SCALE-IT: An Interdisciplinary Graduate Training Program in Computational Biology

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University of Tennessee

JICS/GRS Joint Workshop
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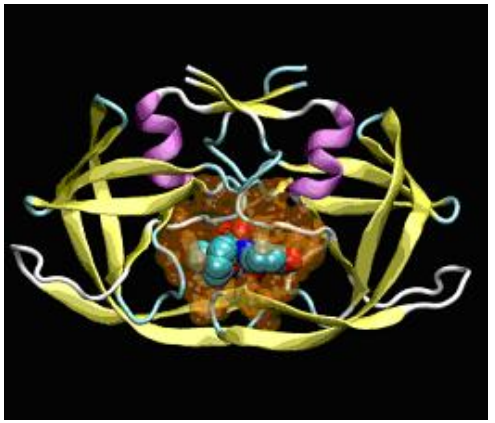
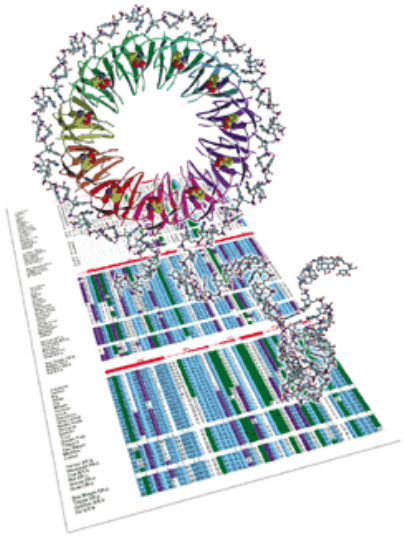
The Genesis: UT/ORNL GST

Bioinformatics

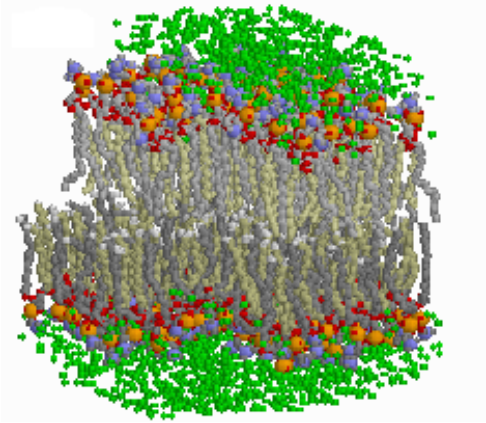
Computational Molecular Biophysics





Molecular Genetics and Systems Biology

Structural and Nanoscale Biology



Analytical Technologies for Bioenergy and the Environment

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Unique Resources at UT/ORNL

A Graduate Training Program

- ***What is IGERT?***
  - Integrative Graduate Education and Research Traineeship
- ***What is the purpose of SCALE-IT?***
  - Scalable Computing and Leading Edge innovative Technologies
  - Create an interdisciplinary, multi-departmental computational biology research community
  - Provide trainees with experiences in high performance computing, quantitative biology, and group research
  - Institutionalize a model for science communication and outreach by students

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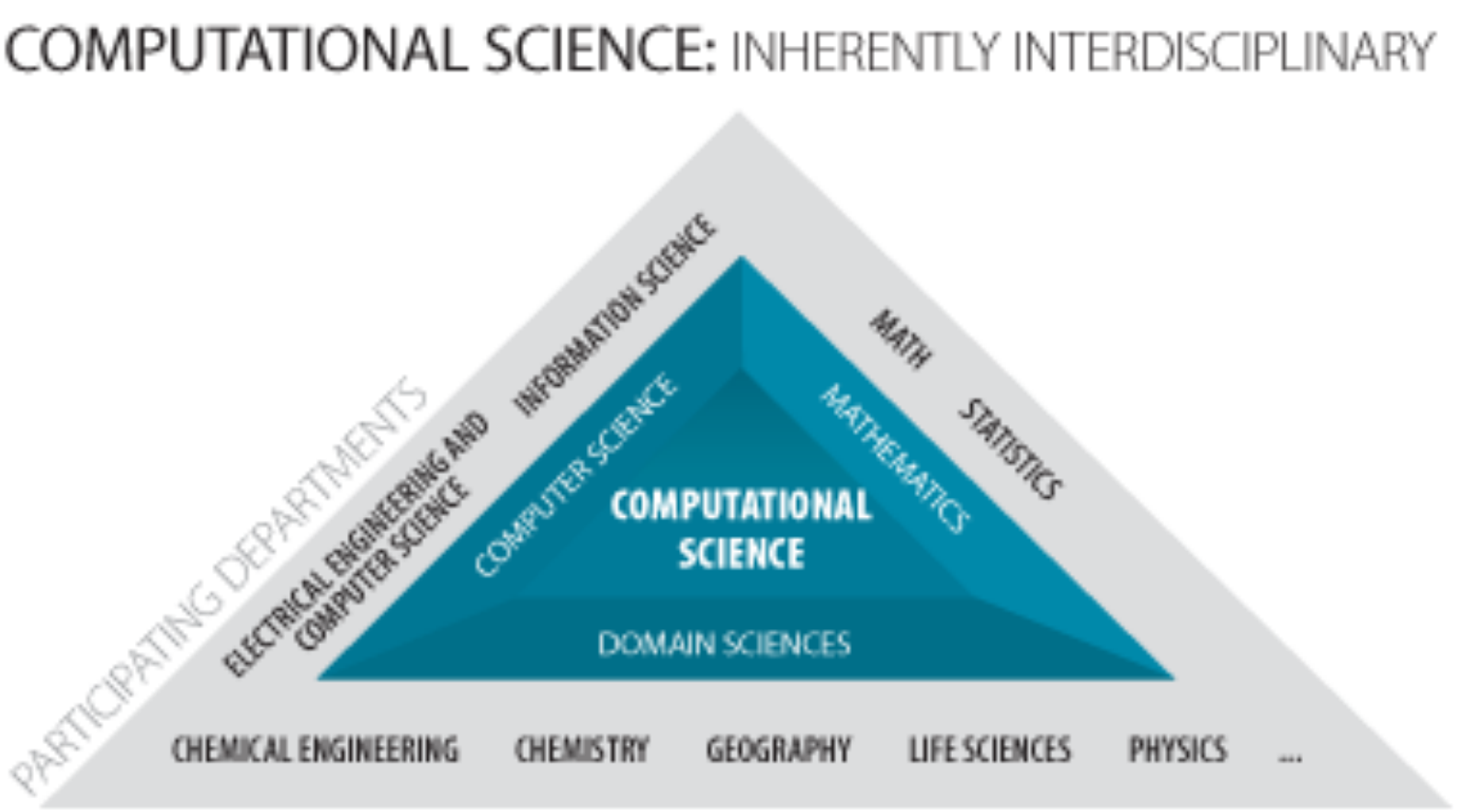
A Graduate Training Program

- ***The Team***
  - PI's: Cynthia Peterson, Elissa Chessler, Jack Dongarra, Mike Langston, Jeremy Smith
  - Program Manager Harry Richards
- ***Strategies***
  - Build on existing framework for education and collaborative research
  - Group projects for cross-training and real-world experience
  - Graduate minor in computational science

Minor in Computational Science (IGMCS)



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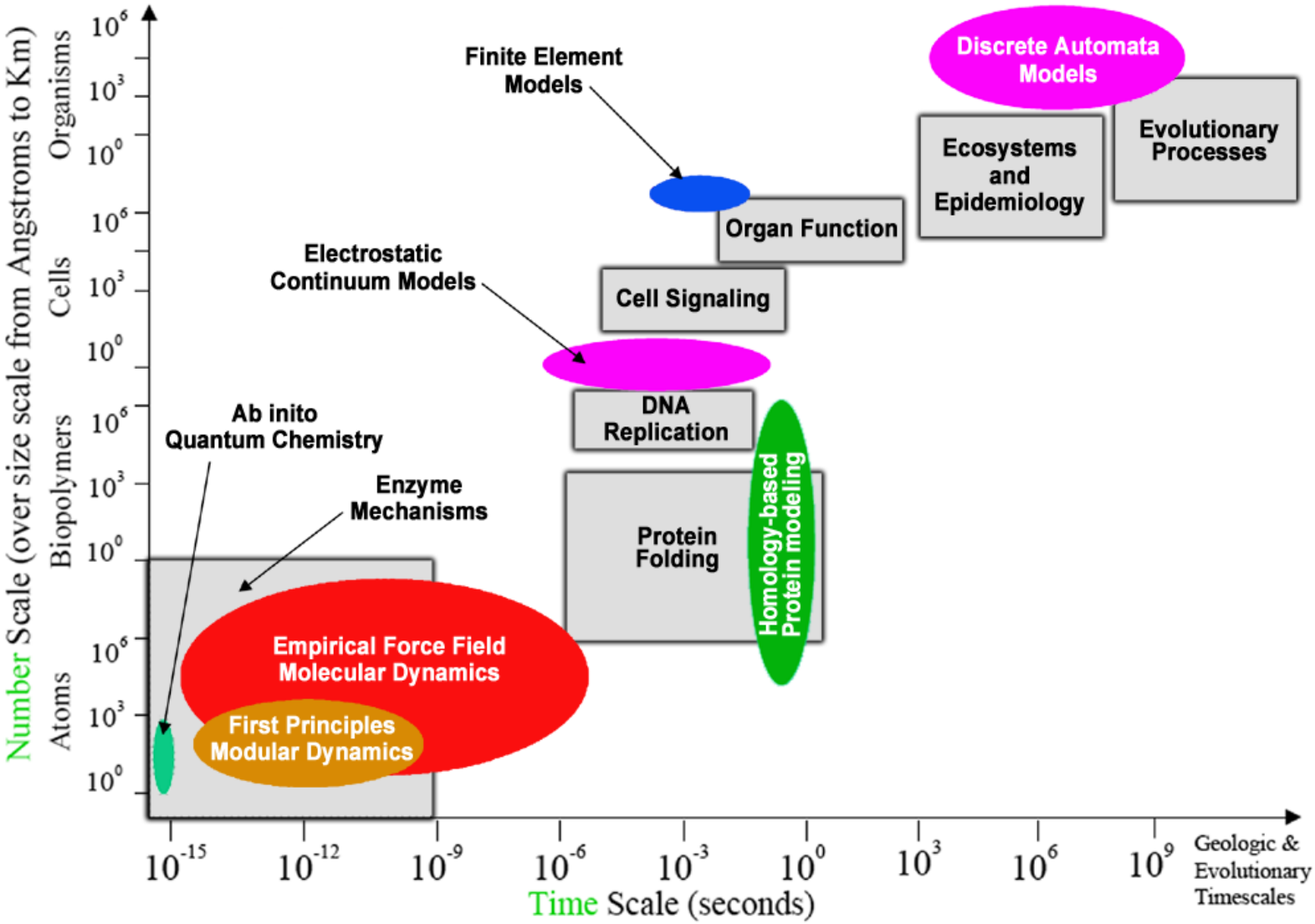
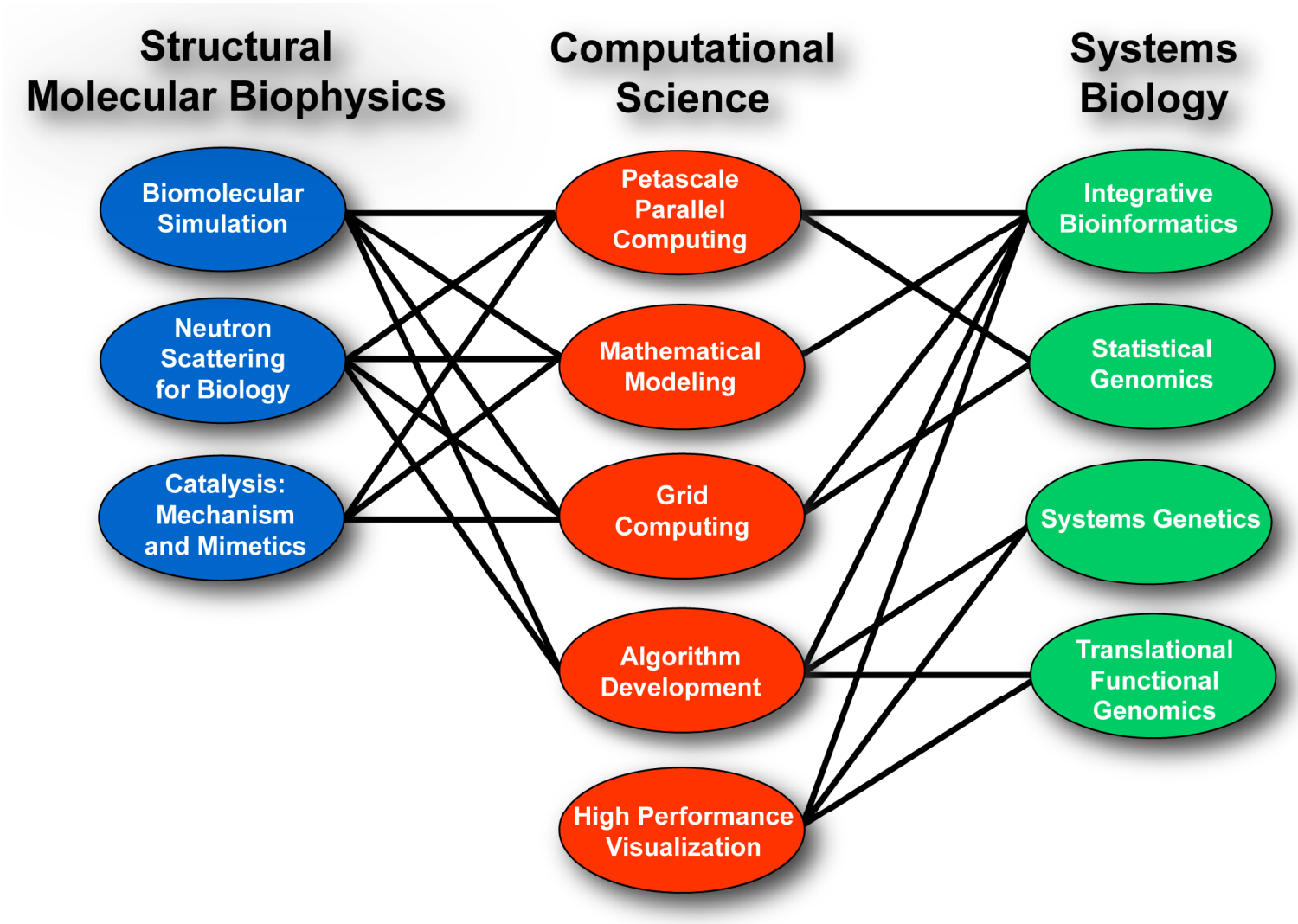
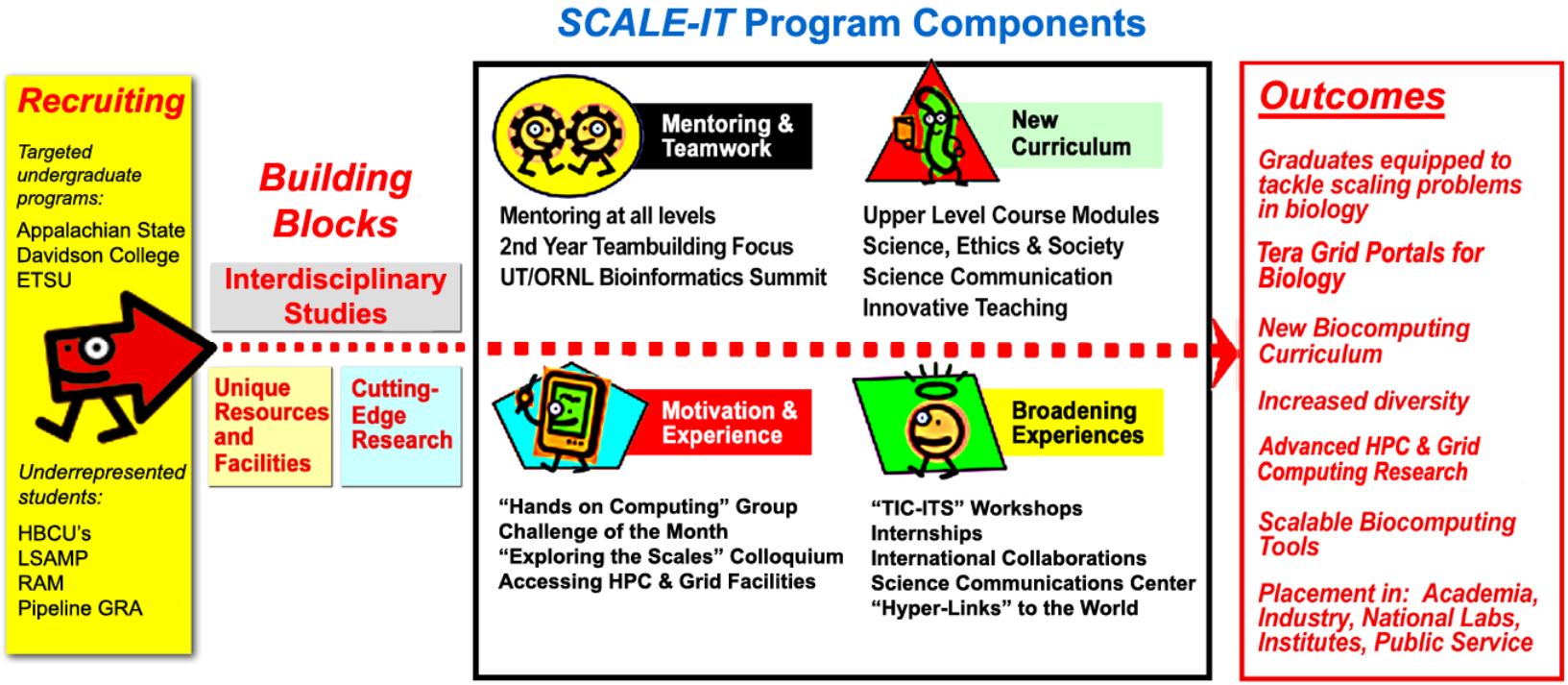
Multiple Scales of Biological Problems



Computational Biology is Interdisciplinary



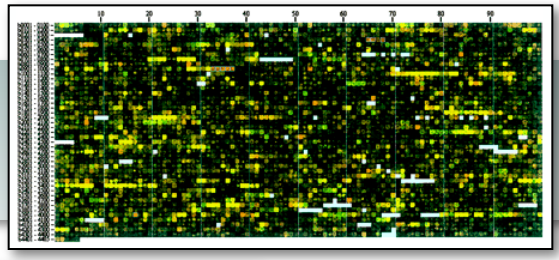
How SCALE-IT Was Envisioned

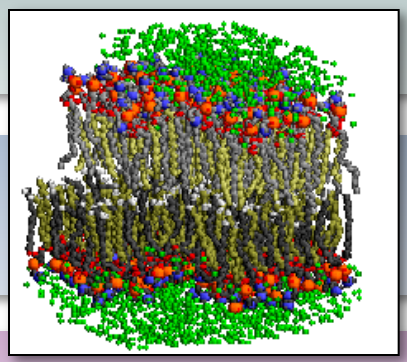


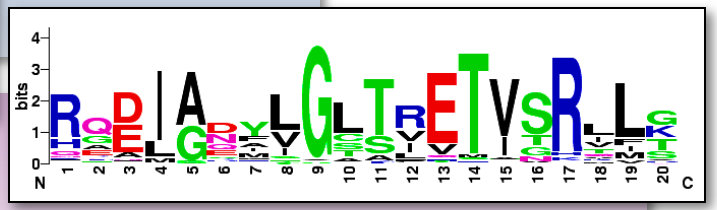
Areas of Expertise in Computational Biology

Areas of Research and Education:

- Computational Systems Biology
- Computational Molecular Biophysics
- Advanced Bioinformatics







http://gst.ornl.gov

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Computational Systems Biology

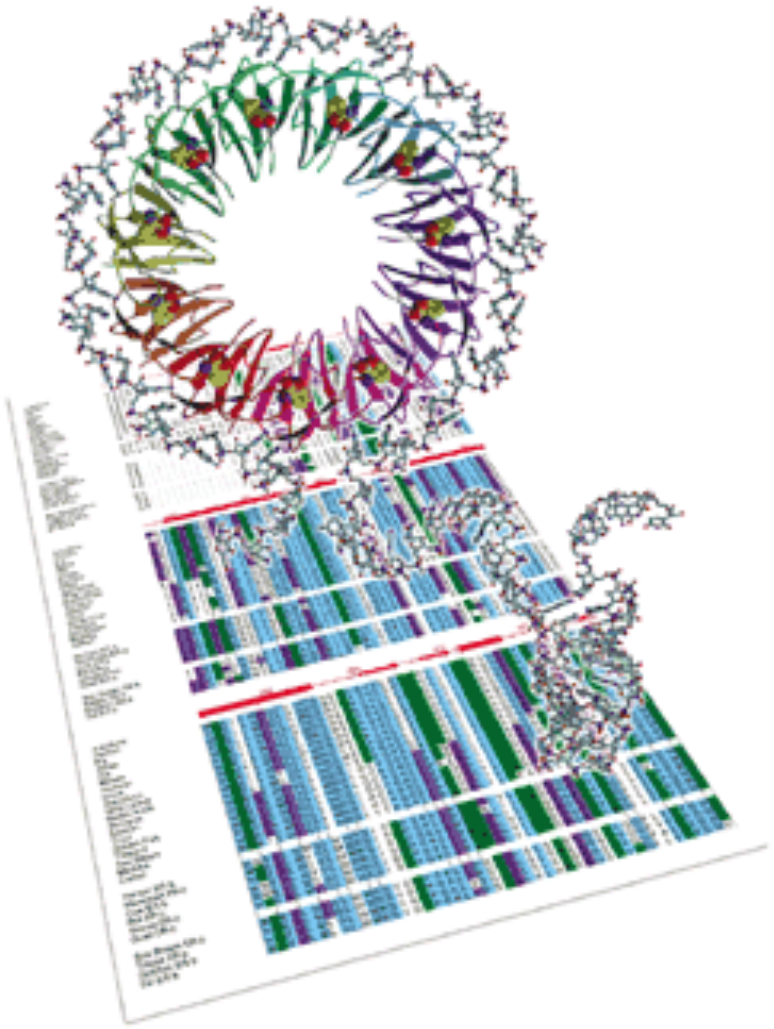
Projects

Integrative Bioinformatics

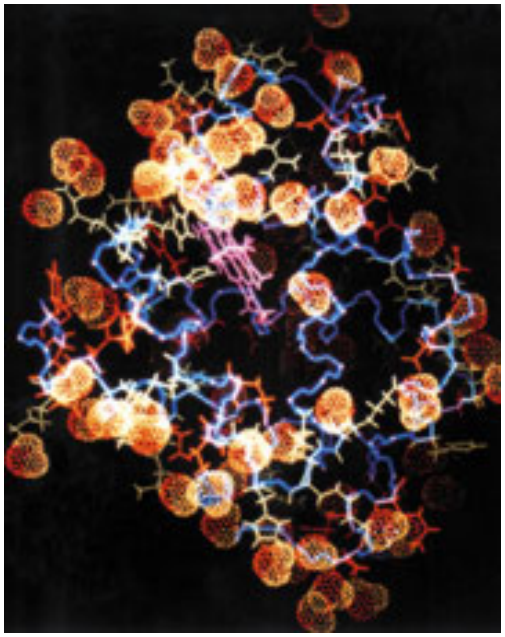
Statistical Genomics

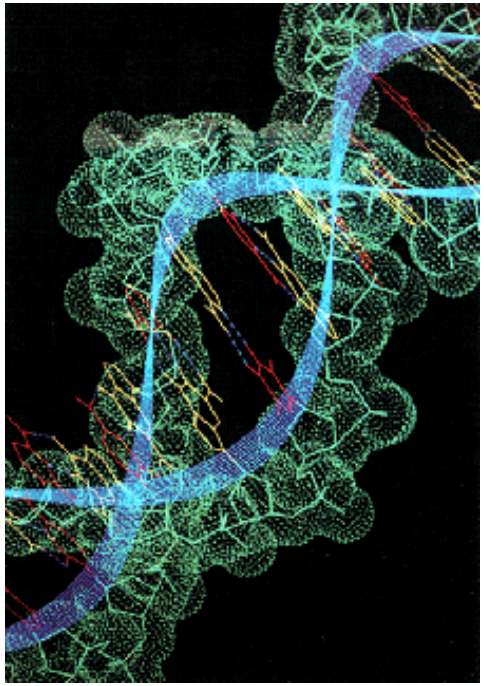
Graph Algorithms

Text Mining for Hypothesis Validation



Structural Molecular Biophysics





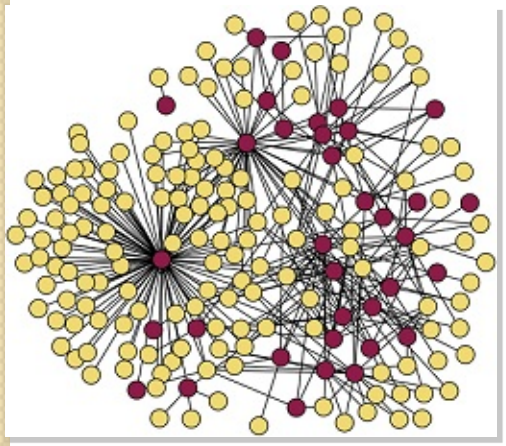
Projects

Neutron Scattering in Biology: Simulation and Experiment

Grand Challenges in High-Performance Biomolecular Simulation: Protein Folding, Binding and Function

Biological Catalysis: Mechanisms and Mimetics

Advanced Bioinformatics



Projects

Whole Genome Science and Gene Interaction Networks

Environmental and Microbial Systems Ecology

Computational Biology Group Research Projects

SCALE-IT

Scalable Computing and Leading Edge Innovative Technologies

- 1st year group projects (begin in spring semester)
  - Teams of 3 – 4 peer level students plus faculty
  - Focus on programming intensive tasks
- 2nd year group projects (primary SCALE-IT commitment)
  - More intensive research project (publications are expected)
  - Student participation in project selection and development
  - Targeted at scalable computing and/or supercomputing tasks

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Science Communication Center

SCALE-IT

Scalable Computing and
Leading Edge Innovative Technologies

- Faculty from the College of Communications
- Monthly workshops focused on communication themes
  - Science journalism and popular science writing
  - Oral communication and speaking to lay audiences
  - Technical writing
- One-to-one assistance for communication projects

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Community Building

- Weekly meetings
- Social activities
- Professional development workshops
  - Orientation bioinformatics workshop
  - Self-assessment skills, Negotiation skills
- Student developed program elements

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Program Outcomes

- ***IRE Grants Program***
- ***Workshops*** *(Orientation, Communication and Newton)*
- ***Team-based Projects***
  - Cation-Anion-Pi Interactions in Proteins (PDB searching, STAAR web interface)
  - Metagenomics to Map the Soil Nitrogen Cycle
  - SPECMASTER-proteomics analysis (using GPUs)
  - Tracking Spatial Information Across Tophic Levels
- ***Student-driven Curriculum***
  - Programming Course for Biologists
  - Bioinformatics Lab (PERL)
  - Journal Club for MatLab
  - Biology for Computer Scientists

Program Outcomes

- ***The Students***
- ***Some Accomplishments***
  - Publications!
  - Sally Ellingson: Grace Hopper Conference on Women in Computing Scholarship; grant through the SuperComputing 2011 Broader Engagement programselected to attend the High Performance Computing 2012 Workshop sponsored in conjunction with XSEDE.
  - Denise Koessler best poster award, TN Women in Computing conference; travel award to attend the WiC national conference.
  - Rachel Adams won the 2011 Martin Keller Award for Excellence from BESC which she will use to fund travel to the HPC 2012 Workshop to which she was also accepted.
  - Dylan Storey was awarded a USDA NIFA-AFRI Graduate Fellowship for 2012-2014.

Web Sites and Contact Information

SCALE-IT: http://web.utk.edu/~scaleit

PI: Cynthia Peterson (cbpeters@utk.edu)

Program Manager: Harry Richards (harry@utk.edu)

PEER: http://web.utk.edu/~peer

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Program Manager: Sekeenia Haynes (shaynes6@utk.edu)

NIMBioS: http://www.nimbios.org

Director: Louis Gross (gross@tiem.utk.edu)

Program Manager: Chris Welsh (cwelsh@utk.edu)

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