
Billion-atom Multiscale Simulations of Nanosystems on a Grid

Priya Vashishta, Rajiv Kalia and Aiichiro Nakano

Collaboratory for Advanced Computing and Simulations (CACS)

**Departments of Materials Science & Engineering,
Computer Science, and Physics & Astronomy**

University of Southern California

priyav@usc.edu rkalia@usc.edu anakano@usc.edu

NSF Division of Materials Research ITR Computational Workshop

University of Illinois_Urbana, June 17-19, 2004

MCC: Duane Johnson

NSF_DMR: Daryl Hess, Bruce Taggart and Tom Weber

CACS

USC

Outline

Research

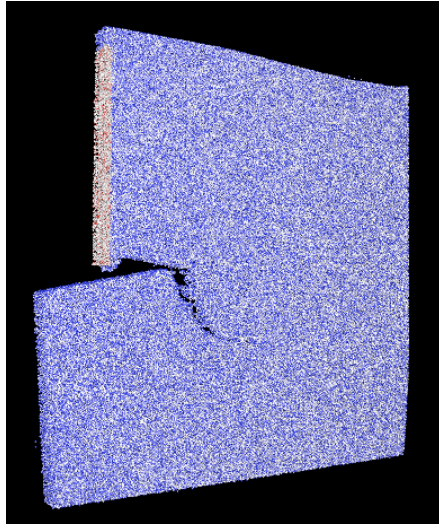
- **Fracture in Compression; Nano-indentation; Grid Computing; Billion Atom Walkthrough**

Education & Outreach

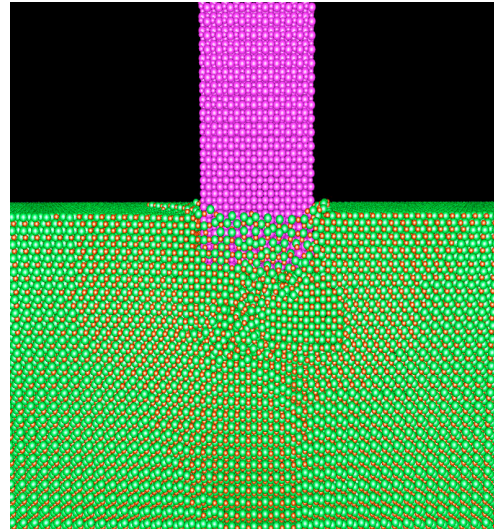
- **Computational Science Workshop for Under Represented Groups**

Overview of accomplishments

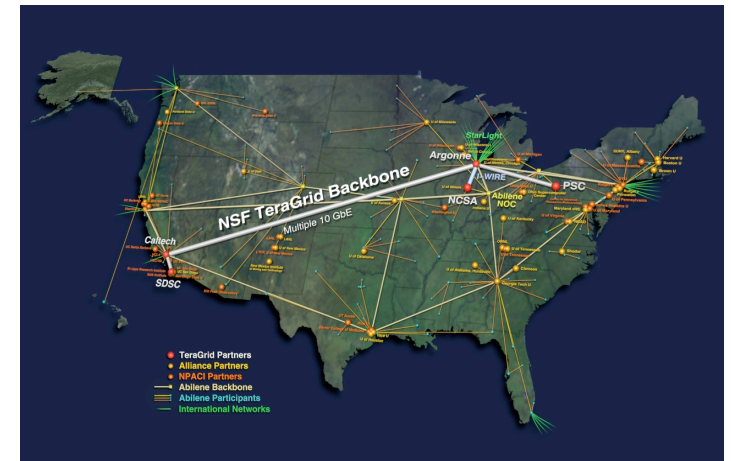
Compressive fracture



Nanoindentation



Grid Computing USA (USC, NSF) - Japan (AIST)



- **Nucleation, growth and healing of wing cracks in silica glass under dynamic compressive loading**
- **Nanoindentation-induced dislocation emission & amorphization in silicon carbide**
- **GRID Computing: Environmentally assisted fracture in silicon using divide & conquer strategy**

Education & Outreach

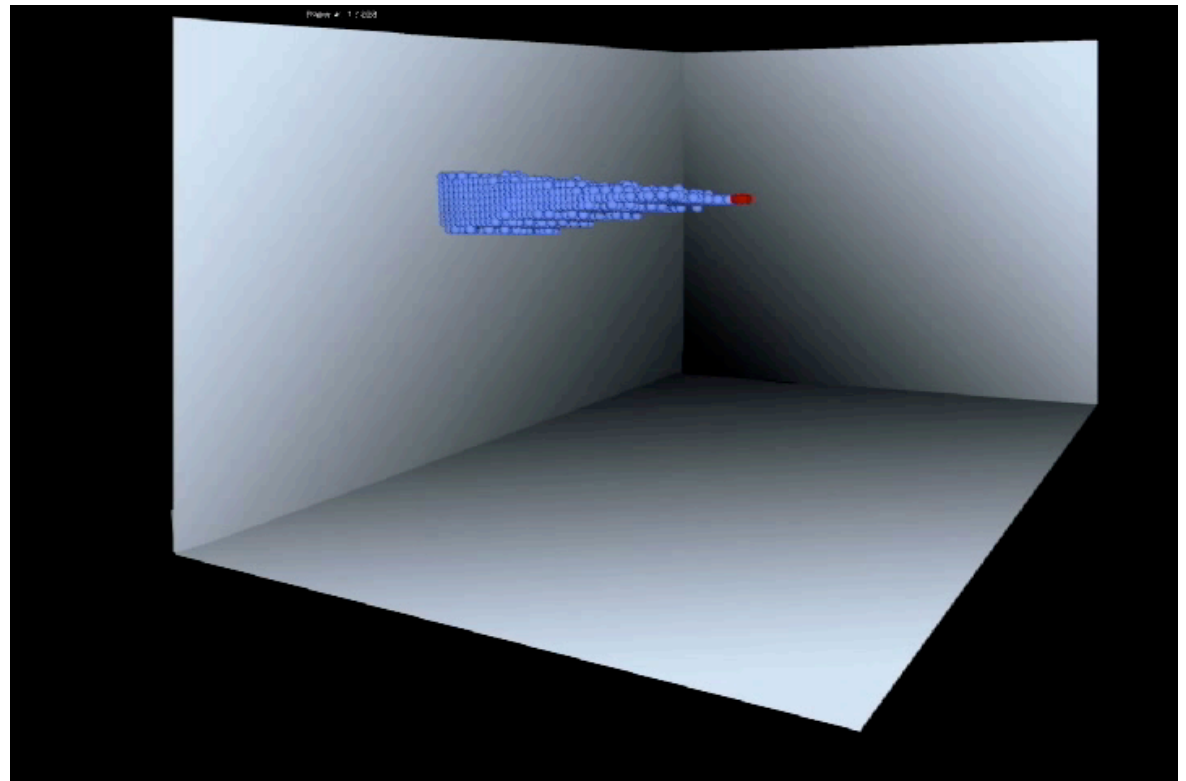
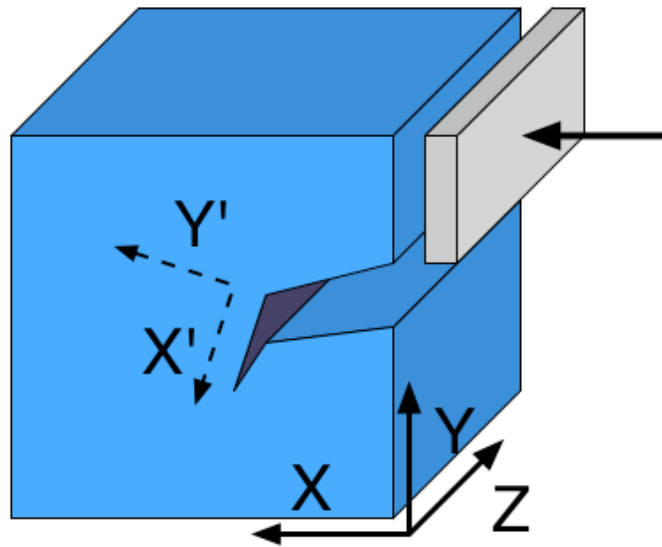
- **Dual Degree Program: PhD (Science or Eng) + MS (CS)**
 - > MS with specialization in Cybersecurity
 - > MS with specialization in High Performance Computing & Simulations
- **Reaching out to underrepresented groups through hands-on computational science workshops**
 - > 21 students and 11 faculty mentors from minority institutions form 12 states (CA, GA, IL, LA, MD, MT, OH, SC, TX, USVI, VA)
 - > Students with varying backgrounds—freshmen through seniors
Applied physics, biology, chemistry, computer science, mathematics, physics, computer engineering, mechanical engineering and school of pharmacy
- **Hands-on experience in parallel computing**
 - > Assembly of PCs nodes from off-the-shelf components, Scientific and simulation Software Scientific and simulation softwar, Connecting them to a Gigabit switch
Algorithmic and simulation exercises in a tutorial setting

Participants from U Texas, Pan-American (Hispanic minority institution) and Norfolk State University (African American minority institution) subsequently built their own clusters.

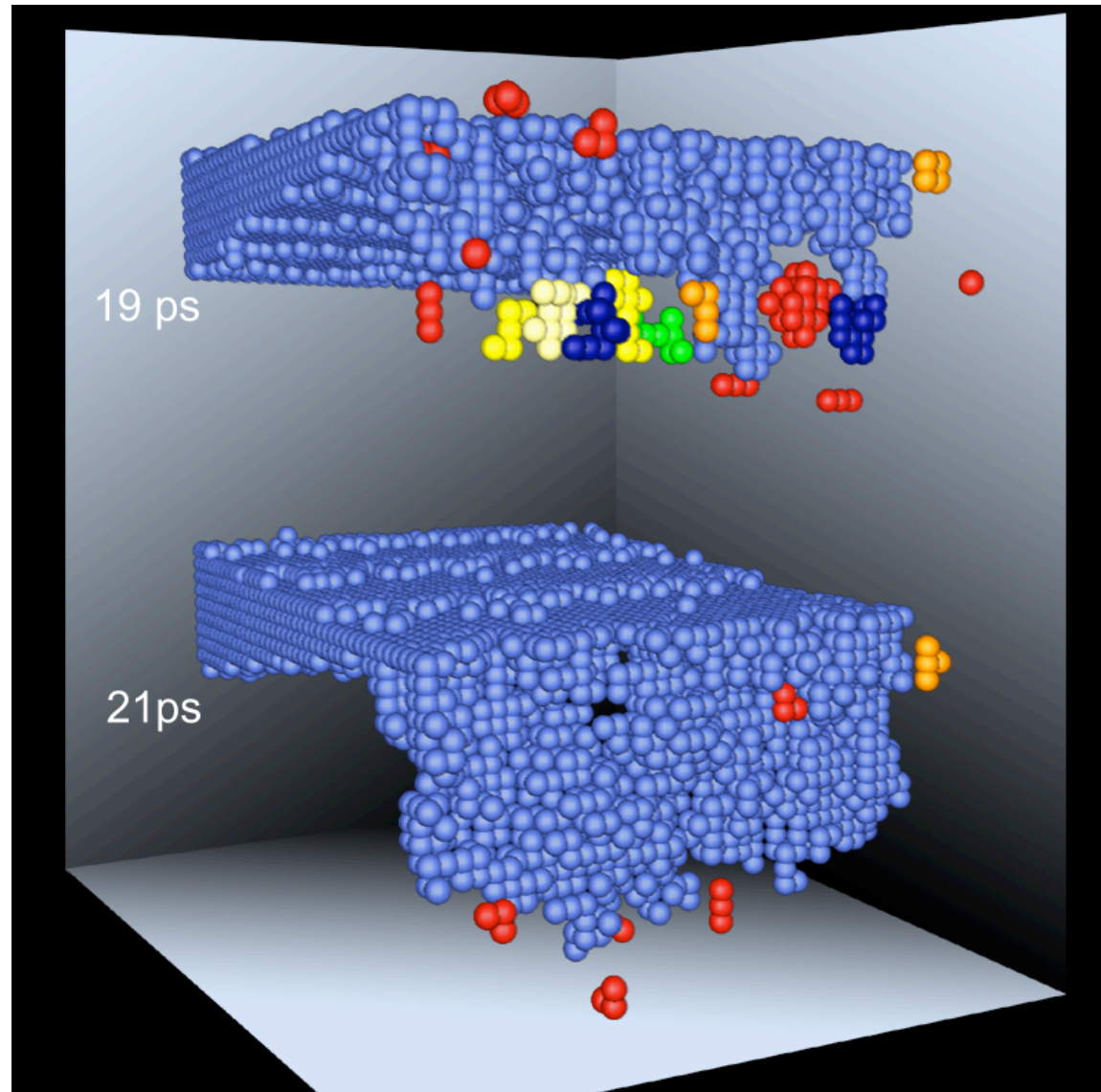
Research

Wing crack dynamics in confined silica glass

Impact speed = 150 m/s

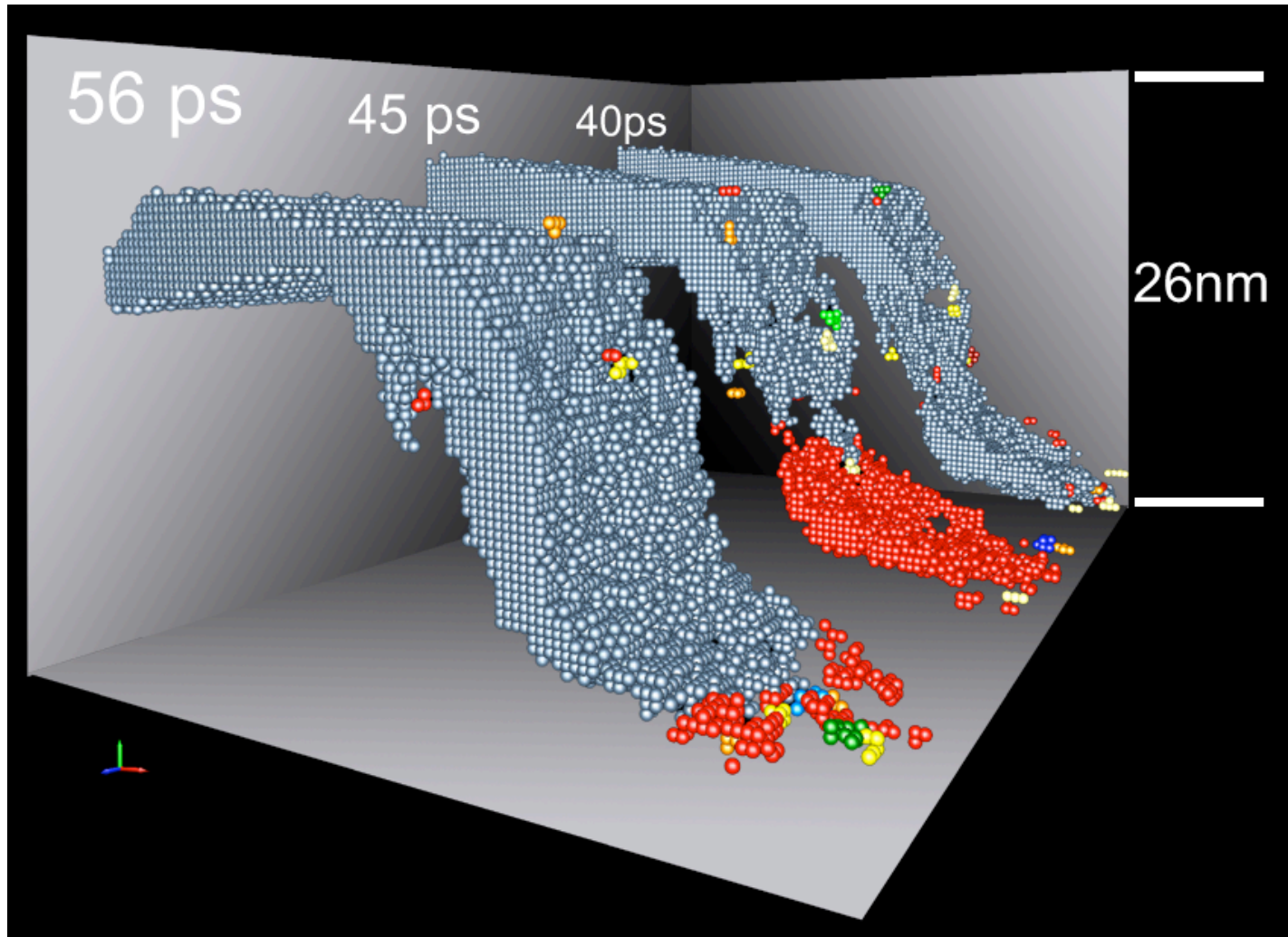


Wing Crack Growth

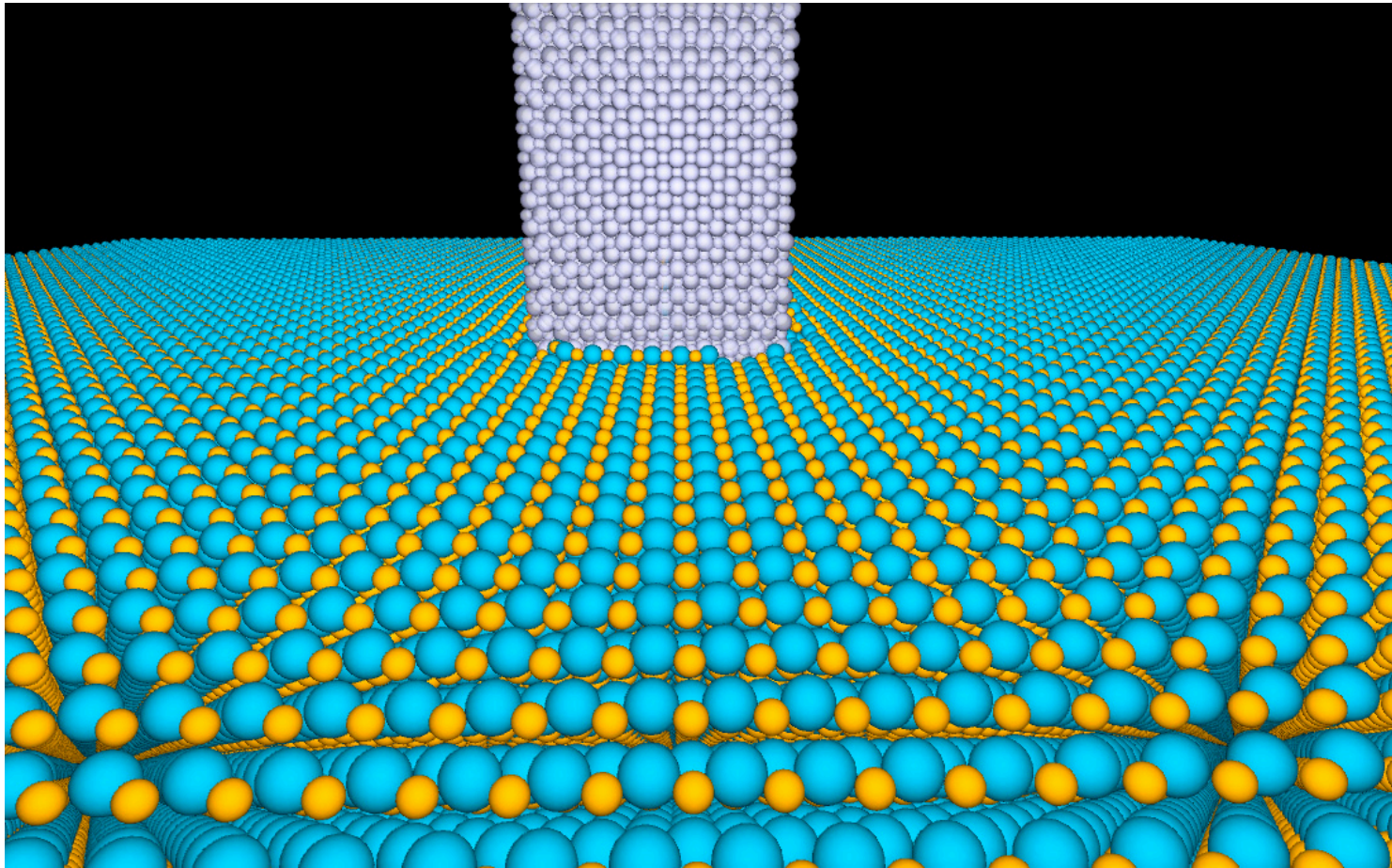


Wing Crack Healing

Impact Speed = 375 m/s

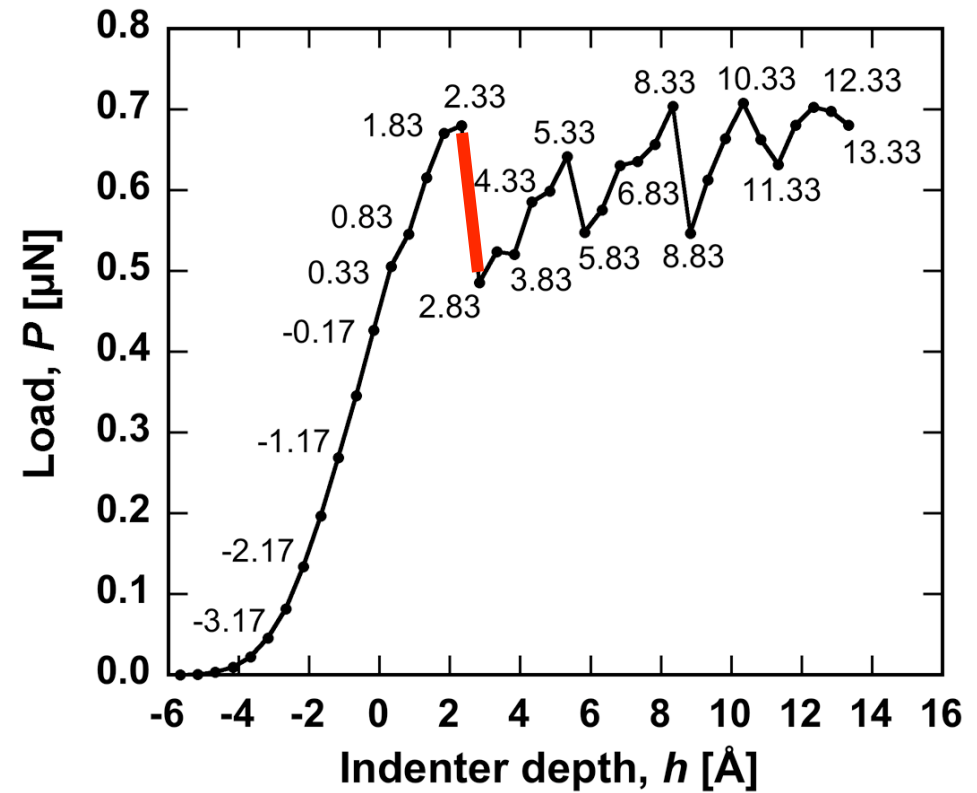
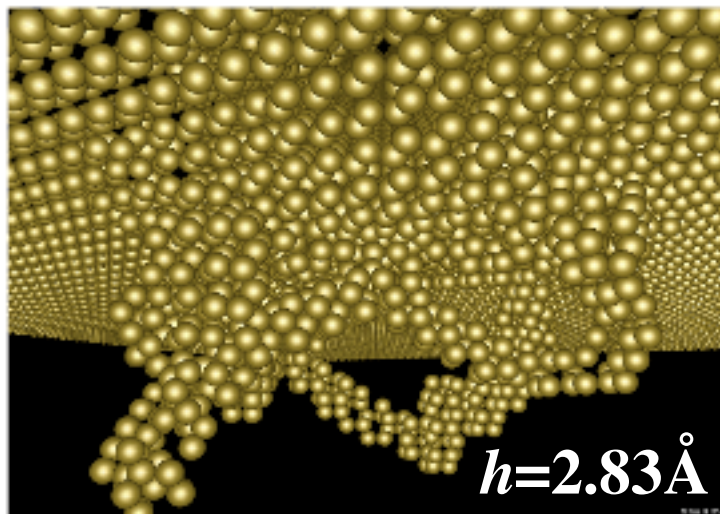
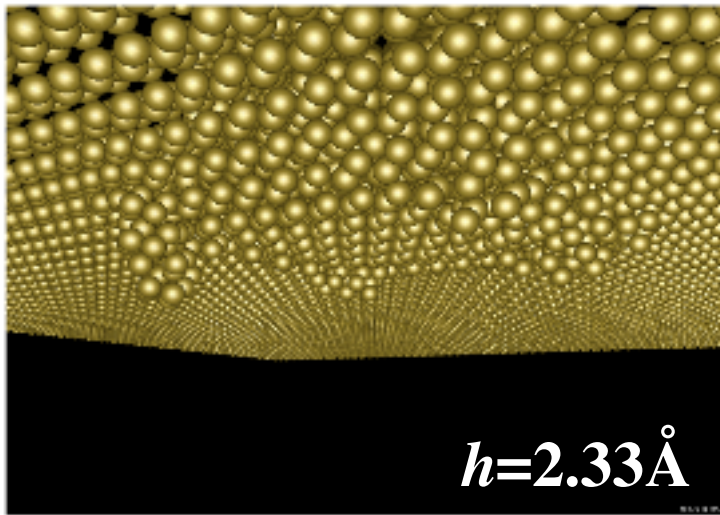


Nanoindentation in Silicon Carbide



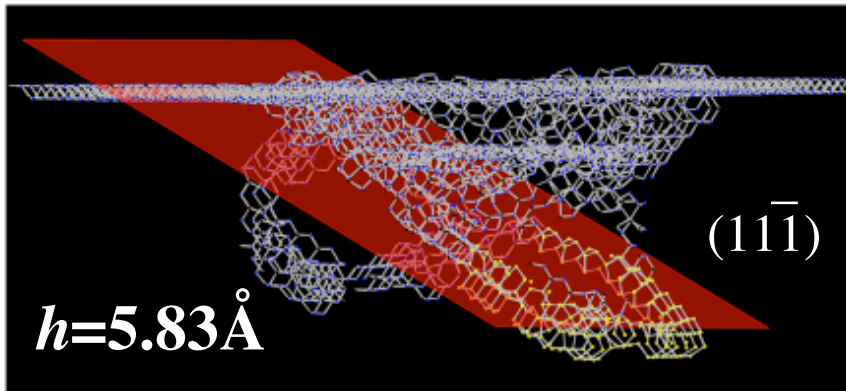
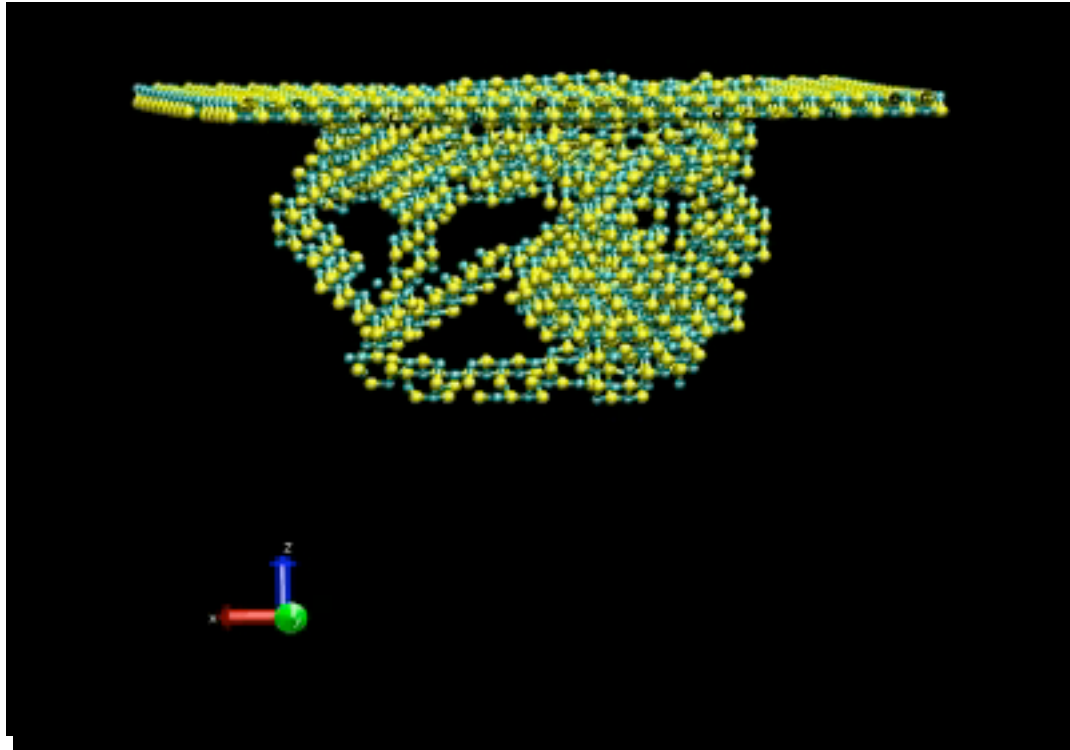
Nanoindentation yields important information about elastic and plastic deformations

Dislocation Analysis Using n-fold Rings

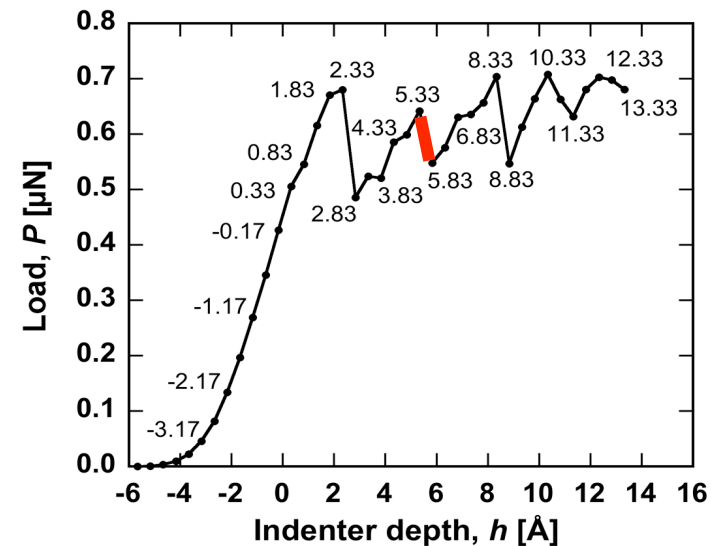


- **Outburst of dislocation loops at the first load drop**

Dislocation Analysis Using n-fold Rings



- Dislocation loops begin to coalesce at $h = 5.83\text{\AA}$
- Before the load drop:
 $h = 5.33\text{\AA}$: (111) , $(11\bar{1})$

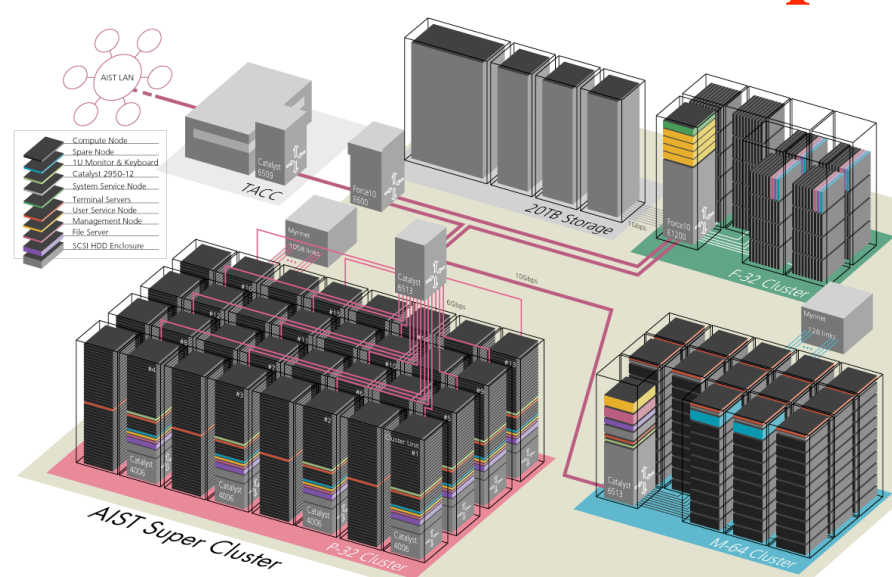


- After the load drop:
 $h = 5.83\text{\AA}$: $(11\bar{1})$

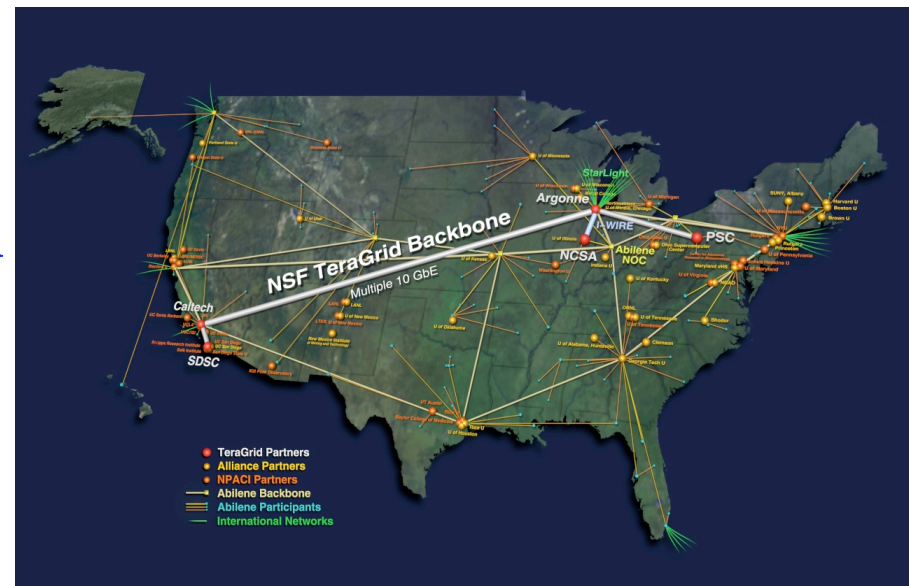
Large-scale Simulations Using GRID

Massively parallel machines in Japan

2000 AMD Opteron Supercluster

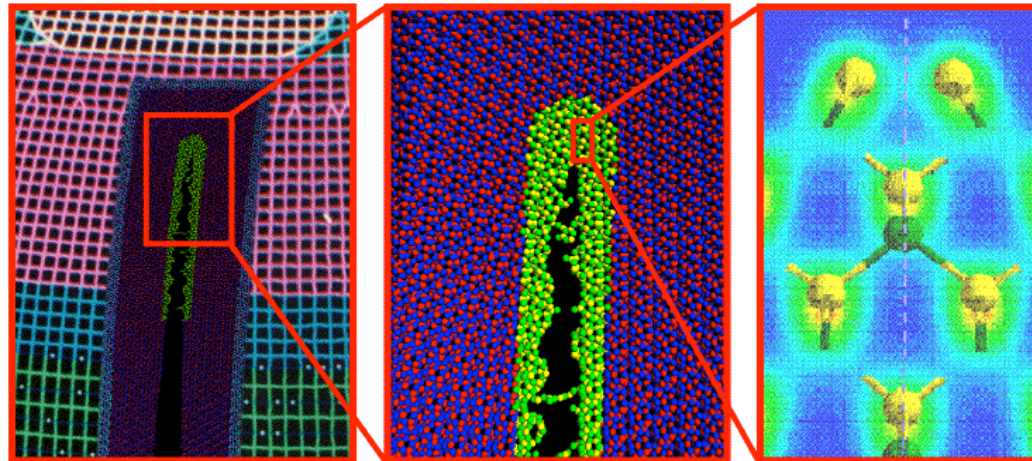


Grid of globally distributed supercomputers



Quantum-to-Atomistic-to-Continuum Simulations

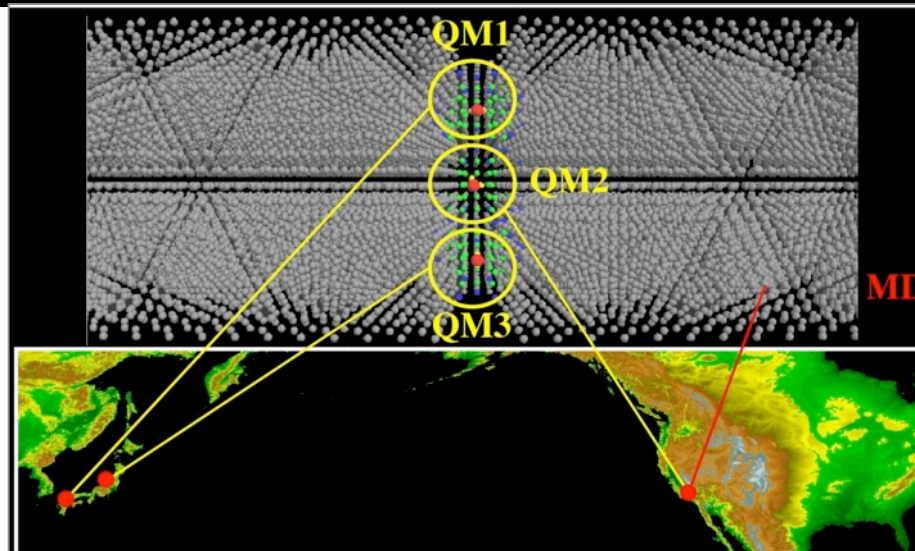
Global Collaborative Simulations on GRID



**Finite
Element**

**Molecular
Dynamics**

**Density
Functional**

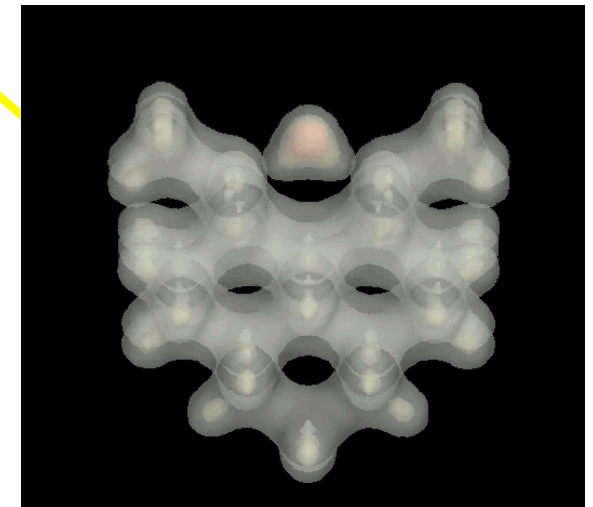
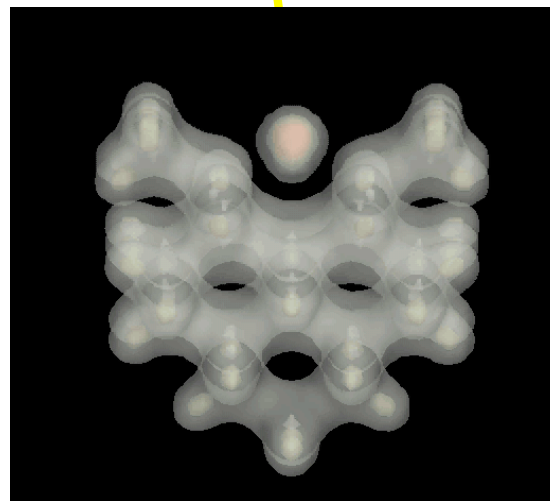
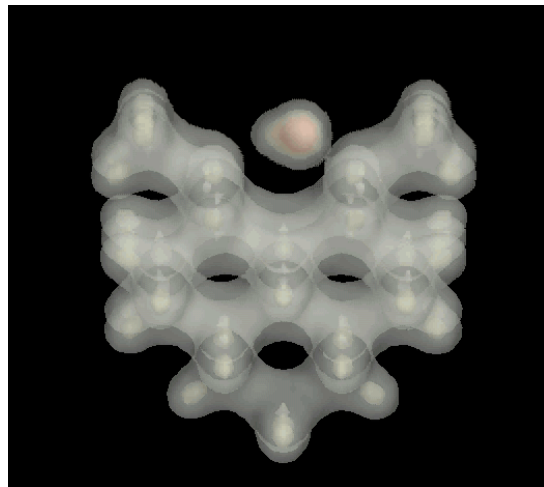
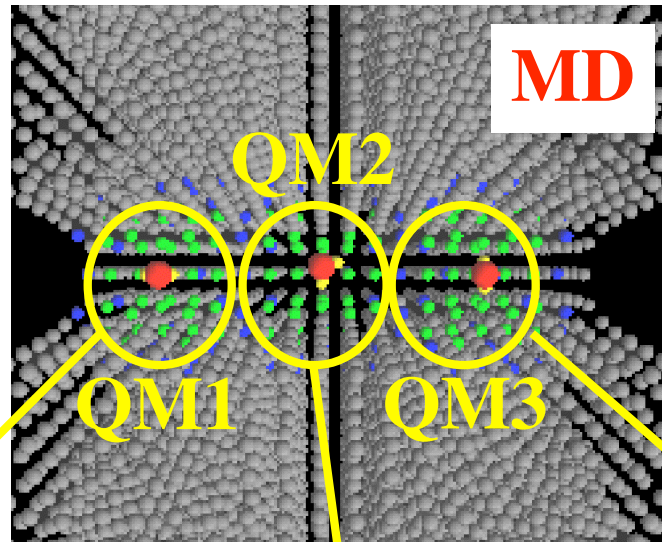


GRID Computing between USA and Japan

Grid Enabling: Multiple QM Partitioning

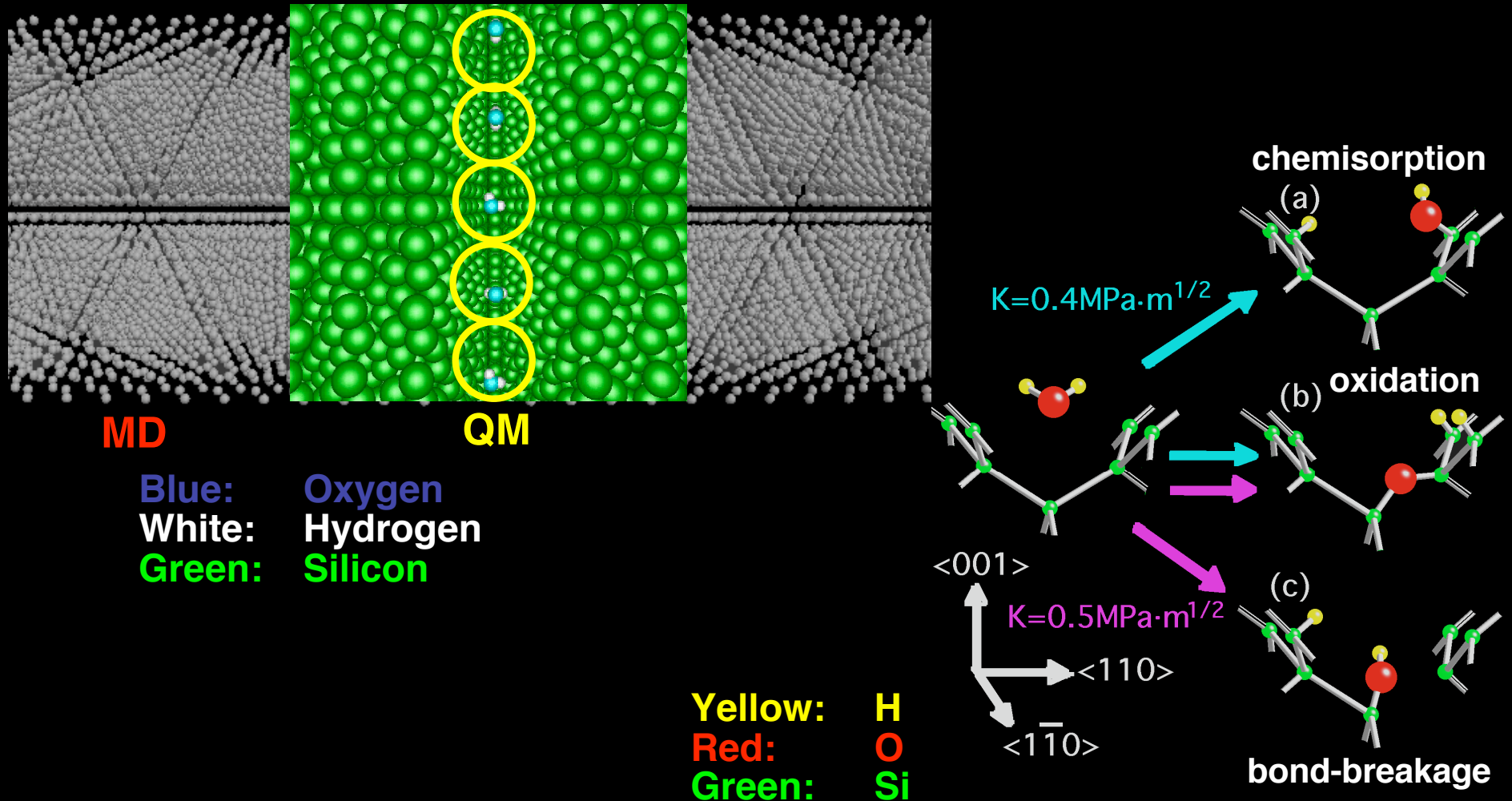
Environmentally assisted fracture:
Reaction of water molecules at the crack tip in silicon

Divide-&-conquer



US-Japan collaboration on environmentally-assisted fracture

Reaction of H₂O molecules at a Si crack tip



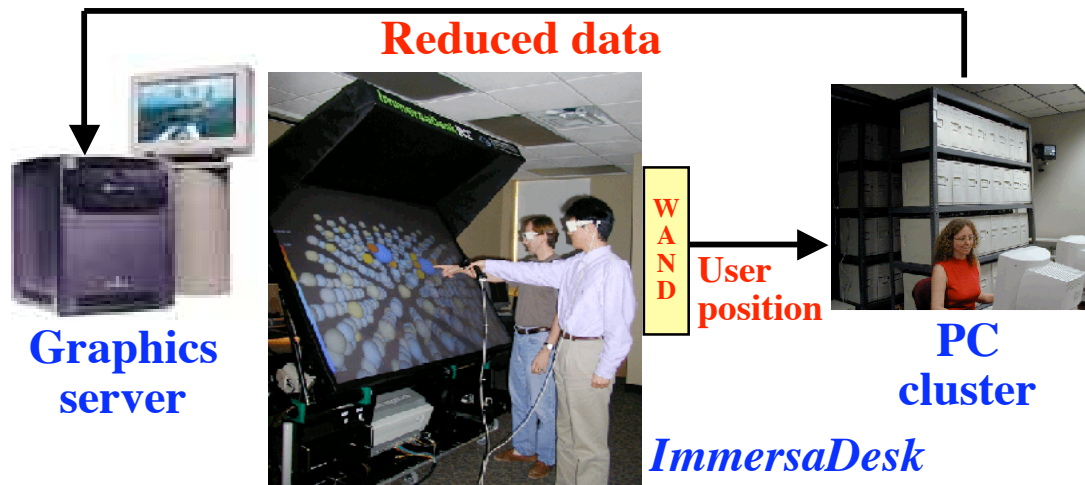
Significant dependence of the reaction on stress intensity factor

Summary_Research

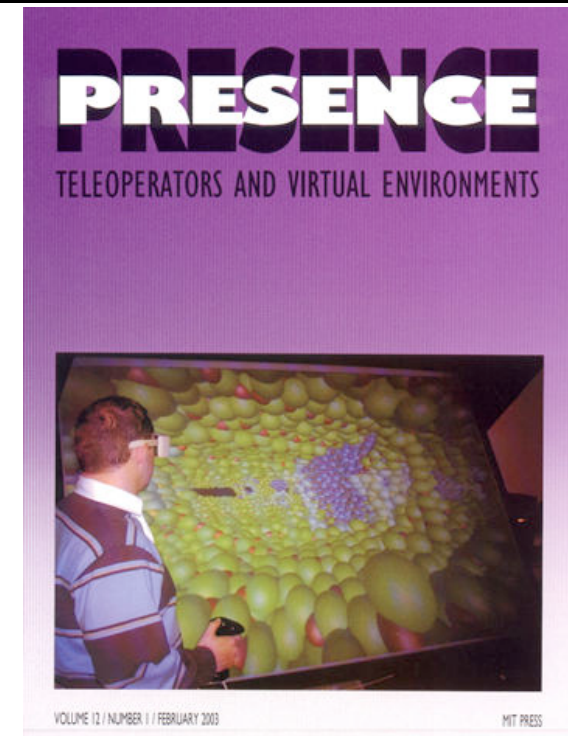
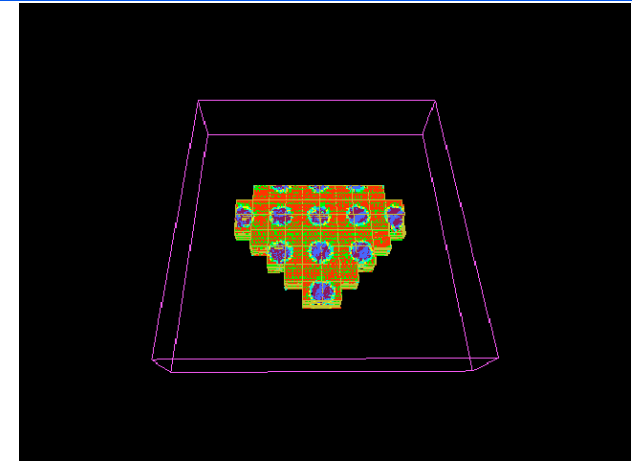
- **Confined silica glass subjected to dynamic compressive loading**
 - > **Kinks at the crack tip coalesce with nanocavities to form a wing crack**
 - > **Wing-crack segments can propagate at supersonic speeds, but the crack heals due to confinement**
- **Nanoindentation in silicon carbide**
 - > **Nucleation of dislocations in crystalline SiC**
 - > **Dislocation loops cause amorphization under the indenter**
- **Collaborative GRID Computing**
 - > **USA and three universities (Niigata, Hiroshima, Yamaguchi) in Japan**
 - > **Environmental assisted fracture in silicon**

Immersive & Interactive Visualization Billion Atom Walkthrough

- Octree-based fast view-frustum culling
- Probabilistic occlusion culling
- Parallel/distributed processing



- Interactive visualization of a billion-atom dataset in immersive environment



Education & Outreach

Education & Outreach: Computational Science Workshop for Underrepresented Groups (CSWUG)

January, 2003 at LSU

January, 2004 at USC

... I want to be able to help inspire others just as all of you in the workshop helped to inspire me...
Tanjalla Purnell, Tougaloo College

2nd Computational Science Workshop for Underrepresented Groups

Report Prepared by Student Participants and Faculty Mentors

Computational Science Workshop for Underrepresented Groups

University of Southern California

January 5-10, 2004

Scope
This workshop provides undergraduate students with hands-on experience in parallel computing, including the construction of a parallel machine, and in interactive and interactive visualization.

Aim
This is the third in a series of annual workshops that involve undergraduate students and faculty members from underrepresented groups in emerging areas of computational science and engineering.

Application Deadline
December 1, 2003

Contact Information
Sabrina Fockey
Telephone: 213-821-2662
Fax: 213-821-2664
E-mail: csoc@usc.edu
Website: <http://www.usc.edu/csoc/workshop.html>

Organizing Committee
Ben Abio, University of California at Newark
Sukun Berman, Middlesex College
Loren Dantz, U.S. Department of Defense
Earl Dierker, Southern University
Samuel Dinko, George Jackson University
Derrick Hillon, Spelman College
Richard Kuhn, Seton Hall University
Doreen Mafira, Caltech
Mike Strong, Mississippi State University
Kareem Yousif, Clark Atlanta University
Daph A. Toufigh, Hampshire University
John Whittall, University of Utah, The American
Matthew F. Ware, Georgia Institute of Technology

Workshop Organizers from USC
Glen Rubin, Dept. of Physics & Astronomy
The-son Chang, Dept. of Physics & Astronomy
Sudhakar Challa, CSE
Stephen Chen, Dept. of Physics & Astronomy
Rafael E. Faller, CSE
Arthur Elster, Dept. of Mechanical Engineering
Dian Lu, Dept. of Electrical Science
William Lee, Dept. of Physics & Astronomy
Joseph Madhala, Dept. of Chemical Science
Huijun Ma, Dept. of Electrical Science
Gerald Knudsen, Dept. of Computer Science
Anthony Kulkarni, Wright Institute
Rudolf Kuznetsov, CSE
Kunlun Li, Dept. of Physics & Astronomy
Tao-Yu Lin, CSE
Wenjun Wang, Dept. of Electrical Science
Chen Wang, Dept. of Chemistry
Cheng Zhang, Dept. of Electrical Science
Shi Zhang, Dept. of Physics & Astronomy

Collaboratory for Advanced Computing & Interactions
School of Engineering
College of Letters, Arts, and Sciences

Success Story of Tangela Purnell, Tougaloo College, Mississippi

“I am one of the students who recently attended your workshop, and I was just writing to sincerely thank you for selecting me to be a part of such an astounding experience. I cannot believe how much I learned in one week, and it was so much fun. I am so glad that I attended the workshop because being in undergraduate school, I do not usually get a chance to do much hands-on work, but I mainly have to do a lot of difficult programming. At one time I was so frustrated with only having to program and not getting any hands-on experience that I almost considered changing my major. However, during the workshop I was so mesmerized by all of the hands-on experience, especially when we built the parallel computer. Your workshop helped me to remember why I wanted to be a computer science major in the first place. I feel so inspired now to go on and get my PhD in computer science. I hope that you will continue the workshop for many years so that other students will be so richly enhanced, just as the workshop enhanced me. I hope that when I obtain my PhD I will be able to return to the workshop no longer as a student but as a mentor for other students. I want to be able to help inspire others just as all of you in the workshop helped to inspire me.”

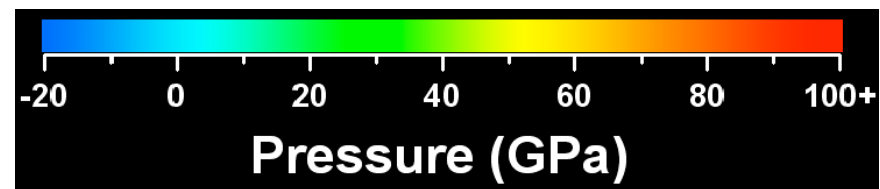
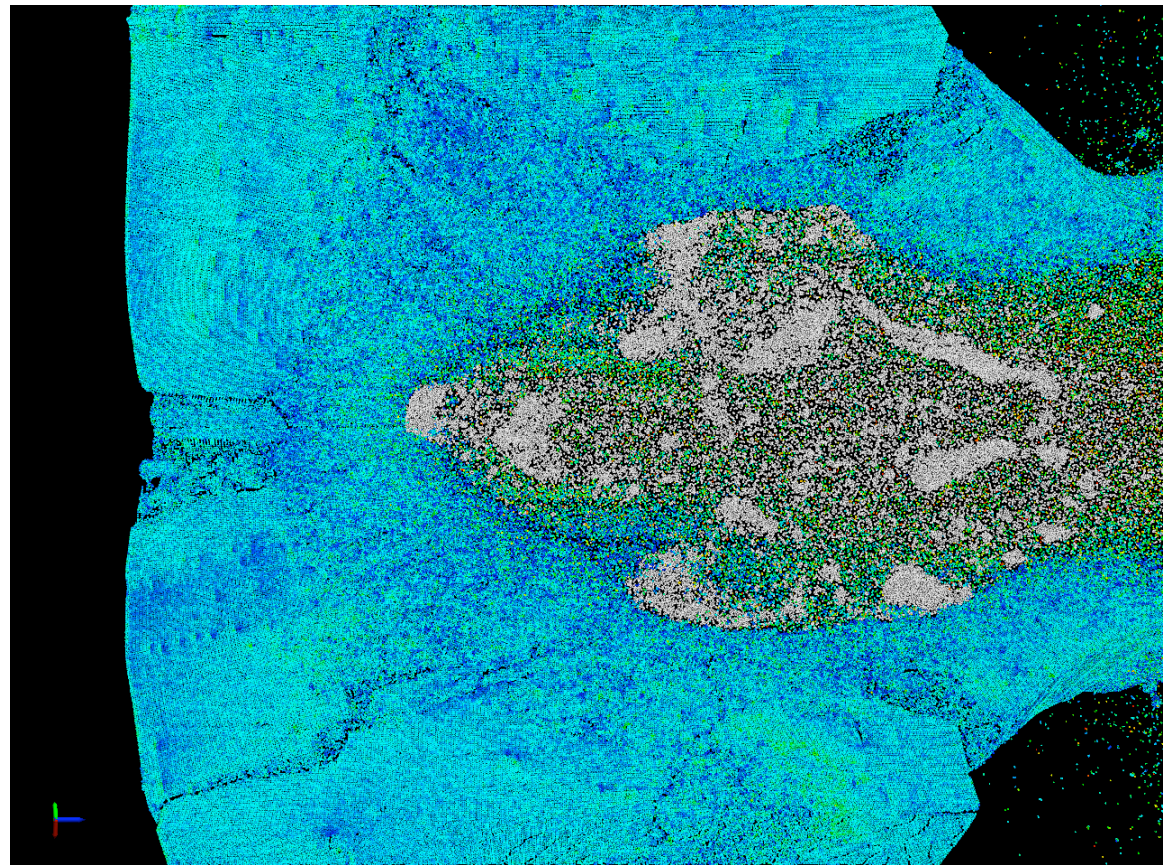
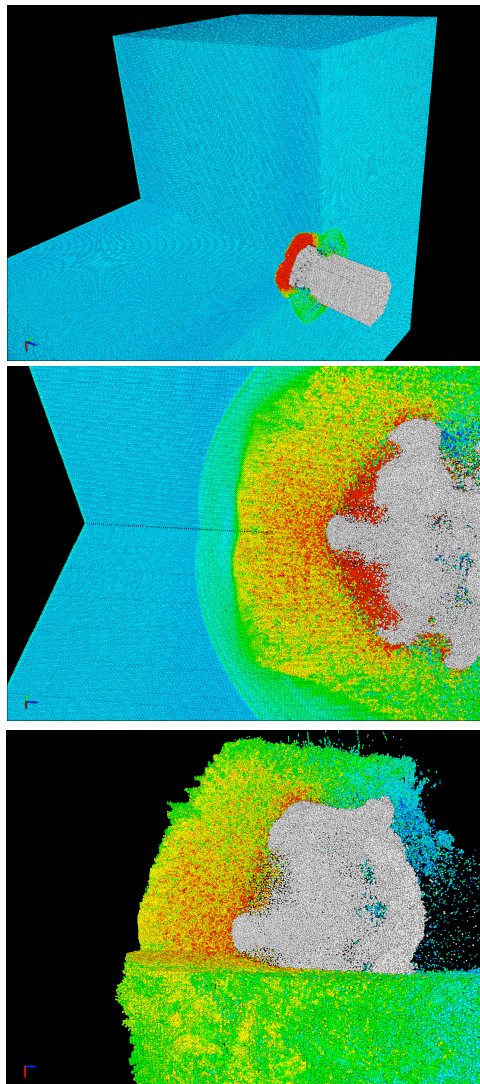
Tanjala Purnell a participant at our
Computational Science Workshop for
Underrepresented Groups, January 5-11, '03.

Summer 2003: Internship at the University of Michigan

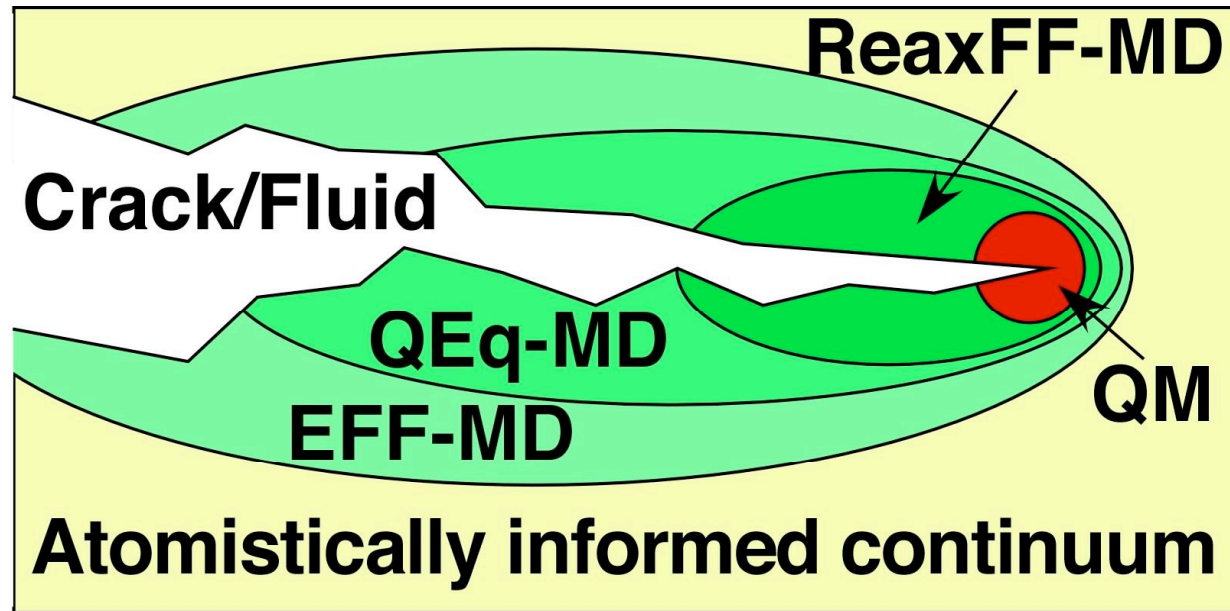
Summer 2004: Internship offers from Michigan, Wisconsin, Chicago, Harvard and NIH

**Research
and
Education & Outreach
In Progress**

Shock-induced structural phase transformation, damage & fracture in AlN

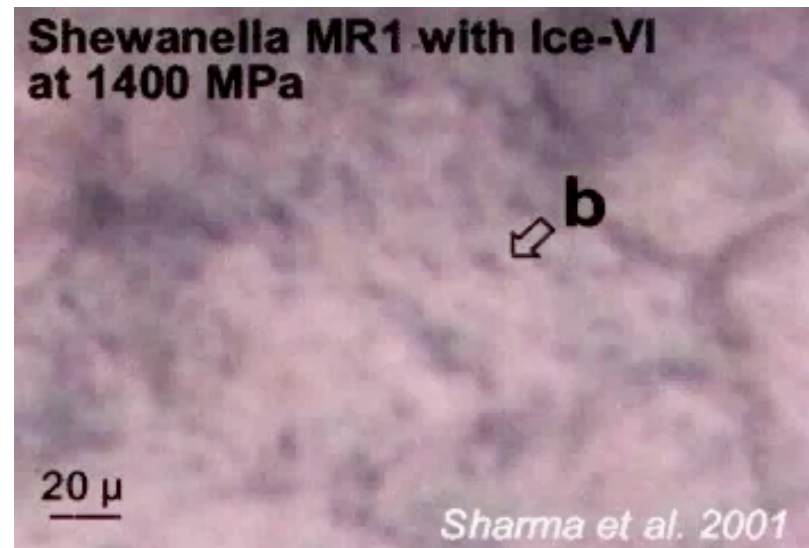


Stress Corrosion Cracking (SCC)



SCC Inhibitors

- Ceramic coatings
- Self-assembled monolayers
- Microorganisms



Education & Outreach: Computational Science Workshop for Underrepresented Groups January 5-11, 2004 at USC



"This workshop will be very beneficial in my future."
- Peter Muhoro

"The workshop at USC has broadened my horizons."
- Jonathan Lee

"The activities of assembling a computer from the ground up and learning about parallel computing has been great."
- Glenn Snyder

3rd COMPUTATIONAL

SCIENCE WORKSHOP
FOR UNDERREPRESENTED GROUPS



Report Prepared by Student Participants and Faculty Mentors



3651 Watt Way, VHE 608
Los Angeles, CA 90089-0242
(213) 821-2662
<http://cacs.usc.edu>

Collaboratory for Advanced Computing and Simulations
Viterbi School of Engineering
College of Letters, Arts, and Sciences

Education & Outreach: Computational Science Workshop for Underrepresented Groups

- **Follow-on activities with participants will include**
 - > **Bringing students back for summer research and to participate in a computational science conference**
 - > **Inviting some students and faculty mentors to help organize and run the next workshop, which will be held at USC during January, 2005**
 - > **Remote research experiences for students facilitated by the loan of the PC nodes they built at the workshop**



Thank you for your attention!