

# Joint Institute for Computational Sciences

Presented by

**Thomas Zacharia**

Associate Laboratory Director  
Computing and Computational Sciences  
Oak Ridge National Laboratory

Director  
Joint Institute for Computational Sciences  
University of Tennessee

**UT-ORNL  
Governor's Chairs**

The University of Tennessee in partnership with the Oak Ridge National Laboratory is recruiting leading scientists to conduct research in the Joint Institute for Computational Sciences with access to some of the most advanced scientific and computational tools available. In addition to working in an exciting atmosphere of intellectual and academic freedom, you would be living in one of the most beautiful areas in the country with easy access to miles of inland waterways, pristine state and national parks, diverse cultural opportunities, and a unique mix of convenient urban and rural living settings.

Find out more at <http://www.tennessee.edu/governorchairs/>

**Governor's Chairs in the UT-ORNL Joint Institute for Computational Sciences**

The State of Tennessee is seeking 20 exceptionally accomplished researchers who will have joint appointments as limited professors at the University of Tennessee (UT) and will have joint appointments as limited professors at the Oak Ridge National Laboratory (ORNL). The Governor's Chair program seeks to catalyze the development of leading edge research under the auspices of four joint institutes between UT and ORNL: Biological Sciences, Computational Sciences, Nuclear Sciences, and Advanced Materials Sciences. The 20 appointments include an ongoing discretionary research fund equal to twelve months salary.

**The Joint Institute for Computational Sciences (JICS)**  
JICS will support both fundamental and applied research and teaching programs in computational sciences, computational mathematics, computer science, high-performance computing, storage and networking, and cyber security.

UT and ORNL have strong research efforts in these areas. The research environment fosters cross-disciplinary, leading-edge efforts that leverage special facilities in the physical and computational sciences. World-class research facilities include the DOE Leadership Computing Facility (LCF). LCF is planning the acquisition and deployment of a 2007 high-performance computing (HPC) system by 2007 and a 2007 HPC system by 2008. It is expected that JICS will focus on application and system software essential to optimal sustained performance of the petascale to enable a range of computationally challenging science and engineering applications.

The UT-ORNL environment nurtures a rich interdisciplinary community of researchers with common interests and collaborative projects. The UT-ORNL research enterprise has more than \$2 billion in investments in some of the world's most advanced research facilities.

There are immediate openings for Governor's Chairs in the following areas:  
Science and engineering applications - Applications are sought from candidates interested in:

- Computational science at the petascale in the physical, biological, and environmental sciences

Computer science applications - Applications are sought from candidates interested in developing:

- Algorithms, methods, and libraries
- Component-based, open-source program development and tools
- Systems software that scale to hundreds-of-thousands of processors
- Scalable systems for moving, storing, and analyzing data

Successful candidates will have an exceptional record of scientific, productivity and accomplishments in research, for example, in high-impact publications, scientific awards, or fellow status in scientific and engineering academies. Successful candidates will also have a demonstrated record of leading cross-disciplinary teams of researchers and of developing substantial externally-funded research programs.

**APPLICATIONS:** Applicants should submit a letter of interest and a curriculum vitae to: Thomas Zacharia, Chair, JICS Governor's Chair Search Committee, Computing and Computational Sciences, Oak Ridge National Laboratory, PO Box 2008, Oak Ridge, TN 37831-0208.

Successful candidates will be named by the University of Tennessee in an official letter of appointment by the University of Tennessee in the process of its education and employment programs and services.

Scientists and engineers at the Oak Ridge National Laboratory and the University of Tennessee conduct basic and applied research and development to create scientific knowledge and technological solutions that strengthen the nation's leadership in key areas of science, increase the availability of clean, abundant energy, improve and protect the environment, and contribute to national security. UT and ORNL provide an environment that encourages collaborative research and development, and provides an environment that encourages collaborative research and development. UT-Battelle manages and operates ORNL under contract DE-AC05-04OR21400.

**UT-BATTELLE**  
**THE UNIVERSITY OF TENNESSEE**  
**OAK RIDGE National Laboratory**



# Joint Institute for Computational Sciences



- State of Tennessee-funded building
- Constructed in 2004 on ORNL's East Campus

# Joint Institute for Computational Sciences



- State-of-the-art distance learning
- Interactive seating
- Conference rooms
- Open meeting space
- Executive offices for distinguished scientists and directors
- Incubator suites for students and visiting staff

- Opened 2005
- 52,000 sq. ft.

# Joint Institute for Computational Sciences

<http://www.jics.utk.edu/research.html>

## Appointments

- Faculty
- Governor's chairs
- Joint faculty
- Postdoctoral
- Student

## Research

- Computer Science
- Computational Chemistry
- Computational Biology
- Computational Materials Science
- Networking
- Astrophysics
- Fusion
- Applied Math
- More . . .



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Summer student poster presentations in JICS lobby

**Research Alliance in Math and Science Program**

<http://www.csm.ornl.gov/Internships/RAMS.html>

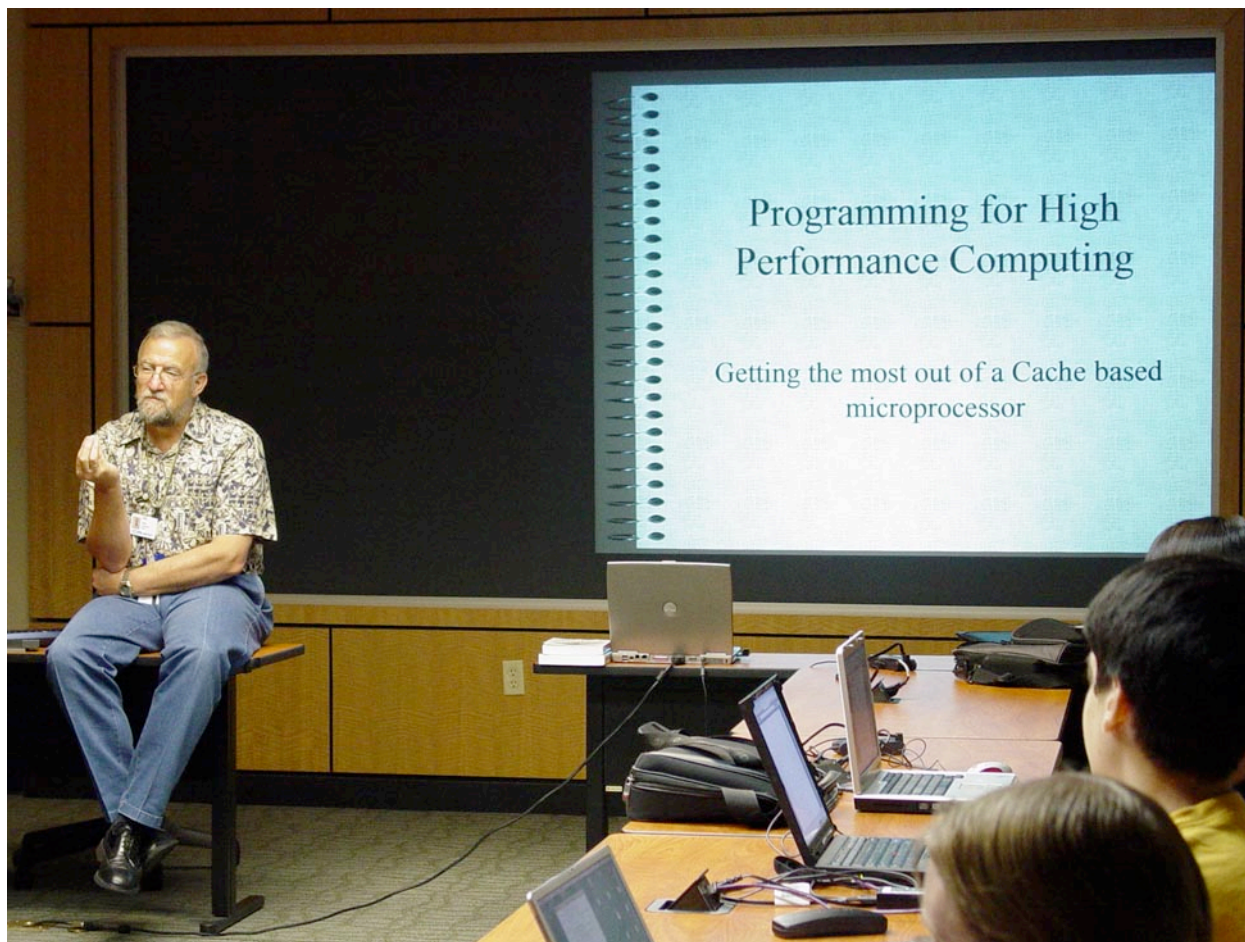
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**Exploratory Visualization Environment for REsearch in Science and Technology (EVEREST)**

<http://www.jics.utk.edu/education.html>

# Joint Institute for Computational Sciences

## Research Areas

- SensorNet
- Geographic Information Science and Technology
- Biomedical Engineering
- Climate Dynamics
- Complex Systems
- Computational Materials Science
- Future Technologies
- Network and Cluster Computing
- Statistics and Data Sciences
- Computational Chemical Sciences
- Vulnerability Analysis
- Computing Applications and Web Technologies
- Grand Challenge Science and Engineering Applications

Student research opportunities through the **Research Alliance in Math and Science (RAMS) Program**



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### Parametric Study of Mechanical Stress in Abdominal Aortic Aneurysms (AAA)

Erin A. Lennartz  
Virginia Polytechnic Institute and State University  
Research Alliance in Math and Science  
Computational Sciences and Engineering Division, Oak Ridge National Laboratory  
Mentors: Kara L. Kruse and Dr. Richard C. Ward  
[http://www.csm.ornl.gov/Internships/rams\\_06/abstracts/e\\_lennartz.pdf](http://www.csm.ornl.gov/Internships/rams_06/abstracts/e_lennartz.pdf)

#### Introduction

- The aorta is the largest human artery, originating from the left ventricle of the heart.
- Aneurysms in the aorta typically occur in the abdominal region due to the decrease of elastin in this area and this region does not have a vaso vasorum, which aids in repair.
- An abdominal aortic aneurysm (AAA) is a disease where the abdominal aorta loses its structural integrity and dilates in a balloon-like manner.


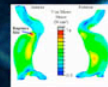
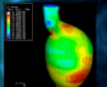


#### Why is this important?

- Abdominal Aortic Aneurysms (AAA) are a leading cause of death in the United States.
- 90% of AAAs that rupture lead to death.
- Currently aneurysms are not treated with intravascular or open surgery until they reach a maximum diameter of 5 to 5.5cm.
- Aneurysms much smaller than 5cm have ruptured, while aneurysms much larger have not.
- An aneurysm ruptures when the stress in the wall exceeds its strength, not when it reaches a certain size.

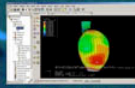
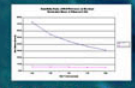


#### What was done before

Two previously created geometries were used for this sensitivity study. One of the geometries includes the bifurcation of the abdominal aorta into the iliac arteries, while the other does not. In both cases the rupture location is known and is accurately predicted using the patient average parameters.



#### Methods

- (1) Geometry model was created from segmented CT scans.
- (2) The AAA geometry model was meshed.
- (3) Stresses were computed for the meshed mode using the finite element (FE) analysis program, Abaqus.
- (4) Values for the wall thickness, elastic properties and blood pressure were varied.
- (5) Stresses were recomputed using the new values.



#### Conclusions

- The hyper-elastic model resulted in higher stress computations compared to the elastic models.
- The von Mises stress was very dependent on the wall thickness and found to be higher and more sensitive in the thinner walls.
- While patient-averaged parameters were accurate in determining site of rupture, changes in these parameters resulted in varying mechanical stresses.
- Higher resolution CT scanning would provide more accurate, patient specific data for calculating wall stress.

**Project Goals**

- Determine the sensitivity of the mechanical stress calculations to changes in the following parameters: wall thickness, elastic properties of both thrombus and artery wall, and blood pressure
- Determine which parameters affect the stress calculations the greatest
- Develop a hyper-elastic model for both AAA models using Abaqus
- Develop a more realistic model for predicting rupture

**Fig. 5: Aortic rupture. Preventing aortic rupture is the ultimate goal of these studies**

**Fig. 6: Sensitivity of the linear elastic model on wall thickness for the bifurcated AAA**

**Fig. 7: Abaqus interface during a hyper-elastic analysis**

The Research Alliance in Math and Science program is sponsored by the Mathematical, Information, and Computational Sciences Division, Office of Advanced Scientific Computing Research, U.S. Department of Energy. The work was performed at the Oak Ridge National Laboratory, which is managed by UT-Battelle, LLC under contract no. DE-AC05-00OR22725. This work has been authorized by a contractor of the U.S. Government, according to the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.

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Mathematical, Information,  
and Computational Sciences

OAK RIDGE NATIONAL LABORATORY  
U.S. DEPARTMENT OF ENERGY



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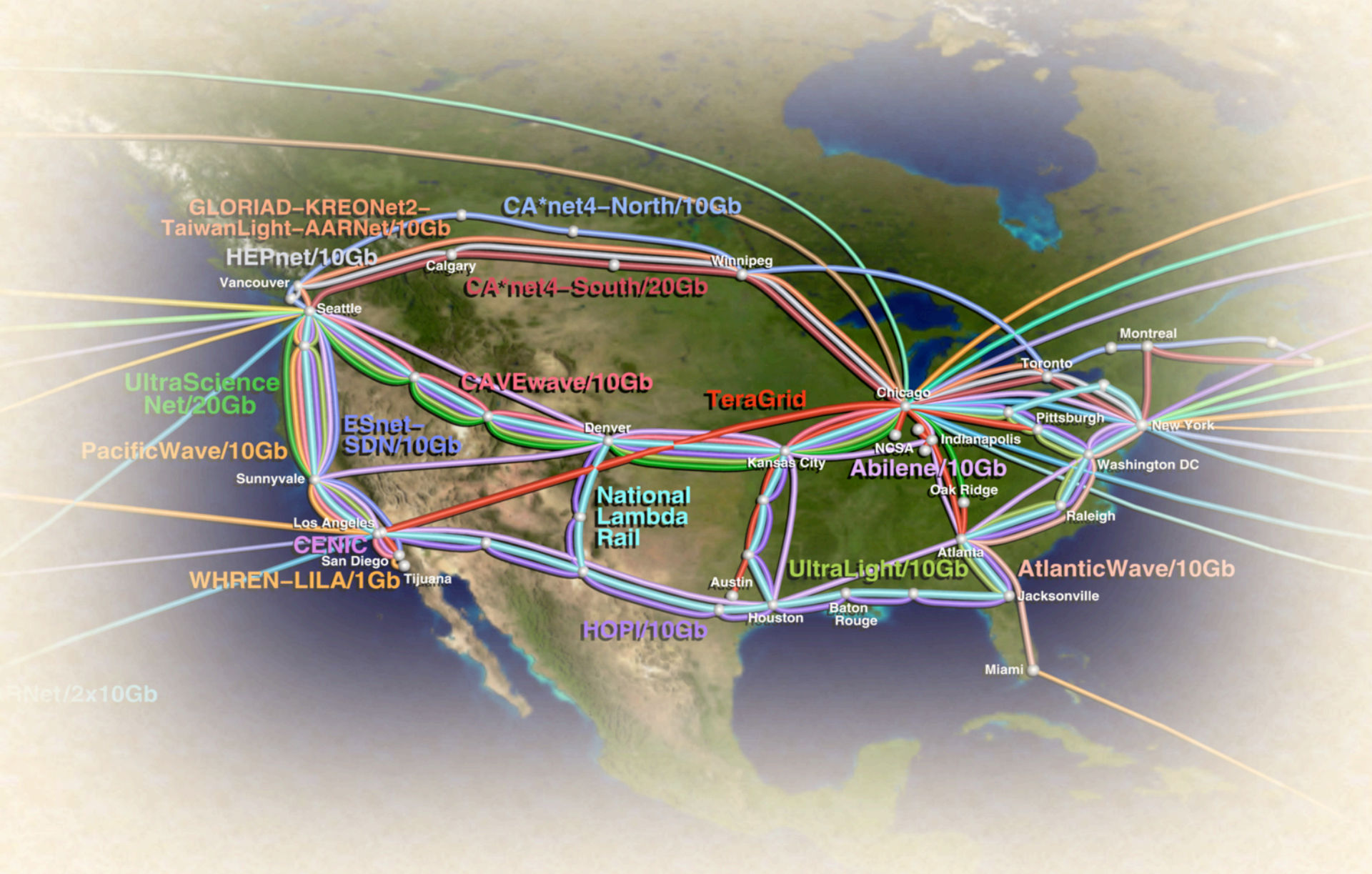
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# Contact

## Thomas Zacharia

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