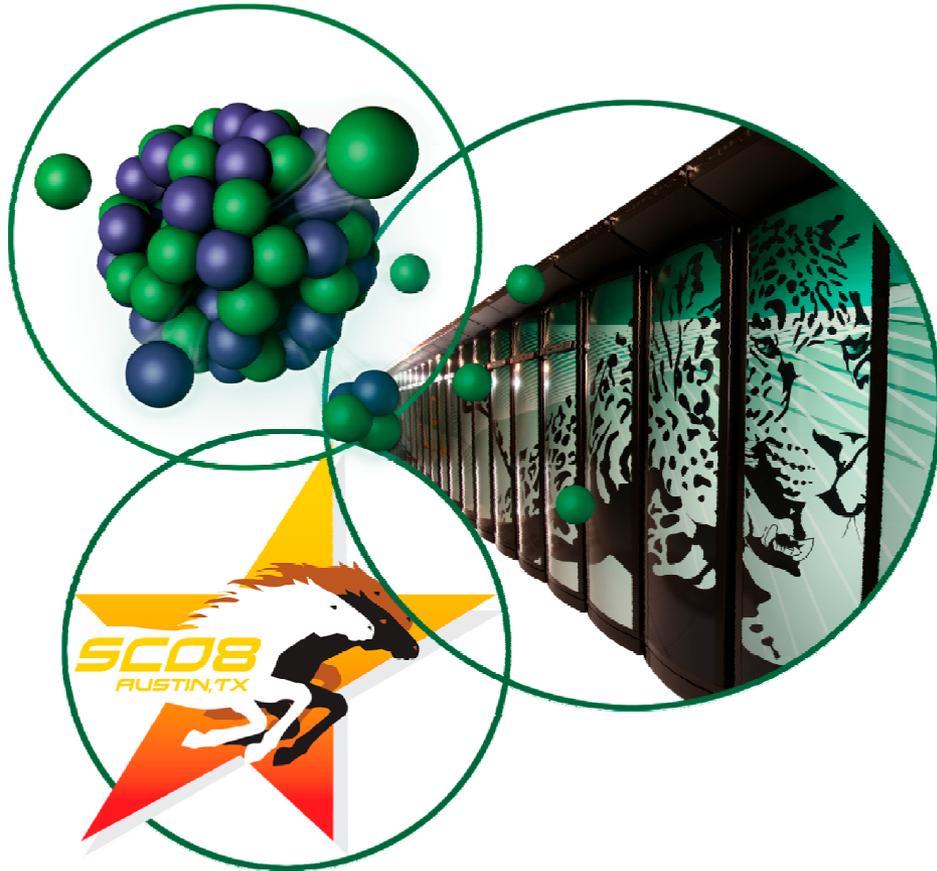


# ORNL–University Partnerships in Computational Biology

Presented by

**Igor B. Jouline (Zhulin)**

Joint Institute for Computational Sciences  
The University of Tennessee–  
Oak Ridge National Laboratory



# ORNL–University partnerships in computational biology

- **Joint Institute for Biological Sciences**

- **Joint Institute for Computational Sciences**

- **Graduate School of Genome Science and Technology**



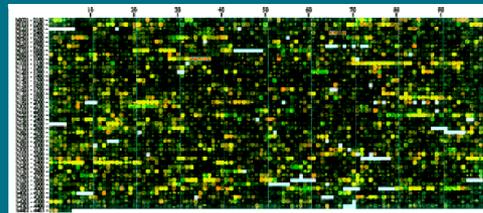
- **School of Biology**
- **College of Computing**
- **Center for Bioinformatics and Computational Biology**

- **Biosciences Division**
- **Computer Science and Mathematics Division**

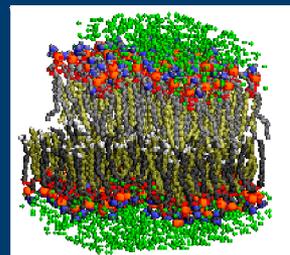
# ORNL-UT Graduate School of Genome Science and Technology

## Areas of research and education

Genetics  
and  
genomics



Structural  
biology and  
proteomics



Computational  
biology and  
bioinformatics



Genome Science & Technology

<http://gst.ornl.gov>

# ORNL-UT Graduate School of Genome Science and Technology

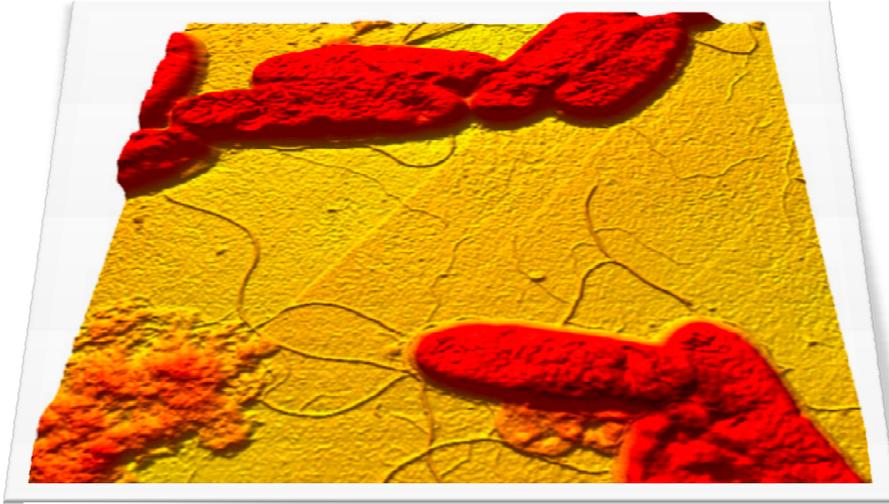


**In August 2008, UT was awarded a \$2M Integrative Graduate Education & Research Traineeship (IGERT) grant: SCALE-IT, Scalable Computing and Leading Edge Innovative Technologies**

**A number of highly competitive stipends for Ph.D. students wishing to work at the intersection of biology and high-performance computing are available. Please direct your inquiries to Dr. Cynthia Peterson at [cbpeters@utk.edu](mailto:cbpeters@utk.edu)**

<http://gst.ornl.gov>

# Shewanella Federation



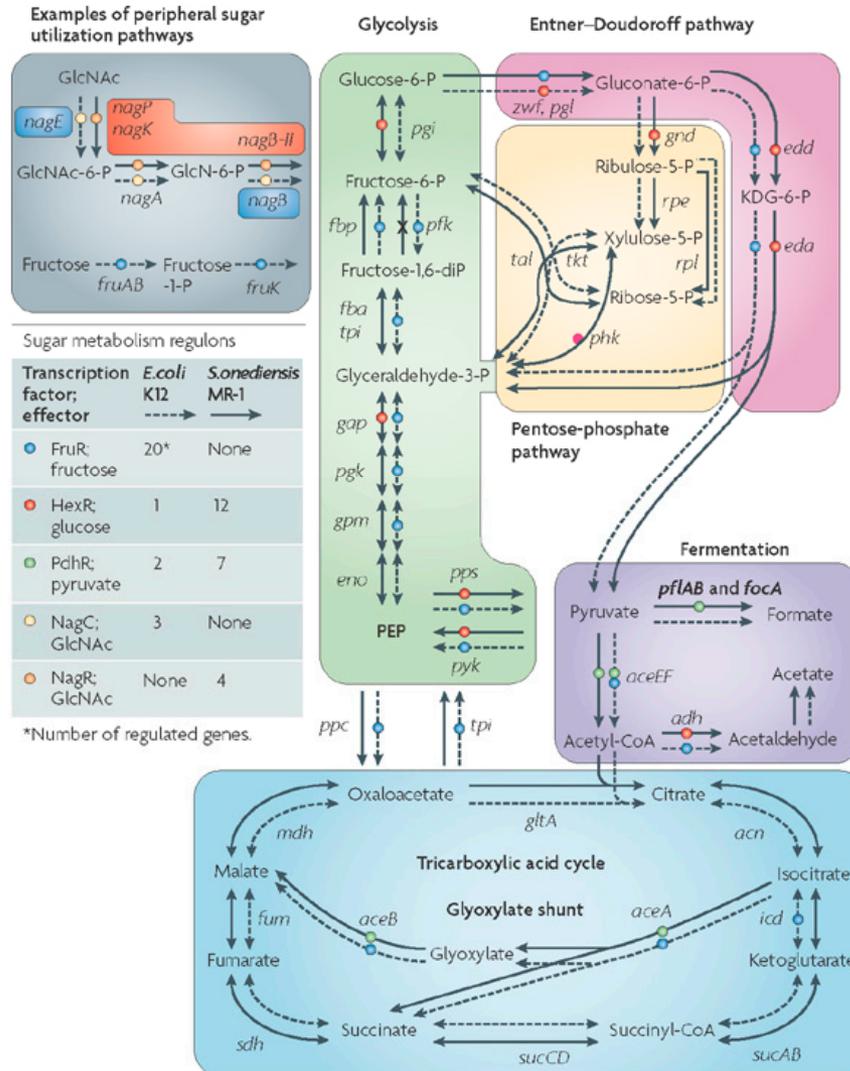
Fredrickson et al., Towards environmental systems biology of *Shewanella*, *Nature Reviews Microbiology* **6**, 592–603 (2008)



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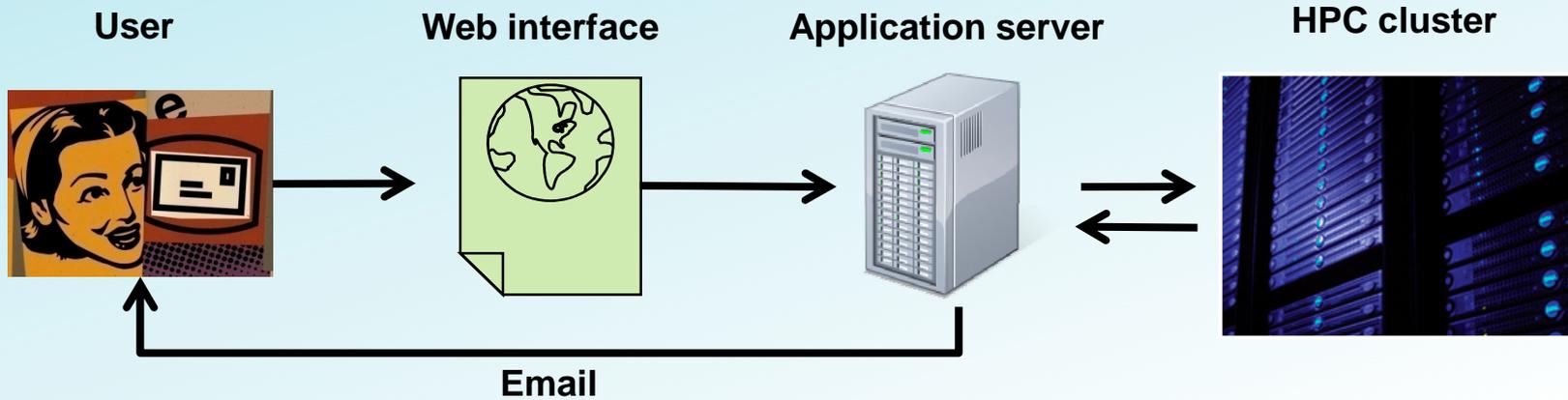


# Computationally reconstructed metabolism of *Shewanella*



# Developing computational biology applications for high-performance computing

## Mid-Scale Analysis



## Large-Scale Analysis

Login node

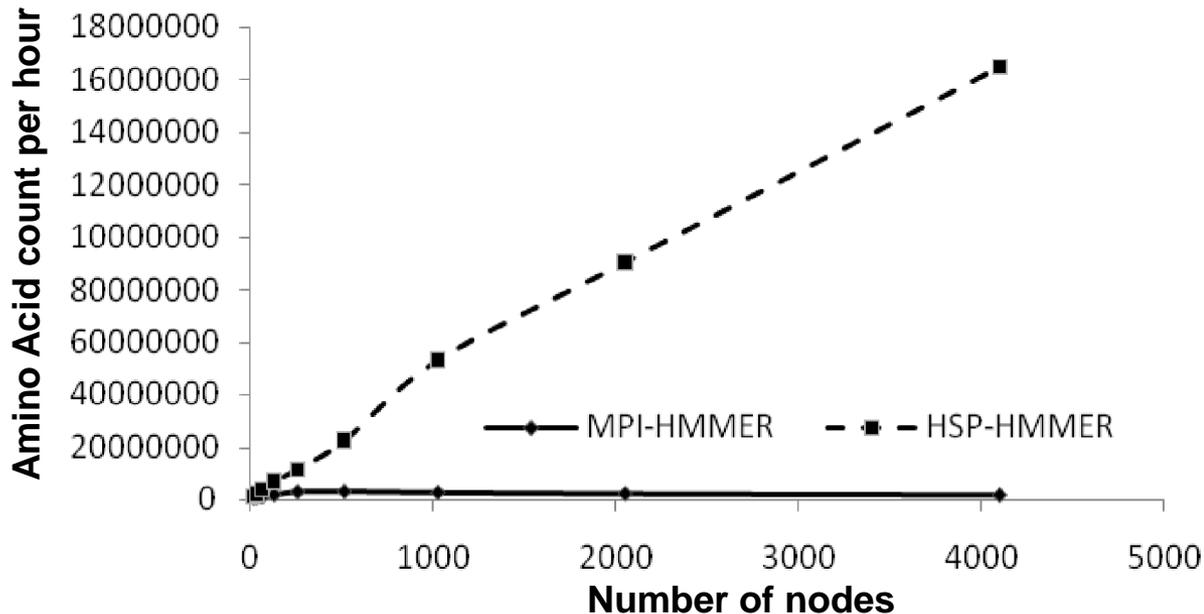


Cray XT4 supercomputer



# Developing computational biology applications for high-performance computing

Traditional MPI versions of popular bioinformatics software, such as HMMER, do not scale and cannot be used on the Cray XT4. We have developed a Highly Scalable Parallel (HSP) version of HMMER, which showed excellent performance on the Cray XT4



# Contact

## **Igor B. Jouline (Zhulin) Ph.D.**

**Joint Institute for Computational Sciences  
The University of Tennessee—Oak Ridge National Laboratory**

**Joint Faculty Professor  
The University of Tennessee  
UTK (865) 974-7687  
ljouline@utk.edu**

**Senior R&D Staff Member  
Oak Ridge National Laboratory  
ORNL (865) 241-3697  
joulineib@ornl.gov**

Postdoctoral positions in computational biology applications for HPC are available: email inquires are welcome; previous experience in biology is not necessary