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National Nuclear Security Administration

# Stewardship Science Today

## Chief Science and Technology Office

Volume 5 | Number 4 | December 2023

*Stewardship Science Today* (SST) highlights the stewardship science and academic programs supported by the Department of Energy/National Nuclear Security Administration (DOE/NNSA). SST is published quarterly by the Defense Programs Chief Science and Technology Office. Questions and comments regarding this publication should be directed to Terri Stone via email at terri.stone@nnsa.doe.gov.

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## Calendar

**12/31/2023**
The James Corones Award in Leadership, Community Building and Communications nominations due

**01/10/2024**
DOE/NNSA Stewardship Science Graduate Fellowship applications due

**01/17/2024**
DOE Computational Science Graduate Fellowship applications due

**01/31 - 2/2/2024**
16th Nuclear Deterrence Summit, Hyatt Regency Crystal City, Arlington, VA

**02/21 - 22/2024**
2024 Stewardship Science Academic Programs (SSAP) Symposium, Hyatt Regency Crystal City, Arlington, VA

**03/13/2024**
DOE/NNSA Laboratory Residency Graduate Fellowship applications due

## Inside



*Contractor Support

A key mission of the National Nuclear Security Administration (NNSA) is to support U.S. leadership in science and technology. The NNSA supports this mission in multiple ways, including through the academic programs that support student development and academic research in areas vital to nuclear security. The support of academic research frequently leads to ground-breaking results.

*Students discuss their research during the Poster Session of the 2023 SSAP Symposium in Santa Fe, New Mexico. The 2024 SSAP Symposium will be held February 21-22, 2024 in Arlington, Virginia. Details are provided below.*

This issue of *Stewardship Science Today* features two articles about recent ground-breaking science. The first discusses an enhanced approach to sensitivity analysis through extending the concept of space splitting to develop a computationally-efficient and stable sensitivity analysis of turbulent flow. This enhanced computational approach is yielding outstanding results and has the potential to be highly impactful to a wide range of turbulence-based challenges that affect nuclear science. The second article highlights recent advances in materials science through experiments that demonstrate the self-healing of metals through spontaneous cold welding. The findings open up new possibilities for designing metals with microstructures that are resistant to fatigue damage. Such metals would have a wide variety of applications within the NNSA.

Our annual Stewardship Science Academic Programs (SSAP) Symposium is fast approaching. Please join us in-person in Arlington, Virginia on February 21-22, 2024 if you are supported by a Stewardship Science Academic Alliances or High Energy Density Laboratory Plasmas award. The SSAP Symposium is a highly-attended event that features graduate student posters, presentations from academic research groups that have been awarded competitive grant funding, talks by NNSA and national laboratory staff, and excellent networking opportunities. We are seeking national laboratory staff volunteers for networking opportunities. If you can volunteer, please contact terri.stone@nnsa.doe.gov. We look forward to seeing you there.

Happy holidays!

Dr. Kevin C. Greenaugh
Chief Science and Technology Officer
Defense Programs

## SAVE THE DATE: Stewardship Science Academic Programs Symposium ♦ February 21-22, 2024

The Department of Energy/National Nuclear Security Administration (DOE/NNSA) is pleased to announce that the 2024 Stewardship Science Academic Programs (SSAP) Symposium will be held at the Hyatt Regency Crystal City in Arlington, Virginia on February 21-22, 2024. This will be an in-person only event, and we look forward to another year with record-breaking attendance.

The SSAP Symposium remains committed to providing you with numerous opportunities to make important connections, exchange research information, and interact with the wide range of scientific communities that SSAP encompasses. As in past years, the symposium will include the following:

- presentations from grantees on their current research efforts,
- talks by NNSA and NNSA national laboratory staff,
- opportunities to connect and network with staff from NNSA,

(continued on page 3)

## Sensitivity Analysis of Chaotic Dynamical Systems and Turbulent Flows *by* Adam A. Śliwiak

(Massachusetts Institute of Technology)

Strategic planning, decision making, and technical design in many areas of engineering are heavily based on advanced simulation techniques. In general, engineers attempt to achieve certain objectives (e.g., improve efficiency or reduce environmental impact) by adjusting several controllable parameters. In other words, they perform sensitivity analysis (SA), i.e., measure the reaction of a system due to the change of input variables. The word *system* should be understood as a combination of physical, environmental, and societal constraints usually expressed in terms of differential equations that affect the design and planning objectives. The physical constraints of turbulent air flows, which are mathematically complex due to their chaotic nature, are critical components of most aerospace systems.

Conventional numerical methodologies for SA of physics-based dynamical (evolving in time) systems directly compute the evolution of system's perturbations introduced intentionally to probe its response.[1] Whereas these methods are conceptually simple and effective in a variety of engineering applications, they are doomed to failure in the presence of chaotic or turbulent motion. The difficulty lies in the fundamental property of chaotic systems, commonly known as the *butterfly effect*. It means that every smallest perturbation of the system monotonically increases in magnitude at an exponential rate (Figure 1). Since the objective quantities are usually expressed in terms of long-time averages or other statistical measures, SA effectively requires summing up these instantaneous perturbations triggering serious computational issues that result in highly inaccurate approximations.

In his doctoral thesis,[2] the author extends the concept of space-splitting[3] to develop computationally-efficient and stable, i.e., immune to the butterfly effect, numerical procedures for SA of high-dimensional, multiscale chaotic models. The proposed methodology, called space-split sensitivity (S3), is derived *abinitio* based on the linear response theory of Ruelle.[4] The method itself does not incorporate any case-specific simplifications, which makes it universal and, thus, applicable to a vast family of chaotic systems.

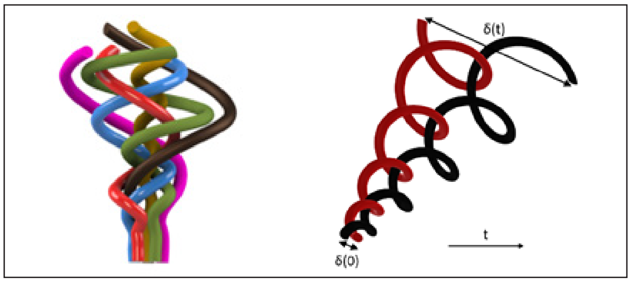


Figure 1. Colored trajectories mimic the time evolution of the same 3D chaotic system initiated at similar, yet different, starting points. Even if the initial distance δ(0) between any pair of trajectories is small, the ratio δ(t) / δ(0) increases exponentially fast with time t.

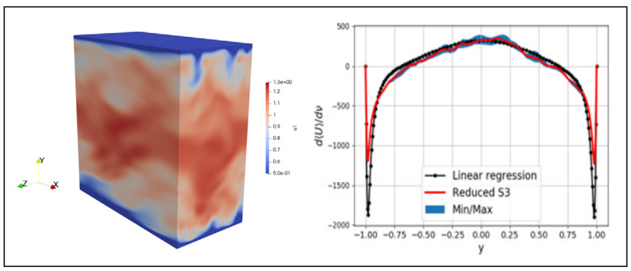


Figure 2. Left: A time snapshot of streamwise velocity (u1) of a turbulent channel flow. Right: Comparison of the sensitivity estimation computed using a simplified version of the S3 method and expensive data-driven linear regression as a reference. The horizontal and vertical axes represent the wall-normal coordinate and sensitivity, respectively. Both plots were taken from reference 2.

Throughout its development process, the S3 method has been proven successful in sensitivity estimation of abstract, low-dimensional systems, climate models, as well as turbulent flows whose dynamics are described by the famous Navier-Stokes equations. Figure 2 illustrates the new method's performance in estimating the sensitivity of a mean velocity profile with respect to the kinematic viscosity of the fluid in a turbulent channel flow. We observe that the relative error does not exceed a few percent almost everywhere throughout the width of the channel, which is an outstanding result compared to the major competitors in the field.

This work provides an advanced simulation tool for design optimization, uncertainty quantification, risk assessment, error analysis, regularity analysis, and grid adaptation. Indeed, a key prerequisite of all of these tasks is the ability to perform accurate sensitivity analysis. S3 merges these complex analytical tools with the universe of chaos and turbulence essential in the aviation industry.

The author is deeply indebted to the present and past members of the Predictive Science Academic Alliance Program III, especially Prof. Qiqi Wang (MIT), Prof. Nisha Chandramoorthy (Georgia Tech), Prof. Johan Larsson (University of Maryland), and the Focused Investigatory Center at the University of Maryland for enlightening discussions, guidance, technical support, and countless opportunities for professional growth. The author's research work was funded by U.S. Department of Energy Grant No. DE-NA-0003993.

### References

[1]A. Jameson, *Aerodynamic Design via Control Theory*, Journal of Scientific Computing 3:233-260, 1988.

[2]A.A. Śliwiak, *Leveraging the Linear Response Theory in Sensitivity Analysis of Chaotic Dynamical Systems and Turbulent Flows*, Ph.D. Thesis, Massachusetts Institute of Technology, 2023.

[3]N. Chandramoorthy, *An Efficient Algorithm for Sensitivity Analysis of Chaotic Systems*, Ph.D. Thesis, Massachusetts Institute of Technology, 2021.

[4]D. Ruelle, *Differentiation of SRB States*, Communications in Mathematical Physics 187: 227-241, 1997.

## Self-Healing of Fatigue Cracks Opens New Prospects for Damage Resistent Metals *by Michael Demkowicz (Texas A&M University)*

Self-healing of metals is a long-standing theme in science fiction. Now, a collaboration between Sandia National Laboratories (SNL) and the Center of Research Excellence on Dynamically Deformed Solids (CREDDS) has shown it to be reality. The SNL team performed cyclic loading experiments inside a transmission electron microscope (TEM) to observe the behavior of nanoscale fatigue cracks. Conventional wisdom states that such cracks should only ever get longer. However, the team observed several cases in which the cracks got shorter, effectively healing themselves. These observations were then explained through atomistic and continuum simulations conducted by CREDDS members at Texas A&M University. The results were published in the journal *Nature*.[1]

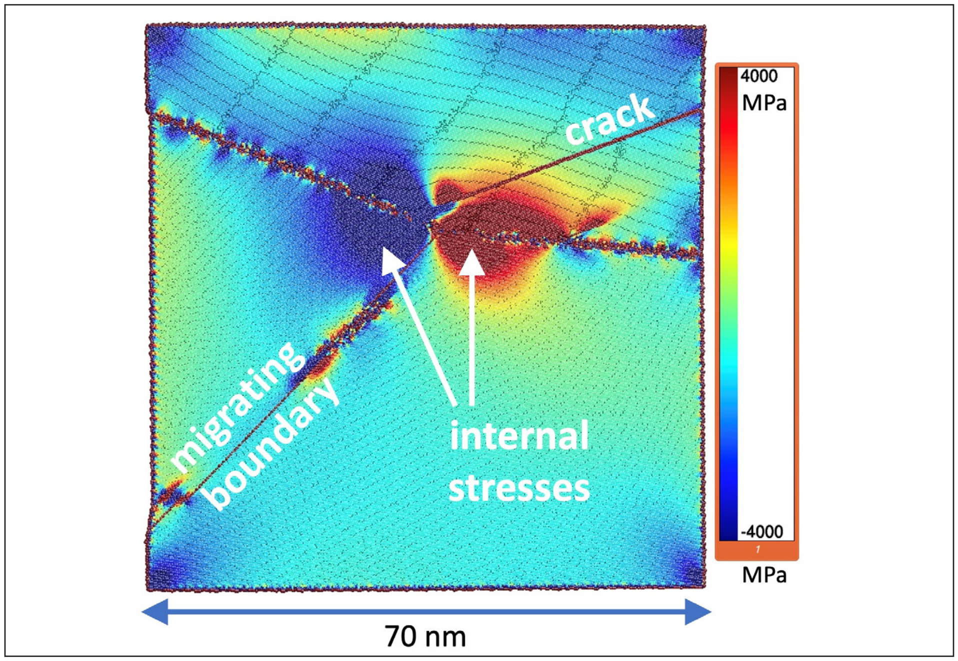

Figure 1. Atomistic simulation of intense internal stresses generated near a crack tip by a migrating grain boundary. These stresses force together the opposing faces of the crack, causing them to cold weld.

The researchers believe that crack healing in their experiments occurred through cold welding: a process whereby flat, contaminant-free surfaces bond spontaneously upon contact. In this case, the opposing surfaces of a crack bonded via cold welding after being forced together by internal stresses in the material. The internal stresses, in turn, originated from changes in the surrounding microstructure, especially stress-induced migration of grain boundaries. Figure 1 shows an atomistic simulation of internal stresses generated near the tip of the crack, immediately prior to healing. The stresses reach levels of ~4 GPa and are concentrated near a triple junction: a line where boundaries between three adjacent crystal grains meet.

These findings challenge current theories of damage initiation and evolution during fatigue loading. They also open new possibilities for designing metals with microstructures that resist fatigue damage by promoting crack healing. The experiments were conducted in vacuum, so early applications of self-healing metals may target airless environments, such as space. However, the authors plan to investigate whether crack healing also takes place in air.

### Reference

[1]Christopher M. Barr, Ta Duong, Daniel C. Bufford, Zachary Milne, Abhilash Molkeri, Nathan M. Heckman, David P. Adams, Ankit Srivastava, Khalid Hattar, Michael J. Demkowicz, and Brad L. Boyce, *Autonomous Healing of Fatigue Cracks via Cold Welding*, Nature 620, 552 (2023).

## Save the Date: 2024 SSAP Symposium *(continued from page 1)*

the national laboratories, the Krell Institute (which manages our fellowship programs), and

- ✧ a Poster Session & Reception.

Always a highlight of the Symposium, there will be multiple opportunities to view and discuss the graduate student posters during the Poster Session the evening of February 21, 2024. The Outstanding Poster Awards ceremony will be held the next day of the Symposium. There will also be several special presentations from NNSA's Academic Programs team not to be missed.

For more information, click here to visit the Symposium website and to register. The deadline to register for the symposium and register a poster is January 29, 2024. We look forward to seeing you in Arlington, Virginia!

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KRELL Institute

**2023 James Corones Award Winner**
Dr. Tammy Ma
*Lawrence Livermore National Laboratory*

## THE JAMES CORONES AWARD

# Now Accepting Nominations

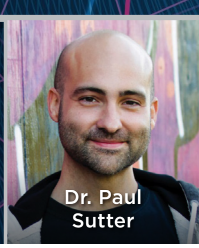
**The James Corones Award in Leadership, Community Building and Communication** recognizes the impact of mid-career scientists and engineers on their chosen fields across a range of areas.

Its namesake, a distinguished researcher and administrator, founded the Krell Institute, a nonprofit organization dedicated to serving the science and education communities. Under his guidance, Krell grew to supervise many projects and programs, most notably two Department of Energy-sponsored education initiatives: the Computational Science Graduate Fellowship (DOE CSGF) and the National Nuclear Security Administration Stewardship Science Graduate Fellowship (DOE NNSA SSGF). Jim retired from the company in December 2016 and passed away in April 2017.

**Broad eligibility:** Mid-career researchers – those having earned a Ph.D. within the past 10 to 20 years – regardless of employment sector.

**Prize:** A cash award of $2,000 and an engraved gift.

For nomination procedures, deadlines and more information, including how to donate to the award fund, please visit **https://www.krellinst.org/about-krell/corones-award.**



Dr. Paul Sutter

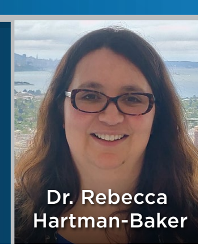
2022 WINNER

Dr. Jeffrey Hittinger

2021 WINNER

Dr. Bethany Goldblum

2020 WINNER



Dr. Rebecca Hartman-Baker

2019 WINNER