Spring 2008

SCS

Integrating Advanced Computing with Science, Engineering and Liberal Arts

School of Computational Science at Florida State University

Understanding Metal Strength by Computational Modeling

INSIDE THIS ISSUE

The smooth and shiny surface of a metal does not reveal its complex inner structure. A look through a microscope is needed to show that a metal consists of large numbers of crystals of sizes ranging from nanometers to hundreds of micrometers.

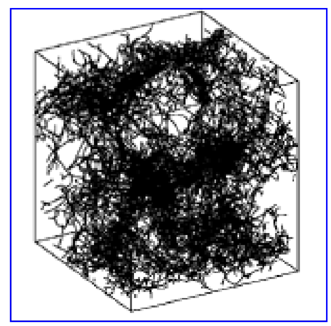
If we could look even closer and see the atomic structure of the metal, we would notice that the crystal is made up of neatly layered atoms. However, the otherwise perfect lattice structure is interrupted by a multitude of irregularities, of which the linear defects called dislocations are very important.

TO THE MOON

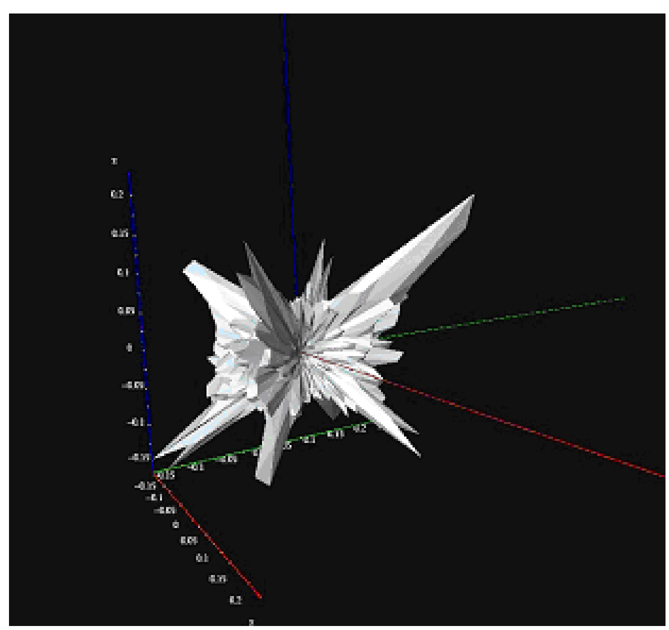
"One cubic centimeter of aluminum contains so many dislocation lines that they would reach from the earth to the moon if we could line them up," says Anter El-Azab, associate professor of computational materials science and mechanical engineering at FSU. He continues:

"Under mechanical stress, dislocations move. They interact with each other and multiply in a complex fashion in the crystal. With enough force applied to the crystal, the dislocations self-organize in the material, and eventually localize the deformation process to form cracks, which may cause the collapse of a metallic structure."

One way to slow down the dislocations motion, and thus make metals stronger, is to make it less pure by mixing one metal with another. For example, while a pure copper crystal can be squished between your fingers, adding some zinc creates the much stronger alloy called brass.



Snapshot of crystal dislocations computed using the method of dislocation dynamics simulation (above), and the result of statistical modeling of the angular distribution of dislocation lines (above).



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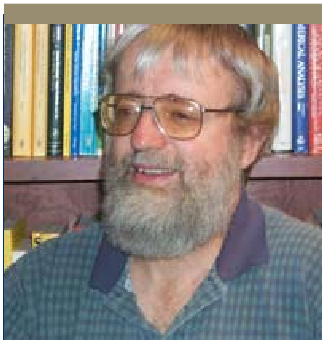

So far, the 07-08 academic year has been an eventful one for the SCS. We greeted new faculty, students, postdocs and staff. The SCS, mostly through the efforts of Jim Wilgenbush (our Associate Director for Computing) was instrumental in the acquisition, deployment, and now the management of a new high performance computing facility at FSU. Our Masters and Ph.D. programs are now in full swing as are a variety of courses that our faculty developed in support of these programs. Janet Peterson is currently offering our first undergraduate course; this is just the beginning of our efforts directed at that segment of the FSU community. We are gearing up for our upcoming Graduate Research Exposition and are looking forward to the arrival of several visiting faculty and research collaborators. Several faculty received prestigious honors and awards, indicative of the very high quality of research going on at the SCS. This edition of our newsletter highlights just a portion of that research, featuring projects devoted to airplane noise reduction, weather forecasting, and metal strength. Undoubtedly, the SCS is well on its way to becoming an integral, even indispensable part of FSU!

Max Gunzburger,
Director, SCS

WHY DOES A METAL BREAK?

Professor El-Azab and his student Jie Deng of Mechanical Engineering are using computer modeling to understand the statistical characteristics of these dislocations in deforming metal. Their goal is to understand how patterns of dislocations form in the crystal and how these patterns evolve during crystal deformation under applied stresses. The overall purpose is to understand what happens before a metallic structure eventually breaks and how that can be prevented.

CLASSIC THEORIES

Dr. El-Azab's approach relies partly on the core principles of the classical kinetic theory, drawn up by Maxwell and Boltzmann in the 19th century. According to this theory, atoms can bounce around in a fluid with a certain freedom, though their movement is restricted by the way that they are attracted to or repelled by other atoms in the same fluid. Each segment of a dislocation line can be compared to atoms in a fluid, and their movement can be modeled in a similar way.

The computer code that Dr. El-Azab uses is called the Parallel Dislocation Simulator (ParaDiS), and has been developed at Lawrence Livermore National Laboratory. This code tracks the dislocation density evolution in crystals, from which various statistical properties of the dislocation system can be predicted, for example, the angular distribution of dislocation density and the dislocation-dislocation correlations.

Typical angular distribution is shown in star shaped graph on the front page, which reflects the highly anisotropic nature of the orientation of the dislocation density in crystals. This statistical information feeds into the kinetic theory of dislocations developed by Dr. El-Azab and his student.

An important finding has been that crystal dislocation systems are both correlated and anti-correlated at short range, but anti-correlated at long range. More results can be found in a recent special issue entitled "Density-Based Modelling of Dislocations," of the Philosophical Magazine journal (issue 8-9, volume 87, 2007), edited by Professor El-Azab and European collaborators.

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Advances in Biophysics

A workshop held earlier this year on Quantitative Computational Biophysics provided an overview of the state of the art in biomolecular computation. The workshop focused on two longstanding, interrelated challenges in computer simulations, namely, (i) how to develop and validate force fields of high accuracy and (ii) how to ensure adequate sampling of conformational space areas of interest in biophysics. The workshop presentations detailed substantial progress in both these areas.

A new generation of force-fields have refined the Ramachandran map and provided an improved representation of the conformational ensemble in folded proteins. The independent assessment of the force-field quality by NMR relaxation, residual dipolar coupling, x-ray diffraction, and other spectroscopic data suggests that the force fields and the simulation methodologies are reaching a level of accuracy that allows quantitative prediction of motional properties. Significant progress was also evident in the extension of current force fields to move beyond the static representation of fixed charges and protonation states.

Enhanced sampling algorithms based on multi-canonical, umbrella sampling and replica exchange methods, are extending the time-scale of events that can be accessed by allowing simulations to overcome energy barriers while maintaining accurate room-temperature ensemble averages. These methods are being coupled with careful analyses of statistical computational error to assess the effects of the finite simulation time and the finite extent of generated ensembles. New metrics for the statistical convergence of properties computed from an ensemble -- analogous to the "error bar" associated with experimental date -- promise the possibility of a more appropriate assessment of computational errors.

These advances in force fields and computational methods are making simulation applicable to an increasing number of problems of practical interest such as modeling charge and proton transfer, the effects of pH, large conformational change, and protein-protein interactions, as well as many others.

PIPE-line for Protein Structures

Professor Huan-Xiang Zhou and his group have developed powerful methods for predicting structural features of proteins and have made these methods widely accessible on web servers. Remote users can access the PIPE website, enter their data in the form of amino acid sequences of proteins, and quickly get results showing the 3D structure of their proteins. The PIPE, or Protein Interface/Interior Prediction Engine analyzes primary, tertiary (3D), and quaternary structures of more than one protein, then analyze superstructures of functioning, multi-component assemblies. For mor information, go to www.pipe.scs.fsu.edu.

SCS History & Hussaini Group Research

Renaissance Scientist

Leonardo da Vinci, Rene Descartes and many other well-known men who were active during the renaissance era in the 15th and 16th century, are known today for their broad interest in different areas of the sciences and arts. Even today we call scientists with a broad interdisciplinary approach Renaissance scientists. In addition to limitless curiosity, a true Renaissance scientist held a firm conviction that everything in nature is based on the laws of mathematics, and can be described in mathematical terms.

Professor Yousuff Hussaini at SCS fits this description very well, and is dedicated to training young scientists in the same open-minded approach to research. His entire group illustrates that example by using their mathematical tools to investigate the most diverse problems – from power system networks to air traffic conflicts, and from hurricane prediction to control of high frequency jet noise.

Dr. Hussaini came to FSU in 1996. His first interview was in 1993, but it took FSU three years to convince him to give up his position at the NASA Langley Research Center in Virginia, where he was the Director of the Institute for Computer Applications in Science and Engineering (ICASE). When he finally accepted the position as Thinking Machines Corporation Scholar Chair in Computational Science and Engineering, it was because of the attraction of the idea to create something new – an interdisciplinary program in computational science.

In 1996, computational science was mostly of interest to the national labs – much less so to universities. At that time, only 12 university-based programs in computational science existed nationwide. The major universities were big enough to have a critical mass of computational scientists within their science and engineering departments, and most did not really see the need for an interdisciplinary program.

Professor Hussaini's position was with SCRI, host of the FSU supercomputers since 1984, and home base for computational science, especially computational physics, at FSU. Professor Hussaini started to make plans for a program in computational science and engineering. His vision was to educate renaissance scientists in a multidisciplinary research atmosphere, since he understood that twenty-first century problems require team efforts to be solved.

SCRI was transformed into CSIT, the School of Computational Science and Information Technology, predecessor of today's SCS, and Professor Hussaini was its first director. However, time was not yet ripe for the new school to actually have students. Not until 2006 did SCS and FSU get a graduate program in computational science. By then, professor Hussaini was no longer involved with the educational matters. Other people at CSIT/SCS had taken over the struggle to establish the graduate program, and Dr. Hussaini could, once again, focus on research.

Today, his multi-disciplinary, multi-national group consists of five post docs and two students. They all have a firm background in applied mathematics, and use their skills in a wide array of fields.

NASA-Funded Research Targets Airplane Noise

Airflow is one of the most critical factors in getting an airplane off the ground. Air, along with a few other things like power and thrust, makes the airplane move. It turns out, though, that the airflow so critical for propelling an aircraft forward is the cause of much consternation among those who live within a certain radius of airports. While jet engine exhaust or airflow makes an airplane move, it also creates a large amount of noise. An ordinary jet engine can create approximately 150 decibels of noise – as a comparison, the Occupational Safety and Health Administration recommends sounds be under 85 decibels to avoid hearing loss.

For years, neighborhoods affected by airplane noise have banded together, marshaled their resources and appealed to airport authorities and city officials for relief. Some local, grassroots-based noise reduction organizations have become more formal, forming national coalitions for reducing noise. They have lobbied to have certain types and weights of aircraft banned, and a decibel limit placed on aircraft noise emissions to help residents whose homes and workplaces are in the noise corridor.
Some cities have built their airports on way outside the city to avoid the problem, but this makes it more difficult, inconvenient, and costly for travelers to get to locations in the city's central business district.

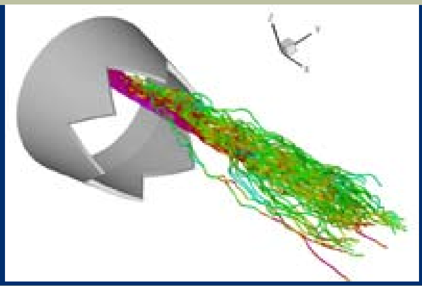
In addition to being a health and quality-of-life issue for affected residents, airplane noise is one of the primary limiters of growth for the aviation and aeronautics industry. Airlines must limit airplane size and flight frequency in an effort to maintain acceptable noise levels. If airplane noise could be sufficiently reduced, larger aircraft could fly passengers to more destinations more often, providing the opportunity for higher profits and optimal travel planning.

Enter Dr. Ali Uzun, SCS Research Associate and expert in aeronautics and astronautics. Ali and his colleagues are working on two NASA-funded research projects that can assist aviation and governmental officials in their quest to find ways to reduce airplane noise. Recognizing the negative economic and health effects of aircraft noise, NASA initiated the Quiet Aircraft Technology Program. The program's mission is to research and develop noise reduction technologies that will cause significant decreases in the amount of airline noise. Because the airlines are a significant contributor to the nation's economy, maintaining its competitiveness in the global marketplace is a high-level priority for the Federal Aviation Administration. Both projects Dr. Uzun is working on are part of the Quiet Aircraft Technology Program.

Understanding the source of the noise and how, when and why it is generated is an important part of the first research project, which focuses on noise from the plane airframe. Airframe noise is generated by the non-propulsive components of an aircraft and is caused by the aerodynamic flow of air around the aircraft fuselage, wings, high-lift device systems and control surfaces. The objective of the project is to perform high-fidelity numerical simulations of various problems of interest in airframe noise. For example, one problem Ali and his colleagues simulate is the noise resulting from the impact of airflow on the wing of the plane (see Figure 1). In the simulations, Ali experiments with slight changes in the shape of the wing to see how these changes affect airflow and whether noise is reduced. The simulations help researchers gain a better understanding of flow physics in the airframe noise problems being studied. The findings from these computations will aid in the development of future airframe noise reduction technologies.

The second research study is a complimentary effort to the first. Instead of analyzing how airflow and wing shape affect noise, the second project focuses on the noise generated by the jet exhaust of the aircraft propulsion system. As in the first project, high fidelity numerical simulations are used to simulate the object of study under certain conditions. In this instance, the simulations are of jet engine exhaust flows interacting with mixing enhancement devices such as chevrons. Chevrons are 'v' or triangular shapes incorporated into the exhaust nozzle of the jet engine. When air travels over exhaust nozzles with the chevron shape, noise is reduced; simulations are being used to study the effect different numbers and sizes of chevrons have on noise. This project also uses an advanced computer simulation program run on supercomputers, so a great deal of flow structure detail is generated. These simulations are help Ali and his colleagues gain a better understanding of the flow physics in chevron nozzle jet flows. The findings from these computations will further aid in the development of chevron nozzles that will have greater jet noise reduction benefits.

Hussaini Group continued on page 8.



Streamlines depicting the noise-reducing enhanced flow mixing in a jet exhausting from a chevron nozzle.

SCS Welcomes New Faculty, Staff & Students

Staff

Cecilia Farmer rejoined SCS and has replaced Debra Crews. You may remember Cecilia in her former position as SCS coordinator before she left to work at the Provost's office.. Cecilia is now Executive Secretary to the Director and Graduate Program Assistant.

Xiaoguang Li, the new Systems Administrator, joined our staff to support the diverse technology and computational research requirements for SCS. Xiaoguang has a Ph.D in Mathematics from Virginia Tech University in Blacksburg, and has a wealth of technology experience, including service as Director of Information Technology, and a professor of mathematics, cryptography and C++.

Master's Students

David Arthur received a BS in Physics from FSU, and while taking a computational physics course, became interested in computational science. He is currently pursuing his master's degree and using his diverse programming background to work with Jim Wilgenbusch handling trouble tickets for PAUP software.

Santosh Dubey is working with Bernd Berg and studying Computational Lattice Gauge Theory. He uses Markov Chain Monte Carlo Simulation to simulate Spin Systems which have been defined by the multi states Potts Model. Santosh became interested in this area because he likes to apply MCMC algorithms to solve real world problems.

Mark Flowers works with Tomasz Plewa and is interested in studying stellar explosions or supernovas. Mark is working on research about he started as an undergraduate on neutron stars. He is interested in the Ph.D. program, and selected SCS because of its interdisciplinary nature. When Mark isn't studying or doing research, he likes to play video games, have sweet tea with friends, and hang out with his wife. Mark is also a certified scuba diver.

Jaime Guzman graduated with a BS in Physics from the University of Florida in Spring 2007, and is now working on his master's degree here at SCS. Jaime is studying fluid dynamics with Yousuff Hussaini this term. When he's not studying, he likes to play Bioshock on his Xbox 360.

Among other things, Steven Henke studied modeling the surface ice on Enceladus, one of the moons of Saturn while obtaining a B.S. in Applied Physics from the University of Wisconsin--Eau Claire. Currently, Steven is looking for an interesting project in engineering, materials science, or fluid mehanics. His free time is spent flying airplanes, being outdoors, and reading.

Doug Jacobsen's interest in scientific computing began as an outgrowth of his undergraduate program in Computational Physics. Currently he is working with the TSG group and will probably study with Professor Wei Yang next year to study Biophysics. Doug is a newly wed, and likes to play board and video games when he can.

PhD Students

While doing his master's work in Mathematics at Nankai University in China, Xi Chen became familiar with Max Gunzburger's research, and decided come here to work with Max and pursue his PhD. Currently, Xi is studying the peridynamic models for studying cracks, fractures, damage in solid mechanics. When he's free, Xi likes to stay phsically active with swimming, running, and soccer. He also likes reading fiction and watching "Friends" on TV.

Dan Lu received her masters in Hydrogeology in China and is working on her PhD under Professor Ming Ye. When she has a few computational science courses under her belt, she plans to use Markov Chain Monte Carlo simulation to continue studying hydrogeology.

Mamdouh Mohamad graduated from Cairo University in 2003 and again in 2007 with degrees in Mechanical Engineering. He is currently studying dislocation dynamics modeling with Anter El-Azab. Mamdouh is married and enjoys spending time with his wife.

Jie Wang is a doctoral student who graduated from the University of Science and Technology of China in 2005, and has come to SCS by way of the FSU College of Engineering. Xiaoqiang Wang is Jie's advisor. Dr. Wang's research and courses inspired Jie to study Phase Field Models and Centroidal Voronoi Tessellation. He also works in the visualization lab learning visualization techniques. When he is not working on his research or in the visualization lab, Jie enjoys reading, talking with friends, snooker, music and movies.

Post Docs

As an undergrad, Vani Cheruvu majored in Mathematics and Chemistry, and both her master's and doctorate degrees are in Applied Math. Vani's research applies wavelets and high-order methods for solving partial differential equations for applications in geophysical flows. Before coming to SCS, Vani was at the University of Colorado - Boulder working at NCAR, the National Center for Atmospheric Research. Vani is also a vocalist and is trained in Indian classical music.

Originally from Morocco, Touria El Mezyani got her Ph.D. in Electircal and Signal Processing from the University of Science and Technology-Lille in Lillie, France. Touria's research focus is detecting and locating faults or flaws in tramission power networks. Her goal is to determine new, more efficient ways to transmit power within these networks. She and her collaborators use simulation software to tests the networks with varying parameters or limits. Her favorite pasttime outside work is spending time with her husband, Sergio.

Hongwu Zhao is a new post doc in Yousuff Hussaini's group who started earlier this year. He comes from the University of Colorado at Boulder, where he began a post doc in 2003. Hongwu will be working with Ali Uzun on jet engine noise and airframe noise research. He received his Ph.D. in 2003 from Old Dominion University in Norfolk, VA where he majored in Aerospace Engineering.

Jill Reese comes to SCS from the North Carolina State University where she completed the Ph.D in December of 2006 in Computational Mathematics. Jill joins Max Gunzburger's group where her research focus is partial differential equations. Jill enjoys traveling domestically and abroad, and spends as much time as she can in outdoor pursuits such as hiking.

Eunjung Lee completed her Ph.D. in Applied Mathematics at CU Boulder in 2005 and is a postdoc in Max Gunzburger's group. She is researching Optimal Control Theory, and is working to combine the information gathered from different images (e.g. a CT scan and an MRI) into a single image for improved use and analysis. Eunjung and her husband Seung Kook Park are from Daegu in South Korea.

Yanzhi Zhang was a visiting fellow at the University of Vienna and a Research Fellow at the National University of Singapore before coming to the SCS. She completed her undergraduate degree in Applied Mathematics in 2002 and the Ph.D. in Mathematics in 2006. Her research interests include computational mathematics, computational physics, numerical analysis and scientific computing. Currently she is doing research on molecular dynamics. Yanzhi enjoys making new friends, traveling, listening to music, shopping, and keeping fit.

Faculty

Adrian Barbu is a new Assistant Professor, and currently holds a joint position in SCS and Statistics. Adrian has a Ph.D. in Computer Science from UCLA and a PhD in Mathematics from Ohio State. He is interested in new learning techniques that integrate statistical models and algorithms for Medical Imaging and Computer Vision.

Tomasz Plewa recently joined SCS as an Associate Professor. Tomasz models the sun and supernovae in his research and is beginning a new major, Astrophysics, through his joint appointment in Physics. In the Fall, he"ll teach a course on Verification & Validation, skills widely applicable to many fields. Tomasz has a PhD in Astrophysics.

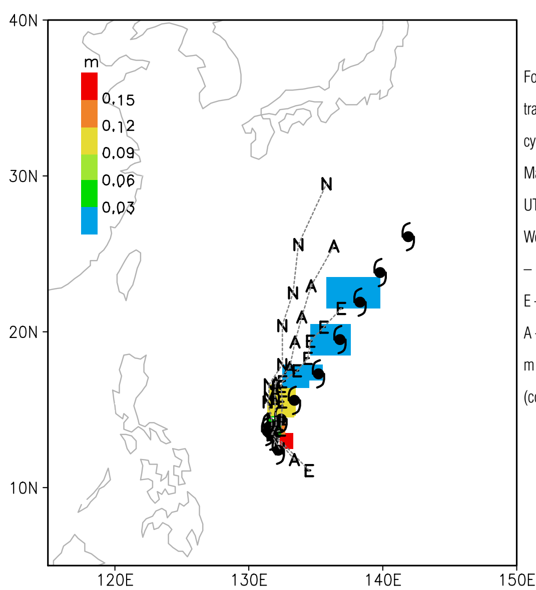
Ming Ye loves warm weather, and came to Florida earlier this year to accept a position as Assistant Professor at SCS. Ming uses his Geology and Hydrology degrees to study groundwater flow and contaminant transport. His research involves quantifying and reducing predictive uncertainty in groundwater numerical modeling.

Forecasting Severe Storms Using Multiple Models

Wouldn't it be good to know when a severe storm such as a hurricane is coming? Although predicting the weather is complex and difficult due to the chaotic and dynamic nature of the atmosphere, knowing when severe storms will occur is highly desirable. Scientists have been trying to forecast with accuracy the occurrence, location and severity of hurricanes for many years. Accurate forecasting is critical for providing early warning assistance to hurricane-prone communities. An early warning system can serve as a life preserver by allowing emergency management officers to streamline evacuation procedures and forewarn residents who are in the storm's path. Property damage may be mitigated by allowing sufficient time for homeowners to board up their homes and adequately prepare. All of the coastal states, particularly those in the Gulf of Mexico, have an especially acute need to understand how hurricanes are formed and to forecast when they will occur.

Dr. Svetlana Poroseva and other members of Dr. Hussaini's group are working on research that develops a new way to predict the track and intensity of hurricanes. A new rigorous multimodel forecast technique allows Dr. Poroseva and her colleagues to combine forecasts produced by different models in a single forecast. Prediction accuracy is considerably enhanced by fusing forecasts produced by different models along with quantified information on the uncertainty in each model's past performance.

The mathematical foundation of this technique is the Dempster-Shafer theory of evidence, and it is completely different from that of current concensus models. For each forecast period, the multimodel prediction is specified as areas where the hurricane position is likely to occur. Each area has the quantitative assessment of "degree of belief" (defined in mathematical terms) in the prediction. Areas with the highest degree of belief for each forecast period forms the final hurricane track forecast. In the future, the application of the techniques developed will be expanded to hurricane intensity, landfall forecasting and other weather-related problems. Moreover, uncertainty is an inherent property of modeling and simulation, therefore any problem that involves different modeling alternatives and has appropriate data will benefit from the multimodel approaches developed in this research.



Forecasts and best track for tropical cyclone that started on May 6, 2000 at 12:00 UTC in the North West Pacific basin. N – NOGAPS forecast, E – ECMWF forecast, A – averaged forecast, m - degree of belief (colored boxes).

SCS — School of Computational Science

The mission of SCS is to be the focal point of computational science at Florida State University. The school supports and develops a variety of high performance computing facilities, accessible to the university community. SCS is designed to overlap with existing departments and schools to provide a venue for interaction among faculty and students across many disciplines. Please visit our website at www.scs.fsu.edu.

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