A NEW PLATFORM FOR PREDICTIVE MODELING: PRIME

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Zoran Djurisic
Michael Gutkin

Supported by:
NSF Chemistry Division (Cyber-infrastructure)
AFOSR (MACCCR)
SERDP
What’s New with PrIME

- PrIME Portal – true 24/7 service; new features
- 2 new PrIME Work Groups: SERDP, MURI / private mode
- “C0-C2” PWG is active – NSF-EVO project
- total registered members: >180

Data Depository
- species records were cleaned: joint MIT-UCB efforts
- new species data are being developed (geometries, frequencies,...): MIT+Stanford
- next: cleaning reaction records

new components of Data Model
- Targets – features of experiments to match / model training
- Instrumental model – separation of experimental facts from experimenters’ opinions/assumption
- next: Optimization variables

PrIME Workflow – new paradigm of data/codes sharing
What does it mean:

“TO ARCHIVE DATA”
PrIME Data Model

- One copy per number
- Complete documentation
  - who, when, what
  - uncertainty
- Extendable and expandable
- Zero-error fetching
- Facts vs opinions
PrIME Data Model

- Bibliography
- Chemical Elements
- Species
- Reactions
- Models
- Experiments
- Targets
- Instrumental models
<chemicalModel primeID="m00000003">
<copyright>©primekinetics.org 2006</copyright>
<preferredKey group="prime">GRI-Mech 3.0</preferredKey>
<bibliographyLink preferredKey="Smith et al., 1999." primeID="b00014718"/>

<speciesSet>
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<thermodynamicDataLink preferredKey="120186" primeID="thp00000001"/>
</speciesLink>
<speciesLink preferredKey="H" primeID="s00009800">
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</chemicalModel>
What does it mean:

“To Compare Models and Data”
TARGET: their ratio
What does it mean:

“Experimental Data”
$\frac{I}{I_0} = e^{-\varepsilon[CN]L}$
PrIME Data Model: Instrumental Model

Beer-Lambert Law

\[ C = \frac{\ln\left(\frac{V_{\text{inf}} - V}{V_{\text{inf}} - V_0}\right)}{\text{Beer-Lambert Law}} \]

Keywords: laser absorption

Diagram showing a graph with two peaks labeled 'N2O-doped' and 'NO-doped', and another diagram with the expression for Beer-Lambert Law.

MathML expression:
\[ C = \frac{\ln\left(\frac{V_{\text{inf}} - V}{V_{\text{inf}} - V_0}\right)}{\text{MathML implicit="true"}} \]

PrimeID for the model: i00000001
What does it mean:

“**AUTOMATE MODEL BUILDING**”
PrIME WORKFLOW

- Collect and curate data
- Share data
- Link data to applications
- Share applications
About PrIMe

PrIMe—Process Informatics Model—is a new approach for developing two-phased coupled chemical reaction systems that is based on the scientific collaboration process. The primary goal of PrIMe are collecting and storing data, validating the data and uncertainties, and assembling the data into predictive models with quantified uncertainties to meet specific user requirements. The principal components of PrIMe data Depository, which is a repository of data provided by the community, a data Library for storage of evaluated data, and a set of computer-based tools to process this data to assemble data into predictive models. Two guiding principles of PrIMe are: open membership—a qualified individual or industrial organization can register to participate in a project; and open source—all submitted data, tools and models will be in the public domain.
3.2.1. *Species Collection.* The following figure is a schematic diagram of the PrIME Warehouse *species* collection.

![Diagram of the PrIME Warehouse *species* collection](image)

Figure 1. A schematic diagram of the PrIME Warehouse *species* collection

The *catalog* files are named starting with the letter *s* followed with the 8-digit number, and this is the PrIME species *primeID* (like s00000001 or s00001234). The same *primeID* is used to name the corresponding subdirectories of *species/data*. These subdirectories contain data files, which can be of any type, as illustrated in the diagram.

3.3. *Data Definition Files.* The XML files of the catalog collections and of some data subdirectories will be validated against *schemas*. XML schemas express shared vocabularies and allow machines to carry out rules made by people. They provide a means for defining the structure, content and semantics of XML documents in more detail. Passing XML validation means that the submitted/created XML documents adhere to the scientific rules set by the PrIME community.
PrIME—Process Informatics Model—is a new approach for developing mathematical reaction systems that is based on the scientific collaborative paradigm. It takes full advantage of existing and developing cyber infrastructure. The primary goals of PrIME are collecting and storing data, validating the data and uncertainties, and assembling the data into predictive models with quantified uncertainties to meet specific user requirements. The principal components of PrIME data Depository, which is a repository of data provided by the community, a data Library for storage of evaluated data, and a set of computer-based tools to process and assemble data into predictive models. Two guiding principles of PrIME are: open membership—a qualified individual or industrial organization can register to participate in any project; and open source—all submitted data, tools and models will be in the public domain.
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GROUPS

- Management
- MURI
- Portal Development
- PRIME Team
- S ERP

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HISTORY

Member for
2 years 18 weeks
Welcome to the SERDP Book

- AFRl Team
- Mechanisms
- Sandia Team
- Stanford team
- Univ of Illinois, Chicago team
- Univ of Utah team

Add new comment | 188 reads

515 reads
AFRL SERDP reports

Folder for Quarterly, Annual reports

Attachment Size
1st Qtr Oct-Dec 07.doc 121 KB

- 3rd Quarterly Report April - June 2008
- AF Quarterly Jan - Mar 07

Add child page | Printer-friendly version | Add new comment | 41 reads
### Group Directory

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<th>Name</th>
<th>Subscribers</th>
<th>Description</th>
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Welcome to the first page of **C0-C2 Book**. Click on the links below to contribute to the various discussions.

- Discussion of organization and procedures
- Kinetics sub-area divisions discussion
- Notices of interest
- REACTIONS
- Voting page

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» 1396 reads
**GROUPS**

- Management
- MURI
- Portal Development
- PrIME Team
- SEROP

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**HISTORY**

**Member for**
2 years 18 weeks
Start: create a new project
- go to “New Project”
- create a network by dragging and connecting the appropriate objects (i.e., Target from Targets, PlugFlow from Processes, etc)
- save the network giving it a distinct name
- execute the network by clicking ‘Run’

Execute saved project
- go to “Open”
- double-click a previously saved project
- execute the network by clicking ‘Run’

Collaborating
- check the “Public” box
Save workflow project

Title: myProject1
Summary:

Author: 2008-09-05 08:45
Status: Submitted 2008-09-05 08:45

Public
Share
Save
Cancel

Matlab application
http://reactionlab.sourceforge.net/

OK Cancel Run
Interval Prediction for Model co psu from Dataset GRIMech 3

**Prediction Interval**
- Outer: 1.56
- Inner: 1.52

**GRIMech 3 targets**
- 

**Constraint Multipliers**
- Multipliers (LB)
- Multipliers (UB)

**Inner Int.** [1.457, 1.557]
**Outer Int.** [1.457, 1.559]

Analysis found feasible parameter values at which the model produces the endpoints of the inner interval.

Constrained by the dataset, the model does not take values outside the outer interval.

**Multipliers**
- Selected Target: 0
- Selected parameter: 0
- LB: 0
- UE: 0

Options:
- Dataset Order
- Sort Right Panel
- Sort Left Panel
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PWA Installation

Note: The present version of the PrIME Workflow Application (PWA) is implemented only for the Microsoft platform: Windows and Internet Explorer.

Adjusting .NET Security Settings
PWA requires certain security configuration settings to work properly within Internet Explorer. These settings apply only to components received from Primekinetics.org web server, and do not relax security measures for any other server.
Run following script to relax security setting for PWA application: run .NET Security Script

Install Matlab Run-Time library
PWA requires Matlab Run-Time library to be installed on your computer to function properly.
To install Matlab run-time click following link "Matlab Installer"

PWA Installation Diagnostics Utility
This utility is designed to help you to examine the configuration of your workstation as needed for working with the PrIME Workflow.
To start, click the link below. When asked, save the file to your workstation and execute it. If you use Vista, right-click the icon of that application and select "Run as administrator". Running this test utility, will open a window. Click the upper-left button "test". The configuration report will be appear. The report contains three sections: .NET configuration, Matlab configuration, firewall issues and list of errors. You may submit the report by clicking the upper-right button "send report" and fill in your PrIME userid and an optional message in the corresponding boxes of the form. Start Diagnostics Utility

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**Future Plans**

- Continue community engagement
  - data submission / analysis
  - application “submission”
  - education
  - mirror site in EU

- Complete Data Model (NSF)
  - targets, instrumental
  - optimization variables

- Workflow interface ($$$?)

- Model development
**Issues/Needs**

- Home for PrIMe Data Warehouse
  - oversight but not possession
  - new job: data-record admission

- Computer hardware
  - storage: data, Work-Group docs
  - running applications

- Professional-level programming