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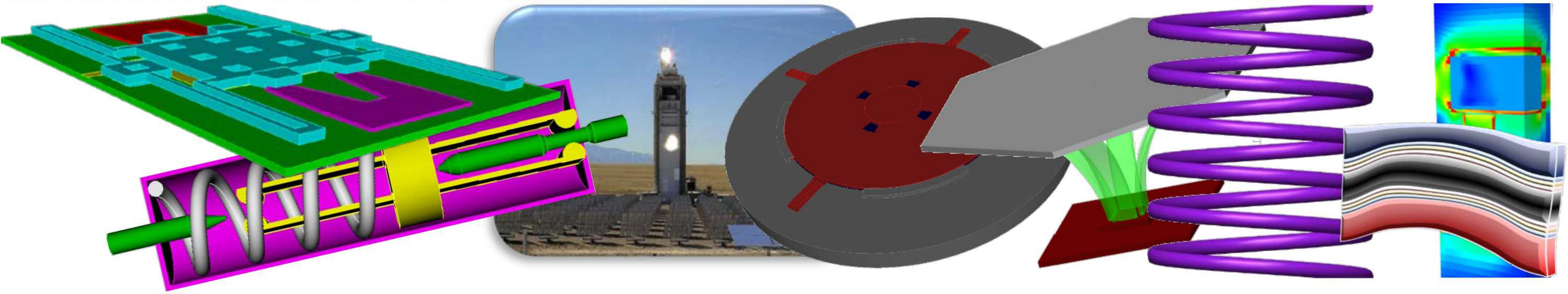


Applied Mathematics at Sandia National Laboratories: A Perspective from an Engineering Scientist

Dr. Jordan E. Massad

Sandia National Laboratories

Albuquerque, NM

College Station, TX

October 17, 2016

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Sandia National Laboratories is a multi-mission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

U.S. DOE National Laboratories

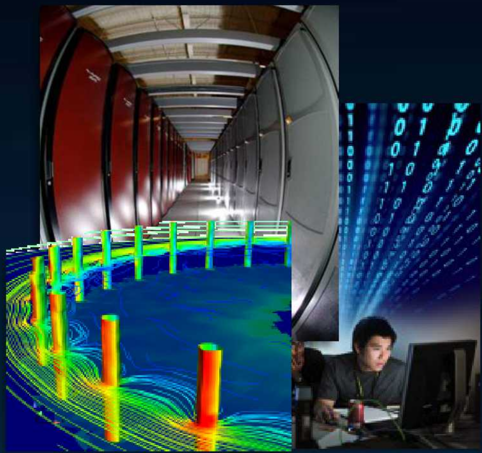
Sandia National Laboratories

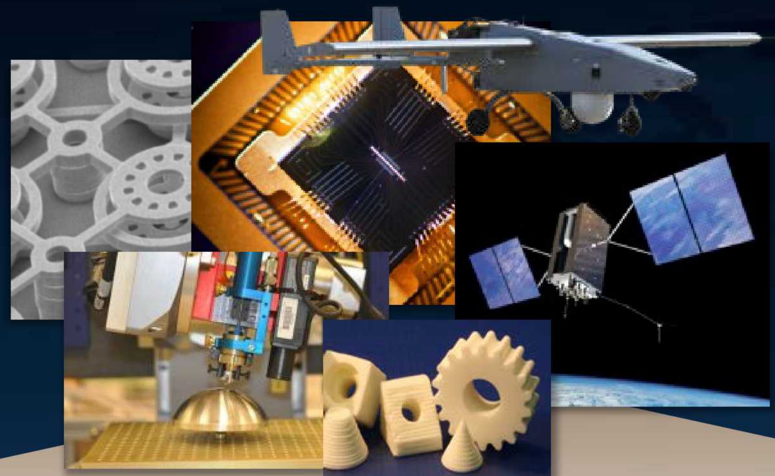
- **Core Purpose**: help our nation secure a peaceful and free world through technology.
- Provide objective, multidisciplinary technical assessments for complex problems.
- Focus on solutions with large science and technology content.
- Create prototypes for production and operation by industry.

Scope & Complexity of National Security

SNL Applies both BREADTH & DEPTH to solving our nation's most challenging problems.

Research Disciplines Drive Capabilities



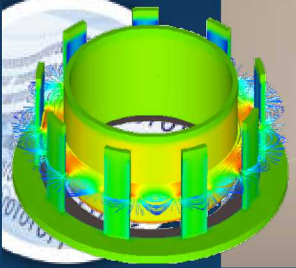


High Performance Computing

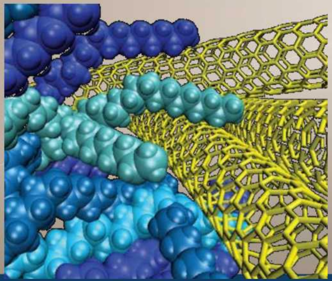
Science & Technology Products

Renewable Systems & Energy Infrastructure

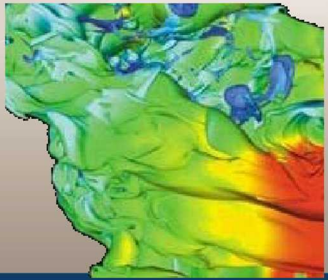
Computer Sciences



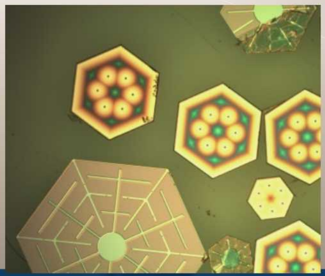
Materials



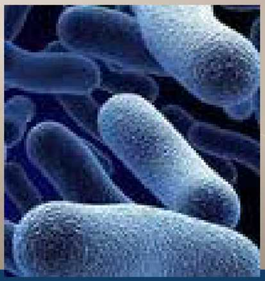
Engineering Sciences



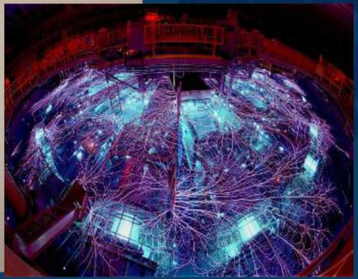
Nanodevices & Microsystems



Bioscience

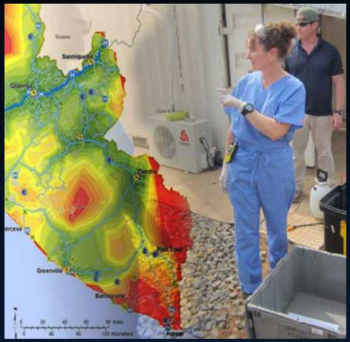


High Energy Density Science



Research Disciplines

Examples of Sandia's Impact



Ebola Outbreak

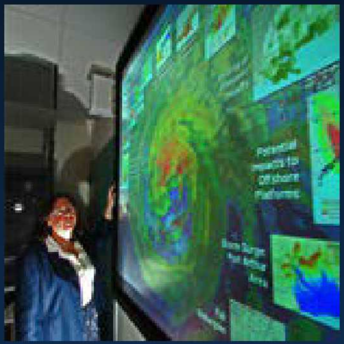
Developed a sample delivery system cutting the wait time and potentially fatal exposure.

Detecting IEDs

Highly modified miniature synthetic aperture radar system helps uncover improvised explosive devices.

Invented Cleanroom 1963

Used in hospitals, laboratories and manufacturing plants today.

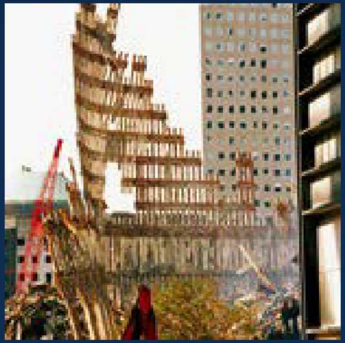


Hurricane Katrina

Assess flooding and infrastructure failures.

Fukushima Quake

Helped clean up radioactive wastewater.



9/11

Planned for subsequent attacks on facilities. Enabled search & rescue K-9s with cameras to allow search of inaccessible spaces.

Sandia Albuquerque (NM)

Sandia National Laboratories

On-site workforce: ~10,800

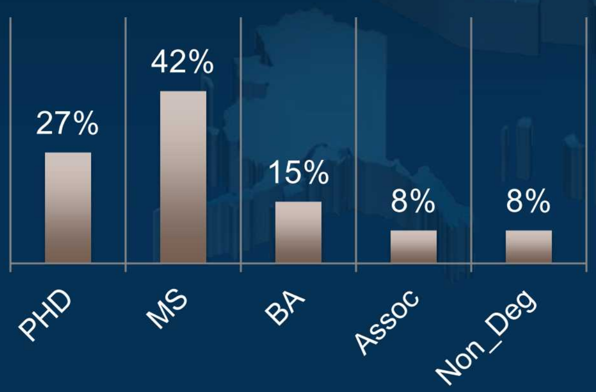
R&D staff: ~3,500

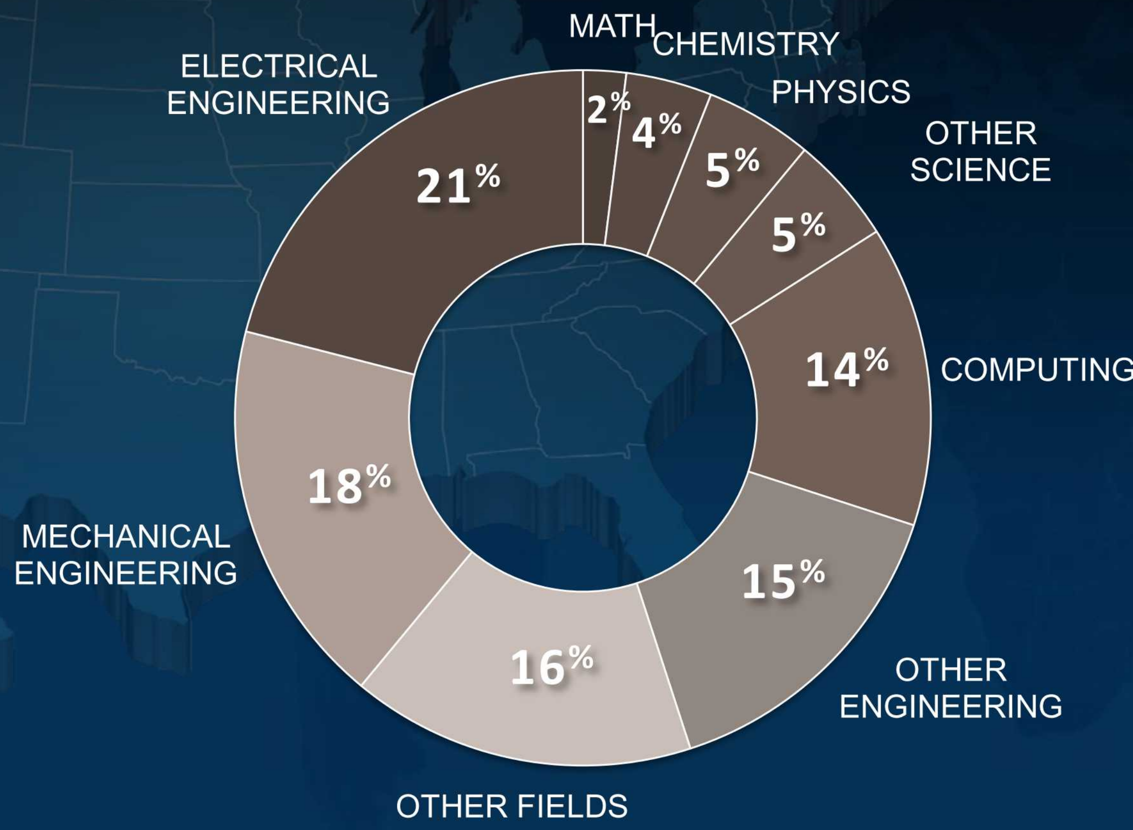
(excluding R&D Tech)

Distinguishing capabilities:

- Renewable Energy
- Microelectronics
- Cyber Security and more

Degree Level





Sandia Livermore (CA)

Sandia National Laboratories

On-site workforce: ~1,300

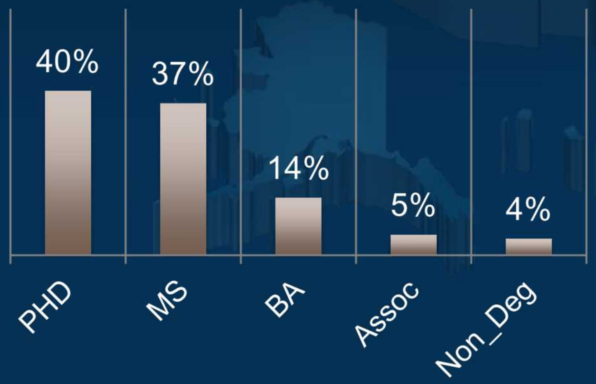
R&D staff: ~500

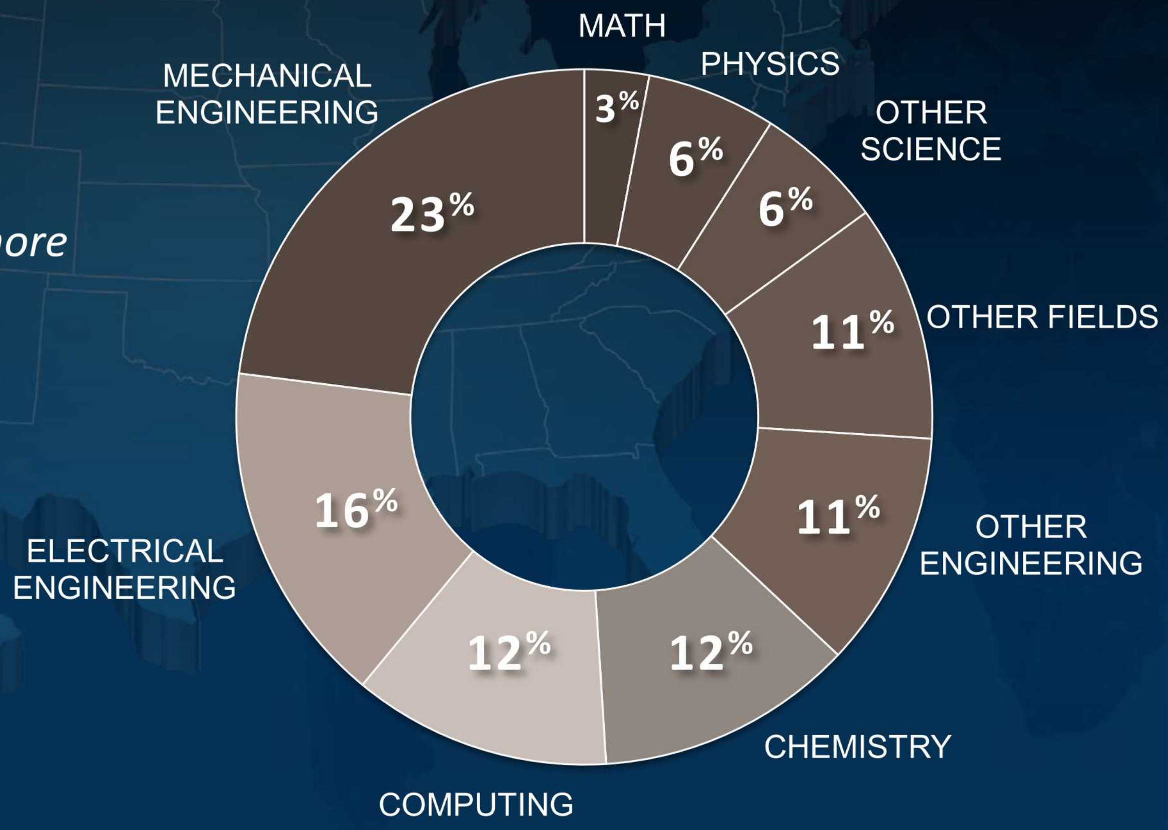
(excluding R&D Tech)

Distinguishing capabilities:

- Applied Biosciences
- Combustion Research
- Information Systems and *more*

Degree Level





Sandia Mathema/Statis-ticians

Sandia National Laboratories

- Work in almost every area across SNL in over 80 organizations.
- Degrees: 50% graduate, 50% undergraduate (graduate in other field).

Center for Computing Research

Discrete Mathematics, Optimization, & Uncertainty Quantification
Scalable System Algorithms, Software, Analysis, & Visualization
Multiscale/Cognitive Science, Data-driven & Neural Computing

Mission Engineering & Information Systems Analysis

Sensor, Data, Imaging Analysis
Data Science, Cyber Security, Cryptography, Analytics
Digital & Quantum Information Sciences & Systems

Engineering Sciences

Diagnostic, Shock, Structural, Climatic, Fluid & Reactive Processes, Fire S&T
Computational Solid/Structural/Thermal/Fluid Mechanics & Dynamics
Verification & Validation, Uncertainty Quantification, Credibility Processes

- Statisticians work mostly in areas of Risk/Reliability Analysis, Quality Engineering, Quantification of Margins and Uncertainty (QMU).

Sandia Aggies (TX)

- ~200 Alumni
- ~9 with degrees from TAMU mathematics and statistics programs.

My Route to SNL Engineering Sciences

Sandia National Laboratories

- **Worcester Polytechnic Institute (B.S.)**
  - Goal was Nuclear *Engineering*, but ended up…
  - Physics (quantum mechanics), Mathematics (Steklov eigenvalues)
  - COMAP Mathematical Contest in Modeling (MRI image analysis) [*Consortium for Mathematics and its Applications*]
- **Headed** for theoretical particle physics (SUNY Stony Brook), but was **diverted** to the Industrial Applied Mathematics Program (NCSU).
- **North Carolina State University (M.S., Ph.D.)**
  - Industrial Mathematical Modeling Workshop (intro. to smart materials).
  - Degrees: Computational/Industrial Applied Mathematics
  - Dissertation: Shape Memory Alloy (SMA) modeling.
  - **Grad. Internships**: The Boeing Company (sparse optimization), SNL (SMAs).
- Applied only to non-academia positions and chose…
- **Sandia National Laboratories, Albuquerque**
  - Adaptive structures, smart materials and metamaterials research.
  - Mechanical design with uncertainty quantification and optimization.
  - Thermal stress analysis, including Finite Element multiphysics.
  - Thermomechanical modeling of micro- and meso-electronics, MEMS.

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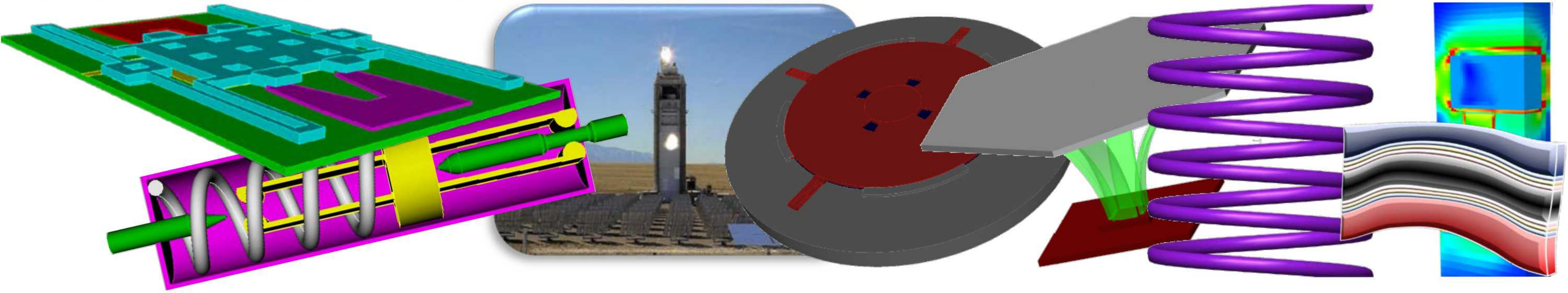

Nonlinear Model for Shape-controlled Corner-supported, Thin Laminates

U.S. DEPARTMENT OF ENERGY

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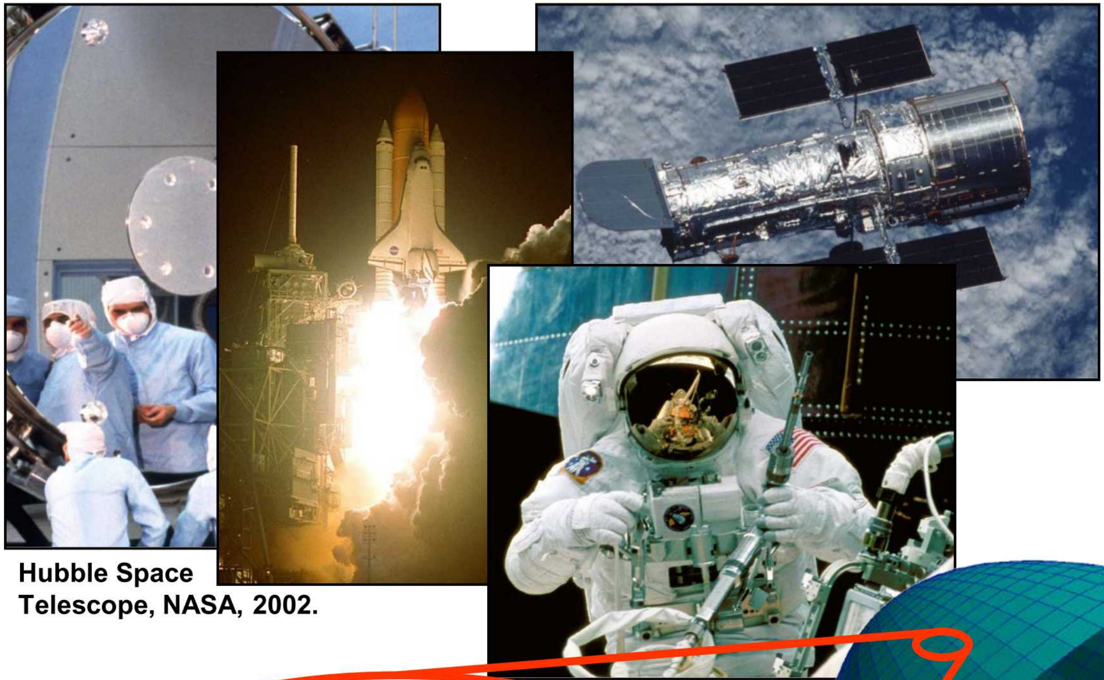
Need for Shape-controlled Reflectors

Traditional Rigid Reflectors

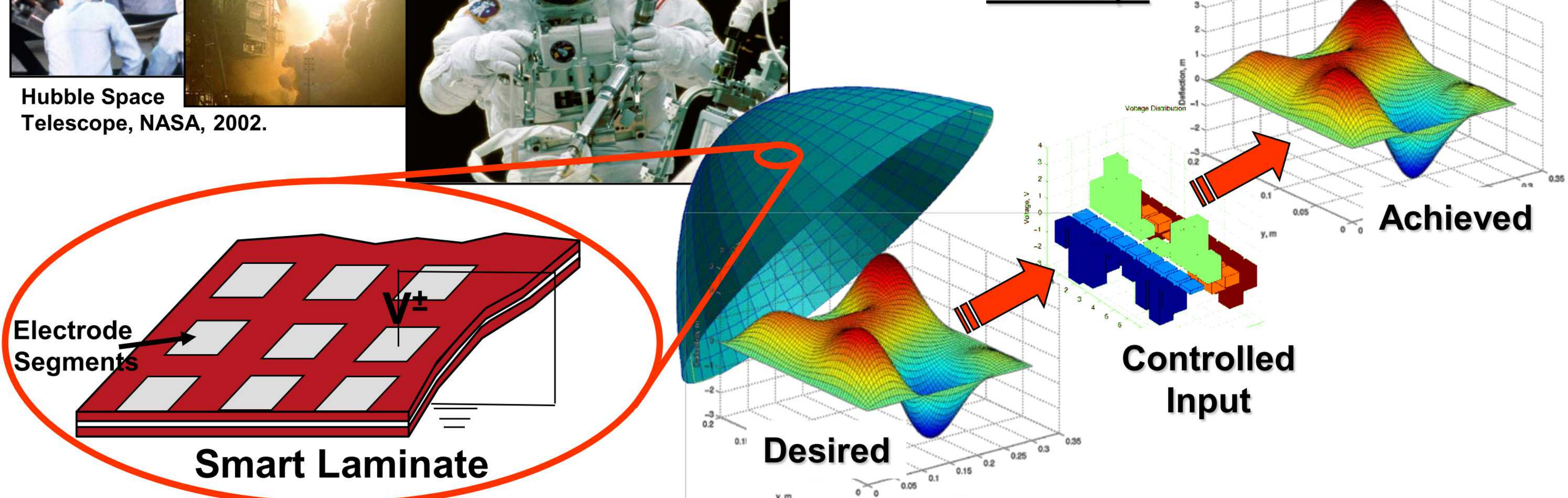


Hubble Space Telescope, NASA, 2002.

Advantages of Flexible Reflectors

- Thin, light.
- Compactly deployed.
- Integrated surface error correction.

Shape-controlled Membrane Concept



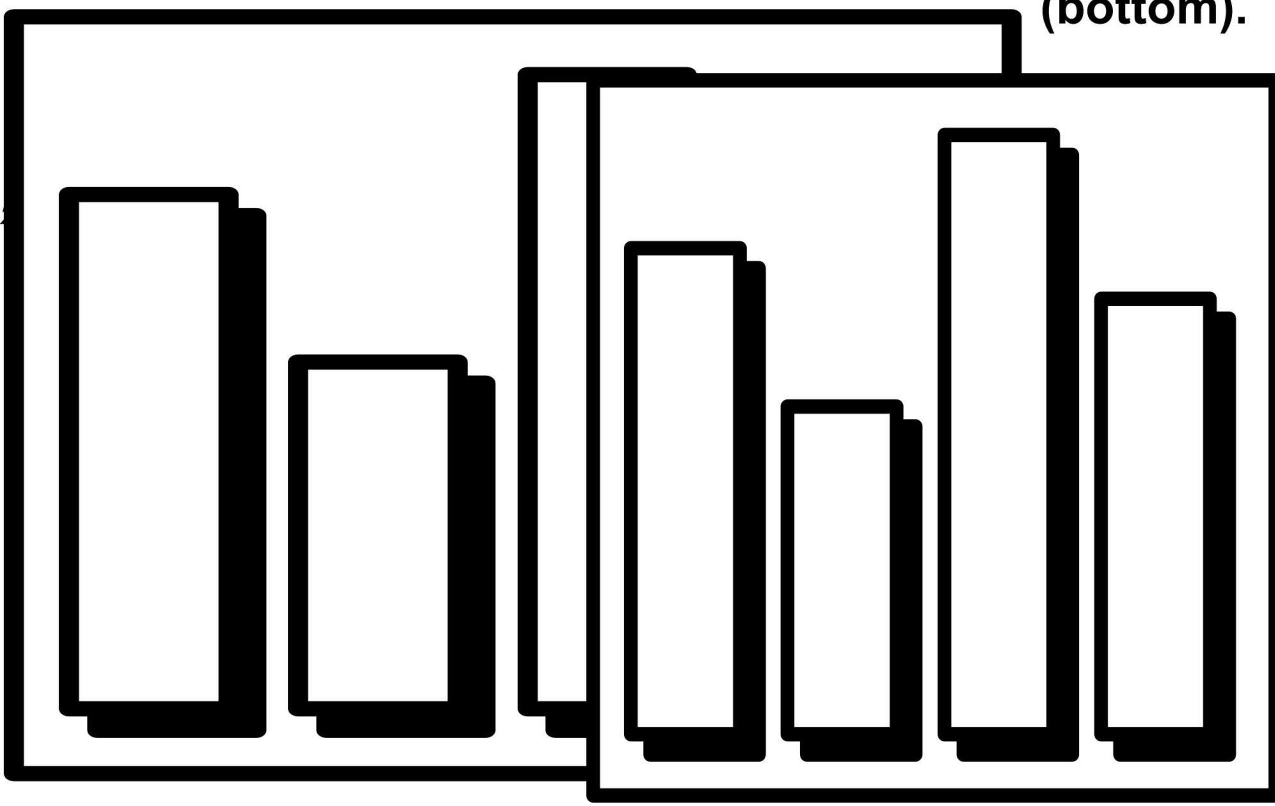
Smart Laminate with Moment Actuators

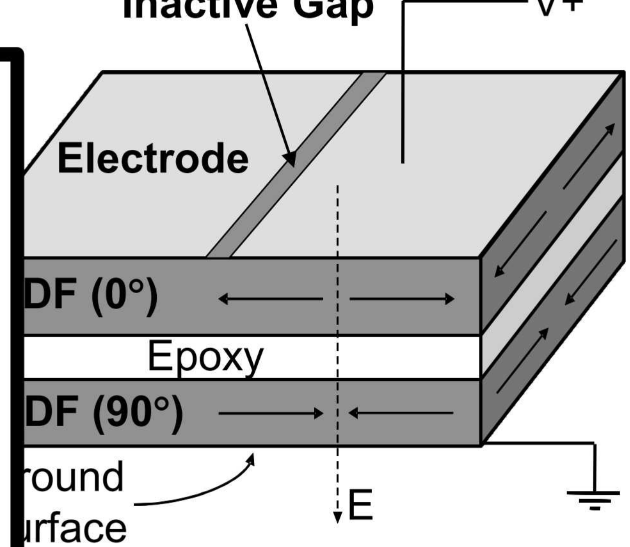
Thin, Square, Membrane with Corner Supports

- Natural actuation into paraboloid,
- Improved flexibility,
- Larger deflections.

Bimorph Action

- PVDF layers have opposing poling directions.
- Positive field induces simultaneous expansion (top) and contraction (bottom).



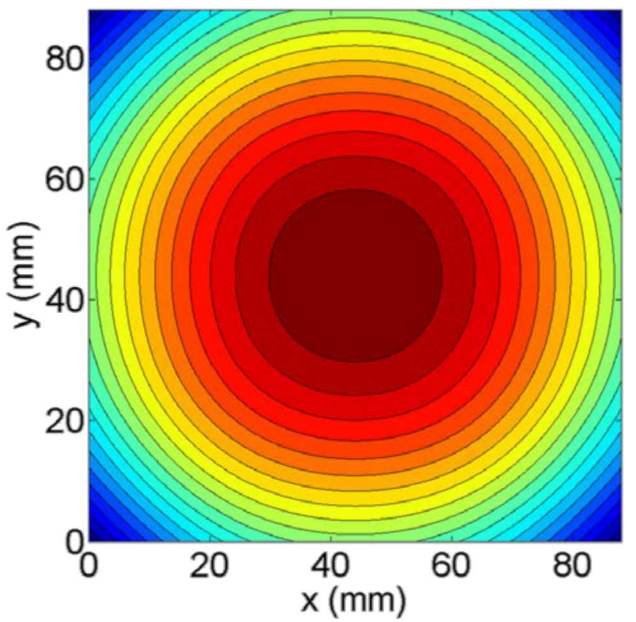


Initial Linear Model

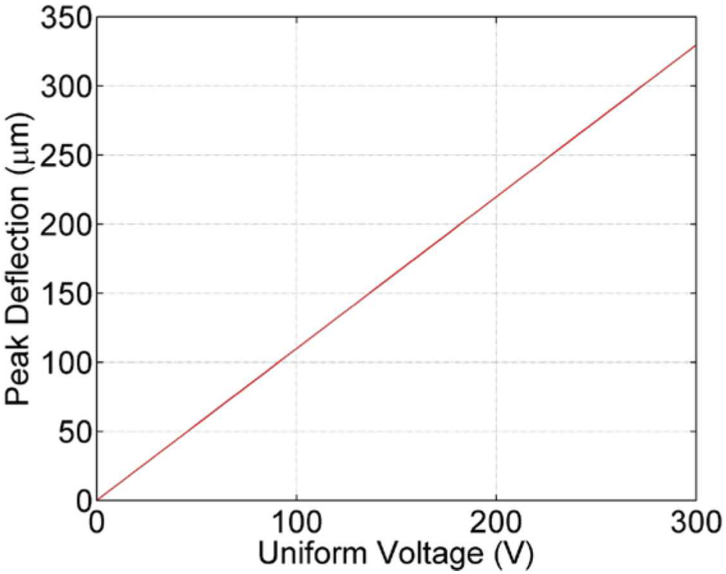
- Corner supports: sliding corners (constrained out-of-plane only).
- Based on Kirchhoff-Love plate theory and Ritz Method:
  - Describes bending-dominated deflection;
  - Yields linear mapping between input voltage to output deflection.
- Formulation facilitates shape control, quick to execute.
- Observations: simulates *uniformly circular contours* and *linear* rise in peak deflection with increasing uniform actuation voltage.

$$\mathbf{R}V = \mathbf{H}u$$

Deflection Contours

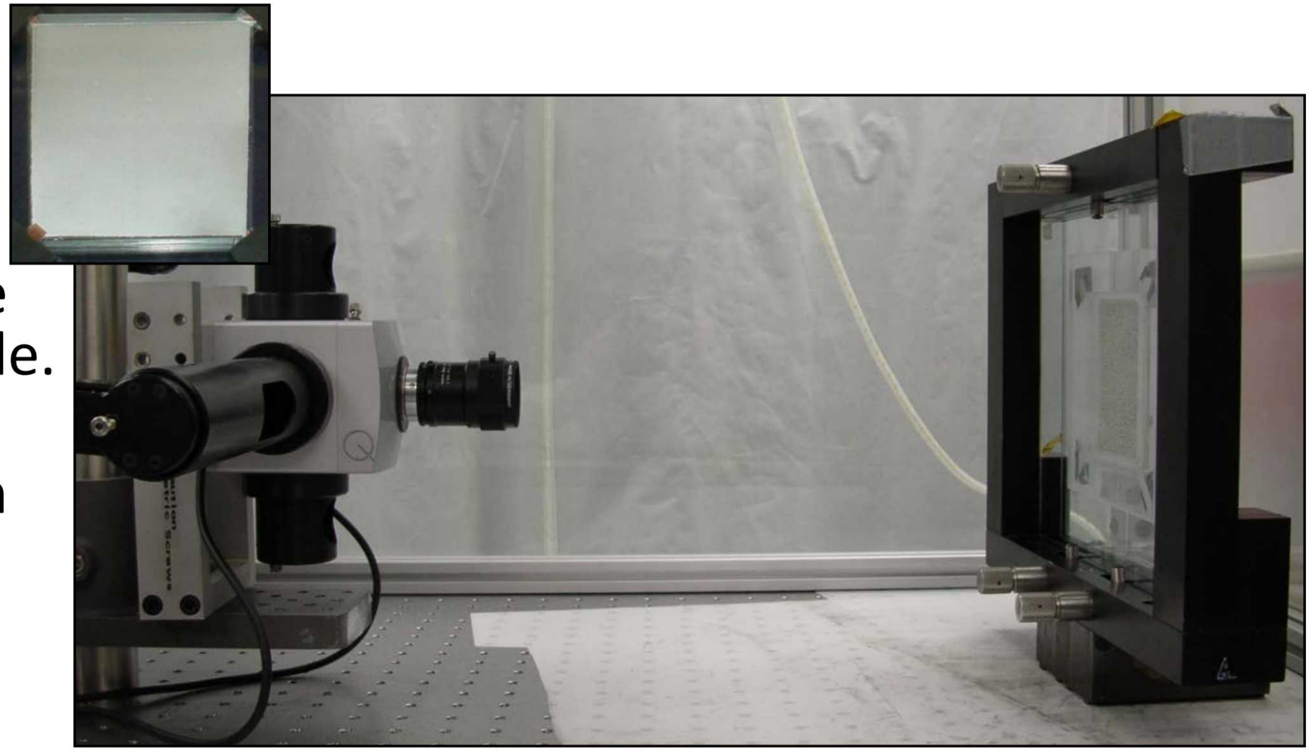


Peak Deflection vs. Uniform Voltage



Smart Laminate Experiments

- Fabricated corner-supported laminate with single electrode.
- Corner-support boundary condition approximated with corner tabs.

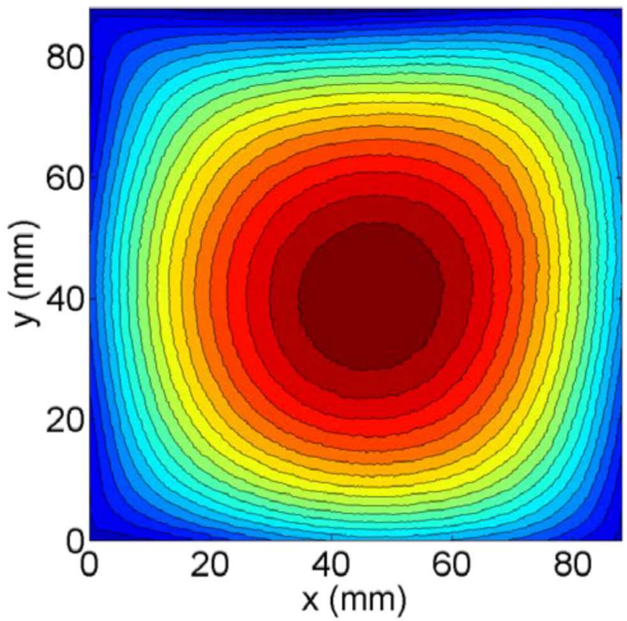


- Electronic Speckle Pattern Interferometry (ESPI): full-field displacement measurements with out-of-plane measurement resolution ≤45 nm.
- Optical fringe measurement is sensitive to vibrations (HVAC, etc.).
  - fixture designed to suppress vibrations;
  - tightened corner supports to facilitate repeatable measurements.

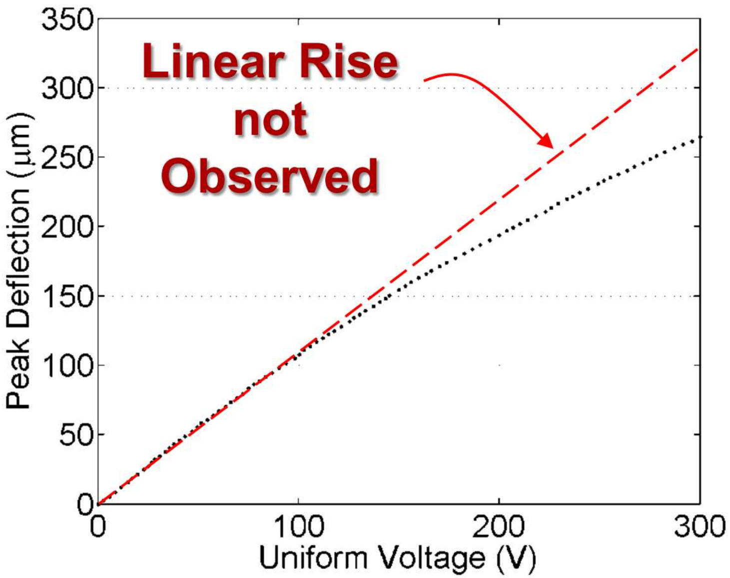
Experiment Results

- Observations:
  - *squared contours* become circular only away from boundary;
  - *nonlinear* rise in peak deflection with increasing uniform actuation voltage.

Deflection Contours



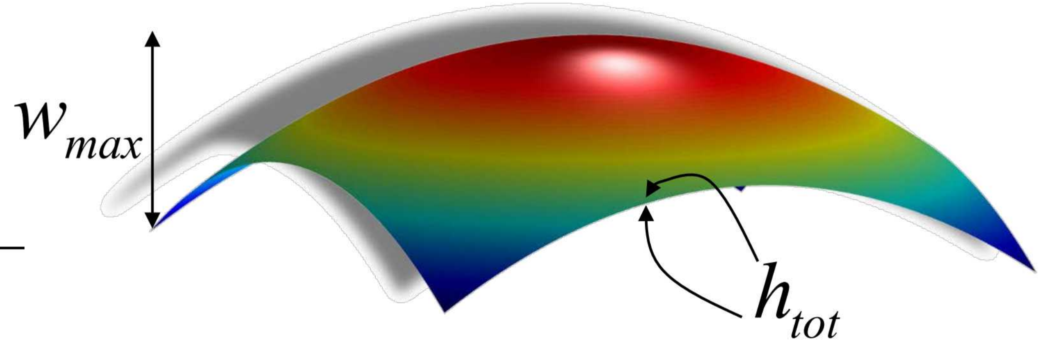
Peak Deflection vs. Uniform Voltage



Why the difference?

- Size of membrane deflections is gauged by the ratio

$$\frac{\textbf{Peak Deflection}\;\; w_{max}}{\textbf{Total Membrane Thickness}\;\; h_{tot}}$$



Small Deflections

$$\frac{w_{max}}{h_{tot}} \leq 0.2$$

- Negligible stretching of middle surface.
- Bending is dominant.
- Kirchhoff linear theory adequate.

Large Deflections

$$\frac{w_{max}}{h_{tot}} \geq 0.3$$

- Significant stretching of middle surface.
- Membrane deformation ≥ bending.
- Nonlinear geometry changes and significant in-plane deformation.

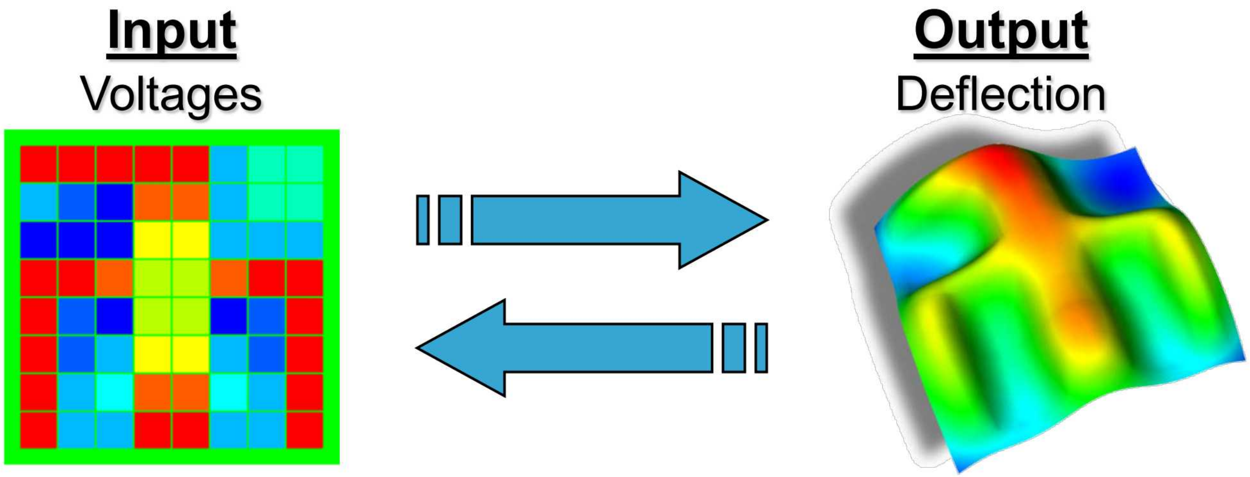
- Desired and measured deflections ≥ 250 μm.
- Typical membrane thicknesses 100 - 250 μm.

$$\Rightarrow \quad \frac{w_{max}}{h_{tot}} \geq 1.0$$

Large deflection theory of membranes must be used to adequately model laminate deflections.

Nonlinear (Large) Deflection Model

- Develop nonlinear model using framework of the initial linear, sliding-corner model.
- Predict large membrane deflections.
- Treat fixed corners.
- Preserve current model formulation as mapping:



Critical: formulate model to be suitable for deflection control.

Energy-based (Ritz) Framework

1. Construct membrane deformation energy in terms of deformations and input voltage.
2. Express deformations in terms of known functions with undetermined constants.
3. Find constants that minimize energy.

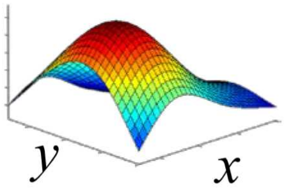
Step 1: Deformation Energy

Total Strain Energy	=	Deflection Energy	+	Actuation Energy

$$U = U_\varepsilon(u, v, w) + U_{act}(u, v, w; V)$$

Deflection

$w(x, y)$



In-plane Deformations

$u(x, y)$

$v(x, y)$

Goal: find energy-minimizing deformation given voltage array V.

Deflection Energy

$$U_\varepsilon = \frac{1}{2}\int_0^a\int_0^b\int_{-h_g-h/2}^{h_{el}+h/2} \boldsymbol{\varepsilon}(x,y,z)^{\mathsf{T}}\boldsymbol{T}(z)\,dz\,dy\,dx$$

Plane Stress

$$\boldsymbol{T}(z) = \boldsymbol{S}(z)\boldsymbol{\varepsilon}(x,y,z)$$

layer-dependent

von Karman Strain Relations

$$\varepsilon = \varepsilon_b + \varepsilon_m + \varepsilon_{nl}$$

Linear Model

Bending Strain

$$\boldsymbol{\varepsilon}_b(z) = -z\boldsymbol{\kappa}$$

Membrane Curvature

$$\boldsymbol{\kappa} = \begin{bmatrix} w_{xx} & w_{yy} & 2w_{xy} \end{bmatrix}^{\mathsf{T}}$$

Membrane Strain

$$\varepsilon_m = \begin{bmatrix} u_x & v_y & u_y + v_x \end{bmatrix}^{\mathsf{T}}$$

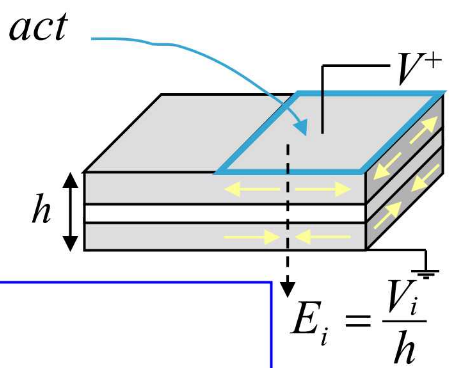
Nonlinear Strain

$$\varepsilon_{nl} = \frac{1}{2}\begin{bmatrix} w_x^2 & w_y^2 & 2w_x w_y \end{bmatrix}^{\mathsf{T}}$$

$$U_\varepsilon = U_b + U_m + U_{lc} + U_{nlc} + U_{nl}$$

Bending, Membrane, Linear-coupled, Nonlinear-coupled, and Nonlinear Energy Components.

Actuation Energy



$$U_{act} = \sum_{i=1}^{i_{max}} \iint_{act_i} \boldsymbol{\kappa}^{\mathsf{T}} \boldsymbol{M}_{act_i} dA$$

Membrane Curvature

$$\boldsymbol{\kappa} = -\begin{bmatrix} w_{xx} & w_{yy} & 2w_{xy} \end{bmatrix}^{\mathsf{T}}$$

Moment

$$\boldsymbol{M}_{act_i} = \int_{act_i} \boldsymbol{S}(z)\boldsymbol{\varepsilon}_{act_i}(z) z dz$$

Actuation Strain

$$\boldsymbol{\varepsilon}_{act_i}(z) = \begin{cases} \begin{bmatrix} d_{31} & d_{32} & 0 \end{bmatrix}^{\mathsf{T}} E_i & \frac{h_{ep}}{2} \le z \le \frac{h}{2} \\ 0 & -\frac{h_{ep}}{2} < z < \frac{h_{ep}}{2} \\ \begin{bmatrix} -d_{32} & -d_{31} & 0 \end{bmatrix}^{\mathsf{T}} E_i & -\frac{h}{2} \le z \le -\frac{h_{ep}}{2} \end{cases}$$

Integrate energy expression thru laminate thickness:

$$U_{act} = \frac{D_{act}}{h} \sum_{i=1}^{i_{max}} V_i \iint_{act_i} \left(w_{xx} + w_{yy}\right) dA$$

Voltages
V_i

Actuation Stiffness Constant
D_{act}

Step 2: Energy Expansion

Assume expansions for tri-axial deformations:

$u(x,y)=\sum_{j=1}^{\infty}\mu_j(x,y)$	$\mu_j(x,y)=a_{u_j}\sin\left(n_j\pi\frac{x}{a}\right)\cos\left(m_j\pi\frac{y}{b}\right)$	Satisfy vanishing strain at edges.
$v(x,y)=\sum_{j=1}^{\infty}\psi_j(x,y)$	$\psi_j(x,y)=a_{v_j}\cos\left(m_j\pi\frac{x}{a}\right)\sin\left(n_j\pi\frac{y}{b}\right)$	
$w(x,y)=\sum_{j=1}^{\infty}\phi_j(x,y)$	$\phi_j(x,y)=a_{w_j}\cos\left(m_j\pi\frac{x}{a}\right)\sin\left(n_j\pi\frac{y}{b}\right)+$ $+b_{w_j}\cos\left(m_j\pi\frac{y}{b}\right)\sin\left(n_j\pi\frac{x}{a}\right)$	Satisfies zero displacement at corners.

Truncate sums, simplify energy in terms of expansions:

$$U(a_u,a_v,c_w,V)=U_\varepsilon(a_u,a_v,c_w)+(\mathbf{R}V)^T c_w$$

Actuation Block Matrix $\mathbf{R}$

Voltage Array V

In-plane Expansion Coefficient Vectors a_u, a_v

Out-of-plane Expansion Coefficient Vector $c_w=[a_w \quad b_w]$

Step 3: Energy Minimization

Find energy-minimizing deformation. → Find energy-minimizing expansion coefficients.

Minimum conditions:

$$\nabla_{a_u} U = 0 \qquad \nabla_{a_v} U = 0 \qquad \nabla_{c_w} U = 0$$

Solve nonlinear system for expansion coefficients:

$$G_\varepsilon\left(a_u, a_v, c_w\right) + \mathbf{R}V = 0$$

Gradient Function

G_ε

couples expansion coefficients nonlinearly

Resulting Map:

Input: V → **Output:** ~~$u(x,y)$, $v(x,y)$~~, $w(x,y)$

- Inverse map requires knowledge of in-plane deformation.
- Typically out-of-plane information is known (e.g., ESPI, error surface), in-plane is *unknown*.

De-couple In-plane Strain

Minimum conditions allow in-plane coefficients (a_u, a_v) to be cast explicitly in terms of out-of-plane coefficients.

$$\nabla_{a_u} U = 0 \quad \Longrightarrow \quad a_u = F_u(c_w)$$

$$\nabla_{a_v} U = 0 \quad \Longrightarrow \quad a_v = F_v(c_w)$$

Recast nonlinear system:

$$\mathbf{H}c_w + G_{nl}(c_w) + \mathbf{R}V = 0$$

<u>Decoupled Energy Hessian</u>

$\mathbf{H}$

<u>Nonlinear Gradient Function</u>

G_{nl}

nonlinear component of decoupled gradient

Resulting Map:

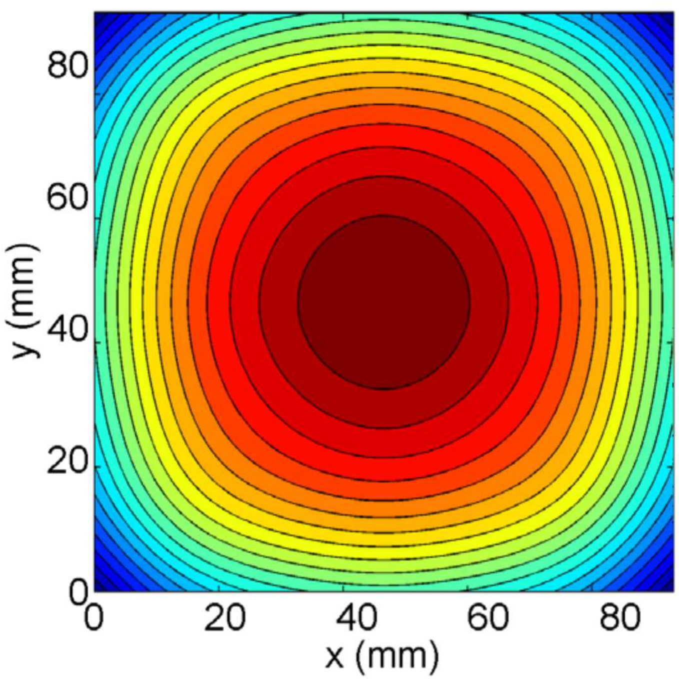
Input: V $\Longrightarrow$ **Output:** $w(x,y)$

- Inverse map requires only *out-of-plane* deformation.
- Deflection control now feasible.

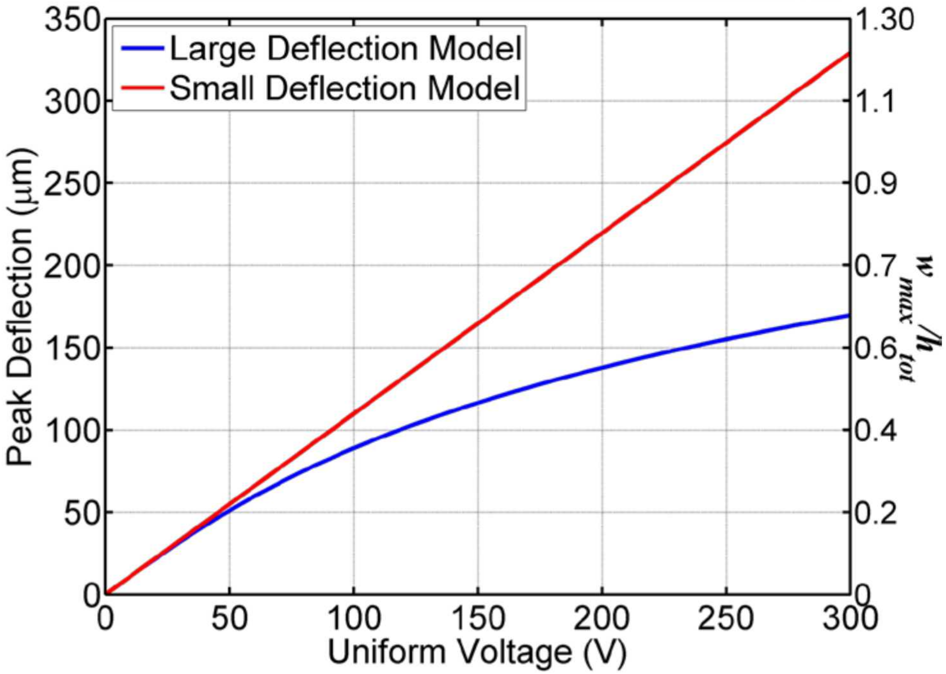
Nonlinear Model Results

- Deflection contours show squaring effects.
- Nonlinear rise in peak deflection predicted.
- Source: nonlinear geometry changes; membrane forces due to large deflections and pinned corners.

Model Deflection Contours



Peak Deflection vs. Uniform Voltage



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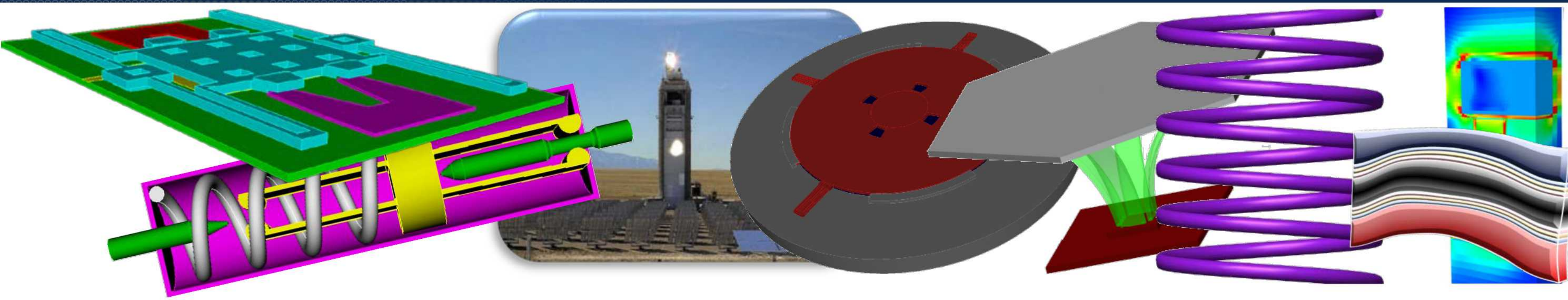

Flexible Optimization and Uncertainty-Enabled Design of Helical Compression Springs in Nonlinear Spring-Mass-Damper Systems

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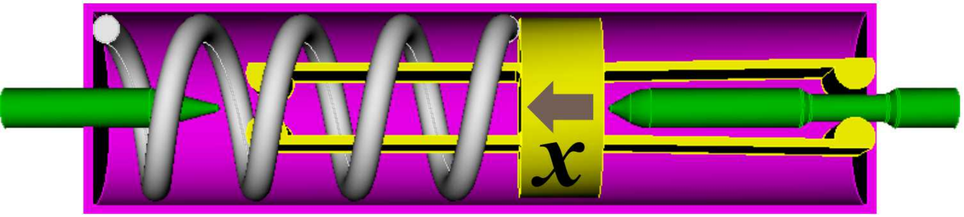
NNSA National Nuclear Security Administration

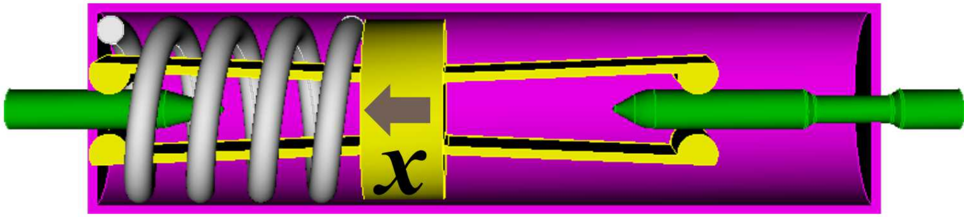
An Acceleration Switch Modeled

Open



An awesome graduate student workshop team at IMSM 2010 analyzed this switch.

Closed



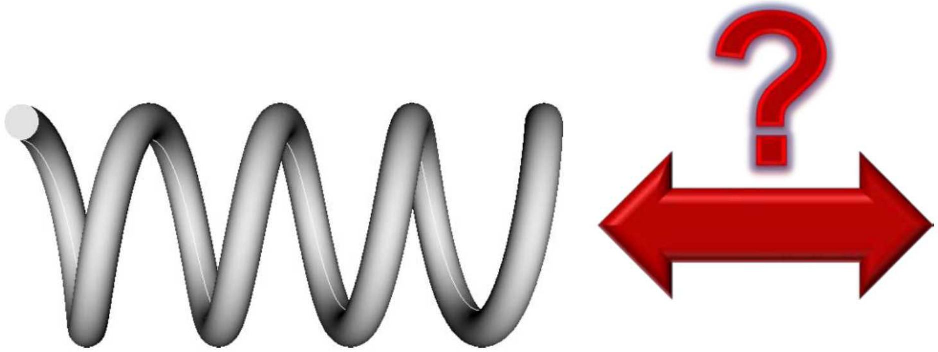
$$m\ddot{x} = F_{accel} - \left(F_{spring} + F_{friction} + F_{contact} + F_{drag} \right)$$

$$x(0) = 0, \dot{x}(0) = 0$$

Critical Parameter: Spring Force

$$m\ddot{x} = F_{accel} - \left(F_{spring} + F_{friction} + F_{contact} + F_{drag} \right)$$

$$F_{spring} = kx + F_{preload}$$

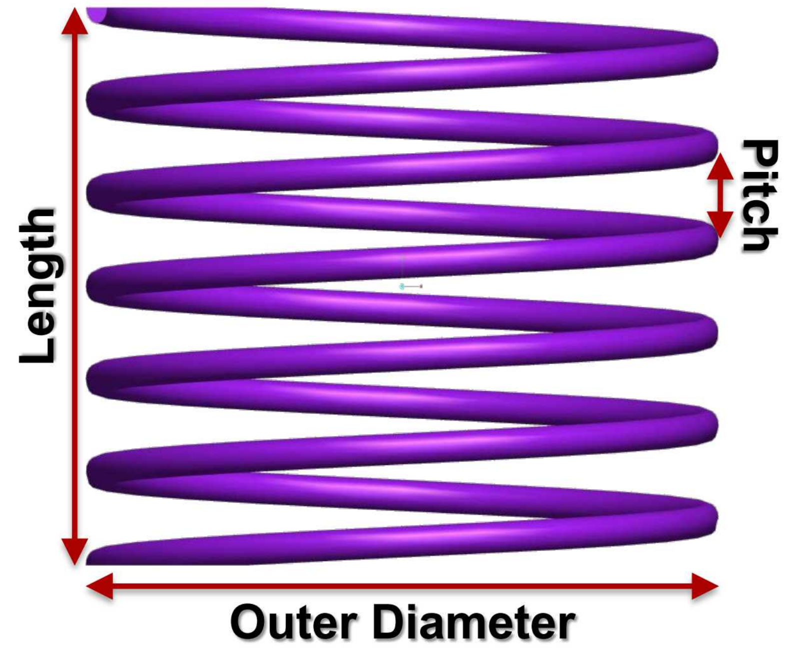


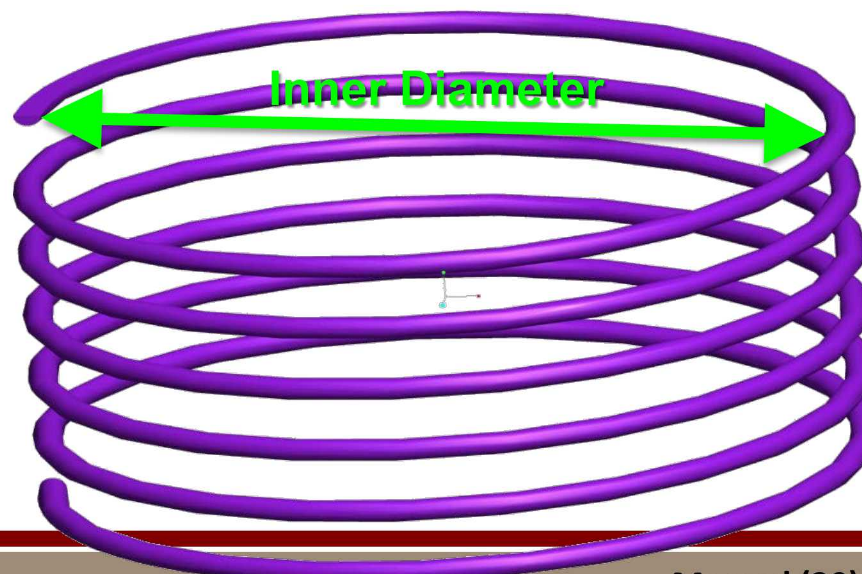
$$k, F_{preload}$$

Helical Spring Anatomy 101

Assuming typical compression spring made of round wire.

- **Free Length**: spring height under no compression.
- **Solid Height**: spring length at full compression (all coils touch).
- **Pitch**: distance between wire centers at free length.
- **Diameters**: wire, spring outer/inner
- **Total Coils**: 1 coil = 360° turn in-plane.
- **End Conditions (ec)**
  - **Ground Ends**: top/bottom coils are ground flat.
  - **Closed/Open Ends**: top/bottom coils attached to adjacent coil.





Key Spring Properties

Spring Rate

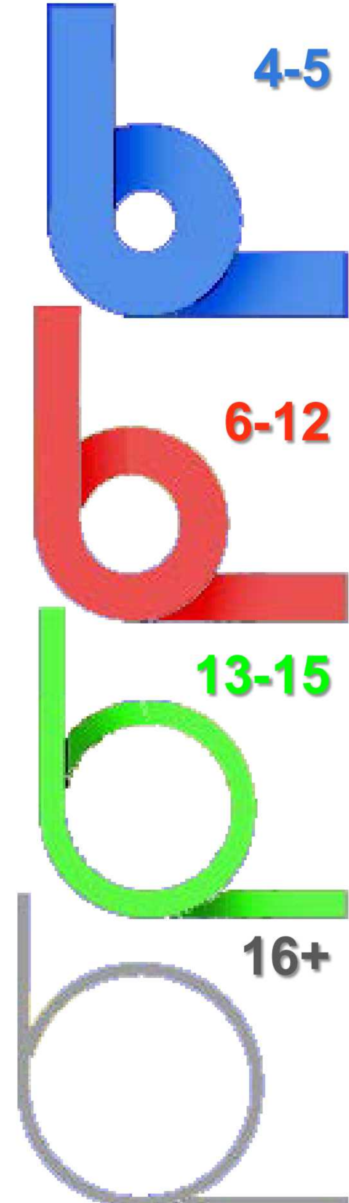
$$k = \frac{G}{8N_a(ec)} \frac{{d_w}^4}{(d_i + d_w)^3}$$

- Effective stiffness of spring in compression.
- Force typically varies linearly with displacement in operating range.
- **Optimal Spring**: specified force when needed, **low Spring Rate** otherwise.

Spring Index

$$C = \frac{d_i}{d_w} + 1$$

- Determines stress distribution and magnitude, and manufacturability and tolerancing.
- **Optimal Spring**: **low Index**.



Optimize the spring?

- Low Rate $\Rightarrow$ High Index
- Low Index $\Rightarrow$ High Rate

$$k = \frac{G}{8N_a(ec)} \frac{d_w^{\,4}}{(d_i + d_w)^3}$$

$$C = \frac{d_i}{d_w} + 1$$

Strategy to keep both k and C low:

- minimize d_i to lower C,
- then increase d_w to reach largest “low” k that is acceptable.
- Also, consider more coils and lower material stiffness.

Simple enough, but…

Design Constraints (*just some!*)

Inner/Outer Diameter Bounds

$$d_i > d_i^{min}$$

$$d_i < d_o$$

$$d_i + 2d_w < d_o^{max}$$

Diametral Expansion

$$d_{expand}\left(d_i, d_w, L_{free}, N_a; \text{ec}\right) < d_o^{max}$$

Maximum Spring Rate

$$\frac{G}{8N_a}\frac{d_w^{\ 4}}{\left(d_i + d_w\right)^3} \le k_{max}$$

Maximum Spring Index

$$\frac{d_i}{d_w} + 1 \le C_{max}$$

Force Requirement

$$\left(L_{free} - L_{reset}\right)\frac{G}{8N_a}\frac{d_w^{\ 4}}{\left(d_i + d_w\right)^3} = F_{reset}$$

Coil Binding Gap

$$\frac{L_{hard} - L_{solid}\left(d_w, N_a; ec\right)}{N_t - 1} \ge g_{min}$$

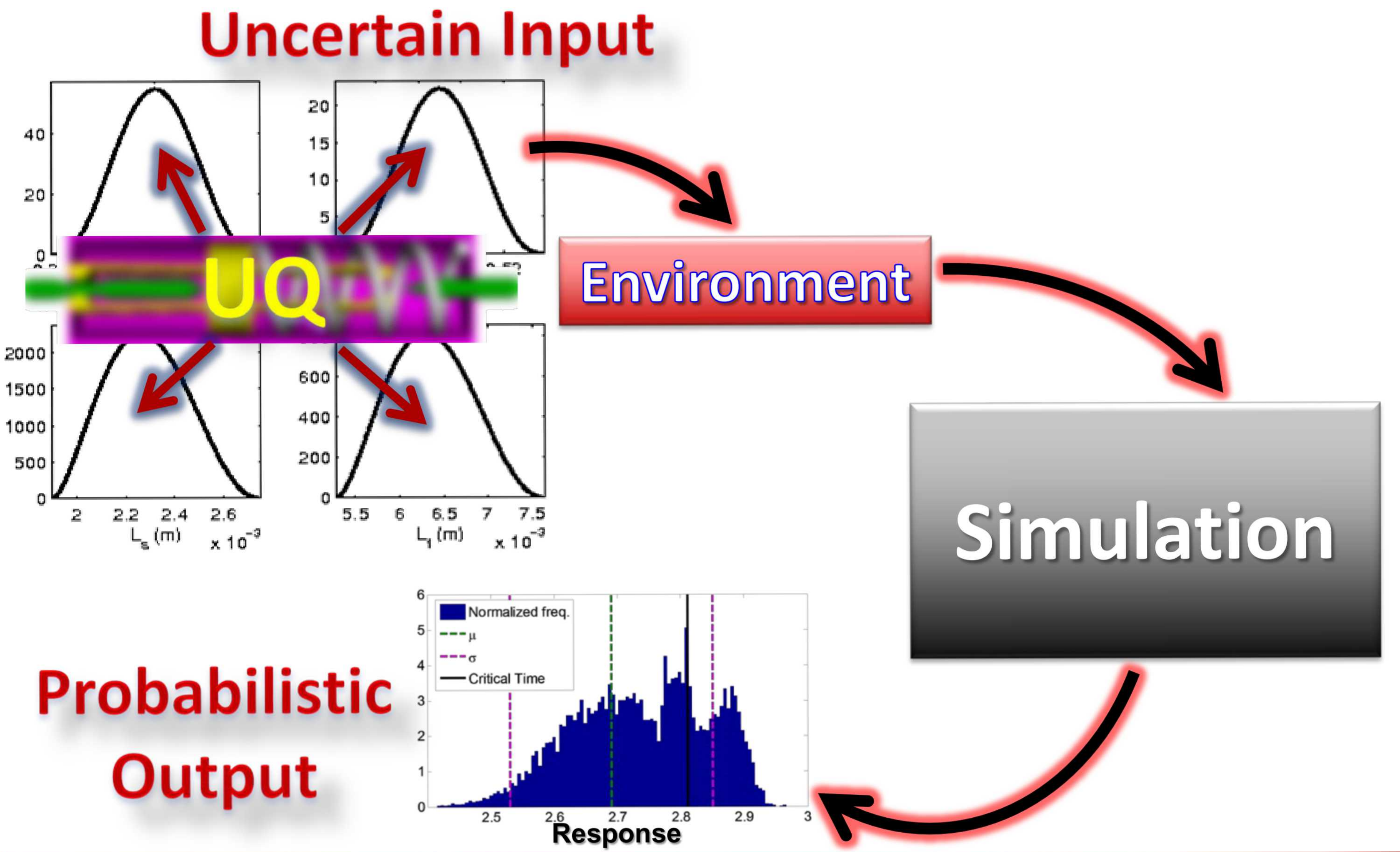
Buckling Slenderness

$$\frac{L_{free}}{d_i + d_w} < \pi\sqrt{\frac{2\left(2\nu + 1\right)}{\nu + 2}}$$

Maximum Shear Stress

$$\text{UTS} > \frac{G\left(L_{free} - L_{hard}\right)}{4\pi N_a\left(ec\right)}\left[\frac{d_w\left(4d_i^{\ 2} + 9.46 d_i d_w + 3d_w^{\ 2}\right)}{d_i\left(d_i + d_w\right)^3}\right]$$

Uncertainty-enabled Design



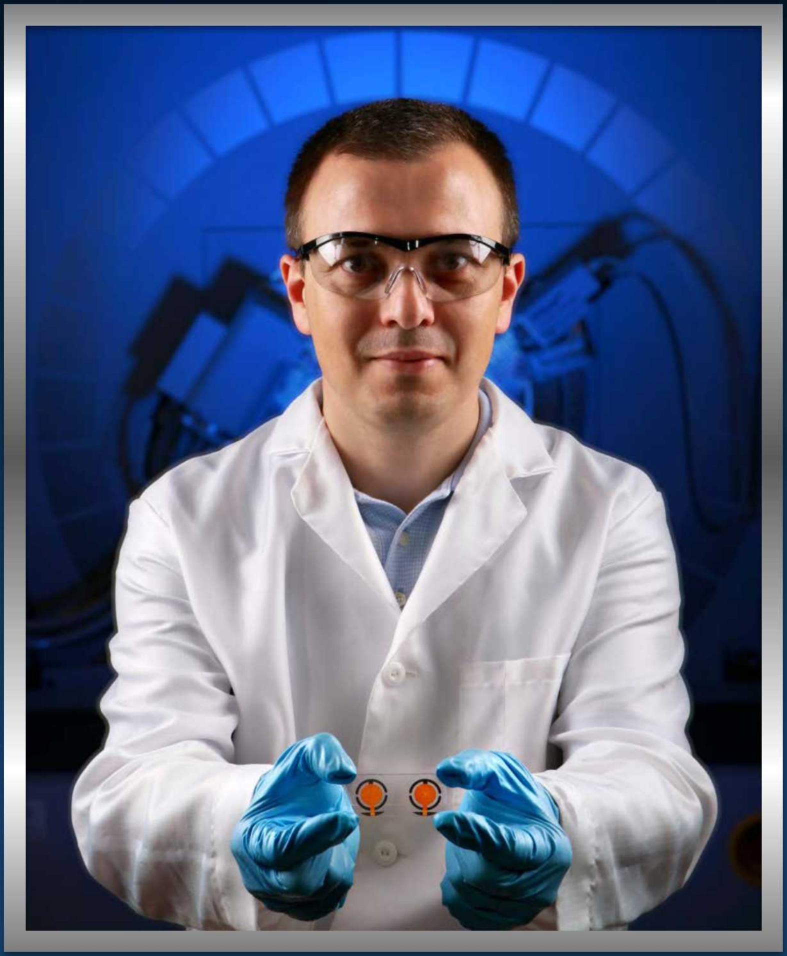
Fulfill the Need, Define the Problem

Given a helical compression spring
within a spring-mass-damper system:
Provide optimal spring designs and do it quickly!

- As an applied mathematician and engineering scientist, my goal is to provide this capability.
- Quantifying "optimal" is non-trivial.
- Differing goals means we need an algorithm that optimizes springs with interchangeable objectives and constraints!
- **Uncertainty-enabled**: design springs that maximize the *probability* of **spring** performance with uncertain conditions/properties. (Optimization Under Uncertainty)
- **Multi-scale**: optimize springs to increase the probability of their parent **components** performing well under uncertain conditions.

The Sandia Work Experience

Sandia National Laboratories

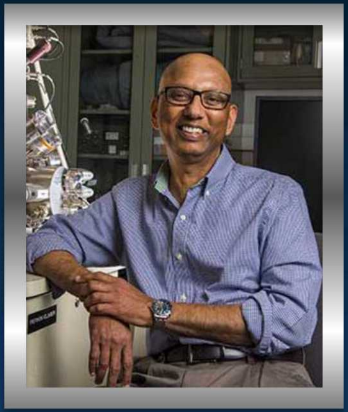


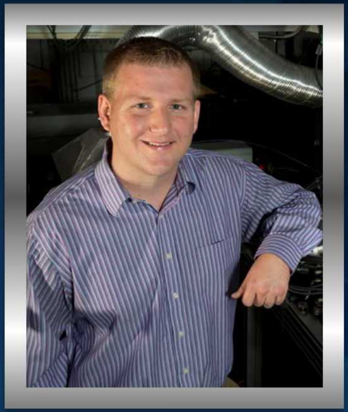
- Challenging assignments
- State-of-the-art research facilities
- Access to outreach and networking groups
- R&D 100 Awards, patent royalties, and more
- Career mobility

Work with Top Minds, Be Recognized

Sandia National Laboratories

Our unique work requires the collective minds of the nation's top scientists, engineers, and support staff, many of which are recognized for developing a range of breakthrough technologies.





Tamara Kolda
Fellow of the Society for Industrial and Applied Mathematics

Somuri Prasad
Asian American Engineer of the Year Award

Jon Madison
Black Engineer of the Year Award

Christopher Kliewer
Early Career Research Program Award

Apply Online! sandia.gov/careers

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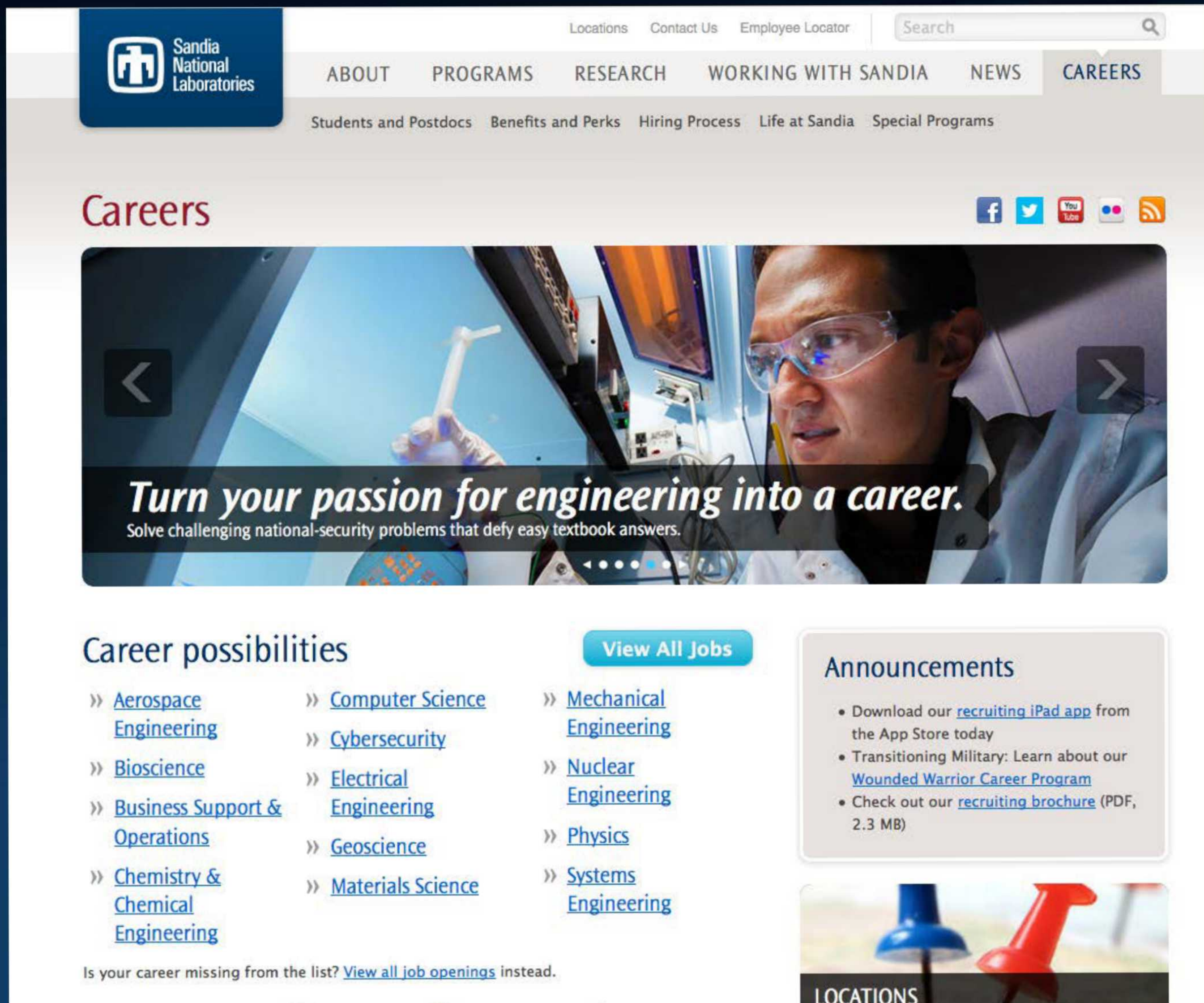


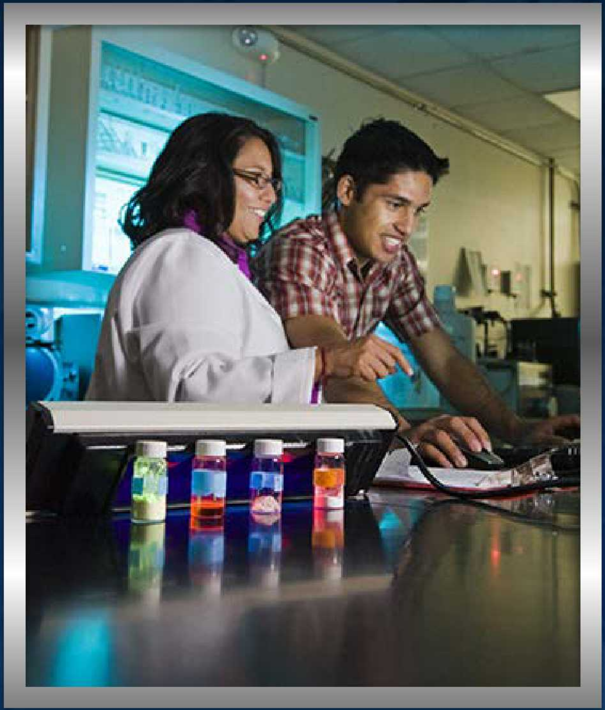
Internships

Encourages qualified students to develop interests in critical skills areas related to our mission, with the ultimate objective of developing our pipeline for our future.

Types: Summer, Year Round and Co-op.

Eligibility Criteria

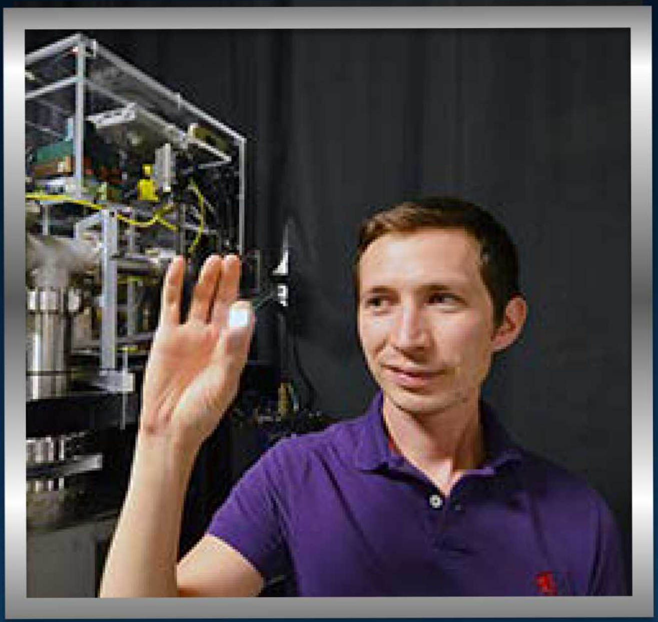
- Min. cumulative GPA: 3.2 Undergraduate, 3.5 Graduate.
- U.S. citizenship for positions that require clearance or as stated in the job posting.
- Full-time enrollment status at an accredited college, university, or local high school.
- At least 16 years of age.



Technical Institute Internships

- Center for Computing Research (CCR)
- Engineering Design and Integration Students (EDIS)
- Nonlinear Mechanics and Dynamics (NOMAD)
- Science of Extreme Environments Research Institute (SEERI)
- SENTINL: Energy Surety Incubator (ESI), Interns for Secruity, Arms Control, and Force Protection Engineering (iSAFE).
- TITANS: Center for Analysis Systems and Applications (CASA), Center for Cyber Defenders (CCD), Monitoring Systems and Technology Intern Center (MSTIC).

Post-doc Opportunities



Key areas for post-docs at Sandia:

- Biosciences and biotechnology
- Chemistry and materials science
- Combustion
- Computational mechanics
- Computer science
- Hydrogen
- Microelectronics and microfluidics
- Nanotechnology
- Physics

Eligibility Criteria

- Recent PhD (awarded within past 5 years) or ability to complete all PhD requirements before beginning.
- No previous post-doc appointments at a national laboratory.

Degree Programs & Fellowships

Special Degree Programs

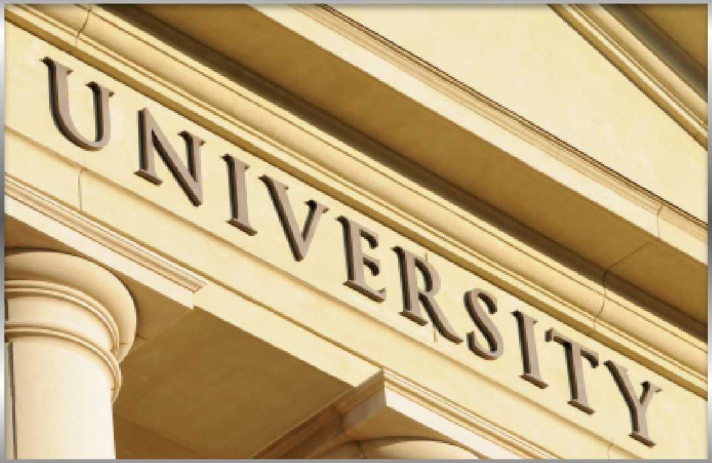
- Critical Skills Master's Fellowship Program
- Master's Fellowship Program

Ph.D. Level Fellowships

- Harry S. Truman Fellowship
- John Von Neumann

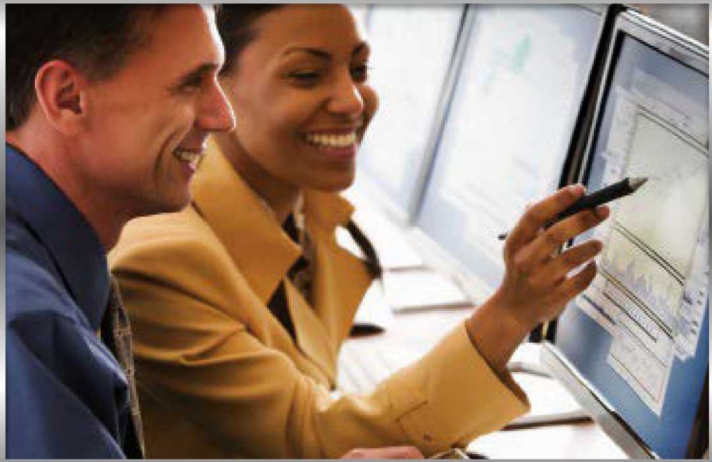
Special Programs, Education & Mentoring

Sandia National Laboratories



University-based Education

- Tuition Assistance Program
- University Part-Time Program
- Special Master's Program
- Doctoral Study Program



In-house Education, Training and Mentoring Programs

- Business
- Communication
- Design and drafting
- Information technology
- Manufacturing
- Marketing
- Project management Sciences

So Why Sandia?

National Security Mission: Work contributes to the security, peace and freedom of our nation and the world.

Uniquely Challenging and Important Work: Work is challenging, and amazing with real-world impact.

Work with Great People: Work with extraordinary people, the top minds in their field.

Research Facilities Like None Other: Access to some of the best tools, equipment, and research facilities in the world.

Healthy Lifestyle, Work-Life Balance: Balance between work life and personal life through flexible schedules, competitive benefits, and convenient amenities.

Videos

Sandia National Laboratories

Sandia Mission Video (4:36)
Sandia Who We Are (3:05)

Location Videos
Sandia New Mexico Location (3:23)
Sandia California Location (3:23)

Black Leadership Outreach

For more Sandia Videos refer to Sandia's YouTube Channel