

GLENN MURRAY, PH.D.

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Primary expertise _____

Technical software and project management skills for advancing scientific research.

Recent Employment History _____

- **Solicited Proposal, CSM/NREL** May 2006-present

Duties and Accomplishments: Writing and managing a data integration project for photovoltaic scientists. The problem here is that PV scientists, using combinatorial techniques, are producing mountains of files with no clear path to their organization. Implemented an architecture including the following:

1. An enterprise service bus (ESB) for automatic data collection and file transfer.
2. Python wrapper scripts to expose legacy application as services available to the ESB.
3. JavaScript/XML/XSLT engine for web forms to collect data.
4. Signed Java applets for more advanced client-side data manipulation.

The backend is a Linux-Apache-MySQL-PHP/Python stack for searching and exporting the data.

- **Solicited Proposal, CSM/NREL** November 2006-present

Duties and Accomplishments: Providing user interface and glue software for a DOE/SciDac petascale systems biology project, integrating existing open source tools for the creation, manipulation, and searchable storage of Systems Biology Markup Language (SBML) files. This is a three-year quarter-time project.

- **Independent Consulting, NREL** January-May 2006

Duties and Accomplishments: Consulting at the National Renewable Energy Laboratory Center for Computational Sciences, providing expertise on architecting software for scientific data management, including work flow management, electronic notebook evaluation, XML, CSS, and JavaScript experiment description prototype, user interface consulting, technology evaluation, and proposal preparation.

- **Independent Consulting, Numerica Technology** March-June 2006

Duties and Accomplishments: Coding Tomcat middleware and rich client (Swing) interface for multiuser access to the Jacobian modeling and optimization software from Numerica Technology, for systems biology modeling. Currently in use at MIT.

- **Independent Consulting, Small Business** January 2006
Duties and Accomplishments: Super simple warehouse inventory recorder for making digital records of old car manuals.
- **Independent Consulting, .NET** December 2005
Duties and Accomplishments: Additional features for the C# .NET project below.
- **Independent Consulting, Remote Computing** July-November 2005
Duties and Accomplishments: For a chemical engineering client, designed and developed a Swing/Tomcat web application to run CPU-intensive programs on remote servers, including batch job submission, status, cancellation, and retrieval.
- **Independent Consulting, NREL** June 2005
Duties and Accomplishments: Consulting with NREL on implementing a LAMP-style architecture for managing and searching databases of experimental data.
- **Independent Consulting, .NET** Feb.-Mar. 2005
Contract position for developing C# ADO.NET code to gather data from Excel spreadsheets to colorize Visio drawings of floor plans imported from CAD drawings. Some UI design.
- **Research Professor, Colorado School of Mines, Golden, Colorado** 2000-2004
Duties and Accomplishments: Research Professor, Dept. of Chemical Engineering.
 Software development, training, and infrastructure manager for the OpenChem Workbench (<http://openchemworkbench.org>, > 100,000 lines of code) and an RDBMS-backed GUI for running models using the ABACUSS solver (for Mitsubishi, > 60,000 lines of code). Responsible for use cases, analysis and design, testing and debugging, CVS repository and website maintenance, and deployment on Linux and Windows. These are distributed cheminformatics desktop tools for chemistry researchers and the chemical process industry. Currently the OpenChem Workbench is being licensed as OpenChem Pro through Numerica Technology (<http://www.numericatech.com/>).

 - *Project management:* Managing Ph.D. students and undergraduates in object-oriented software development, agile methodology evangelism (emphasis on Test Driven Development using JUnit tools and close integration with users), source code style and metrics management, code reviews.
 - *Project infrastructure management:* UNIX server administration (mostly Linux, some Solaris) with MySQL and PostgreSQL, Apache, CVS, mailing lists, bug-tracking, firewall, etc.; CVS and SSH training, multi-platform build scripting with Ant, Bash and DOS, new technology evaluation.
 - *Enterprise application development:* J2EE three-tier Swing rich client/relational database application, EJB with BMP using JDBC/SQL for Windows and Linux RDBMS, data modeling and database refactoring, XML processing, user interface design, remote

computing, algorithm development (graph isomorphism), legacy (C, C++, FORTRAN) integration, help system, use case development, specifications, documentation, encryption and security.

- *Ph.D. committee member and supervisor*: Cheminformatics pedagogical and dissertation advising for Devin Hodgson (Ph.D. 2003, currently doing similar work for Reaction Design in San Diego CA) and Zhiwei Zhang (Ph.D. 2003, currently doing similar work for NumericalTech in Cambridge MA).

Monte Carlo polymer molecular dynamics simulation software, in Java and C++, employing XML formatting and high-performance Java tuning.

Flame image statistical analysis application for the CSM Water Mist experiment aboard the NASA Columbia space shuttle, in MATLAB, including a GUI. (<http://www.msfc.nasa.gov/news/news/photos/2002/STS107-MIST.html>).

Teaching: Ordinary Differential Equations

- **Independent Consulting, Training at NIST** 1998-1999
Duties and Accomplishments: Workshops in *Mathematica* for engineering, scientific, and mathematical investigations.
- **Teaching Faculty, Metropolitan State College of Denver** 1995-2000
Duties and Accomplishments: Adjunct Professor of Mathematics and Computer Science: full-time faculty position. Technical teaching experience in mathematics and computer science to a diverse student body, including Computer Networks, Computer Architecture, Calculus, Math for Poets, College Algebra, etc. as full-time faculty member, including curriculum development, lecturing, evaluation, etc. Development of *Mathematica* curricular materials for a course.
- **Teaching Faculty, Colorado School of Mines, Golden, Colorado** 1994-1995
Duties and Accomplishments: Adjunct Assistant Professor, Dept. of Mathematics; part-time faculty position.
- **Aerospace Engineer, El Segundo CA** 1980-1981
Duties and Accomplishments: Member of the Technical Staff. Real time programming in assembler for target tracking and controlling large lasers, Kalman filtering, simulation in FORTRAN, original statistical analysis of IR sensor data in FORTRAN; award for cost improvements.

- **Colorado Software Summit**, Keystone, Colorado, 2001-2003, 2006.
Intensive six-day all-tutorial immersions in Java technology (<http://www.softwaresummit.com/>).
- **Short Course in UML**, Greenbriar and Russell, Denver, 2000.
Five-day course in UML (Unified Modeling Language), architecture, design, analysis, and RUP (the Rational Unified Process).
- **Ph.D. and M.S., Algebraic Geometry**, Colorado State University, 1994.
Advisor: Rick Miranda (<http://www.math.colostate.edu/~miranda/>).
- **B.A., Mathematics and B.A. Physics**, Grinnell College, Grinnell, Iowa.
Graduated in three years.

Publications

My publications have appeared in a variety of formats and venues.

Cheminformatics: The two Ph.D. students on whose committee I served have not yet prepared and submitted their cheminformatics theses for peer review. The theses titles are *Computational Chemistry Reaction Engineering Software Integration* (Devin Hodgson) and *OpenChem Workbench - An Integrated Chemical Information System and an Example of its Application* (Zhiwei Zhang).

Miscellaneous Web How-To's and Documents: Several linked to from my home page at <http://www.mines.edu/~gmurray>. Also, unpublished articles on Notes on data mining topics (decision trees, entropy and information gain, linear regression, neural networks) and grid computing (PBS, MPI, Globus Toolkit), available on request.

Software: Much of my software has been released under open source licences and is visible on the web. Please ask me for links.

Mathematics: *The Gaussian Map for Smooth Toric Surfaces*, Mathematische Zeitschrift, 227(2): 187-210, 02/1998.

Some Easy Manifolds, Denver Metropolitan Journal of Mathematics and Computer Science, Spring 1998.