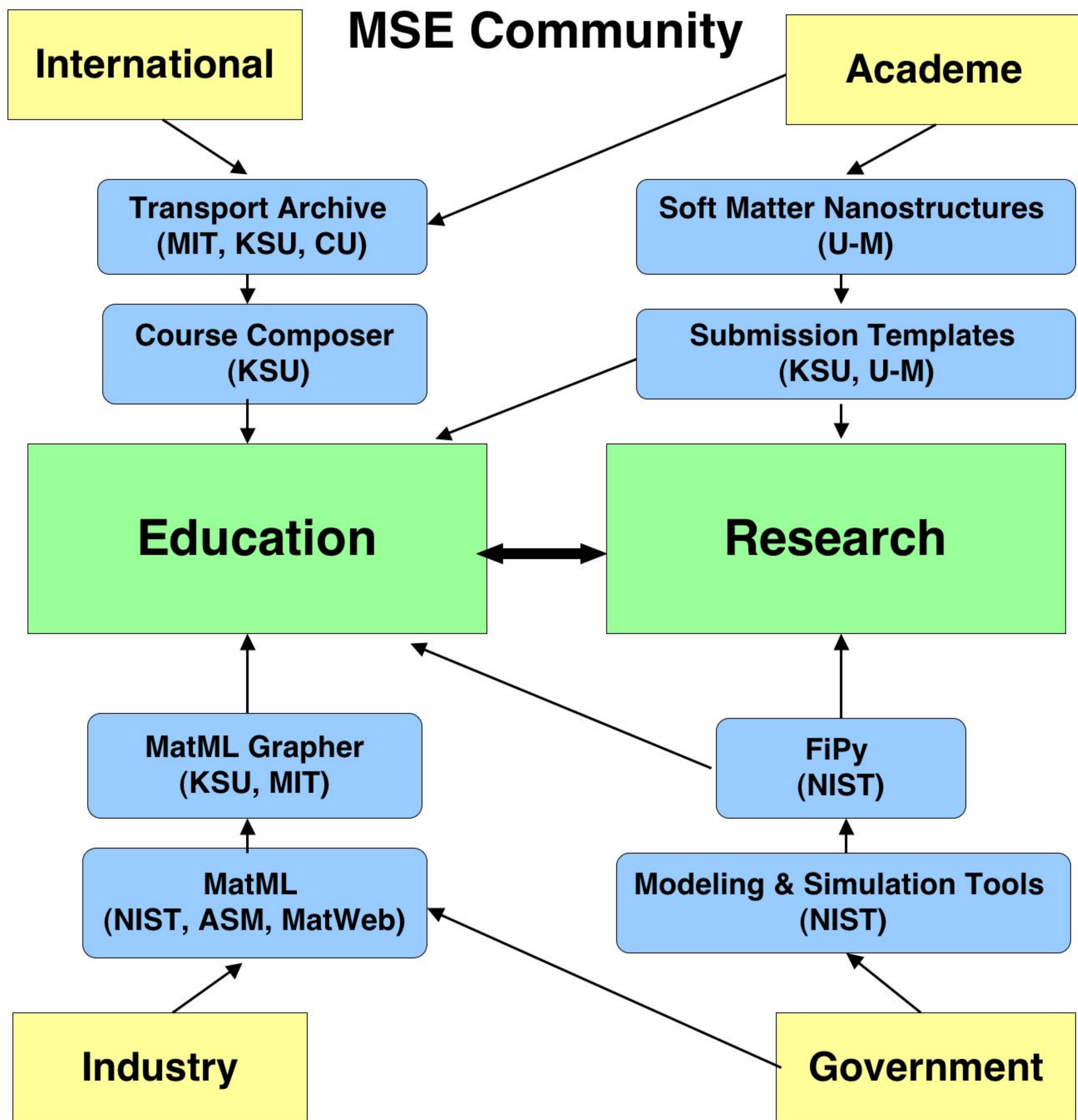
Materials Property Sheet

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



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.



Submission Tool for Soft Matter Nanostructures

Submission Template

Add A New Item to MatDL
Please Enter the Following Information. When finished click the "Begin Import" Button at the bottom of this page.
* Required Fields.

Title: DPD cylinders Time E *

Author (Last, First): Iacovella, Chris
Add Another Author

Simulation Type: DPD simulation of a block copolymer

Number of Building Blocks: 2700 *

Dimensions of Building Block: 3 - 7 *

Concentration: 5 *

Delta A: 6

Run Temperature: 1 *

Number of Time Steps: 100000 *

Final Phase: cylindrical

Description
A system of 2700 building blocks of composition 3 - 7 at a concentration of 5, was run starting at a disordered state at high temperature, then instantaneously quenched to a temperature of 1. The system was then run for 100000 time steps forming a cylinders phase. Time evolution.

Give a citation to a published paper (and url, if available) that describes how you did this work.
Citation: _____
URL: _____

Keywords: Dissipative Particle Dynamics, DPD, DPD Particle Bead Spring, FENE

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Please choose one of the following Creative Commons licenses to specify on which you wish to distribute your work.
I do not wish to specify a license for general public usage
Attribution [more info] →
Attribution-NonCommercial [more info]
Attribution-NonCommercial-ShareAlike [more info]

Alternatively, you may enter...
A URL to the license you want to use: _____
Or your own license text: _____

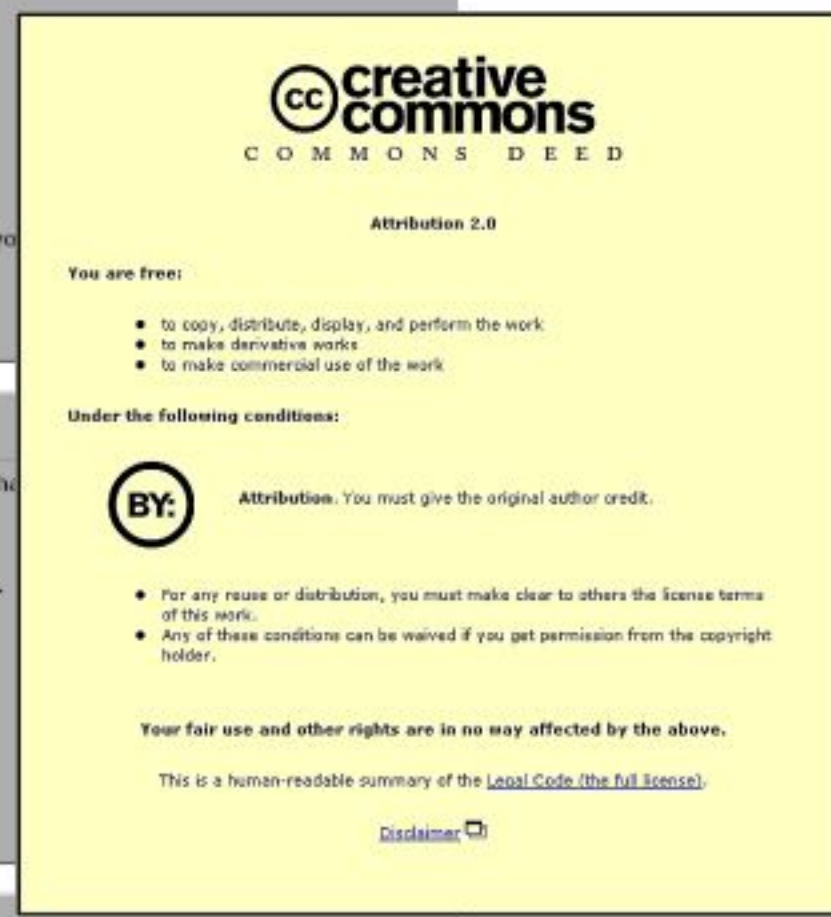
Files
Please Select Your File(s) to Upload
If you are uploading more than one file, please enter a description for each file.

C:\DPD_cyl_time_evo_50k.jpg	Browse...	File Description:
C:\DPD_cyl_time_evo_100k.jpg	Browse...	File Description:
C:\DPD_cyl_time_evo_400k.jpg	Browse...	File Description:
C:\DPD_cyl_time_evo_700k.jpg	Browse...	File Description:
C:\DPD_cyl_time_evo_1000k.jpg	Browse...	File Description:

Click "Begin Import" when Finished

Begin Import

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

MatDL.org Materials Digital Library NSDL NIST

Search DSpace: DSpace at MatDL.org > U-M Repository of Soft Materials Nanostructures > Lab for Computational Nanoscience and Soft Matter Simulation >

Please use this identifier to cite or link to this item: <http://hdl.handle.net/1862/1443>

Title: DPD cylinders Time Evolution
Authors: Iacovella, Chris
Keywords: Particle Bead Spring with Soft Potential, Dissipative Particle Dynamics, FENE, DPD
Issue Date: 6-Jul-2004
Description: A System of 2700 building blocks of composition 3 - 7 at a concentration of 5, was run starting at a disordered state at high temperature, then instantaneously quenched to a temperature of 1. The system was then run for 100000 time steps forming a cylinders phase. Time evolution.
Delta A: 6
Simulation Software: Glotzer Group Code
Simulation Method: Dissipative Particle Dynamics
Simulation Model: DPD Particle Bead Spring with Soft Potential and FENE
rights: <http://creativecommons.org/licenses/by/2.0/>
URI: <http://hdl.handle.net/1862/1443>

Appears in Collections: Lab for Computational Nanoscience and Soft Matter Simulation

File	Size	Format
50k.jpg	46kb	JPEG View/Open
100k.jpg	47kb	JPEG View/Open
400k.jpg	46kb	JPEG View/Open
700k.jpg	48kb	JPEG View/Open
1000k.jpg	45kb	JPEG View/Open

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

Finite Volume Method

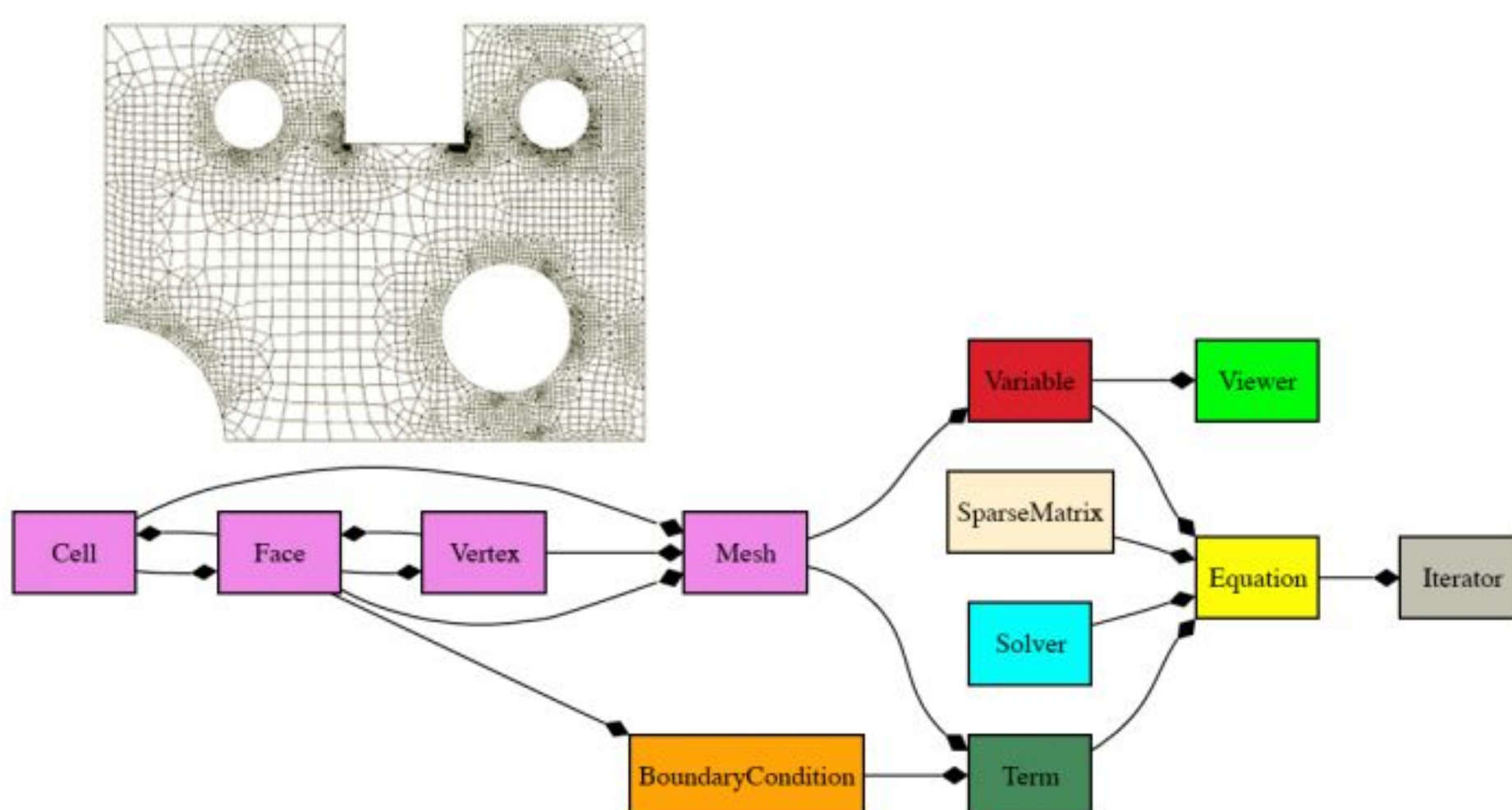
- Solve a general PDE on a given domain for a field ϕ
- Integrate PDE over arbitrary control volumes
- Evaluate PDE over polyhedral control volumes
- Obtain a large coupled set of linear equations in ϕ

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

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

FiPy Design - Objects



Example Problem - Grain Impingement Governing Equations

• Phase field variable

$$0 \leq \phi \leq 1$$

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

transient diffusion source

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

• Orientation variable

$$-\pi \leq \theta \leq \pi$$

$$P(\phi, \nabla\theta) \frac{\partial\theta}{\partial t} = \nabla \cdot \left[h\epsilon^2 \nabla\theta + g_s \frac{\nabla\theta}{|\nabla\theta|} \right]$$

transient diffusion

