MatForge: Collaborative Computational Materials Research & Education

UMC Workshop on Computational Materials Education
Northwestern University, June 23-24, 2010

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Outline

- Introduction
- Open source
- Community building
  - Partnerships & Workshops
  - Hosting/Mirroring
- Research-based curriculum aids
- Easy authoring and broad dissemination
- Participating in MatForge
- Concluding remarks

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What is MatForge (http://matforge.org) ?

- **Provides** a branded, trusted, non-commercial, and neutral host/mirror site supporting materials code development.

- **Promotes** interaction between materials research, code development, and education by supporting:
  - materials code developers;
  - materials community to use code; and
  - **faculty to integrate code & aids into their courses**.

Open Source

- **MatForge platform**: Choice of software repositories with a web interface - Redmine
  - Subversion, Git, Mercurial, Bazaar – manage source code (version control, downloading services, and privacy control)
  - Redmine – communication tools
    - Wiki
    - Issue tracker
    - Interface to code repository
    - Forum
- **Code projects**:
  - Open source at your discretion
  - Effective instructional vehicle
  - Ways to work with proprietary codes

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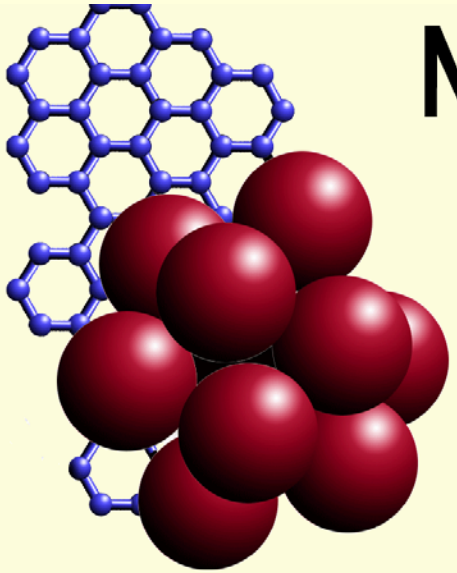
Community Building

A Community Platform supports synergy to:



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As part of the NSF NSDL, MatDL Pathway provides a branded, trusted, non-commercial, and neutral site supporting open source, collaborative, materials code development.

Projects:

- NIST MSEL CTCMS
  - FiPy
  - Teaching with FiPy
- Carnegie Mellon Computational Materials Science
  - Mesoscale Microstructure Simulation Project (MMSP)
  - Microstructure Builder (coming soon)
  - Parallel Grain Growth 3D (PGG-3D)
  - Texture subroutines
- Department of Energy Computational Materials Science Network Cooperative Research Team
  - Dynamics and Cohesion of Materials Interfaces and Confined Phases Under Stress
- FDA Computational Materials Science
  - TheraPy
- Gibbs
- Lab for Computational Nanoscience and Soft Matter Simulation
  - GlotZilla
  - Image Processing GlotZilla (IPGZ)
  - Transition Path Sampling (TPS)
- Powell Research Group
  - Julian
  - RheoPlast
  - Illuminator
  - EBaporate
  - Ternary
- Thornton Research Group, University of Michigan
  - Li Battery cathode development (coming soon)
  - Topological Analysis with Level Set Method (coming soon)
  - Phase Field Modeling of Lipid Membranes (coming soon)
  - Simulation of Solid Oxide Fuel Cell Electrodes with Complex Microstructure (coming soon)
- Voorhees Research Group, Northwestern University
  - VLS-Growth (coming soon)

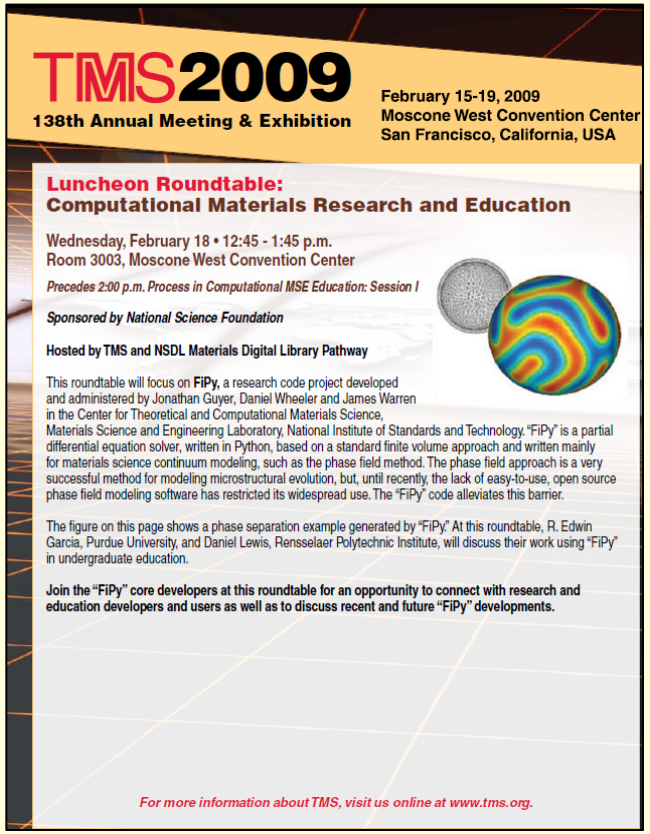
MatForge Live CDs:

- FiPy (Download Now. 655MB)
- Ternary (Download Now. 648MB)

- Promote U.S. innovation & competitiveness in development & use of materials
- Develop a pool of users ready to transfer the technology to industry, academia, and government labs
- **Train next generation of scientists to use and develop computational materials tools**

Community building with Materials Partners: TMS & ICME Committee

- TMS Committees
  - CoChair, ICME Education
  - Member, Education
- Education Symposia
- Roundtables
  - Spotlight materials codes
  - Discuss development & testing of curriculum aids
- MS&T 2010 TMS/MatDL
  - Oct 19-20, noon time



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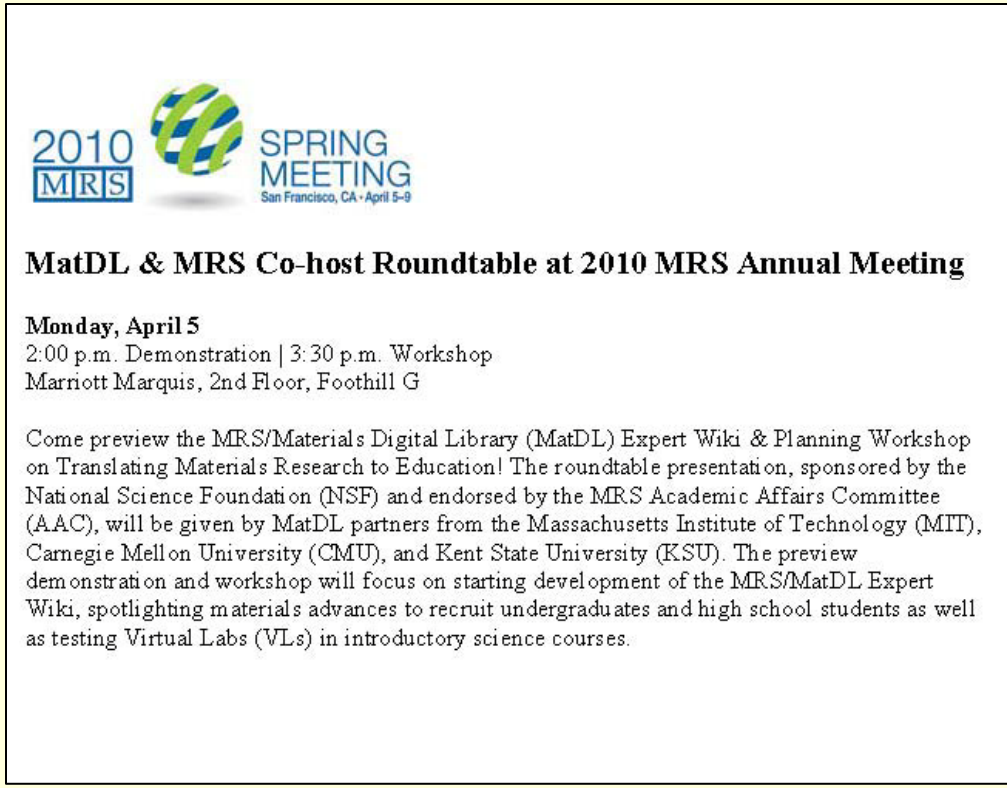
Community building with Materials Partners: MRS & AAC

- MRS Committee
  - Collaborate with Academic Affairs
- Education Symposia
  - Presented & Chaired
- Workshops
  - Brief presentations
  - Curriculum discussions



2010 MRS SPRING MEETING
San Francisco, CA • April 5–9

MatDL & MRS Co-host Roundtable at 2010 MRS Annual Meeting

Monday, April 5
2:00 p.m. Demonstration | 3:30 p.m. Workshop
Marriott Marquis, 2nd Floor, Foothill G

Come preview the MRS/Materials Digital Library (MatDL) Expert Wiki & Planning Workshop on Translating Materials Research to Education! The roundtable presentation, sponsored by the National Science Foundation (NSF) and endorsed by the MRS Academic Affairs Committee (AAC), will be given by MatDL partners from the Massachusetts Institute of Technology (MIT), Carnegie Mellon University (CMU), and Kent State University (KSU). The preview demonstration and workshop will focus on starting development of the MRS/MatDL Expert Wiki, spotlighting materials advances to recruit undergraduates and high school students as well as testing Virtual Labs (VLs) in introductory science courses.

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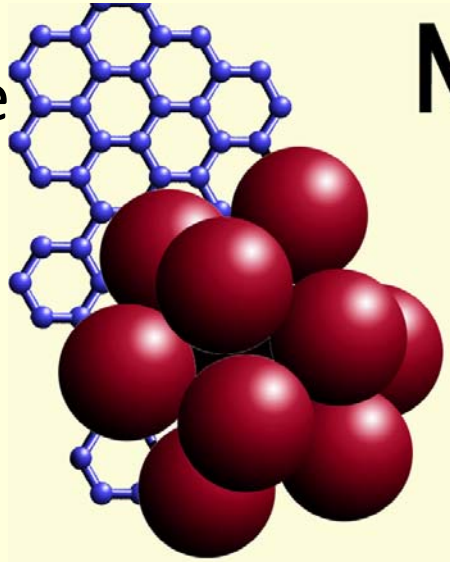
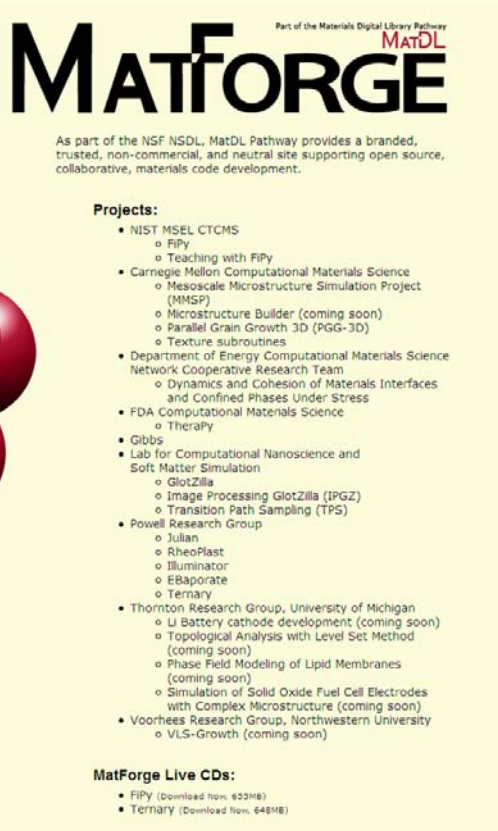
Community building by Hosting & Mirroring

- Hosting:
  - Develop on your machines, tools & timetable
  - Check in your code changes
  - Roll your code back
  - back up daily
  - Communicate over encrypted channels
- Mirroring



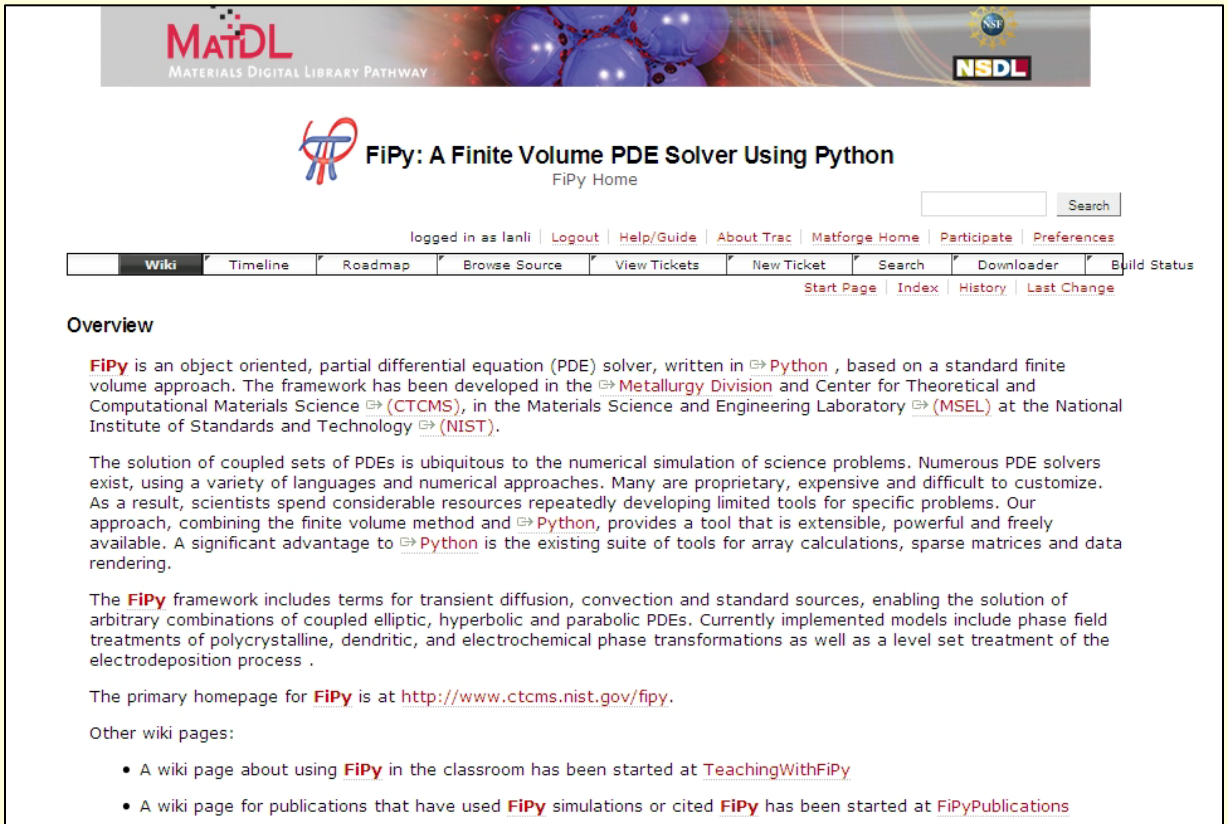


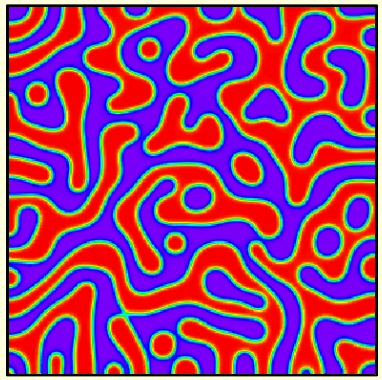
Developing Research-based Curriculum Aids

Example: FiPy Research Code

- *Guyer, Wheeler, Warren, NIST*

A partial differential equation (PDE) solver, written in Python, based on a standard finite approach.





Cahn-Hilliard

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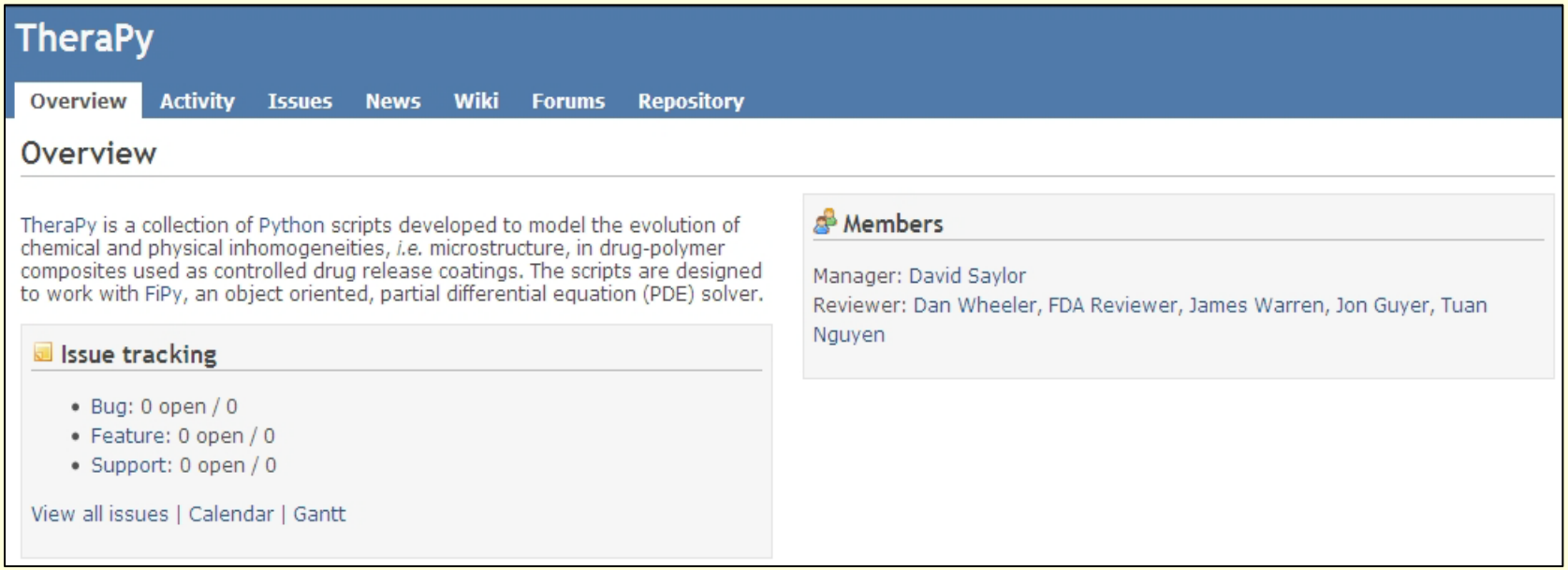
Developing Research-based Curriculum Aids

- Using FiPy in research, *David Saylor, Food & Drug Administration*

TheraPy: a collection of Python scripts, designed to work with FiPy, developed to model the evolution of chemical and physical inhomogeneities in drug-polymer composites used as controlled drug release coatings.



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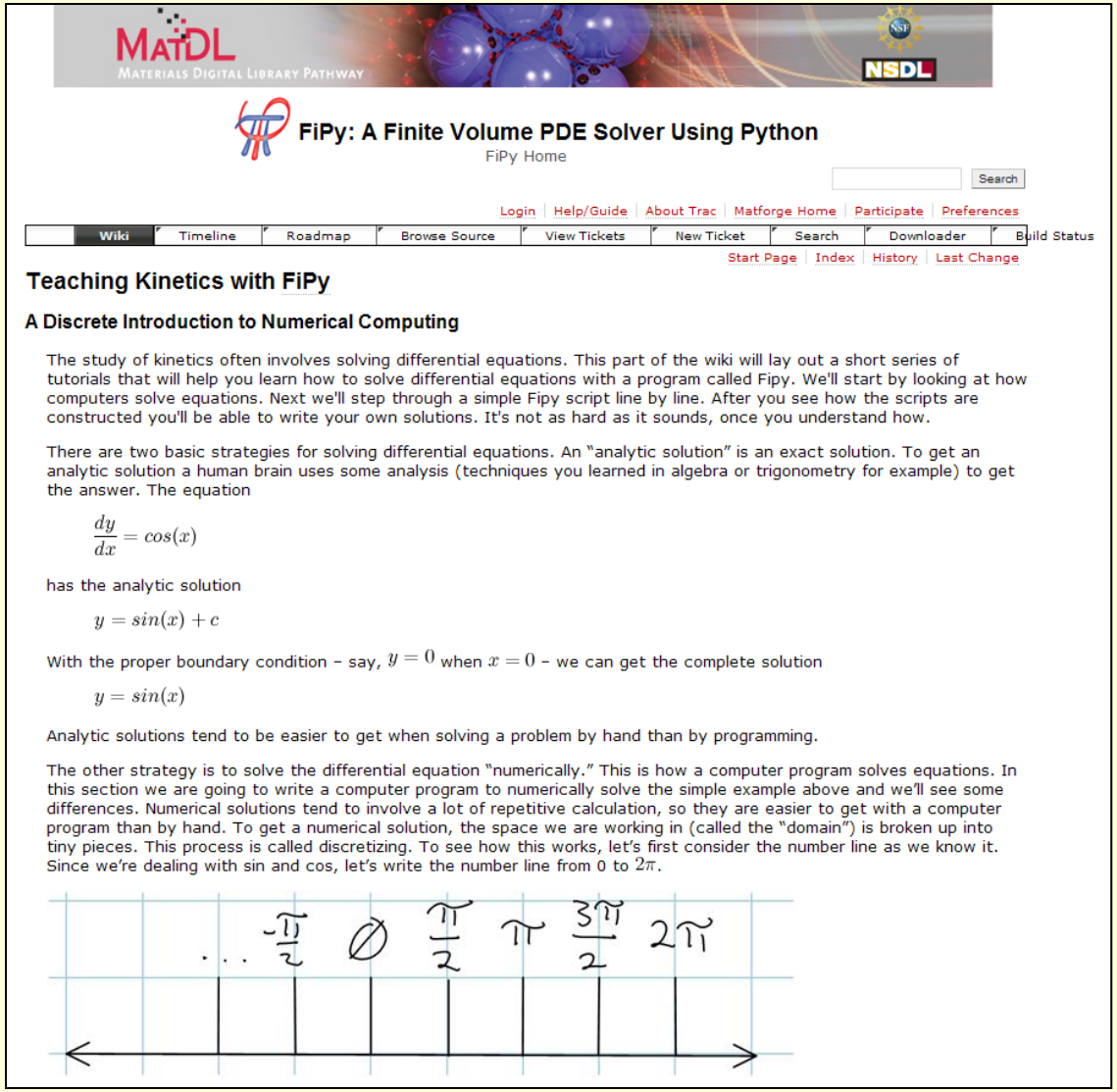
Developing Research-based Curriculum Aids

- Teaching with FiPy



FiPy Workbook: Teaching Kinetics with FiPy

Daniel Lewis, RPI

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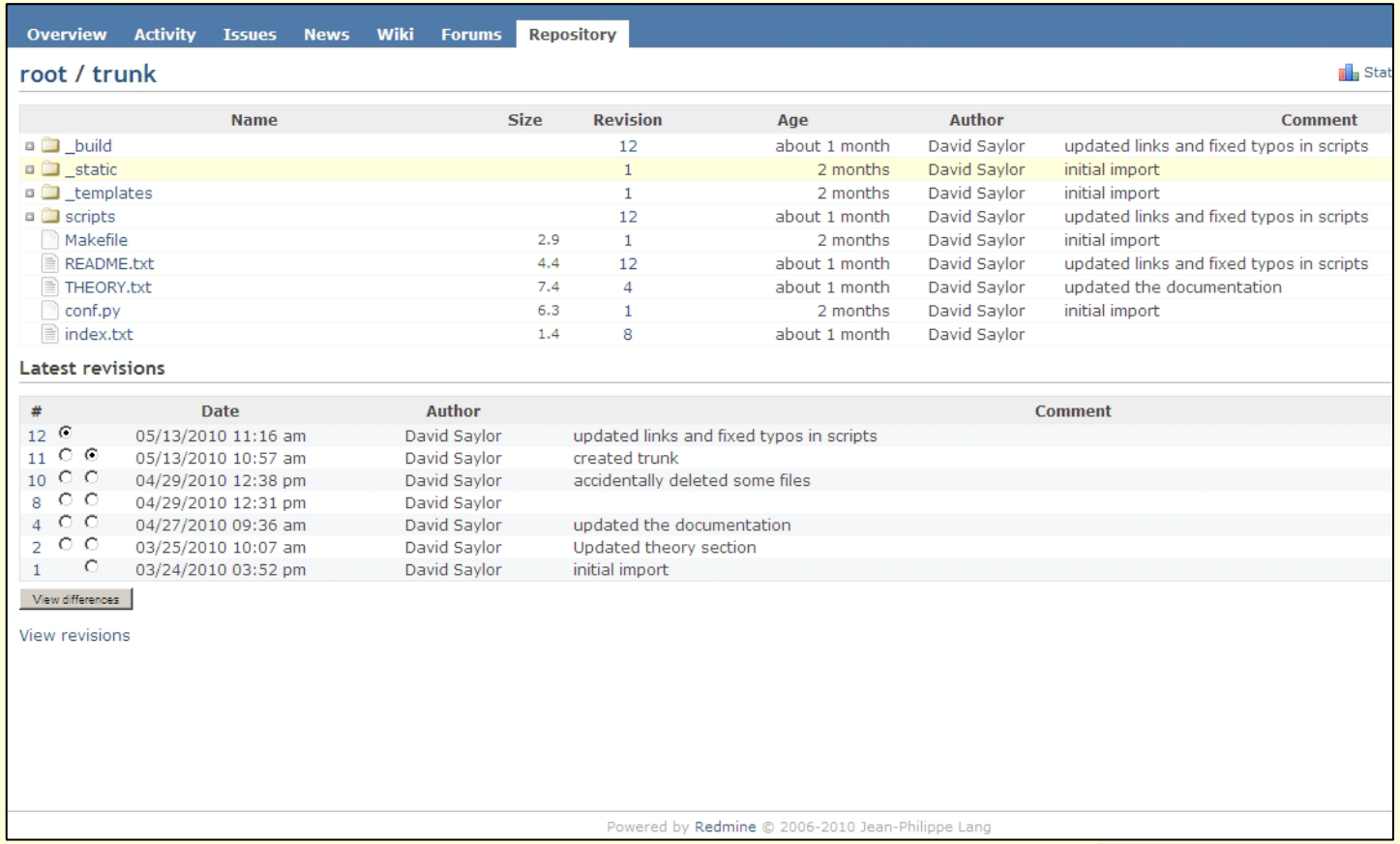
Code repository



Overview | Activity | Issues | News | Wiki | Forums | Repository

root / trunk

Name	Size	Revision	Age	Author	Comment
_build		12	about 1 month	David Saylor	updated links and fixed typos in scripts
_static		1	2 months	David Saylor	initial import
_templates		1	2 months	David Saylor	initial import
scripts		12	about 1 month	David Saylor	updated links and fixed typos in scripts
Makefile	2.9	1	2 months	David Saylor	initial import
README.txt	4.4	12	about 1 month	David Saylor	updated links and fixed typos in scripts
THEORY.txt	7.4	4	about 1 month	David Saylor	updated the documentation
conf.py	6.3	1	2 months	David Saylor	initial import
index.txt	1.4	8	about 1 month	David Saylor	

Latest revisions

#	Date	Author	Comment
12	05/13/2010 11:16 am	David Saylor	updated links and fixed typos in scripts
11	05/13/2010 10:57 am	David Saylor	created trunk
10	04/29/2010 12:38 pm	David Saylor	accidentally deleted some files
8	04/29/2010 12:31 pm	David Saylor	
4	04/27/2010 09:36 am	David Saylor	updated the documentation
2	03/25/2010 10:07 am	David Saylor	Updated theory section
1	03/24/2010 03:52 pm	David Saylor	initial import

View differences

View revisions

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Wiki

TheraPy

Overview | Activity | Issues | News | **Wiki** | Forums | Repository

TheraPy

History

Overview

TheraPy is a collection of Python scripts developed to model the evolution of chemical and physical inhomogeneities, *i.e.* microstructure, in drug-polymer composites used as controlled drug release coatings. This includes the development of microstructure during the process of casting drug eluting coatings, as well as the microstructural changes that occur during use or after the coating is immersed in the release medium. Therefore, these scripts provide tools to predict the relationships between materials and process variables, microstructure, and performance. Establishing these relationships can reduce empiricism in materials selection and process design, providing a facile and efficient means to tailor the underlying microstructure and achieve a desired drug release behavior.

The TheraPy scripts were developed in the Division of Chemistry and Materials Science (DCMS) in the Office of Engineering Laboratories (OSEL) at the Food and Drug Administration's (FDA) Center for Devices and Radiological Health (CDRH). The scripts are designed to work with FiPy, an object oriented, partial differential equation (PDE) solver. As described below, these scripts can be used much in the same way as the examples provided with the FiPy distribution.

Currently, scripts are provided to predict the microstructure development during casting in both 1D and 2D of systems composed of three components: drug, polymer, and solvent, as well as drug release behavior in 2D. In the future, we intend to add scripts that extend the current model to material systems that:

- are 3D
- contain arbitrary number of components
- exhibit crystallization
- form chemical bonds between constituents
- contain components that may undergo chemical degradation.

Download

A tarball of the TheraPy scripts and documentation can be downloaded from export:release/therapy0.1.tar.gz. Alternatively, you can checkout the latest version from the repository:

```
$ svn checkout https://matforge.org/svn/therapy/trunk therapy
```

To browse the source code on-line, click here.

Documentation

Online versions of detailed documentation including the underlying theory and specific usage instructions can be found here (html) or source:trunk/_build/latex/TheraPy.pdf (pdf).

Alternatively, after downloading and unpacking the tarball or in a version obtained directly from the repository, you will have local copies of the documentation. Under the main "therapy" directory, the html version is in "_build/html" and the pdf version can be found in "_build/latex".

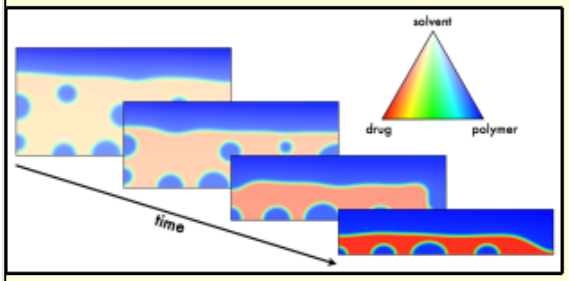
Support

The forum for open discussion of all issues related to the TheraPy scripts can be accessed by clicking the "Forums" tab at the top of the page. If you find a bug or have a specific feature request, please enter it using the "New Issue" tab.

Terms of Use

This software and documentation (the "Software") were developed at the Food and Drug Administration (FDA) by employees of the Federal Government in the course of their official duties. Pursuant to Title 17, Section 105 of the United States Code, this work is not subject to copyright protection and is in the public domain. Permission is hereby granted, free of charge, to any person obtaining a copy of the Software, to deal in the Software without restriction, including without limitation the rights to use, copy, modify, merge, publish, distribute, sublicense, or sell copies of the Software or derivatives, and to permit persons to whom the Software is furnished to do so. FDA assumes no responsibility whatsoever for use by other parties of the Software, its source code, documentation or compiled executables, and makes no guarantees, expressed or implied, about its quality, reliability, or any other characteristic. Further, use of this code in no way implies endorsement by the FDA or confers any advantage in regulatory decisions. Although this software can be redistributed and/or modified freely, we ask that any derivative works bear some notice that they are derived from it, and any modified versions bear some notice that they have been modified.

Also available in: HTML | TXT



Microstructure evolution in controlled drug delivery systems for medical device applications

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Easy Authoring and Broad Dissemination

- Matforge live CDs are
  - un-official “re-spin” of the Ubuntu 9.10 live CDs;
  - designed to help students & researchers “jump start” using a code without having to install the code and all of its dependencies.

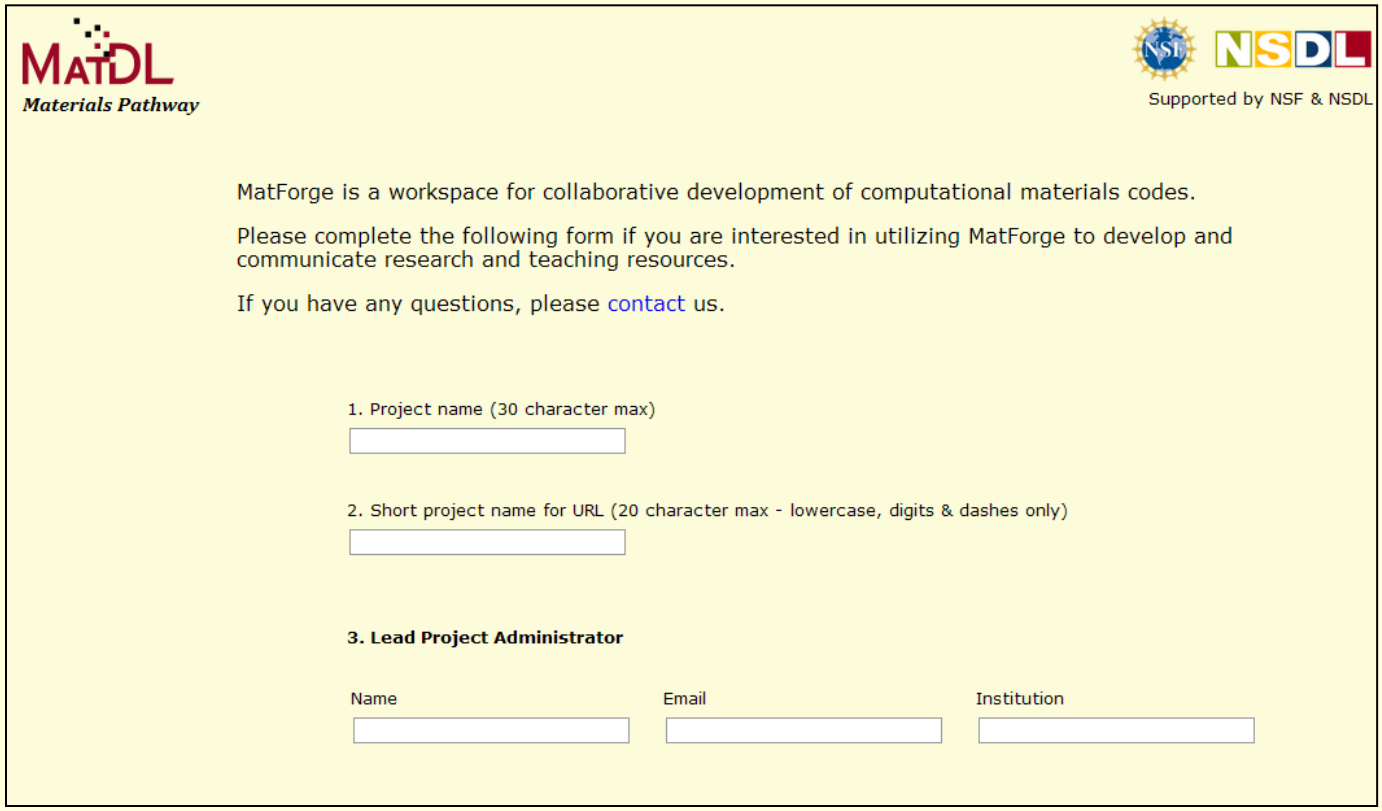
To use the live CD,

- download and burn the ISO image into a CD;
- reboot computer from the CD.

The ISO image can also be used in a virtualization environment (like VirtualBox, VMWare, Parallels, KVM, Qemu, etc.) without needing to reboot the host computer.

How to participate?

http://matforge.org/signup



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Concluding Remarks

- Need to integrate computational materials research codes into undergraduate coursework
  - compelling/integral/advantageous to students
  - preparing next generation materials code developers
- Collaborative computational mat'l research & education
  - bring together significant research code and vetted undergraduate teaching resources
  - Establish consortial academe/gov't/industry materials community center with a sustainability plan
- MatForge: a collaborative partner

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Contact Info

- MatForge http://matforge.org

Questions? Please contact:

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