Final Report

DE-FG02-00ER45828

DOE EPSCoR Initiative in Structural and Computational Biology/Bioinformatics

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OVERVIEW

The overall goal of the DOE EPSCoR Initiative in Structural and Computational Biology was to enhance the competiveness of Vermont research in these scientific areas. To develop self-sustaining infrastructure, we increased the critical mass of faculty, developed shared resources that made junior researchers more competitive for federal research grants, implemented programs to train graduate and undergraduate students who participated in these research areas and provided seed money for research projects. During the time period funded by this DOE initiative: (1) four new faculty were recruited to the University of Vermont using DOE resources, three in Computational Biology and one in Structural Biology; (2) technical support was provided for the Computational and Structural Biology facilities; (3) twenty-two graduate students were directly funded by fellowships; (4) fifteen undergraduate students were supported during the summer; and (5) twenty-eight pilot projects were supported. Taken together these dollars resulted in a plethora of published papers, many in high profile journals in the fields and directly impacted competitive extramural funding based on structural or computational biology resulting in 49 million dollars awarded in grants (Appendix I), a 600% return on investment by DOE, the State and University.

RELATIONSHIP TO THE STATE SCIENCE AND TECHNOLOGY RESEARCH PLAN

The infrastructure to support EPSCoR in the State of Vermont is well developed primarily because of the EPSCoR awards initiated by the National Science Foundation in 1985. The State of Vermont has been the recipient of EPSCoR grants not only from the National Science Foundation but NASA, EPA, the NIH and the DOE. Vermont is a small state of only 600,000 people, with a single research university, the University of Vermont, allowing for a clear vision of the route to research infrastructure enhancement. In 1992 the Vermont Technology Council was started as a privately organized nonprofit group to bring together the high quality research of (the State's) colleges and university with the entrepreneurial capacity of its business sector. In 1993 the Vermont Technology Council became the EPSCoR State Board and was charged with developing a science and technology plan for the State as well as policy guidance to the Vermont EPSCoR program. Dr. Christopher Allen was the Vermont State EPSCoR Director; Dr. Judith VanHouten took over in 2005. Lillian Gamache is the EPSCoR Project Coordinator. When the first science and technology plan was presented to the Governor in 1994, biotechnology was one of the four areas of emphasis proposed, an emphasis in which Structural and Computational Biology play a pivotal role. At the time there were no resources nor facilities in the State devoted to these scientific areas. Because of this need the DOE EPSCoR Initiative in Structural and Computational Biology was begun and supported by the State of Vermont.

PROGRAM COORDINATION

Since Vermont has only a single research university, program coordination was relatively straightforward. At the time Dr. Christopher Allen was the State EPSCoR Director and he and DOE EPSCoR Director had an effective working relationship. Table 1 shows the composition of the DOE EPSCoR Board and Table 2 shows the composition of the DOE EPSCoR Structural and Computational Biology Executive Committee. The Principal Investigator chaired the DOE EPSCoR Board which made major decisions regarding budgetary appropriations while the Executive Committee solicited applications for pilot projects and established review committees to make recommendations to the DOE EPSCoR Board as to which project should be funded and which students should be directly supported. Over the duration of the DOE EPSCoR funding for Structural and Computational Biology the Executive Committee held a number of retreats at the Bishop Booth Conference Center, Burlington, Vermont. The DOE EPSCoR Executive Committee also developed an External Advisory Board of structural and computational biologists (Table 3) who communicated with the senior leaders by phone and with the entire group of faculty, postdoctoral fellows, graduate and undergraduate students at the retreats. DOE EPSCoR also supported a seminar series which brought internationally renowned structural and computational biologists to campus to give talks to this same contingent of scholars.

Table 1 DOE EPSCoR Board	
Christopher Allen, Ph.D.	Professor of Chemistry, Vermont State EPSCoR Project Director, Project Director DOD and NSF EPSCoR, Project Co-Director, NIH EPSCoR
John Burke, Ph.D.	Vice-Provost for Research, Professor of Microbiology and Molecular Genetics
William Lakin, Ph.D.	Professor of Mathematics & Statistics, Associate Project Director, NASA EPSCoR
Susan Lowey, Ph.D.	Professor of Molecular Physiology and Biophysics
Kenneth Mann, Ph.D.	Professor and Chair of Biochemistry
Alan McIntosh, Ph.D.	Professor, School of Natural Resources, Projector Director, EPA EPSCoR
Judith VanHouten, Ph.D.	Professor and Chair of Biology, Associate State EPSCoR Project Director, Co-Director NIH EPSCoR
Susan Wallace, Ph.D., Chair	Professor and Chair of Microbiology and Molecular Genetics, Project Director, DOE EPSCoR

Table 2 DOE EPSCoR Structural and Computational Biology Executive Committee	
Jeffrey Bond, Ph.D., Co-Chair	Research Assistant Professor of Microbiology and Molecular Genetics
Sylvie Doublié, Ph.D., Co-Chair	Assistant Professor of Microbiology and Molecular Genetics
Stephen Everse, Ph.D.	Assistant Professor of Biochemistry
Christopher Francklyn, Ph.D.	Associate Professor of Biochemistry
Scott Morrical, Ph.D.	Associate Professor of Biochemistry
Robert Snapp, Ph.D.	Professor of Computer Science

Table 3 External Advisory Board		
Charles Carter, Ph.D.	Professor of Biochemistry and Biophysics	University of North Carolina at Chapel Hill
Robert Sweet, Ph.D.	Scientist, Biology Department	Brookhaven National Laboratory
George Rose, Ph.D.	Professor of Biophysics	Johns Hopkins University

HUMAN RESOURCES

1. Faculty Development

In the first phase of the DOE EPSCoR Program in Structural and Computational Biology, two computational biologists were recruited into tenure track positions in the Department of Computer Sciences, Dr. Margaret Eppstein in 2001 and Dr. Abdullah Arslan in 2002. Dr. Eppstein has made significant national contributions in the areas of optical imaging and evolutionary computational biology. In 2006 she was made founding Co-Director of the Complex Systems Center here at the University of Vermont. An extensive publication list, as well as awards and honors are included in her Curriculum Vitae (Appendix 2). The second recruit in Computational Biology, Dr. Abdullah Arslan, was recruited from the University of California, Santa Barbara. His research interests include algorithms on strings, graphs, similarity search problems, computational problems and bioinformatics. He also has a substantial list of publications since his appointment as noted in his Curriculum Vitae (Appendix 2). In 2004, during the second phase of support, a biostatistician, Dr. Richard Single, was recruited to the tenure track in the Department of Mathematics and Statistics. His research focuses on genotypic analysis of proteins involved in immunobiology. Dr. Single has numerous publications in this area and is supported by a variety of funding mechanisms (Appendix 2). The recruitment of these individuals significantly contributed to the critical mass of faculty working in Computational Biology (Table 4).

Table 4 Cluster Primary Faculty	
Abdullah Arslan	Assistant Professor, Computer Science
Daniel Bentil, Ph.D.	Associate Professor, Mathematics and Statistics and Molecular Physiology and Biophysics
Jeffrey Bond, Ph.D.	Research Assistant Professor, Microbiology and Molecular Genetics
Margaret Eppstein, Ph.D.	Assistant Professor, Computer Science
Douglas Green, Ph.D.	Professor, Biology, Saint Michael's College
James Hoffmann, Ph.D.	Associate Professor, Botany and Agricultural Biochemistry
Alan Ling, Ph.D.	Assistant Professor, Computer Science
Richard Single, Ph.D.	Assistant Professor, Mathematics and Statistics
Robert Snapp, Ph.D.	Associate Professor of Computer Science and Mathematics and Statistics
Xindong Wu, Ph.D.	Professor and Chair, Computer Science

To add to the structural biology faculty, Dr. Robert Hondal was recruited into the Biochemistry Department in 2002. The main focus of Dr. Hondal's laboratory is the investigation of the enzyme mechanism of eukaryotic thioredoxin reductases. Dr. Hondal's group uses NMR spectroscopy and X-ray crystallography to undertake structure/function studies of these selenocystein-containing proteins. He also has an excellent publication list and is currently supported by an NIH R01 grant (Appendix 2). Dr. Hondal was a significant addition to the primary faculty working in the structural biology area (Table 5).

Table 5	
Kelvin Chu, Ph.D.	Assistant Professor, Physics
Sylvie Doublié, Ph.D.	Assistant Professor, Microbiology and Molecular Genetics
Stephen Everse, Ph.D.	Assistant Professor, Biochemistry
Robert Hondal, Ph.D.	Assistant Professor, Biochemistry
Barbara Lyons, Ph.D.	Assistant Professor, Biochemistry
Mark Rould, Ph.D.	Assistant Professor, Molecular Physiology and Biophysics

Taken together, the hires into Computational and Structural Biology have been successful; the faculty members are productive and interactive.

2. Student Support

Twenty-two graduate research fellowships were awarded to students in eight different programs and four different colleges at the University of Vermont (Appendix 3). Of these, five were awarded the Masters Degree, ten the Ph.D. Degree, one left the program, and four are still in residence and working toward completing the requirements for the Ph.D. As can be seen, many excellent publications resulted from the students' work and the students who have graduated have gone on to prestigious postdoctoral academic positions or to industry.

Fifteen undergraduate students were also supported with summer stipends by DOE EPSCoR. other institutions in the State were represented. Announcements for the DOE EPSCoR Summer Internships were sent to all undergraduate institutions in the State of Vermont. Although most came from the University of Vermont, other institutions of higher learning in the State were represented.

3. Summary

Table 6 summarizes the total number of individuals supported by the DOE EPSCoR Initiative in Structural and Computational Biology.

Table __ DOE EPSCoR Support of Human Resources

Supported by DOE EPSCoR	**Total Number**
Undergraduate Students	15
Graduate Students	47
Postdoctoral Associates	8
Faculty	36
Technicians	15
Underrepresented Minorities	
Black	7
Hispanic	1
Asian or Pacific Islander	21
Women	22
University Departments Represented	12
University Colleges Represented	4
State Institutions Represented	3

INFRASTRUCTURE

1. Facilities

During the DOE EPSCoR Phase I, substantial progress was made in developing computer infrastructure for use by Vermont Structural and Computational biologists. This included not only hardware resources but support for using existing Computational Biology/Informatics applications and for novel web application development. During Phase II substantial effort was made in developing the UVM Biodesktop which supports private management of data using a graphical folder tree interface to an object/relational database of biological sequences, structures, alignments, trees and enzyme kinetics data. It provides a bioinformatics platform that supports the efficient use of computational toolkits such as those distributed by the NCBI and the Bioperl project. The Biodesktop also provides for a variety of bioinformatics applications for microarray data analysis, sequence analysis and publication quality graphics.

In the UVM X-ray Facility, the Director, Dr. Mark Rould, and an X-ray technician were supported by DOE EPSCoR over the entire duration of the grant. Dr. Rould designed the X-ray Facility and was in charge of ensuring the equipment and related software was up to date. The technician trained users on how to use the x-ray equipment, the crystallization robot and the dynamic light scattering apparatus. The technician was also in charge of routine and emergency maintenance of the generator, detectors, and cryogenic system. A technician who provided support for the NMR equipment was also funded part-time.

2. Research Projects

Over the duration of the DOE EPSCoR initiative, twenty-eight pilot projects were funded (Appendix 4). These were competed state-wide, reviewed by appropriate scientific committees and recommended for funding to the Principal Investigator and the DOE EPSCoR Executive Board (Table 1). The projects focused on either Computational or Structural Biology and most had multiple PIs and were interdisciplinary in nature. Almost half of the projects included principal investigators from different departments. Four colleges were represented, the College of Medicine, the College of Mathematics and Engineering, the College of Arts and Sciences and the College of Agriculture and Life Sciences. Also one project had a principal investigator from another institution of higher learning in the State, St. Michael's College. As shown, these pilot projects generated numerous publications in superb journals and almost eleven million dollars in extramural funding, which represents about 17-fold return on investment.

Current Assessment of Computational Biology/Bioinformatics in the State of Vermont

The current state of computational biology/bioinformatics in Vermont has been heavily influenced by the DOE EPSCoR initiative. Successful applications to NASA for the Vermont Advanced Computing Center and to the NIH for the Vermont Genetics Network included substantial portions based directly on activities, infrastructure, and experience directly associated with DOE EPSCoR support. Both of these enterprises serve interests statewide. More recently, activities supported by both DOE EPSCoR funds and the Vermont Genetics Network will provide infrastructure for the proposed Vermont Clinical Health Information Exchange (VCHIX), part of the Center for Clinical and Tranlational Science, which will make clinical information from sources across the state available to researchers in a form that protects patient privacy. The DOE EPSCoR initiative worked seamlessly with developing interests, representing four colleges of UVM, in complex systems and evolutionary computation, and we feel that DOE funding played a role in the development of UVM's Complex Systems Center, a central part of the Spire of Excellence in Complex Systems Analysis and Engineering that is being built in the College of Engineering and Mathematical Sciences. Dr. Margaret Eppstein, a DOE EPSCoR initiative recruit, is co-director of the center and Dr. Richard Single, a second recruit, is a member. Three graduate student fellowships and four research projects were awarded to activities involving complex systems or evolutionary computing. More generally, we feel that financial support for *fifteen* faculty members with appointments in the College of Engineering or research programs in computational biology, in the form of pilot awards or graduate student fellowships, played an indirect role in development of the new PhD program in Computer Science.

Current Assessment of Structural Biology in the State of Vermont

The DOE-EPSCoR grant supported the fledging structural biology program when it needed it most, providing funds for running the X-ray facility as well as for graduate student fellowships and research projects. The success/legacy/impact of the DOE-EPSCoR grant is probably best exemplified by the sustained growth of the number of students and postdoctoral fellows in the structural biology laboratories. Fifteen students and postdocs are actively solving structures using X-ray crystallography. This year a critical mass of students was reached and Mark Rould taught for the first time a graduate level course on the subject of macromolecular crystallography. This course will be offered every other year. Structural biology students are also publishing in high impact journals and are invited to give talks at international conferences, such as the Cold Spring Harbor RNA Processing meeting. Moreover, this critical mass of investigators, postdoctoral fellows and graduate students has fostered the growth of extramural funding that supports the research efforts in structural biology.

Appendix 1

Awarded Grants Directly Resulting from Structural and Computational Biology Human Resources and Infrastructure

Awarded Grants Directly Resulting from Structural and Computational Biology Human Resources and Infrastructure

1. **U.S. Department of Agriculture-Hatch (Hoffmann, J.)**
   A Novel Approach for Developing and Evaluating PDE Models of the Spatial Spread of Invasive Species
   2000-2003
   $45,000

2. **R01 HL064891 (Everse, S)**
   NIH/NHLBI
   Structures of coagulation cofactors
   The major goal of this award is to solve the crystal structures of bovine and human factors V & Va.
   02/01/2000-04/30/2004
   $755,000

3. **UCSF P0313SC (Doublié, S.)**
   Pew Scholars Program
   Structural Studies of pre-mRNA Processing and Editing
   The aim of the project is to solve the crystal structures of factors involved in mRNA 3'-end processing and RNA editing.
   01/01/2000-06/30/2005
   $240,000

4. **PHS R01 GM62239/1-5 (Doublié, S.)**
   NIH/NIGMS
   Crystallographic Studies of Eukaryotic Poly(A) Polymerase
   The long term goal of this project is to understand the molecular mechanisms of eukaryotic mRNA polyadenylation
   12/18/2000-02/28/2008
   $1,312,316

5. **Lake Champlain Cancer Research Organization (Dostmann, W.)**
   Protein Transduction: Membrane translocation signals and their possible roles in cancer therapy
   8/30/2001 – 7/31/2002
   $ 10,000

6. **LCCRO 01 JWJ Scholar (Doublié, S., P.I.)**
   Vermont Cancer Center/LCCRO
   Structural Study of BRCA1-Associated BARD1 with CstF
   08/01/01-07/31/03
   $75,000

7. **R01 CA096536/1-3** (**Greenblatt, M**)
   NIH/NCI
   Computational and Laboratory Study of P16/INK4 Mutations
   09/01/2002-08/31/2005
   $738,420
8. **PHS R01 HL68991-01 (Dostmann, W.)**
   NIH
   Exploring vasomotor mechanism using new PKG inhibitors
   2002 – 2006
   $1,925,000

9. **R01 HL38113 (Trybus, K.)**
   NIH, NHLBI
   Myosin Motors and their Interaction with Actin
   One aim of this grant was to express and isolate a small oligomer of actin for crystallization studies.
   01/01/2002-06/30/2007
   $1,887,500

10. **R01 DK021739/20-24 (Mason, A.)**
    NIH/NIDDK
    Iron Delivery via Blood; Structural role of Transferrin
    The major goals of this project are to define the structure/function relationships of the blood transport protein transferrin.
    05/01/2002-06/30/2007
    $524,471

11. **VT-BO-01005 (Hoffmann, J.)**
    U.S. Department of Agriculture-Hatch
    Using Genetic Programming to Evolve Optimally Specified Process Models of Biological Systems
    2003-2007
    $35,000

12. **RG P22/2003 (Doublié, S., Izaurralde, E.)**
    Human Frontier Science Program
    A Molecular, Structural and Functional Analysis of RNP-Complexes Controlling Gene Expression
    The goal of this international collaborative project is to develop a systematic approach of investigating the biochemical composition, structure and function of large ribonucleoprotein (RNP) assemblies.
    07/01/2003-06/30/2007
    $262,500

13. **Vt. EPSCoR (Chu, K.)**
    Computation in biotechnology, materials science and astrophysics

2004
$20,000

14. R01 HL034575/20-24 (Mann, K.G.)
NIH/NHLBI
Primary structure of prothrombin
Studies will include evaluation of catalytic and binding functions and include contributions to the elucidation of the crystal structure of factor Va and its complexes.
01/01/2004-12/31/2008
$1,663,539

15. R01 GM070742 (Hondal, PI)
NIH-NIGMS
Selenium-Thioredoxin Reductase Studies by Semisynthesis
The major goals of this project are (i) make small molecule mimics of TR active site (ii) produce a semisynthetic TR (iii) characterize a cysteine-TR.
4/1/2004 – 3/13/2009
$750,000

16. R01 CA033657/23-27 (**Wallace, SS**)
NIH/NCI
Repair of DNA Damage by Ionizing Radiation
The overall goal of this research program since its inception is to elucidate, at the molecular level, the processing and consequences of free radical-induced DNA lesions which account for 70% of the DNA damages produced by ionizing radiation.
08/20/2004-07/31/2009
$2,211,389

17. P01 CA098993-01/05 (Wallace, S.S.)
NIH/NCI
Structure, Function, and Evolution of DNA Repair Enzymes
The purpose of this Program Project is to understand the function of DNA repair enzymes using computational, biochemical, and structural approaches.
Project: *Structural Basis of Substrate Specificity in BER enzymes* (PI: Doublié, S)
Project: *Structure & Function of Homologous Recombination Enzymes* (PI: Morrical, S)
09/03/2004-08/31/2009
$7,523,282 + $397,691 = $7,920,973

Project 1 (**Wallace, S)**: $1,492,006
Project 2 (**Doublié, S**): $1,290,047
Project 3 (**Morrical, S)**: $1,530,595
Project 4 (**Pederson, D)**: $ 397,691
Core A (**Bond, J**): $1,219,935

Core B (**Bond, J, Doublié, S, Morrical, S**): $1,613,159
Core C (**Wallace, S)**: $ 377,536

18. **P01 HL059408/6-10 (Warshaw, D.)**
    NIH, NHLBI
    Molecular Basis of Dilated & Hypertrophic Cardiomyopathy
    Project #2: "Effect of Cardiomyopathy Mutations on Myosin and Actin" (Trybus PI, Lowey Co-PI)
    This grant examines the structural effects of actin point mutations implicated in heart disease. Crystallography is one technique proposed to detect structural changes in actin.
    12/01/2004-11/30/2009
    Project 1 (**Trybus, K, Lowey, S**): $1,887,500

19. **Vermont Advanced Computing Center (Chu, K.)**
    Planning Grant: *Computation in the Physical Sciences and Mechanical Engineering*
    2005
    $5,000

20. **Vermont Advanced Computing Center (Eppstein, M.,** Co-PIs: Molofsky, Rizzo, Stevens, Goodnight, Hoffmann)
    Planning Grant: Focal research area in Biocomplexity
    9/1/2005-5/31/2006 (no cost extension through 5/31/07)
    $5,000

21. **CCF-0514819 (PI Wu, X.**; Co-PIs: Arslan, A.N. Zhu, X.)
    NSF
    Pattern Matching with Wildcards and Length Constraints
    7/15/2005 – 6/30/2008
    $200,000

22. **P20 RR016462/5-9** (**VanHouten, J**)
    NIH/NCRR
    Vermont Genetics Network – Vermont IMBRE
    07/01/2005-06/30/2010
    $16,624,372

23. **NSF – 0536773 (Chu, K)**
    NSF
    Undergraduate Labs for Biological Physics
    2006-2008
    $150,000

24. **2007-35206-17983** (**McFadden, T**)
    USDA CSREES

Unilateral frequent milking: a powerful model for identifying biological mechanisms involved in enhanced milk production efficiency
06/01/2007-05/31/2009
$282,594

25. **NSF EPSCoR** (Research Infrastructure Improvement program)**(VanHouten, J.)**
Core faculty include Eppstein
Complex Systems Thinking and Modeling for Ecosystem Analysis
8/15/2007-6/30/2010
$6,692,531

26. **PHS R01CA52040/14-17 (Wallace, S.S.)**
NIH/NCI
Processing of Damage by Translesion DNA Synthesis
The long-term goal of this grant proposal is to use a combination of structural and biochemical approaches to study processing of oxidative damage by translesion DNA synthesis.
08/29/2007-04/30/2011
$1,317,772

27. **1RO1 DE017474 (Ruiz, T.)**
Structure of oral bacterial adhesins
The major goals of this project are to solve the structure of oral bacterial adhesins from *S. parasanguis* and *A. Actinomycetemcomitans* by electron microscopy and image processing techniques.
3/1/2008 – 2/28/2013
$1,631,125

Appendix 2

CV

Abdullah Arslan

Margaret J. Eppstein

Robert J. Hondal

Richard Single

ABDULLAH N. ARSLAN

LEGAL STATUS Turkish Citizen, US Green-Card Holder

TITLE Assistant Professor

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EDUCATION

2002 Ph.D. Computer Science, University of California, Santa Barbara (UCSB)
Dissertation Title: *Algorithms for String Similarity with Constraints.*
Dissertation Committee: Omer Egecioglu (Chair), Oscar H. Ibarra, Teofilo F. Gonzalez, Ming Li, Peter Cappello

1996 M.S. Computer Science, University of North Texas (UNT), Denton, Texas

1990 B.S. Computer Engineering, Middle East Technical University, Ankara, Turkey

RESEARCH INTERESTS

Algorithms on strings, algorithms on graphs, similarity search problems, fractional programming, computational biology, bioinformatics

APPOINTMENTS

2002-present Assistant Professor (tenure-track). Department of Computer Science, University of Vermont (UVM)
Courses Taught: Advanced Topics in Theory of Computation: Computation and Approximation, Theory of Computation, Bioinformatics, Analysis of Algorithms, Operating Systems, Computer Organization

1996 – 2002 Department of Computer Science at UCSB
Research Assistant of Prof. Omer Egecioglu
Associate: Taught Theory of Computation in Spring 2001.
Teaching Assistant: Introduction to Programming (Fortran and Java as two separate courses), Introduction to C and Unix, Programming Methods, Introduction to Computer Systems, Foundations of Computer Science, Foundations of Scientific Computing, Theory of Computation

1994 – 96	Department of Computer Science at UNT Teaching Fellow: Taught Structured Programming in Fall 1995, and Program Development in Spring 1996. Teaching Assistant: Data Structures, Analysis of Computer Algorithms (Graduate level)
1991 – 94	Programmer in the Central Bank of Turkey: Participated in all phases of life cycles of several internal software projects. Administered database. Participated in research/survey on topics such as system disaster recovery techniques.

AWARDS AND HONORS

1994-2000	Selected after a nation-wide exam for all CS graduates in Turkey for full financial support of Turkish Ministry of Education for graduate study in computer science.
1985-1990	Financial support of Turkish Education Foundation for undergraduate study
1985	Ranked 1st in the city of Corum, 3rd in Black Sea Region in Nationwide University Entrance Exam in Turkey taken by approximately 600,000 students.
1985	In High School Level Regional Science Competitions sponsored by The Scientific and Technical Research Council of Turkey (TUBITAK): Individually: ranked 2nd in physics, and earned a special award in mathematics; member of the team ranked 1st in physics, 3rd in chemistry.
1983-85	High School Scholarship from TUBITAK

PUBLICATIONS

Book Chapters

BC2. **Arslan, A. N.** (2008) *Guided Sequence Alignment*. Encyclopedia of Data Warehousing and Mining - 2nd Edition, Edited by John Wang, Professor, Department of Management & Information Science, Montclair State University, scheduled for publication by Idea Group Reference in 2008 (a peer-reviewed chapter)

BC1. **Arslan, A. N.** and Egecioglu, O. (2007) *Chapter 76. Dynamic and fractional programming approximation algorithms for local alignment with constraints.* Handbook of Approximation Algorithms and Metaheuristics, Edited by: Teofilo F. Gonzalez, Chapman & Hall/CRC in the Computer & Information Science Series, Volume 13, ISBN: 9781584885504

Journal Papers

In the following list of journal publications impact factors are included whenever this information is available. Impact factors are typically about 1.00 or less for many top journals in theoretical computer science and algorithms.

J11. **Arslan, A. N.** (in press) An algorithm with linear expected running time for string editing with substitutions and substring reversals. *Information Processing Letters* (available online: DOI 10.1016/j.ipl.2007.11.017) (impact factor: 0532)

J10. **Arslan, A. N.** (2007) Regular expression constrained sequence alignment. *Journal of Discrete Algorithms,* Elsevier, 5(4), 647-661 (published online: http://dx.doi.org/10.1016/j.jda.2007.01.003) (a new journal by the publisher of *Journal of Algorithms*, which is a top journal in algorithms; the work in this paper has been cited in papers in Nucleic Acids Research, Information Processing Letters, and Discrete Applied Mathematics)

J9. He, D., **Arslan, A. N.**, and Ling, A. C. H. (2006) A fast algorithm for the constrained multiple sequence alignment problem. *Acta Cybernetica*, 17: 701-717 (a reputable international journal)

J8. Chen, G., Wu, X., Zhu, X., **Arslan, A. N.**, and He, Yu. (2006) Efficient string matching with wildcards and length constraints. *Knowledge and Information Systems,* 10(4):399-419 (available also online DOI: 10.1007/s10115-006-0016-8) (impact factor: 0.862; the paper reports results from an NSF-funded project in which I have been participating as a Co-PI)

J7. He, D and **Arslan, A. N.** (2005) A space-efficient algorithm for the pairwise sequence alignment algorithm. *Genome Informatics,* 16(2): pp. 237–246 (a known publication venue for current research in bioinformatics)

J6. **Arslan, A. N.** and Egecioglu, O. (2005) Algorithms for the constrained longest common subsequence problems. *International Journal of Foundations of Computer Science*, (16)6:1099-1111, December 2005 (impact factor: 0.5)

J5. **Arslan, A. N.** and Egecioglu, O. (2004) Dynamic programming based approximation algorithms for sequence alignment with constraints. *INFORMS Journal on Computing, Special issue on Computational Molecular Biology/Bioinformatics,* Vol. 16, No. 4, pp. 441-458, Fall 2004 (impact factor: 0.833)

J4. **Arslan, A. N.** and Egecioglu, O. (2004) Dictionary look-up within small edit distance. *International Journal of Foundations of Computer Science,* Vol. 15, No 1, pp. 57-71, February 2004 (impact factor: 0.5)

J3. **Arslan, A. N.** and Egecioglu, O. (2002) Approximation algorithms for local alignment with length constraints. *International Journal of Foundations of Computer Science* 13:751-567 (impact factor: 0.5)

J2. **Arslan, A. N.,** Egecioglu, O. and Pevzner, P.A. (2001) A new approach to sequence alignment. *Bioinformatics* 17:327-337 (impact factor: 4.894; the work in this paper has been cited so far in 56 articles in venues including many top journals and conferences in computational biology and bioinformatics, and computer science)

J1. **Arslan, A. N.** and Egecioglu, O. (2000) Efficient algorithms for normalized edit distance. *Journal of Discrete Algorithms* (Special Issue on Matching Patterns) 1:3-20 (the work in this paper has been cited so far in 17 articles in many top venues in computer science)

Refereed Conference Papers

All conference publications in this section are peer-reviewed papers.

C24. **Arslan, A. N.** (2007) Sequence alignment guided by common motifs described by context free grammars (accepted to the 4th Biotechnology and Bioinformatics Symposium (BIOT) 2007), October 19-20, Colorado Springs, CO (acceptance rate: 80%; the highest acceptance rate in this list; the conference received an unusually small number of very high quality submissions in 2007)

C23. **Arslan, A. N.** and Bizargity, P. (2007) Phylogeny by top down clustering using a given multiple alignment. *The Proceedings of the 7th IEEE Symposium on Bioinformatics and Biotechnology (BIBE 2007)*, Vol. II, pp. 809-814, Boston, Massachusetts, October 14-17, 2007 (acceptance rate: 13%, 65 regular-length papers were accepted from ~500 submissions)

C22. He, D., **Arslan, A. N.,** He, Y. and Wu, X. (2007) Iterative refinement of repeat sequence specification using constrained pattern matching. *The Proceedings of the 7th IEEE Symposium on Bioinformatics and Biotechnology (BIBE 2007)*, Vol. II, pp. 1199-1203, Boston, Massachusetts, October 14-17, 2007 (acceptance rate: 65 regular-length papers and a small number of short papers were accepted from ~500 submissions; this is a short paper; the paper reports results from an NSF-funded project in which I have been participating as a Co-PI; I have been the lead author and I have done all the technical writing in this paper)

C21. **Arslan, A. N.** (2007) A largest common d-dimensional subsequence of two d-dimensional strings. *The 16th International Symposium on Fundamentals of Computation Theory (FCT 2007)*, Budapest, Hungary, August 2007, Lecture Notes in Computer Science (LNCS) 4639, Erzsebet Csuhaj-Varju, Zoltan Esik (Eds.), Springer, pp. 40-51 (acceptance rate: 26%; 39 papers were accepted from 147 submissions; the website http://www.cs-conference-ranking.org/conferencerankings/topicsiv.html assigns for FCT 0.86 as the EIC value (Estimated Impact of Conference, which is normalized to be in the range 0.00-1.00 (the closer the number to 1.00, the better the conference))

C20. He, Y., Wu, X., Zhu, X. and **Arslan, A. N.** (2007) Mining Frequent Patterns with Wildcards from Biological Sequences. *Proc. of the IEEE International Conference on Information Reuse and Integration (IEEE IRI-07)*, pp. 329-334, Las Vegas, August 13-15, 2007 (acceptance rate: between 48% and 53%; the paper reports results from an NSF-funded project in which I have been participating as a Co-PI)

C19. **Arslan, A. N.** (2006) An algorithm with linear expected running time for string editing with substitutions and substring reversals. The Proceedings of the Biotechnology and Bioinformatics Symposium (BIOT-2006), pp. 90-96, Provo, Utah, October 20-21, 2006 (acceptance rate = 40%)

C18. **Arslan, A. N.** and He, D. (2006) An improved algorithm for the regular expression constrained multiple sequence alignment problem. The Proceedings of the 6th IEEE Symposium on Bioinformatics and Biotechnology (BIBE 2006), pp. 121-126, Washington, DC, October 16-18, 2006 (acceptance rate: 49%, 38 regular-length, and 10 short papers were accepted from 98 submissions; this is a short paper)

C17. **Arslan, A. N.** (2006) An algorithm for string edit distance allowing substring reversals. The Proceedings of the 6th IEEE Symposium on Bioinformatics and Biotechnology (BIBE 2006), pp. 220-226, Washington, DC, October 16-18, 2006 (acceptance rate: 39%, 38 papers were accepted from 98 submissions)

C16. He, D. and **Arslan, A. N.** (2006) FastPCMSA: An Improved Parallel Algorithm for the constrained multiple sequence alignment problem. FCS'06 - The 2006 International Conference on Foundations of Computer Science, pp. 88-94, Monte Carlo Resort, Las Vegas, Nevada, June 26-29, 2006 (acceptance rate = 38%; the website http://www.cs-conference-ranking.org/conferencerankings/topicsiv.html assigns for FCS 0.56 as the EIC value (Estimated Impact of Conference, which is normalized to be in the range 0.00-1.00 (the closer the number to 1.00, the better the conference))

C15. He, D. and **Arslan, A. N.** (2006) Space-efficient algorithms for the constrained multiple sequence alignment problem. BIOCOMP'06- The 2006 International Conference on Bioinformatics & Computational Biology, pp. 10-16, Monte Carlo Resort, Las Vegas, Nevada, June 26-29, 2006 (acceptance rate = 33%; the website http://www.cs-conference-ranking.org/conferencerankings/topicsiv.html assigns for BIOCOMP 0.62 as the EIC value (Estimated Impact of Conference, which is normalized to be in the range 0.00-1.00 (the closer the number to 1.00, the better the conference))

C14. He, D. and Arslan, A. N. (2006) A* algorithms for the constrained multiple sequence alignment problem. ICAI'06 - The 2006 International Conference on Artificial Intelligence, pp. 465-479, Las Vegas, Nevada, June 26-29, 2006. (acceptance rate = 46%)

C13. Zheleva, E. and **Arslan, A. N.** (2006) Fast motif search in protein sequence databases. International Computer Science Symposium in Russia (CSR 2006), *Lecture Notes in Computer Science 3967*, pp. 670-681, St.Petersburg, Russia, June 8-12, 2006 (acceptance rate = 30 / 159 = 19%)

C12. **Arslan, A. N.** (2006) Efficient approximate dictionary look-up for long words over small alphabets. *Lecture Notes in Computer Science 3887*, pp. 118-129, Latin American Theoretical Informatics LATIN'06, Valdivia, Chile, March 20-24, 2006 (acceptance rate = 66 / 224 = 29%)

C11. Singh, D. R. , **Arslan, A. N**, and Wu, X. (2006) Using an extended suffix tree to speed-up sequence alignment. *IADIS International Conference on Applied Computing*, pp. 655-660, San Sebastian, Spain, February 25-28, 2006 (acceptance rate: N/A)

C10. **Arslan, A. N.** (2005) Multiple sequence alignment containing a sequence of regular expressions, Proc. *IEEE Symposium on Computational Intelligence in Bioinformatics and Computational Biology (CIBCB'05)*, pp. 230-236, La Jolla, November 14-15, 2005 (acceptance rate: N/A)

C9. He, Dan and **Arslan, A. N.** (2005) A parallel algorithm for the constrained multiple sequence alignment problem, Proc. *IEEE the 5th Symposium on Bioinformatics and Biotechnology (BIBE'05)*, pp. 258-262, Minneapolis, Minnesota, October 19-21, 2005 (acceptance rate: 28%)

C8. **Arslan, A. N.** (2005) Regular expression constrained sequence alignment, *Lecture Notes in Computer Science* 3537, pp. 322-333, Combinatorial Pattern Matching (CPM), Jeju Island, Korea, June 19-22, 2005 (acceptance rate = 37 / 129 = 29%; the web-site http://cs.conference-ranking.net/Computer_Science_Conference_Ranking.html includes CPM in their short list of first-rank conferences)

C7. He, Dan and **Arslan, A. N.** (2005) A fast algorithm for the constrained multiple sequence problem. Proceedings. *11th International Conference on Automata and Formal Languages (AFL 2005)*, Zoltan Esik, Zoltan Fulop (Eds.) Institute of Informatics, University of Szeged, pp. 131-143, Dobogoko, Hungary, May 17-20, 2005 (acceptance rate: 40%)

C6. **Arslan, A. N.** and Egecioglu, O. (2004) Algorithms for the constrained longest common subsequence problems, Proceedings of the *Prague Stringology Conference 2004*, pp. 24-32, Edited by Milan Simanec and Jan Holub, Prague, Czech Republic, August 30-September 1, 2004 (acceptance rate: N/A)

C5. **Arslan, A. N.** and Egecioglu, O. (2002) Efficient computation of long similar subsequences. *Lecture Notes in Computer Science* 2476:77-90, String Processing and Information Retrieval, 9th International Symposium (SPIRE 2002), Lisbon, Portugal, September 11-13, 2002 (acceptance rate: N/A)

C4. **Arslan, A. N.** and Egecioglu, O. (2002) Dictionary look-up within small edit distance. *Lecture Notes in Computer Science* 2387:127-136, 8th Annual International Computing and Combinatorics Conference (COCOON), Singapore, August 15-17, 2002 (acceptance rate: N/A; the website http://www.cs-conference-ranking.org/conferencerankings/topicsiv.html assigns for COCOON 0.85 as the EIC value (Estimated Impact of Conference, which is normalized to be in the range 0.00-1.00 (the closer the number to 1.00, the better the conference))

C3. **Arslan, A. N.** and Egecioglu, O. (2001) An improved upper bound on the size of planar convex-hulls. *Lecture Notes in Computer Science* 2108:111-120, COCOON, Guilin, China, August 20-23, 2001 (acceptance rate: N/A; the website http://www.cs-conference-ranking.org/conferencerankings/topicsiv.html assigns for COCOON 0.85 as the EIC value (Estimated Impact of Conference, which is normalized to be in the range 0.00-1.00 (the closer the number to 1.00, the better the conference))

C2. **Arslan, A. N.** and Egecioglu, O. and Pevzner, P.A. (2001) A new approach to sequence alignment. *The Fifth Annual International Conference on Computational Molecular Biology (RECOMB 2001)*, pp. 2-11, Montreal, Canada,, April 22-25, 2001 (acceptance rate: N/A; the website http://www.cs-conference-ranking.org/conferencerankings/topicsiv.html assigns for RECOMB 0.99 as the EIC value (Estimated Impact of Conference, which is normalized to be in the range 0.00-1.00 (the closer the number to 1.00, the better the conference))

C1. **Arslan, A. N.** and Egecioglu, O. (1999) An efficient uniform-cost normalized edit distance algorithm. *IEEE Computer Society 6th International Symposium on String Processing and Information Retrieval (SPIRE 1999)*, pp. 8-15, Cancun, Mexico, September 22-24, 1999 (acceptance rate: N/A)

Other Selected Publications

O3. **Arslan, A. N.** (2004) Algorithmic methods in bioinformatics, Biyoinformatik-II (Bioinformatics Graduate Summer School II, Sile/Turkey), pp. 1-11, August,2004 (Editors: Azmi Telefoncu, Fikrettin Sahin, Ali Kilinc), ISBN=975-483-637-X

O2. **Arslan, A. N.** (2004) Sequence alignment, Biyoinformatik-II (Bioinformatics Graduate Summer School II, Sile/Turkey), pp. 101-114, August,2004 (Editors: Azmi Telefoncu, Fikrettin Sahin, Ali Kilinc), ISBN=975-483-637-X

O1. **Arslan, A. N.** (2002) Algorithms for string similarity with constraints. Ph.D. Thesis at University of California, Santa Barbara. Published by UMI, Ann Arbor.

Papers Under Review

Extended version of Conference Paper C12 with an additional coauthor Johannes Nowak (a PhD student in Germany) has been under review in *Pattern Recognition* since February 2007

Papers Currently Under Preparation for Submission to Journals

Extended versions of Conference Papers C21 and C17,

Extended version of Conference Paper C18 (with additional co-author Drew DeHaas, one of my former MS students)

PROJECTS

Funded Projects

AP1. Pattern Matching with Wildcards and Length Constraints

Sponsor: NSF, Award No. CCF-0514819
PI: Xindong Wu; Co-PIs: **Abdullah N. Arslan** and Xingquan Zhu
Duration: July 15, 2005 - June 30, 2008 ($200K)

The computational problem tackled in this project: in a given text, find maximal occurrences of a given pattern described as a sequence of letters, where between any two consecutive letters there is a pair that specifies minimum and maximum numbers of acceptable wildcards. A pattern can occur only in a given text within a window whose length is within a given range. No letter in the text can be used by more than one occurrence.

Contributions made:
At proposal preparation level: Explained difficulties of the problem in comparison with other well-known computational problems, found counter-examples for algorithms proposed by others, provided a graph-based formulation of the problem that requires finding maximal cliques, raised the question if the problem is NP-hard.
In research results to date: Co-authored and contributed in algorithm analyses in Journal Paper J8, Conference Papers C22 and C20. Took the lead in writing Conference Paper C22, where special cases of the pattern matching problem are solved in polynomial time.

MS THESES/PROJECTS SUPERVISED

MS3. DeHaas, Drew. (2007) Project: *Programs For Constrained Sequence Alignment* (Advisor: Arslan, A. N.)

MS2. Zheleva, Elena (2005) Thesis: *Restricted Regular Expression Pattern Matching Using Suffix Trees* (Advisor: Arslan, A. N.)

MS1. Singh, Divya R. (2005) Thesis: *Faster Sequence Alignment Using Suffix Tree and Data-Mining Techniques* (Advisor: Arslan, A. N., co-advisor: Wu, X.)

CURRENT STUDENT-SUPERVISION

MS Projects

Vicky W. Jambhore. Project: *Effcient Approximate Look-Up Problems*

Sirisha Punugu. Project: *Sequence Alignment Guided By Motifs Defined By Context-Free-Grammars*

Renu Sharma: *Sequence Alignment With Block Inversions*

Independent Readings & Research

Betsy George (MS student in the Department of Mathematics and Statistics)
Project: Complexity study and algorithm design for problems in Funded NSF Project AP1 in this CV

Kirsten Stor (PhD student in the Department of Mathematics and Statistics)
Project: Complexity study and algorithm design for problems in Funded NSF Project AP1 in this CV

TEACHING

At U. of North Texas taught Structured Programming in Fall 1995, and Program Development in Spring 1996

At U. of California at Santa Barbara taught Theory of Computation to a class of 57 in Spring 2001

At U. of Vermont taught courses shown in the following table (the numbers in this table are my ratings on Questions 6 of the evaluation form used at the CS Department of the U. of Vermont which asks the student to rate the overall performance of the instructor. These scores are between 0-5 with the following classification: 1:poor, 2:unsatisfactory, 3:satisfactory, 4:good, 5:excellent):

Course	Fall'02	Spring'03	Fall'03	Spring'04	Fall'04	Spring'05	Fall'05	Spring'06	Fall'06	Spring'07	My Average-Rating
CS 101 Computer Organization								2.92		5	3.96
CS 201 Operating Systems	3.93				3.45				3.94		3.77
CS 224 Analysis of Algorithms		3.47		3.80				3.96			3.74
CS 243 Theory of Computation			4.24				3.89				4.07
CS 231 Bioinformatics						4.75					4.75
CS 295 & CS 395 Computation and Approximation										5	5
CS 346 Advanced Theory of Computation						4.25					4.25

PROFESSIONAL ACTIVITIES

Service to the CS Department at UVM

Currently serving on the CS graduate admissions committee

Have served on the CS curriculum committee

Served as the library liaison for the CS department between Fall 2002-Fall 2005

Served as the webmaster for the CS department between 2002-2007

Prepared parts of the CS MS and PhD Comprehensive Exam course contents, guidelines, and sample exams for CS 201, Operating Systems, CS 224, Analysis of Algorithms, and CS 243, Theory of Computation

Prepared, proctored, and graded parts of all CS Comprehensive Exams to date since 2002

Service to my Profession

In October 2007, provided input for classifying publication venues (refereed journals and conferences) in computational biology and bioinformatics to aid the tenure and advancement review process in Brigham Young University (I was among the few external experts in this area chosen and contacted by the Computer Science Department Chair of Brigham Young University for this purpose)

Served/Currently Serving On:

Advisory Committee of the 4th Annual Biotechnology and Bioinformatics Symposium (BIOT 2007), Colorado Springs, CO, October 19-20, 2007

Program Committee of:

- IEEE Symposia on Computational Intelligence in Bioinformatics and Computational Biology (CIBCB):
  - CIBCB 2007, Honolulu, Hawaii, USA, April 1-5, 2007
  - CIBCB 2006, Toronto, Ontario, Canada, September 28-29, 2006
- International Symposia on Health Informatics and Bioinformatics (HIBIT):
  - HIBIT 2007, Belek, Atalya, Turkey, April 30 – May 2, 2007
  - HIBIT 2005, Belek, Antalya, Turkey, 10-12 November 2005
- The IEEE International Conference on Bioinformatics and Biomedicine (BIBM 2007), Silicon Valley, California, USA, Nov. 2-4, 2007

On the Reviewer Committee of HIBIT 2008, Istanbul, Turkey, 18-20 May, 2008

On the **permanent Steering Committee** of Biotechnology and Bioinformatics Symposium (BIOT)

Inivited lecturer: Bioinformatics Graduate Summer School (August 15-21, 2004, Sile/Turkey) (http://sci.ege.edu.tr/~biyoinformatik2/eng/ogruyeleri.htm) organized by Ege University, Yeditepe University of Turkey, and Berlin Technical University of Germany. Attended by undergraduate, graduate students, researchers, and faculty members from various disciplines, and from multiple countries including Turkey, Germany, England, and Hungary

Reviewed for journals: IEEE Transactions on Pattern Analysis and Machine Intelligence (TPAMI), IEEE/ACM Transactions on Computational Biology and Bioinformatics (TCBBSI), Knowledge and Information Systems (KAIS): An International Journal, Journal of Mathematical Biology (JMB), Bioinformatics, Theoretical Computer Science (TCS), IEEE Transactions on Knowledge Engineering (TKDE), Information Processing Letters (IPL), Pattern Recognition (PR), Information Sciences (INS), Information and Computation

Reviewed for Conferences: Combinatorial Pattern Matching Symposium (CPM), Research in Computational Molecular Biology (RECOMB), International Conference on Implementation and Application of Automata (CIAA), International Conference on Parallel and Distributed Computing Systems (PDCS), and Symposium on Health Informatics and Bioinformatics Health (HIBIT), IEEE Symposium on Computational Intelligence in Bioinformatics and Computational Biology (CIBCB), IEEE International Conference on Bioinformatics and Biomedicine (BIBM), Bioinformatics and Biotechnology Symposium (BIOT)

SOFTWARE DEVELOPED

Several applications for internal use by Turkish Central Bank such as accounting and payroll. Each developed by a team of 3 to 15. Multi-user, time-sharing environment. Number of users from 5 to 200

SSS Authoring Tool: Senior project completed during undergraduate study. Spent two years (1989-90) to design and implement an authoring tool with a classmate. The tool included a text editor, a graphics editor, and an interpreter for a language we designed. Using the tool, one could either record the history of actions such as sequence of events (e.g., drawings, new positions of objects moved, prompts for user's answers, etc.), and generate a code which the user could edit or execute later, or allow the experienced user to directly write programs in the language. Several courses at middle and high school level were prepared by this tool as a pilot project for the Turkish Ministry of Education by the company Yumak Bilgisayar

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Table of Contents

Education

B.S. in Zoology, with High Honor
Honors College, Michigan State University, 1978.

Graduate Study in Zoology
University of Washington, 1980-81.
University of Vermont, 1981-82.

M.S. in Computer Science
University of Vermont, 1983.

Ph.D. in Civil & Environmental Engineering
Dissertation: "Efficient Data Inversion for Large Multi-Dimensional Problems Using an Approximate Extended Kalman Filter with Data Driven Zonation"
Advisor: Dr. David E. Dougherty
University of Vermont, 1997.

Continuing Education

- New England Complex Systems Institute Summer School (5-day): Complex Physical, Biological and Social Systems, MIT, Cambridge, MA, June 2005.
- New England Complex Systems Institute Summer School (5-day): Modeling, Networks and Evolution of Complex Systems, MIT, Cambridge, MA, June 2005.
- New Directions in Bioinformatics and Biotechnology Workshop, Chautauqua Short Course #65 (3-day), RPI, July 2002.
- NPACI Parallel Computing Workshop (1-day), San Diege Supercomputer Center, San Diego, CA. January, 2002
- Inter-Institute Workshop on In Vivo Optical Imaging at NIH (2-day), October, 1999.
- Parallel Virtual Machine Workshop (1-day) at the 6th SIAM Conference on Parallel Processing for Scientific Computing, Norfolk, VA, March, 1993.
- Follow-up Parallel Processing Workshop (4-day), Colgate University, Hamilton, NY. 1992.
- Parallel Processing for Undergraduate Educators (2-week), Colgate University, Hamilton, NY. 1991.
- Workshop for the Foundations of Artificial Intelligence (2-day), New Mexico State University, Las Cruces, NM. 1986.

Awards and Honors

- Best Student Paper Award (my graduate student is 1st author, I am 2nd author), IEEE Symposium on Artificial Life, 2007.
- The American Association of Physicists in Medicine Sylvia Sorkin Greenfield Award for the best paper (other than radiation dosimetry) published in Medical Physics in 2004.
- Outstanding Student Paper Award, American Geophysical Union, Fall 1996.
- American Association of University Women Career Development Award, 1993.
- Finalist for the U.V.M. Kroepsch-Maurice Teaching Award, 1992.
- U.V.M. graduate student travel mini-grants, 1982 and 1994.
- National Science Foundation 3-year graduate fellowship, 1980-1983.
- Initiated as Member, Upsilon Pi Epsilon, Computer Science Honor Society, 1983.
- Member, Michigan State University Honor's College, 1974-1979
- Initiated as Member Phi Kappa Phi Honor Society, 1978.

Professional Positions

(in reverse chronological order)

- 2002-present **Assistant Professor (*Primary Appointment*),** Department of Computer Science, University of Vermont, Burlington, Vermont.
- 2006-present **founding co-Director**, Complex Systems Center at the University of Vermont. College of Engineering and Mathematical Sciences, University of Vermont, Burlington, Vermont.
- 2006-present **Adjunct Member**, Computational Genetics Laboratory, Dartmouth College, Lebanon, NH.
- 2005-present **Assistant Professor (*Secondary Appointment*)**, Department of Biology, University of Vermont, Burlington, VT.
- 2001-2003 **Adjunct Assistant Professor**, Department of Chemical Engineering, Texas A&M University, College Station, TX.
- 2001-present **Member**, Vermont Cancer Center.
- 1997-2002 **Research Assistant Professor (*Primary Appointment 1998-2002*)**, Department of Computer Science, University of Vermont, Burlington, VT.
- 1998-2003 **Research Assistant Professor (*Secondary Appointment*)**, Department of Civil & Environmental Engineering, University of Vermont, Burlington, VT.

- 1983-2001 **Lecturer (*Primary Appointment 1983-1998*)**, Department of Computer Science, University of Vermont, Burlington, VT.
- 1993-1997 **Graduate Research Assistant**, Department of Civil & Environmental Engineering, University of Vermont, Burlington, VT.
- 1990 **Consultant**, Digital Equipment Corporation, S. Burlington, VT.
- 1987-1988 **Bioinformatics Software Engineer,** International Biotechnologies, Inc., New Haven, CT (telecommuted).
- 1986 **System Graphics Software Engineer**, Vermont Microsystems, Inc., Winooski, VT.
- 1986 **Consultant**, Computing Research Laboratory, New Mexico State University, Las Cruces, NM.
- 1982 **Graduate Teaching Assistant**, Department of Computer Science, University of Vermont, Burlington, VT.
- 1982 **Programmer**, Academic Computing Center, University of Vermont, Burlington, VT.
- 1981-1982 **Graduate Teaching Assistant**, Department of Zoology, University of Vermont, Burlington, VT.
- 1979-1980 **Research Associate**, Department of Zoology, Michigan State University, E. Lansing, MI.
- 1977 **Undergraduate Teaching Assistant**, Department of Mathematics, Michigan State University, E. Lansing, MI.
- 1975-1979 **Archaeologist** for various institutions, including the Department of Anthropology at Michigan State University, the Tennessee Valley Authority, the State of Tennessee, and the U.S. Army Corps of Engineers.

Research

Research Interests

In keeping with my interdisciplinary educational background in biology, computer science, and environmental engineering, my research interests involve computational forward and inverse modeling and analysis of biological and environmental problems. Most of my research has focused on developing novel computational methods for large-scale, nonlinear, multi-scale tomographic inverse image reconstruction problems in subsurface hydrology, geophysics, and deep-tissue near-infrared fluorescence imaging. However, in the past couple of years I have shifted my research towards modeling and analysis of complex adaptive systems in a variety of biological and environmental systems. This **deliberate recent shift in research direction** is supported by the College, as we are seeking to develop a Spire of Excellence in Complex Systems. Current projects include developing, studying, and using novel evolutionary and agent-based computational approaches for a wide range of important problems, including plant species' invasiveness in ecological communities, biological speciation, the impact of spatial topologies on information flow through complex interaction networks, identifying nonlinear interactions between single nucleotide polymorphisms that predispose for complex disease traits, and agent-based integrated assessment modeling of transportation energy alternatives.

Publications

Refereed Journal Publications

Number of "non-self" citations shown do not include any citations in articles co-authored by any of the co-authors, according to the ISI Citation Index, for a total of 273 non-self citations, as of 10 Aug 2007.

In review:

1. Payne, J.L. and **Eppstein, M.J.** "Modeling Takeover Dynamics with Pair Approximations in Regular Population Structures", *Evolutionary Computation (in review).*

Published or accepted:

1. **Eppstein, M.J.,** Payne, J.L., White, B.C., and Moore. J.H. "Genomic mining for complex disease traits with 'Random Chemistry'", *Genetic Programming and Evolvable Machines (special issue on Medical Applications),* 8:395-411, 2007. (DOI 10.1007/s10710-007-9039-5).
2. Zhu, B., **Eppstein, M.J**., Sevick-Muraca, E.M., and Godavarty, A. "Noise pre-filtering techniques in fluorescence-enhanced optical tomography", *Optics Express,* **15**(18):11285-11300, 2007.
3. **Eppstein, M.J**. and Molofsky, J. "Invasiveness in plant communities with feedbacks". *Ecology Letters*, **10**:253-263, 2007.
4. **Eppstein, M.J.**, Bever, J.D., and Molofsky, J., "Spatio-temporal community dynamics induced by frequency dependent interactions", *Ecological Modelling*, **197**:133-147, 2006. (1 non-self citation)
5. Fedele, F., **Eppstein, M.J**., Laible, J.P., Godavarty, A., and Sevick-Muraca, E.M., "Fluorescence Photon Migration by the Boundary Element Method", *J. Computational Physics,* **210**(1):109-132, 2005. (1 non-self citations)
6. Godavarty, A., Sevick-Muraca, E.M., and **Eppstein, M.J.** "Three-dimensional fluorescence lifetime tomography", *Medical Physics,* **32**(4): 992-1000, 2005. (12 non-self citations)
7. Godavarty, A., **Eppstein, M.J.**, Zhang, C., and Sevick-Muraca, E.M., "Detection of single and multiple targets in tissue phantoms using fluorescence-enhanced optical imaging", *Radiology*, **235**: 148-154, 2005. (10 non-self citations)
8. Godavarty, A., Thompson, A.B., Roy, R., Gurfinkel, M., **Eppstein, M.J.,** Zhang, C., and Sevick-Muraca, E.M., "Diagnostic imaging of breast cancer using fluorescence-enhanced optical tomography: phantom studies," *J. Biomed. Opics*.: Special edition on Biomedical Optics and Women's Health **9**:488-496, 2004. (12 non-self citations)
9. Godavarty, A., Zhang, C., **Eppstein, M.J.,** and Sevick-Muraca, E.M., "Fluorescence-enhanced optical imaging of large phantoms using single and simultaneous dual point illumination geometries", *Medical Physics* **31**(2):183-190, 2004. (Awarded the American Association of Physicists in Medicine Sylvia Sorkin Greenfield Award for the best paper published in Medical Physics in 2004) (1 non-self citations)
10. **Eppstein, M.J**., Fedele, F., Laible, J.P., Zhang, C., Godavarty, A., and Sevick-Muraca, E.M., "A comparison of exact and approximate adjoint sensitivities in fluorescence tomography", *IEEE Transactions on Medical Imaging,* **22**(10):1215-1223*, 2003.* (3 non-self citations)

11. Godavarty, A., **Eppstein, M.J.,** Zhang, C., Thompson, A.B., Gurfinkel, M., Theru, S., and Sevick-Muraca, E.M., "Fluorescence-enhanced optical imaging in large tissue volumes using a gain modulated ICCD camera, *Physics in Medicine and Biology,* **48**:1701-1720, 2003. (20 non-self citations)
12. Fedele, F. Laible, J. P., and **Eppstein, M.J.**, "Coupled complex adjoint sensitivities for frequency-domain fluorescence tomography: theory and vectorized implementation", *J Computational Physics,* **187**(2):597-619*,* 2003*.* (3 non-self citations)
13. Godavarty, A., Hawrysz, D.J., Roy, R., Sevick-Muraca, E.M., and **Eppstein, M.J., "**The influence of the refractive index-mismatch at the boundaries measured in fluorescence-enhanced frequency-domain photon migration imaging", *Optics Express,* **10**(15):653:662, 2002. (4 non-self citations)
14. **Eppstein, M.J.,** Hawrysz, D.J., Godavarty, A., and Sevick-Muraca, E.M., "Three-dimensional, Bayesian image reconstruction from sparse and noisy data sets: Near-infrared fluorescence tomography", *Proc. Natl. Acad. Sci. USA,* **99**(15):9619-9624, 2002. (32 non-self citations)
15. Hawrysz, D.J., **Eppstein, M.J.,** Lee, J., and Sevick-Muraca, E.M., "Contrast Enhanced Three Dimensional Optical Tomography", *Optics Letters,* **26**(10):704-706, 2001. (5 non-self citations)
16. **Eppstein, M.J.**, Dougherty, D.E., Hawrysz, D.J., Sevick-Muraca, E.M., "3-D Bayesian optical image reconstruction with domain decomposition", *IEEE Transactions on Medical Imaging,* **20**(3):147-163, 2001. (18 non-self citations)
17. **Eppstein, M.J.,** Dougherty, D.E., Troy, T.L, and Sevick-Muraca, E.M., "Biomedical optical tomography using dynamic parameterization and Bayesian conditioning on photon migration measurements", *Applied Optics*, **38**:2138-2150, 1999 (cover article). (22 non-self citations)
18. **Eppstein, M.J.** and Dougherty, D.E., "Efficient 3-D data inversion: Soil characterization and moisture monitoring from crosswell GPR at a Vermont test site", *Water Resources Research*, **34**(8):1889-1900, 1998. (28 non-self citations)
19. **Eppstein, M.J.** and Dougherty, D.E., "Optimal 3-D traveltime tomography", *Geophysics*, **63**(3):1053-1061, 1998. (9 non-self citations)
20. **Eppstein, M.J.** and Dougherty, D.E., "Simultaneous estimation of transmissivity values and zonation", *Water Resources Research,* **32**(11):3321-3336, 1996. (18 non-self citations)

21. **Eppstein, M.J.** and Dougherty, D.E., "A comparative study of PVM workstation cluster implementations of a two-phase subsurface flow model", *Adv. In Water Resources,* **17**:181-195, 1994. (3 non-self citations)
22. Heinrich, B. and **Heinrich (née Eppstein), M.J.E.,** "The pit-trapping foraging strategy of the ant lion, *Myrmeleon immaculatus*", *Behav. Ecol. and Sociobiol.,* **14**:151-160, 1984. (31 non-self citations)
23. Heinrich, B. and **Heinrich (née Eppstein), M.J.E.,** "Size and caste in temperature regulation by bumblebees", *Phys. Zool.*, **56:**552-562, 1983. (21 non-self citations)
24. Heinrich, B. and **Heinrich (née Eppstein), M.J.E.,** "Torpor in foraging workers and drones of the bumblebee *Bombus terricola*", *Phys. Zool.*, **56**: 563-567, 1983. (19 non-self citations)

Published Refereed Conference Proceedings

1. Payne, J.L, and **Eppstein, M.J.** "Using Pair Approximations to Predict Takeover Dynamics in Spatially Structured Populations", *Genetic and Evolutionary Computation Conference (GECCO),* late-breaking papers pp. 2557-2563*,* 2007.
2. Payne, J.L. and **Eppstein, M.J.**, "Takeover Times on Scale-Free Topologies", *Genetic and Evolutionary Computation Conference (GECCO),* pp. 308-315, 2007.
3. Payne, J.L., **Eppstein, M.J.**, and Goodnight, C.J. "Sensitivity of Self-Organized Speciation to Long Distance Dispersal", *Proceedings of the 2007 IEEE Symposium on Artificial Life (Alife'07)*, pp. 1-7, 2007 (best student paper award).
4. **Eppstein, M.J.,** Payne, J.L., White, B.C., and Moore. J.H., "Hill-climbing through 'random chemistry' for detecting epistasis", *Genetic and Evolutionary Computation Conference (GECCO), late-breaking papers, 2006.*
5. **Eppstein, M.J**., Payne, J.L, and Goodnight, C.J. "Speciation by Self-Organizing Barriers to Gene Flow in Simulated Populations with Localized Mating", *Workshop Proceedings for Genetic and Evolutionary Computation Conference (GECCO), 2006.*
6. J.L. Payne and **M.J. Eppstein**, "Emergent Mating Topologies in Spatially Structured Genetic Algorithms", *Proceedings of Genetic and Evolutionary Computation Conference (GECCO) 2006, pp. 207-214.*
7. J.L. Payne and **M.J. Eppstein**, "A Hybrid Genetic Algorithm with Pattern Search for finding Heavy Atoms in Protein Crystals", *Genetic and Evolutionary Computation Conference (GECCO) 2005*, Part 1, Eds. H-G Bayer *et al*., pp. 377-384, 2005. (nominated for a best-paper award).

8. Godavarty, A., **Eppstein, M.J.**, Zhang, C., and Sevick-Muraca, E.M., "Fluorescence-enhanced optical tomography on large phantoms using dual point illumination geometry", *OSA Biomedical Topical Meetings*, OSA Technical Digest, Optical Society of America, Washington, DC, April, 2004.
9. Godavarty, A., **Eppstein, M.J.**, and Sevick-Muraca, E.M., "Fluorescence-enhanced optical tomography: Absorption and lifetime contrast studies", *OSA Biomedical Topical Meetings*, OSA Technical Digest, Optical Society of America, Washington, DC, April, 2004.
10. Fedele, F., Laible, J.P., and **Eppstein, M.J**., "Boundary Element Solution of the Coupled Fluorescence Diffusion Equations", *OSA Biomedical Topical Meetings*, OSA Technical Digest, Optical Society of America, Washington, DC, April, 2004.
11. Gilbert, J., and **Eppstein, M.J.,** "Codons in Evolutionary Computation", *Genetic and Evolutionary Computation Conference (GECCO) 2003*, Part 1, Eds. E. Cantu-Paz *et al*., *Lecture Notes in Computer Science*, **2723**:967-978, 2003.
12. **Eppstein, M.J.,** Zhang, C., Godavarty, A., and Sevick-Muraca, E.M.,"Advances in 3-D frequency domain fluorescence tomography", *Proc SPIE* **4955**:211-218*,* 2003.
13. Zhang, C., **Eppstein, M.J.**, Godavarty, A., and Sevick-Muraca, E.M., "A hybrid approach to Bayesian image reconstruction", *SPIE* 2003 *ProcSPIE* **4955**:591-599*,* 2003.
14. **Eppstein, M.J.,** and Laible, J.P., "The benefits of vectorization in optical tomography", *Proc SPIE* **4955**:59-69*,* 2003.
15. Godavarty, A., Sevick-Muraca, E.M., **Eppstein, M.J.**, Zhang, C., "Fluorescence-enhanced tomographic imaging in large phantoms using gain-modulated ICCD camera", *SPIE* **4949**:433-443*,* 2003.
16. **Eppstein, M.J.**, Hawrysz, D.J., Godavarty, A., and Sevick-Muraca, E.M., “Experimental Frequency Domain Fluorescence Tomography”, *OSA Biomedical Topical Meetings*, OSA Technical Digest, Optical Society of America, Washington, DC, pp. 510-512, April, 2002.
17. Godavarty, A.., Sevick-Muraca, E.M., and **Eppstein, M.J.**, “Minimizing mismatch of forward model and experimental measurements for fluorescence-enhanced optical imaging”, *OSA Biomedical Topical Meetings*, OSA Technical Digest, Optical Society of America, Washington, DC, pp. 516-518, April, 2002.
18. Joshi, A.., Sevick-Muraca, E.M., and **Eppstein, M.J**., “A Method to Determine the Optimal Number of Measurements for Three-Dimensional Optical Tomography for a Physiologically Realistic Geometry”, *OSA Biomedical Topical Meetings*, OSA Technical Digest, Optical Society of America, Washington, DC, pp. 128-130, April, 2002.

19. Fedele, F., Laible, J.P., and **Eppstein, M.J.**, "Generalized Adjoint Sensitivities of the Coupled Frequency Domain Fluorescence Diffusion Equations", *OSA Biomedical Topical Meetings*, OSA Technical Digest, Optical Society of America, Washington, DC, pp. 371-373, April, 2002.
20. Hawrysz, D.J., **Eppstein, M.J.,** and E.M. Sevick-Muraca, "Measurement and Model Error Assessment of a Single Pixel, Frequency Domain Photon Migration Apparatus and Diffusion Model for Imaging Applications." European Biomedical Optics and Spectroscopy Conference, Amsterdam, 2000.
21. **Eppstein, M.J.** and Rizzo, D.M., "Rapid 3-D Bayesian site characterization: A tandem strategy", *Proceedings of the XIII International Conference on Computational Methods in Water Resources,* L.R. Bentley, J.F. Sykes, C.A. Brebbia, W.G. Gray, and G.F. Pinder, eds., Vol 1: Computational Methods for Subsurface Flow and Transport, Balkema, Rotterdam, The Netherlands, pp. 491-494, 2000.
22. **Eppstein, M.J.**, "Three-dimensional fluorescence absorption imaging with domain decomposition", *in Biomedical Topical Meetings, OSA Technical Digest,* Optical Society of America, Washington, DC, pp. 173-176, 2000.
23. **Eppstein, M.J**., Dougherty, D.E., Hawrysz, D.J., and Sevick-Muraca, E.M., "Three-dimensional optical tomography", *Optical Tomography and Spectroscopy of Tissue III,*Chance, B., Alfano, R.R., and Tromberg, B.J., eds., *SPIE Proceedings,* **3597**:97-105, 1999.
24. **Eppstein, M.J.,** Dougherty, D.E., Troy, T.L., and Sevick-Muraca, E.M., "Stochastic optical tomography using beta-distributed parameters to model absorption, lifetime, and quantum efficiency", *Biomedical Imaging: Reporters, Dyes, and Instrumentation,* Bornhop, D.J., Contag, C.H., and E.M. Sevick-Muraca, *SPIE Proceedings*, **3600**:230-236, 1999.
25. **Eppstein, M.J.** and Dougherty, D.E., "3-D computed subsurface tomography", *Proceedings of the XII International Conference on Computational Methods in Water Resources"*, Vol. **2**, pp. 329-336, 1998.
26. **Eppstein, M.J.** and Dougherty, D.E., "Optimal 3-D geophysical tomography", *Proceedings of the Symposium on the Application of Geophysics to Environmental and Engineering Problems (SAGEEP)*, pp. 249-256, 1998.
27. **Eppstein, M.J.** and Laible, J.P., "A practical parallel retrofit of a 3-Dimensional surface water model", *Proceedings of the 2nd International Conference on Computer Modeling of Seas and Coastal Regions: COASTAL 95*, Cancun, Mexico, September, 1995.

28. **Eppstein, M.J.** and Dougherty, D.E., "Parameter estimation with data-driven zonation", *Proc. of the 10th International Conference on Computational Methods in Water Resources*, Vol. 1, pp. 727-734, Heidelberg, Germany, June, 1994.
29. **Eppstein, M.J.,** Guarnaccia, J.F., and Dougherty, D.E., "Parallel groundwater computations using PVM", *Proc. of the 9th International Conference on Computational Methods in Water Resources,* Vol. 1, pp. 713-720, Denver, CO, 1992.

Other Conference Presentations, Papers, and Published Abstracts

1. Payne, J.L. and **Eppstein, M.J.**, "Why your mates shouldn't date", poster and published extended abstract accepted for *Genetic and Evolutionary Computation Conference (GECCO),* 2007.
2. DeHaas, D., Craig, J., Rickert, C., Haake, P., Stor, K., **Eppstein, M.J.** "Feature Selection and Classification in Noisy Epistatic Problems using a Hybrid Evolutionary Approach", poster and published extended abstract accepted for *Genetic and Evolutionary Computation Conference (GECCO),* 2007.
3. **Eppstein, M.J.** and Molofsky, J. Predicting invasion vs. naturalization in plant communities. Poster presentation at the *2007 Annual meeting of the Weed Science Society of America (WSSA)*, San Antonio, TX, Feb 2007.
4. Molofsky, J. and **M. J. Eppstein**. Naturalization versus invasion in plant communities. *91st Ecological Society of America annual meeting.* Memphis, TN August 2006
5. **Eppstein, M.J.**, Payne, J.L., White, B.C., and Moore, J.H. "A "Random Chemistry" Algorithm for Detecting Epistatic Genetic Interactions", International Conference on Complex Systems (ICCS), Boston, MA, June, 2006.
6. **Eppstein, M.J**., Payne, J.L, and Goodnight, C.J. "Speciation by Self-Organizing Barriers to Gene Flow in Simulated Populations with Localized Mating", poster presentation at *Evolution 2006*; Joint National Meetings of the Society for the Study of Evolution (SSE), the Society of Systematic Biologists (SSB), and the American Society of Naturalists (ASN) June 23-27, 2006.
7. **Eppstein, M.J.** and J. Molofsky. Modeling non-competitive and competitive ecological interactions: Implications for coexistence, invasion, and the importance of spatial scale of interactions, abstract published and talk presentated at *90th Ecological Society of America annual meeting*, Montreal, August, 2005.

8. **Eppstein, M.J.** and Hoffmann, J.P. Crystallographic Case Study in an Interdisciplinary Evolutionary Computation Course, presented in the Evolutionary Computation in Practice Track, *Proc. GECCO*, (2005).
9. **Eppstein, M.J.**, Payne, J.L., F. Fedele, Laible, J.P., Godavarty, A., and E.M. Sevick-Muraca, "Validation of the Boundary Element Method for Fluorescence Photon Migration", Fourth Inter-Institute Workshop on Optical Diagnostic Imaging from Bench to Bedside, National Institutes of Health, Bethesda, MD, Sept., 2004.
10. Godavarty, A., **Eppstein, M.J.**, and E.M. Sevick-Muraca, "Three-dimensional fluorescence-enhanced absorption and lifetime tomography",Fourth Inter-Institute Workshop on Optical Diagnostic Imaging from Bench to Bedside, National Institutes of Health, Bethesda, MD, Sept., 2004.
11. Laible, J.P., Fedele, F., and **Eppstein, M.J.**, "A boundary element approach to optical and fluorescence tomography", *SPIE 4955-33,* 2003.
12. **Eppstein, M.J.**, Godavarty, A., Zhang, J., Laible, J., and Sevick-Muraca, E.M.,"3-D Fluorescence Tomography for Breast Imaging", 17th Vermont Cancer Center Cancer Research Symposium: Cancer in a Post-Genomic Era, Burlington, VT, Oct, 2002.
13. May, S.T., **Eppstein, M.J.**, Tang, M.E., and Yandell, D.W., "The human retinoblastoma gene mutation spectrum: Analyses of 240 independent mutations." Presented at the 17th Vermont Cancer Center Cancer Research Symposium: Cancer in a Post-Genomic Era, Burlington, VT, Oct, 2002 and the American Society of Human Genetics, Baltimore, MD, October, 2002.
14. **Eppstein, M.J.**, Godavarty, A., Zhang, J., Laible, J., and Sevick-Muraca, E.M., "Three-dimensional Bayesian tomography using sparse fluorescence frequency domain photon migration measurements on clinically relevant phantom volumes", Third Inter-Institute Workshop on Diagnostic Optical Imaging and Spectroscopy: The Clinical Adventure, National Institutes of Health, Bethesda, MD, Sept., 2002.
15. Godavarty, A, Roy, R., Hawrysz, D., Sevick-Muraca, E.M., and **Eppstein, M.J.,** "Accuracy of 3D forward solvers and precision of frequency domain photon migration measurements for fluorescence enhanced optical imaging", United Engineering Foundation conference on Advances in Optics for Biotechnology, Medicine, and Surgery, Banff, Canada, July, 2001.
16. Hawrysz, D.J., **Eppstein, M.J.,** and E.M. Sevick-Muraca, "Deterministic errors in frequency domain, photon migration imaging", *SPIE*, **4250**, 2001.

17. Hawrysz, D.J., **Eppstein, M.J.**, Lee, J., Roy, R., and E.M. Sevick-Muraca, "Three-dimensional optical imaging using frequency domain photon migration", 10th Inverse Problems in Engineering Seminar, June 2000.
18. Hawrysz, D.J., **Eppstein, M.J.**, and E.M. Sevick-Muraca, "Bayesian approach to the inverse problem in biomedical imaging by photon migration", American Institute of Chemical Engineers Annual Meeting, October, 1999.
19. **Eppstein, M.J.,** Dougherty, D.E., Hawrysz, D.J., and Sevick-Muraca, E.M., "Rapid Bayesian 3-d Biomedical Optical Imaging", Inter-Institute Workshop in *In Vivo* Optical Imaging at the NIH, National Institutes of Health, Bethesda, MD, September, 1999.
20. Hawrysz, D.J., **Eppstein, M.J.**, and E.M. Sevick-Muraca, "Optical Imaging with a Bayesian Inversion Technique using Frequency Domain Photon Migration Measurements", Advances in Optics for Biotechnology, Medecine, and Surgery: United Engineering Foundation Conferences, August, 1999.
21. **Eppstein, M.J.,** Dougherty, D.E., Hawrysz, D.J., and Sevick-Muraca, E.M., "Three-dimensional optical tomography using APPRIZE", Conference on Lasers and Electro-Optics, Germany, June, 1999.
22. **Eppstein, M.J.,** Dougherty, D.E., and Sevick-Muraca, E.M., "Spectroscopic and imaging reconstructions in near infrared optical tomography", VT EPSCoR Annual Conference on Science and Technology, UVM, October, 1998.
23. Rizzo, D.M., Yu, M., and **Eppstein, M.J.,** "Distributed parameter estimation using three inverse methods", VT EPSCoR Annual Conference on Science and Technology, UVM, October, 1998.
24. **Eppstein, M.J.** and Dougherty, D.E., "Efficient three-dimensional parameter estimation using cross-hole seismic and hydrologic data", American Geophysical Union Fall Meeting, December, 1996. (awarded an Outstanding Student Paper Award)
25. **Heinrich (née Eppstein), M.J.E.** and Heinrich, B., "Pit-trapping as an optimal foraging strategy by ant lions", *Amer. Zool.,* **21**(4):995, 1981.

Patents

1. **Eppstein, M.J.** and Dougherty, D.E., "*Three-dimensional stochastic tomography with upscaling*", U.S. Patent #6,067,340, 2000.

Invited Talks

1. "*Predicting naturalization vs. invasion in plant communities using stochastic cellular automata models*", NKS 2007 Wolfram Science Conference, Burlington, VT, July 14, 2007.
2. "*Genomic mining for complex disease traits with 'Random Chemistry'*", Computational Genetics Laboratory, Dartmouth College, Hanover, NH, Dec 1, 2006.
3. *"A 'Random Chemistry' algorithm for detecting epistatic genetic interactions"*, Department of Computer Science, Middlebury College, Middlebury, VT, April 7, 2006.
4. *"Molecularly-targeted imaging with diffuse fluorescence tomography for biomedical diagnostics"*, Vermont Lung Center, University of Vermont College of Medicine, Burlington, VT, Sept. 30, 2003.
5. *"The benefits of vectorization in Matlab: obtaining speedups without parallelism",* Department of Computer Science, Rochester Institute of Technology, Rochester, NY, May 6, 2003.
6. *"Algorithm Development for Biomedical Fluorescence Tomography",* Department of Imaging Science, Rochester Institute of Technology, Rochester, NY, May 5, 2003.
7. *"Fluorescence Tomography for Biomedical Diagnostics: Mathematical and Computational Challenges",* Departments of Mathematics, Rensselaer Polytechnic Institute, Troy, NY, March, 31, 2003.
8. *"3-D Bayesian fluorescence tomography from sparse and noisy frequency domain photon migration data sets",* Harvard Medical School, Photon Migration Seminar Series, Massachusetts General Hospital Imaging Center, Boston, MA, September, 2001.
9. *"Recursive, Minimum-Variance Optical Imaging with Domain Decomposition",*Optical Society of America spring meeting "Advances in Optical Imaging and Photon Migration 2000", Miami, Florida, April, 2000.
10. *"Rapid Bayesian 3-D Biomedical Optical Imaging*", Biomedical Computation Group, Thayer School of Engineering, Dartmouth College, Hanover, NH, November, 1999.
11. *"3-D Site Characterization Using APPRIZE*", Center for Geophysical Investigations of the Shallow Subsurface, Distinguished Lecture Series, Boise State University, May, 1999.
12. "*Using PVM to Implement Grand-Challenge Problems in Environmental Engineering: a Case Study of a Finite-Element Groundwater Model*", Workshop in

Parallel Processing for Undergraduate Educators, Colgate University, Hamilton, NY, January, 1993.

Funding: (**Total Funding Awarded $1,338,667)**

(plus an additional **$499,992** recommended for funding, for a total of **$1,838,659**)

Research Grants: ($1,207,705 awarded plus $499,992 recommended)

1. P.I. for "*Recursive Bayesian Optical Tomography for Imaging Tissues*", DBI/CBA 987-0779, National Science Foundation, Division of Biological Infrastructure/Computational Biology Activities, $290,043, 09/15/98-8/31/01. Supplemented with an additional $27,000, 10/1/00-4/31/01.
2. P.I. for "*3-D Frequency-Domain NIR Diagnostic Breast Imaging with APPRIZE*", R01 EB 002763 (formerly R01 CA 88082), National Institutes of Health, National Institute for Biomedical Imaging and Bioengineering and National Cancer Institute, Bioengineering Research Grants, $805,662, 4/3/01-3/31/04 (no-cost extension to 3/31/05).
3. P.I. (with J. Molofsky) for "Disentangling the mechanisms of species diversity in landscapes", DOE EPSCoR Computational Biology pilot project (funded out of DE-FG02-00ER45828, P.I.: S. Wallace), $35,000, 7/1/02-6/31/04 (no-cost extension to 6/30/07).
4. P.I. (originally, with M. Rould, who later left the project) for "A Bayesian Genetic Algorithm Approach to Crystallographic Phasing"; later generalized to “Evolutionary Computational Approaches to Complex Biological Problems”, DOE EPSCoR Computational Biology pilot project (funded out of DE-FG02-00ER45828, P.I.: S. Wallace), $40,000, 9/1/03-8/31/05 (no-cost extension to 6/30/07).
5. Equal co-I. (with J. Marshall and D. Rizzo) for “Regulatory Control Prediction for Transportation Alternative Energy Usage via a Multiscale Agent-Based Model”, University of Vermont Transportation Center, recommended for funding for $499,992 on 8/28/07; final award is pending. Anticipated dates: 7/1/2008-6/30/2011.

Research Infrastructure Grants: ($6,692,531 total; see below)

1. P.I. is EPSCoR director J. VanHouten. “Complex Systems Thinking and Modeling for Ecosystem Analysis”, National Science Foundation EPSCoR Research Infrastructure Improvement (RII) Grant, $6,692,531 from 8/15/07-6/30/10. Note: this amount is not included in my funding total since I am not a listed P.I. However, I am a funded core faculty and made significant contributions to writing the science portions of this grant related to complex systems analysis and modeling.

Equipment Grants: ($20,000 total)

1. Co-P.I. (with G.Pinder, T.Keller, F. Sansoz, D. Rizzo) for "Enabling Technology for High Speed Computing", UVM Faculty Equipment Acquisition funded by NSF EPSCoR, $20,000, awarded 3/31/04.

Grants Specifically To Fund Graduate Students: ($66,892 total)

1. Supervisor for "Computational Modeling in Ecology and Evolution", DOE EPSCoR Computational Biology graduate research fellowship to fund Ph.D. student Joshua Payne, (funded out of DE-FG02-00ER45828, P.I.: S. Wallace), $20,000, 7/1/05-6/30/06. Renewed for $20,722, 7/1/06-6/30/07.
2. P.I. for "Biomedical Fluorescence Tomography using the Boundary Element Method", Vermont Genetics Network graduate research assistantship to fund Ph.D. student Francesco Fedele, (funded out of NIH grant NCRR, 1 P20 RR16462, P.I.: C. Allen), $22,000, 6/1/03-5/31/04.
3. P.I. for "Application of Proper Orthogonal Decomposition to Biomedical Fluorescence Tomography", DOE EPSCoR Computational Biology summer graduate research fellowship to fund M.S. student Scott Wakefield, (funded out of DE-FG02-00ER45828, P.I.: S. Wallace), $4170, 6/15/03-8/15/03.

Grants to Support Teaching: ($8,165 total)

1. P.I. (with J. Hoffmann) for "Developing Cross-Disciplinary Learning Experiences in Evolutionary Computation", University of Vermont Center for Teaching and Learning, $3,165, 7/1/04-6/31/05.
2. P.I. for "A novel computational science course for life science majors", University of Vermont Center for Teaching and Learning, $5000, 7/1/07-6/30/08.

Planning Grants: ($5,000 total)

1. P.I. (with D. Rizzo, L. Stevens, C. Goodnight, J. Molofsky, and J. Hoffmann) for "Proposed VACC focal research area in Biocomplexity", Vermont Advanced Computing Center; $5,000, 9/1/05-5/31/06 (no cost extension through 5/31/07).

Contracts: ($96,839 total)

1. P.I. for contract "*Tools for Inversion and Imaging*", from Subterranean Research, Inc., as subaward of a U.S. Department of Energy SBIR Phase II (P.I. D.M. Rizzo); contract amount $51,839, 01/01/99-08/31/99; renewal amount $30,000, 01/01/00-05/31/00.
2. P.I. for contract "*Professional Development Course on Inversion and APPRIZE",* Subterranean Research, Inc., contract amount $15,000, 01/01/00-06/30/00.

Teaching and Advising

Courses Taught

I have independently developed and taught the following courses at UVM. **Courses taught since appointment as Assistant Professor are shown in Boldface**.

Level	Course	Semester	Title
literacy	CS 2	S '89	Microcomputer Applications Software
	CS 3	F'83, S'84, F'87, S'88	Computer Literacy
programming	CS 11	F '91(×3), S'92 (×2), F'92, S'93	Computer Programming I
	CS 12	S'85, S'86, F'86, Sum'87,F'88, S'89, F'89, F'90, S'91	Computer Programming II
	CS 16	F'94, S'95, F'95, S'96, F'96, S'97, **S'04**	**Programming in MATLAB for Engineers and Scientists**
	CS 95	F'88	C Programming for Pascal Programmers
	CS 27	F'96, S'97	C++ for C Programmers
Sophomore/junior	CS 195	**F'07**	**Data Analysis, Modeling, & Visualization for Life Scientists**
	CS 100	F'97, F'00, S'01	Object-Oriented Programming
	CS 103	F'83, F'84, F'90, S'92	Programming Languages
	CS 104	S'85, S'86, S'87, S'90, S'91, F'92, S'93, **S'05, F'05, S'06, F'06**	**Data Structures**
	CS 105	S'96	Software Engineering
Senior/graduate	CS 260	**S'03, S'05**	**Parallel Algorithms and Prog. Techniques**
	CS 381	**S'04**	**Graduate Seminar in Evolutionary Computation**
	CS 295/Bot 295, CS 395 /Biol 395.	**F'04, F'06**	**Evolutionary Computation**
	CS 295	**S'06**	**Intro to Scientific Computing: Modeling Complex Nonlinear Dynamic Systems**

Graduate Student Thesis/Dissertation Supervision

Ongoing:

1. Supervisor of Ph.D. student, Joshua L. Payne, "Interaction topologies and the flow of information in complex adaptive systems", Department of Computer Science, UVM, 2004-present.
2. Supervisor of M.S. student, Joshua Gilbert, “Bayesian evolutionary algorithms for locating heavy atoms in protein crystals”, Department of Computer Science, UVM, 2003-present (ABT).
3. Supervisor of M.S. student, Paul Haake, "Detecting Large Supersets of SNPs that contain small epistatically interacting subsets", Department of Computer Science, UVM, 2006-present.
4. Supervisor of M.S. student, Peter Duval, "Canonical Disjunctive Normal Form Genetic Programming for nonlinear-SNP Association Studies". Department of Computer Science, 2006-present.
5. Supervisor of Ph.D. student, Jeff Sprenger, “Rapid sound recognition and recall using spiking neural networks grown from a single neurode using a multi-objective evolutionary algorithm”, Department of Computer Science, 2007-present.
6. Co-Supervisor (with R. Costanza) of Ph.D. student, Karim Chichakly, who is working on research into development and implementation of multiscale models for ecosystem services, Department of Computer Science, 2007-present.

Completed:

1. Co-supervisor (with J. Laible) of Francesco Fedele, "Novel Numerical Techniques for Problems in Engineering Science", Department of Civil & Environmental Engineering, UVM, 2001-2004. Ph.D. granted 2004. Post-doctoral associate in the Global Modeling and Assimilation Office, NASA Goddard Space Flight Center, Greenbelt, Md, 2004-2006. Currently, assistant professor, Dept. of Civil & Environmental Engineering, Georgia Institute of Technology, Savannah.
2. Co-supervisor (with E.M. Sevick-Muraca) Anuradha Godavarty, "Fluorescence enhanced optical tomography in breast phantoms with measurements using a gain modulated intensified CCD imaging system", Department of Chemical Engineering, Texas A&M Univ, 2001-2003. Ph.D. granted 2003. Currently, assistant professor in Biomedical Engineering at Florida International University.
3. Funded and unofficially helped to co-supervise (with E.M. Sevick-Muraca) Daniel J. Hawrysz, "Bayesian approach to the inverse problem in contrast-enhanced, three-dimensional, biomedical optical imaging using frequency domain photon migration", Department of Chemical Engineering, Purdue Univ., 1998-2001. Ph.D. granted 2001. Currently, research scientist at Exxon Mobil.

Post-Doctoral Supervision

1. Funded and supervised Dr. Anuradha Godavarty as a postdoctoral research associate in computer science, UVM, 2003-2004. Currently, assistant professor in Biomedical Engineering at Florida International University.
2. Funded and supervised Dr. Chaoyang Zhang as a research assistant professor in computer science, UVM, 2001-2003. Currently, assistant professor in the School of Computing at University of Southern Mississippi.

Other Student Research Supervision

1. Chair, Undergraduate Honor's Thesis Committee, Kyle John Palmer, Thesis on aggressive behavior in individual workers of 6 different species of harvester ant whose colony-level aggressive behaviors differ dramatically, Environmental Science, CAS, UVM, spring 2007.
2. Supervised M.S. student, Scott Wakefield, research in biomedical fluorescence tomography, funded through DOE EPSCoR summer research grant, Department of Computer Science, UVM, summer 2003.
3. Supervised undergraduate Joshua Gilbert (Computer Science Major, University of Vermont) through the SURE program (funded by the UVM Dept of Biochemistry and NIH) for research in evolutionary algorithms in structural biology, summer 2003.
4. Co-supervised (with J. Molofsky), undergraduate Chris Pyman (Mathematics major, Computer Science minor) for research in computational modeling of plant species interactions (funded by DOE EPSCoR pilot project), summer 2003.
5. Supervised M.S. student, Tyler Carr, research in phylogenetic tree algorithms, Department of Computer Science, UVM, spring 2003.
6. Supervised undergraduate Scott Wakefield (Computer Science Major, University of Vermont), funded through my discretionary funds, for exploratory research in DNA folding algorithms and their application to mutation spectra analysis, spring 2003.
7. Supervised undergraduate Joshua Gilbert (Computer Science Major, University of Vermont) through the HELIX program (funded by DOE EPSCoR summer internship) for research on use of codons for genetic representation in genetic algorithms, summer 2002
8. Supervised M.S. student, Zheng Zheng Wei, independent study in mutation spectra analysis, Department of Computer Science, UVM, spring 2002.

Graduate Student Committees

1. Karim Chichakly, Member Ph.D. Studies Committee, Department of Computer Science, UVM, 2007-present.
2. Jeffrey Sprenger, Member Ph.D. Studies Committee, Department of Computer Science, UVM, 2007-present.
3. Casey Greene, Ph.D. Dissertation Committee, Department of Genetics, Dartmouth College, Hanover, NH, 2007-present.
4. Ryan Urbanowicz, Ph.D. Dissertation Committee, Department of Genetics, Dartmouth College, Hanover, NH, 2007-present.
5. Casey Korecki, Member Ph.D. Dissertation committee, Mechanical Engineering, School of Engineering, UVM, 2007-present.
6. Brittny Starford, Member Ph.D. Studies committee, Department of Biology, UVM, 2006-present.
7. Zhiqaing, Li, Chair Ph.D. Dissertation Defense Committee, Civil & Environmental Engineering Program, UVM, Defended, Dec. 2006.
8. Robin Collins, Member Ph.D. Studies committee and Comprehensive Examination Committee, Department of Plant Biology, UVM, 2005- present.
9. Thomas Weicht, Member Ph.D. Studies committee, Department of Biology, Univ. of Toledo, 2005- present.
10. Joshua Gilbert, Chair M.S. Project committee, Department of Computer Science, UVM, 2005- present.
11. Joshua Payne, Member Ph. D. Studies committee, Comprehensive Examination Committee, Department of Computer Science, UVM, 2004- present.
12. Nagi Basha, Member Ph. D. Studies committee, Comprehensive Examination Committee, Department of Computer Science, UVM, 2004- present.
13. Tri Tran, Member Ph. D. Studies committee, Department of Computer Science, UVM, 2004- present.
14. Thomas Tucker, Member, M.S. Comprehensive Examination Committee, Department of Biology, UVM, January, 2004.
15. Francesco Fedele: Member, Ph.D Dissertation Defense Committee, Dept. of Civil & Environmental Engineering, defended Dec 2004.
16. Charles Mark: Chair, MS Thesis Defense Committee, Department of Civil & Environmental Engineering, defended October, 2004.
17. Linda Mayer: Chair, MS Thesis Defense Committee, Department of Electrical & Computer Engineering, defended July 2004.
18. Norman Kennedy: Chair, Ph.D. Dissertation Defense Committee, Department of Cellular and Molecular Biology, UVM, November, 1999.

19. Mengchun Yu: Member, Ph.D. Dissertation Defense Committee, Department of Civil & Environmental Engineering, UVM, September, 1998.
20. Henry Tufo: Member, M.S. Thesis Defense Committee, Department of Computer Science, UVM, June 1995.

Service

National Service

Federal Agency Reviews

- Panel Member, Biomedical Imaging Technology Study Section (BMIT), National Institutes of Health, 2005.
- Panel Member, Physical Imaging 2 Review Panel of the U.S. Army Breast Cancer Research Program, 2004.
- Panel Member, National Science Foundation Review Panel for Information Technology Bioinformatics, 2001.
- Panel Member, National Science Foundation Review Panel for Computational Biological Activities, 1999.
- Mail Reviewer for several *National Science Foundation Grant Proposals*, 1997-present.

Conference Service (Program Committees, Conference Peer Reviewing, and Session Chairing)

- Conference Organizing Committee, Complex Systems in Transportation Conference, 2007-2008.
- Member, Standing Program Committee, OSA Biomedical Topical Meetings, Advances in Optical Imaging and Photon Migration, 2003-2008.
- Program Committee Member for the 6th European Conference on EvolutionaryComputation, Machine Learning and Data Mining in Bioinformatics (EvoBIO), 2008.
- Program Committee Member for the 3rd International IEEE Workshop on Software Evolvability at the IEEE International Conference on Software Maintenance (ICMS), 2007.
- Program Committee Member for the Biological Applications Track, Genetic and Evolutionary Computation Conference, 2007.

  - Reviewer for 2nd IAPR Workshop on Pattern Recognition in Bioinformatics (PRIB), 2007.
  - Reviewer for IEEE Symposium on Computational Intelligence in Bioinformatics and Computational Biology, 2005 and 2006.
- Session chair, Optical Tomography and Spectroscopy of Tissue IV at Photonics West (International Society for Optical Engineering), San Jose, CA, January 2000.
- Session chair, XII International Conference on Computational Methods in Water Resources, Crete, Greece, 1998.

Editorial Boards

  - Editorial Board Member for BioData Mining, published by BioMed Central, 2007-present

External Peer Reviewer for Grants, Journals, Book Chapters

  - External peer reviewer for book chapter in *Stochastic Methods in Subsurface Contaminant Hydrology,* 1999.
- External peer reviewer for the following journals, 1997-present.
  - *Water Resources Research*
  - *Geophysics*
  - *Advances in Water Resources*
  - *Optics Letters*
  - *Optics Express*
  - *Optics Communications*
  - *Medical Physics*
  - *Journal of the Optical Society of America A*
  - *Journal of Biomedical Optics*
  - *Physics in Medicine and Biology*
  - *IEEE Transactions in Medical Imaging*
  - *Journal of Soft Computing*
  - *Ecological Modelling*
  - *Evolutionary Computation*
  - *American Journal of Human Genetics*
  - *Inverse Problems*
  - *Engineering in Biology and Medicine Magazine*

University Level Service

- Member, Vermont Advanced Computing Center Director Search Committee (2007-08).
- Biosciences PhD Umbrella Steering Committee (2007-present).
    - Aiken Lecture ‘08-‘09 Planning Committee (2007-present).
    - University Diversity Curriculum Committee (2005).
    - Member of the VT EPSCoR SBIR Phase 0 proposal review committee, (2005).
    - Member of the DEPSCoR Pre-proposal review committee, (2003).

College Level Service (*CEMS is College of Engineering and Mathematical Sciences*)

    - CEMS Curriculum Committee member (1994-present) and Chair (1994-1996, 2000-present).
    - Founding co-Director, Complex Systems Center (2006-present).
- Dean’s Faculty Advisory Committee, (2006-present).
    - Bioengineering Faculty Search Committee (2007-08).
    - Bioengineering & Computational Biology PhD Track Director (2007-present).
    - CEMS Bioengineering Advisory Committee (2005).
- Electrical and Computer Engineering Chair Search Committee (2003-04).
    - CEMS Studies Committee (1986-1994).

Department Level Service (*CS is Department of Computer Science*)

    - CS Curriculum Committee member (1983-present) and Chair (1997-2005).
    - CS Faculty Search Committee (2005-06).
    - UPE (CS Honor Society) Faculty Advisor (1983-2006).
    - CS Computational Biology Faculty Search Committee (2001-02).
    - CS certificate coordinator (1983-2001).
    - CS Interim Chair Search Committee (1999)
    - CS Co-op advisor (1983-1990).
    - CS Open Houses/Visitation Days: I regularly participate in approximately 2 sessions per year.

Robert J. Hondal

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Robert.Hondal@uvm.edu

CURRICULUM VITAE

EDUCATION

1982-1986	Berlin-Brothersvalley High School, Berlin, PA.
1989-1991	B.S. Chemistry, University of Pittsburgh, Pittsburgh, PA.
1991-1997	Ph. D., Chemistry, The Ohio State University, Columbus, OH.

POST-DOCTORAL APPOINTMENTS

Oct. 1997- Oct .1998	Post-Doctoral Fellow, Vanderbilt University
Jan. 1999- June 2002	NIH Post-Doctoral Fellow, University of Wisconsin (1 F32 GM20180-01)

CURRENT APPOINTMENT

Aug 1 2002 to present	Asst. Professor of Biochemistry, University of Vermont, Burlington, VT.

MILITARY SERVICE

U.S. Army Reserves 1988-1992

HONORS AND AWARDS

The Paul D. Boyer Memorial Award for Post-Doctoral Fellows (2001). This was a new award given by a Biochemistry Department faculty committee at the University of Wisconsin in 2001. This award is given on an annual basis to the post-doctoral fellow in the department determined to be the "most outstanding" post-doctoral scientist.

PROFESSIONAL ORGANIZATIONS

American Chemical Society
American Peptide Society

OTHER PROFESSIONAL ACTIVITIES:

Member, Cell Signaling and Environmental Pathology Training Program (2004 to present)
Member, Hemostasis and Thrombosis Training Program (2003 to present)
Member, UVM Graduate College (2004 to present).

PEER-REVIEWED PUBLICATIONS

1) Ruggles EL, Flemer SJ, & **Hondal RJ** (2008) A Viable Procedure for the Synthesis of *N*-Methyl Cysteine. *Biopolymers 90*, 61-68.

2) Flemer SJ, Lacey BM & **Hondal RJ** (2008) Synthesis of peptide substrates for mammalian thioredoxin reductase. *J. Pept. Sci. In Press*.

3) Eckenroth BE, Lacey BM, Lothrop AP, Harris KM, & **Hondal RJ** (2007) Investigation of the C-terminal Redox Center of High M_r Thioredoxin Reductases by Protein Engineering and Semisynthesis. *Biochemistry 46*, 9472-9483.

4) Eckenroth BE, Rould MA, **Hondal RJ**, & Everse SJ (2007) Structural and biochemical studies reveal differences in the catalytic mechanisms of mammalian and *Drosophila melanogaster* thioredoxin reductases. *Biochemistry 46*, 4694-4705.

5) Harris KM, Flemer S & **Hondal RJ**. (2007) Studies on deprotection of cysteine and selenocysteine side chain protecting groups. *J. Pept. Sci 13*, 81-93.

6) Eckenroth BE, Harris K, Turanov AA, Gladyshev VN, Raines RT, & **Hondal, RJ.** (2006) Semisynthesis and characterization of mammalian thioredoxin reductase. *Biochemistry 45*, 5158-5170.

7) Ruggles EL, & **Hondal RJ**. (2006) Synthesis and properties of disulfide-bond containing eight-membered rings. *Tet. Lett. 47*, 4281-4284.

8) Lacey BM, & **Hondal RJ**. (2006) Characterization of mitochondrial thioredoxin reductase from *C. elegans*. *Biochem. Biophys. Res. Commun. 346*, 629-636.

9) Hondal RJ. (2005) Incorporation of selenocysteine into proteins using peptide ligation. *Protein and Peptide Letters 12*, 757-764.

10) Nilsson BL, **Hondal RJ**, Soellner MB, & Raines RT. (2003) Protein assembly by orthogonal chemical ligation methods. *J. Am Chem. Soc. 125,* 5268-9.

11) Hondal RJ, & Raines RT. (2002) Semisynthesis of proteins containing selenocysteine. *Methods Enzymol. 347,* 70-83.

12) Kubiak RJ, Yue X, **Hondal RJ**, Mihai C, Tsai M.-D., & Bruzik K.S.(2001) Involvement of the Arg-Asp-His Catalytic Triad in Enzymatic Cleavage of the Phosphodiester Bond *Biochemistry 40,* 5422-5432.

13) Hondal RJ, Nilsson BL, & Raines RT, (2001) Selenocysteine in Native Chemical Ligation and Expressed Protein Ligation. *J. Am Chem. Soc. 123,* 5140-5141.

14) Hondal RJ, Ma, S Caprioli RM, Hill KE, & Burk RF. (2001) Identification of Heparin-Binding Histidine and Lysine Residues of Rat Selenoprotein P. *J. Biol. Chem. 276,* 15823-31.

15) Hondal RJ, Motley AK, Hill KE, & Burk RF. (1999) Failure of Selenomethionine Residues in Albumin and Immunoglobulin G to Protect against Peroxynitrite. *Arch. Biochem. Biophys. 371,* 29-34.

16) Kubiak RJ, **Hondal RJ**, Yue X, Tsai M.-D., & Bruzik KS. (1999) Identification of a Novel Catalytic Triad with Dual Functions in Enzymatic Cleavage of the P-O Bond. *J. Am. Chem. Soc. 121,* 488-489.

17) Hondal RJ, Zhao Z, Kravchuk AV, Liao H, Riddle SR, Bruzik KS, & Tsai M.-D. (1998) Mechanism of Phosphatidylinositol-Specific Phospholipase C: A Unified View of the Mechanism of Catalysis" *Biochemistry 37,* 4568-4580.

18) Hondal RJ, Riddle SR, Kravchuk AV, Zhao Z, Liao H, Bruzik KS, & Tsai M.-D. (1997) Phosphatidylinositol Phospholipase C: Kinetic and Stereochemical Evidence for an Interaction between Arginine-69 and the Phosphate Group of Phosphatidylinositol. *Biochemistry 36,* 6633-6642.

19) Hondal RJ, Bruzik KS, Zhao Z, & Tsai M.-D. (1997) Mechanism of Phosphatidylinositol-Phospholipase C. 2. Reversal of a Thio Effect by Site-Directed Mutagenesis. *J. Am. Chem. Soc. 119,* 5477-5478.

20) Hondal RJ, Zhao Z, Riddle SR, Kravchuk AV, Liao H, Bruzik KS, & Tsai. M.-D. (1997) Phosphatidylinositol-specific Phospholipase C. 3. The Catalysis Combines both the General Acid-General Base Mechanism and the Triester-like Mechanism. *J. Am. Chem. Soc. 119,* 9933-9934.

21) Werneburg BG, Ahn J, Zhong X, **Hondal RJ**, Kraynov VS, & Tsai M.-D. (1996) DNA Polymerase β: Pre-Steady-State Kinetic Analysis and Roles of Arginine-283 in Catalysis and Fidelity: *Biochemistry 35,* 7041-50.

22) Hondal RJ & Ulsh RC. (1992) Studies on the Coprophageal Behavior of the Domestic Rabbit Using Adiabatic Calorimetry. *J. Penn. Acad. Sci. 66,* 107-110.

Conference Proceedings:

1) Harris KM & **Hondal RJ.** Deprotection of the *p*-methoxybenzyl group of selenocysteine by neighboring group participation. (2006). *In Understanding Biology Using Peptides: Proceedings of the 19th American Peptide Symposium* (Sylvie E. Blondelle, Ed.). Springer, New York, pgs 91-92.

2) Flemer S & **Hondal RJ.** An efficient on-resin protocol for on-resin, vicinal disulfide formation: Applications to thioredoxin reductase (2008). *In Peptides for Youth: Proceedings of the 20th American Peptide Symposium* (Emanuel Escher, William D. Lubell, Susan Del Valle (Eds.). Springer, New York, *In Press.*

3) Schroll A & **Hondal RJ.** Further development of new deprotection chemistry for cysteine and selenocysteine side chain protecting groups (2008). *In Peptides for Youth: Proceedings of the 20th American Peptide Symposium* (Emanuel Escher, William D. Lubell, Susan Del Valle (Eds.). Springer, New York, *In Press.*

Book Chapters:

1) Hondal RJ, Zhao Z, Kravchuk AV, Liao H, Riddle SR, Bruzik KS, & Tsai, M.-D. (1998) The Mechanism of Phosphatidylinositol-Specific Phospholipase C Revealed by Protein Engineering and Thio-PI Analogs. *In Phosphoinositides: Chemistry, Biochemistry and Biomedical Applications*, K. S. Bruzik, Ed. *ACS Symp. Ser. 718,* 109-120.

Papers in Preparation:

1) Flemer SJ, Schroll A, & Hondal RJ, (2007) Cysteine and Selenocysteine Deprotection Chemistry in Peptide Synthesis. *In Preparation for Minireviews in Organic Chemistry*

2) Deker PB, & **Hondal RJ**. (2007) Eight-Membered Ring Structures of Thioredoxin Reductases:Implications for the Mechanism of Catalysis. *In Preparation for Biochemistry*

3) Lacey BM, Flemer SJ, & **Hondal RJ** (2007) Selenium in Thioredoxin Reductase: A Mechanistic Perspective. *In Preparation for Biochemistry*

4) Ruggles EL, & **Hondal RJ** (2007) Synthesis, Redox, and Conformations of Cyclocystine Mimics. *In Preparation for Tetrahedron.*

INVITED LECTURES

•**Hondal, RJ** *Selenium vs. Sulfur in Enzymes: The Case of Thioredoxin Reductase.* College of Pharmacy, University of Wisconsin-Madison, Madison,WI. October 12th, 2007.

•**Hondal, RJ** *LEGO Proteins: The Use of Protein Building Blocks to Study Protein Function*. State University of New York-Plattsburgh, Platsburgh, NY. September 7th, 2007.

•Eckenroth BE & **Hondal RJ**. Selenium vs. Sulfur Thioredoxin Reductases: A Conformation Switching Mechanism Explains Differences in the Catalytic Mechanisms. *Gordon Research Conference – Enzymes, Coenzymes, and Metabolic Pathways.* University of New England, July 8-13, (2007).

•**Hondal, RJ** *Selenium in Proteins: The Case of Thioredoxin Reductase.* Department of Chemistry, The Ohio State University, Columbus, OH. March 29th, 2007.

•**Hondal, RJ** *Selenium vs. Sulfur Thioredoxin Reductases: Structure studies by X-ray crystallography and functional analysis using semisynthesis.* Department of Chemistry & Biochemistry, The Florida State University, Tallahassee, FL. January 30th, 2007.

•Flemer, SF, Harris, KM, & **Hondal RJ** A New Method for Deprotecting *p*-Methoxybenzyl and Acetamidomethyl Groups from Cysteine and Selenocysteine. *Northeast Regional Meeting of the American Chemical Society,* Binghamton, NY, October 5-7, (2006)

•Eckenroth BE, & **Hondal RJ**. Structure-Function Relationships of the Conserved GCUG Tetrapeptide Motif of Thioredoxin Reductase Investigated by Protein Semisynthesis. *The 8th International Symposium on Selenium in Biology and Medicine*, Madison, WI. July 25-30, (2006).

•**Hondal, RJ** *I. New orthogonal deprotection strategies for cysteine and selenocysteine. II. Semisynthetic selenoproteins.* Department of Biochemistry, University of Nebraska, Lincoln, NE. October 11, 2005.

•**Hondal, RJ** *Inserting Selenocysteine into Proteins – Problems and Advances*. New England Biolabs, Beverly, MA. November 4th, 2005.

•**Hondal, RJ** I. *Mechanism of thioredoxin reductase studied by semisynthesis.* Department of Chemistry and Biochemistry, Baylor University, Waco, TX. January 30th, 2004.

•**Hondal, RJ**. *The mechanism of thioredoxin reductase studied by semisynthesis.* Cell Signaling/Environmental Seminar Series, University of Vermont. February 9th, (2004).

•**Hondal, RJ**. *The mechanism of thioredoxin reductase studied by semisynthesis.* 8th International Congress on Amino Acids and Proteins. Rome, Italy. September 5 –9, (2003).

•**Hondal, RJ**. *Insertion of Non-natural Amino Acids into Proteins by Semi-synthesis: Structural and Functional Studies.* Department of Chemistry Seminar Series, University of Vermont. February 6th, (2003).

•**Hondal, RJ**, Nilsson, BL, & Raines, RT. *Selenocysteine in Native Chemical Ligation and Expressed Protein Ligation.* ACS National Meeting, Chicago, IL. August 26-30. (2001), AN2001:637020.

•**Hondal, RJ**. *Selenocysteine in Native Chemical Ligation and Expressed Protein Ligation.* FASEB Summer Research Conference: Trace Elements. Whitefish, MT. (2001)

•**Hondal, RJ**. *Semisynthesis of Proteins with Selenocysteine and Other Unusual Amino Acids.* Oregon Health Sciences University Portland, OR. (2001).

•Hill, KE, Ma, S., **Hondal, RJ**, & Burk, RF. *Physical and Chemical Characterization of Rat Selenoprotein P Isoforms*. Selenium 2000: 7th International Symposium On Selenium In Biology and Medicine. Venice, Italy. (2000).

•**Hondal, RJ**, Hill, KE, & Burk, RF. *Identification of Heparin-Binding Histidine and Lysine Residues by Chemical Modification*. Annual Meeting of the American Society for Experimental Biology. Washington D.C. July 17-21, (1999), Abstract #662.3, pg A875, *FASEB Abstracts*.

ABSTRACTS PRESENTED AS POSTERS

•Ruggles EL, & **Hondal RJ**. Viable construction of *N*-methyl cysteine and its use in peptide synthesis. *234th Meeting of the American Chemical Society*. Boston, MA. Aug 19th – 23rd. (2007) AN2007: 884125

•Lacey BM, Flemer, S. & **Hondal RJ**. Contribution of ring strain to catalysis: Comparison of cyclic and acyclic forms of octapeptides as substrates for high M_r thioredoxin reductases. *234th Meeting of the American Chemical Society*. Boston, MA. Aug 19th – 23rd. (2007) AN2007: 878899

•Stevenson Flemer Jr. & **Hondal RJ**. An Efficient Protocol for On-Resin, Vicinal Disulfide Formation: Applications to Thioredoxin Reductase. *20th American Peptide Society Symposium: Peptides for Youth.* Montreal, Canada. June 26-30, (2007).

•Alayne L Schroll & **Hondal RJ**. Further Development of New Deprotection Chemistry for Cysteine and Selenocysteine Side Chain Protecting Groups. *20th American Peptide Society Symposium: Peptides for Youth.* Montreal, Canada. June 26-30, (2007).

•Ruggles EL, **Hondal RJ**, & Deker, PB. Synthesis and properties of cyclocystine subunits (CCS): Application to thioredoxin reductase and hepcidin. *233rd Meeting of the American Chemical Society*. Chicago, IL. Mar 25th – 29th. (2007) AN2007: 295763

•P. Bruce Deker & **Hondal RJ**. Conformational Switching at the C-terminus of Thioredoxin Reductase? *The 8th International Symposium on Selenium in Biology and Medicine*, Madison, WI. July 25-30, (2006).

•Eckenroth BE, Harris, KM, & **Hondal RJ**. Structure-Function Investigation of the C-terminal Redox-Active Tetrapeptide of Mammalian Thioredoxin Reductase by Semisynthesis. *Gordon Research Conference – Enzymes, Coenzymes, and Metabolic Pathways.* University of New England, July 16-21, (2006).

•Lacey, B. & **Hondal RJ**. Purification and Characterization of Mitochondrial Thioredoxin Reductase from *Caenorhabditis elegans*: A Non-Selenium Containing Enzyme. *Northeast Regional Meeting of the American Chemical Society,* Fairfield, CT. July 14-17, (2005), AN2005:663401.

•Eckenroth, BE, Everse, SJ, Adams, TE, & **Hondal, RJ**. Crystallization of mammalian thioredoxin reductase for structural studies using synthetic active site peptides. *FASEB Meeting*. April 2-6 (2005), San Diego, CA. Abstract #2600. *FASEB Abstracts.*

•Ruggles, EL, Deker, P.B., & **Hondal, RJ**. Synthesis and properties of disulfide-bond containing eight-membered rings. *230th Meeting of the American Chemical Society*. Washington, D.C. Aug. 28-Sep. 1, (2005), AN2005:74088.

•Harris, KM & **Hondal RJ.** Deprotection of the *p*-methoxybenzyl group of selenocysteine by neighboring group participation.19th *American Peptide Symposium*. San Diego, CA. (2005).

•**Hondal, RJ** *The Functional Role of the C-Terminus of Mammalian Thioredoxin Reductase Investigated by Peptide Complementation*. Selenium Biochemistry 2003. Bethesda, MD. September 17-19, (2003)

•**Hondal, RJ** *The mechanism of thioredoxin reductase studied by semisynthesis.* (2003) *Amino Acids 25*, 185.

•**Hondal, RJ**, Nilsson, BL, & Raines, RT. *Incorporation of Unnatural Amino Acids into Ribonuclease A by Semisynthesis.* 17th Enzyme Mechanism Conference, Marco Island, FL. (2001).

•**Hondal, RJ**, Abel, RL, & Raines, RT. *Stereochemical Consequences of Catalysis by Ribonuclease A: Non-natural Variants and Phosphorothioate Substrates.* ACS National Meeting, Chicago, IL. Aug. 26-30, (2001), AN2001:637183.

•Abel, RL, **Hondal, RJ**, & Raines, RT. Active Site Variants of Ribonuclease A. ACS National Meeting, Chicago, IL. Aug. 26-30, (2001), AN2001:637192.

•**Hondal, RJ**, & Burk, R. F. *Evidence for Thiol Redox States of Selenoprotein P*. Annual Meeting of the American Society for Experimental Biology. San Francisco, CA. April 18-20, (1998), Abstract#3040, pg A523, *FASEB Abstracts*.

•**Hondal, RJ**, Kravchuk, AV, & Tsai, M.-D. *Using Protein Engineering and Thio-PI Analogs to Probe the Mechanism of PI-PLC.* ACS National Meeting, Las Vegas, Nevada. (1997), AN1997:485974.

•Liao, H., **Hondal, RJ**, & Tsai, M.-D. *Site-directed mutagenesis studies of phosphoatidylinositol-specific phospholipase C: the substrate binding residues.* 17th International Congress of Biochemistry and Molecular Biology. Annual Meeting of the American Society for Biochemistry and Molecular Biology. San Francisco, CA. Aug. 24-29, (1997). Abstract #2628, pg A1307, *FASEB Abstracts.*

Ongoing Research Support

NIH-NIGMS R01 GM070742 (Hondal, PI) 4/1/04 – 3/13/09 40% $750,000

Selenium-Thioredoxin Reductase Studies by Semisynthesis

The major goals of this project are (i) make small molecule mimics of TR active site (ii) produce a semisynthetic TR (iii) characterize a cysteine-TR.

College of Medicine 08/01/02 – 07/31/05

New Faculty start-up funds: To initiate research and support personnel.

Instrumentation Grants

1 S10 RR017743-01 A1. $179,094

NIH Shared Instrumentation Grant – Symphony Multiplex Peptide Synthesizer w/VISION Workstation

This grant received a priority score of 149 and was funded in March of 2004. I was the Co-PI on this grant because at the time, I did not have my own R01 and could not be the PI. I was in fact the primary author of this grant. This money was used to purchase a Symphony peptide synthesizer and two HPLC systems. We have established a peptide core lab at UVM. I am the director of this facility. More information can be obtained at http://proteins.uvm.edu

Vermont EPSCoR

Small Equipment Grant $12,079

Lyophilizer for Use in Making Proteins by Total Chemical Synthesis.

Pending Grants

NIH-NHLBI 2R01 HL068865 (van der Vliet, PI) 4/1/08 – 3/13/13 5% $1,125,000

Toxic Aldehydes as Modulators of Lung Inflammation

Role: co-PI – My role for this project is to supply thioredoxin reductase to Dr. van der Vliet so that various electrophiles could be tested as modifying agents for the enzyme.

Completed Research Support

NIH/NIGMS NRSA F32 GM20180 07/01/99 – 12/31/02

Synthesis of PDI Mimics

This project involved synthesizing small molecules that mimicked the action of the enzyme Protein Disulfide Isomerase. These molecules were then characterized by various biophysical techniques and subsequently tested for their ability to replace PDI in yeast knockouts.
Role: Postdoctoral Fellow.

DOE EPSCoR DE-FG02-00ER45828 (Wallace, PI) 08/01/02 - 06/30/03 $112,000

DOE EPSCoR Initiative in Structural Biology and Computational Biology/Bioinformatics – New Faculty Start-up

These funds were part of my initial start-up package.

DOE EPSCOR DE-FG02-00ER45828 (Wallace, PI) 7/1/03 – 6/30/05 $70,000

Structural Studies of Mammalian Thioredoxin Reductase

The goal of this project is to crystallize a truncated form of TR with a synthetic peptide substrate. We have produced a preliminary structure and are working on finishing the refined structure.

Mentored Grants

DOE/EPSCoR Graduate Research Fellowship 07/01/05 – 06/30/07 $40,100

Structure Determination of Mouse Thioredoxin Reductase-3 and the Thioredoxin Reductase/Thioredoxin Complex by X-Ray Crystallography.

Brian E. Eckenroth was awarded a two-year graduate fellowship by the Structural Biology Initiative of DOE/EPSCoR to continue work on the crystal structure of mTR3 and the mTR3/thioredoxin complex.

RUBY Summer 2004 $5,000

Synthesis of a Phosphorothioate Substrate Analog to Investigate the Role of His119 of RNase A in Catalysis.

This grant was funded for $5,000 dollars to Adam Lothrop (St. Michael's College, Colchester, VT) The program was entitled RUBY, which stands for **R**esearch **U**ndergraduates in your **B**ack **Y**ard. This grant paid Adam a salary of $3,500 for the summer and my lab received $1,500 for supplies for this project. The purpose of this program was to attract Vermont students to UVM for graduate studies. Adam was required to write a mini-grant in order to obtain funding.

HELiX Summer 2005 $5,000

Crystallization of Thioredoxin Reductase/Thioredoxin Complex.

This grant was funded by HELiX for Ms. Erin Chicoine (UVM) to work in my lab for the summer of 2005. Erin worked on crystallizing the TR/Trx complex. HELiX stands for **H**ughes **E**ndeavor for **Li**fe Science E**x**cellence. The HELiX program is designed to support students doing undergraduate research and provides funding for the summer and academic year research. This is a highly competitive program and students are required to write a mini-grant that is reviewed by a panel to obtain funding.

URECA! Spring 2006 $4,000

Biosynthesis of Selenocysteine using *O*-Acetylserine Sulfhydrylase.

Dov Pechenick was funded by URECA! (**U**ndergraduate **R**esearch **E**ndeavors **C**ompetitive **A**wards) to do his his honors thesis in my laboratory. The goals of this project were to: (i) clone *O*-acetylserine sulfhydrylase, (ii) Use this enzyme to make the amino acid selenocysteine biosynthetically. The entire award was used for supplies for this project.

VGN 06/01/06 – 05/31/07 $10,000

Synthesis, Characterization, and Use of New Selenocysteine Derivatives.

Dr. Alayne Schroll, St. Michael's College applied for sabbatical research support to work in my laboratory during the 2006-07 academic year from the **V**ermont **G**enetics **N**etwork (VGN). Dr. Schroll and I worked jointly on this proposal as part of a broader proposal we subsequently submitted to the National Science Foundation (NSF). This grant was funded for $10,000.

RESEARCH COLLABORATIONS

Dr. Jose Madalengoitia (UVM, Dept. of Chemistry) – I have a collaboration with Dr. Madalengoitia as part of my NIH grant to synthesize peptide bond isosteres. These synthetic moieties will be placed into a protein structure. The enzyme we are studying forms a disulfide bond between adjacent cysteine residues to form an 8-membered ring. The geometry of this peptide bond is important for chemical catalysis. In order to determine which conformation this peptide bond has in the enzyme, we have proposed as part of my grant to synthesize isosteres which restrict the peptide bond to a single conformation. Dr. Madalengoitia and a graduate student of his have been working on this project for the past year. Once he finishes this synthesis, we will incorporate these isosteres into our semisynthetic enzyme to study the enzyme mechanism.

Dr. Stephen Everse (UVM, Dept. of Biochemistry) – I have a collaboration with Dr. Everse as part of an EPSCoR grant to crystallize thioredoxin reductase-3 (TR). We have a preliminary structure and we plan to submit an R01 based on this structure. A particular focus of this project is to look at the conformation of the C-terminus of TR.

Dr. Alayne Schroll (St. Michael's College) – I have a collaboration with Dr. Schroll to synthesize new protecting groups for selenocysteine to be used in solid-phase peptide synthesis. Dr. Schroll is planning on spending a sabbatical year in my lab starting in the summer of 2006. She will also be working on our new orthogonal protecting strategies that we have developed for cysteine. This research is part of a planned grant submission to NSF as described above

Dr. Vadim Gladyshev (Univ. of Nebraska, Redox Biology Center) – I am collaborating with Dr. Gladyshev in synthesizing a semisynthetic version of thioredoxin reductase. Dr. Gladyshev has provided expertise in synthesizing selenium containing proteins by an alternative recombinant method.

Dr. Elias Arner (Karolinska Institute) – I have provided Dr. Arner with selenocysteine-containing peptides . Dr. Arner wish to determine the redox potential of these peptides so that he can understand how thioredoxin reductase reduces its substrate.

Dr. Mark Rould – (UVM, Dept. of Molecular Physiology & Biophysics) Total synthesis of engrailed, which is a DNA binding protein involved in organismic development. As described above, we are taking a total synthetic approach to producing this protein because of its small size and difficulty in producing using *E. coli*. We have devised a cassette system in which we can introduce many mutations by using total peptide synthesis.

Dr. Watson Lees (Florida International University, Dept. of Chemistry) Dr. Lees is synthesizing aromatic disulfides to be used in an enzymatic assay for TR. These disulfides are to be used in a linear free energy relationships study to determine how the activity of the enzyme varies with leaving group pK_a.

Dr. Albert van der Vliet (UVM, Dept. of Pathology) I am collaborating with Dr. van der Vliet in his study of inflammation by providing him with semisynthetic thioredoxin reductase. He has developed the hypothesis that thioredoxin reductase becomes modified with electrophiles during inflammation.

TEACHING EXPERIENCE

BIOC205 (1 hour)	Proteomics	Fall 2002
BIOC351 (1.5 hours)	Protein semisynthesis	Fall 2002
BIOC381 (14 hours)	Graduate Seminar (protein engineering)	Spring 2003
BIOC207 (entire course)	Biochemistry Laboratory	Fall 2003
BIOC207 (entire course)	Biochemistry Laboratory	Spring 2004
BIOC207 (entire course)	Biochemistry Laboratory	Fall 2004
BIOC351 (1.5 hours)	Peptide synthesis & sequencing	Fall 2004
BIOC207 (entire course)	Biochemistry Laboratory	Spring 2005
BIOC371 (4.5 hours)	NMR theory & applications	Spring 2005
BIOC381 (14 hours)	Graduate Seminar (oxidative stress & cell signaling)	Spring 2005
BIOC207 (entire course)	Biochemistry Laboratory	Fall 2005
BIOC353 (15 hours)	Enzyme mechanism	Fall 2005
BIOC207 (entire course)	Biochemistry Laboratory	Spring 2006
BIOC381 (14 hours)	Graduate Seminar (translational control mechanisms)	Spring 2006
MMG198 (3 credits)	Undergraduate Research	Spring 2006
BIOC207 (entire course)	Biochemistry Laboratory	Fall 2006
BIOC351 (12 hours)	Protein structure & function	Fall 2006
BIOC291 (3 credits)	Undergraduate Research	Spring 2006
CHEM291 (2 credits)	Undergraduate Research	Spring 2006
BIOC371 (6 hours)	NMR theory & applications	Fall 2007
BIOC353 (18 hours)	Enzyme mechanism	Spring 2008
BIOC381 (14 hours)	Graduate Seminar (highly cited papers-JBC/Biochem)	Spring 2008

Graduate Student Laboratory Rotations

All first year graduate students in the Department of Biochemistry are required to do four laboratory rotations. These rotations are the basis for the grade a student receives in BIOC309 and BIOC310. Each rotation is worth 1.5 graduate credits. They are required to write a paper about their project and give an oral presentation about their project to the Department. The following students have rotated in my laboratory and the title of their project is listed below:

Fall 2002
Ethan Guth – Optimization of Expression and Purification of Human Thioredoxin Reductase from a Recombinant *E. coli* Construct.

Spring 2003
Marque St. John – Examination of the Activity of a Novel Mutant of Thioredoxin Reductase

Brian Eckenroth – Expression and Characterization of a Mammalian Thioredoxin Reductase Mutant Containing a Cysteine Substitution for the Selenocysteine at Residue 489.

Spring 2004
Brian Lacey – Characterization of Thioredoxin Reductase Mutants.

Jon Ramsey – Mouse thioredoxin reductase shows a selenocysteine requirement in the terminal redox center for catalytic efficiency.

Fall 2004
Shaina Byrne – Creation of a Semisynthetic Thioredoxin Reductase

Nicholas James – Optimizing the Expression of Thioredoxin Reductase.
Fall 2005
Adam Lothrop – Synthesis of a Phosphorothioate Substrate Analog to Investigate the Role of His119 of RNase A in Catalysis.

Spring 2006
Amy Branagan **-** The Dependence of Thioredoxin Reductase Catalysis on Substrate pK_a.

Fall 2007
Todd Byrne – Redox potential of a vicinal disulfide

GRADUATE STUDENTS

Brian Eckenroth – (2002 –2007) Ph.D. Biochemistry 2007 – The Mechanism of High M_r Thioredoxin Reductase Investigated by Semisynthesis and Crystallography

Brian Lacey – (2003 – 2007) M.S. Biochemistry 2007 – Investigation into the Role of the C-Terminal Vicinal Cysteine Residues in High M_r Thioredoxin Reductases.

Adam Lothrop – (2005 to present) Ph.D. Biochemistry candidate

UNDERGRADUATE STUDENTS

Erin. Chicoine – (2005 –2006) B.S. Biosciences – Crystallization of TR/Trx complex

Dov Pechenick – (2005 –2006) B.S. Microbiology – Biosynthesis of Selenocysteine Using *O*-Acetylsulfhydryl Synthetase (honors thesis).
MMG Award – Warren R. Stinebring Outstanding Senior Award
Distinguished Undergraduate Research honors thesis from CALS for work in my laboratory

Alejandro Lopez – (Spring 2007) – Methods for making disulfide bonds,

Christine Fitzsimmons (2007 – present)– Methods for making disulfide bonds, Currently working on honors thesis from CALS

SUMMER STUDENTS

Adam Lothrop (St. Michael's College, VT)	Summer 2003(**SURE**)*****	Synthetic substrates for RNase A
Kevin Laxton (Oregon State University, OR)	Summer 2004 (**SURE**)*****	Purification of thioredoxin.
Adam Lothrop (St. Michael's College, VT)	Summer 2004(**RUBY**)	Synthetic substrates for RNase A
Erin Chicoine (UVM)	Summer 2005 (**HELiX)**	Crystallization of TR complex.
Sarah Abdallah (SUNY-Plattsburgh)	Summer 2007	Synthesis of Hepcidin.

***SURE (S**ummer **U**ndergraduate **R**esearch **E**xperience**)** – This was a NIH funded program (Dr. Christopher Francklyn, PI) to train students from engineering, mathematics, and computer sciences in the biochemical sciences. Every faculty member of my Department took a summer student for 9 weeks. Each student received a stipend of $4500 and the preceptor received $500 for supplies for the project.

SERVICE

DEPARTMENTAL SERVICE:

Graduate Student Recruitment Committee 2003-current Chair 2007 – current.

Graduate Student Recruiting Trips:
2002 Boston ACS Undergraduate Day
2003 Boston ACS Undergraduate Day
2003 SUNY-Plattsburgh recruiting trip with Dr. Scott Morrical.
2004 Boston ACS Undergraduate Day
2005 Boston ACS Undergraduate Day

Organized Recruiting Visit by St. Michael's College – The Department has a tradition of hosting students and faculty from St. Anselm's College on a yearly basis to try and recruit undergraduate students into our graduate program. To extend this idea I organized a visit of interested students from St. Michael's College in Colchester, VT. This will be an annual event.

Organized Recruiting Visit of SUNY-Plattsburgh Students – Organized a visit of nine students from SUNY-Plattsburgh to visit the Department and the College of Medicine. I organized a series of talks from faculty members and human resources. I also gave a tour to the students of the campus core scientific facilities. April 27th 2007.

Graduate Teaching Assistant Committee Chair 2005-current. –This committee evaluates what courses in the Department need a teaching assistant and then assigns a student to that course based on their individual talents.

Ad hoc Committees
Master's Program. I served as chairman of a committee charged with revising the requirements for the M.S. degree. The submitted plan was adopted by the faculty as our current policy on the Master's degree program.

Teaching Assistants. I served as chairman of a committee charged with writing job descriptions for teaching assistants and to devise a plan to integrate our new undergraduate courses (especially the laboratories) into our teaching rotation. The submitted plan was adopted as Departmental policy for graduate students as teaching assistants.

COLLEGE OF MEDICINE:

Director of UVM Protein Core Facility – I was able to develop this new core facility at UVM when the NIH Shared Instrumentation Grant that I wrote was funded. Major equipment in the core consists of a Symphony peptide synthesizer, one analytical HPLC system, one preparative HPLC system, and a Virtis freeze-dryer. The core also manages the PE Voyager Pro MALDI-TOF mass spectrometer. Our main mission is to synthesize peptides on a fee for use basis and provide them at a low cost to UVM researchers. Please see our website at http://proteins.uvm.edu.

Faculty Nominating Committee (2005-2008)

UNIVERSITY SERVICE:
University Committees –

AD-HOC

DEPSCoR Review Panel (Fall 2005) – We selected grants to be Vermont's representatives to the DoD EPSCoR competition for fiscal year 2006. A total of twelve grants were reviewed.

HELiX Fall Mini-Grant Committee Meeting (Fall 2007) – We reviewed HELiX grant applications that will be awarded in the Spring of 2008.

VT EPSCoR Review Panel (Fall 2007) This review panel met on December 7th, 2007 to review 16 proposal for SBIR Phase (0) review.

Assessment of Library and Information Needs of Basic Science Researchers – Participated in a one hour interview with Laura Haines (PI) of the Dana Medical Library to help asses and improve the library's services. January 4th, 2008.

Standing

Faculty Senate – Curricular Affairs Committee (2007 - 2010)

Faculty Advisor for UVM Biochemical Society. This club began in the all of 2005 and was subsequently recognized by the Student Government Association (SGA) at UVM. The club is open to all undergraduates interested in biochemical sciences. The purpose of the club is to facilitate student's interest in research and to provide a forum for undergraduates to learn about careers in the biochemical sciences. This club was initiated by myself, Dr. Margaret Daugherty (no longer at UVM), and enthusiastic biochemistry undergraduates. The club has created a website which can be found at http://www.uvm.edu/~nmahany/ and our constitution can be found on the SGA website at http://www.uvm.edu/~sgaclubs/club_detail.php?CID=177. The club has been dormant for the past 1.5 years and we are waiting for enthusiastic undergraduates to reactivate it.

Activities that I helped mentor:

1. Organized UVM Faculty-Student Fora as an event for undergraduates to come and meet faculty (October 3rd, 2005). The purpose of the event was to allow undergraduates to come and identify and research mentors. This was attended by ~15 faculty members and close to 40 undergraduate students. Each faculty member presented a poster and students were able to chat with faculty members about their research in an informal setting. The event was a huge success.

2. Organized a student trip to New England Biolabs (November 4th, 2005). New England Bioloabs is a biotechnology company located in Beverly, MA and is the largest producer of DNA restriction enzymes in the United States. Please see their website at http://www.neb.com. The purpose of the visit was to educate students about careers in the biotechnology industry.

3. Accompanied club officers to ACS Undergraduate Day (November 5th, 2005). The club president and treasurer attended this meeting with me to learn about other clubs and careers in science.

4. Invited Don Malenfant of Fisher Scientific to speak to club. Don spoke to the students about careers in scientific sales.

5. Invited Dr. Sean Field of the UVM History Department to give a talk on the "Black Death". His talk was entitled *The Black Death: Tales from a Fourteenth-Century Pandemic.* His talk was received with great enthusiasm by the students present.

NATIONAL SERVICE

Ad-hoc Peer Review for Granting Agencies

NIH Small Business Initiative Study Section (2003)
Petroleum Research Fund (American Chemical Society) (2005)
NIH Respiratory Integrative Biology and Translational Research (RIBT) Study Section (2007)
NIH (MSFE) Study Section (2008)

Ad-hoc Reviewer for the following journals:
1. *Journal of the American Chemical Society*
2. *Cellular and Molecular Life Sciences*

3. *Life Sciences*
4. *Nucleic Acids Research*
5. *Biochemistry*
6. *Antioxidants and Redox Signaling*
7. *Journal of Organic Chemistry*

Symposia

Northeast Regional Meeting of the American Chemical Society (NERM) 2008 Symposium Chair – Organizing and Chairing a Symposium at NERM 2008 entitled “Peptides as Tools to Study Protein Function”

Richard MacLeod Single

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Education

Ph.D. Statistics, State University of New York at Stony Brook, 1995
Thesis in Statistical Genetics, titled “An Application of Robust Estimation to Linkage Analysis”
Advisor: Stephen Finch

M.S. Applied Mathematics, State University of New York at Stony Brook, 1992

B.S. Mathematics, *summa cum laude*, State University of New York at Albany, 1990
Minors: Physics, Music. Phi Beta Kappa

Work Experience

University of Vermont, Burlington VT (2001 – present)
Assistant Professor, Department of Mathematics and Statistics (2004 – present)
Research Assistant Professor, Department of Medical Biostatistics (2001 – 2004)

St. Michael’s College, Colchester, VT (2000 – 2001)
Assistant Professor, Department of Mathematics

University of California at Berkeley, Berkeley, CA (1999 – 2000)
Postdoctoral Research Associate, Department of Integrative Biology

Environmental Risk Analysis, San Mateo, CA (1998 – 1999)
Research Scientist

St. Olaf College, Northfield, MN (1995 – 1998)
Assistant Professor, Department of Mathematics
Director of Statistics Program (1996 – 1998)

Software Developed

EMhaplofreq: software for the estimation of multilocus haplotype frequencies and linkage disequilibrium. Copyright © 2003 **–** 2007. The Regents of the University of California, under the terms of the GNU General Public License.

PyPop: A Software Framework for Population Genomics. Copyright © 2003 **–** 2007. The Regents of the University of California, under the terms of the GNU General Public License **(**http://www.pypop.org/ or http://www.uvm.edu/~pypop/).

Refereed publications in print and in press

The publications listed below are organized by the three major areas of my research and scholarship: 1) Immunogenetics and Statistical Genetics, 2) Medical Biostatistics, 3) Education and Program Evaluation. A one page overview of my research is available at *www.uvm.edu/~rsingle/summary.pdf* .

1) Immunogenetics and Statistical Genetics

Kulkarni S, Single RM, Martin MP, Joshi N, Badwe R, and Carrington M. Comparison of the Rapidly Evolving KIR Locus in Parsis and Natives of India. *Immunogenetics*. In press.

Single RM*, Martin MP*, Gao X, Meyer D, Yeager M, Kidd JR, Kidd KK, Carrington M. Global diversity and evidence for co-evolution of KIR and HLA genes. *Nature Genetics,* 2007; 39(9): 1114-1119. *joint first authors.

Single RM, Meyer D, Mack SJ, Lancaster A, Erlich HA, Thomson G. Biostatistics and Anthropology/Human Genetic Diversity joint report: Overview of progress in methodology, data collection, and analyses. *Tissue Antigens,* 2007; 69: 185-187.

Mack SJ, Sanchez-Mazas A, Single RM, Meyer D, Hill J, Dron HA, Jani AJ, Thomson G, Erlich HA. Biostatistics and Anthropology/Human Genetic Diversity joint report: Population samples and genotyping technology. *Tissue Antigens*, 2007; 69: 188-191.

Lancaster AK, Single RM, Nelson MP, Solberg O, Thomson G. PyPop update - a software pipeline for large-scale multi-locus population genomics. *Tissue Antigens*, 2007; 69: 192-197.

Gourraud PA, Cambon-Thomsen A, Dauber EM, Feolo M, Hansen J, Mickelson E, Single RM, Thomsen M, Mayr WR. Nomenclature for HLA microsatellites. *Tissue Antigens*, 2007; 69: 210-213.

Meyer* D, Single* RM, Mack SJ, Erlich H, and Thomson G. Signatures of demographic history and natural selection in the human MHC loci. *Genetics,* 2006; 173: 2121-2142. *joint first authors.

Gao X, Single RM, Karacki P, Marti D, O'Brien SJ, and Carrington M. Diversity of MICA and linkage disequilibrium with HLA-B in two North American populations. *Human Immunology,* 2006; 67: 152-158.

Malkki* M, Single* R, Carrington M, Thomson G, and Petersdorf E. MHC microsatellite diversity and linkage disequilibrium among common HLA-A, HLA-B, DRB1 haplotypes: Implications for unrelated donor hematopoietic transplantation and disease association studies. *Tissue Antigens*, 2005; 66: 114-124. *joint first authors.

Chen JJ, Duan T, Single RM, Mather KA, and Thomson G. Hardy-Weinberg testing of a single homozygous genotype. *Genetics,* 2005; 170: 1439-1442.

Williams F, Meenagh A, Single R, McNally M, Kelly P, Nelson MP, Meyer D, Lancaster A, Thomson G, and Middleton D. High resolution HLA-DRB1 identification of a Caucasian population. *Human Immunology*, 2004 Jan; 65(1): 66-77.

Cao K, Moormann AM, Lyke KE, Masaberg C, Sumba OP, Doumbo OK, Koech D, Lancaster A, Nelson M, Meyer D, Single R, Hartzman RJ, Plowe CV, Kazura J, Mann DL, Sztein MB, Thomson G, and Fernandez-Viña M. Diversity of HLA class I-A, B and C alleles and haplotypes in five African populations. *Tissue Antigens*, 2004; 63(4):293-325.

Nicklas JA, Brooks EM, Hunter TC, Single R, and Branda RF. Development of a quantitative PCR (TaqMan) assay for mitochondrial DNA copy number and the common mitochondrial DNA deletion in the rat. *Environmental and Molecular Mutagenesis,* 2004; 44:313-320.

Lancaster A, Nelson MP, Meyer D, Thomson G, and Single RM. PyPop: A software framework for population genomics: Analyzing large-scale multi-locus genotype data. *Pacific Symposium on Biocomputing*, 2003; 514-25.

Single RM, Meyer D, Hollenbeck J, Nelson M, Noble JA, Erlich HA, and Thomson G. Haplotype frequency estimation in patient populations: The effect of departures from Hardy-Weinberg proportions and collapsing over a locus in the HLA region. *Genetic Epidemiology,* 2002; 22:186-195.

Gordon D, Finch SJ, Jacobs AL, Mendell NR, Single RM and Marr TG. Association of posterior p-values of S.A.G.E. SIBPAL proportion-IBD and Haseman-Elston statistics for ACTHR 112. *Genetic Epidemiology*, 1997; 14:629-634.

Single RM and Finch SJ. Gain in efficiency from using Generalized Least Squares in the Haseman Elston procedure. *Genetic Epidemiology*, 1995; 12:889-894.

2) Medical Biostatistics

Privette A, McCahill L, Borrazzo E, Single RM, Zubarik R. Laparoscopic approaches to resection of suspected gastric gastrointestinal stromal tumors based on tumor location. *Surgical Endoscopy*, 2007/8; [Epub ahead of print].

McCahill LE, Ahern JW, Gruppi LA, Limanek J, Dion GA, Sussman JA, McCaffrey CB, Leary DB, Lesage MB, and Single RM. Enhancing compliance with Medicare guidelines for surgical infection prevention: Experience with a cross-disciplinary quality improvement team. *Archives of Surgery*, 2007 142: 355-361

Cook AD, Single R, and McCahill LE. Utilization of surgical resection of primary tumors in patients presenting with Stage IV colorectal cancer: An analysis of SEER data, 1988-2000. *Annals of Surgical Oncology*, 2005; 12(8): 637-645.

Krag, DN, Julian, TB, Harlow, SP, Weaver, DL, Ashikaga, T, Bryant, J, Single, RM, and Wolmark, N. NSABP-32: Phase III, Randomized trial comparing auxiliary resection with sentinel lymph node dissection: A description of the trial. *Annals of Surgical Oncology,* 2004; 11: 208S-210.

Krag D and Single RM. Breast cancer survival according to number of nodes removed. *Annals of Surgical Oncology*, 2003; 10: 1152-1159.

Stokes IA, Henry SM, and Single RM. Surface EMG Electrodes do not accurately record from lumbar multifidus muscles. *Clinical Biomechanics*, 2003 Jan; 18(1):9-13.

3) Education and Program Evaluation

Kasprisin CA, Single PB, Single RM, Muller CB, and Ferrier, JL. Improved mentor satisfaction: Emphasizing protégé training for adult age mentoring dyads. *Mentoring and Tutoring*, in press.

Single, PB and Single, RM. E-mentoring for social equity: Review of research to inform program development. *Mentoring and Tutoring*, 2005; 13(2): 303-322.

Single PB, Muller CB, Cunningham CM, Single RM, and Carlsen WS. MentorNet: E-mentoring for women students in engineering and science. *Journal of Women and Minorities in Science and Engineering*, 2005; 11(3), 295-309.

Kasprisin CA., Single PB, Single RM, and Muller CB. Building a better bridge: Testing e-training to improve e-mentoring programs in higher education. *Mentoring and Tutoring*, 2003; 11(1): 67-78.

Single RM. 52,467 + 57,204 = 254,281,227? Using the National Health Interview Survey and the 2000 Census to introduce statistical sampling and weights. *Journal of Statistics Education*, 2000; 8. (http://www.amstat.org/publications/jse/v8n1_abstracts.html)

Single PB, Muller CB, Cunningham CM, and Single RM. Electronic communities: A forum for supporting women professionals and students in technical and scientific fields. *Journal of Women and Minorities in Science and Engineering*, 2000; 6:115-129.

Single RM. Difference quotients, derivates, and data through modeling. *PRIMUS: Problems, Resources, and Issues in Mathematics Undergraduate Studies*, 1999; 9:279-288.

Refereed Book Chapters

Single, PB and Single, RM. Mentoring and the technology revolution: A literature review on how face-to-face mentoring set the stage for e-mentoring. In: F. K. Kochan & J. T. Pascarelli, eds., Creating successful telementoring programs. Greenwich, CT: Information Age Press, 2005; 7-27.

Single RM, Meyer D, and Thomson G. Statistical methods for analysis of population genetic data. In: J.A. Hansen, ed: Immunobiology of the Human MHC. Proceedings of the 13th International Histocompatibility Workshop and Conference. Vol I, IHWG Press, Seattle, 2007; 518-522.

Single RM, Meyer D, Mack SJ, Lancaster A, Nelson MP, Fernández-Viña M, Erlich H, and Thomson G. Haplotype Frequencies and Linkage Disequilibrium among classical HLA genes. In: J.A. Hansen, ed: Immunobiology of the Human MHC. Proceedings of the 13th International Histocompatibility Workshop and Conference. Vol I, IHWG Press, Seattle, 2007; 705-746.

Single RM, Malkki M, Thomson G, Mather KA, Carrington M, and Petersdorf E. Linkage disequilibrium and HLA-A: B: DRB1 haplotype probabilities for Class I, II, III microsatellite markers in unrelated donor hematopoietic stem cell transplantation. In: J.A. Hansen, ed: Immunobiology of the Human MHC. Proceedings of the 13th International Histocompatibility Workshop and Conference. Vol I, IHWG Press, Seattle, 2007; 1372-1377.

Meyer D, Single RM, Mack SJ, Lancaster A, Nelson MP, Fernández-Viña M, Erlich H, and Thomson G. Single locus polymorphism of classical HLA genes. In: J.A. Hansen, ed: Immunobiology of the Human MHC. Proceedings of the 13th International Histocompatibility Workshop and Conference. Vol I, IHWG Press, Seattle, 2007; 653-704.

Lancaster A, Nelson MP, Single RM, Meyer D, and Thomson G. Software framework for the Biostatistics Core. In: J.A. Hansen, ed: Immunobiology of the Human MHC. Proceedings of the 13th International Histocompatibility Workshop and Conference. Vol I, IHWG Press, Seattle, 2007; 510-517.

Mack SJ, Sanchez-Mazas A, Meyer D, Single R, Tsai Y, and Erlich HA. Methods used in the generation and preparation of data for analysis in the 13th International Histocompatibility Workshop. In: J.A. Hansen, ed: Immunobiology of the Human MHC. Proceedings of the 13th International Histocompatibility Workshop and Conference. Vol I, IHWG Press, Seattle, 2007; 564-579.

Thomson G, Hongzhe L, Dorman J, Lie BA, Mignot E, Steenkiste A, Thorsby E, Akey J, McWeeney S, and Single RM. Statistical approaches for analyses of HLA-associated and other complex diseases. In: J.A. Hansen, ed: Immunobiology of the Human MHC. Proceedings of the 13th International Histocompatibility Workshop and Conference. Vol I, IHWG Press, Seattle, 2007; 782-787.

Mickelson E, Damodaran A, He P, Malkki M, Smith A, Petersdorf E, Carrington M, Harding A, Cambon-Thomsen A, Gagne K, Bignon J-D, Gebuhner L, Dubois V, Dormoy A, Tongio M-M, Bois M, Concannon P, Martin B, Lie B, Thorsby E, Bétard C, Lathrop M, Mignot E, Schroeder M, Reveille J, Feolo M, Inoko H, Thomson G, Single R, and Hansen JA, on behalf of the IHWG Microsatellite Project and participating laboratories. Standardization of Microsatellite Data: Comparative Analysis of Results from 13th IHWS Participating Laboratories and Establishment of a Microsatellite Reference Panel and Standard Nomenclature. In: J.A. Hansen, ed: Immunobiology of the Human MHC. Proceedings of the 13th International Histocompatibility Workshop and Conference. Vol I, IHWG Press, Seattle, 2007; 1277-1314.

Reports and manuals

Single RM, Mather KA, Mack SJ, Maiers M, Gragert L. A Comparison of HLA and Informative Microsatellite Markers for Population Group Assignment in Clustering. National Marrow Donor Program (NMDP) technical report, 2008.

Lancaster A, Nelson MP, Meyer D, and Single RM. PyPop User Guide: User Guide for Python for Population Genetics, Version 0.6.0. Available at http://www.uvm.edu/~pypop/docs and http://www.pypop.org/docs , Copyright © 2003-2007. Regents of the University of California.

Single PB, Cunningham CM, Single RM, Nepton CN, and Kirk L. 2000-01 MentorNet Research Project Evaluation Report, 2002; March; University of Vermont: Burlington, VT. Retrieved on February 4, 2004, from http://www.mentornet.net/documents/about/results/evaluation/00-01/00.01.YearEnd.Eval.Report.appendices.pdf

Single RM and Finch SJ. Properties of the Null Distribution of the GLS Test Statistic Applied to the Haseman-Elston Procedure. American Statistical Association Proceedings of the Epidemiology Section 1997.

Finch SJ, Yu Q, Lipfert FW, Baxter LA, Mendell NR, Thode HC Jr, Single RM and Gong H. Review of External Costs of Air Pollution with Respect to Human Health Effects. Technical Report, 1995; AMS Report 95-11.

Mendell NR, Lipfert FW, Finch SJ, Baxter LA, Grimson R, Larsen U, Single RM, Thode HC Jr, and Yu Q. Ozone Pollution and Human Mortality: A Review of Studies Applicable to Estimating the External Health Costs of Pollution. Technical Report, 1994; AMS Report No. 9413.

Papers in Progress

Single RM, Mack SJ, Lancaster AK, Erlich HA, Thomson G. A multi-locus asymmetric extension of the r-squared measure of linkage disequilibrium: Application to amino acid correlations in classical HLA genes. In preparation.

Single RM, Martin MP, and Carrington M. Statistical and population genetic methods for KIR genes typed for presence/absence. To be submitted to the journal *Immunogenetics*. In preparation.

Kennedy LJ, Modrell A, Groves P, Wei Z, Single RM, and Happ GM. Genetic diversity of the Major Histocompatibility Complex in Alaskan Caribou herds. Submitted to Tissue Antigens.

Solberg OD, Mack SJ, Lancaster AK, Single RM, Sanchez-Mazas A, Tsai Y, and Thomson G Meta-analysis of population-specific HLA allele-count data reveals further evidence for balancing selection. In preparation.

Privette A, McCahill LE, Borrazzo E, Zubarik R, Nicole Messier N, Single RM. Endoscopically assisted laparoscopic resections of submucosal gastric and GE junction tumors - A novel approach based on tumor location. Submitted to *Surgical Endoscopy*.

James TA, McCahill LE, Ratliff J, Ashikaga T, Single R, Sheehey-Jones H, Messier N, Stanley M, Krag D, Harlow S. Neoadjuvant therapy as a quality indicator in breast conservative surgery: Barriers to implementation. Submitted to *Archives of Surgery*.

Recent Presentations and Abstracts

“Global Diversity of KIR and HLA: Population-Level Evidence for Co-Evolution, Natural Selection, and Signatures of Demographic History” Richard M. Single, Maureen P Martin, Xiaojiang Gao, Diogo Meyer, Meredith Yeager, Judith R Kidd, Kenneth K Kidd, and Mary Carrington. American Society for Histocompatibility and Immunogenetics (ASHI), October 2007.

“KIR genes and risk of melanoma.” Maria Teresa Landi, Melissa Rotunno, Maureen P. Martin, Richard M. Single, Daniel Geraghty, Mary Carrington. American Association for Cancer Research. April 2007.

“Measuring Individual Surgeon Performance in Breast Cancer Surgery.” McCahill LE, James TA, Ratliff J, Single R, Sheehey-Jones H, Messier N, Stanley M, Krag D, Harlow S. The Society of Surgical Oncology 60th Annual Cancer Symposium, Washington DC, March 2007.

“Statistical methods for Population Genetics.” An invited presentation for the audio conference lecture series, Current Topics in Histocompatibility and Transplantation (http://www.ctht.info/), sponsored by the American Board for Histocompatibility and Immunogenetics and Georgetown University. August 2006.

“Haplotype Specific Heterozygosity (HSH) and an application to Unrelated Donor Search” An invited presentation for the National Marrow Donor Program (NMDP) Geocoding meeting. Minneapolis, MN. March 2006.

“Enhancing Compliance with Medicare Guidelines for Surgical Infection Prevention (SIP)- An institutional experience with a cross disciplinary quality improvement team.” Laurence E McCahill, John Ahern, Linda Gruppi, Jim Limanek, Jessica Sussman, Gail Dion, Christina McCaffrey, Richard Single. New England Surgical Society 87th Annual Meeting, Groton, CT. September 2006.

“Detection of statistical and functional correlates in HLA protein sequences using PyPop: a multi-locus population genomics software.” Alex Lancaster, Steven J. Mack, Richard M. Single, Owen Solberg, Henry A. Erlich, and Glenys Thomson. Society for Molecular Biology and Evolution. Tempe, Arizona. May 2006.

“Demographic history and natural selection in the MHC loci.” RM Single, D Meyer, SJ Mack, A Lancaster, H Erlich, M Fernandez-Viña, G Thomson. Australian Society for Immunology. Melbourne, Australia. December 2005.

“Analysis of microsatellite markers in unrelated HLA identical hematopoietic stem cell transplantation.” 14th International HLA and Immunogenetics Workshop. Richard M. Single. Melbourne, Australia. November 2005.

“Population genetic analyses: their contribution to disease studies.” 14th International HLA and Immunogenetics Workshop. Richard M. Single. Melbourne, Australia. November 2005.

“Signatures of demographic history and natural selection – a comparative study.” 14th International HLA and Immunogenetics Workshop. Richard M. Single. Melbourne, Australia. November 2005.

“Population genetic analyses of the 13th IHW anthropology data.” Glenys Thomson, Richard Single, Alex Lancaster, Diogo Meyer, Owen Solberg, Steven Mack, Henry Erlich. American Society for Histocompatibility and Immunogenetics. Washington, DC. October 2005.

“Worldwide polymorphism in classical human major Histocompatibility (HLA) genes.” Diogo Meyer, Richard Single, Steven J. Mack, Alex Lancaster, Mark P. Nelson, Henry Erlich, Marcelo Fernandez Viña, Glenys Thomson. American Society of Human Genetics. Toronto, Canada, October 2004.

“Potential role of MCM7 and Ki67 labeling indices in diagnosis and prognosis of low and high grade gliomas including glioblastoma multiforme (GBM).” Luo P, Single RM, Simmons-Arnold L, Pendlebury WW, Elhosseiny A, Leiman G, 25th Congress of the International Academy of Pathology. Brisbane, Australia. October 2004.

“Selection and demographic history in HLA genes.” Laboratory of Genomic Diversity, NCI-FCRC, Fredrick, MD. September 2003.

“Signatures of selection and demographic history in genes of the human MHC.” Meyer D, Single R, Mack S, Lancaster A, Nelson M, Fernandez-Vina M, Erlich H, and Thomson G. Joint Meeting of the Society for the Study of Evolution, Society of Systematic Biologists, and American Society of Naturalists, Chico, CA. June 2003.

Research Support

Donor Genetic Clustering. PI: Richard Single; Agency: National Marrow Donor Program (NMDP); $42,700; 1/1/07-12/31/07.

Computational Infrastructure for the Relocation, Maintenance, and Expansion of the PyPop Software Development Project for the Analysis of Large-Scale Genomic Data at UVM. PI: Richard Single; Vermont Advanced Computer Center Research Planning Grant; $5,000; 10/1/05-7/31/07.

Initiative in Structural Biology and Computational Biology/Bioinformatics, Phase II. PI: Susan Wallace, UVM; DOE EPSCOR-FG0200ER45828; Support: 2004 - 32% FTE, 2005 - 50% FTE; 9/1/04-6/30/06.

International Histocompatibility Working Group: Core B Biostatistic, PI: Richard Single for subcontract with Fred Hutchinson Cancer Research Center (John Hansen, PI); NIH/NIAID-U24AI49213; $99,788 (subcontract); 1/1/03-6/30/05.

International Histocompatibility Working Group. PI: John Hansen, Fred Hutchinson Cancer Research Center, Richard Single, consultant through UVM Bioinformatics facility; NCI/R24CA84497; $72,560; 7/1/01-12/31/02.

Cancer Center Core Support Grant (Biostat Core). PI: David Yandell, UVM; NCI/P30CA22435; Support: 2001-2002 – 35% FTE, 2003 - 25% FTE; 9/1/01-8/31/04

Sentinel Node versus Axillary Dissection in Breast Cancer. PI: David Krag; NCI/UO1CA74137; Support: 20% FTE; 9/1/01-6/30/03

Proposals Under Review

Comparative genomic analysis of selection and demographic history in immune-related genes in worldwide populations, with a focus on Amerindian populations. Fellowship application submitted to the Fulbright Scholar Program in response to award #8528 (São Paulo Science/Technology, Brazil).

Statistical methods for population genetic analysis of the human immune genes and the Immunology Database and Analysis Portal (ImmPort). PI: Richard Single; Agency: Northrop Grumman Information Technology, Inc. (under NIH-NIAID-NO1-A1-40076); $45,000; Status: submitted.

Examining Models of Persistence for Women in College Engineering: Analysis of a National Longitudinal Database; Co-PI: Richard Single; Agency: U.S. Department of Education, Institute of Education Sciences - RFA# IES-NCER-2008-01, CFDA# 84.305; $366,000; Status: submitted.

Modeling the Coagulation Proteome. PI: Ken Mann, UVM; Agency: NIH/NHLBI; Role: co-investigator, $560,790 (Project 3); Status: declined (Priority Score: 195) after re-submission to the Special Emphasis Panel Exploratory Program in Systems Biology (R33). To be revised and submitted as an NIH Program Project Grant 01/2008.

Service

Department

Member of the Steering Committee for the Statistics program (2002 – present).

Member of Statistics Program curriculum committee (2002 – present).

Coordinator for the Statistics Student Association’s Journal Club (2004 – present).

College

Member of the College of Engineering and Mathematics Studies Committee (2003 – present).

University

Member of a National Cancer Institute Data Safety and Monitoring Committee, UVM (2001 – 2005).

Reviewer for the Protocol Review Committee of the Vermont Cancer Center (VCC) (2002 – 2004).

Member of the Genome Stability and Expression Program of the VCC (2004 – present).

State/National/International

Member of the editorial board for *Human Immunology*.

Invited member of a National Marrow Donor Program (NMDP) expert panel on Population Genetics for projecting optimal donor and cord blood registry sizes and predicting match rates for potential transplant recipients (Fall, 2007).

15th International Histocompatibility and Immunogenetics Workshop (IHIW) (2006 – present).

- Member of the Scientific Advisory Committee.
- Co-chair of the Anthropology/Human Genetic Diversity and Biostatistics Project.

Co-chair of the Biostatistical Analysis Project for the 14th IHIW (2002 – 2006).

Co-chair of the Microsatellite Working Group session at the 14th IHIW (2005).

Assisted with questionnaire design and analysis for the Vermont State Department of Education on the School Readiness Assessment Initiative, 2002 - 2003.

Assisted with questionnaire design and analysis for the Vermont Agency of Human Services on Vermont's Youth Risk Behavior Survey and a project investigating mediators of child well-being in lowincome families, 2002 - 2003.

Reviewer for *Genetic Epidemiology, American Journal of Human Genetics, Human Immunology, European Journal of Human Genetics, Tissue Antigens, Genes and Immunity, the American Statistician,* and the *Journal of Statistics Education*.

Graduate Advising

Chairperson of the Ph.D. Dissertation Examination Committee for Yan Zhang: “Noise Modeling and Correction for Supervised Learning”. Advisor: Xindong Wu, Computer Science. 2007.

Chairperson of the Ph.D. Dissertation Examination Committee for Juan Carlos Pizarro: “Ecogenetics of Triatoma infestans, The main vector of Chagas disease in Chuquisaca, Bolivia”. Advisor: Lori Stevens, Biology. 2006.

Advisor for Doug Dickey on a master’s research project on the impact of collapsing over low frequency alleles in tests of Hardy-Weinberg proportions for multi-allelic data. UVM, 2006-2007.

Advisor for Brien Aronov on a master’s research project on the Markov Chain Monte Carlo approximation of the exact test for deviation from Hardy-Weinberg proportions for multi-allelic data. This project involved assessing the convergence of the Markov chain for sparse tables and determining the sensitivity of results to chain length. UVM, 2005-2006.

Advisor for Joan Mongeon on a master’s research project – “A comparison of two measures of linkage disequilibrium” at UVM, 2004.

Statistical Advisor for Amy Poisson on a Master’s Thesis – “Recombination hot spots are associated with diminished levels of linkage disequilibrium within the human MHC” at Hood College and the Laboratory of Genomic Diversity at NCI Frederick, 2004.

Advisor for Scott Wakefield, an Accelerated Master’s Program student in CS, for his project in Parallel Algorithms and Programming Technique – “Parallelization of a program for haplotype frequency estimation” at UVM, 2003.

Consulting

Consulting for the Richmond Southeast Shoreline Area (RSSA) Community Advisory Group (CAG) Toxics Committee (Jean Rabovsky, Ph. D. & Michael Esposito, Ph.D., chairs) on sampling procedures to determine background levels of arsenic, PCB, radionuclide, and other toxins at a former industrial site adjacent to residential area in Richmond, CA. A technical report was issued in March 2007 addressing issues related to a proposed residential expansion onto the contaminated site.

Consulting with Dr. Beverley Wemple in the Department of Geography at UVM on two projects. The first involved a spatial model of atmospheric deposition in the NE US. The second involved the use of regression tree analysis for a study of soil nitrification rates, vegetation, and topographic properties at sampling sites for 10 watersheds across New England.

Consulting with Lisa Barcellos on T1DGC

Updated 1/04/2008

Appendix 3

Graduate Fellowships Awarded Phase I and Phase II

Graduate Fellowships Awarded Phase I and Phase II

1. Student: **Ty Adams** (2000-2002)
   Project: Understanding coagulation through structure – the crystal structure of bovine factor Va
   Mentor: Stephen Everse, Ph.D.
   Program: Biochemistry
   Publications: **Adams, T.E.**, Everse, S.J., and Mann, K.G. Predicting the Pharmacology of Thrombin Inhibitors. *J Thromb Haemost.* 2003 1(5):1024-7.
   Adams, T.E., Mason, A.B., Halbrooks, P.J., Briggs, S.K., Smith, V.C., MacGillivray, R.T., and Everse, S.J. The Position of Arginine 124 Controls the Rate of Iron Release from the N-lobe of Human Serum Transferrin: A Structural Study. *J. Biol. Chem.* 2003 278(8):6027-33.
   Degree Awarded: Ph.D., 2004
   Present Position: Postdoctoral Associate, Department of Haematology Cambridge Institute for Medical Research, Cambridge, United Kingdom

2. Student: **Anthony Aidoo** (2000-2002)
   Project: Studies on a prototype channel geometry for acetylcholine receptor channel.
   Mentor: Daniel Bentil, Ph.D.
   Program: Mathematics and Statistics
   Publications: **Aidoo A.** (2003) The Effect of Channel Geometry on the Electrostatic Potential in Acetylcholine Channels. *Mathematical Biosciences,* 186(2) 175-189.
   Aidoo, A. (2004) Prototype acetylcholine channel geometry. *Mathematical and Computer Modelling.* 40(3-4) 271-283.
   Degree Awarded: Ph.D., 2002
   Present Position: Assistant Professor, Mathematics and Computer Science, Eastern Connecticut State University,

3. Student: **Peter Brescia** (2000-2001)
   Project: Solution structure of the human Grb7-SH2 domain
   Mentor: Barbara Lyons, Ph.D.
   Program: Biochemistry
   Publications: **Brescia, P.J**., Ivancic, M. and Lyons, B.A. (2002) Assignment of backbone 1H, 13C, and 15N resonances of human Grb7-SH2 domain in complex with a phosphorylated peptide ligand. *J Biomol NMR.* **23**:77-78.
   Degree Awarded: M.S., 2007
   Present Position: Technical Engineer, BioTek, Winooski, Vermont

4. Student: **Karen Champagne** (2001-2003)
   Project: Novel regulatory functions of the Class II aaRS catalytic domain: a crystallographic analysis
   Mentor: Christopher Francklyn, Ph.D.
   Program: Microbiology and Molecular Genetics

Publications: Bovee, M., **Champagne, K.**, Demeler, B. and Francklyn, C.S. (2002) The quaternary structure of the HisZ-HisG *N*-1-(5'-Phosphoribosyl)-ATP transferase from *Lactococcus lactis*. *Biochemistry* 41:11838-11846.

Champagne, K.S., Sissler, M., Larrabee, Y., Doublie, S., and Francklyn, C.S. (2005) Activation of the hetero-octameric ATP phosphoribosyl transferase through subunint interface rearrangement by a tRNA synthetase paralog. *Journal of Biological Chemistry*. 280(40):34096-104.

Champagne, K.S., Piscitelli, E., and Francklyn, C.S. (2006) Substrate Recognition by the Hetero-octameric ATP phosphoribosyltransferase from *Lactococcus lactis*. *Biochemistry*. 45(50):14933-43.

Degree Awarded: Ph.D., 2005
Present Position: Postdoctoral Associate, University of California at Santa Cruz

5. Student: **Ben Millard** (2000-2001)
Project: Differential and combinatorial crystallography applied to the design of SH2 domain inhibitors
Program: Cell and Molecular Biology
Mentor: Mark Rould, Ph.D.
Publications: **Millard, B.J.**, Connolly, J.P., and Rould, M.A. Crystallographic Determination of the Ligand Binding Constellation of the Grb7 SH2 domain. In preparation.
Degree Awarded: M.S., 2002
Present Position: Biotech company in Wisconsin

6. Student: **Hang Xu** (2001-2002)
Project: Crystal structure of UvsY, a recombination mediator protein in bacteriophage T4
Mentor: Scott Morrical, Ph.D.
Program: Biochemistry
Publications: Bleuit, J.S., **Xu, H.**, Ma, Y., Wang, T., Liu, J. and Morrical, S.W. (2001) Mediator proteins orchestrate enzyme-ssDNA assembly during T4 recombination-dependent DNA replication and repair. *Proc. Natl. Acad. Sci. USA* **98**(15):8298-305.

Xu, H., Wang, Y., Bleuit, J.S. and Morrical, S.W. (2001) Helicase assembly protein Gp59 of bacteriophage T4: fluorescence anisotropy and sedimentation studies of complexes formed with derivatives of Gp32, the phage ssDNA binding protein. *Biochemistry* **40**(25):7651-7661.

Degree Awarded: Ph.D., 2005
Present Position: Staff Scientist, National Laboratory of Biomacromolecules, Institute of Biophysics, Chinese Academy of Science, P.R. China

7. Student: **James C. Morris** (2002)
Project: Magnetic labeling of protein substructures with Fe(III) probes
Mentor: Scott Gordon-Wylie, Ph.D.
Program: Chemistry

Publications: Gordon, S., **Morris, J.C.**, Lyons, B.A., Ivancic, M., Rould, M. and Hayes, E. Magnetic labeling of lysozyme substructures with Fe(III) probes. In preparation.
Degree Awarded: Ph.D. 2007
Present Position: Lecturer, Department of Chemistry, University of Vermont

8. Student: **Tom Tucker** (2002)
   Project: Evolutionary algorithms for host pathogens coevolution
   Mentor: Lori Stevens, Ph.D.
   Program: Biology
   Publications: **Tucker, T.** M. and Stevens, L. Geographic variation and sexual dimorphism pf phenoloxidase in Japanese beetles *(Popillia japonica)*. *Proceedings of the Society of London, Series B.* 270:S245-7.
   Degree Awarded: M.S., 2004
   Present Position: Cytogenetic Technologist II, Nebraska Medical Center, University of Nebraska

9. Student: **Wei Zhang** (2000-2001, 2003-2004)
   Project: Estimation of DNA sequence context-dependent mutation rates using Markov Chain Monte Carlo method
   Mentor: Jeffrey Bond, Ph.D.
   Program: Microbiology and Molecular Genetics
   Publications: **Zhang, W.**, Bouffard, G.G., Wallace, S.S., NISC Comparative Sequencing Program, and Bond, J.P. Estimation of DNA sequence context-dependent mutation rates using primate genomic sequences. *J. Mol. Evol.* **65**(3):207-14.
   Zhang, W., Wallace, S.S. and Bond, J.P. Somatic amino acid substitutions in TP53: Separation of DNA mutation bias and bias based on protein functional selection. *Human Mutation.* Under Review.
   Degree Awarded: Ph.D., 2004
   Present Position: Postdoctoral Associate, University of Chicago

10. Student: **Yin Guo** (2003-2004)
    Project: Expression of four paralogs of the Fpg/Nei family in *Mycobacterium tuberculosism* determine their substrate specificities and enzymatic properties, and to determine the crystal structure of one or more of these proteins.
    Mentor: Susan Wallace, Ph.D.
    Program: Microbiology and Molecular Genetics
    Publications: **Guo, Y.** The successful use of a bicistronic vector in overexpressing a *Mycobacterium tuberculosis* Fpg/Nei homolog in *Escherichia coli*. In preparation
    Guo, Y. Characterization of *Mycobacterium tuberculosis* Fpg/Nei homologs. In preparation.
    Degree Awarded: Ph.D., expected 2008

11. Student: **Matthew Hogg** (2003-2004)
    Project: Error Dedetction by the Replicative DNA Polymerase from Bacteriophage RB69
    Mentor: Sylvie Doublié, Ph.D. and Susan Wallace, Ph.D.
    Program: Microbiology and Molecular Genetics
    Publications: **Hogg, M.**, Wallace, S.S., Doublié, S. Crystallographic snapshots of a replicative DNA polymerase encountering an abasic site. *EMBO J.* Apr 7;23(7):1483-93, 2004.
    Hogg, M., Wallace, S.S., Doublié, S. Bumps in the road: how replicative DNA23w3 polymerases see DNA damage. *Curr Opin Struct Biol.* **15**:86-93, 2005.
    Hogg, M., Cooper, W., Reha-Krantz, L., and Wallace, S.S. (2006) Kinetics of error generation in homologous B-family DNA polymerases. *Nucleic Acids Res.* **34**(9):2528-2535.
    Hogg, M., Aller, P., Konigsberg' W., Wallace, S.S. and Doublié, S. (2007) Structural and biochemical investigation of the role in proofreading of a beta hairpin loop found in the exonuclease domain of a replicative DNA polymerase of the B family. *J. Biol. Chem.* **282**:1432-1444.
    Aller, P., Rould, M.A., **Hogg, M.**, Wallace, S.S. and Doublié, S. (2007) A structural rationale for stalling of a replicative DNA polymerase at the most common oxidative thymine lesion, thymine glycol. *Proc. Natl. Acad. Sci. USA.* **104**:814-818. (selected by Faculty of 1000)
    Degree Awarded: Ph.D., 2005
    Present Position: Postdoctoral Associate, Microbiology and Molecular Genetics, University of Vermont

12. Student: **Osei Bonsu** (2003-2004)
    Project: Biological applications of evolutionary computation
    Mentor: James Hoffmann, Ph.D.
    Program: Botany
    Publications: Bentil, D.E., Ellingwood, C.D., **Osei, M.B**. and Hoffmann, J.P. On a unified model for growth based upon Schnute's postulates. Submitted to *Mathematical Biosciences*.
    Osei, B.M, Hoffmann, J.P., Ellingwood, C.D., Bentil, D.E. Probabilistic Uncertainty in Population Dynamics. *WSEAS Transactions on Biology and Biomedicine* 2(1): 51-56, 2005.
    Hoffmann, J.P., Ellingwood, C.D., **Bonsu, O.M**. and Bentil, D.E. Ecological model selection via evolutionary computation and information theory. Invited paper for special issue on biological applications of evolutionary computation. *Journal of Genetic Programming and Evolvable Machines* 5(2): 229-241, 2004.
    Bentil, D.E., **Bonsu O.M**., Ellingwood, C.D., Hoffmann, J.P. 2003. Deterministic uncertainty in population Growth, 4th IEEE International Symposium on Uncertainty Modeling and Analysis (ISUMA), CA, IEEE Computer Society Press, Los Alamitos, pp. 274 – 278, 2004.
    Hoffmann, J.P., Ellingwood, C.D., **Bonsu, O.M.** and Bentil, D.E. Turning genes off and on: Using genetic algorithms with complexity-based fitness

for model selection in ecology. Proceedings of the Genetic and Evolutionary Computation Conference (GECCO-2002), Workshop Special Session on Biological Applications of Evolutionary Computation, pp 38-40, 2002.

Degree Awarded: Ph.D., 2005

Present Position: Faculty member, Eastern Connecticut University

13. Student: **Peter Halbrooks** (2002-2003)

Project: Structural and functional investigation of human serum transferrin.

Mentor: Stephen Everse, Ph.D. and Anne Mason, Ph.D.

Program: Biochemistry

Publications: Mason, A. B., He, Q. Y., **Halbrooks, P. J.**, Everse, S. J., Gumerov, D. R., Kaltashov, I. A., Smith, V. C., Hewitt, J., and MacGillivray, R. T. A. (2002) Differential effect of a His tag at the N-and C-termini: Functional studies with recombinant human serum transferrin, *Biochemistry* 41, 9448-9454.

Adams T.E., Mason, A. B., He, Q.-Y., **Halbrooks, P. J.**, Briggs, S. K., Smith, V. C., MacGillivray, R. T. A., and Everse, S. J. (2003) The position of arginine 124 controls the rate of iron release from the N-lobe of human serum transferrin: A structural study, *J. Biol. Chem.* 278, 6027-6033.

Halbrooks, P. J., He, Q. Y., Briggs, S. K., Everse, S. J., Smith, V. C., MacGillivray, R. T. A., and Mason, A. B. (2003) Investigation of the Mechanism of Iron Release from the C-Lobe of Human Serum Transferrin: Mutational Analysis of the Role of a pH Sensitive Triad, *Biochemistry* 42, 3701-3707.

Halbrooks, P. J., Mason, A. B., Adams, T. E., Briggs, S. K., and Everse, S. J. (2004) The oxalate effect on release of iron from human serum transferrin explained, *J. Mol. Biol.* 339, 217-226.

Mason, A. B., **Halbrooks, P. J.**, Larouche, J. R., Briggs, S. K., Moffett, M. L., Ramsey, J. E., Connolly, S. A., Smith, V. C., and MacGillivray, R. T. A. (2004) Expression, purification, and characterization of authentic monoferric and apo-human serum transferrins, *Protein Expr. Purif.* 36, 318-326.

Mason, A. B., **Halbrooks, P. J.**, James, N. G., Connolly, S. A., Larouche, J. R., Smith, V. C., MacGillivray, R. T. A., and Chasteen, N. D. (2005) Mutational analysis of C-lobe ligands of human serum transferrin: insights into the mechanism of iron release, *Biochemistry* 44, 8013-21.

Lambert L. A., Perri H., **Halbrooks P. J.**, and Mason A. B. (2005) Evolution of the transferrin family: conservation of residues associated with iron and anion binding. *Comp. Biochem. Physiol. B Biochem. Mol. Biol.*, 142, 129-41.

Giannetti A. M., **Halbrooks P. J.,** Mason A. B., Vogt T. M., Enns C. A., and Bjorkman P. J. (2005) The molecular mechanism for receptor-stimulated iron release from the plasma iron transport protein transferrin. *Structure*, 13, 1613-23.

Halbrooks P. J., Giannetti A. M., Klein J. S., Bjorkman P. J., Larouche J. R., Smith V. C., MacGillivray R. T., Everse S. J., and Mason A. B. (2005) Composition of pH-sensitive triad in C-lobe of human serum transferrin. Comparison to sequences of ovotransferrin and lactoferrin provides insight into functional differences in iron release. *Biochemistry,* 44, 15451-60.

Wally, J., **Halbrooks, P. J.**, Vonrhein, C., Rould, M. A., Everse, S. J., Mason, A. B., and Buchanan, S. K. (2006) The crystal structure of iron-free human serum transferrin provides insight into inter-lobe communication and receptor binding. *J. Biol. Chem.* 281, 24934-44.

Degree Awarded: Ph.D., 2004
Present Position: Postdoctoral Fellow at Wyeth Pharmaceuticals, Cambridge, MA

14. Student: **Divya Singh** (2005)
    Project: Faster Sequence Alignment Using Suffix Tree and Data-Mining Techniques
    Mentor: Xindong Wu, Ph.D. and Abdullah Arslan, Ph.D.
    Program: Computer Science
    Publications: **Singh, D. R.** , Arslan, A. N, and Wu, X. (2006) Using an extended suffix tree to speed-up sequence alignment. IADIS International Conference on Applied Computing, pp. 655-660, San Sebastian, Spain, February 25-28, 2006
    Degree Awarded: M.S., 2005
    Present Position: IBM

15. Student: Na Qian (2003-2004)
    Project: Presynatpic filament assembly in T4 phage
    Mentor: Scott Morrical, Ph.D.
    Program: Biochemistry
    Publications: Liu J, **Qian N,** Morrical SW. Dynamics of bacteriophage T4 presynaptic filament assembly from extrinsic fluorescence measurements of Gp32-single-stranded DNA interactions. J Biol Chem. 2006 Sep 8;281 (36): 26308-19.
    Degree Awarded: M.S., 2005
    Present Position: Unknown

16. Student: **Lydia Nausch** (2003-2004)
    Project: Crystal structure of human poly(A) polymerase gamma
    Mentor: Sylvie Doublié, Ph.D.
    Program: Microbiology and Molecular Genetics (transferred from program)
    Publications: None
    Degree Awarded: Ph.D., 2007
    Present Position: Postdoctoral Associate, Pharmacology, University of Vermont

17. Student: **Brian Eckenroth** (2004-2006)
    Project: Structural studies of mammalian thioredoxin reductase
    Mentor: Robert Hondal, Ph.D.
    Program: Biochemistry
    Publications: **Eckenroth, BE,** Everse, SF, Adams, TE and Hondal, Rj. Crystallization of mammalian thioredoxin reductase for structural studies using synthetic active site peptides. *FASEB Meeting.* April 2-6 (2005), San Diego, CA. Abstract #2600. *FASEB Abstracts.*
    Eckenroth, BE, Rould, MA, Hondal, RJ and Everse, SF (2006) Structural and Biochemical Studies Reveal Differences in Catalytic Mechanisms between Mammalian and *Drosophila melanogaster* Thioredoxin Reductases. *Biochemistry 46*, 4694-4705.
    Eckenroth BE, Lacey BM, Lothrop AP, Harris KM, & **Hondal RJ** (2007) Investigation of the C-terminal Redox Center of High *M*r Thioredoxin Reductases by Protein Engineering and Semisynthesis. *Biochemistry 46*, 9472-9483.
    Eckenroth BE, Harris K, Turanov AA, Gladyshev VN, Raines RT, & Hondal, RJ. (2006) Semisynthesis and characterization of mammalian thioredoxin reductase. *Biochemistry 45*, 5158-5170.
    Degree Awarded: Ph.D., 2007
    Present Position: Postdoctoral Associate, Biochemistry, University of Vermont

18. Student: **Jie Liu** (2003-2004)
    Project: A dynamic view of T4 presynaptic filament assembly
    Mentor: Scott Morrical, Ph.D.
    Program: Biochemistry
    Publications: **Liu J,** Qian N, Morrical SW. Dynamics of bacteriophage T4 presynaptic filament assembly from extrinsic fluorescence measurements of Gp32-single-stranded DNA interactions. *J Biol Chem.* 2006 Sep 8;281(36):26308-19.
    Liu J, Bond JP, Morrical SW. Mechanism of presynaptic filament stabilization by the bacteriophage T4 UvsY recombination mediator protein. *Biochemistry.* 2006 May 2;45(17):5493-502.
    Bleuit JS, Xu H, Ma Y, Wang T, **Liu J,** Morrical SW. Mediator proteins orchestrate enzyme-ssDNA assembly during T4 recombination-dependent DNA replication and repair. *Proc Natl Acad Sci U S A.* 2001 Jul 17;98(15):8298-305. Review.
    Liu J, Berger C, Morrical SW.Kinetics of presynaptic filament assembly in the presence of SSB and mediator proteins. Submitted to *PNAS,* Jan. 2008
    Liu J, Morrical SW.Presynaptic filament dynamics in homologous recombination and DNA repair. Invited review in preparation for *CRC Crit. Rev. Biochem. Mol. Biol.,* February, 2008
    Degree Awarded: Ph.D., 2006
    Present Position: Postdoctoral Associate, University of California, Davis

19. Student: **Molly Coseno** (2004-2006)
    Project: Investigation of 3’ pre-mRNA processing factors by crystallographic techniques
    Mentor: Sylvie Doublié, Ph.D.
    Program: Microbiology and Molecular Genetics
    Publications: **Coseno, M.E.,** Martin, G., Gilmartin, G., Keller, W. and Doublié, S. Crystal structure of the 25 kDa subunit of human cleavage factor Im. *Nucleic Acids Res.* In press.
    Degree Awarded: Ph.D. expected 2008

20. Student: **Chunxiao Yu** (2004-2006)
    Project: Functional and structural analysis of EmaA (extracellular matrix protein adhesion A) from *Actinobacillus actinomycetemcomitans*
    Mentor: Keith Mintz, Ph.D.
    Program: Microbiology and Molecular Genetics
    Publications: **Yu, C.,** Lenox, C., Mintz, K. and Ruiz, T. (2006) Structural analysis of an extracellular matrix protein adhesion (EmaA) of *Acintobacillus actinomycetemcomitans.* 64th Annual Meeting of the Microscopy Society of America.
    Degree Awarded: Ph.D. expected 2008

21. Student: **Dan He** (2004-2006)
    Project: Development of a personalized PubMed entry recommender
    Mentor: Jeffrey Bond, Ph.D.
    Program: Computer Science
    Publications: None
    Degree Awarded: Left program

22. Student: **Joshua Payne** (2004-2006)
    Project: Computational modeling in ecology and evolution
    Mentor: Maggie Eppstein, Ph.D.
    Program: Computer Science
    Publications: Eppstein, M.J., **Payne, J.L.**, & Goodnight, C.J. “Underdominance, Multiscale Interactions, and Self-Organizing Barriers to Gene Flow.” *Submitted to* Artificial Life.
    Eppstein, M.J., **Payne, J.L.**, White, B.C., & Moore, J.H. “Genomic mining for complex disease traits with 'Random Chemistry.’” *Submitted to* Genetic Programming and Evolvable Machines.
    Payne, J.L., Eppstein, M.J., & Goodnight, C.J., “Sensitivity of Self-Organized Speciation to Long-Distance Dispersal.” Proceedings of the IEEE Symposium on Artificial Life, 2007, *in press*.
    Eppstein, M.J., **Payne, J.L.**, White, B.C., & Moore, J.H., "Hill-climbing through 'random chemistry' for detecting epistasis." Proceedings of the Genetic and Evolutionary Computation Conference, GECCO-2006, late-breaking papers.
    Eppstein, M.J., **Payne, J.L.**, & Goodnight, C.J. "Speciation by Self-Organizing Barriers to Gene Flow in Simulated Populations with Localized Mating."

Proceedings of the Genetic and Evolutionary Computation Conference, GECCO-2006, CODESOAR workshop.

Payne, J.L., Eppstein, M.J. "Emergent Mating Topologies in Spatially Structured Genetic Algorithms." Proceedings of the Genetic and Evolutionary Computation Conference, GECCO-2006. Eds. Keijzer, M. et al. pp.207-214.

Degree Awarded: Ph.D. expected 2009

23. Student: **Minmin Liu** (2006-2007)
    Project: Cloning, characterization and structure of mammalian DNA repair glycosylase, Neil3
    Mentor: Susan Wallace, Ph.D.
    Program: Microbiology and Molecular Genetics
    Publications: None
    Degree Awarded: Ph.D. expected 2009

Appendix 4

Research Projects Funded

Research Projects Funded

1. Algorithms for genetic rearrangement and mapping (07/01/00-06/30/01)
Investigators: Charles J. Colbourn, Ph.D., Department of Computer Science
Guoliang Xue, Ph.D., Department of Computer Science
Publications:

Alon, N., **Colbourn, C.J.,** Ling, A.C.H. and Tompa, M. (2001) Equireplicate Balanced Binary Codes for Oligo Arrays. *SIAM Journal on Discrete Mathematics* **14**:481-497.

Colbourn, C.J., **Ling, A.C.H.** and Tompa, M. (2002) Construction of Optimal Quality Control for Oligo Arrays. *Bioinformatics* **18**:529-535.

2. Structural characterization of cGMP-dependent protein kinase Ia and its complexes with high affinity inhibitors (7/1/00-6/30/02)
Investigators: Wolfgang Dostmann, Jose Madalengoitia, Mark Rould
Participants: Christian Nickl, Technician
Publications:

Dostmann WRG, Nickl CK, Taylor MS, Brayden JE, Frank R and Tegge WJ. Highly specific, membrane permeant peptide blockers of cGMP-dependent protein kinase Iα inhibit NO-induced cerebral dilation, *Proc Natl Acad Sci USA,* 97: 14772-14777 (2000)

Dostmann WRG, Nickl CK, Taylor MS, Brayden JE, Frank R and Tegge WJ A new class of cGMP-dependent protein kinase peptide inhibitors and their role in elucidating vasomotor mechanisms, *Pharm Ther,* 93: 203-215 (2002)

Dostmann WRG. Inhibitors of cyclic nucleotide dependent protein kinases, *Handbook of Cell Signaling,* 201: 487-493 (2003)

Taylor MS, Okwuchukwuasanya C, Nickl CK, Brayden JE and **Dostmann WRG,** Unique inhibitory properties of the cell-permeable cGMP-dependent protein kinase inhibitor DT-2 reveal a novel mechanism of vasoregulation, *Mol Pharm*, 65: 1111-1119 (2004)

Krieg T, Philipp S, Cui L, **Dostmann WR**, Downey JM, Cohen MV. Peptide blockers of PKG inhibit ROS generation by acetylcholine and bradykinin in cardiomyocytes but fail to block protection in the whole heart. *Am J Physiol* 288:H1976-81 (2005)

Zhu CB, Carneiro AM, **Dostmann WR,** Hewlett RA, and Blakely, RD, p38 MAPK Activation Elevates Serotonin Transport Activity via a Trafficking-Independent, PP2A-Dependent Process**,** *J Biol Chem,* 280: 15649-58, (2005)

Foley KF, De Frutos S, Laskovski KE, Tegge W and **Dostmann WR**. Culture conditions influence uptake and intracellular localization of the membrane permeable cGMP-dependent protein kinase peptide inhibitor DT-2, *Front Biosci* 10: 1302-1312 (2005)

Dey N, Foley KF, Lincoln TM and **Dostmann WR.** Inhibition of cGMP-dependent protein kinase-I attenuates contractile protein expression and contractile morphology in cultured rat aortic smooth muscle cells, *J Cardiovasc Pharm,* 45: 404-4123, (2005) Zhang R, Nickl CK, Mamai A, Flemer S, Natarajan A, **Dostmann WR, Madalengoitia JS,** Poly-L-Proline Type II Peptide Mimics as Probes of the Active Site Occupancy Requirements of cGMP Dependent Protein Kinase, *J Peptide Res*, 66:151-9, (2005)

Hou Y, Wong E, Martin J, Schoenlein P, **Dostmann WR** and Browning DD, A Role for cyclic-GMP dependent protein kinase in Anoikis, *Cell Signal,* 18:882-888 (2006)

Bove PF, Wesley UV, Greul AK, Hristova M, **Dostmann WR,** van der Vliet A. Nitric Oxide Promotes Airway Epithelial Wound Repair through Enhanced Activation of MMP-9, *Am J Respir Cell Mol Biol.* 2007 Feb;36(2):138-46.

Scholten A, Fuss H, Heck, AJR, **Dostmann, WR** The hinge region operates as a stability switch in cGMP-dependnt protein kinase I alpha, *FEBS J,* 2007 May;274(9):2274-86.

Extramural Funding:

Lake Champlain Cancer Research Organization (LCCRO):
Protein Transduction: Membrane translocation signals and their possible roles in cancer therapy.

$ 10,000	2001 – 2002

National Institutes of Health, NIH RO1 Public Health Service Grant,
HL68991-01 (PI): Exploring vasomotor mechanism using new PKG inhibitors

$ 1,540,000	2002 – 2006

3. Structural studies of TPBF1: A unique and repressor of the TBP gene (7/1/00 – 6/30/02)
Investigators: Erik Bateman and Mark Rould
Participants: Zhihua Peng, Ph.D., Peter Brescia, Technician

4. A Novel Approach for Developing and Evaluating PDE Models of the Spatial Spread of Invasive Species (7/1/00-6/30/02)
Investigators: James Hoffmann & Daniel Bentil
Participants: Osei Mensah Bonsu, Graduate Student
Adam Dow, Undergraduate Student

Publications:

Bentil, D.E., Ellingwood, C.D., Osei, M.B. and **Hoffmann, J.P**. 2007. Analysis of a Schnute Postulate-based Unified Growth Model for Model Selection in Evolutionary Computations. *BioSystems* 87: (In Press).

Hoffmann, J.P. 2006. Simultaneous Inductive and Deductive Modeling of Ecological Systems via Evolutionary Computation and Information Theory. Transactions of the Society for Modeling and Simulation International – Special Issue on Ecological and Environmental Simulation. *Simulation* 82 (7): 439-450.

Hoffmann, J.P. 2005. Darwin and Computational Ecology: How Simple Computational Models of Evolution Help our Search for Better Models of Ecological Systems. Keynote Address: In Proceedings of Open International Conference on Modeling and Simulation - *OICMS* 2005, Hill, D. R. C., V. Barra., and M. K. Troer (Eds.), Blaise Pascal University, France, pp 27-39.

Osei, B. M., **Hoffmann, J. P.** Ellingwood, C. D., and **Bentil, D.E.** 2005. Probabilistic Uncertainity in Population Dynamics. *WSEAS Transactions on Biology and Medicine* 1(2):51-56.

Hoffmann, J.P., Ellingwood, C.D., Bonsu, O.M. and **Bentil, D.E.** 2004. Ecological model selection via evolutionary computation and information theory. Invited paper for special issue on biological applications of evolutionary computation. *Journal of Genetic Programming and Evolvable Machines* 5(2): 229-241.

Bentil, D. E., Bonsu O. M., Ellingwood, C. D. **Hoffmann, J. P.** 2003. Deterministic uncertainty in population growth. 4th IEEE International Symposium on Uncertainty Modeling and Analysis (*ISUMA*). IEEE Computer Society Press, Los Alamitos, CA. pp 274 - 278

Hoffmann, J.P., Ellingwood, C.D., Bonsu, O.M. and **Bentil, D.E.** 2002. Turning genes off and on: Using genetic algorithms with complexity-based fitness for model selection in ecology. . Proceedings of the Genetic and Evolutionary Computation Conference (*GECCO-2002*) – Workshop Special Session on Biological Applications of Evolutionary Computation, pp 38-40.

Extramural Funding:
A Novel Approach for Developing and Evaluating PDE Models of the Spatial Spread of Invasive Species.
U.S. Department of Agriculture-Hatch
2000-2003 $45,000

5. Two novel methods to aid in the assignment of functions to open reading frames (07/01/00-06/30/02)

Investigators: Jeffrey P. Bond, Ph.D., Department of Microbiology and Molecular Genetics
Christopher Francklyn, Ph.D., Department of Biochemistry
Douglas S. Green, Ph.D., Department of Computer Science, St. Michael's College
Participants: Rama Kocherlakota, Research Associate, Microbiology and Molecular Genetics
Ramiro Barrantes-Reynolds, Information Systems Specialist, Microbiology and Molecular Genetics
Mingyuan Shao, Graduate Student, Microbiology and Molecular Genetics

6. Modeling the dynamics of solute exchange in the hemodialyzer domain: Applied mathematics and computational science (07/01/00-06/30/02)

Investigators: Daniel E. Bentil, Ph.D., Departments of Mathematics and Statistics, Computer Science, and Molecular Physiology & Biophysics

Participants: Edward Boamah, Graduate Student, Mathematics and Statistics
Vera Amponsah, Graduate Student, Electrical and Computer Engineering
Samuel Asiedu-Addo, Lecturer
Anthony Aidoo, Graduate Student, Mathematics and Statistics
Julius Dasah, Undergraduate Student

Publications:

Bentil, D.E. On the pseudo--steady state approximation model for diffusible enzyme-substrate and enzyme--inhibitor reactions with two intermediates. /Journal of Theoretical Medicine (Submitted)

7. Novel regulatory functions of the class II aaRS catalytic domain: a crystallographic analysis (7/1/00 – 6/30/03)

Investigators: Sylvie Doublié & Christopher Francklyn

Participants: Michael Bovee, Ph.D., Postdoctoral Research Associate, Karen Champagne, Graduate Student, Marque St. John, Graduate Student

Publications:

Bovee, M.L, Champagne, K.S., Demeler, B., & **Francklyn, C. S**. (2002) The HisZ-HisG N'-5-phosphoribosyl ATP transferase from *Lactococcus lactis* is an octamer. *Biochemistry* **41**: 11838-11846

Francklyn, C. (2003) tRNA Synthetase Paralogs: evolutionary links in the transition from tRNA-dependent amino acid biosynthesis to de novo biosynthesis. *Proc. Natl. Acad. Sci. U.S.A.* **100**: 9650-9652.

Francklyn, C.S. (2005) "tRNA Synthetase-like Proteins", in *The Aminoacyl-tRNA Synthetases.* (Ibba, M., Cusack, S., and **Francklyn, C.**, eds.) Landes Biosciences Publishing. Georgetown, Texas.

Champagne, K.S., Sissler, M., Larrabee, Y., **Doublie, S.**, and **Francklyn, C.S**. (2005) Activation of the hetero-octameric ATP phosphoribosyl transferase through subunint interface rearrangement by a tRNA synthetase paralog. *Journal of Biological Chemistry.* **280**(40):34096-104.

Champagne, K.S., Piscitelli, E., and **Francklyn, C.S**. (2006) Substrate Recognition by the Hetero-octameric ATP phosphoribosyltransferase from *Lactococcus lactis*. *In press*, *Biochemistry*.

8. Bioremediation of halogenated hydrocarbons: a structure-based mechanism (7/1/00-6/30/03)

Investigators: Kelvin Chu, Thomas Lewis

Participants: Scott Gordon-Wylie, Assistant Professor, Shanti Jeedigunta, Technician, James Morris, Graduate Student, Lisa Sitek, Graduate Student

Publications:

Schlichting, I. and **Chu K.** (2000) Trapping intermediates in the crystal: ligand binding to myoglobin. *Curr. Opin. Struct. Biol.* **10**:744-752.

Schlichting, I., Berendzen, J., **Chu, K.**, Stock, A.M., Maves, S.A., Benson, D.E., Sweet, R.M., Ringe, D., Petsko, G.A., Sligar, S.G. (2000) The catalytic pathway of cytochrome P450cam at atomic resolution. *Science* **287**:1615-1622.

Brunori, M., Vallone, B., Cutruzzola, F., Travaglini-Allocatelli, C., Berendzen, J., **Chu, K.**, Sweet, R. M. and Schlichting, I. (2000) The role of cavities in protein dynamics: crystal structure of a novel photolytic intermediate of myoglobin. *Proc. Natl. Acad. Sci. USA* **97**:2058-2063.

Lewis, T.A., Paszcynski, A., Gordon-Wylie, S.W., Jeedigunta, S., Lee, C.-H., and Crawford, R.L. (2001) Carbon tetrachloride dechlorination by the bacterial transition metal chelator pyridine-2,6-bis(thiocarboxylic acid). *Environ. Sci. Technol.* **35**:552-559.

Lewis, T.A., Gordon-Wylie, S.W., Jeedigunta, S., and **Chu, K.** Environmental factors affecting reactivity of copper(II):pyridine-2,6-bis(monothiocarboxylic acid) (PDTC) with polyhalomethanes. In preparation.

9. Quality control of manufacturing oligo arrays via combinatorial designs (7/1/01-6/30/02)
Investigators: Alan Ling
Participants: Charles Colbourn
Publications:

C.J. Colbourn, **A.C.H. Ling** and M. Tompa, Construction of optimal quality control for Oligo arrays, *Bioinfomatics* 18 (2002), 529-535.

N. Alon, **C.J. Colbourn, A.C.H. Ling** and M. Tompa, Equireplicate balanced binary codes for Oligo arrays, *SIAM J. on Discrete Math.* 14 (2001), 481-497.

10. Analysis of functional protein interactions in *Drosophila* flight muscles through the study of mutant proteomes (7/1/01-6/30/02)
Investigators: Jim Vigoreaux and Xindong Wu
Participants: Joshua Henkin, Graduate Student, Qijun Chen, Graduate Student, Jeff Stone, Graduate Student, Jamie Lemus, Undergraduate Student

Publications:

Ying Yang, **Xindong Wu**, and Xingquan Zhu, Mining in Anticipation for Concept Change: Proactive-Reactive Prediction in Data Streams, *Data Mining and Knowledge Discovery*, 13(2006), 3: 261-289.

Xingquan Zhu, **Xindong Wu**, and Ying Yang, Effective Classification of Noisy Data Streams with Attribute-Oriented Dynamic Classifier Selection, *Knowledge and Information Systems*, 9(2006), 3: 339-363.

Ying Yang and **Xindong Wu**, Parameter Tuning for Induction Algorithm Oriented Feature Elimination, *IEEE Intelligent Systems*, 19(2004), 2: 40-49.

Ying Yang, **Xindong Wu,** and Xingquan Zhu, Combining Proactive and Reactive Predictions for Data Streams, *Proceedings of the 11th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD-2005)* (acceptance rate: 40 full papers + 36 short papers, out of 358 research-track submissions), Chicago, IL, USA, August 21-24, 2005, 710-715.

Xingquan Zhu, **Xindong Wu**, and Ying Yang, Error Detection and Impact-Sensitive Instance Ranking in Noisy Datasets, *Proceedings of the 19th National Conference on Artificial Intelligence (AAAI-04)* (acceptance rate: 121/453), July 25-29, 2004, San Jose, California, 378-383.

Ying Yang, **Xindong Wu**, and Xingquan Zhu, Dealing with Predictive-but-Unpredictable Attributes in Noisy Data Sources, *Proceedings of the 8th European Conference on Principles and Practice of Knowledge Discovery in Databases (PKDD)* (acceptance rate: 39/301 for regular papers), Pisa, Italy, September 20-24, 2004, 471-483.

Xingquan Zhu, **Xindong Wu**, and Ying Yang, Dynamic Classifier Selection for Effective Mining from Noisy Data Streams, *Proceedings of the Fourth IEEE International Conference on Data Mining (ICDM '04)* (acceptance rate: 39/451 for regular papers), Brighton, UK, November 1 - 4, 2004, 305-312.

Ying Yang, Geoff I. Webb, and **Xindong Wu**, Discretization Methods (Book Chapter), In O. Maimon and L. Rokach (eds.), *Data Mining and Knowledge Discovery Handbook: A Complete Guide for Practitioners and Researchers*, Springer, 2005, 113-130.

Henkin, J., Jennings, M. E., Matthews, D. E., and **Vigoreaux, J. O.** (2004) Mass Processing^2 – An improved technique for protein identification with MS data. *J. Biomolecular Tech*., 15: 227-233.

Maughan, D. Henkin, J., and **Vigoreaux, J.** (2005) Concentrations of glycolytic enzymes and other cytosolic proteins in the diffusible fraction of a vertebrate muscle proteome. *Mol. Cell Proteomics* 4.10: 1541-1549.

Henkin, J. and **Vigoreaux, J.** (2006) Mapping myofibrillar protein interactions by mutational proteomics, in *Nature's Versatile Engine: Insect Flight Muscle Inside and Out*, Vigoreaux, J. editor, Springer/Landes Bioscience, New York/Georgetown. pp 270-283.

11. Crystallization of the transferrin-transferrin receptor complex (07/01/01-06/30/03)
Investigators: Stephen J. Everse, Ph.D., Department of Biochemistry
Anne B. Mason, Ph.D., Department of Biochemistry
Participants: Sara K. Briggs, Technician
Peter J. Halbrooks, Graduate Student, Biochemistry
Publications:

Giannetti, AM., P.J. Halbrooks, **A.B. Mason**, T.M. Vogt, C.A. Enns and P.J. Bjorkman, The molecular mechanism for receptor-stimulated iron release from the plasma iron transport protein , transferrin *Structure* 13, 1613-1623 (2005).

Mason, A.B., P.J. Halbrooks, N. G. James, S.A.Connolly, J.R. Larouche, V.C. Smith, R.T.A. MacGillivray and N.D. Chasteen, Mutational analysis of C-lobe ligands of human serum transferrin: Insights into the mechanism of iron release, *Biochemistry* 44, 8013-8021 (2005).

Halbrooks P.J., **A.B. Mason**, T.E. Adams, S.K. Briggs, and **S.J. Everse,** The oxalate effect on release of iron from human serum transferrin explained, *J Mol. Biol.* 339, 217-226 (2004).

Adams, T.E., **A.B. Mason**, Q-Y. He, P.J. Halbrooks, S.K. Briggs, V.C. Smith, R.T.A. MacGillivray and **S.J. Everse,** The Position of Arginine 124 Controls the Rate of Iron Release from the N-lobe of Human Serum Transferrin: A Structural Study, *J. Biol Chem.* 278, 6027-6033 (2003).

Halbrooks, P.J., Q-Y. He, S.K Briggs, **S.J. Everse**, V.C. Smith, R.T.A. MacGillivray and **A.B.Mason**, Investigation of the Mechanism of Iron Release from the C-lobe of Human Serum Transferrin: Mutational Analysis of the Role of a pH Sensitive Triad, *Biochemistry* 42, 3701-3707 (2003).

Mason, A.B., Q-Y He, P.J. Halbrooks, **S.J. Everse**, D.R.Gumerov, I.A. Kaltashov, V. C. Smith, J.Hewitt and R.T.A. MacGillivray, Differential Effect of a His tag at the N- and C-termini: Functional Studies with Recombinant Human Serum Transferrin, *Biochemistry* 41, 9448-9454 (2002).

12. Numerical simulation of skeletal structural adaptation (07/01/01-06/30/02)

Investigators: Tony S. Keller, Ph.D., Professor, Department of Mechanical Engineering

Participants: R.D. Prabhu, Ph.D., Post-doctoral Associate
Victor Kosmopoulos, M.S., Graduate Student, Mechanical Engineering

Publications:

Kosmopoulos, V. and **Keller, T.S.** Finite element modeling of trabecular bone damage. *Computer Methods in Biomechanics and Biomedical Engineering.* Submitted.

Keller, T.S., Kosmopoulos, V., and Liebschner, M.A.K. Modeling of bone loss and fracture in osteoporosis. (In: Vertebral Compression Fractures. From Conservative Treatment Over Surgery to Vertebroplasty, R. Gunzburg and M. Szpalski, Eds). Lippencott-Raven, Philadelphia, 2002.

Keller, **T.S.,** Harrison, D.E., Colloca, C.J., Harrison, D.D., Janik, T.J. Prediction of osteoporotic spinal deformity. *Spine* 28(5):455-462.

13. Disentangling the mechanisms responsible for species diversity in landscapes (7/1/02-6/30/04)

Investigators: Margaret J. Eppstein and Jane Molofsky

Participants: Joshua Gilbert, Undergraduate

Publications:

Eppstein, M.J. and **Molofsky, J.** "Invasiveness in plant communities with feedbacks". *Ecology Letters*, in press, 2007. *(published in the Ideas and Perspectives section of the journal designed to be read by all ecologist because of the importance of the result, journal ranked 4 out of 161 ecological journals, Impact factor 5).*

Eppstein, M.J., Bever, J.D., and **Molofsky, J.**, "Spatio-temporal community dynamics induced by frequency dependent interactions", *Ecological Modelling*, **197**:133-147, 2006.

Extramural Funding:

“Planning Grant for Biocomplexity Center”
9/1/05-5/31/06 (no cost extension through 5/31/07) $5,000
VACC
PI: Eppstein, Co-PIs: Molofsky, Rizzo, Stevens, Goodnight, Hoffmann

“Complex Systems Thinking and Modeling for Ecosystem Analysis
8/15/07-6/30/10 $6,692,531
NSF EPSCoR (Research Infrastructure Improvement program)
PI: Judith VanHouten, Core faculty include Eppstein

14. A digital library system for computational biologists (7/1/02-6/30/04)
Investigators: Xindong Wu and Marc Greenblatt
Participants: Jeff Stone, graduate student
Publications: Jeff Stone, Graduate Student

Jeffrey Stone, **Xindong Wu,** and **Mark Greenblatt,** A Semantic Network for Modeling Biological Knowledge in Multiple Databases, *Communications of the IIMA*, 4(2004), 4: 41-57.

Jeffrey Stone, **Xindong Wu,** and **Mark Greenblatt,** An Intelligent Digital Library System for Computational Biologists (a poster paper; abstract refereed), Proceedings of the 2004 IEEE Computational Systems Bioinformatics Conference (CSB2004), Stanford, CA, August 16-19, 2004, 491-492.

15. Crystallographic screening and structural characterization of small molecule binding (7/1/02-6/30/04)
Investigators: Mark Rould, Jose Madalengoitia & Kathleen Trybus
Participants: Michael Sperber, Graduate Student
Stephenson Flemer, Graduate Student
Alexander Wurthmann, Graduate Student
Jian Wang, Graduate Student
Amy Bowser, Graduate Student
Rakesh Ganorkar, Graduate Student

Publications:

Bowser, A.M. and **Madalengoitia, J.S**. Synthesis of Highly Substituted Ureas and Thioureas Through a 1,3-Diaza-Claisen Rearrangement. *Tetrahedron Lett.* Accepted for publication.

Bowser, A.M. and **Madalengoitia, J.S.** A 1,3-Diaza-Claisen Rearrangement that Affords Guanidines" *Org. Lett.*, *6*, 3409, 2004.

Rould M.A, Wan Q., Joel P.B., Lowey S., **Trybus K.M.** (2006) Crystal Structures of Expressed Non-polymerizable Monomeric Actin in the ADP and ATP States. *J Biol Chem* 281, 31909-31919.

Rould M.A. (2006) The Same but Different: Isomorphous Methods for Phasing and High-Throughput Ligand Screening. *Methods in Molecular Biology,* 364, 159-181.

Nair U.B., Joel P.B., Wan Q., Lowey S., **Rould M.A., Trybus K.M.** (2008) Crystal Structure of Monomeric Actin Bound to Cytochalasin D, *Journal of Molecular Biology* (accepted pending revision).

16. Specificity determinants of the Grb7 protein family
Investigators: Barbara Lyons (7/1/02-6/30/04)
Participants: Paul Schaarf, graduate student

17. SL1: Carving out the structure of the TAFs (7/1/02-6/30/04)
Investigators: Margaret Daugherty and Stephen Everse
Participants: Jon Ramsey, Technician

18. A structural approach to the coupling of transcription, mRNA processing and DNA repair (7/1/02-6/30/04)
Investigators: Gregory Gilmartin and Sylvie Doublié
Participants: Kirk Brown, graduate student, Krishnan Venkataraman, graduate student
Publications:

Brown, K.M., **Gilmartin, G.M.** A mechanism for the regulation of pre-mRNA 3' processing by human cleavage factor Im. *Mol Cell.* **12**:1467-76, 2003.

19. Stability and optimal growth of disturbances in pulsatile pipe flow (7/1/03-6/30/05)
Investigators: Darren Hitt
Publications:

Fedele F. and **Hitt D.L.**, 2006, Transport, Growth and Stability of Weakly Rarefied Pulsatile Channel Flows, *J. Comp. Theo. Nanoscience* Vol. (3), 1-9.

Fedele F., **Hitt D.L**., and Prabhu R.D., 2005, Revisiting the linear stability of pulsatile pipe flow, *Eur J Mech B - Fluids,* Vol. 24 (2), 237-254.

Fedele F. and **Hitt D.L.**, 2005, Linear Stability of Pulsatile Slip Flows in Microchannels, *Far East J. Appl. Math.*, Vol. 21(1), 31-41.

Fedele F. and **Hitt D.L.,** 2005, Transport, Growth and Stability of Weakly Rarefied Channel Flows, in Computational Solid and Fluid Mechanics 2005, K.J. Bathe, ed. Elsevier Publishing

Fedele F. and **Hitt D.L.**, 2005, On the Linear Stability of Weakly Rarefied Flows in Microchannels, AIAA Paper 2005-5031, American Institute of Aeronautics & Astronautics.

Fedele F., **Hitt D.L.** and Prabhu, R.D., 2003, A Complete Set of Eigenfunctions for the Stability of Pulsatile Pipe Flow, Proceedings of the 2003 Mediterranean Conference on Modeling and Simulation, Reggio Calabria, Italy.

20. Modifying the genetic programming algorithm for discovering novel process models of biological systems (7/1/03-6/30/05)

Investigators: James Hoffmann, Suzanne Levine and Timothy Perkins

Publications:

Hoffmann, J.P. 2006. Simultaneous Inductive and Deductive Modeling of Ecological Systems via Evolutionary Computation and Information Theory. Transactions of the Society for Modeling and Simulation International – Special Issue on Ecological and Environmental Simulation. *Simulation* 82 (7): 439-450.

Hoffmann, J.P. 2005. Darwin and Computational Ecology: How Simple Computational Models of Evolution Help our Search for Better Models of Ecological Systems. Keynote Address: In Proceedings of Open International Conference on Modeling and Simulation - OICMS 2005, Hill, D. R. C., V. Barra., and M. K. Troer (Eds.), Blaise Pascal University, France, pp 27-39.

Extramural Funding:

Using Genetic Programming to Evolve Optimally Specified Process Models of Biological Systems.
U.S. Department of Agriculture-Hatch
$35,000 2003-2007

21. Evolutionary computational approaches to biological problems (9/1/03-6/30/05)

Investigators: Margaret J. Eppstein & Mark Rould

Publications:

Eppstein, M.J., Payne, J.L., White, B.C., and Moore. J.H. "Genomic mining for complex disease traits with 'Random Chemistry'". Genetic Programming and Evolvable Machines (special issue on Medical Applications), 8:395-411, 2007.

Payne, J.L. and **Eppstein, M.J.**, “Takeover Times on Scale-Free Topologies”, submitted to *Genetic and Evolutionary Computation Conference (GECCO)* pp. 308-315, 2007.

Payne, J.L. and **Eppstein, M.J.**, “Why your mates shouldn’t date”, poster and published extended abstract, *Genetic and Evolutionary Computation Conference (GECCO)* 2007.

DeHaas, D., Craig, J., Rickert, C., Haake, P., and **Eppstein, M.J.**, "Feature Selection and Classification in Noisy Epistatic Problems using a Hybrid Evolutionary Approach", poster and published extended abstract, *Genetic and Evolutionary Computation Conference (GECCO)* 2007.

Payne, J.L., **Eppstein, M.J.**, and Goodnight, C.J. "Sensitivity of Self-Organized Speciation to Long Distance Dispersal", Proceedings of the 2007 IEEE Symposium on Artificial Life (Alife'07) pp. 1-17, 2007 (best student paper award).

Eppstein, M.J., Payne, J.L., White, B.C., and Moore. J.H., "Hill-climbing through "random chemistry" for detecting epistasis", *Late-breaking papers, Genetic and Evolutionary Computation Conference (GECCO) 2006.*

Eppstein, M.J., Payne, J.L, and Goodnight, C.J. "Speciation by Self-Organizing Barriers to Gene Flow in Simulated Populations with Localized Mating", *Workshop Proceedings for Genetic and Evolutionary Computation Conference (GECCO) 2006.*

J.L. Payne and **M.J. Eppstein,** "Emergent Mating Topologies in Spatially Structured Genetic Algorithms", *Proceedings of Genetic and Evolutionary Computation Conference (GECCO) 2006, pp. 207-214.*

J.L. Payne and **M.J. Eppstein,** "A Hybrid Genetic Algorithm with Pattern Search for finding Heavy Atoms in Protein Crystals", *Genetic and Evolutionary Computation Conference (GECCO) 2005*, Part 1, Eds. H-G Bayer *et al*., pp. 377-384, 2005. (nominated for a best-paper award)

Extramural Funding:
"Planning Grant for Biocomplexity Center"
9/1/05-5/31/06 (no cost extension through 5/31/07) $5,000
VACC
PI: Eppstein, Co-PIs: Molofsky, Rizzo, Stevens, Goodnight, Hoffmann

"Complex Systems Thinking and Modeling for Ecosystem Analysis
8/15/07-6/30/10 $6,692,531
NSF EPSCoR (Research Infrastructure Improvement program)
PI: Judith VanHouten, Core faculty include Eppstein

22. Structural studies of mammalian thioredoxin reductase (7/1/03-6/30/05)
Investigators: Robert Hondal, Stephen Everse and Jose Madalengoitia
Participants: Brian Eckenroth, graduate student
Publications:

Eckenroth, BE, **Rould, MA, Hondal, RJ** and **Everse, SF** (2006) Structural and Biochemical Studies Reveal Differences in Catalytic Mechanisms between Mammalian and *Drosophila melanogaster* Thioredoxin Reductases. *Biochemistry 46*, 4694-4705.

23. Correlation between structure and mechanism in the modified human hemoglobin Hbαβ YQ (7/1/04-6/30/06)

Investigators: Kelvin Chu
Participants:
Publications:

K. Chu, A. Laughney and J. Williams, (2007) Undergraduate Labs for Biological Physics: Brownian Motion and Optical Trapping. *Bull. Am. Astr. Soc.* 38:134.

K. Chu (2007) “Determination of Reaction Intermediate Structures in Heme Proteins.” Meth. Molec. Biol., Macromolecular Crystallography Protocols. The Humana Press, NJ, USA. 19-30.

Kuehnel, K., Schlichting, I., Brunori, M., Vallone, B., Sweet, R., **Chu, K.** (2005) Photolysis-induced structural changes in the Hb-- -YQ. *Biophys. J.* 88:85-90.

Extramural Funding:

2006-08 PI, Undergraduate Labs for Biological Physics
(NSF, $150,000) (NSF – 0536773)

2005 PI, Planning Grant: Computation in the Physical Sciences and Mechanical Engineering
(Vermont Advanced Computing Center, $5,000)

2004 PI, Computation in biotechnology, materials science and astrophysics
(Vt. EPSCoR, $20,000).

24. D_2E: The fundamental structural unit of a clot (7/1/04-6/30/06)

Investigators: Stephen Everse
Participants: Sara Briggs, Technician

25. Crystal structure of the eukaryotic $tRNA^{His}$ guanylyltransferase THG1 (7/1/04-6/30/06)

Investigators: Nick Heintz, Sylvie Doublié, Chris Francklyn, David Pederson
Publications:

T.S. Rice, M. Ding, **D.S. Pederson** and **N.H. Heintz.** The highly conserved $tRNA^{His}$ guanylyltransferase Thg1p interacts with ORC and is required for the G2/M phase transistion in yeast. *Eukaryotic Cell* 4:832-835, 2005.

26. Clotspeed-III (7/1/05-6/30/06)

Investigators: Kathleen Brummel-Ziedins, Thomas Orfeo
Participants:
Publications:

Orfeo T, Kathleen E. Brummel-Ziedins, Saulius Butenas, and Kenneth G. Mann (2006) Simulating blood coagulation: the contribution of α_2-macroglobulan and α_1-antitrypsin.

FASEB J 20(4):A64. Abstract at 2006 American Society of Biochemistry and Molecular Biology.

Extramural Funding:

RFA HL-07-005	7/01/07- 6/30/10
NIH-NIHLBI	$600,000

Modeling the Coagulation Proteome

This project aims to develop biologically realistic, mathematically robust models of the processes involved in hemostasis that will permit predictions of the behavior of the coagulation system in normal and pathologic states (Pending)

27. Determination of the three-dimensional structure of EmaA (Extracellular Matrix Protein Adhesin A) from *Actinobacillus actinomycetemcomitans* (7/1/05-6/30/07)

Investigators: Keith Mintz

Participants:

Publications:

C. Yu, C. Lenox, **K. Mintz**, T. Ruiz. (2006) Structural Analysis of an Extracellular matrix protein adhesin (EmaA) of *Actinobacillus actinomycetemcomitans. 64th Annual Meeting of the Microscopy Society of America*. Poster presentation. Microscopy and Microanalysis. Chicago, Illinois. Microscopy and Microanalysis, (2006), Vol. 12, Suppl. 2, 310.

Extramural Funding:

1RO1 DE017474, T. Ruiz (PI)	3/1/08 – 2/28/13	$1,631,125

Structure of oral bacterial adhesins

The major goals of this project are to solve the structure of oral bacterial adhesins from *S. parasanguis* and *A. Actinomycetemcomitans* by electron microscopy and image processing techniques.

28. Numerical computation of the temperature-time evolution in the human eye exposed to various energy sources

Investigators: Antonio Campo, El Hassan Ridouane

Publications:

Ridouane, EH and **Campo, A.** (2006) Numerical Computation of the Temperature Evolution in the Human Eye *Heat Transfer Research* 37(7):607-617.