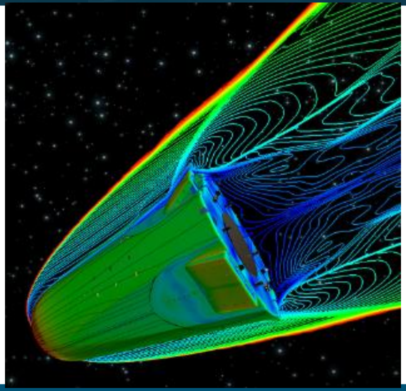
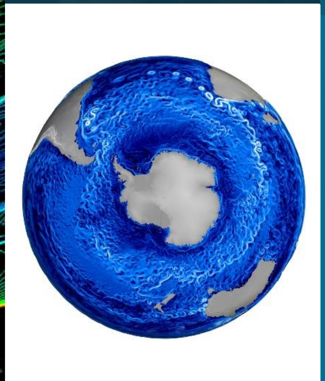
SAND2021-4318PE

My Career as a Computational Scientist at Sandia National Labs





PRESENTED BY

Irina Tezaur, Principal Member of Technical Staff

Quantitative Modeling & Analysis Department
Sandia National Laboratories, Livermore, CA

STEM Career Seminar
April 15, 2021

Casper College
Casper, Wyoming

Outline

1. A little bit about me and my background

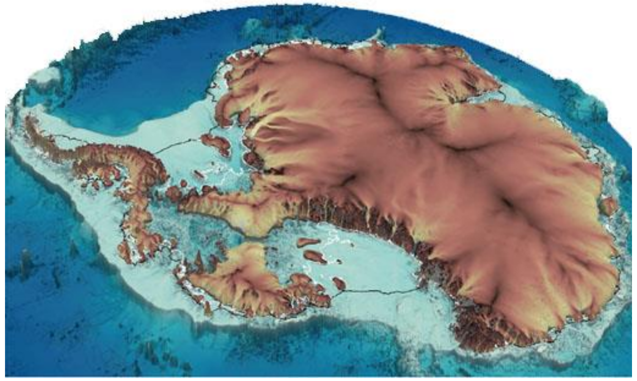
2. A little bit about Sandia National Laboratories

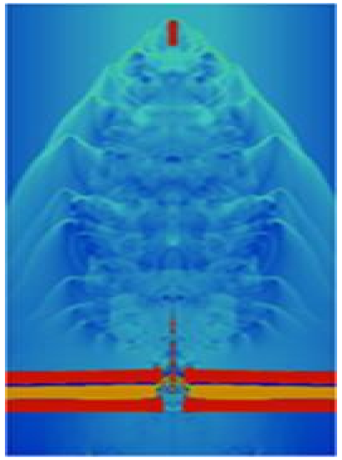
3. Physics-based computational modeling & simulation in a nutshell

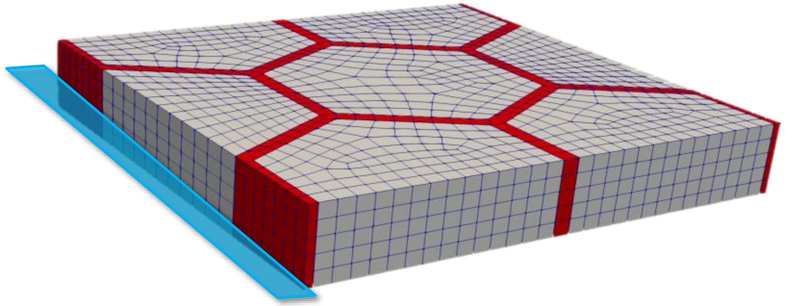
4. A few research highlights
    - Ice sheet modeling
    - Multi-material impact simulations

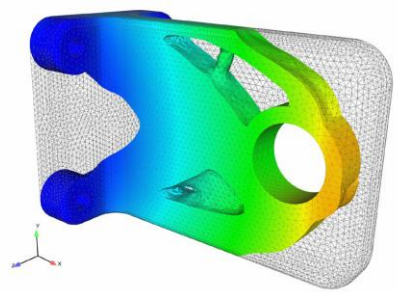
5. Career & educational tips

6. Question & answer (Q&A)









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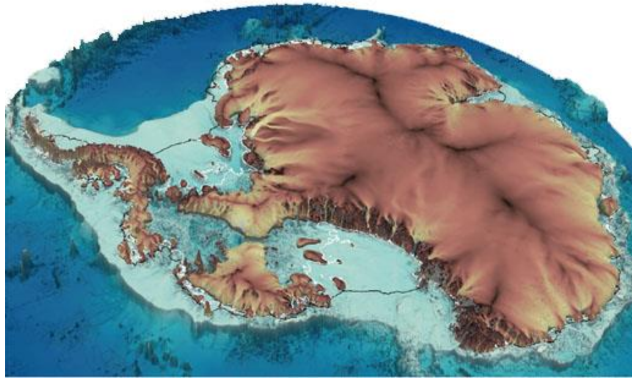
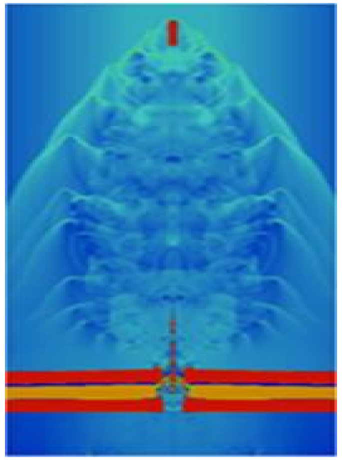
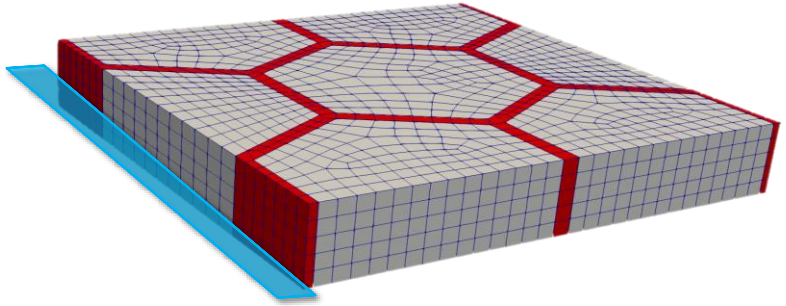
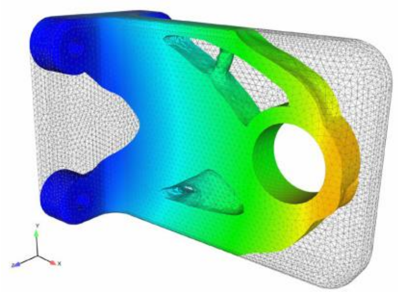




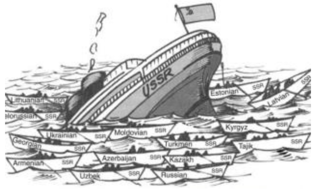




About me

1984

Born in
Moscow, USSR



Dissolution of
the USSR

1991

1992

Immigrated to U.S.
Settled in metro
Detroit area

1999

Naturalized as
U.S. citizen

Graduated High School
Started College at Penn

2002

2006

Graduated from Penn
(B.A., M.A. Mathematics)
Started Ph.D. at Stanford

Graduated from Stanford
(Ph.D. Comp. Math. Engng.)
Started Staff Scientist
Position at SNL

2011

Sandia National Laboratories

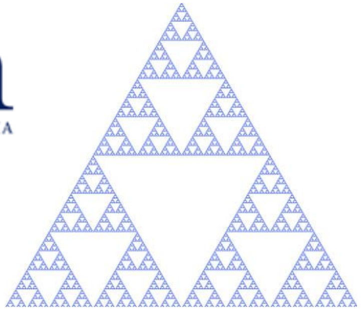
Education

Childhood:

- Had interest/aptitude in ***math/science***
- Both of my parents had been ***scientists*** in Moscow…
  …but when they came to U.S., they had to ***start over*** effectively ***at the bottom***
  - ➢ ***Failure*** was ***not an option for me***, having seen all the sacrifices my parents made trying to create a better future for me

2002-2006: University of Pennsylvania (B.A., M.A.)

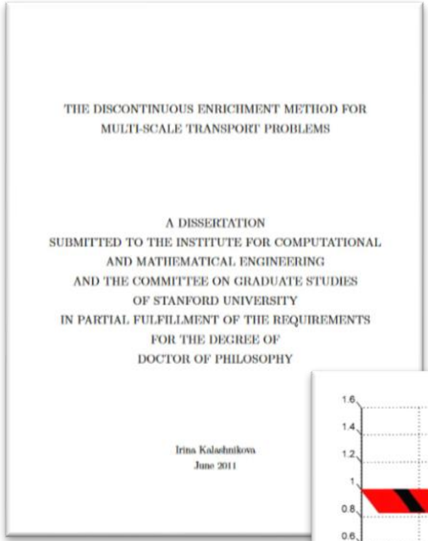
- Liked ***math*** but did not known what I wanted to do with it
- Majored in ***Mathematics*** with a minor in ***Actuarial Science***
  - ➢ Initially interested in career as an ***Actuary***
  - ➢ ***Internship*** at Watson Wyatt Worldwide → decided career as an Actuary is not for me
- Submatriculated into the ***Masters*** program in ***Mathematics***
  - ➢ Wanted to experience ***research/teaching***
  - ➢ ***Masters thesis*** on harmonic functions on the Sierpinski gasket → decided pure math is not for me



Education

2006-2011: Stanford University (Ph.D.)

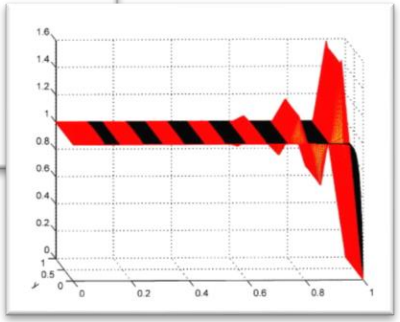
- Ph.D. in ***Computational & Mathematical Engineering (CME)***
  - ➢ Interdisciplinary applied/computational math program
  - ➢ ***Ph.D. advisor***: Prof. Charbel Farhat (Aero/Astro Dept. Chair)
  - ➢ Worked on new discretization method for solving ***advection-dominated (high-speed) flow problems***
  - ➢ Met my now ***husband***, Radek Tezaur
- Concurrently a ***Year-Round Graduate Technical Intern*** in ***Aerosciences Department*** at ***Sandia National Labs*** in New Mexico (2007-2011)
  - ➢ Spent ***4 summers*** in ***Albuquerque*** working on a project ***different*** from my Ph.D. thesis topic
  - ➢ Experience put national labs on the ***radar*** for me

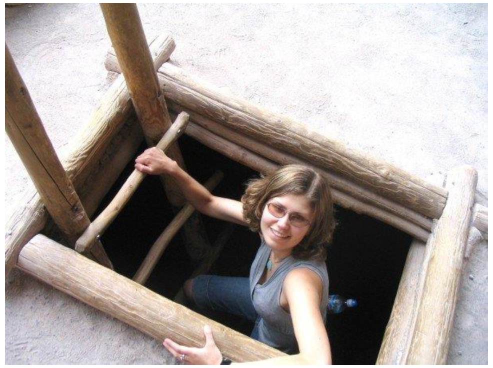

THE DISCONTINUOUS ENRICHMENT METHOD FOR MULTI-SCALE TRANSPORT PROBLEMS

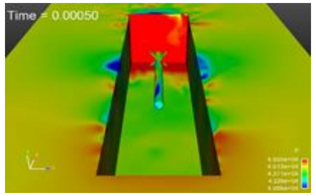
A DISSERTATION SUBMITTED TO THE INSTITUTE FOR COMPUTATIONAL AND MATHEMATICAL ENGINEERING AND THE COMMITTEE ON GRADUATE STUDIES OF STANFORD UNIVERSITY IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY

Irina Kalashnikova
June 2011

Stanford ENGINEERING

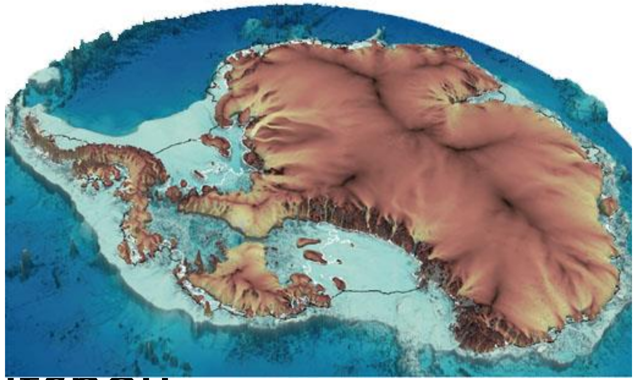






Sandia National Laboratories

Outline



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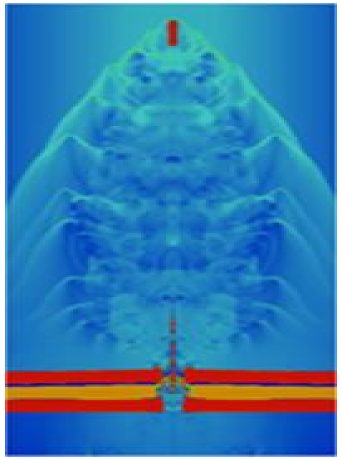

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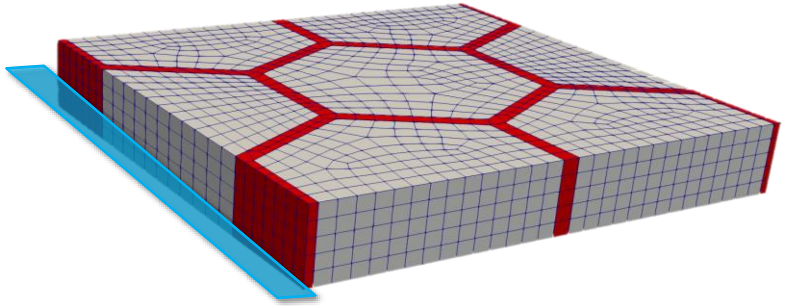
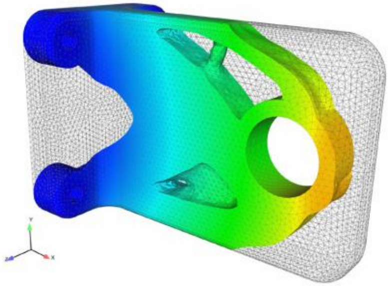




Career at Sandia National Laboratories

2007-2011:

- ***Year-Round Graduate Technical Intern***: Aerosciences Dept. (Albuquerque, NM)

2011-2014:

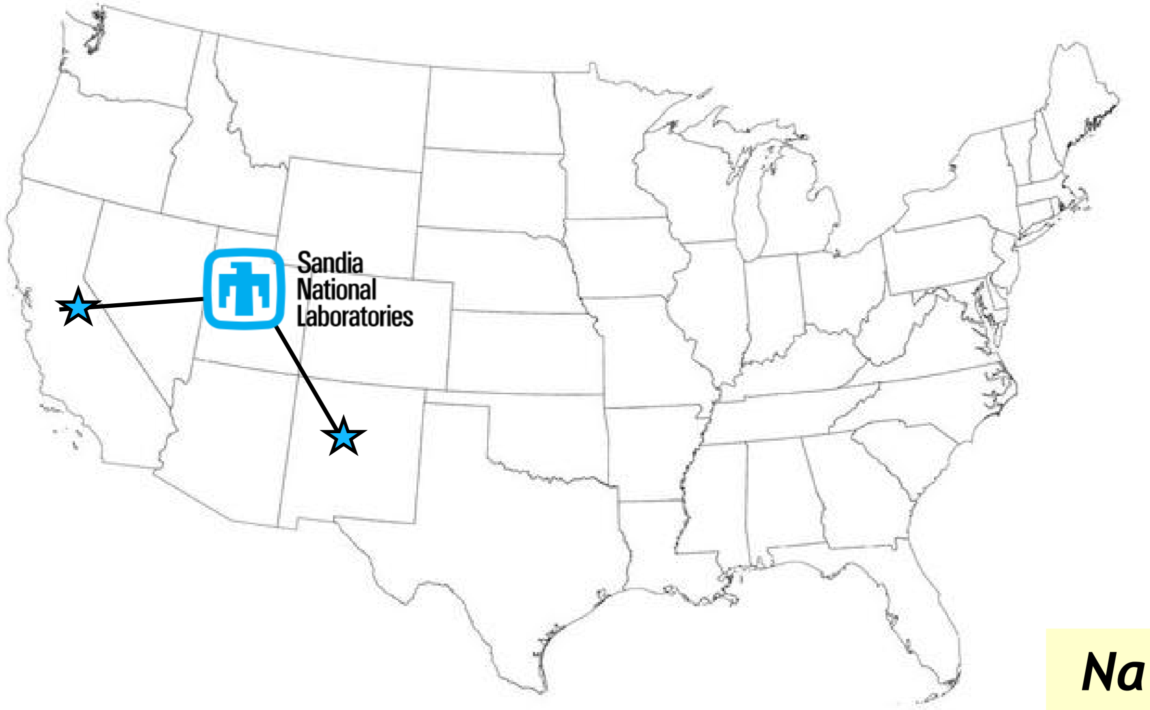
- ***Senior Member of Technical Staff***: Computational Math. Dept. (Albuquerque, NM)

2014-present:

- ***Principal Member of Technical Staff***: Quantitative Modeling & Analysis Dept. (Livermore, CA)
- Moved to California due to ***multi-body problem*** with my ***husband*** and two ***stepsons***

My research has focused on developing **algorithms & software** to enable **computational modeling** of complex **multi-scale & multi-physics** problems.

About Sandia National Laboratories (SNL)



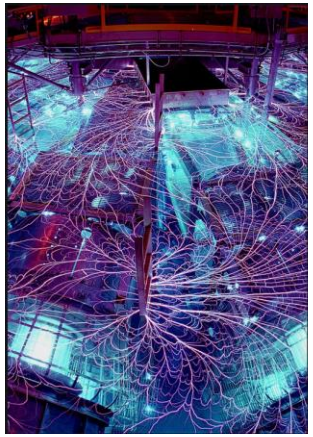
Sandia's **primary mission** is ensuring the U.S. nuclear arsenal is safe, secure and reliable, and can fully support our nation's deterrence policy

We have **programs** in the following areas:

- Nuclear Deterrence
- Defense Nuclear Nonproliferation
- National & Global Security
- Energy & Climate
- Advanced Science & Technology

National labs are in between academia and industry

- Sandia is a **multidisciplinary** national lab and Federally Funded Research & Development Center (FFRDC)
- Contractor for the U.S. DOE's National Nuclear Security Administration (**NNSA**)
- **Two main sites**: Albuquerque, NM and Livermore, CA (above)



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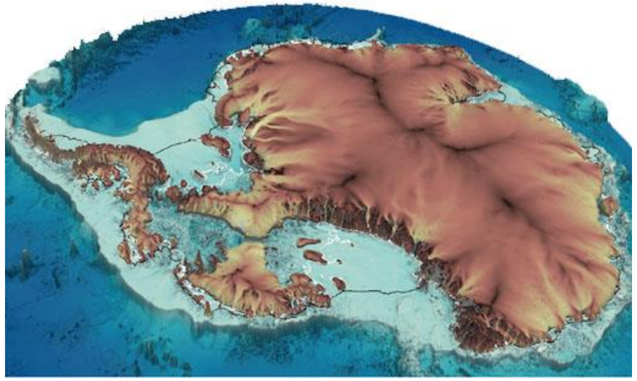
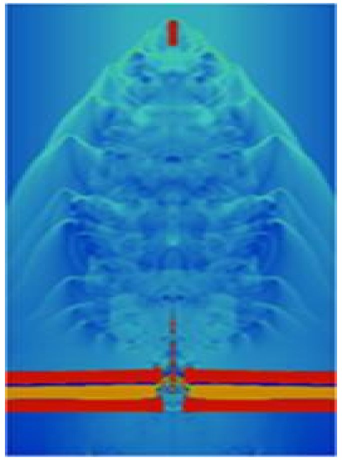
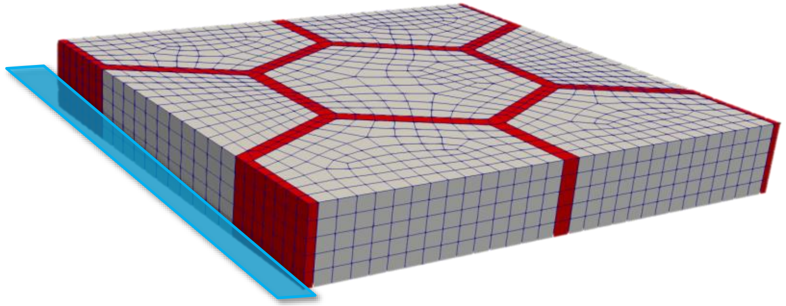
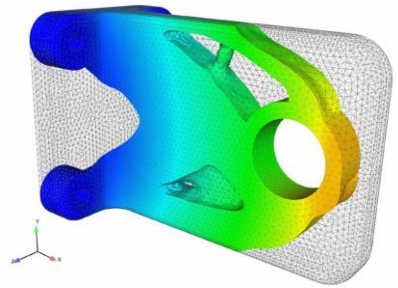








Physics-based computational modeling & simulation

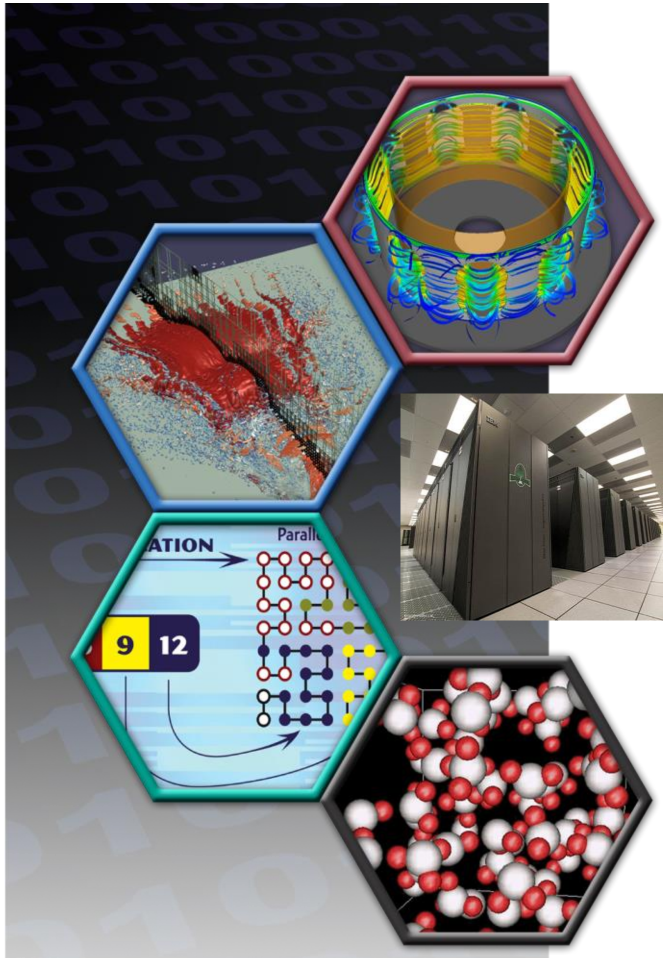


Image from SNL's Center for Computing Research (CCR) homepage

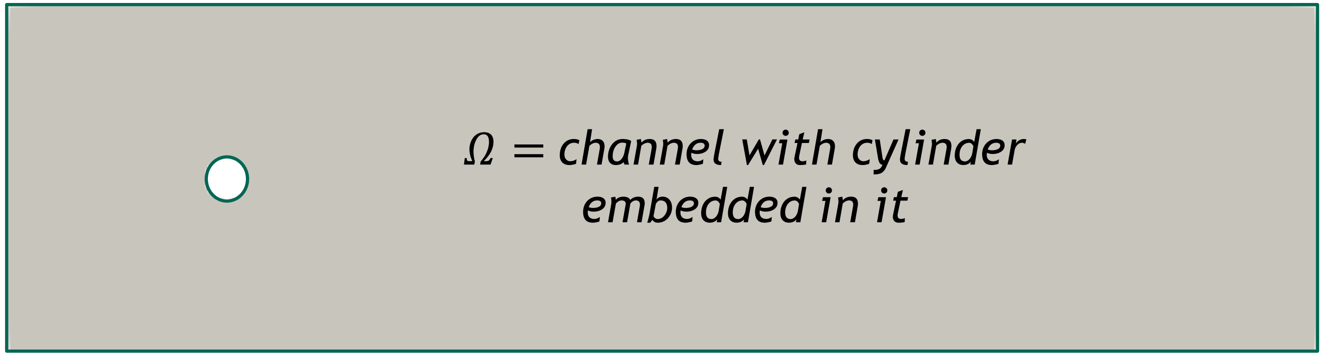
Computational science = mathematics + computer science + physics

- Physics-based computational mod/sim can ***replace*** and/or ***enhance*** laboratory/field experiments, which can be costly, dangerous and time-consuming
  - ➢ Allows one to explore and evaluate ***multiple configuration settings*** for engineering designs
- Physics-based computational mod/sim can help ***predict possible future scenarios*** of interest worldwide that cannot be studied experimentally (e.g., disease outbreaks, climate change)
  - ➢ Can provide ***actionable*** information to support ***public policy*** and ***decision making***
- Physics-based computational mod/sim is ***ubiquitous*** even ***outside the fields of science/engineering***
  - ➢ CGI in video games, movies
  - ➢ Animation (Dreamworks, Pixar, etc.)
  - ➢ Virtual reality

How physics-based computational mod/sim works

Computational science = mathematics + computer science + physics

- Start **physical geometry**, which we will refer to as the physical domain Ω



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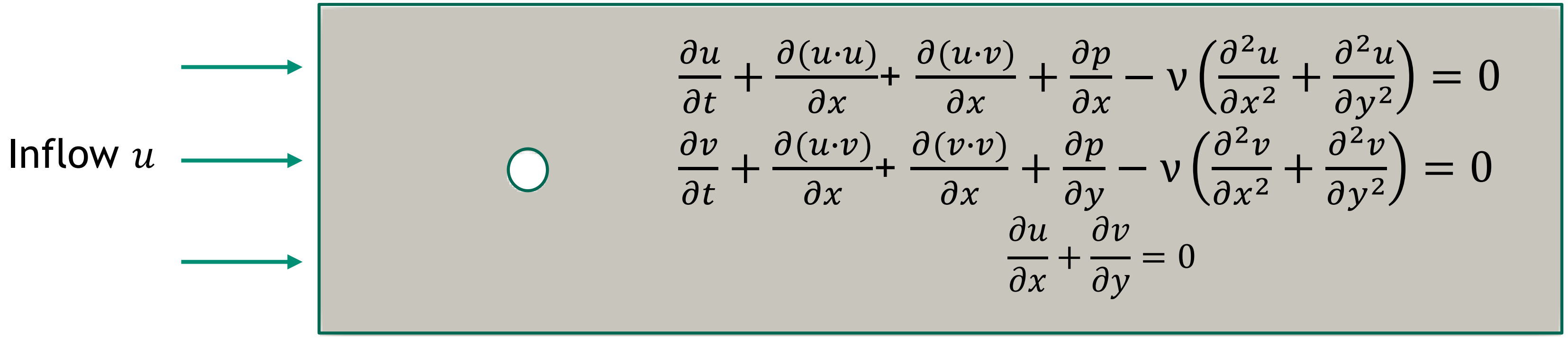

$$\frac{\partial u}{\partial t}+\frac{\partial(u\cdot u)}{\partial x}+\frac{\partial(u\cdot v)}{\partial x}+\frac{\partial p}{\partial x}-\nu\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right)=0$$

$$\frac{\partial v}{\partial t}+\frac{\partial(u\cdot v)}{\partial x}+\frac{\partial(v\cdot v)}{\partial x}+\frac{\partial p}{\partial y}-\nu\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}\right)=0$$

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0$$

Incompressible Navier-Stokes equations for fluid flow

- Write down the continuous equations (typically **partial differential equations**, or **PDEs**, + initial and boundary conditions) that describe the **physics** in/of Ω (e.g., fluid flow).
  - ➢ Often, this is a set of "**conservation laws**" (conservation of mass, momentum, energy).
  - ➢ Often it's **impossible** to solve the equations **analytically** – need computational modeling.

How physics-based computational mod/sim works

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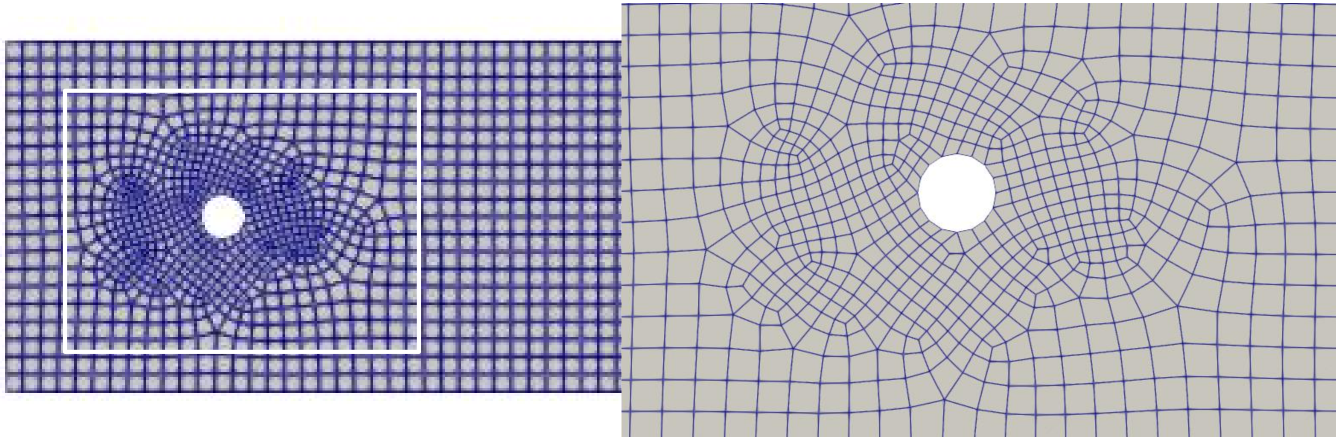

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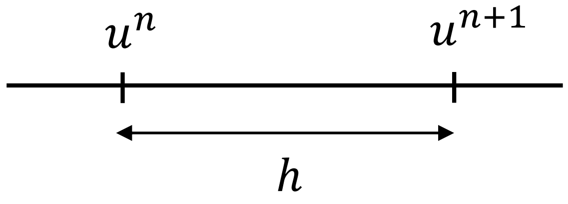
  - ➢ Often, this is a set of "**conservation laws**" (conservation of mass, momentum, energy).
  - ➢ Often it's **impossible** to solve the equations **analytically** - need computational modeling.
- Create a "**mesh**" (discrete representation) of the geometry, call it Ω_h (h = "mesh size")
  - ➢ Triangles, **quadrilaterals**, tetrahedra, hexahedra, etc.
  - ➢ As $h \to 0$, numerical solution → analytical solution.

How physics-based computational mod/sim works

Computational science = mathematics + computer science + physics

- "**Discretize**" the continuous equations on the mesh (approximate them in each grid cell), e.g.,

$$\frac{\partial u}{\partial x} \approx \frac{u^{n+1} - u^n}{h}$$



  - Common "**discretization methods**": finite differences, finite volumes and finite elements
  - Assemble contributions in each cell into large **discrete (nonlinear) global system**

$$\begin{cases} \frac{\partial u}{\partial t} + \frac{\partial (u \cdot u)}{\partial x} + \frac{\partial (u \cdot v)}{\partial x} + \frac{\partial p}{\partial x} - \nu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = 0 \\ \frac{\partial v}{\partial t} + \frac{\partial (u \cdot v)}{\partial x} + \frac{\partial (v \cdot v)}{\partial x} + \frac{\partial p}{\partial y} - \nu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) = 0 \\ \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \end{cases}$$

Continuous PDEs

$$\Rightarrow$$

$$\begin{pmatrix} \boldsymbol{M} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{pmatrix} \begin{pmatrix} \dot{\boldsymbol{u}} \\ \dot{\boldsymbol{p}} \end{pmatrix} + \begin{pmatrix} \boldsymbol{K_{uu}(u)} & \boldsymbol{K_{up}} \\ \boldsymbol{K_{up}} & \boldsymbol{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{u} \\ \boldsymbol{p} \end{pmatrix} = \begin{pmatrix} \boldsymbol{0} \\ \boldsymbol{0} \end{pmatrix}$$

Discrete PDEs

- **Code** up the discretized system of equations.

How physics-based computational mod/sim works

Computational science = mathematics + computer science + physics

- **Solve** the large discrete system to obtain an **approximate solution** to your original equations

Known as **"Incompressible Flow around a Cylinder"** or **"Vortex Shedding"** problem*

* From Albany open-source multi-physics finite element code: www.github.com/SNLComputation/Albany

How physics-based computational mod/sim works

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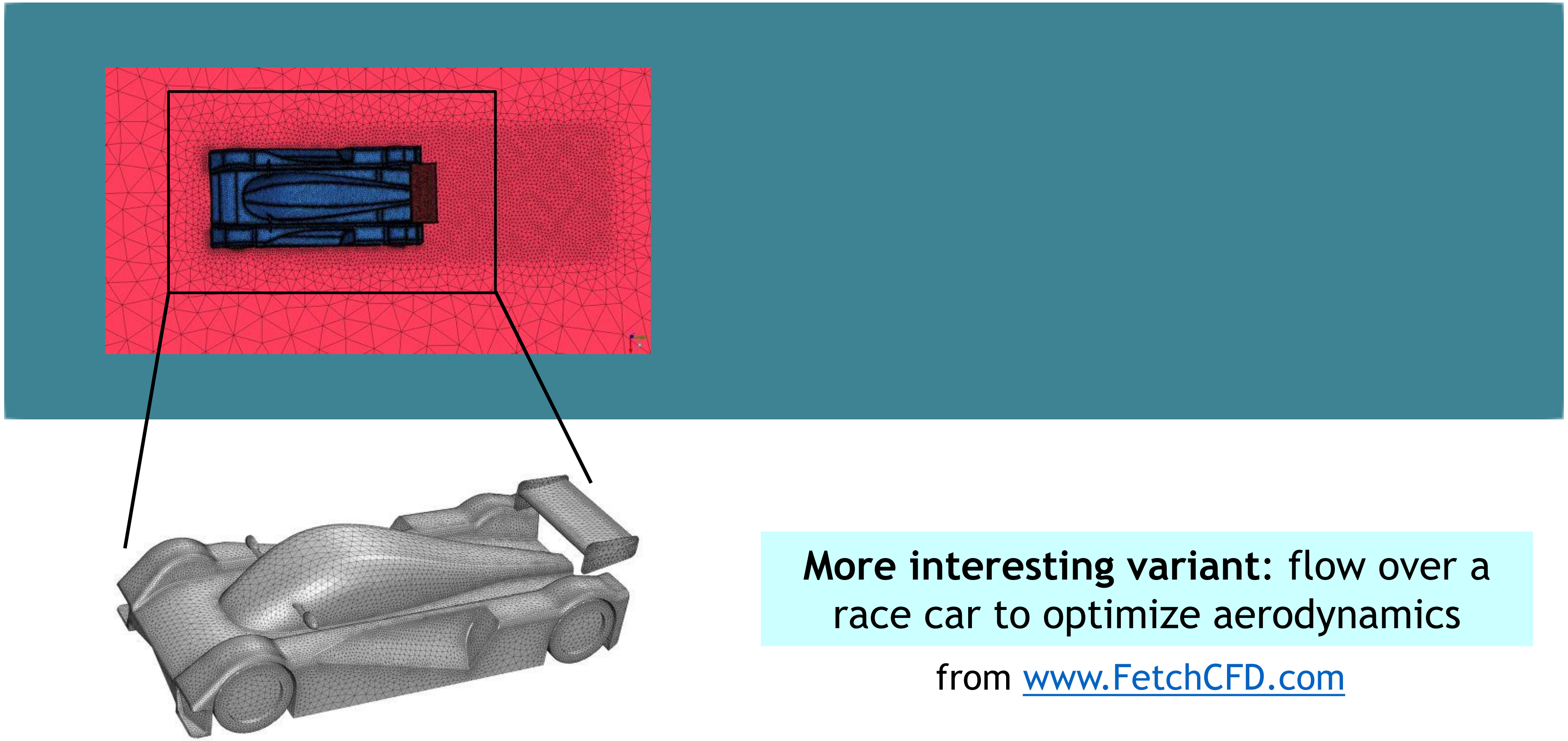


More interesting variant: flow over a race car to optimize aerodynamics

from www.FetchCFD.com

What do computational scientists work on?

Discretizations

- ***Meshing*** technologies for arbitrarily complex 3D geometries, including ***mesh adaptation***
- Methods to handle ***difficult features*** (sharp gradients, shocks, discontinuities, fracture, failure, etc.)
- Methods to ensure ***stability***, ***consistency***, ***accuracy***, ***convergence***
- ***Load balancing*** algorithms for parallel processing
- ***Model reduction***

My area of expertise,
though I dabble in many of the others…

Solver technologies

- Efficient ***linear*** and ***nonlinear solvers*** for problems arising in discretizations

Analysis approaches

- ***Optimization*** algorithms
- ***Uncertainty Quantification (UQ)***
- ***Data assimilation*** methods (calibrating models using observational data)
- ***Data analytics*** approaches (including ***machine-learning***)

Computational science is ***much more*** than just math + CS + physics!

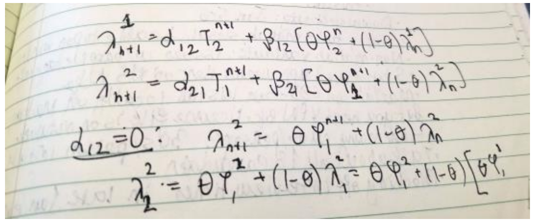
Enabling software technologies

- Libraries providing ***performance portability*** to new HPC architectures
- ***GPU*** computing, ***quantum*** computing
- Writing scalable and efficient ***HPC codes***

…including a good deal of software development

What does a computational scientist at SNL do?

Fundamental research in computational mathematics ("pencil-and-paper"):



- Develop ***new algorithms*** to ***enable new capabilities***, improve existing algorithms to provide ***better performance*** and/or extend algorithmic capabilities
- Prove ***theoretical properties*** about algorithms

Software development:

- Software to ***prototype*** new algorithms
- Develop/maintain ***"production" software*** (both open-source and Sandia proprietary codes)

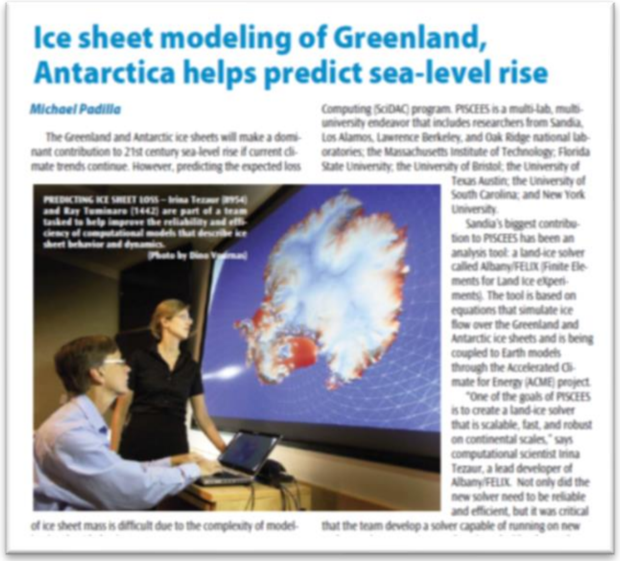
Proposal writing:

- ***Seek funding*** (internal and external) for new research ideas

Publicizing R&D and outreach:

- Conference/University ***presentations/outreach***
- Journal ***publications***
- General-audience ***article*** interviews


ELSEVIER
Computer Methods in Applied Mechanics and Engineering
Volume 319, 1 June 2017, Pages 19-51
The Schwarz alternating method in solid mechanics
Alejandro Mota [a], Irina Tezaur [b], Coleman Alleman [a]


Ice sheet modeling of Greenland, Antarctica helps predict sea-level rise
Michael Padilla

Supporting scientific studies:

- ***Run software*** on HPC architectures
- ***Support*** domain scientists' ***science runs***

Collaborative meetings:

- Support ***collaborations*** in the above

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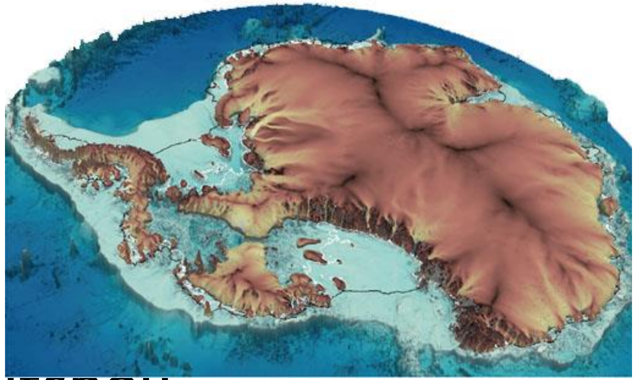
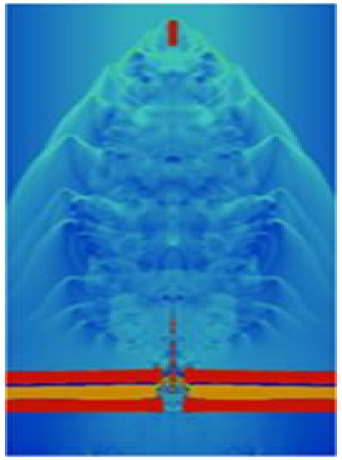
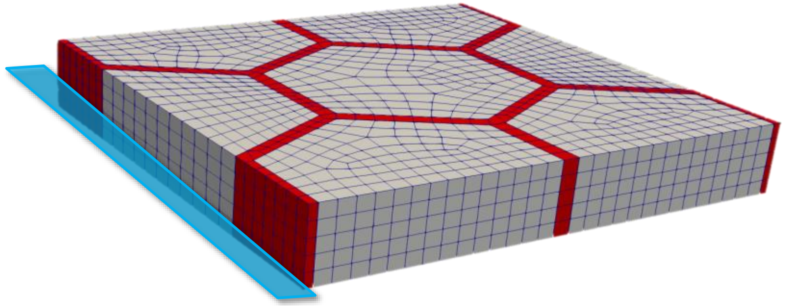
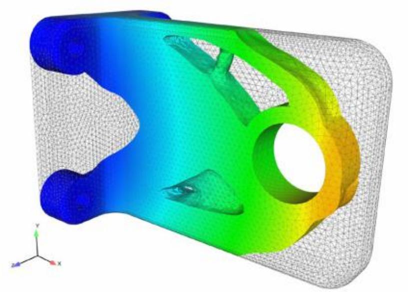








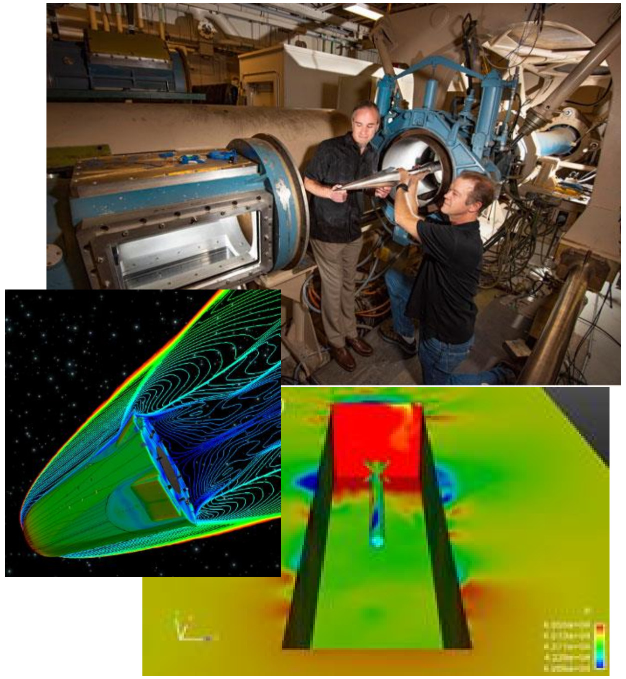
Modeling & simulation project highlights

My research focuses on improving ***computational modeling & simulation*** of complex ***multiscale & multiphysics*** problems of interest to the SNL, DOE and US nuclear deterrence, national security and climate missions.

Pressio

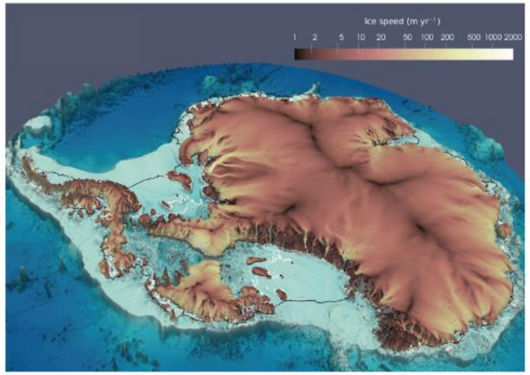
Trilinos

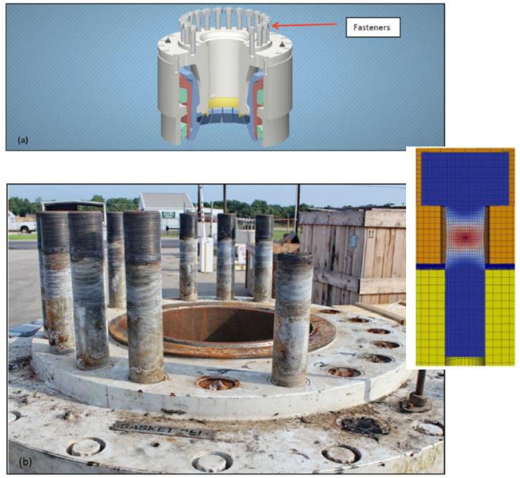
Albany



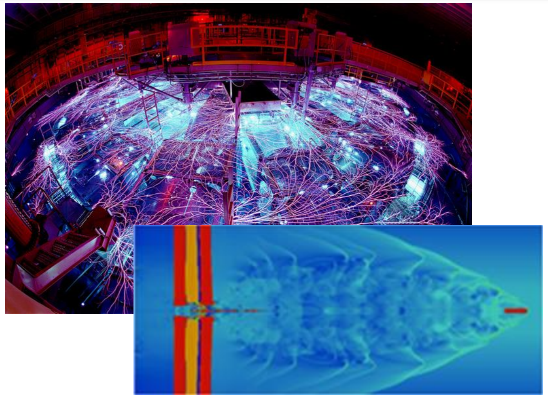
Model Order Reduction of Captive-Carry and Re-Entry Environments

Climate Modeling





Multi-Scale Methods for System/ Component Failure Analyses



Shock Multi-Physics for Z-Machine Implosion and Multi-material impact

SIERRA

E3SM
Energy Exascale Earth System Model

ALEGRA

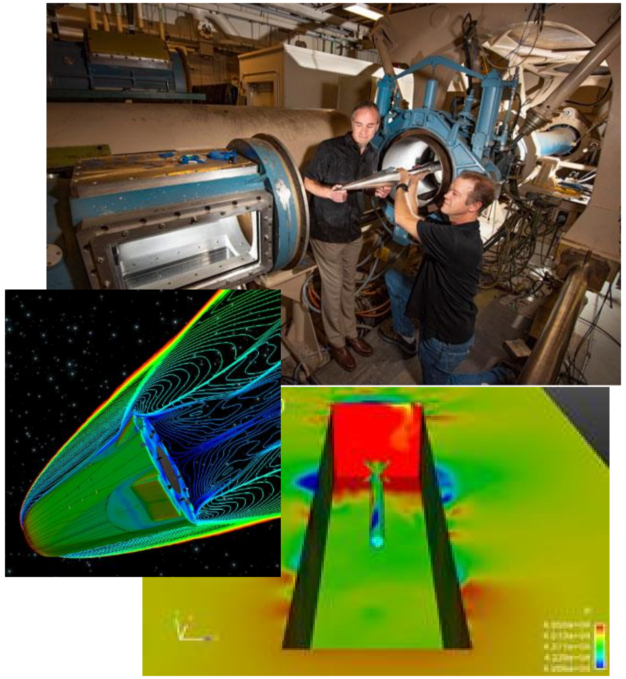
Modeling & simulation project highlights

My research focuses on improving ***computational modeling & simulation*** of complex ***multiscale & multiphysics*** problems of interest to the SNL, DOE and US nuclear deterrence, national security and climate missions.

Pressio

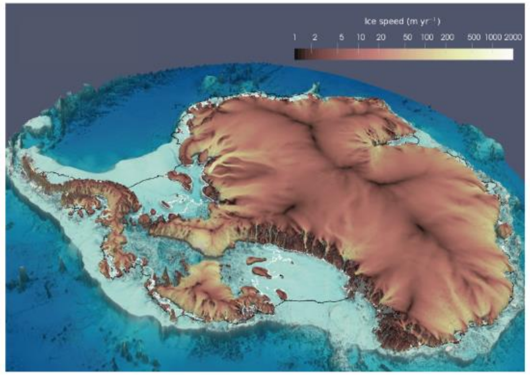
Trilinos

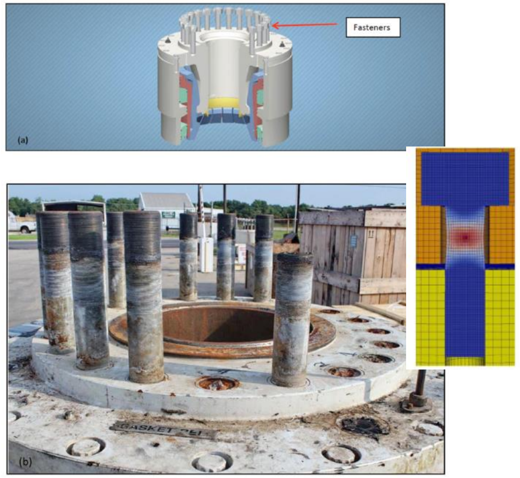
Albany



Model Order Reduction of Captive-Carry and Re-Entry Environments

Climate Modeling





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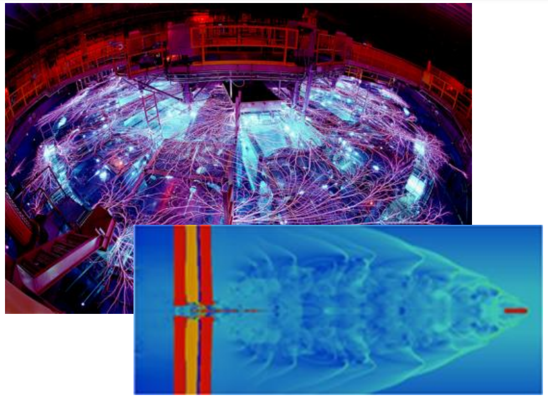


Shock Multi-Physics for Z-Machine Implosion and Multi-material impact

SIERRA

E3SM Energy Exascale Earth System Model

ALEGRA

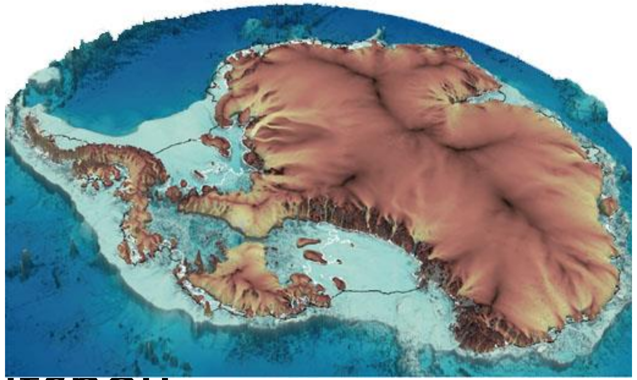
Deep dives!

Outline

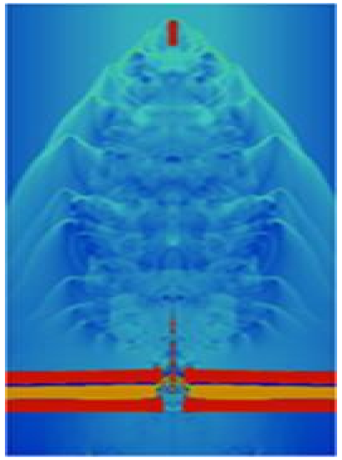
1. A little bit about me and my background

2. A little bit about Sandia National Laboratories

3. Physics-based computational modeling & simulation in a nutshell

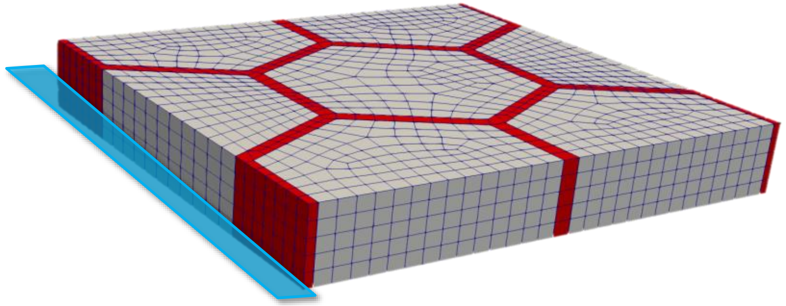


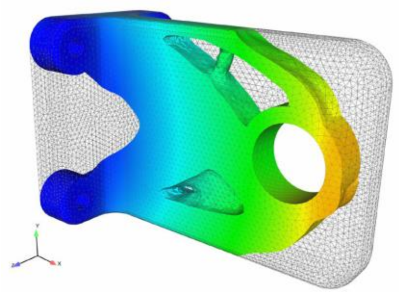
4. **A few research highlights**
    - **Ice sheet modeling**
    - Multi-material impact simulations



5. Career & educational tips

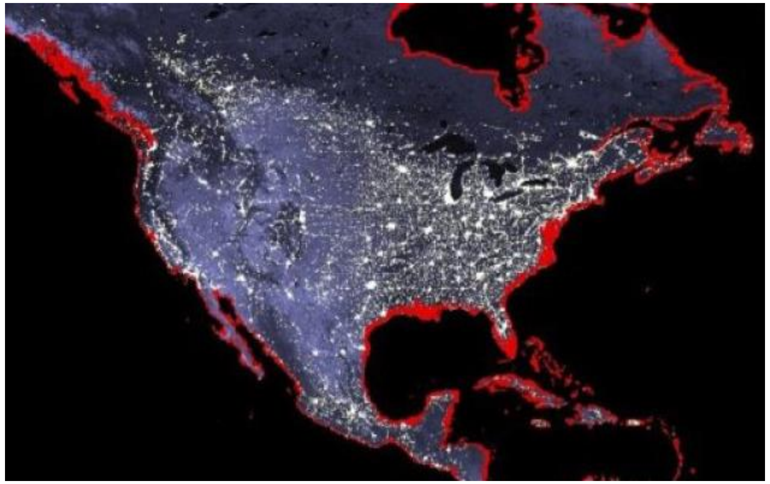
6. Question & answer (Q&A)



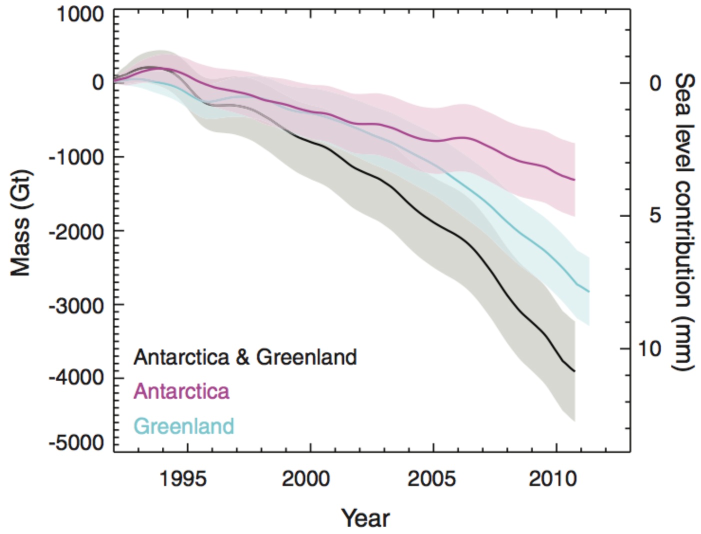


Ice sheet modeling: motivation

- **Climate change** has been declared a "**national security issue**" by President Joe Biden.
- Global mean sea-level is rising at the rate of **3.2 mm/year** and this rate is **increasing**, with the latest studies suggesting a possible increase in sea-level of **0.3-2.5 m** by 2100.
  - ➢ Due to **melting of the polar ice sheets** (Greenland, Antarctica).
- **Full deglaciation***: sea level could rise up to ~65 m (Antarctica: 58 m, Greenland: 7 m)



Map of North America showing 6 m SLR (NASA)

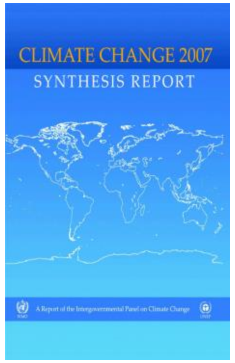


Total mass loss of ice sheets b/w 1992-2011

Modeling of ice sheet dynamics is **essential** for providing estimates of expected **sea-level change**, towards understanding the local/global effects of **climate change**.

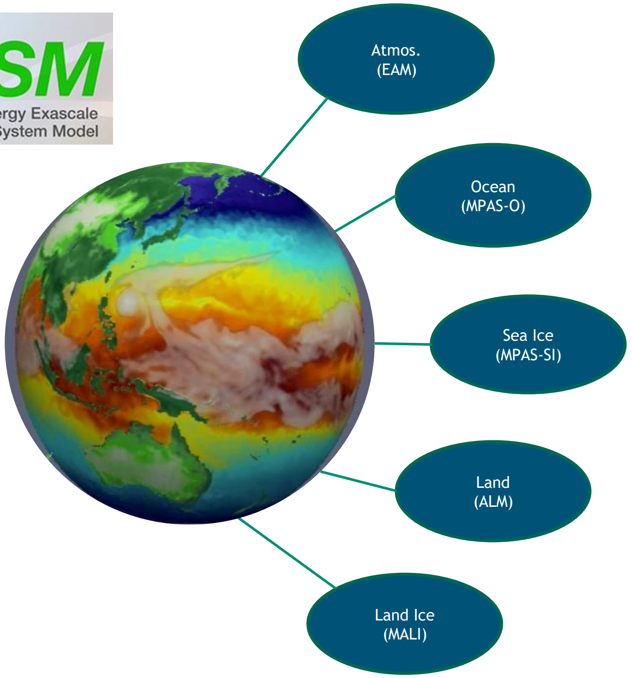
*Estimates given by Prof. Richard Alley of Penn State.

Ice sheet modeling: ProSPect* project



Motivation: *2007 Intergovernmental Panel on Climate Change (IPCC) Assessment Report* ***declined*** *to include estimates of future sea-level change from ice sheet dynamics due to* ***deficiencies*** *in ice sheet models.*

E3SM Energy Exascale Earth System Model



We are developing a ***next-generation*** land ice model known as ***MALI*** that will provide ***actionable predictions*** of 21st century ***sea-level change*** and supports ***national security missions*** as part of DOE Energy Exascale Earth System Model (E3SM).

Probabilistic Sea-Level Projections from Ice Sheet and Earth System Models (ProSPect):** ***multi-institution project involving mathematicians, climate scientists, and computer scientists.

Ice sheet modeling: equations and codes

Momentum Balance: *First-Order Stokes* PDEs

$$\begin{cases} -\nabla \cdot (2\mu \dot{\boldsymbol{\epsilon}}_1) = -\rho g \dfrac{\partial s}{\partial x} \\ -\nabla \cdot (2\mu \dot{\boldsymbol{\epsilon}}_2) = -\rho g \dfrac{\partial s}{\partial y} \end{cases}, \quad \text{in } \Omega$$

with ***Glen's law*** viscosity $\mu = \frac{1}{2} A(T)^{-\frac{1}{3}} \left(\frac{1}{2} \sum_{ij} \dot{\boldsymbol{\epsilon}}_{ij}{}^2\right)^{\left(-\frac{2}{3}\right)}$

Energy Balance: *temperature* advection-diffusion PDE

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) - \rho c \boldsymbol{u} \cdot \nabla T + 2 \dot{\boldsymbol{\epsilon}} \boldsymbol{\sigma}$$

Conservation of Mass: *thickness* evolution PDE

$$\frac{\partial H}{\partial t} = -\nabla \cdot (\overline{\boldsymbol{u}} H) + \dot{b}$$

Codes:

Albany =multi-physics PDE code*

Albany Land-Ice (ALI)

Trilinos

MALI = MPAS + ALI

MPAS Model for Prediction Across Scales

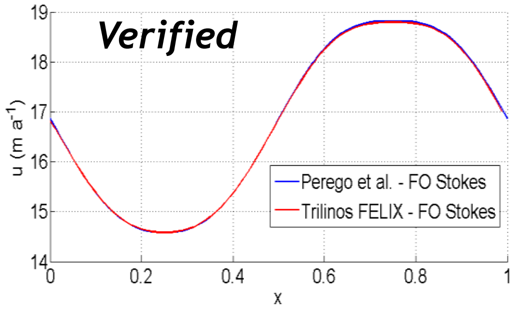
Model for Prediction Across Scales

E3SM Energy Exascale Earth System Model

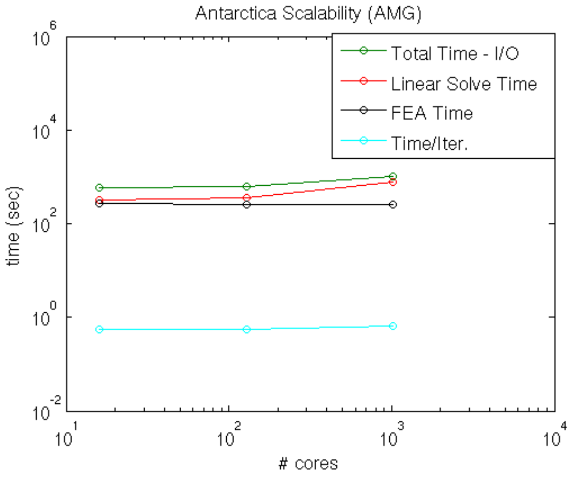
* https://github.com/SNLComputation/Albany

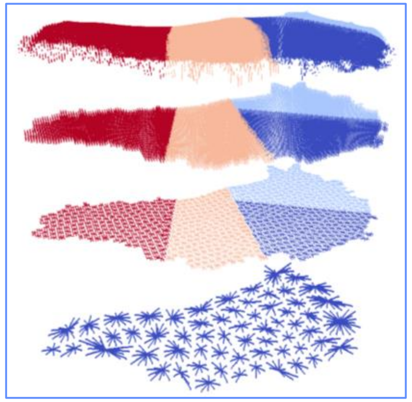
Ice sheet modeling: key capabilities of MALI

Component-based **code development approach enabled** ***rapid*** **development of MALI code.**

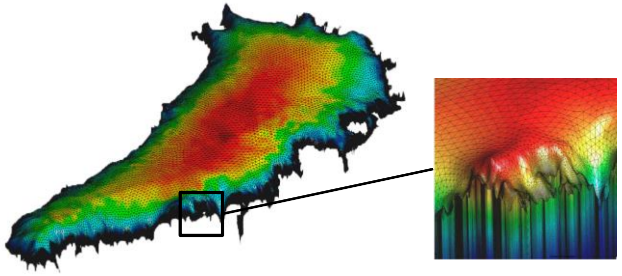


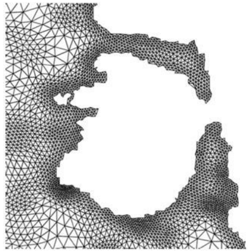
Scalable & fast multi-level linear solver (to 1.12B dofs, 16K cores)



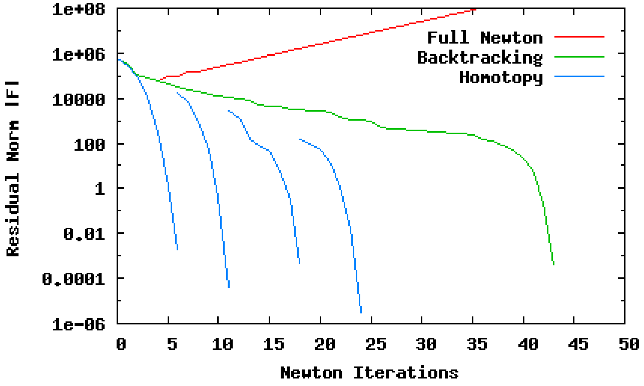


Unstructured meshes with real data





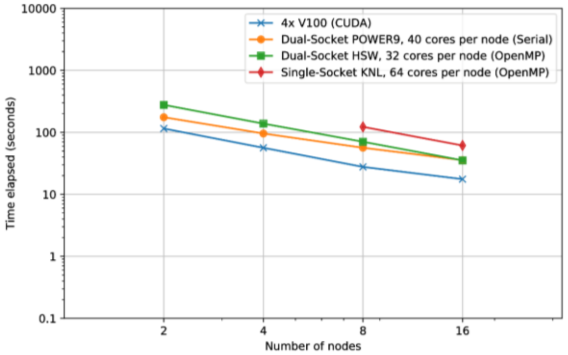
Robust non-linear solver with automatic differentiation and homotopy continuation



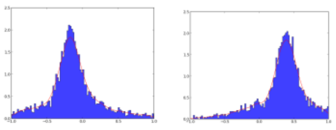
Ice sheet modeling: key capabilities of MALI

MALI is equipped with ***advanced analysis*** and ***next-generation*** capabilities.

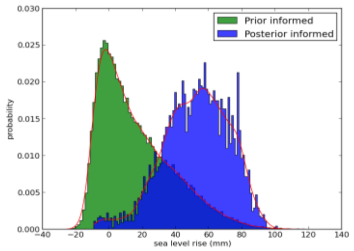
Performance portability to new architecture machines (multi-core, many-core, GPUs) using *Kokkos Trilinos* library and programming model



Uncertainty quantification algorithms and workflow for sea-level change is being developed



Step 1: Bayesian Calibration



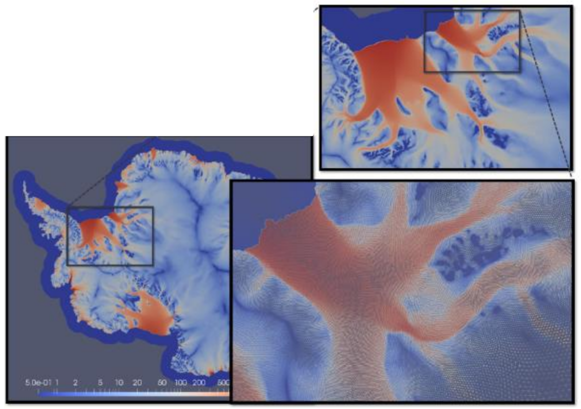
Step 2: Uncertainty propagation

PDE-constrained optimization for generating ice sheet initial conditions

$$\min_{\beta,H} \left(\frac{1}{2} \alpha_v \int_{\Gamma_{top}} |\boldsymbol{u} - \boldsymbol{u}^{obs}|^2 ds \right)$$

s.t. FO Stokes PDEs

Objective: find ice sheet initial state that matches observations, matches present-day geometry and is in "equilibrium" with climate forcings.

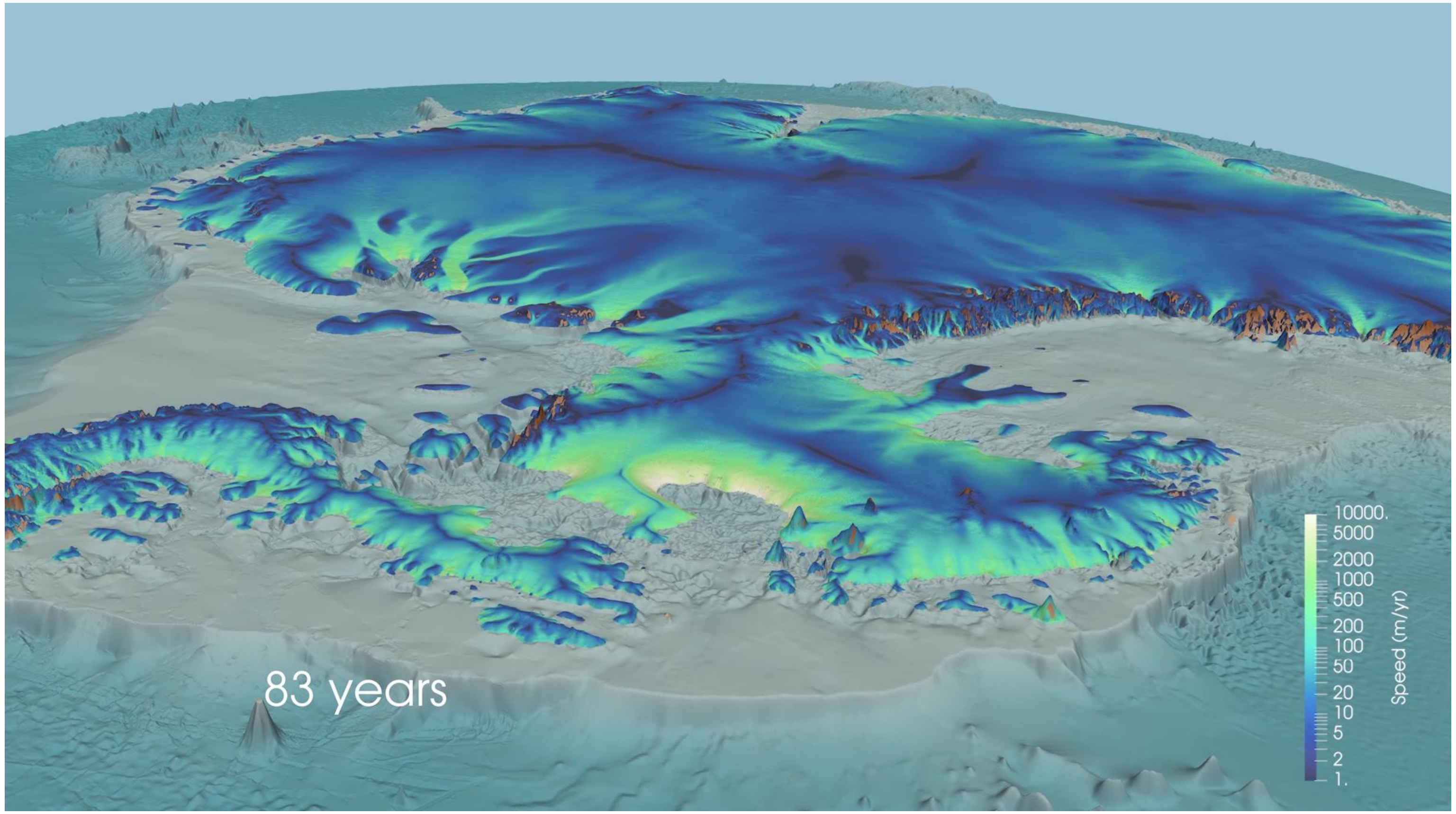


We have inverted for up to ***1.6M parameters***.

Ice sheet modeling: ABUMIP* simulation

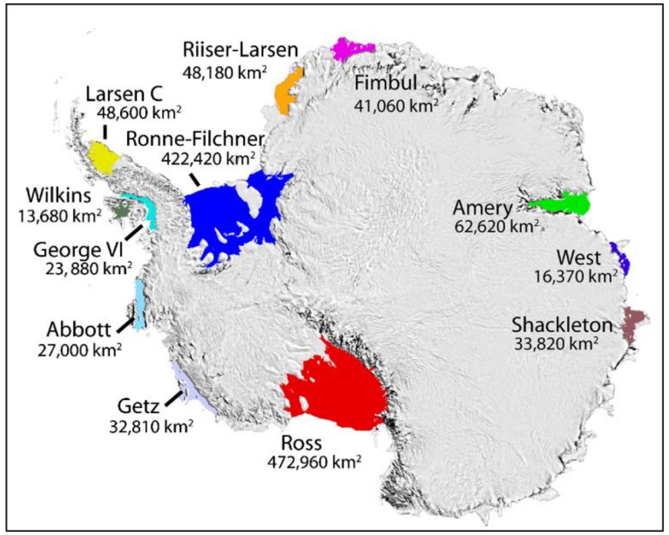
Basic idea: instantaneously remove all ice shelves and see what happens in the next 200 years, preventing any floating ice from ever forming again

* Antarctic BUttressing Model Intercomparison Project



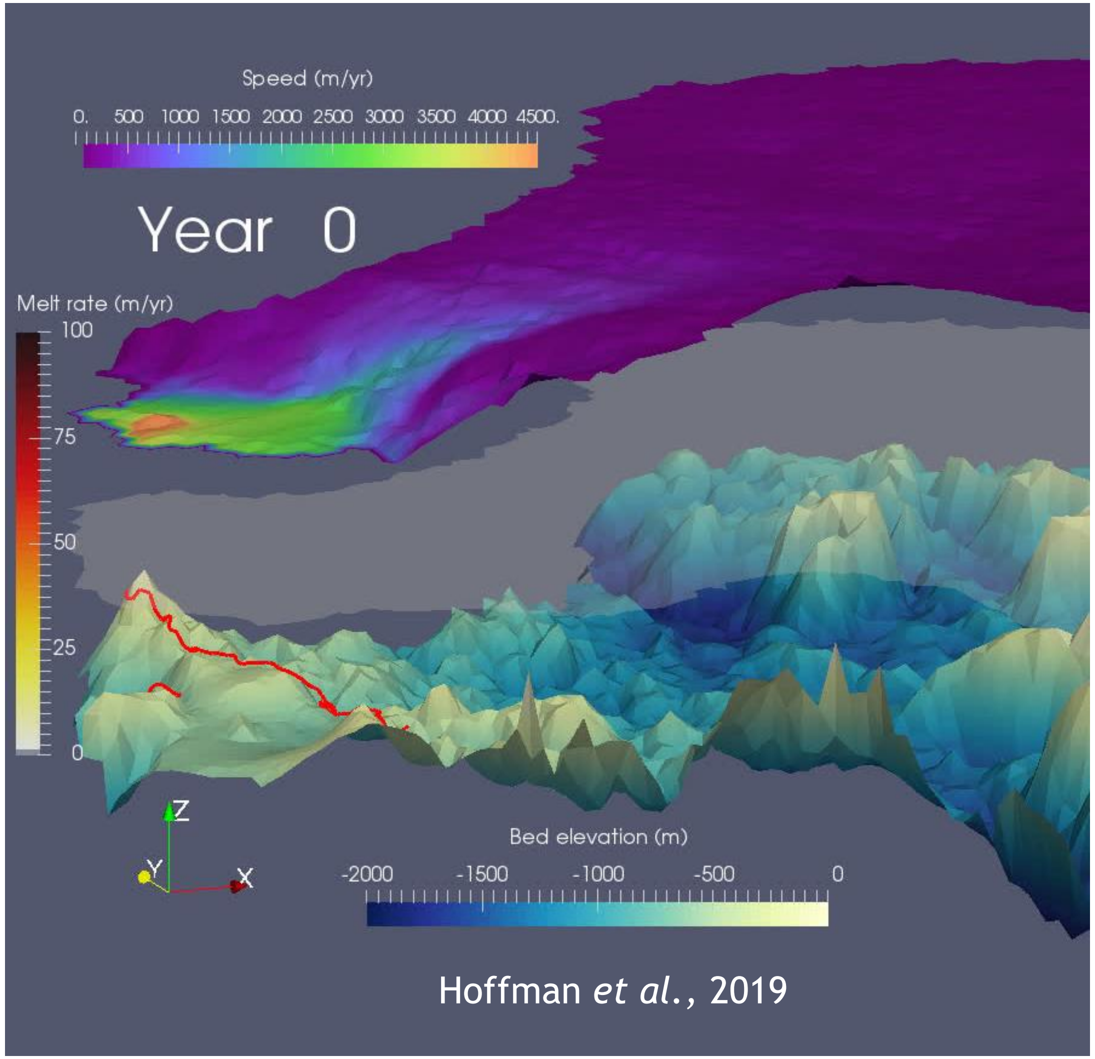
Provides an ***extreme upper bound*** on SLR contributions from Antarctica

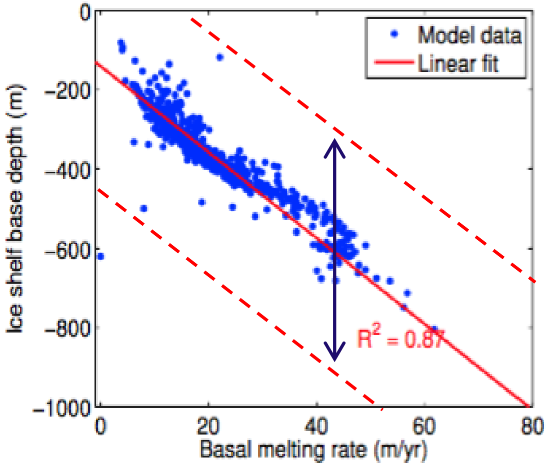
~32M unknowns solved for on **6400 procs**, with average model throughput of **~120 simulated yrs/wall clock day.**



https://www.youtube.com/watch?v=Wt0TvNjYsOs&feature=youtu.be

Ice sheet modeling: Thwaites glacier simulation





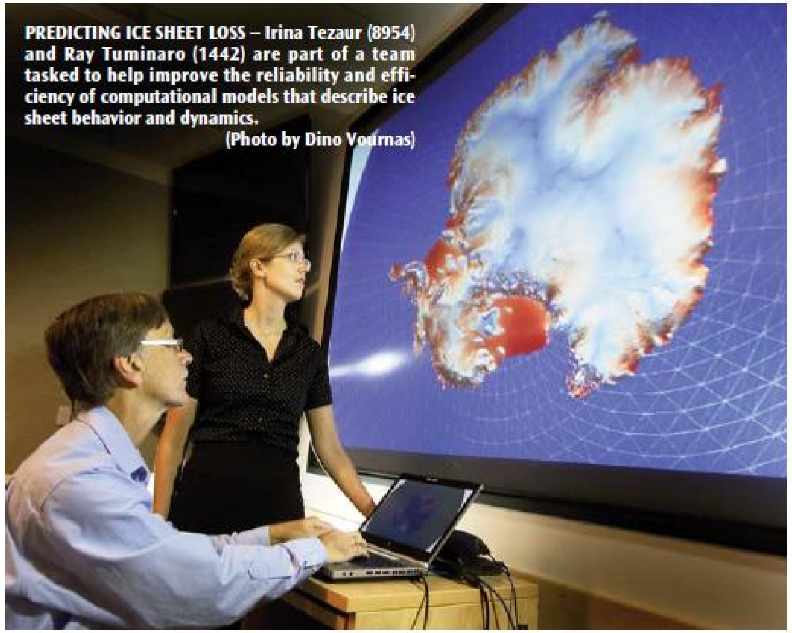
- Movie shows ***Thwaites Glacier*** retreat simulation under parameterized submarine melting.
- 250 year ***regional simulation*** with "present day" initial condition.
- Investigate importance of ***CDW* depth changes*** due to climate variability.
- When ***climate variability*** in sub-shelf forcing is accounted for, we get a ***distribution*** of possible SLR curves.

Ice sheet modeling: In-the-News*

Ice sheet modeling of Greenland, Antarctica helps predict sea-level rise

Michael Padilla

The Greenland and Antarctic ice sheets will make a dominant contribution to 21st century sea-level rise if current climate trends continue. However, predicting the expected loss of ice sheet mass is difficult due to the complexity of modeling ice sheet behavior.



PREDICTING ICE SHEET LOSS – Irina Tezaur (8954) and Ray Tuminaro (1442) are part of a team tasked to help improve the reliability and efficiency of computational models that describe ice sheet behavior and dynamics. (Photo by Dino Vournas)

Computing (SciDAC) program. PISCEES is a multi-lab, multi-university endeavor that includes researchers from Sandia, Los Alamos, Lawrence Berkeley, and Oak Ridge national laboratories; the Massachusetts Institute of Technology; Florida State University; the University of Bristol; the University of Texas Austin; the University of South Carolina; and New York University.

Sandia's biggest contribution to PISCEES has been an analysis tool: a land-ice solver called Albany/FELIX (Finite Elements for Land Ice eXperiments). The tool is based on equations that simulate ice flow over the Greenland and Antarctic ice sheets and is being coupled to Earth models through the Accelerated Climate for Energy (ACME) project.

"One of the goals of PISCEES is to create a land-ice solver that is scalable, fast, and robust on continental scales," says computational scientist Irina Tezaur, a lead developer of Albany/FELIX. "Not only did the new solver need to be reliable and efficient, but it was critical that the team develop a solver capable of running on new and emerging computers, and equipped with advanced

ProSPect has been a high-profile project for SNL with lots of **general-audience articles.**

RAPID DEVELOPMENT OF AN ICE SHEET CLIMATE APPLICATION USING THE COMPONENTS-BASED APPROACH

ANDREW SALINGER, PI
IRINA TEZAUR
MAURO PEREGO
RAYMOND TUMINARO
Sandia National Labs

STEPHEN PRICE
Los Alamos National Labs

PROCESSING HOURS
1,000,000

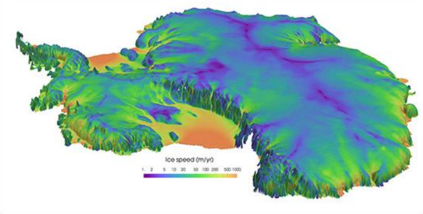
agsalin@sandia.gov

"As computational scientists with expertise in math and algorithms, it is challenging to get deep enough into a new science application area to make an impact. This team has made a sustained effort in learning about ice sheets and building relationships with climate scientists, and has been rewarded seeing our code on the critical path of DOE's climate science program."

– Andy Salinger

Climate

A land-ice simulation code



An Albany/FELIX simulation of Antarctica shows surface velocities draped over a surface topography computed on a variable resolution mesh.

As part of the five-year multi-institution DOE/SciDAC [Scientific Discovery Through Advanced Computing] project PISCEES, Sandia has developed a land-ice simulation code that has been integrated into DOE's Accelerated Climate Model for Energy earth system model for use in climate projections. The Albany/FELIX code enables the calculation of initial conditions for land-ice simulations, critical for stable and accurate dynamic simulations of ice sheet evolution and the quantification of uncertainties in 21st century sea level rise. With NASA, the team has successfully validated simulations in comparison to actual Greenland ice sheet measurements. (8900,1400)

CleanTechnica

Forecasting, Not Fearing, Sea-Level Rise

August 28th, 2016 by Robyn Purchia

This week, the *Washington Post* reported a widening 80-mile crack threatening one of Antarctica's biggest ice shelves. A large chunk of Larsen C, the most northern major ice shelf, may break off in the coming years.

Of course, the probable loss of Larsen C is a terrifying reminder that climate change is real and happening now. But what consequence will it have on Antarctic glaciers and sea-level rise? Researchers know ice shelves have a buttressing effect on interior ice because they restrain the flow of glaciers from the land to the sea. However, researchers can't predict how the glaciers will behave once the shelf is gone.

How to Fit a Planet Inside a Computer: Developing the Energy Exascale Earth System Model

JULY 12, 2018

Home » How to Fit a Planet Inside a Computer: Developing the Energy Exascale Earth System Model

The Earth was apparently losing water.

Ruby Leung, a scientist from the Department of Energy's (DOE) Pacific Northwest National Laboratory (PNNL), and her team were baffled by their results.

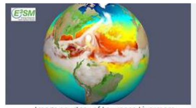


Image courtesy of Lawrence Livermore National Laboratory

* Article URLs can be found on my website: https://www.sandia.gov/~ikalash

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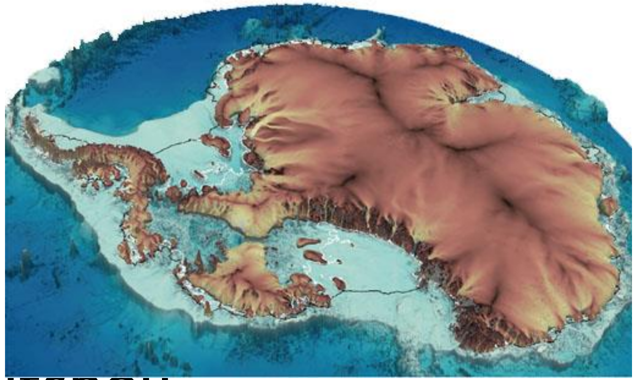
2. A little bit about Sandia National Laboratories



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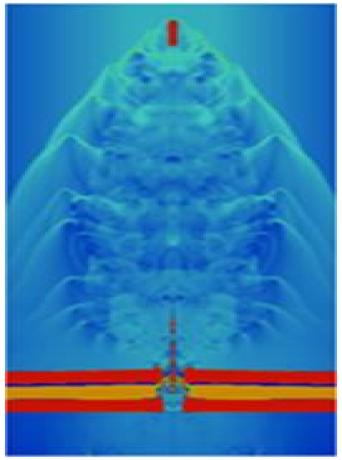
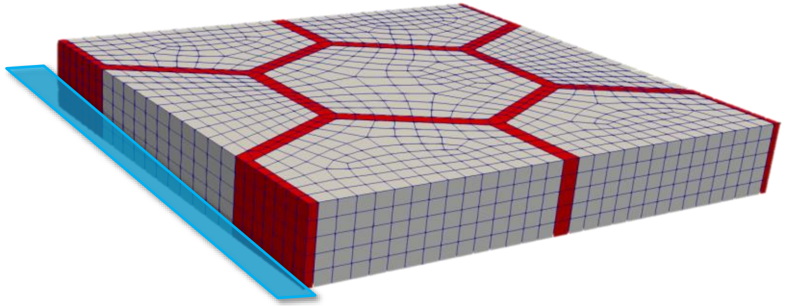
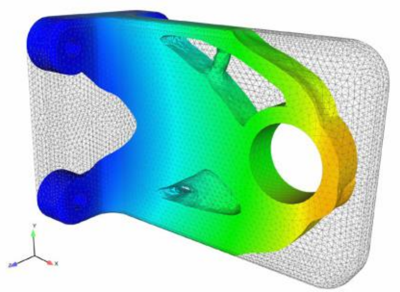


4. **A few research highlights**
   - Ice sheet modeling
   - **Multi-material impact simulations**

5. Career & educational tips

6. Question & answer (Q&A)





Multi-material impact simulations: motivation

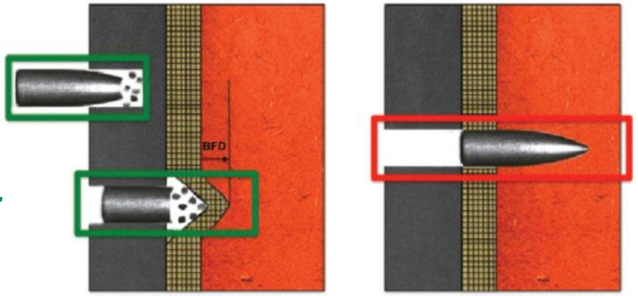
ALEGRA: a multi-material ALE (Arbitrary Lagrangian-Eulerian) **finite element** code that models large distortions and shock propagation in multiple materials.

ALEGRA can simulate:

- Large deformations
- Strong shock dynamics
- Magnetohydrodynamics (MHD)*
- Electromechanics
- Multi-material impact

Highlight

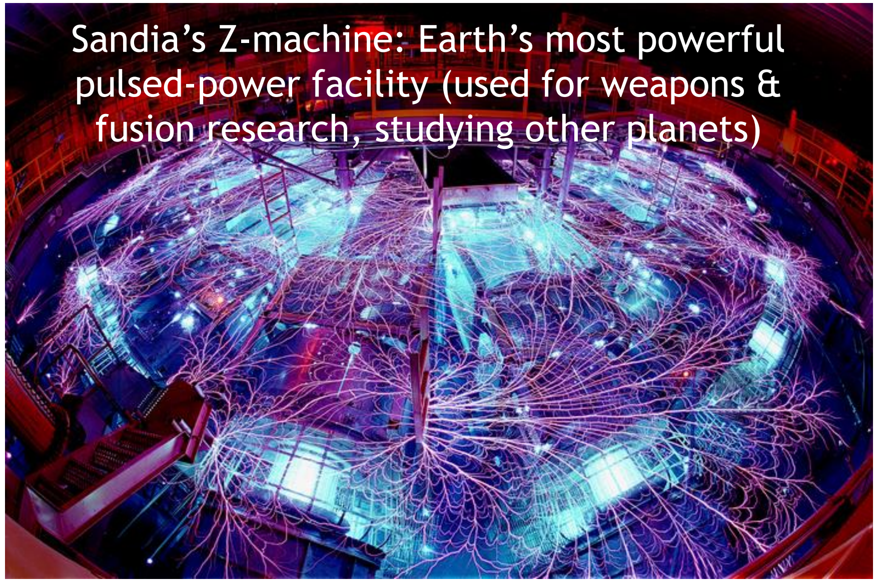
- Detonations



* The study of the magnetic properties and behavior of electrically conducting fluids (e.g., plasmas).

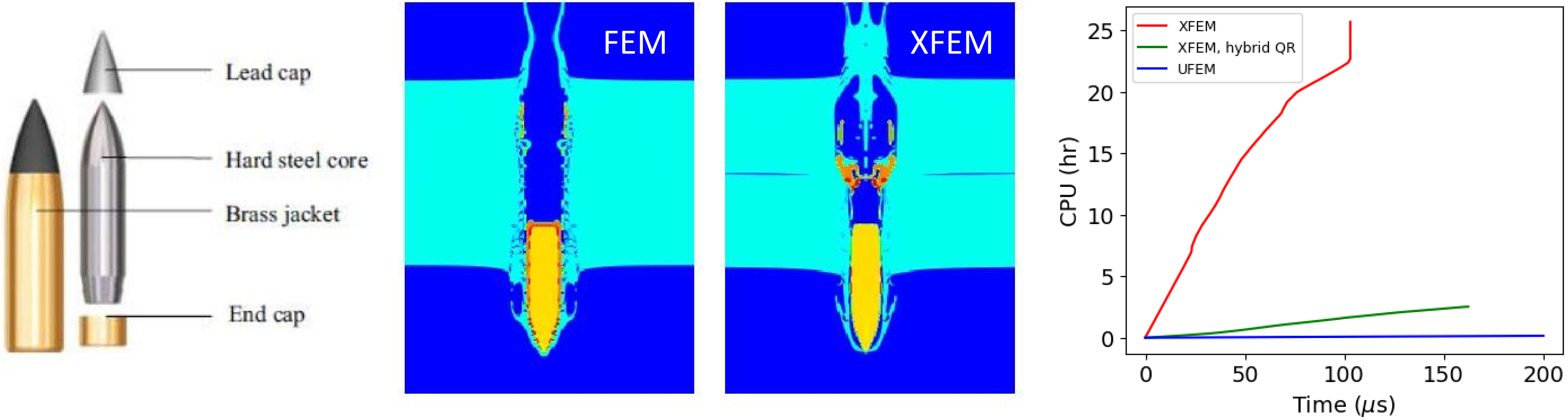
Customers:

- Scientists operating the ***Z-machine***
- ***Army Research Lab (ARL)*** – use ALEGRA to study advanced armor concepts


Sandia's Z-machine: Earth's most powerful pulsed-power facility (used for weapons & fusion research, studying other planets)

Multi-material impact simulations using XFEM

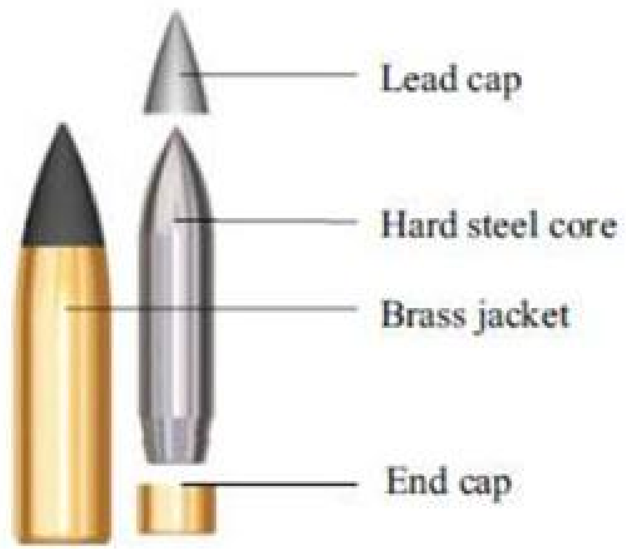
- The eXtended Finite Element Method (XFEM) endows **different materials** with **independent velocity fields** (via FE space enrichment), enabling frictionless separation b/w objects in impact simulations.
- Classical Eulerian FEM discretizations can manifest a **non-physical "sticking"** phenomenon due to materials being forced to travel at the same velocity.

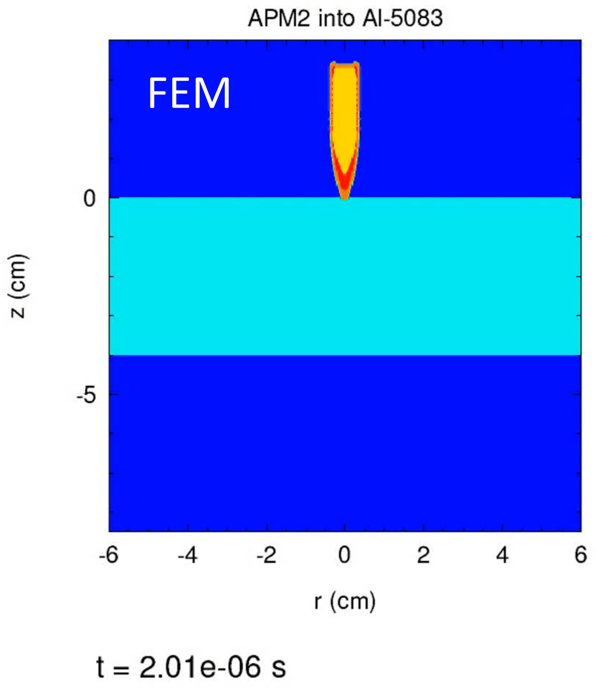


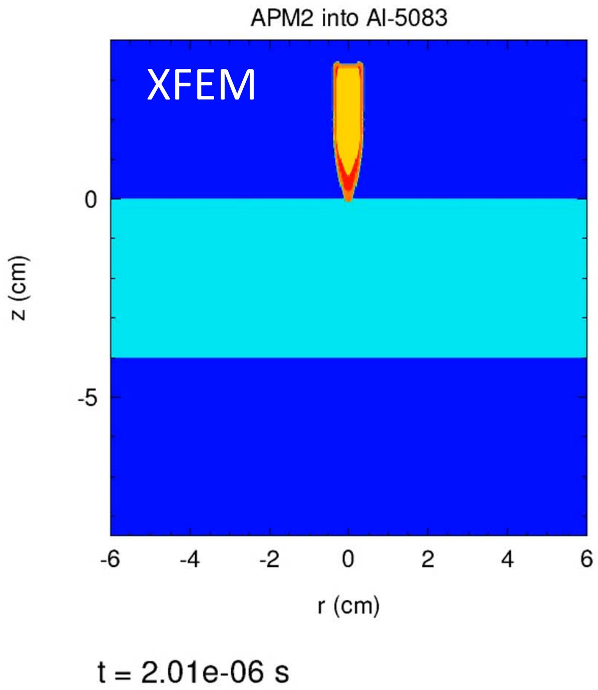
*<u>Figure</u>: Simulation of armor piercing projectile impacting two stacked aluminum plates using the standard FEM vs. XFEM in ALEGRA. Only XFEM captures the **physically correct behavior** in which the projectile jacket separates from the plates. New stabilized formulation (shown in green in the right-most subfigure) achieves a **CPU-time savings of ~13x** over the standard XFEM implementation in ALEGRA and enables the simulation to run to completion.*

Multi-material impact simulations using XFEM

Algorithmic improvements enabled us to run **XFEM** problems that had been **abandoned** years ago!

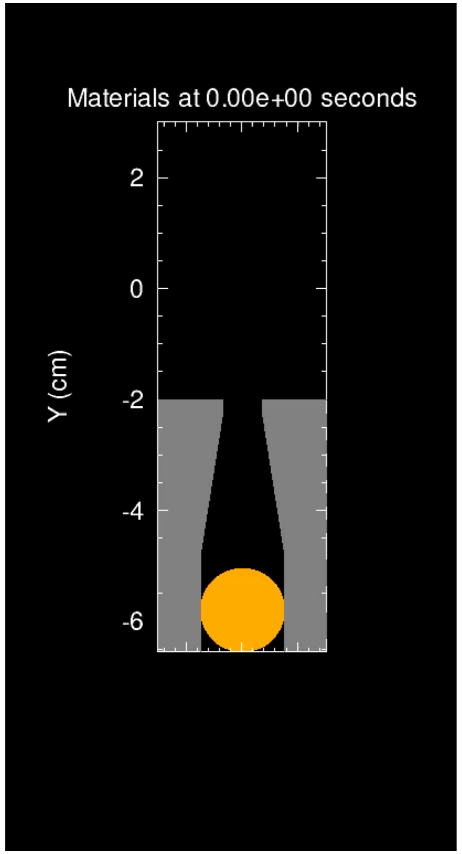






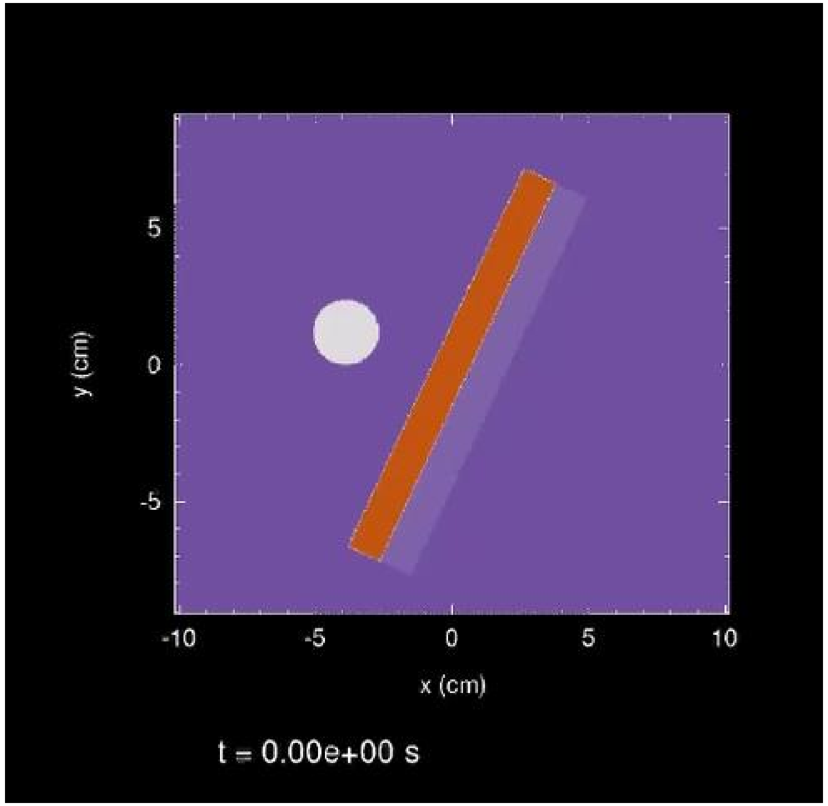
XFEM simulation runs to ***completion*** and captures the ***physically correct*** behavior (separation of projectile jacket).

Multi-material impact simulations using XFEM



DTEX problem (left):
projectile pushed through and ejected from die

Oblique impact problem (right):
projectile impacting layered target (parallel plates)



XFEM simulation runs to ***completion*** and captures the ***physically correct*** behavior for these problems as well.

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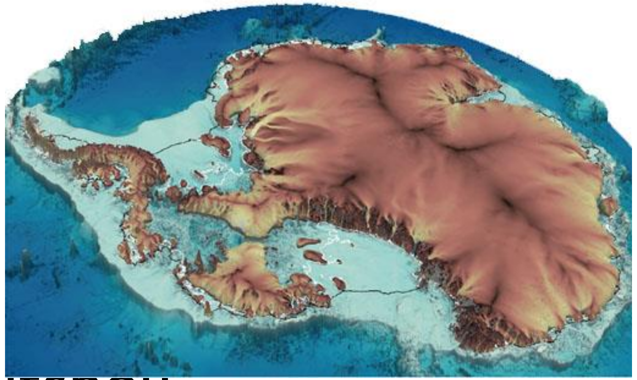
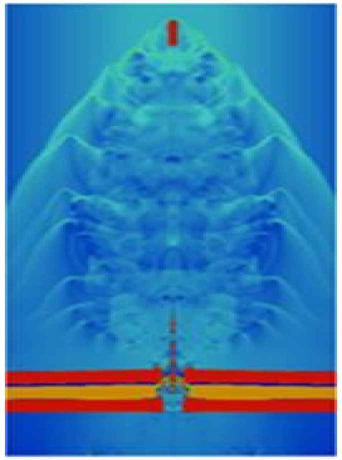
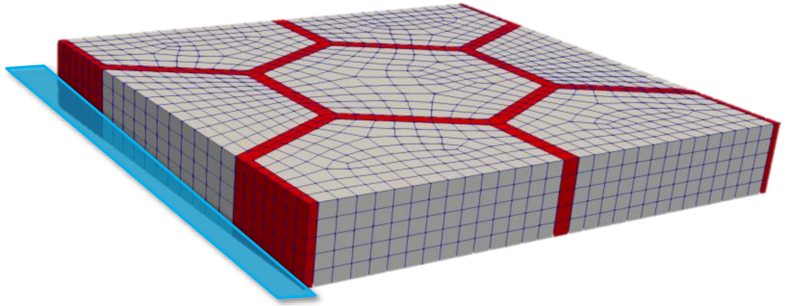
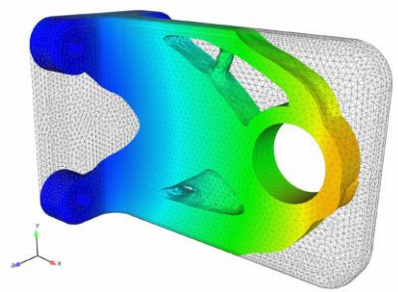








Career and educational tips: general

Be open to exploring opportunities that come your way

- This is how I found out about Sandia and ended up there!

Do internships outside of academia

- You never know what a career is truly like until you experience it first-hand
- Useful for expanding your knowledge base and building connections

Work at building connections and a professional network

- At your university and beyond (conferences, internships, reaching out to researchers, etc.)

Take initiative

- In general, opportunities will not come to you – you need to seek them out
- Superiors will notice

Never stop learning

Develop good time-management skills!

You don't need to decide what to do "with the rest of your life"!

- Life is a journey… all you need to decide is what to do next!

Insights from my experiences and additional tips

I never had a life plan

- I took things one step at a time, and figured out what I liked/disliked along the way

I never tried to "optimize" my career to get ahead

- My approach has always been to:
  - (1) work on things I like, and
  - (2) do them as well as I can

Advice for women in STEM:

- Women are under-represented in STEM fields.
  - ➢ Don't let this intimidate you!
  - ➢ There is a growing number of opportunities in STEM for women.
- Female mentors/role models are key to increasing diversity in STEM fields.

Additional advice
(things I would tell my younger self):

Don't be intimidated about reaching out to senior researchers for help/advice

- "Big shot" professors/researchers are people just like you!

Having a support system is extremely important

- Friends/family and technical/professional role models/mentors

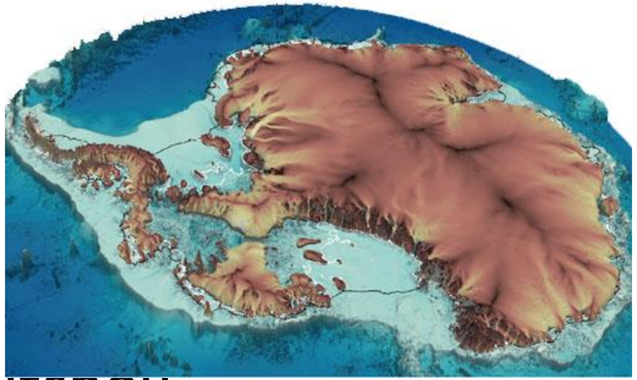
Work-life balance is extremely important

Be resilient! Don't be phased by setbacks

Outline

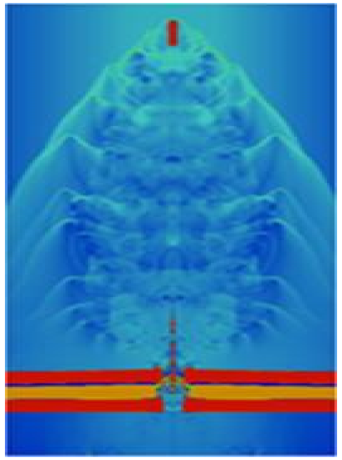
1. A little bit about me and my background

2. A little bit about Sandia National Laboratories



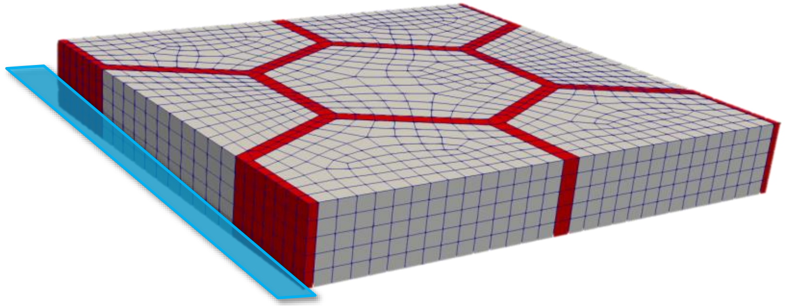
3. Physics-based computational modeling & simulation in a nutshell

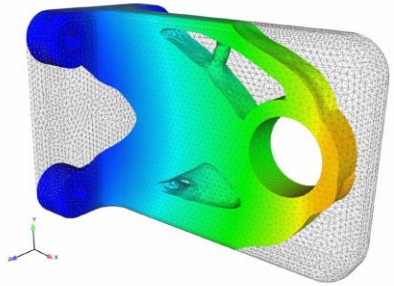
4. A few research highlights
   - Ice sheet modeling
   - Multi-material impact simulations



5. Career & educational tips

6. Question & answer (Q&A)





Thank you! Questions?

Contact: ikalash@sandia.gov
URL: www.sandia.gov/~ikalash

Backup Slides

Labs vs. academia

University/Academia

- Most of work is ***individual/independent***
- ***Collaboration*** can be ***difficult***
- ***Single*** (or few) ***projects/research*** grants
- ***Must*** publish, write proposals, attend conferences

Sandia National Laboratories

- Work as a part of ***interdisciplinary team*** (mix of independent and group work, e.g. pair programming, on a day-to-day basis)
- ***Very collaborative environment***: collaboration is expected and most projects require interdisciplinary collaboration for success
- ***Multiple (many) projects/research grants*** (time management is critical!)
- ***Can*** publish, write proposals, attend conferences (balanced with internal R&D projects/commitments)

Labs vs. academia

University/Academia

- Timescales can be ***slow***
- ***Metrics of success/deliverables*** are not always clearly defined
- Teaching and advising students/post docs is ***required***
- ***Software development*** is often ***dumped*** on students, codes can be a mess
- ***Limited access*** to people with expertise, equipment, HPC resources

Sandia National Laboratories

- ***Faster timescales*** driven by project deliverables (faster than academia, slower than industry)
- ***Clearly defined deliverables/metrics of success*** with multiple checkpoints throughout process
- Teaching and advising students/post docs is ***possible*** but not required
- ***Software development***, testing, maintenance, bug fixes is often a ***key part*** of the job
- People with expertise, equipment and HPC resources are there ***at your fingertips***

Labs vs. academia

University/Academia

- Focus on ***technical depth***
- Maintaining ***work-life balance*** can be ***challenging***
- Possible to ***make a name for yourself*** and ***determine your own projects***
- Evaluated on ***reputation***, ***publications***, ***grants***
- ***Open-ended research*** upon attaining tenure (at least in theory)

Sandia National Laboratories

- Technical depth is important, but so is ***breadth***
- Various programs in place (e.g. flexible schedules) to ***promote work-life-balance***
- Possible to ***make a name for yourself*** and ***determine your own projects*** (but ***not required***)
- Evaluated on ***reputation***, ***publications***, ***grants***, ***behaviors*** and ***how well you work with others***
- Research ***driven by mission-critical problems relevant*** to the U.S. government – can be fundamental (low TRL*) or applied (high TRL)

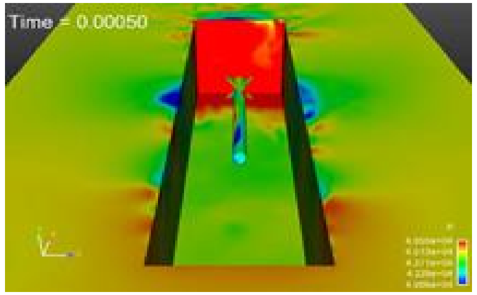
*Technical Readiness Level

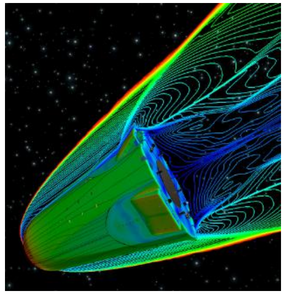
Projection-based reduced order modeling (pROM)

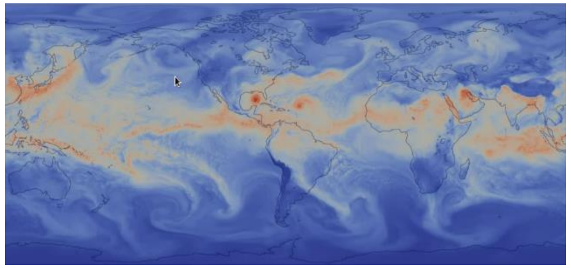
Despite improved algorithms and powerful supercomputers, **"high-fidelity" models** are often too expensive for use in a design or analysis setting.

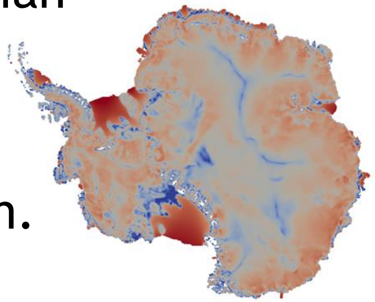
Application areas in which this situation arises:

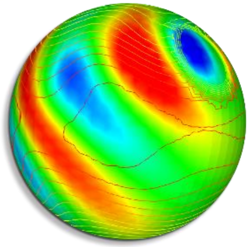
- **Captive-carry** and **re-entry environments:** Large Eddy Simulations (LES) runs require very fine meshes and can take on the order of ***weeks***.
- **Climate modeling** (e.g., land-ice, atmosphere): high-fidelity simulations too costly for uncertainty quantification (UQ); Bayesian inference of high-dimensional parameter fields is ***intractable***.
- **Wind plant simulations:** wind turbines need to be controlled in ***real-time*** to attain optimal energy capture for wind plant system.











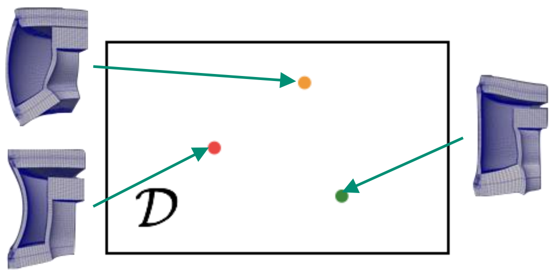
Projection-based reduced order modeling (pROM): a promising approach that can ***dramatically reduce*** the CPU-time requirement for simulations such as these and ***enable real-time*** and ***multi-query analyses*** by combining ***data*** (computational, experimental, observational) with the ***governing equations and physics***.

pROM workflow*

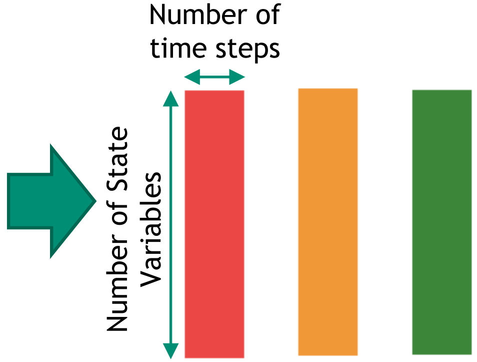
High-fidelity simulation = Ordinary Differential Equation (ODE): $\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}; t, \boldsymbol{\mu})$

Pressio

1. Acquisition



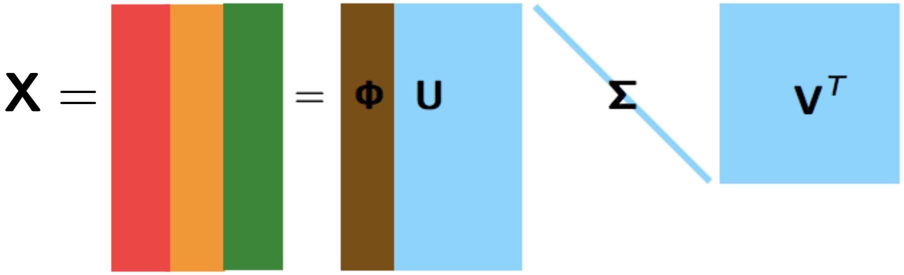
Solve ODE at different design points



Save solution data

2. Learning

Unsupervised Learning with Principal Component Analysis (PCA):



3. Reduction

Choose ODE Temporal Discretization

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}; t, \boldsymbol{\mu})$$

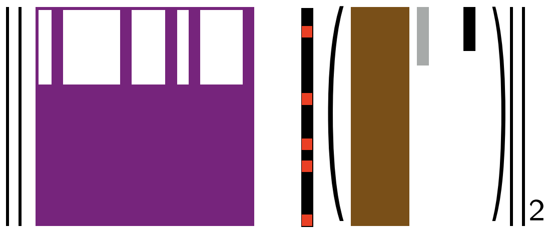
$$\mathbf{r}^n(\mathbf{x}^n; \boldsymbol{\mu}) = \mathbf{0}, \quad n = 1, \ldots, T$$

Reduce the number of unknowns

$$\mathbf{x}(t) \approx \tilde{\mathbf{x}}(t) = \boldsymbol{\Phi}\,\hat{\mathbf{x}}(t)$$

Minimize the Residual

$$\underset{\hat{\mathbf{v}}}{\text{minimize}} \| \mathbf{A} \, \mathbf{r}^n(\boldsymbol{\Phi}\,\hat{\mathbf{v}}; \boldsymbol{\mu}) \|_2$$

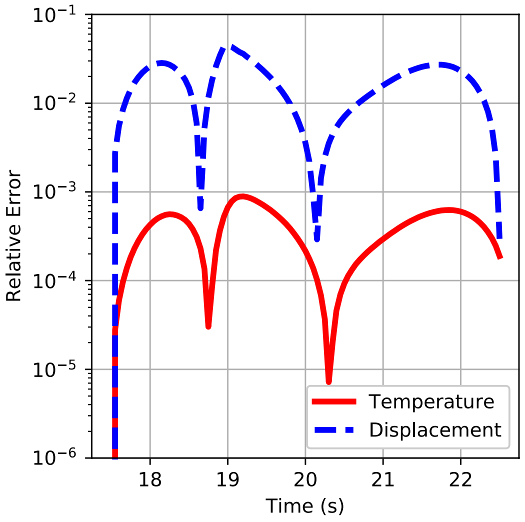


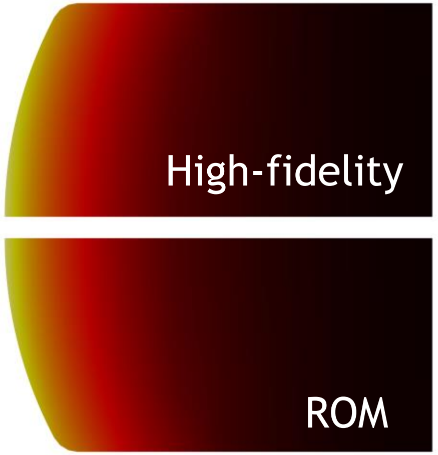
*Least-Squares Petrov-Galerkin (LSPG) Projection [Carlberg, Bou-Mosleh, Farhat, 2011; Carlberg, Barone, Antil, 2017]

pROMs: recent successes at SNL

ROM accelerates **ablation** simulation with SPARC compressible flow solver

- First applications of ROMs to ablation
- Large differences in scales (7 orders of magnitude)
- Iso-q with prescribed axisymmetric heat- and mass-transfer boundary conditions

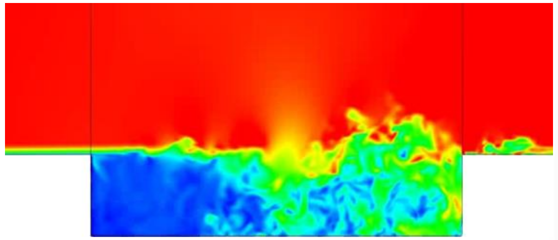


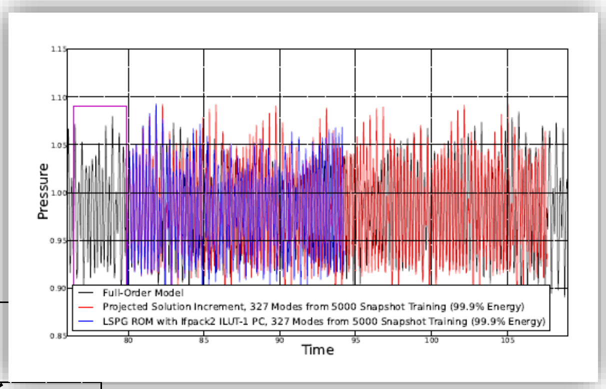


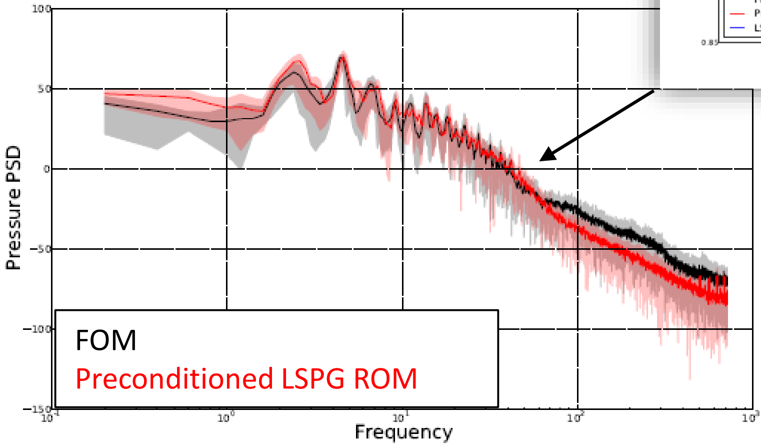
~17x savings in core-hours
<0.1% error in temp, <4% error in disp

Time-predictive preconditioned **captive-carry** ROM in SPARC demonstrated to have sufficiently accurate pressure PSD

- Laminar compressible cavity problem (Ma = 0.6, Re = 3000).
- Primarily interested in prediction in time.



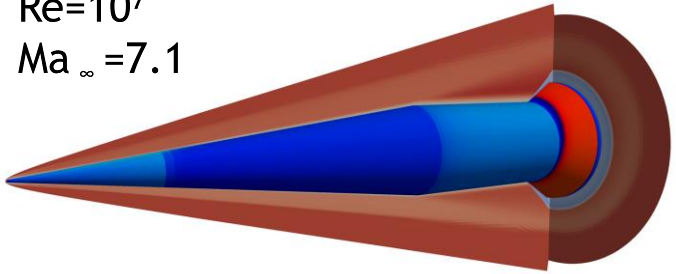




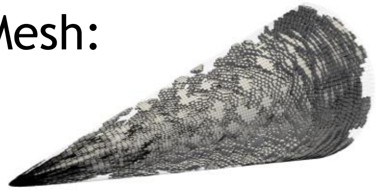
ROM PSD is within FOM PSD range!

pROMs: recent successes at SNL

ROM accelerates **hypersonics** simulation (HiFIRE-1 experiment) using in-house compressible flow solver (SPARC)



- Prediction across param space (Ma, ρ)
- POD-LSPG + Sample Mesh:



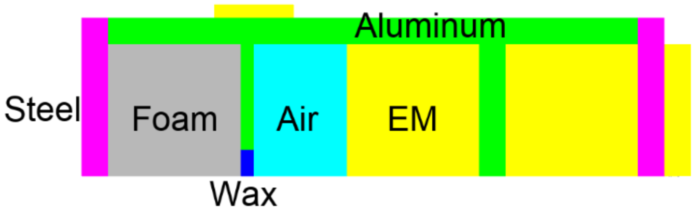
~300-1000x savings in core-hrs
<1% error in density, momentum, energy
~1-2% error in integrated wall heat flux

[Blonigan, Carlberg, Rizzi, Howard, Fike, 2020]

ROM accelerates **transient conduction/thermochemistry** in Aria

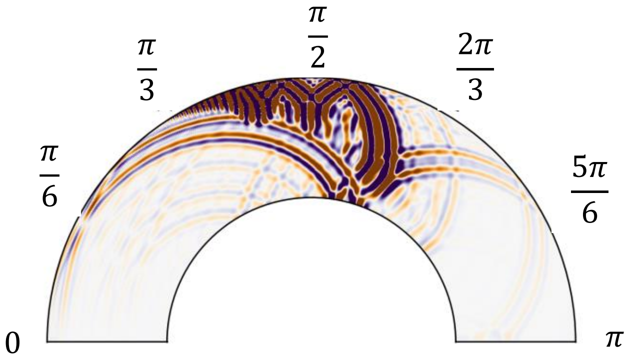
- Transient thermochemistry test
  - ➢ Foam decomposition
  - ➢ Heat conduction
  - ➢ Exothermic chemical reactions

~9000x savings in core-hrs
<1°C error in temp.

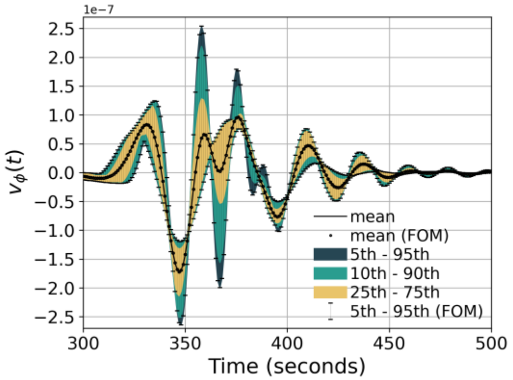


ROM accelerates **seismic wave propagation**

- Synthetic seismogram data
- One shot UQ: simultaneous simulation of many trajectories



~950x savings in wall-time
<1% error



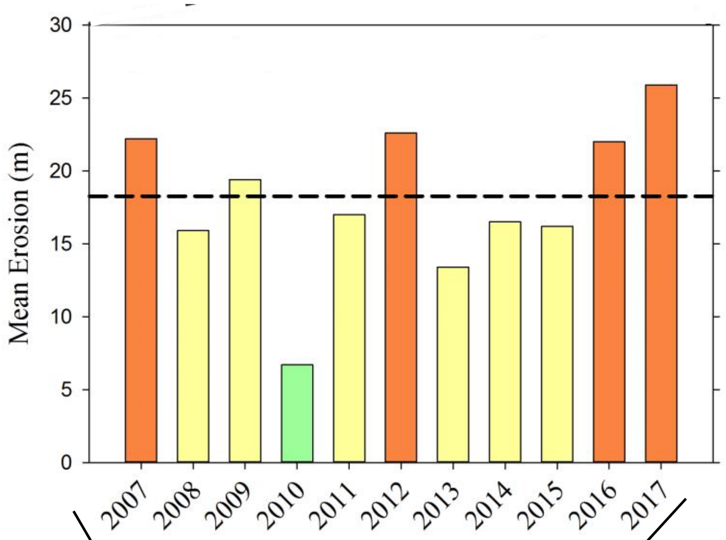
Arctic coastal erosion (ACE) modeling: motivation

The Arctic is warming at **2-3 times** the rate of the rest of the U.S. resulting in **accelerated rates of coastal erosion**!

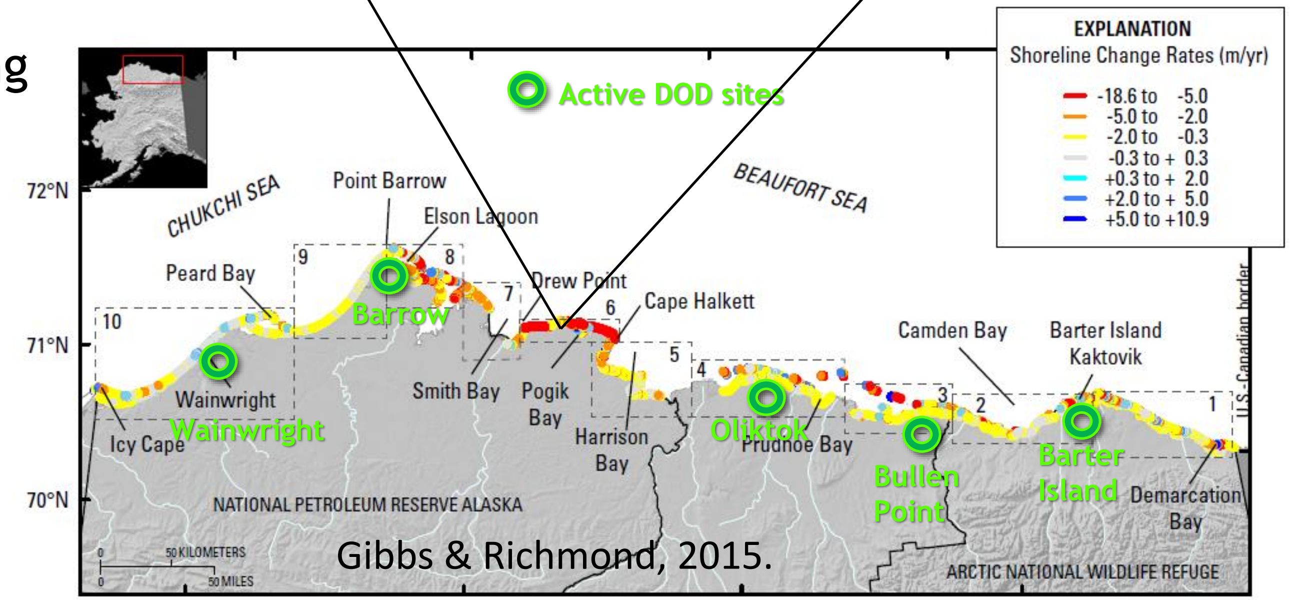
- Since 1979 **sea-ice** has lost 51% in area, 75% in volume
  - ➢ Increasing **ice-free season**
  - ➢ Increasing **wave energy** and **storm surge**
- Increasing **sea water** temperatures
- Warming **permafrost**
  - ➢ **Coastal erosion rates** in Alaskan Arctic among the **highest** in the world and **accelerating.**

Erosion is threatening:

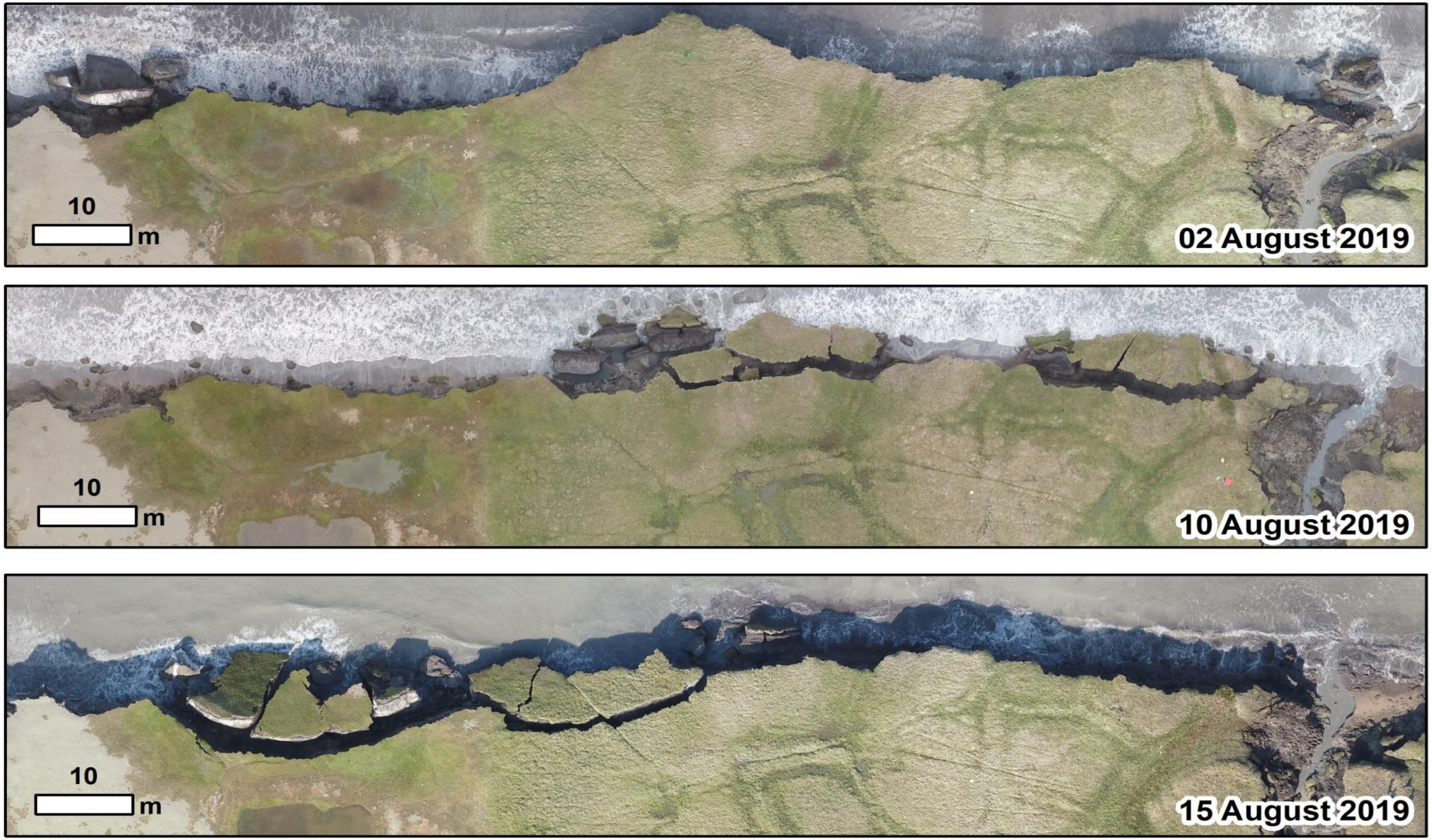
- ➢ Displacement of coastal communities
- ➢ Coastal infrastructure (DoD sites, toxic waste sites)
- ➢ Global carbon balance (GH gas release)



~200 m (~2 football fields in length) in a decade!



ACE modeling: 2019 UAV studies*



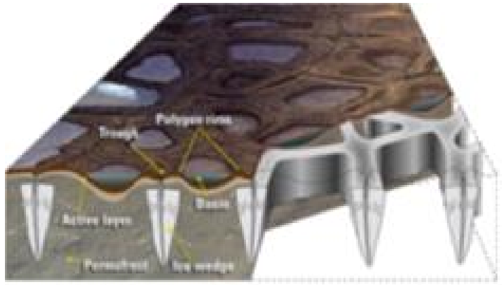
Fallen blocks can disintegrate in near-shore environment **within 1-2 weeks!**

*Images courtesy of Ben Jones, UAF

ACE modeling: permafrost erosion

What is permafrost?

- Ground that remains frozen for 2 or more consecutive years.
- Comprised of soil, rock, silt, clay and sand, held together by ice.
- 24% of ice-free land area in Northern Hemisphere and 85% of Alaska, Greenland, Canada and Siberia sits on top of permafrost.



Martin *et al*. 2009.

Left: schematic illustrating formation of ice wedges and ice-wedge polygon landscapes. *Right*: map of permafrost distribution in Arctic

Brown *et al*. 1998.

Unique coastal permafrost erosion process in Arctic:

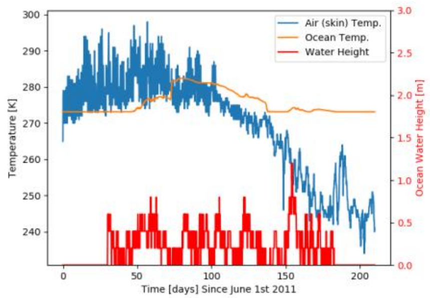
- Predominant geomorphology: **ice-wedge polygons**
  - ➢ Ice acts to **bind** unconsolidated soils in permafrost forming ice wedges.
  - ➢ Ice wedges **grow/expand** up to ms wide and 10s meters deep.
- Melting ice causes permafrost **failure**.
  - ➢ **Storm surges** accelerate ice melt by delivering **heat** to ice/permafrost*.

* Thermo-abrasion: permafrost material is warmed by ocean and removed by mechanical action of waves.

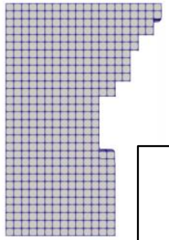
ACE terrestrial model

Unique capabilities of ACE model:

- ***Tightly coupled mechanical*** and ***thermal states***: coupling happens at ***material model*** level
- ***Failure modes*** develop from ***constitutive relationships*** in numerical model (no empirical models!)
- ***Observational & experimental data*** from Drew Point, AK used to estimate ***model params***



- Model uses ***realistic atmospheric & oceanic boundary conditions***
- Elements ***removed*** to simulate ***erosion***
- Encompasses all possible ***failure mechanisms***

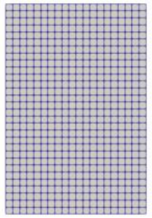


$$(\overline{\rho c_p} + \widetilde{\Theta})\frac{\partial T}{\partial t} = \nabla \cdot (\boldsymbol{K} \cdot \nabla T)$$

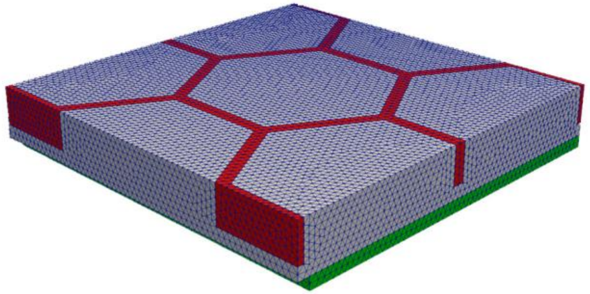
Thermal:

Inputs: geometry, sediment type, ice volume, water volume, pore size, salinity

Outputs: temperature field, ice saturation



Eroded geometry



Albany

Ice saturation

Mechanical:

Inputs: ice saturation, strength relationship as function of thermal state, stress-strain relationships of permafrost and ice

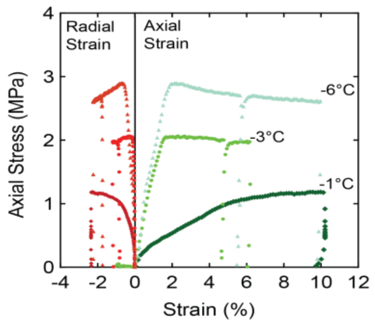
Outputs: displacements, eroded geometry

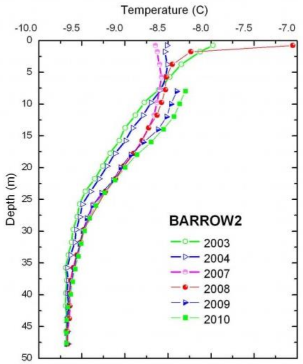
$$\Phi[\boldsymbol{\varphi}] := \int_{\Omega} A(\boldsymbol{F}, \boldsymbol{Z})\, dV - \int_{\Omega} \rho \boldsymbol{B} \cdot \boldsymbol{\varphi}\, dV - \int_{\partial_{\boldsymbol{T}}\Omega} \boldsymbol{T} \cdot \boldsymbol{\varphi}\, dS$$

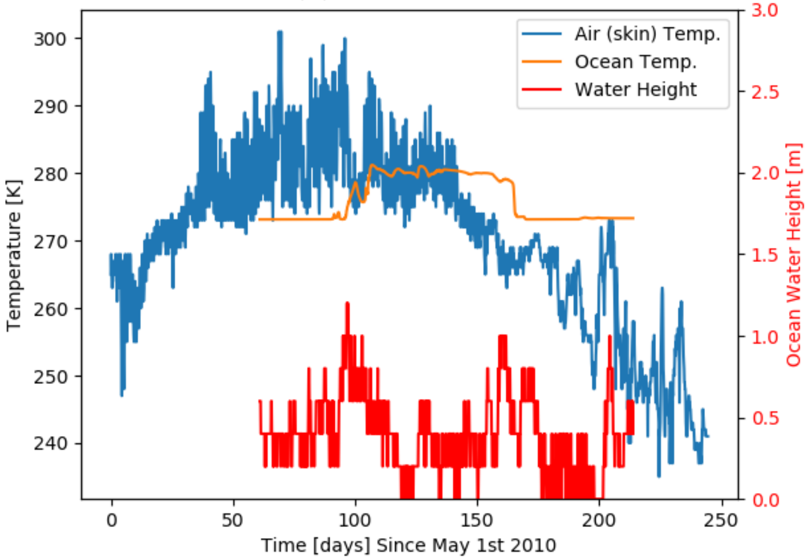
ACE terrestrial model: 2.5D slice experiment

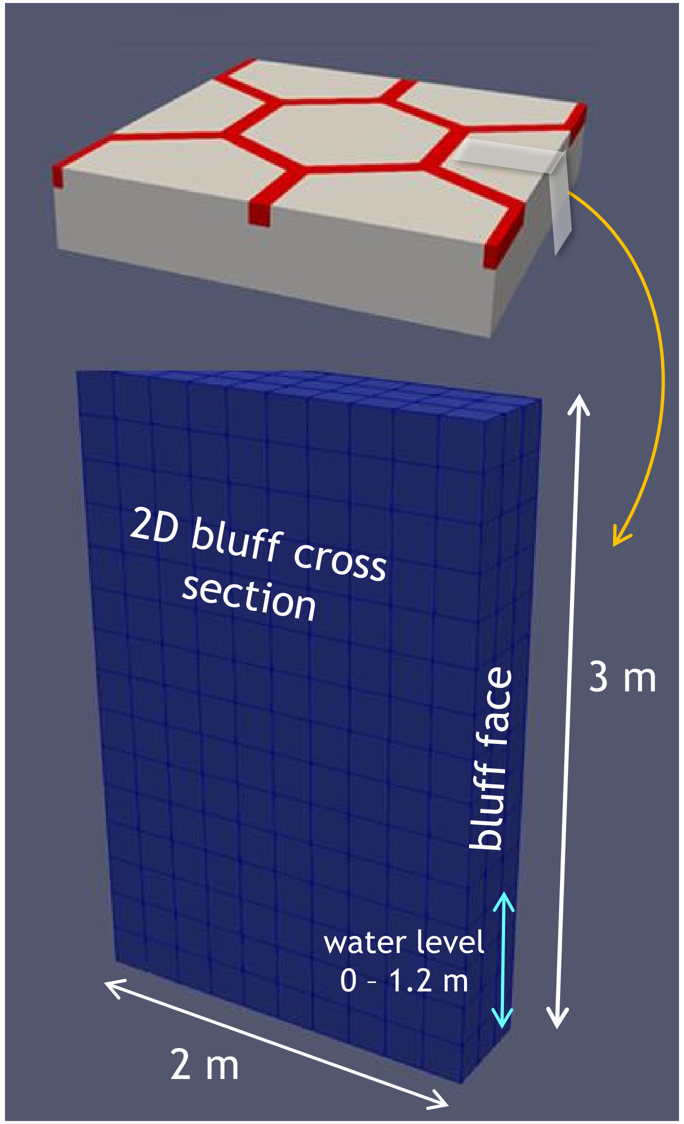
- Computational domain is ***2.5D cross-section*** of archetypal 3D bluff geometry
- ***Air (skin) temperature*** from ASR dataset at 3hr resolution
- ***Ocean temp*** & ***height*** from WW3+SWAN at 20 min resolution
- ***Time period***: May-December 2011
- ***Ice-free period***: July-October
- ***Material properties***: from laboratory experiments

Our ***initial verification study*** uses real oceanic/atmospheric boundary condition data but assumes material is ***ice only***.

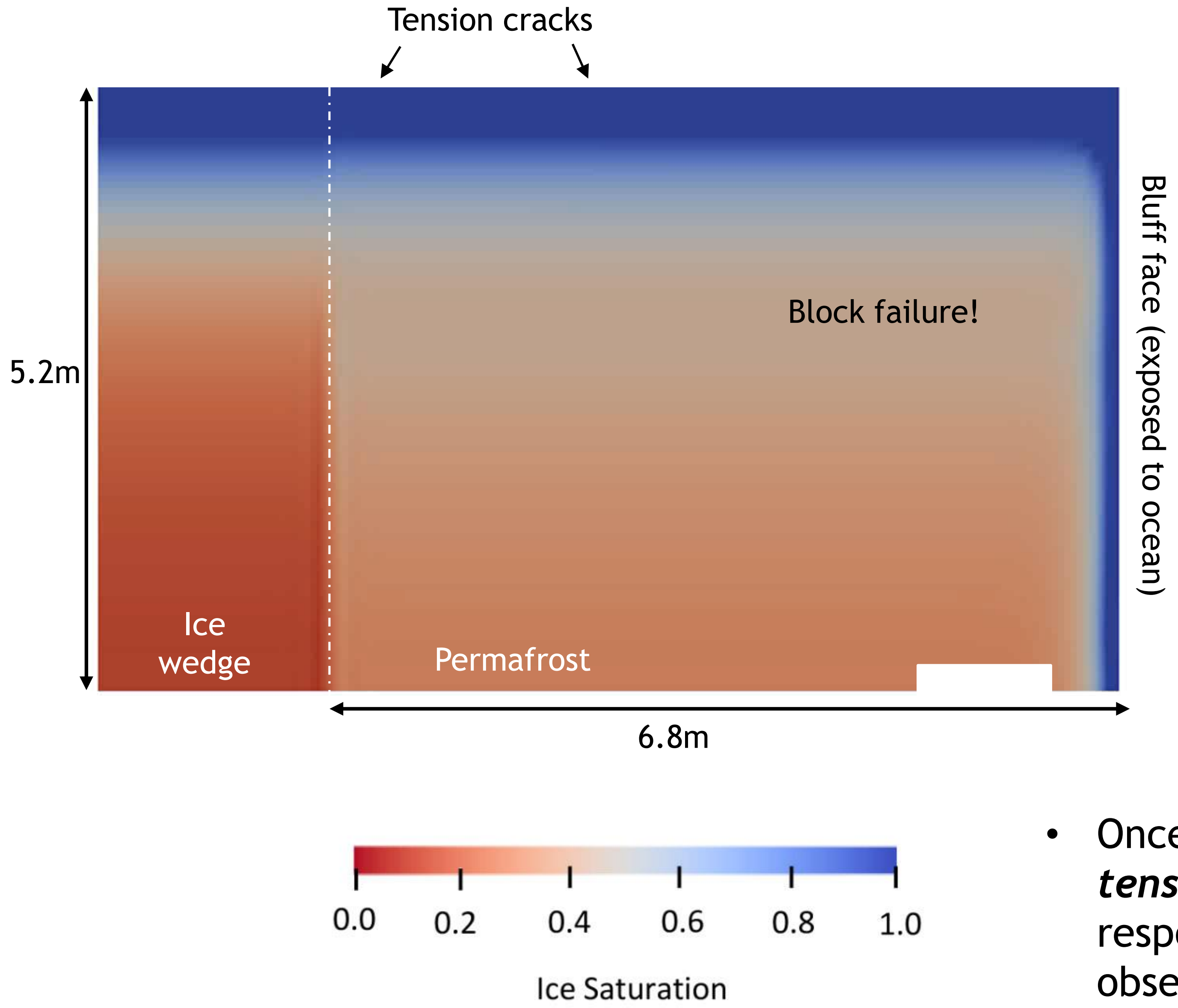




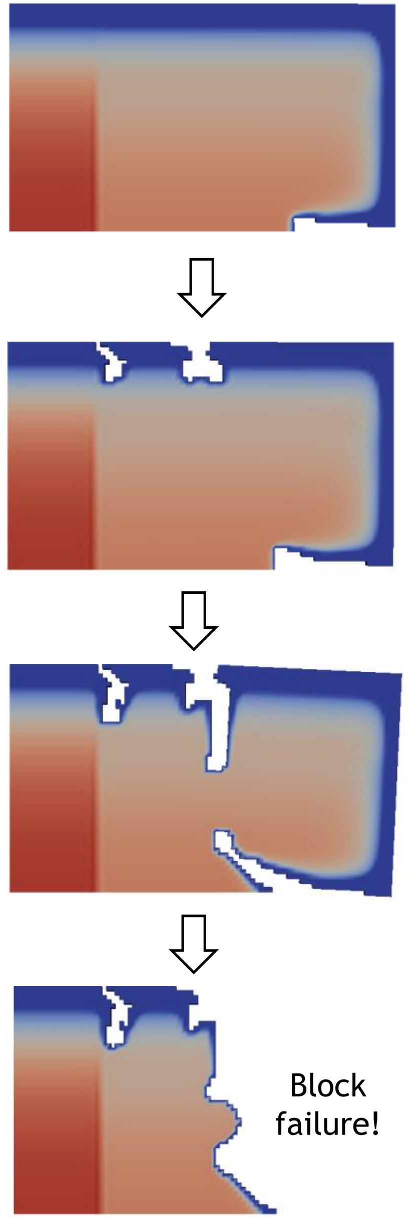




ACE terrestrial model: 2.5D slice experiment



Simulation showing **niche progression** beginning at the bluff toe, followed by **block failure/ collapse event**

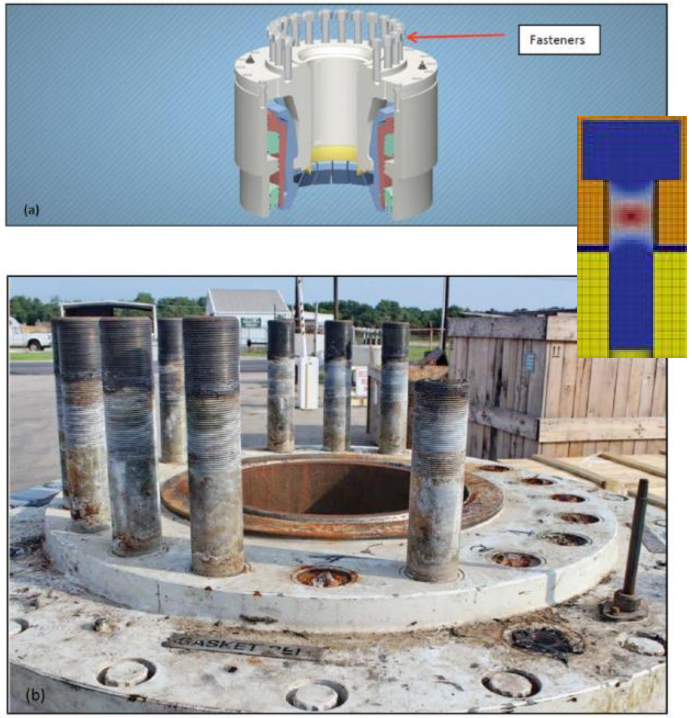


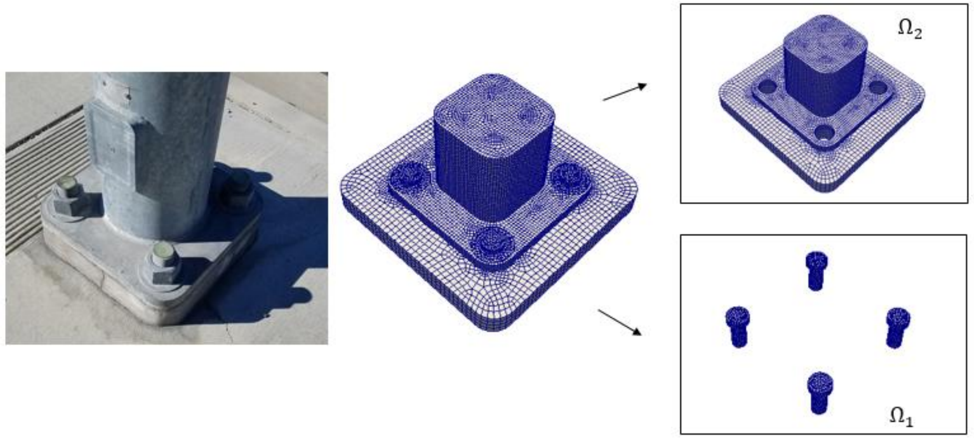
- ***Niche*** that is ~3m deep forms before a ***block collapse event*** similar to observed collapse event at Drew Point, Alaska in early fall 2018.
- Once niche advanced far enough, ***tension crack development*** in response to niche formation is observed

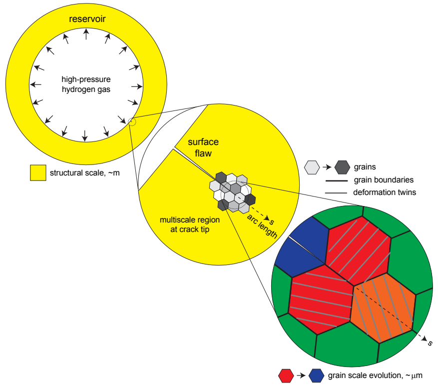
Multi-scale failure simulations: motivation

- ***Small-scale*** defect/microcrack often leads to ***large-scale*** structural failure (e.g. components held together by fasters).
- Presence of multiple scales is ***challenging*** and ***expensive*** to simulate.
  - ➢ ***Meshing*** a multi-scale object can take weeks and needs to be repeated for each new design configuration!
  - ➢ Discrete multiscale models can be very difficult to ***solve***.
  - ➢ Existing methods for multiscale coupling are ***deficient***: provide only ***one-way coupling***, ***hard to implement*** in HPC codes.

Roof failure of Boeing 737 aircraft due to fatigue cracks.

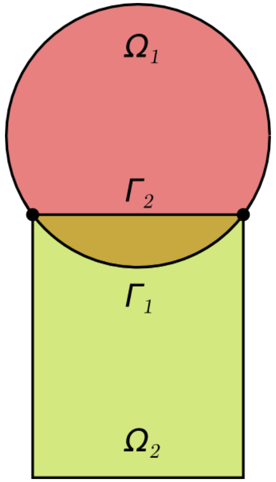






Multi-scale failure simulations

Our novel multi-scale coupling approach is based on the ***alternating Schwarz method*** and enables the simulation of ***many more scenarios*** than afforded using existing technologies by breaking up system into pieces and "gluing" them together.



Basic Schwarz Algorithm

Initialize:

- Solve PDE by any method on Ω_1 w/ initial guess for Dirichlet BCs on Γ_1.

Iterate until convergence:

- Solve PDE by any method (can be different than for Ω_1) on Ω_2 w/ Dirichlet BCs on Γ_1 that are the values just obtained for Ω_1.
- Solve PDE by any method (can be different than for Ω_2) on Ω_1 w/ Dirichlet BCs on Γ_1 that are the values just obtained for Ω_2.

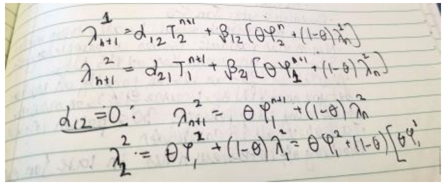

Getting to the nuts and bolts of nuts and bolts

BY MICHAEL ELLIS LANGLEY | PHOTOGRAPHY BY MICHAEL ELLIS LANGLEY

THURSDAY, AUGUST 29, 2019

FINDING SOLUTIONS — Alejandro Mota, left, and Irina Tezaur explain how their new computer modeling system can solve problems for each piece of something, like bolts in a lamppost, reducing the time it takes to render the model.

- We have been able to see this method through from ***pencil-and-paper*** to ***prototyping*** to ***production***!



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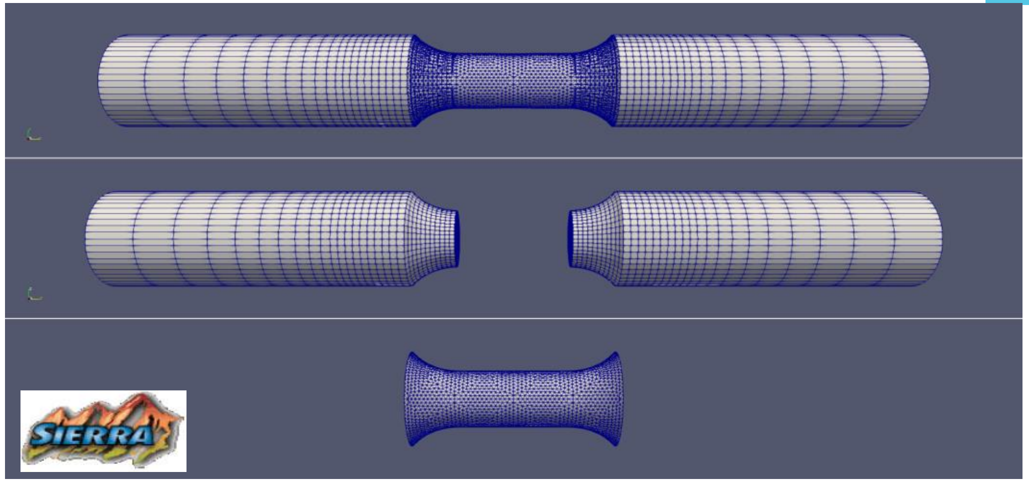
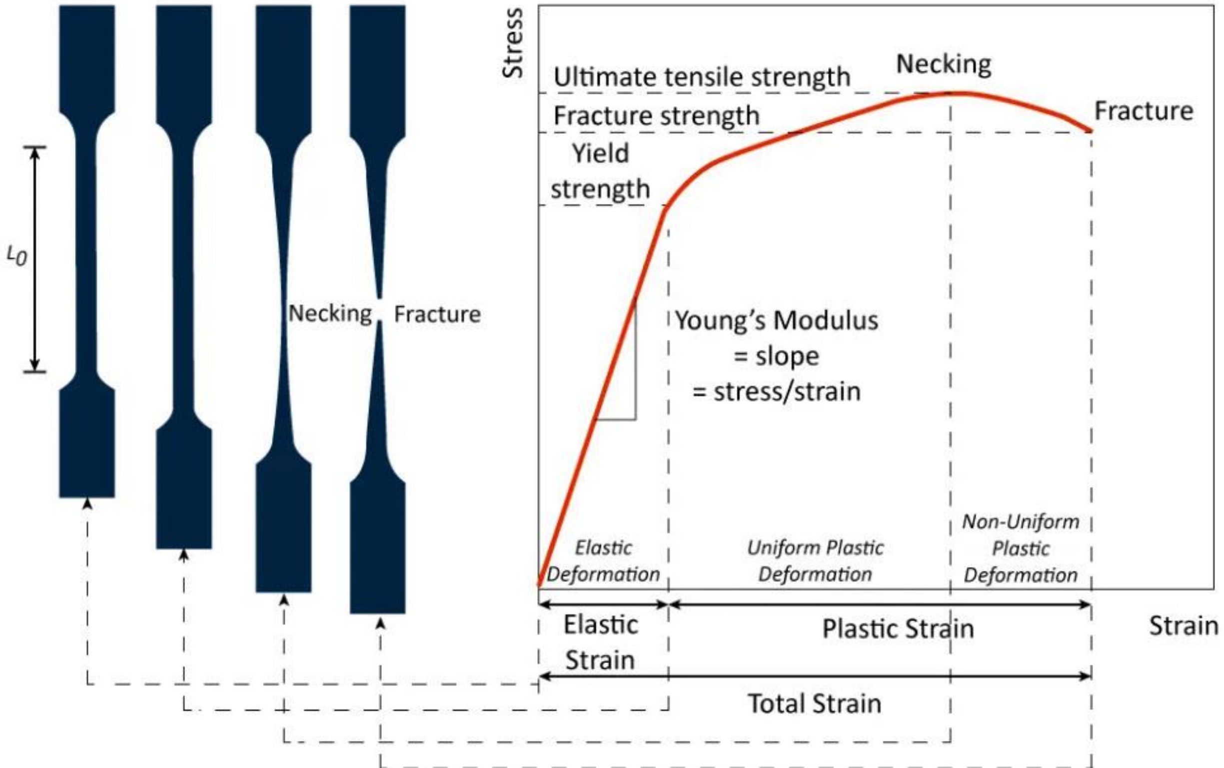
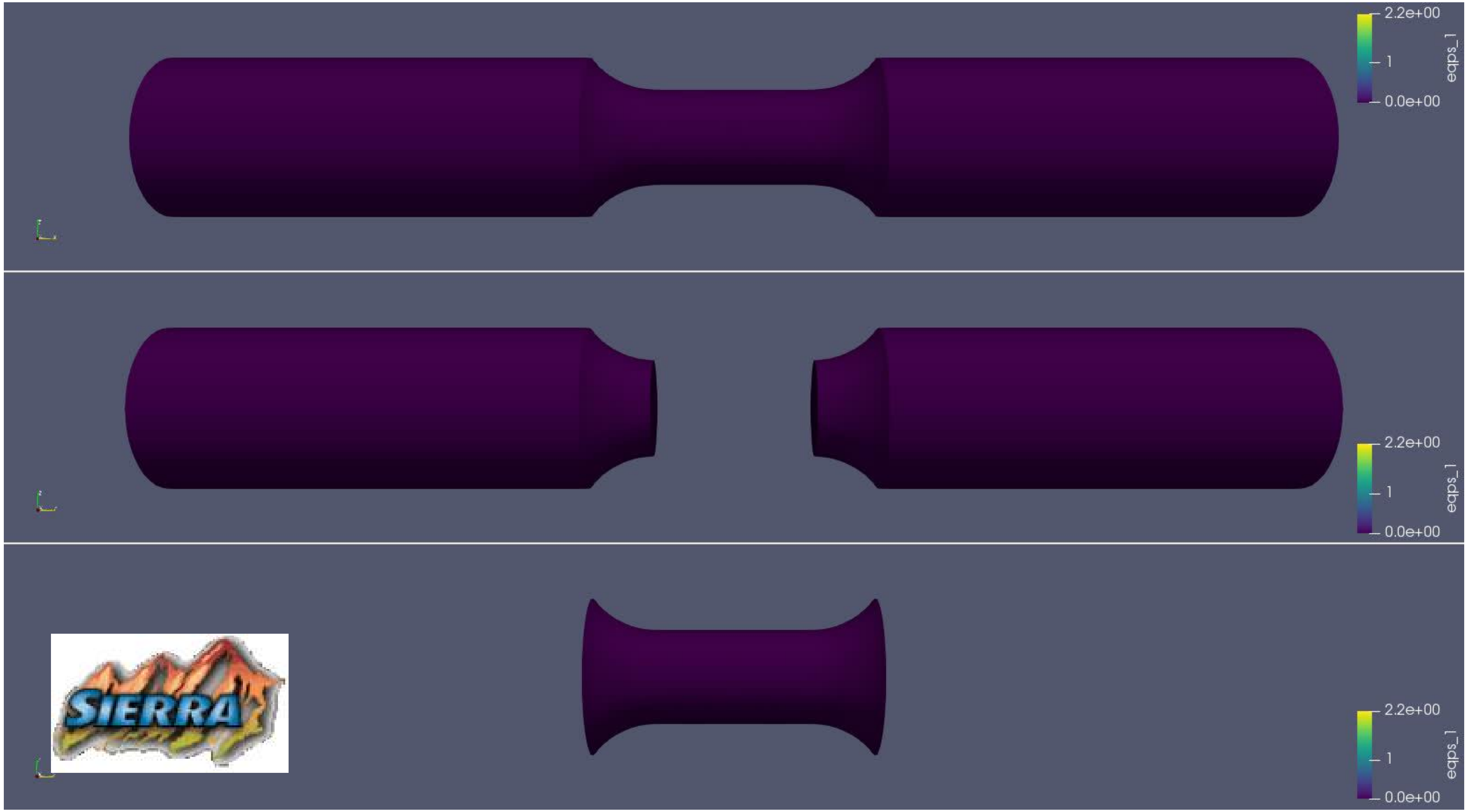
Multi-scale failure simulations: tension specimen



- Uniaxial aluminum cylindrical tensile specimen with ***inelastic J_2 material model***.
- Domain decomposition into ***two subdomains*** (right): Ω_0 = ends, Ω_1 = gauge.
- ***Nonconformal HEX + composite TET10*** coupling via Schwarz.
- ***Implicit*** Newmark time-integration with ***adaptive time-stepping*** algorithm employed in both subdomains.
- Slight ***imperfection*** introduced at center of gauge to force ***necking*** upon pulling in vertical direction.



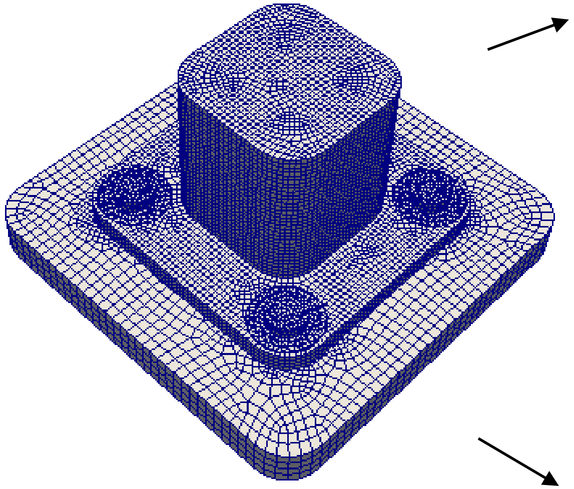
Multi-scale failure simulations: tension specimen

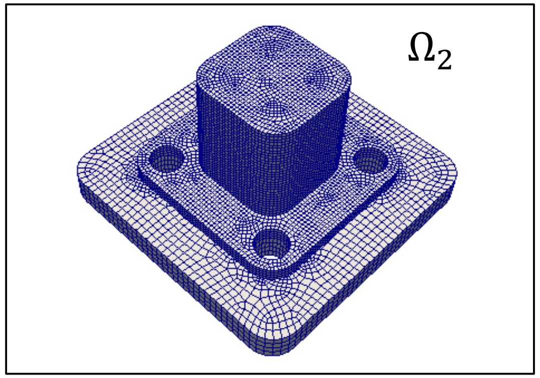


Multi-scale failure simulations: bolted-joint problem

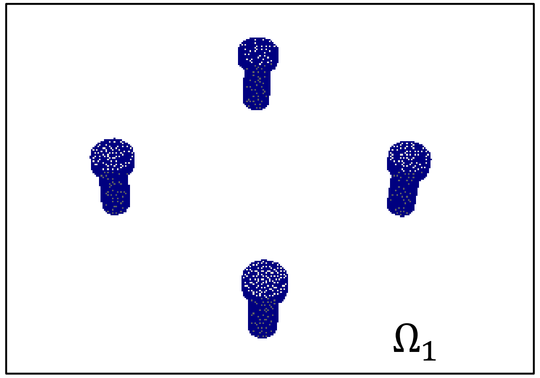
Problem of ***practical scale***.

- Schwarz solution compared to single-domain solution on composite TET10 mesh.



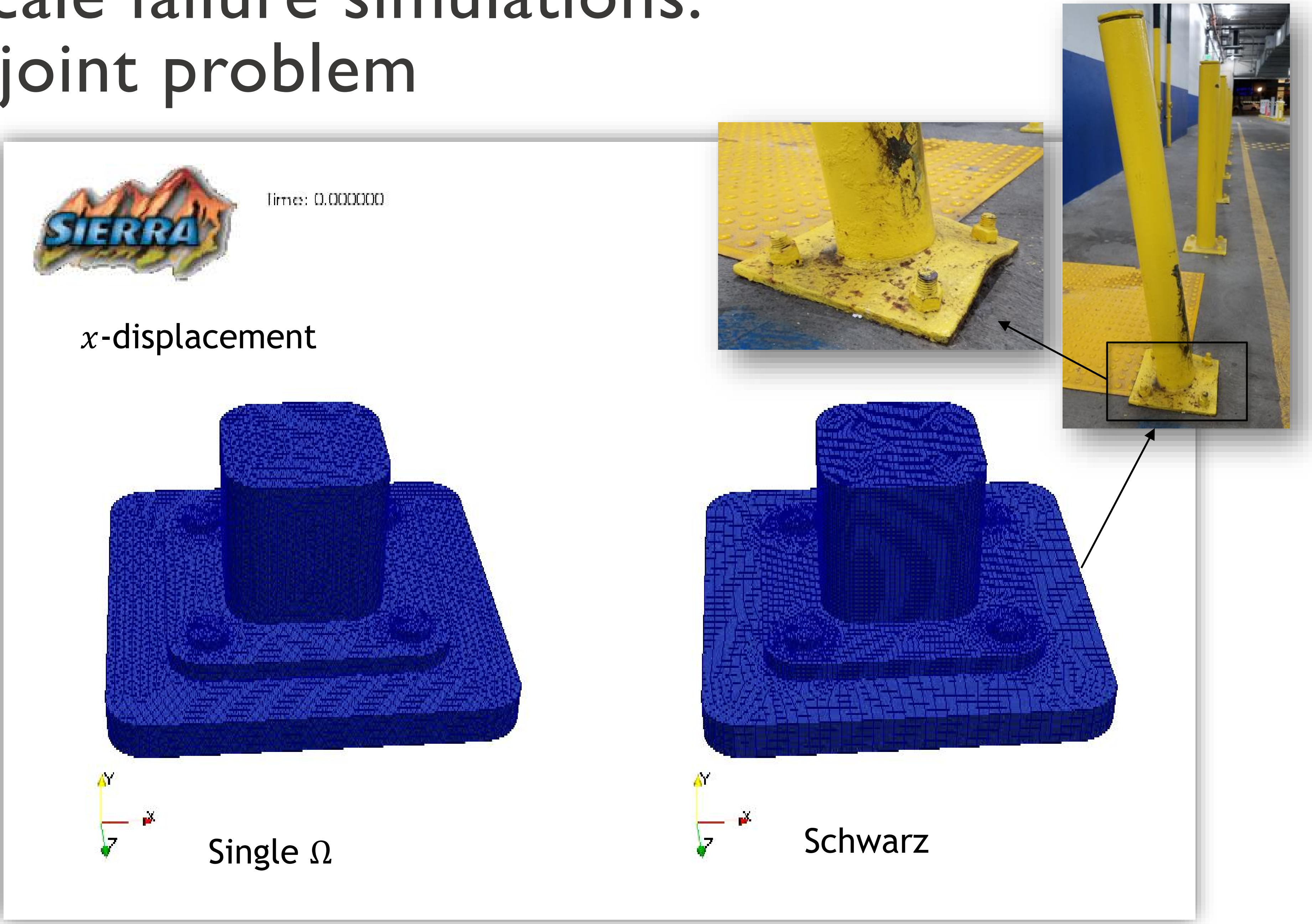


- BC: x-disp = 0.02 at T = 1.0e-3 on top of parts.
- Run until T = 5.0e-4 w/ dt = 1e-5 + implicit Newmark with analytic mass matrix for composite tet 10s.

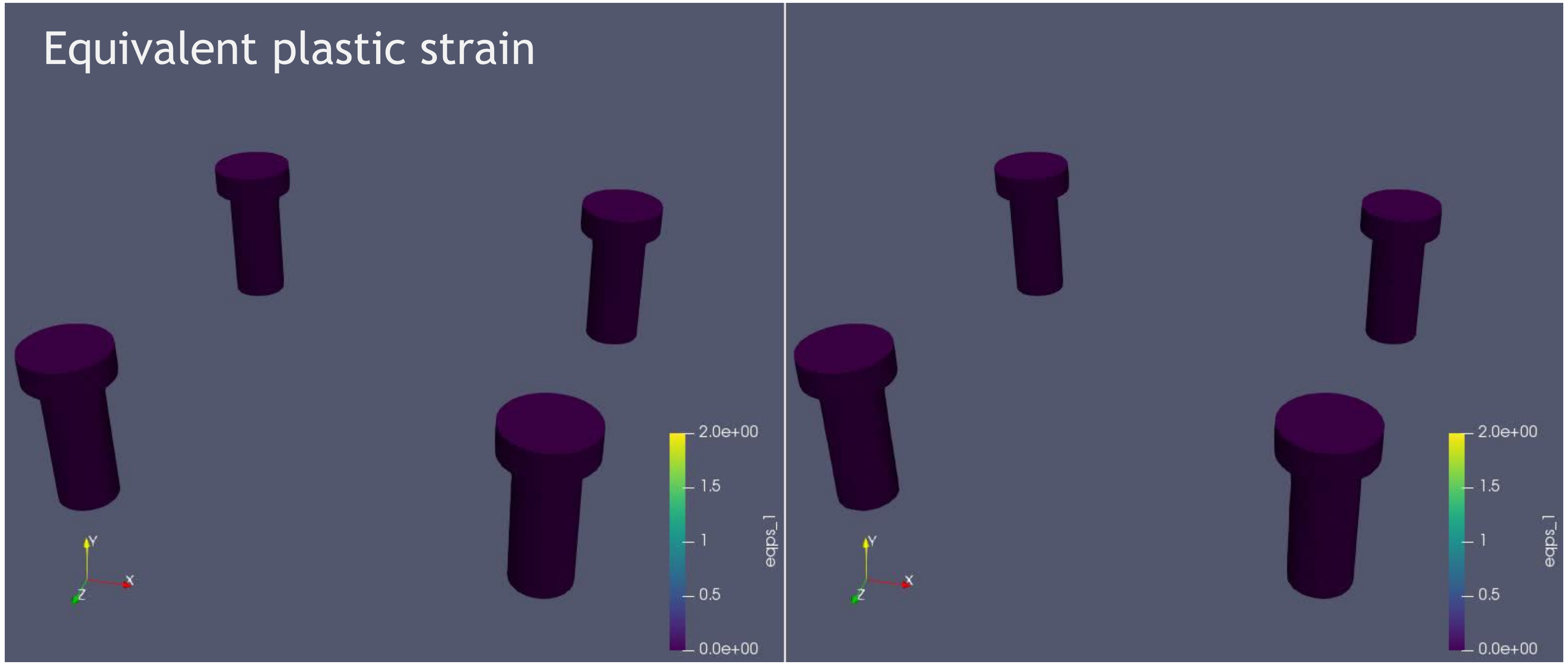


- Ω_1 = bolts (Composite TET10), Ω_2 = parts (HEX).
- ***Inelastic J_2 material model*** in both subdomains.
  - Ω_1: steel
  - Ω_2: steel component, aluminum (bottom) plate

Multi-scale failure simulations: bolted-joint problem



Multi-scale failure simulations: bolted-joint problem



Single Ω

Schwarz

Career and educational tips: courses

Useful courses I took in undergrad/grad school:

- Calculus
- Ordinary differential equations (ODEs)
- Partial differential equations (PDEs)
- Functional analysis
- Numerical analysis
- Linear algebra/numerical linear algebra
- Optimization/numerical optimization
- Object-oriented (C++) programming
- Time-integration methods
- Discretization methods: finite difference, finite elements, finite volumes, spectral methods
- Computational fluid mechanics
- Numerical solution to PDEs
- Software development for science and engineers
- Intro to parallel processing

Courses I wish I had taken in undergrad/grad school:

- Software engineering for large HPC codes
- Programming for heterogeneous architectures/GPUs*
- Advanced optimization topics, e.g., adjoint-based optimization
- Uncertainty Quantification (UQ)
- Machine Learning (ML)/Artificial Intelligence (AI)*
- Computational solid mechanics

* Had not taken off yet while I was in school!

Careers at Sandia National Laboratories

<u>Students:</u> please consider Sandia and other national labs as a potential employer for summer internships and when you graduate!

Sandia is a great place to work!

- Lots of ***interesting*** problems that require ***fundamental research*** in applied math/computational science and impact ***mission-critical applications***.
- Great ***work/life balance***.

Opportunities at Sandia:

- Internships (summer, year-round)
- Post docs + several prestigious post doctoral fellowships (von Neumann, Truman, Hruby)
- Staff scientists (with Bachelors, Masters, Ph.D.s)

Please see: www.sandia.gov/careers for info about current opportunities.