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National Nuclear Security Administration

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Office of Defense Programs

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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 NNSA Office of Defense Programs. 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

12/31/2022
The James Corones Award in Leadership, Community Building and Communications nominations due

1/11/2023
DOE/NNSA Stewardship Science Graduate Fellowship applications due

1/18/2023
DOE/NNSA Computational Science Graduate Fellowship applications due

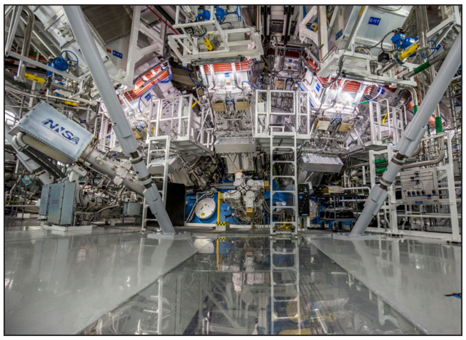
2/14-15/2023
DOE/NNSA Stewardship Science Academic Programs Symposium, Santa Fe, New Mexico

3/15/2023
DOE/NNSA Laboratory Residency Graduate Fellowship applications due

Inside

*Contractor Support

Welcome to the December issue of *Stewardship Science Today*. As you will see from this issue—and from national news—scientific achievements at the National Nuclear Security Administration (NNSA) are at an all-time high! With Lawrence Livermore National Laboratory's (LLNL's) recent achievement of ignition, delivering 2.05 megajoules (MJ) of energy to the target and yielding 3.15 MJ of fusion energy output, and the construction of a next-generation enhanced capability for subcritical experiments that will enable the United States to carry out and diagnose experiments involving plutonium's response to influences of aging, modern manufacturing techniques, and modern materials, NNSA has cemented its legacy as the premier agency for federally-sponsored research and development.



The target chamber of LLNL's National Ignition Facility, where 192 laser beams delivered more than 2 million joules of ultraviolet energy to a tiny fuel pellet to create fusion ignition on December 5.

The scientific research performed, and the diagnostics developed, in our programs continue to advance the frontiers of science. An example featured in this issue is Neutron Diagnosed Subcritical Experiments (NDSE). There was a time when the very concept of NDSE seemed far-fetched, and the ability to diagnose the experiments and extract meaningful data, unattainable. Yet, here we are today doing it all and contributing greatly to advancing the security of nuclear weapons without underground nuclear explosive tests. Likewise, you'll read about breakthroughs in understanding material response to high pressure environments and how the impact that this understanding has on the nuclear stockpile has reached a new high, thanks to experiments undertaken by the Chicago/Department of Energy Alliance Center at the Advanced Photon Source.

Clearly, now is the time to join NNSA's scientific goldrush. We are pleased to announce that the 2023 Stewardship Science Academic Programs Symposium will be held in person for the first time in three years on February 14-15, 2023 (see page 4) and that applications for NNSA's Fellowship Programs are now being accepted (although some deadlines are fast approaching).

Please enjoy this issue, engage with NNSA programs, and have a healthy and happy holiday. We look forward to seeing you in Santa Fe, New Mexico in February 2023!

Dr. Njema J. Frazier
Assistant Deputy Administrator (Acting)
Strategic Partnership Programs

NNSA Academic Programs
Fellowship Programs

World-class scientists and engineers in areas critical to stockpile stewardship and national security are vital to the national security enterprise. The National Nuclear Security Administration (NNSA) is committed to helping train the next generation of stockpile stewards through its Academic Programs. In addition to research programs at the Nation's most prestigious universities and educational institutions, NNSA also attracts, trains, and supports top-tier science, technology, engineering, and mathematics (STEM) doctoral students through its highly competitive fellowship programs. Focused on areas related to stockpile stewardship, these programs showcase the important work of NNSA and the national laboratories and have proven to be a successful recruiting tool. In the sections that follow, we highlight select NNSA fellowship programs. Some of the NNSA fellowships are currently accepting applications (see the calendar in the far left column).

(continued on page 4)

Neutron Diagnosed Subcritical Experiments on Static Uranium

by Madison Andrews and John Lestone (Los Alamos National Laboratory)

With the conclusion of underground nuclear tests, subcritical experiments (subcrits) allow scientists to explore fissile material behavior in the relevant regimes. Such measurements include Dense Plasma Focus (DPF) Neutron Diagnosed Subcritical Experiments (NDSE) which infer properties of special nuclear materials by measuring fission decay signatures referred to as die-away. Key elements of these experiments include a DPF source capable of rapidly producing over a trillion neutrons, the uranium object under evaluation, and an array of diagnostics recording the object's response (Figure 1). The gamma response of the fissile material to the incident neutron flux is dependent on how close the object is to sustaining a chain reaction, which can be characterized by the object's k_{eff} value. By analyzing the die-away measurement, an object's k_{eff} can be inferred precisely with just a few hundred nanoseconds of data.

Recent NDSE measurements at the Nevada National Security Site (NNSS) have demonstrated the precision of the technique with several static uranium objects with k_{eff} values ranging from ~0.91-0.95. The measurements were compared to the simulated response of an array of uranium configurations generated with Los Alamos National Laboratory's Monte Carlo N-Particle (MCNP) code to infer each object's k_{eff} (Figure 2). As the goal is to infer k_{eff} with a high degree of precision, identifying and mitigating sources of uncertainties has been the focus of recent static measurements.

In 2018, NDSE measurements from individual DPF shots were used to infer the k_{eff} of a static uranium object for the first time. However, the overall precision was outside of the static precision goals (Table 1). These measurement campaigns identified the largest contributors to the technique's uncertainty, namely: (1) degraded DPF anode performance resulting in non-ideal neutron pulses and (2) discrepancies between the measured DPF pulse and the true time dependence of the neutrons reaching the object. Both sources of uncertainty were mitigated in 2019 by replacing the aging DPF anode and fielding new diagnostics that achieved precise measurements of the time dependence of the DPF neutrons that impinge on the object of interest. With these changes implemented in the most recent static series, precision goals were met (Table 1). NDSE static measurements will continue with Series VII which will include new and optimized in-beam diagnostics and will use the ZEUS DPF high-voltage drive designed by Lawrence Livermore National Laboratory. Success in executing and interpreting these static NDSE experiments paves the way for future subcritical experiments in Nevada.

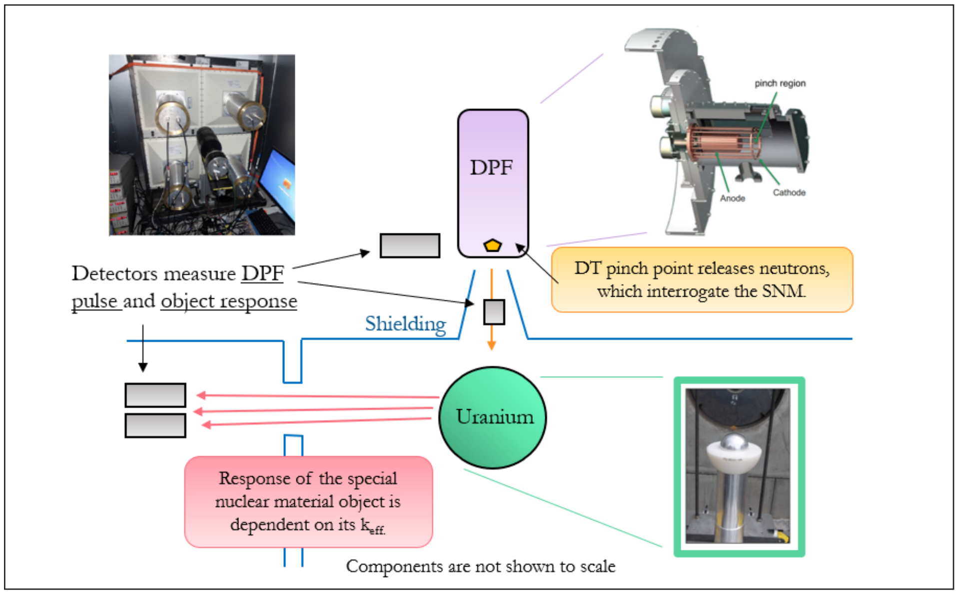


Figure 1. Static NDSE measurements interrogate uranium with DT neutrons, and the response of the object is recorded by an array of detectors.

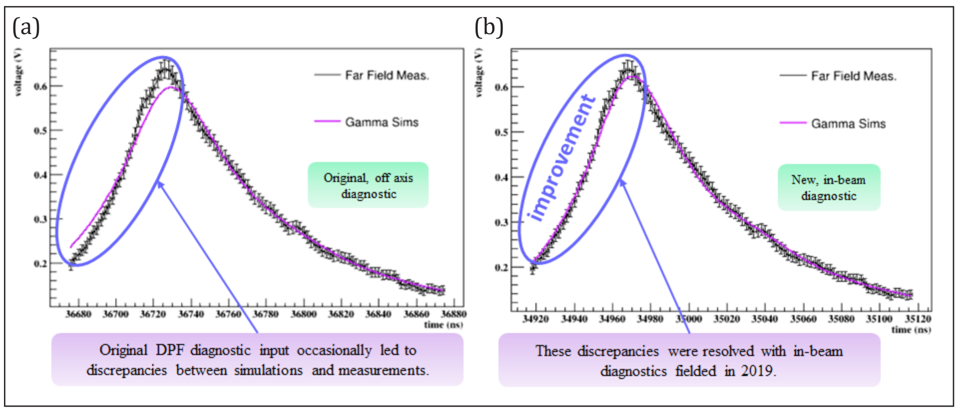


Figure 2. Original DPF diagnostic input occasionally led to discrepancies between measurements and simulations (a) which were resolved in 2019 with diagnostic upgrades (b).

Date	k_{eff} Precision (1σ)	Key Developments
Before 2018	N/A	Not yet able to analyze individual shots
February 2018	0.004 – 0.005	Initial characterization of k_{eff} precision
June 2018	0.009 – 0.011	Simulations and analysis identified DPF degradation
May 2019	0.002 – 0.003	New DPF anode and diagnostics met precision goals
November 2019	0.002 – 0.003	Diagnostic performance verified in repeat experiment

Table 1. Static precision goals of < 0.0034 were achieved in 2019, enabled by improvements in diagnostics and DPF anode replacement.

Imaging of Atoms at Ultrahigh Pressures *by Stephen Gramsch (University of Illinois Chicago, Chicago/ Department of Energy Alliance Center)*

A common perception of atoms is that they are hard spheres that join together by way of rigid chemical bonds to form molecules. Similarly, the conventional view of solids is that they are formed from close-packed arrays of spherical atoms or ions, sometimes with smaller atoms occupying interstitial spaces. As applied pressure forces atoms much closer than an equilibrium separation, however, a modified view is often necessary to understand how atoms at high pressure accommodate decreasing volume. Since crystalline materials consist of periodic variations of electron density, is it possible to use X-ray diffraction to “image” the shapes of atoms in a solid at high pressures?

New work from a collaboration of Chicago/Department of Energy Alliance Center (CDAC) scientists from UC Berkeley and Northwestern University and the High Pressure Collaborative Access Team (HPCAT) at the Advanced Photon Source shows that iron atoms undergo a significant change in shape associated with the change in their spin state at pressures characteristic of Earth’s mantle. This pressure-induced "spin transition" is canonically described as arising from a competition between the energetic penalty associated with pairing electrons versus the energy required to leave them unpaired when the difference in energy between available states becomes too large as a result of increasing pressure. Numerous laboratory experiments attest to the significant changes in a wide variety of physical properties that result when compounds containing iron experience deep-Earth pressures and undergo a change from a high-spin to a low-spin state.

Using diamond-anvil cell compression, former CDAC graduate student Matthew Diamond (UC Berkeley, now a postdoctoral researcher at the University of Illinois Chicago), CDAC Academic Partners Raymond Jeanloz (UC Berkeley) and Steven Jacobsen (Northwestern University), and Guoyin Shen, Dmitry Popov, and Changyong Park from HPCAT report X-ray-determined electron-density changes in (Fe,Mg)O, a major phase in Earth’s deep mantle, at pressures up to 74 GPa. Measurements were carried out at HPCAT beamline 16-BM-D on single crystals with two different (Fe,Mg)O compositions, i.e., $(Fe_{0.53}Mg_{0.47})O$ and $(Mg_{0.85}Fe_{0.15})O$, that reveal changes in trends in X-ray intensity at approximately 56 GPa and 45 GPa, respectively. These pressures are within the spin-transition pressure regimes established previously by independent analytical techniques. In the $(FeO_{53}Mg_{0.47})$ data, the changes in X-ray intensities are rendered as electron density difference maps (Figure 1) across the spin transition at Fe^{2+}.” Discontinuities in the pressure-volume equations of state at the same pressures in the present work support the claim that the intensity observations reflect the spin-transition behavior.

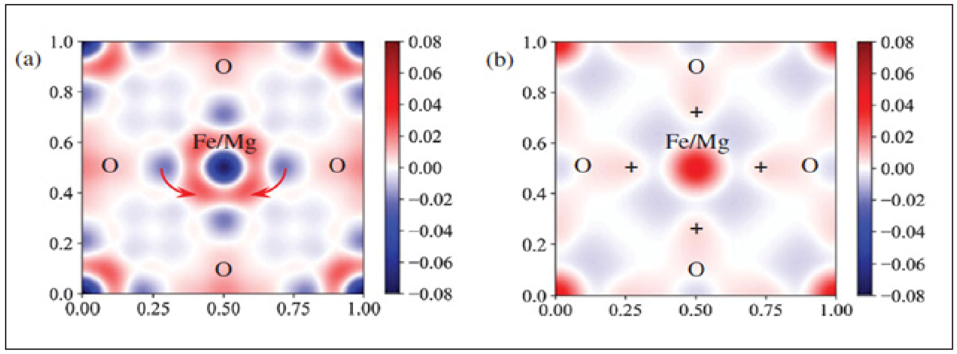


Figure 1. Electron density distribution difference maps for the composition $(Fe_{0.53}Mg_{0.47})O$. Red shades represent an increase, and blue shades a decrease, in electron density across the high- to low-spin transition. (a) End-transition compression (56 GPa) minus minimum compression (18 GPa). Arrows indicate direction of transfer of electron density. (b) Maximum compression (74 GPa) minus end-transition compression (56 GPpa). Increases in covalency is indicated with the + sign. Scale relative to maximum electron density at 18 GPa.

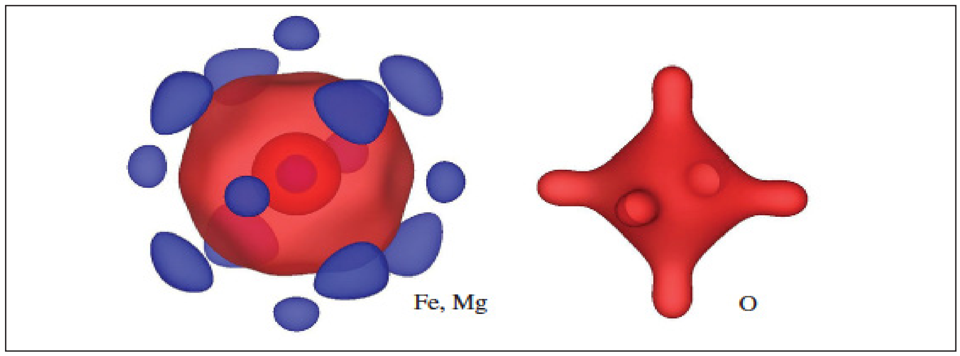


Figure 2. Contours of change in electron density across the high-to-low spin transition in $(Fe_{0.53}Mg_{0.47})O$ from 18 GPa to 56 GPa for (Fe,Mg) sites (left) and O sites (right). Red regions—increasing electron density; blue regions—decreasing electron density.

Another key observation on (Fe,Mg)O is that the (Fe,Mg)–O bond becomes less ionic and more covalent with increasing pressure, resulting in an apparent change in the shape of the electron density around the oxygen atom site (Figure 1 and Figure 2).

Beyond imaging the shapes of atoms, the new measurements described here provide direct tests of modern quantum simulations, because the electron density is a quantum mechanical observable, and the distribution of electrons within crystals is among the key results derived from atomistic theory. A paper[1] describing this work has recently been published.

Reference

[1]M.R. Diamond, G. Shen, D.Y. Popov, C. Park, S.D. Jacobsen, and R. Jeanloz, *Electron Density Changes Across the Pressure-Induced Iron Spin Transition*, Physical Review Letters 129, 025701 (2022).

NNSA Academic Programs: Fellowship Programs *(continued from page 1)*

There is also information about a new award that is accepting nominations though the end of the year. For more information, visit the fellowship program websites.

Stewardship Science Graduate Fellowship

The Stewardship Science Graduate Fellowship provides outstanding benefits and opportunities to students pursuing a PhD in areas of interest to stewardship science, such as properties of materials under extreme conditions and hydrodynamics, nuclear science, and high energy density physics. The fellowship includes a 12-week research experience at one of the NNSA national laboratories: Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), or Sandia National Laboratories (SNL). Click here to learn more.

Applications due: 1.11.2023

Computational Science Graduate Fellowship

The Computational Science Graduate Fellowship (CSGF) is open to senior undergraduates and students in their first year of doctoral study. It provides up to four years of financial support for students pursuing doctoral degrees in fields that use high-performance computing to solve complex problems in science and engineering. The program also funds doctoral candidates in applied mathematics, statistics, and computer science who are pursuing research that will contribute to more effective use of emerging high-performance systems. Details and a full listing of applicable research areas can be found on the CSGF website.

Applications due: 1.18.2023

Laboratory Residency Graduate Fellowship

Launched in 2017, the Laboratory Residency Graduate Fellowship (LRGF) provides outstanding benefits and opportunities to U.S. citizens who are pursuing a doctoral degree in fields of study of great importance to stewardship science. Through the LRGF program, Fellows will work and study with laboratory scientists at one or more of NNSA's premier national laboratories. LRGF includes at least two 12-week research residencies at LLNL, LANL, SNL, or the Nevada National Security Site. Longer stays are highly encouraged, up to or including pursuit of thesis studies at a chosen site. More details are available here.

Applications due: 3.15.2023

2023 Stewardship Science Academic Programs Symposium

The National Nuclear Security Administration's Office of Strategic Partnership Programs is pleased to announce the 2023 Stewardship Science Academic Programs (SSAP) Symposium will be held on February 14-15, 2023. The exciting news is that this symposium will be the first one to be held in person since the start of the pandemic! To be held at the Hilton Santa Fe Buffalo Thunder Resort in Sante Fe, New Mexico, the symposium will be spread over two days with an optional third day for those who sign up in advance to take tours of key facilities at one of NNSA's national laboratories, the nearby Los Alamos National Laboratory.

Our goal remains to provide you with numerous opportunities to make important connections, exchange research information, and interact with the wide range of scientific communities the 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, the national laboratories, the Krell Institute (who manage 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 14. The Outstanding Poster Awards ceremony will be held the next day of the Symposium.

For more information, click here to visit the Symposium website and to register. An important date to note is the January 20, 2023 deadline to register for the symposium and to register a poster. We look forward to seeing you in Santa Fe!

Save the Date!

Stewardship Science Academic Programs Symposium

February 14-15, 2023

2022 James Corones Award Winner
Dr. Paul M. Sutter
Stony Brook University and the Flatiron Institute

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.

Nominations Due
12.31.2022

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. Jeffrey Hittinger
2021 Winner

Dr. Bethany Goldblum
2020 Winner

Dr. Rebecca Hartman-Baker
2019 Winner

SSGF

STEWARDSHIP SCIENCE GRADUATE FELLOWSHIP

APPLICATIONS DUE

1.11.2023

WWW.KRELLINST.ORG/SSGF

DEPARTMENT OF ENERGY

NATIONAL NUCLEAR SECURITY ADMINISTRATION

STEWARDSHIP SCIENCE GRADUATE FELLOWSHIP

The Department of Energy National Nuclear Security Administration Stewardship Science Graduate Fellowship (DOE NNSA SSGF) provides outstanding benefits and opportunities to students pursuing a Ph.D. in areas of interest to stewardship science, such as properties of materials under extreme conditions and hydrodynamics, nuclear science, or high energy density physics. The fellowship includes a 12-week research experience at Lawrence Livermore National Laboratory, Los Alamos National Laboratory or Sandia National Laboratories.

The DOE NNSA SSGF is open to U.S. citizens who are senior undergraduates or students in their first or second year of doctoral study.

BENEFITS

+ $38,000 yearly stipend
+ Payment of full tuition and required fees
+ Yearly program review participation
+ Annual professional development allowance
+ 12-week research practicum experience
+ Renewable up to four years

SCAN TO LEARN HOW TO APPLY

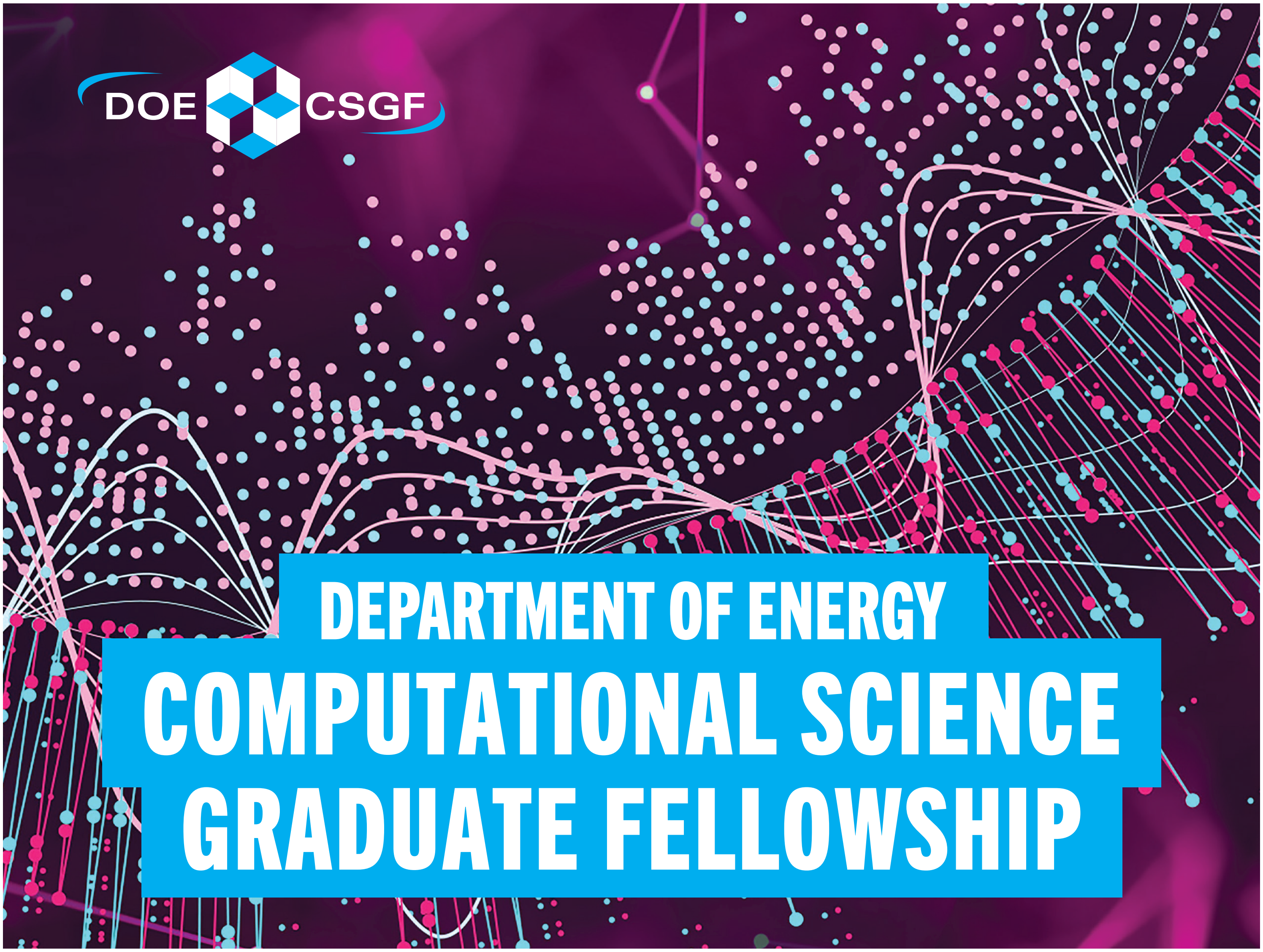
__Top:__ Image courtesy of Galloway et al.; captured at Sandia National Laboratories' Z-Petawatt laser facility.
__Bottom:__ Sandia's High Energy Radiation Megavolt Electron Source (HERMES) III pulsed power facility.

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

KRELL institute

This equal opportunity program is open to all qualified persons without regard to race, color, national origin, sex, disability, or any other characteristics protected by law.



DEPARTMENT OF ENERGY
COMPUTATIONAL SCIENCE GRADUATE FELLOWSHIP

The Department of Energy Computational Science Graduate Fellowship (DOE CSGF) provides up to four years of financial support for students pursuing doctoral degrees in fields that use high-performance computing to solve complex problems in science and engineering.

The program also funds doctoral candidates in applied mathematics, statistics, computer science or computational science – in one of those departments or their academic equivalent – who undertake research in enabling technologies for emerging high-performance systems. Complete details and a listing of applicable research areas can be found on the DOE CSGF website.

BENEFITS

- $45,000 yearly stipend
- Payment of full tuition and required fees
- Yearly program review participation
- Annual professional development allowance
- 12-week research practicum experience
- Renewable up to four years

Applications Due
1.18.2023

SCAN TO LEARN HOW TO APPLY

The DOE CSGF is open to senior undergraduates and those in their first year of graduate study.

www.krellinst.org/csgf

Image courtesy of the Pacific Northwest National Laboratory, operated by Battelle for the U.S. Department of Energy.

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NNSA National Nuclear Security Administration

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Then-fellow Raspberry Simpson working at Lawrence Livermore National Laboratory's Jupiter Laser Facility in 2019.

Applications Due
3.15.2023
www.krellinst.org/lrgf

DEPARTMENT OF ENERGY NATIONAL NUCLEAR SECURITY ADMINISTRATION

LABORATORY RESIDENCY GRADUATE FELLOWSHIP

The Department of Energy National Nuclear Security Administration Laboratory Residency Graduate Fellowship (DOE NNSA LRGF) provides outstanding benefits and opportunities to U.S. citizens who are entering their second (or later) year of doctoral study to work at premier national laboratories while pursuing degrees in fields relevant to the stewardship of the nation's nuclear stockpile.

LAB RESIDENCY Fellowships include at least two 12-week research residencies at Lawrence Livermore National Laboratory, Los Alamos National Laboratory, Sandia National Laboratories, or the Nevada National Security Site. Fellows are encouraged to extend these residencies to carry out thesis research and other studies at the four DOE NNSA facilities.

BENEFITS

- $38,000 yearly stipend
- Payment of full tuition and required fees
- Yearly program review participation
- Annual professional development allowance
- Two or more 12-week-minimum national laboratory residencies
- Renewable up to four years

FIELDS OF STUDY

ENGINEERING & APPLIED SCIENCES
pulsed power; particle accelerator physics and design; detector and data processing; fluid mechanics

PHYSICS atomic, nuclear and plasma physics; shock physics

MATERIALS additive materials; dynamic materials; energetic materials physics and chemistry

MATHEMATICS AND COMPUTATIONAL SCIENCE
multiscale, multiphysics theory and numerical simulation; PIC/fluid hybrid simulation

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