Advertisement: ESD Special Issue on Ensemble Design/Implementation in Climate Science

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Theoretical and computational aspects of ensemble design, implementation, and interpretation in climate science (ESD/GMD/NPG inter-journal SI)

Editor(s): Francisco de Melo Virissimo, Irina Tezaur, Eviatar Bach, David Stainforth, and Christian Franzke

Special issue jointly organized between Earth System Dynamics, Geoscientific Model Development, and Nonlinear Processes in Geophysics

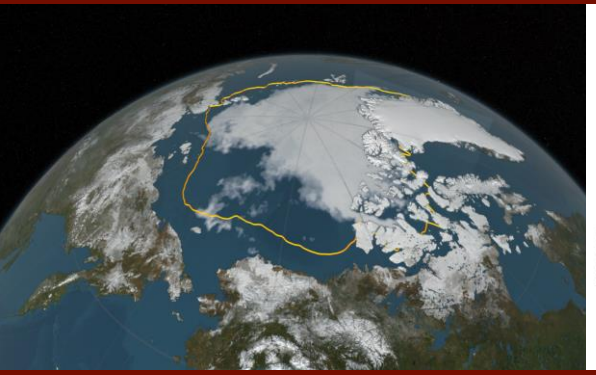
The purpose of this special issue is to review and report on recent advances in the design, implementation, and interpretation of ensembles in climate science. This includes theoretical, mathematical, and computational aspects, therefore bringing together contributions from mathematicians, computational scientists, model users and developers, and climate scientists alike.

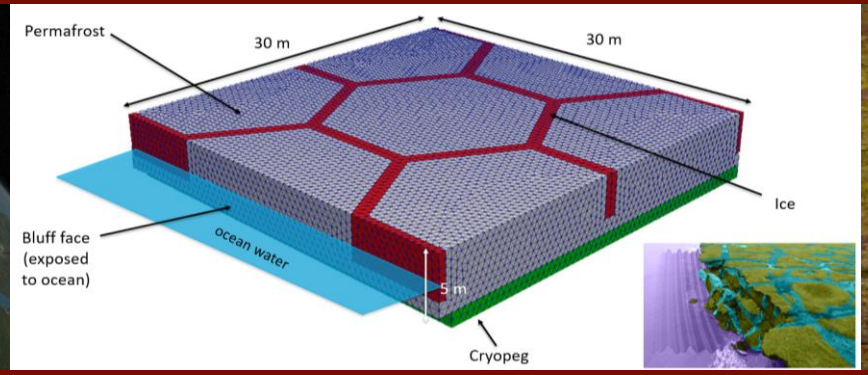
Climate science, in particular climate prediction and projection, are heavily dependent on the use of Earth system models (ESMs), which are nonlinear, complex, and chaotic representations of the Earth's spheres. As such, ESMs are susceptible to various sources of uncertainty. These include uncertainty in the initial state, parameter values, model formulation, structure, and external forcing. Ensembles have become a key tool to quantify these uncertainties and improve predictions. However, challenging questions remain regarding how to design and interpret such ensembles within the constraints of limited computational power and the lack of a rigorous framework for their design. Therefore, this special issue will be a valuable resource to climate scientists working on both theoretical and practical aspects of prediction ahead of Phase 7 of the Coupled Model Intercomparison Project (CMIP7) and future assessments.

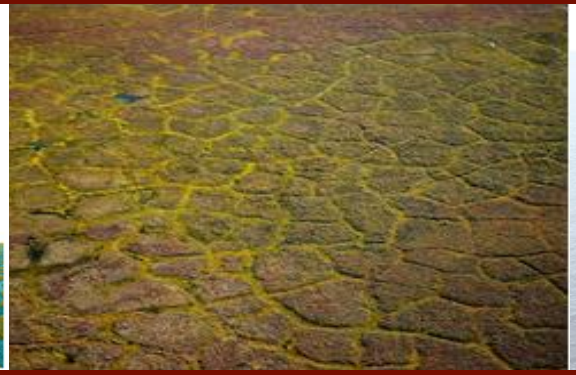
This issue arises from the minisymposium "Theoretical and Computational Aspects of Ensemble Design and Interpretation in Climate Science and Modelling" hosted during the SIAM Conference on Mathematical & Computational Issues in Geosciences in Bergen, Norway (19–22 June 2023). It will feature works by participants as well as external contributions.

- **Earth System Dynamics (ESD)/ Geoscientific Model Development (GMD)/ Nonlinear Processes in Geophysics (NPG)** inter-journal special issue
- **Editors:** Francisco de Melo Virissimo, Irina Tezaur, Eviatar Bach, David Stainforth, Christian Franzke
- Papers due **July 31, 2024**
- More **info** found here: https://esd.copernicus.org/articles/special_issue1278.html
- **Contact:** ikalash@sandia.gov

Exceptional service in the national interest







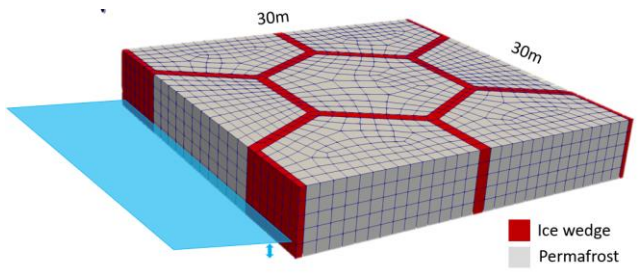
Development and Calibration of the Arctic Coastal Erosion (ACE) Model, Towards UQ of Climate Change-Induced Arctic Permafrost Degradation

Jenn Frederick, Alejandro Mota, **Irina Tezaur**, Charles Choens, Diana Bull, Elyce Bayat
Sandia National Laboratories, USA

Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. SAND2019-7899 C

Outline

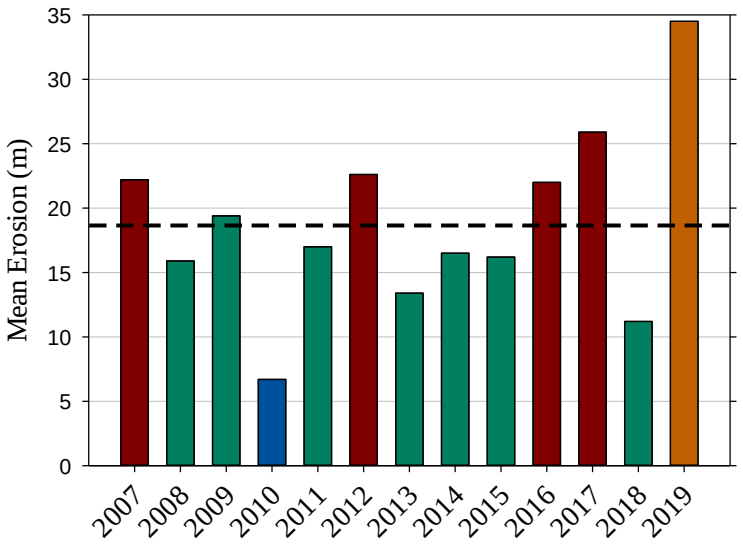
- Motivation and background
- The Arctic Coastal Erosion (ACE) model
  - Birds-eye-view of ACE
  - Thermo-mechanical terrestrial component of ACE
- Numerical results
  - Sensitivity study for 3D elastic mechanics-only simulation
  - Calibration/validation of thermo-mechanical coupling for pseudo-realistic 2.5D slice problem
- Summary
- Current and future work



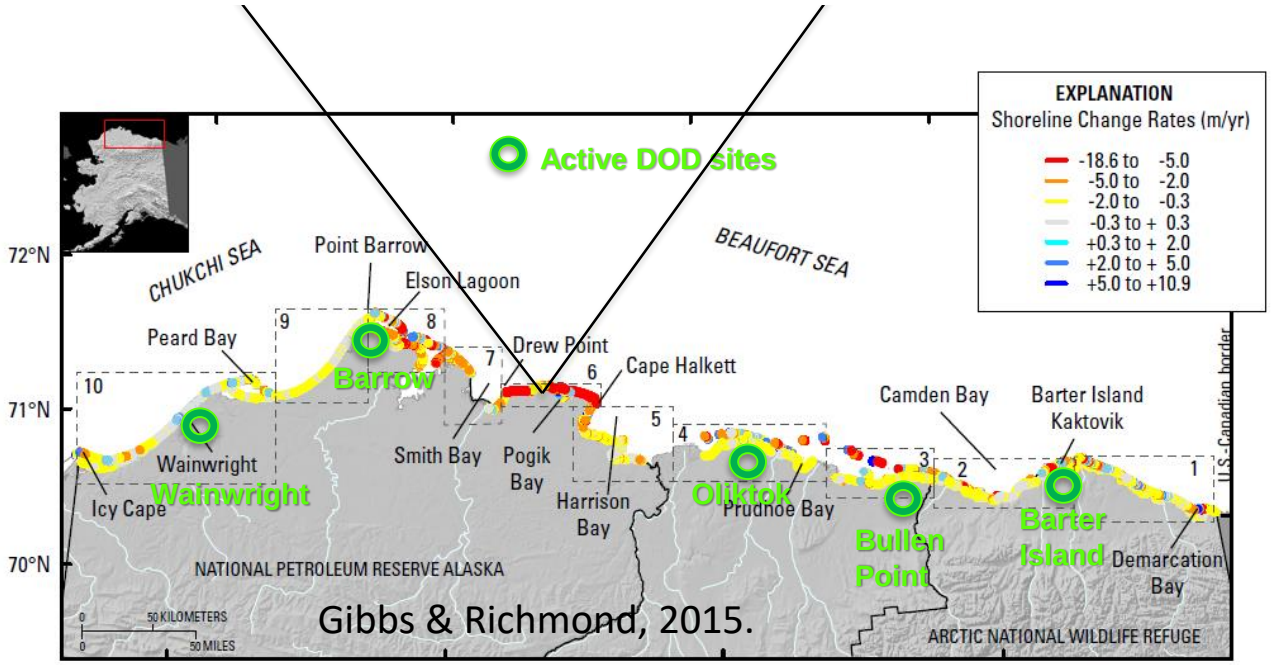
Motivation

The Arctic is warming at **4 times** the rate of the global average resulting in **accelerated rates of coastal erosion**!

- Primary culprit is **loss of Arctic sea ice**: since 1979 sea ice has lost 51% in area and 75% in volume
  - Increasing **ice-free season**
  - Increasing **wave energy** and **storm surge**
  - Increasing **sea water** temperatures



Certain locations lost >250 m (~2 football fields in length) b/w 2007-2019!



Gibbs & Richmond, 2015.

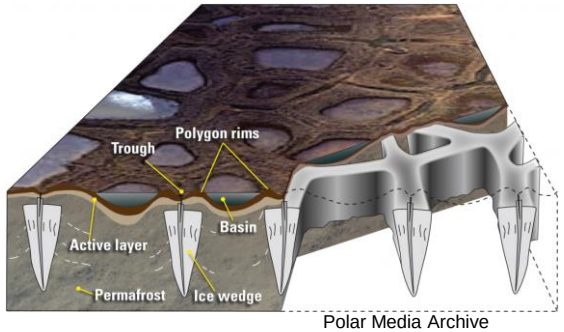
Erosion is threatening:

- **Coastal communities**: threatened with displacement
- **Coastal infrastructure**: active DoD sites, including toxic waste sites, in northern Alaska
- **Global carbon balance**: permafrost stores greenhouse gases (CO_2, CH_4, NO_2).

Permafrost thaw & erosion

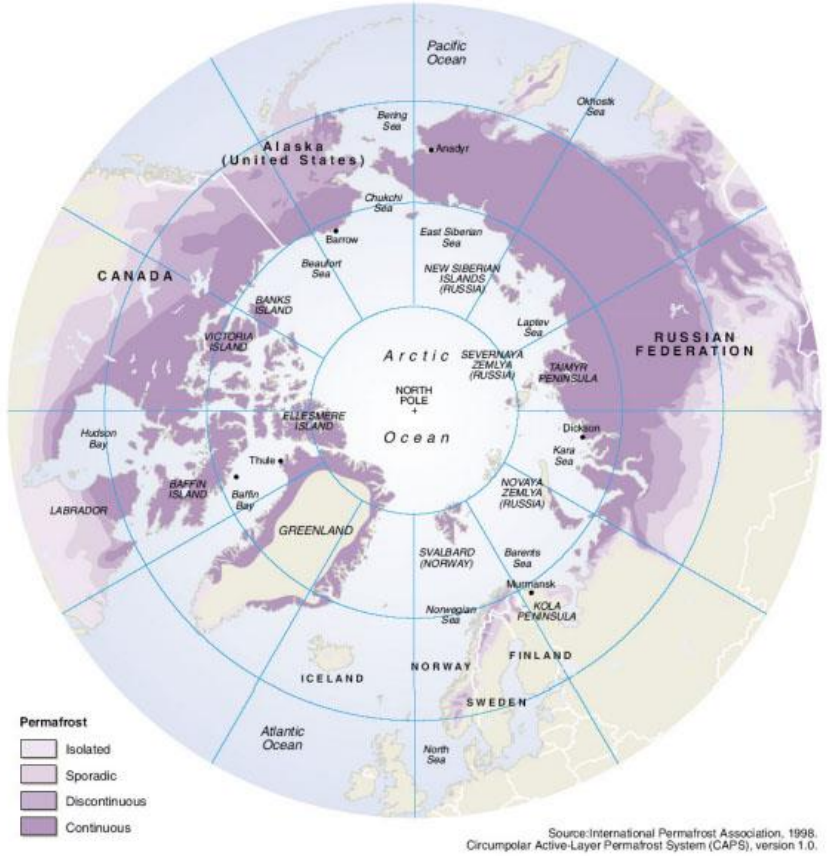
What is permafrost?

- Ground that remains frozen for 2+ consecutive years.
- 24% of ice-free land area in Northern Hemisphere and 85% of Alaska, Greenland, Canada and Siberia contains permafrost.
- 34% of global coastline is permafrost.



Polar Media Archive

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



Brown *et al.* 1998.

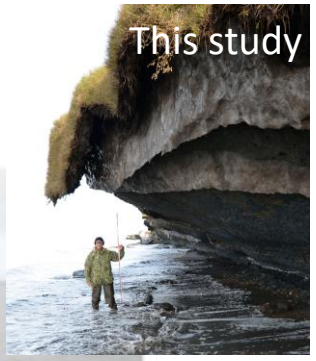
Martin *et al.* 2009.

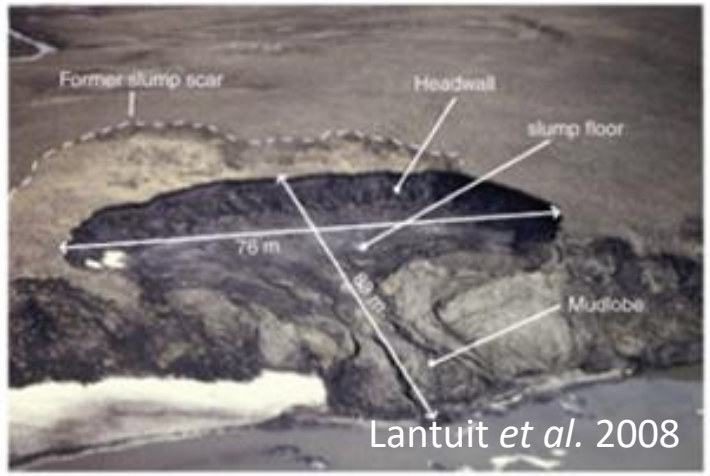
Unique coastal permafrost erosion process in Arctic:

- Predominant geomorphology: **ice-wedge polygons**
  - Ice acts to **bind** unconsolidated soils in permafrost.
  - Ice wedges **grow/expand** up to 10s meters wide and deep.
  - Permafrost thaw can cause subsidence, slumping, **weakening**.

Coastal permafrost failure mechanisms

- **Retrogressive thaw slumping**: a slope failure characterized by thaw of exposed ground ice and slumping of thawed soil, typically caused by thermo-denudation[1].
- **Active layer detachment**: failures are translational landslides that occur in summer in thawing soil overlying permafrost, typically caused by thermo-denudation[1].
- **Block failure**: a niche (recess at bluff base) progresses landward until the overhanging material fails in a shearing or toppling mode known as block failure, caused by thermo-abrasion[2].
  - ➢ Fallen blocks can disintegrate in the near-shore environment **within 1-2 weeks**!





Retrogressive thaw slumping

Active layer detachment

Block failure

[1]Thawing of permafrost bluffs that proceeds under the influence of gravity. [2]Undercutting of permafrost bluff by warming ocean.

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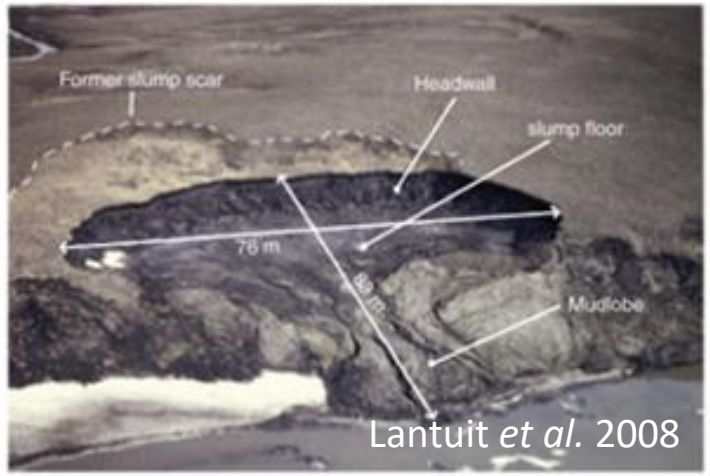

Retrogressive thaw slumping

Active layer detachment

Block failure

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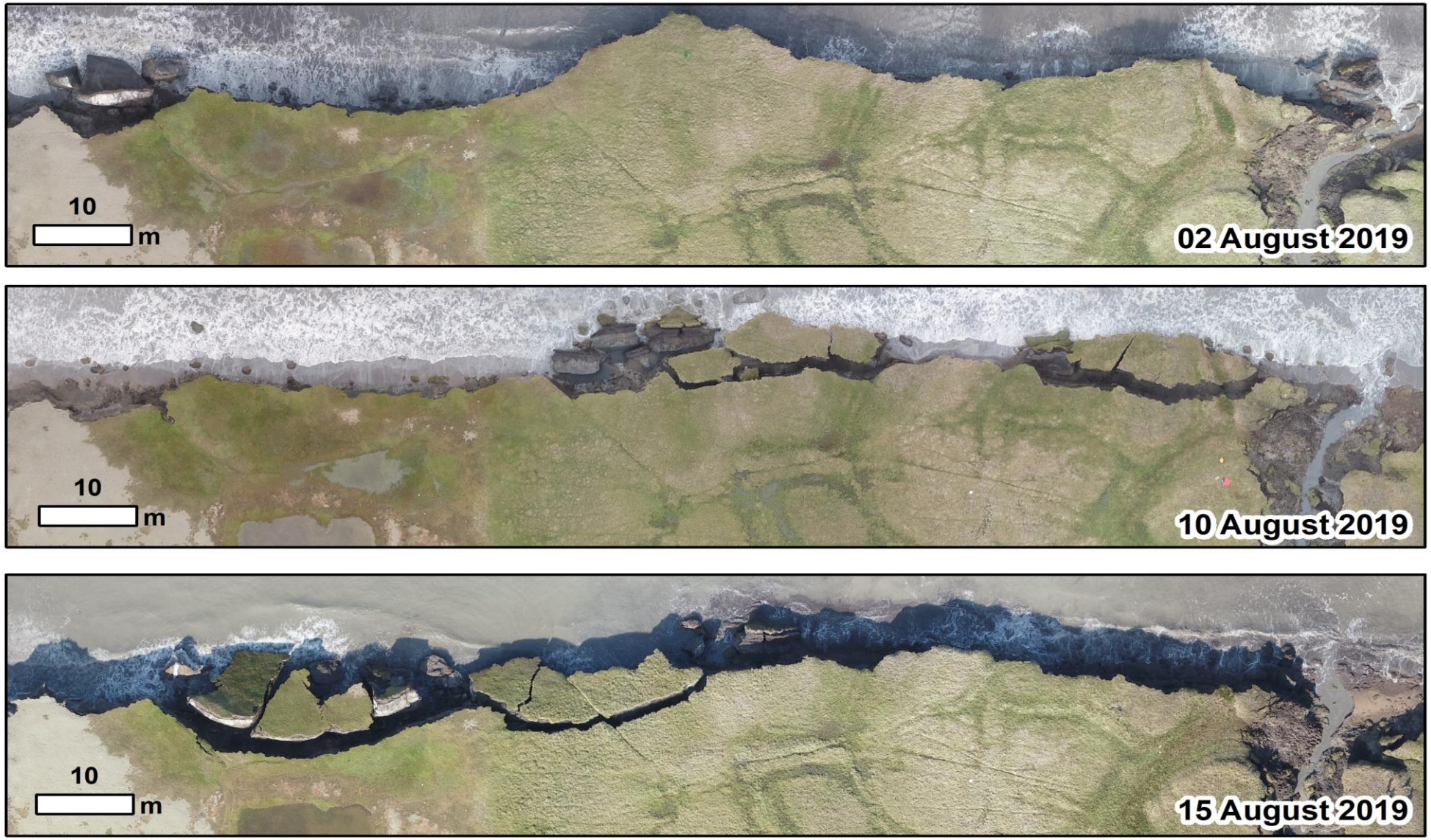
Example of bluff erosion during 2019 UAV surveys*



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

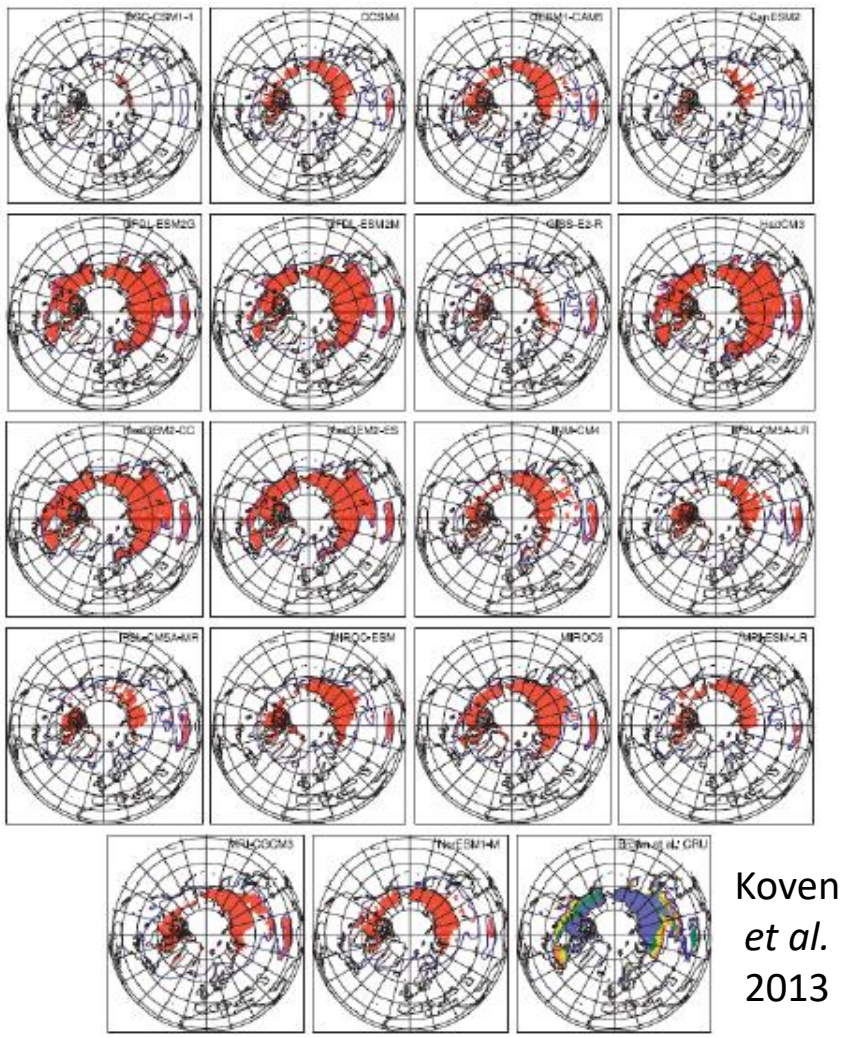
*Images courtesy of Ben Jones, UAF

State-of-the-art in permafrost modeling

Most **existing permafrost models*** (including Earth System Model-, or ESM-, coupled models) are fairly **primitive**!

- Most models were based on **trend projection** and/or **empirical relationships**
- **Limited PDE-based models**: primarily **thermal models**, e.g., 1D steady state heat flow (no mechanics/deformation)
- Most models assumed a **particular type** of **erosion** (e.g., block failure)
- Models **did not** include **realistic boundary conditions** and **did not** account for permafrost **geomorphologies** or **geophysics**.

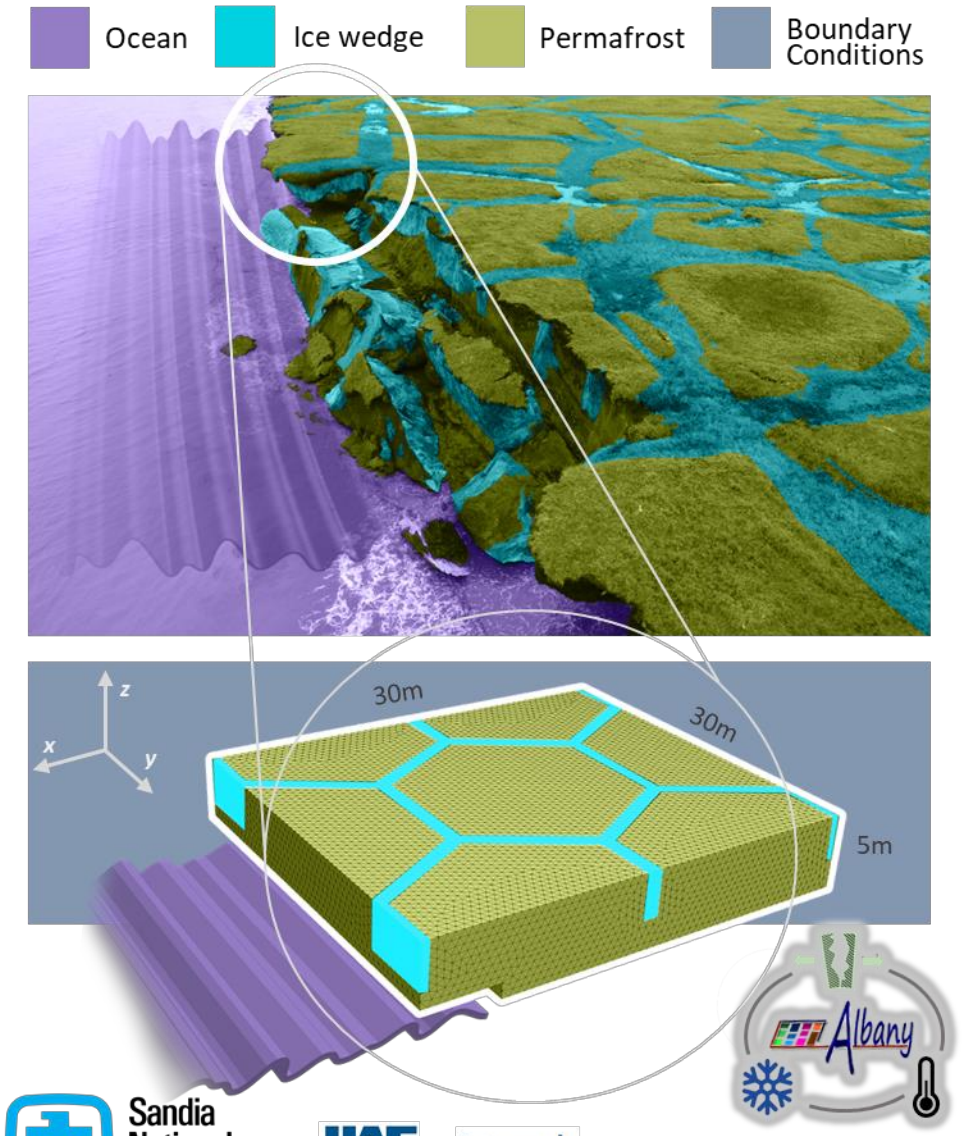
Premise behind ACE: an accurate, **predictive** Arctic coastal erosion model must **couple** the influences of evolving **wave dynamics**, **thermodynamics** and **mechanics**.



Koven *et al.* 2013

* See (Frederick *et al.* 2016), Chapter 5, for extensive overview.

Arctic Coastal Erosion (ACE) model



LOCATION SPECIFIC DATA

BOUNDARY CONDITIONS

Reanalysis (ASR & ERA) *(Historic)*

HYCOM *(Historic)*

SNAP Downscaled RCP 8.5 Earth System Models *(Projections)*

- WIND SPEED / DIRECTION
- ATMOSPHERIC TEMP
- PERMAFROST TEMP
- OCEAN ICE EXTENT
- OCEAN CURRENTS
- OCEAN TEMP

TERRESTRIAL \ TERRESTRIAL

Albany: 3-D multi-physics based finite element model

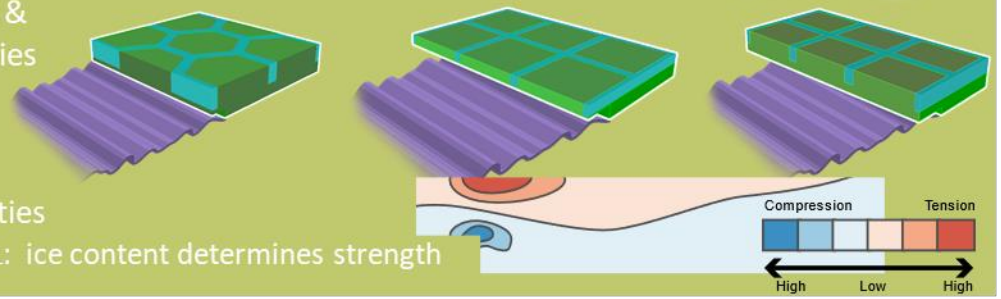
MECHANICAL: finite deformation plasticity model

THERMAL: transient temperature and ice saturation evolution

Geomorphology & Material Properties

Strength Properties

MATERIAL: ice content determines strength

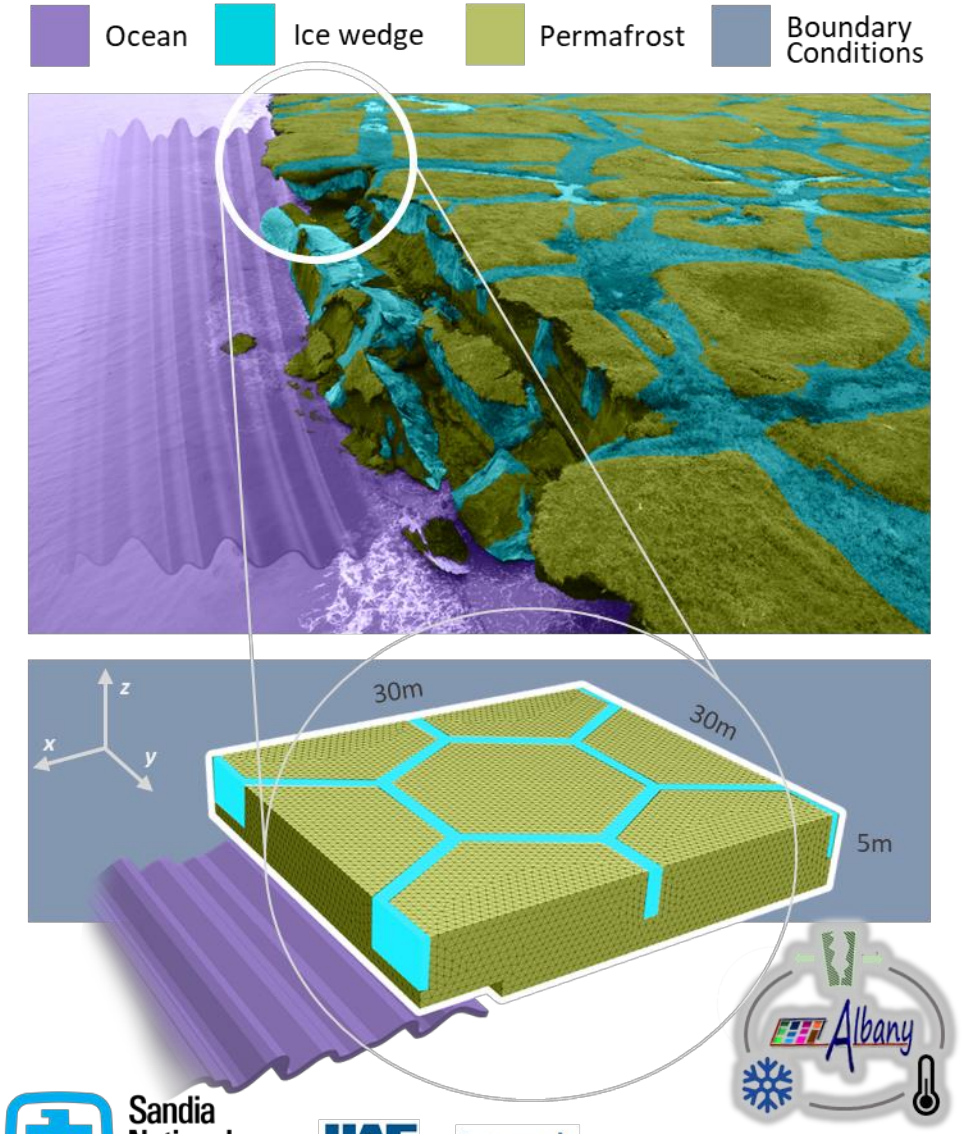


OCEAN

Circum-Arctic: wave energy

Nearshore: coupled wave & circulation

Arctic Coastal Erosion (ACE) model



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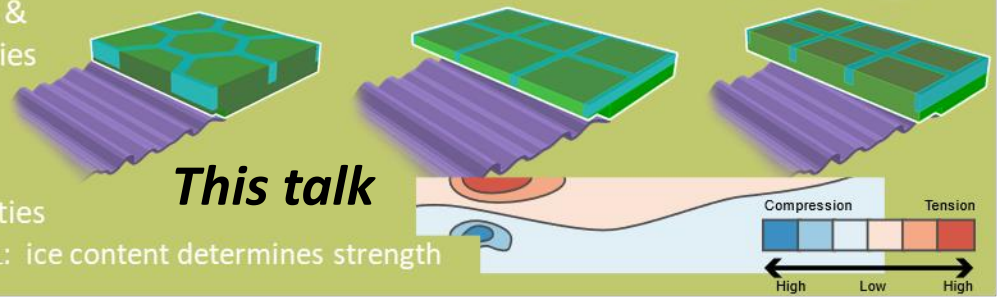
This talk



OCEAN

Circum-Arctic: wave energy

Nearshore: coupled wave & circulation

Finite element implementation in Albany-LCM

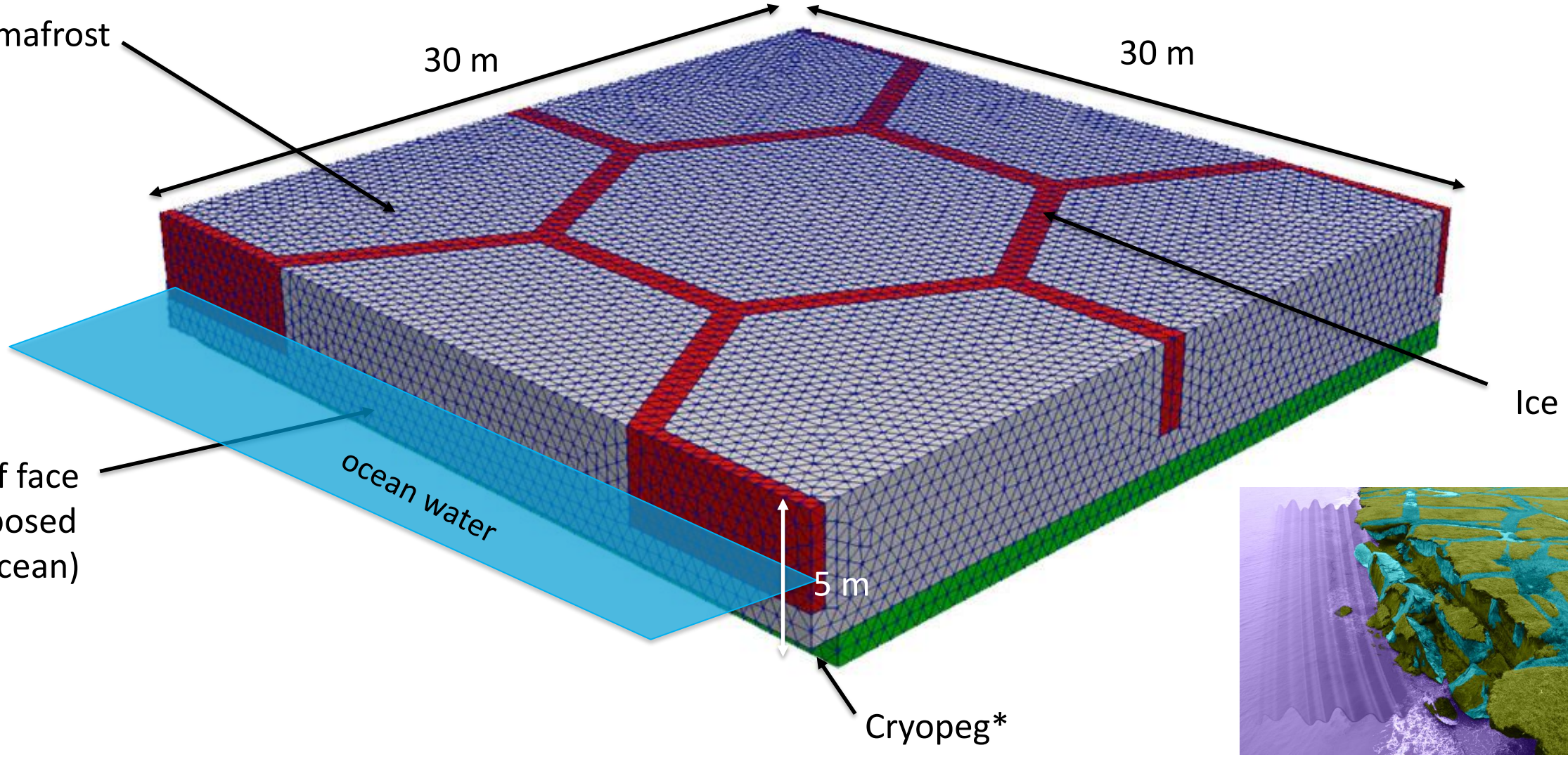
The ***thermo-mechanical Arctic Coastal Erosion (ACE)*** model is implemented within the ***LCM project*** in Sandia's open-source parallel, C++, multi-physics, finite element code, ***Albany***.

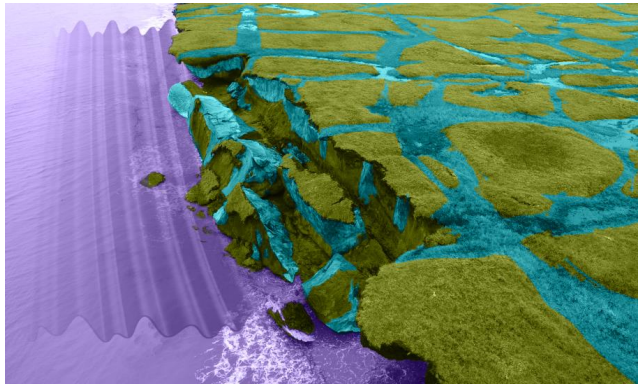
https://github.com/sandialabs/LCM

- ***Component-based*** design for rapid development.
- Contains a wide variety of ***constitutive models***.
- Extensive use of libraries from the open-source ***Trilinos*** project.
  - Use of the ***Phalanx*** package to decompose complex problem into simpler problems with managed dependencies.
  - Use of the ***Sacado*** package for ***automatic differentiation.***
- All software available on ***GitHub***.

https://github.com/trilinos/trilinos

Anatomy of a canonical computational domain





* Layer of unfrozen ground that is perennially cryotic (forming part of the permafrost) in which freezing is prevented.

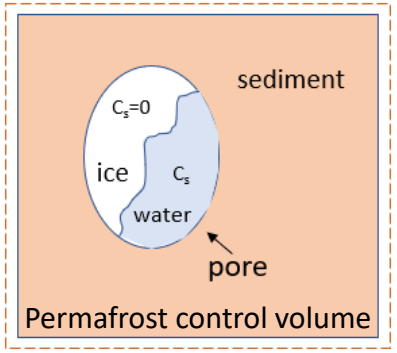
Thermal model

- ***Transient heat conduction*** in a non-homogeneous porous media with water-ice phase change:

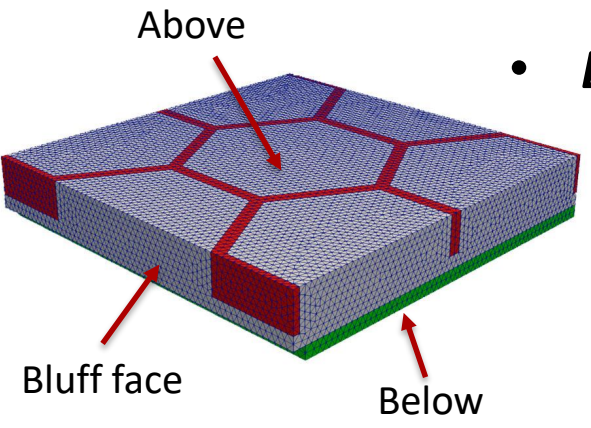
$$(\overline{\rho c_p} + \widetilde{\Theta})\frac{\partial T}{\partial t} = \nabla \cdot (\boldsymbol{K} \cdot \nabla T)$$

where $\widetilde{\Theta} := \rho_f L_f \frac{\partial f}{\partial T}$ incorporates phase changes through soil freezing curve, $\frac{\partial f}{\partial T}$.

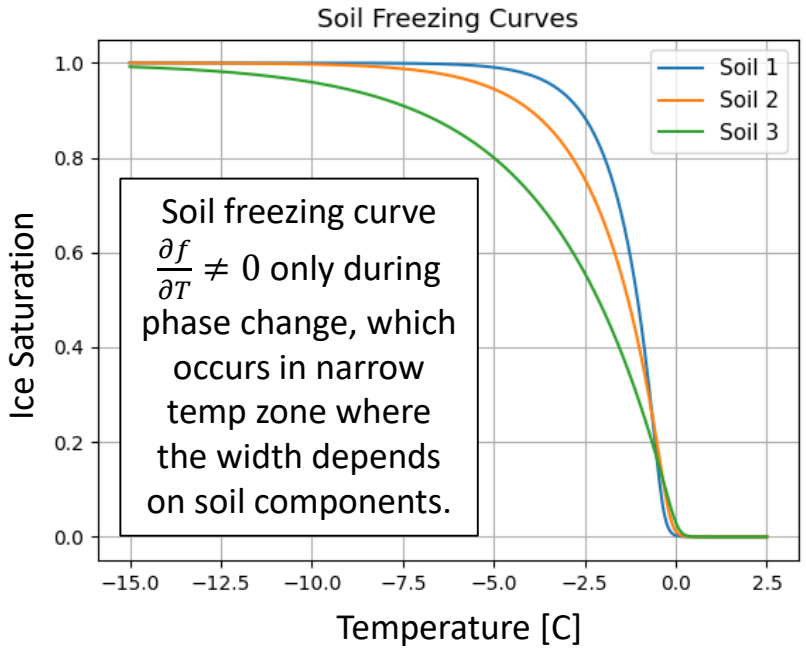
➢ Computes ***temperature*** T and ***ice saturation*** f



$\bar{\rho}$: density from mixture model
$\overline{c_p}$: specific heat from mixture model
$\boldsymbol{K}$: thermal diffusivity tensor
ρ_f: ice density
L_f: latent heat of water-ice phase change
f: ice saturation ($\in [0,1]$)
$\frac{\partial f}{\partial T}$: soil freezing curve (depends on salinity)



- ***Boundary conditions*** (from wave model/data)
  - ➢ Local geothermal heat flux from below
  - ➢ Air temp* from above
  - ➢ Air/ocean temp at bluff face
  - ➢ Ocean salinity at bluff face**



* Or, alternatively surface ground temperature (if available). ** Used to modify melting temperature of ice.

Mechanical model

- Finite deformation ***time-dependent*** variational formulation for ***solid mechanics problem*** obtained by minimizing the energy functional:

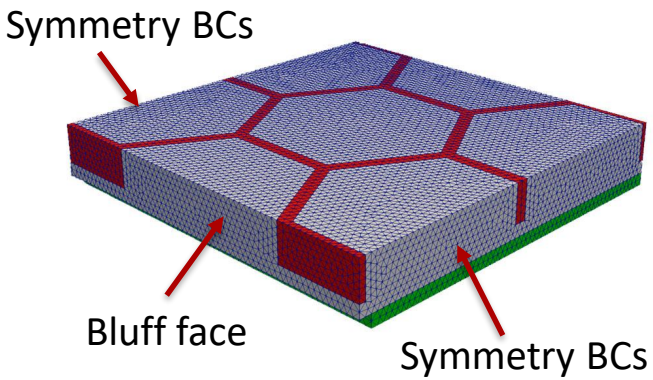
$$\Phi[\boldsymbol{\varphi}] := \int_{\Omega} A(\boldsymbol{F}, \boldsymbol{Z})\, dV - \int_{\Omega} \rho \boldsymbol{B} \cdot \boldsymbol{\varphi}\, dV - \int_{\partial_{\boldsymbol{T}}\Omega} \boldsymbol{T} \cdot \boldsymbol{\varphi}\, dS$$

$A(\boldsymbol{F}, \boldsymbol{Z})$: Helmholtz free-energy density
$\boldsymbol{Z}$: material variables
$\boldsymbol{F}$: deformation gradient ($\nabla \boldsymbol{\varphi}$)
ρ: density
$\boldsymbol{B}$: body force
$\boldsymbol{T}$: prescribed traction

  - Computes ***displacements*** and ***new computational geometry*** (following erosion)

- ***J_2 plasticity*** extended to large-deformation regime ***constitutive model*** for ***ice*** and ***permafrost***
  - ***Incorporates all mechanisms*** that lead to deformation and plastic flow of polycrystalline materials like ice; ***minimal*** calibration ***parameters***; ***simplest*** material model w/ plastic behavior
  - Constitutive model is a function of f, the ***ice saturation***, which comes from the ***thermal problem***

- ***Boundary conditions:***
  - ***Symmetry BCs*** on lateral sides
  - ***Wave pressure Neumann BC*** on bluff face* (from wave model)
  - **Damage variable** on bluff face in contact with ocean (introduces softening due to dissolution by lowering elastic modulus E)



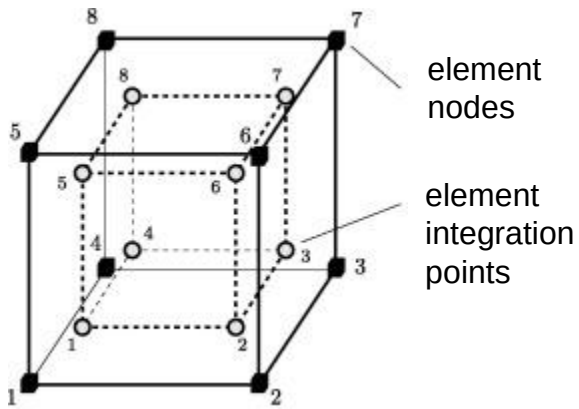
* Holthuijsen 2007.

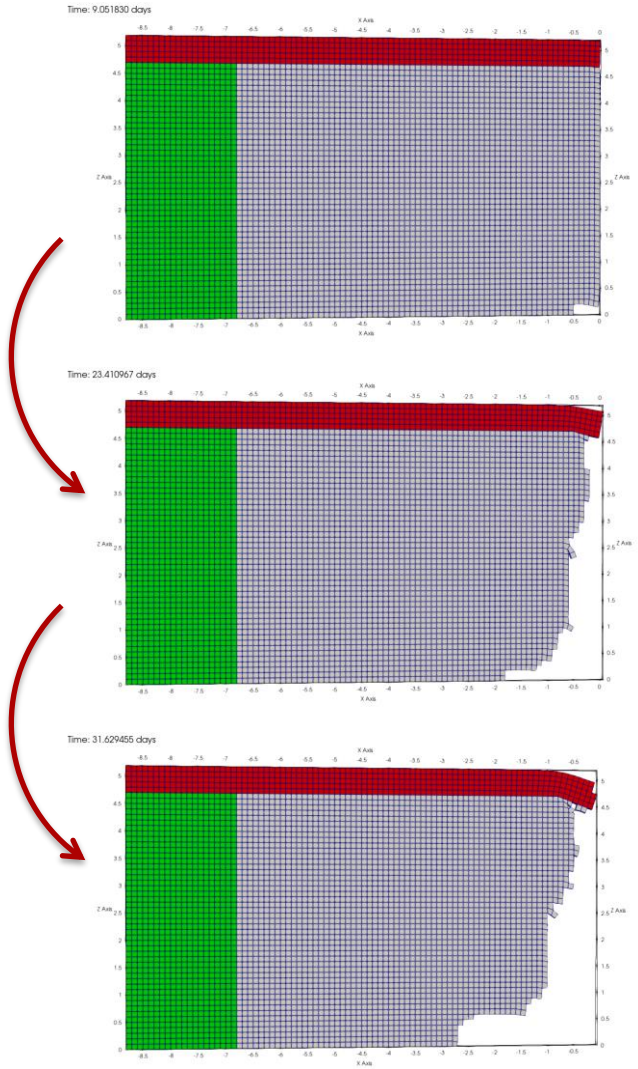
Erosion failure criteria

- **Stress criterion:** when material reaches a critical value of the stress in tension or compression.

- **Strain criterion:** when material reaches a critical strain limit defined as a function of peat content (distortion).

- **Kinematic criterion:** when material has tilted excessively, or exceeded a maximum physical displacement, it is assumed to have fallen as part of block erosion.





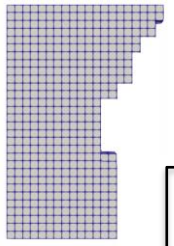
When any of the **failure criteria** are reached for all integration points within an element, “failed” elements are **removed** from mesh.

Coupled thermo-mechanical formulation

Potential key advantages:

- Failure modes develop from **constitutive relationships** in FEM model (no empirical relationships!)
- 3D unsteady heat flow can include **chemistry**
- Thermal and mechanical problems can be advanced using **different time-steppers** (e.g., implicit-explicit coupling)
- **Coupled** mechanical + thermal states

Unique characteristic of coupled model: coupling happens at the level of material model

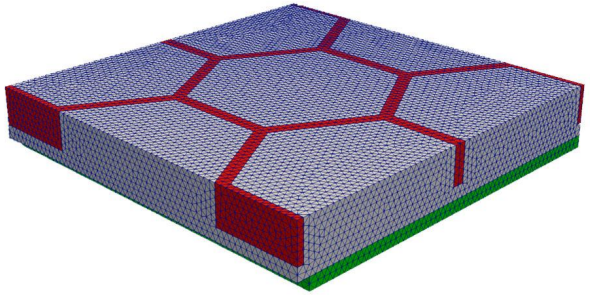


Thermal:

Inputs: geometry, sediment type, porosity, salinity

Outputs: temperature field, ice saturation

Eroded geometry



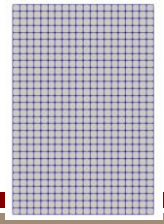
Albany-LCM

Ice saturation

Mechanical:

Inputs: ice saturation, mechanical parameter relationships as function of sediment type and ice saturation

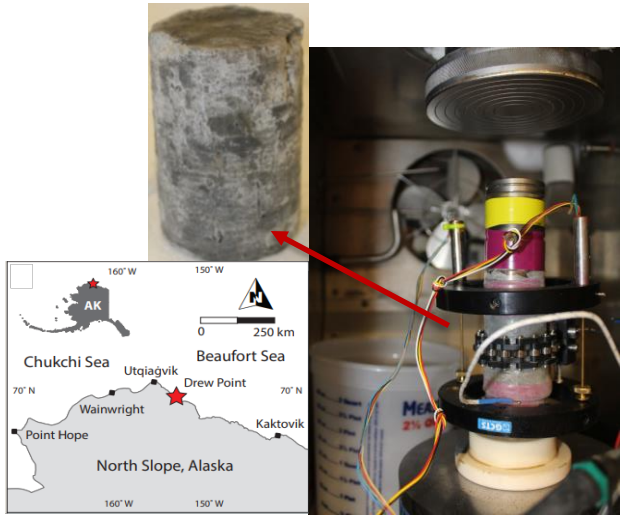
Outputs: displacements, eroded geometry

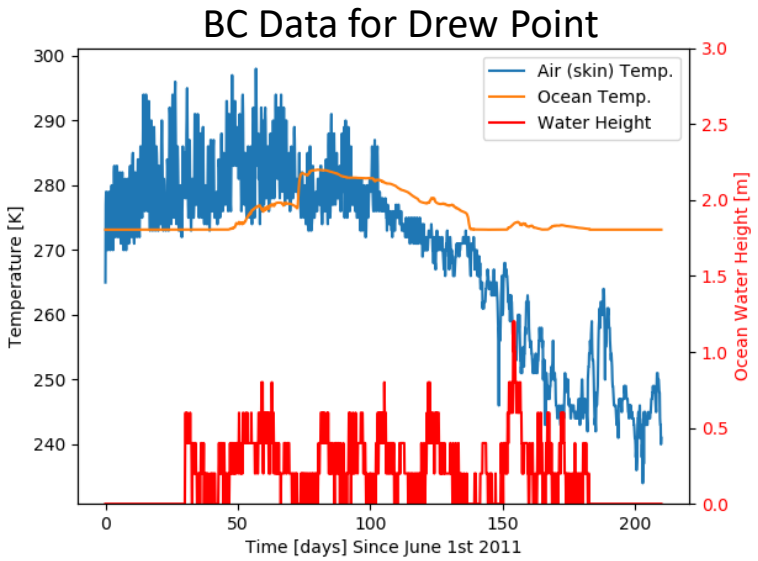


Parameters & inputs

Parameters estimated from core lab experiments:

- Elastic modulus, Poisson's ratio, yield strength
- Sand/silt/clay/peat fractions with depth
- Porosity with depth
- Salinity with depth



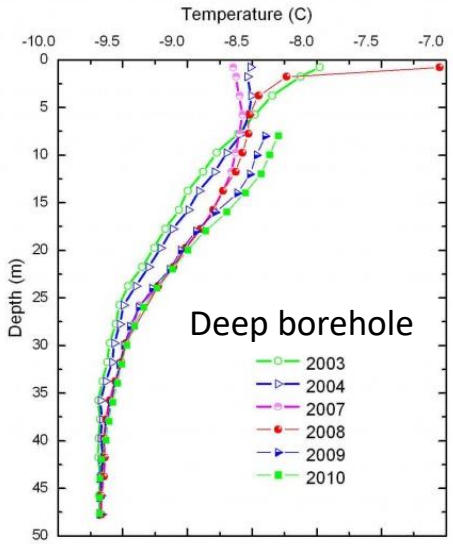


Parameters from literature:

- Ice/water/sediment densities, thermal conductivities, heat capacities
- Freezing curve/width as function of sediment type

Parameters estimated from observational data at Drew Point, AK:

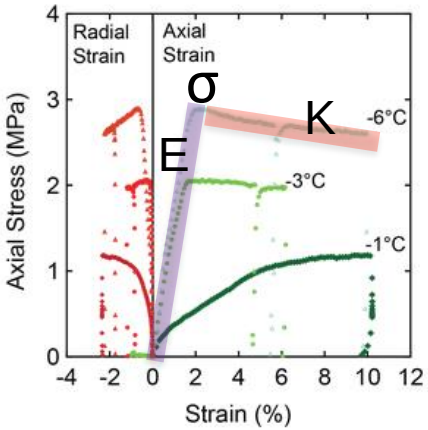
- Air temp w/ time, initial bluff temp (USGS weather station data)
- Geothermal heat flux (borehole at Barrow, AK)
- Polygon dimension, ice wedge thickness and depth, bluff height, organic layer (peat) thickness (Aug. 2019 field campaign)

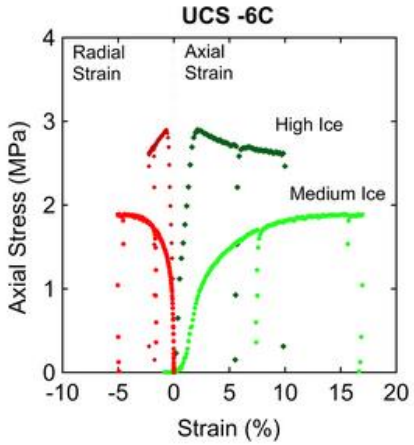


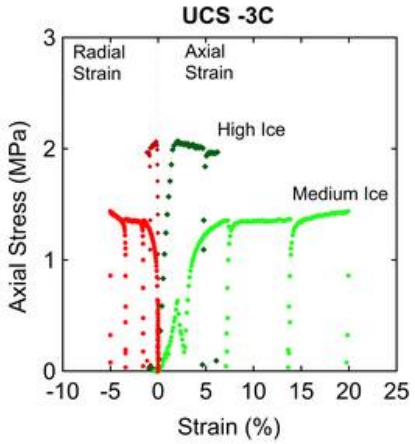
Parameters from wave model (WW3+SWAN+Delft3D):

- Ocean temperature, salinity and sea-level w/ time (for thermal and wave pressure mechanical BCs)

Material model calibration to experimental data





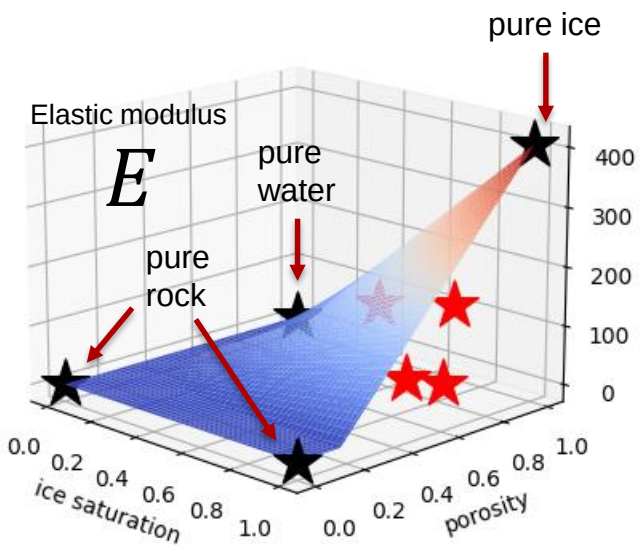


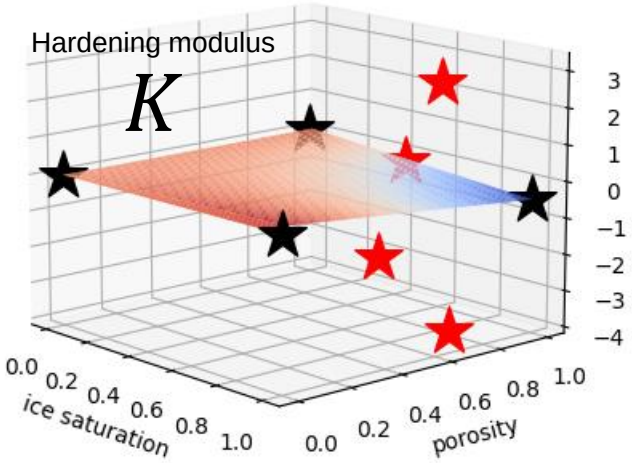
Experimental results on permafrost core samples used to create fits for E, K, σ as a function of **ice saturation** and **porosity**.

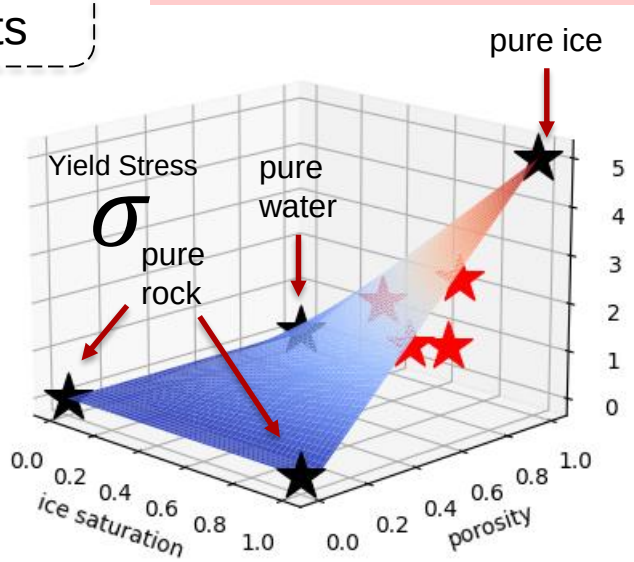
Experiments are very **challenging** to perform and provide **limited data**!

★ experimental data points

★ theoretical data points







3D elastic mechanics-only sensitivity study

<u>Goal:</u> assess ***impact*** of ***bluff geometry*** and ***material variability*** on stress states leading up to bluff failure, and use results to ***inform thermo-mechanical*** analyses

- **Geometric parameters varied**: niche height (N_H), niche depth (N_D), bluff height (B_H), permafrost block size (B_S), ice wedge thickness (I_W), ice wedge depth (I_D)
- **Mechanical properties varied:** bulk density (ρ_b), Young's modulus (E), Poisson's ratio (υ)
- **Parameter ranges:** informed by field observations, visual inspection of UAV-based aerial photography and mechanical testing of permafrost samples (see Thomas *et al.*, 2020)
- **Output QOIs**: location (indicated by star) and magnitude of simulated maximum tensile stress ($\sigma_{T_{\max}}$)


frontiers in Earth Science

ORIGINAL RESEARCH
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Geometric and Material Variability Influences Stress States Relevant to Coastal Permafrost Bluff Failure

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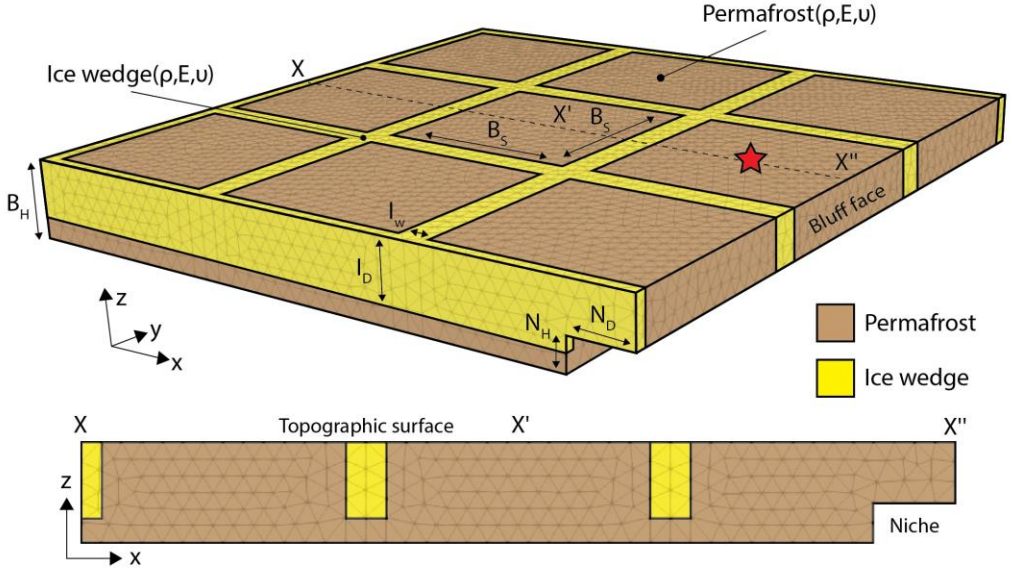
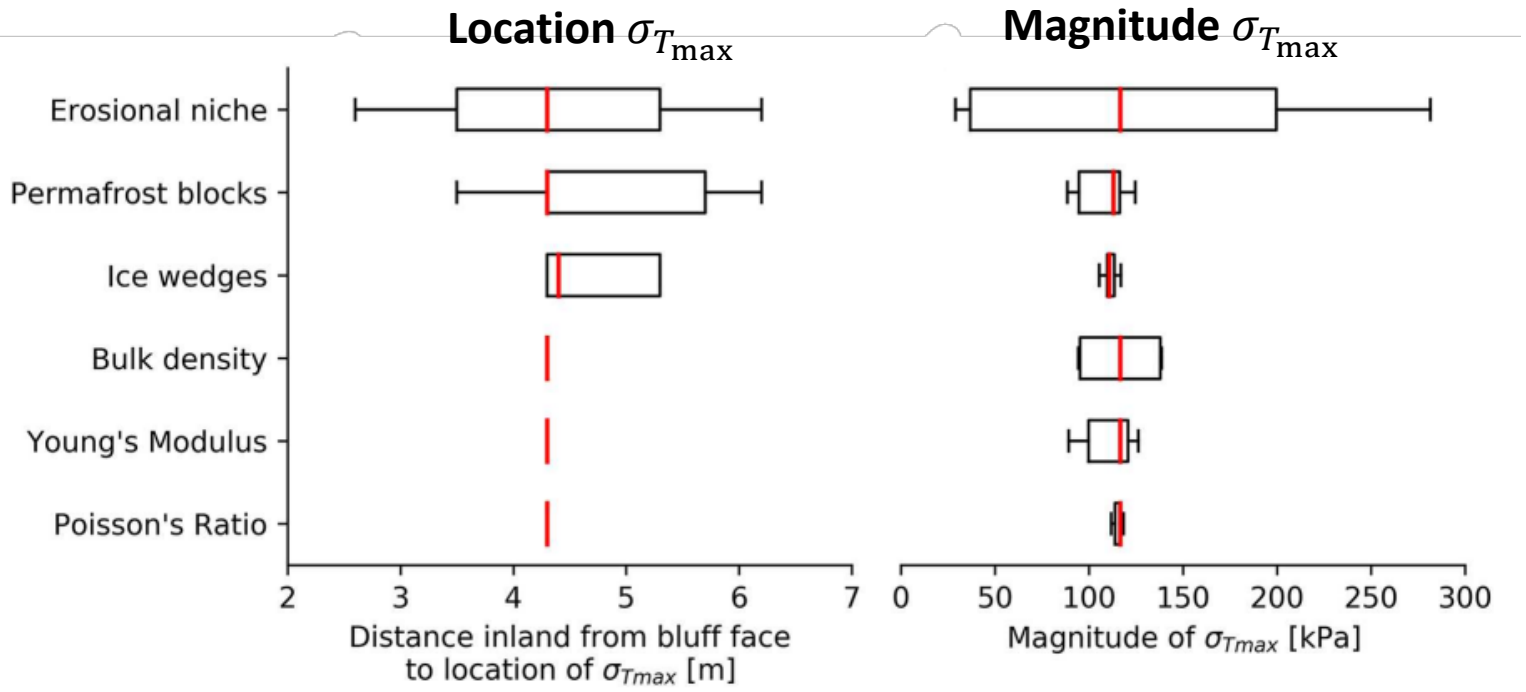


3D elastic mechanics-only sensitivity study



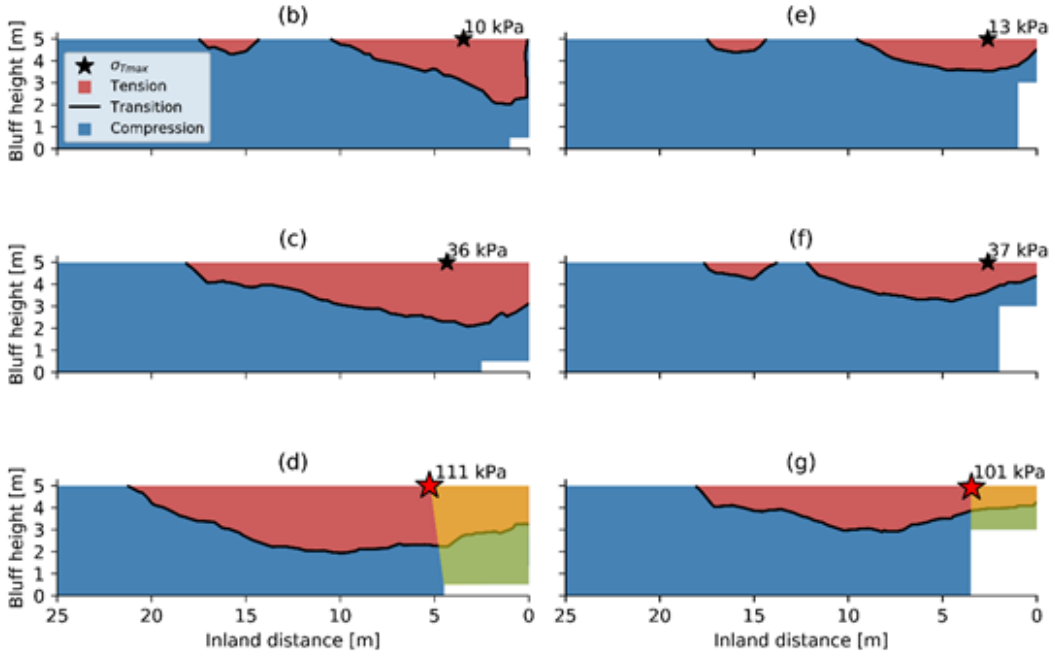
Erosional niche properties: N_H & N_D
Permafrost blocks: B_H & B_S, Ice wedges: I_W & I_D

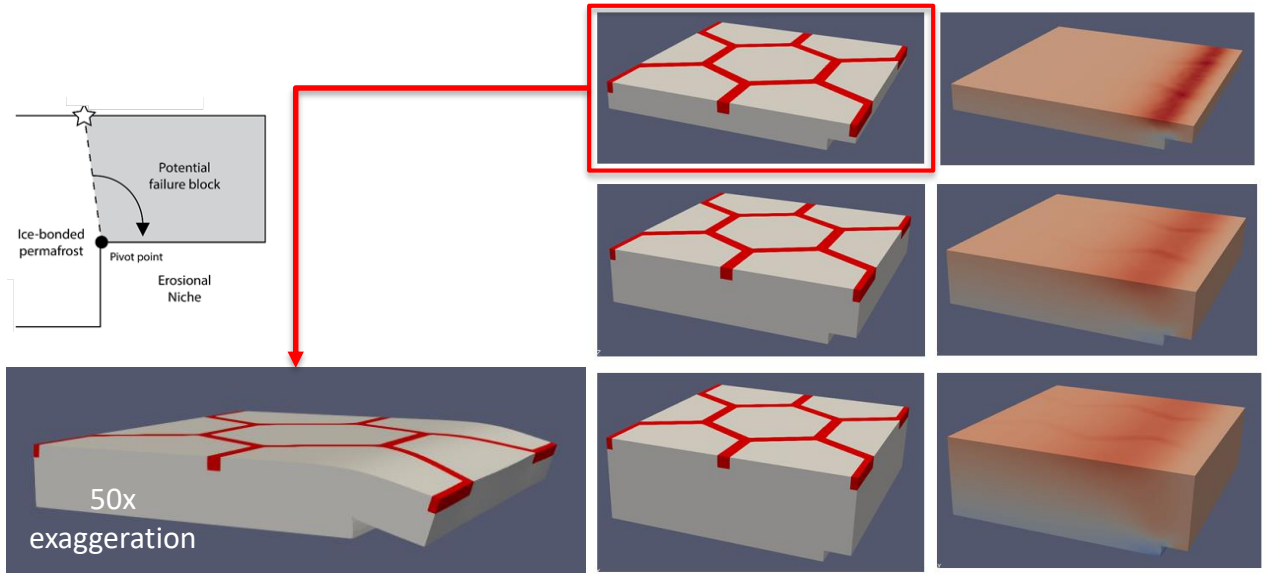
- ***Niche characteristics*** exert the largest impact on the ***location*** and ***magnitude*** of $\sigma_{T_{\max}}$
- Variability in ***material properties*** influences ***magnitude*** of $\sigma_{T_{\max}}$ but not its ***location***

Parameter	Unit	Min	Max	Base
N_H	m	1	3	2
N_D	m	2	6	4
B_H	m	2.5	7.5	5
B_S	m	10	20	15
I_W	m	1	3	3
I_D	m	50%B_H	100%B_H	75%B_H
ρ_b permafrost	kg/m^3	1000	1500	1250
E permafrost	Pa	1e8	1e9	5e8
υ permafrost	–	0.1	0.4	0.25
ρ_b ice	kg/m^3	871	963	917
E ice	Pa	5e8	1e9	7.5e8
υ ice	–	0.1	0.4	0.25

3D elastic mechanics-only sensitivity study

Niche dimension affects location and magnitude of simulated **max tensile stress** ($\sigma_{T_{\max}}$) more than the bluff height, ice wedge polygon size, ice wedge geometry, bulk density and Poisson's ratio



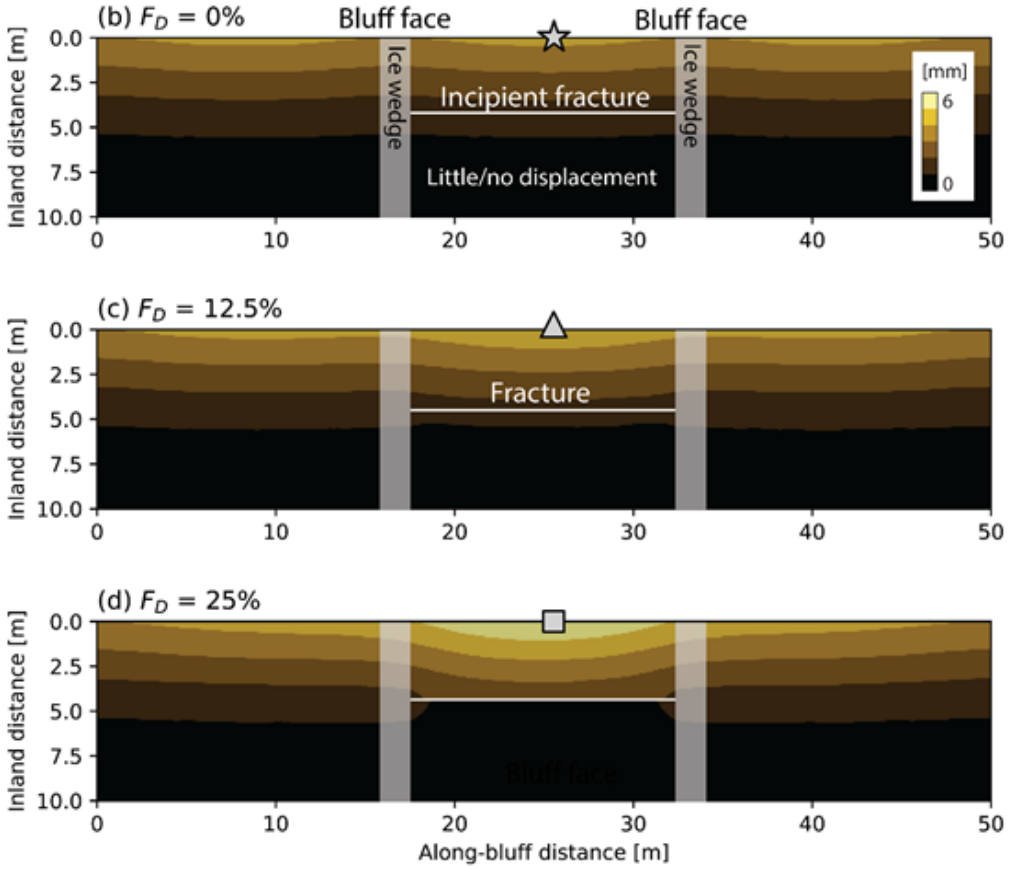


Figures plot tensile stress. Lower bound for failure: 100 kPa (from lab measurements).

- ***Taller*** and ***narrower*** erosional ***niches*** promote ***smaller failure masses*** compared to those with ***shorter*** and ***deeper niches***. Orange/green shading highlights potential ***failure areas*** (left figure).
- As niche advances into the block, an overhanging section in the block acts as ***cantilever*** (right figure).
- Highest ***tensile stresses*** develop on top surface where cantilever meets rest of block (right figure).

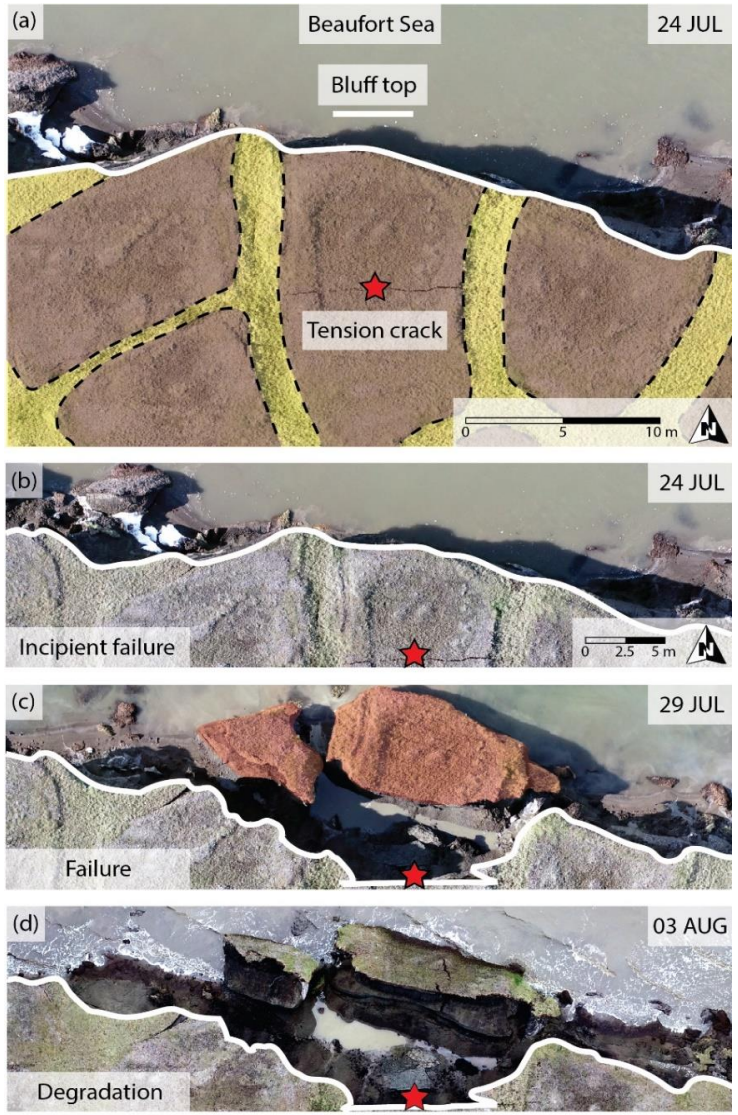
3D elastic mechanics-only sensitivity study

- **Observations** have shown that **failure** can occur **along tension cracks** in ice wedge polygon centers
- ***Additional sensitivity study:*** introduce **vertical fractures** having fracture depth F_D from 0 to 25% B_H



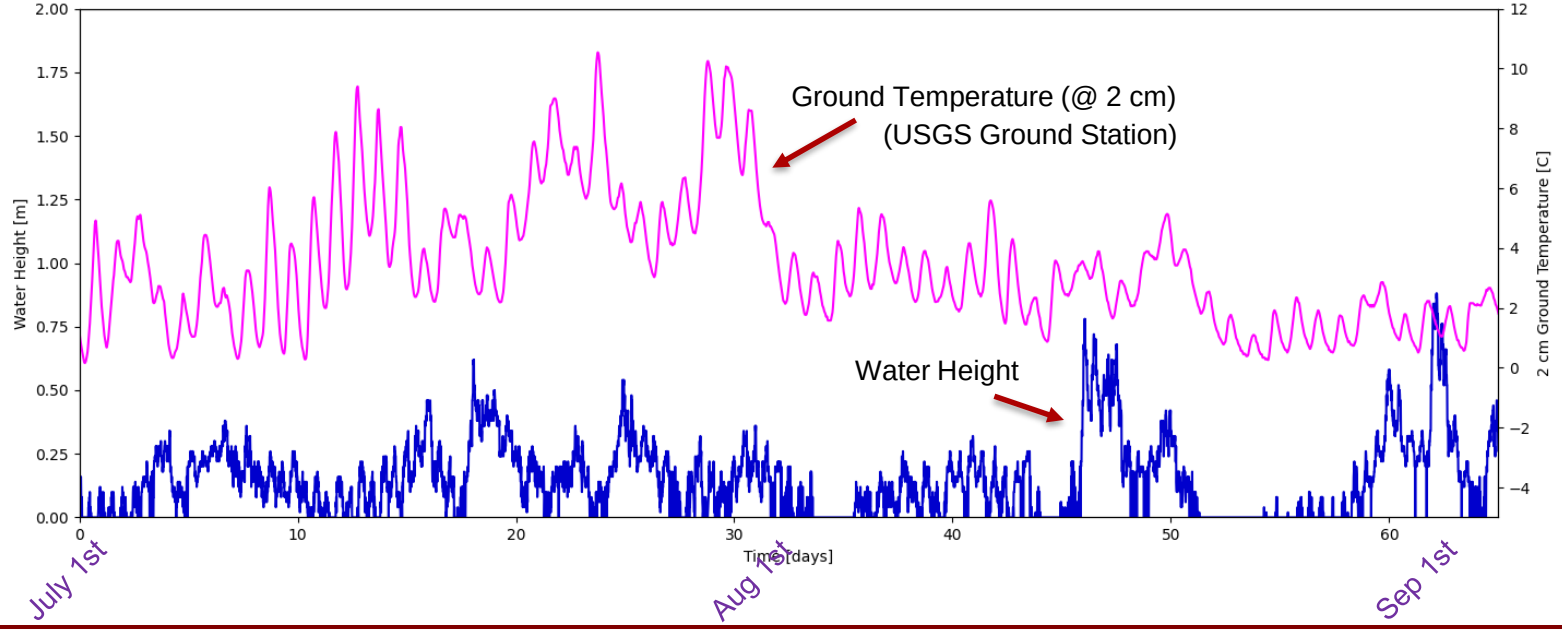
Left figure: highest F_D produces ~40% **more displacement** than lowest F_D, suggesting that the presence of a **tension crack** prior to failure can **induce localized displacement**

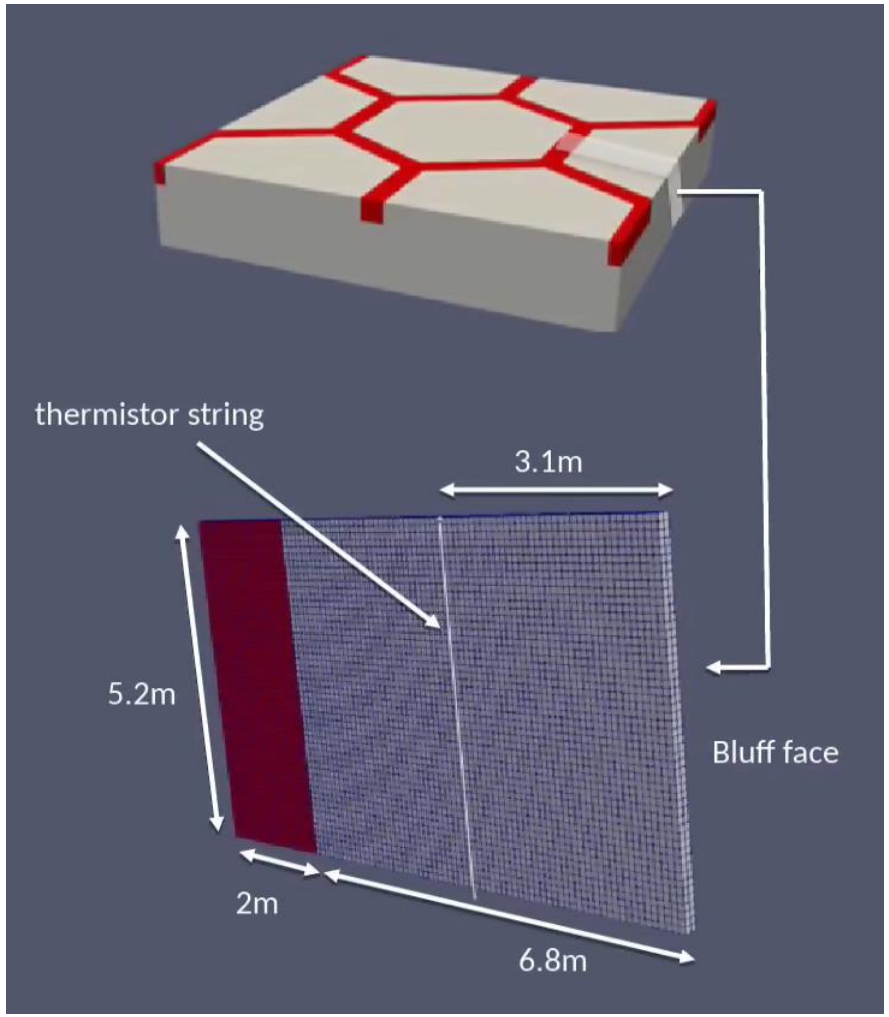
<u>Takeaway:</u> even relatively **shallow vertical cracks** can **concentrate strain** within ice-bonded permafrost bluffs.



Thermo-mechanical coupling: 2.5D slice

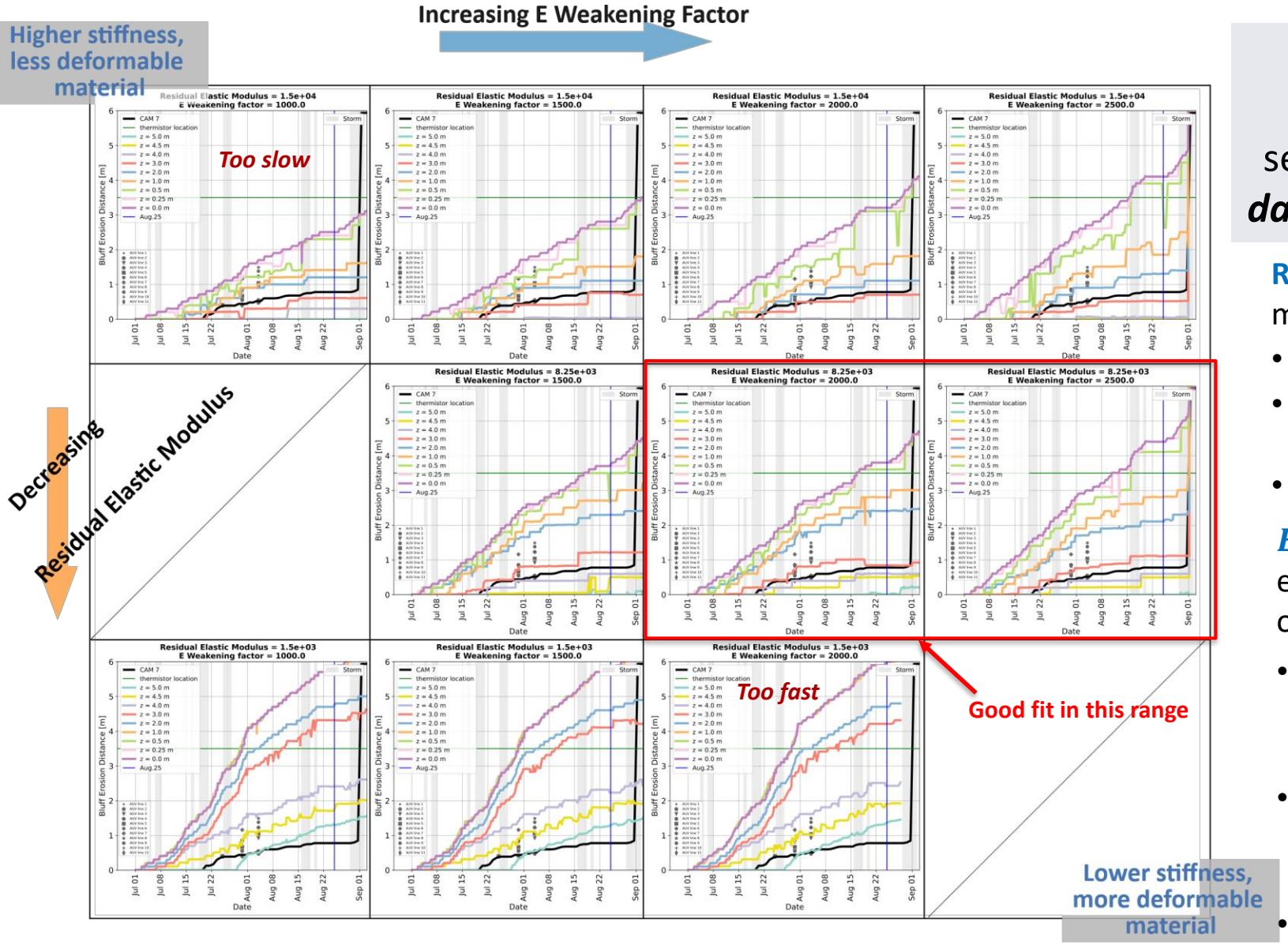
- Computational domain is ***2.5D cross-section*** of archetypal 3D bluff geometry discretized using a uniform hex grid
  - ***Pseudo-realistic problem*** with ***realistic oceanic and atmospheric forcing BC data*** occurring at Drew Point, AK in summer 2018
  - ***Initial temperature field*** obtained from vertical thermistor string placed into DP1-1 ice core at Drew Point





2.5D slice thermo-mechanical sensitivity study

Sandia National Laboratories



E weakening factor and redidual E parameters ***hand-calibrated*** through sensitivity studies s.t. ***niche growth*** and ***day/time of collapse*** match ***observations***

Residual Elastic Modulus: lowest value the elastic modulus, $E = f(\textit{ice saturation}, \textit{porosity})$, can take

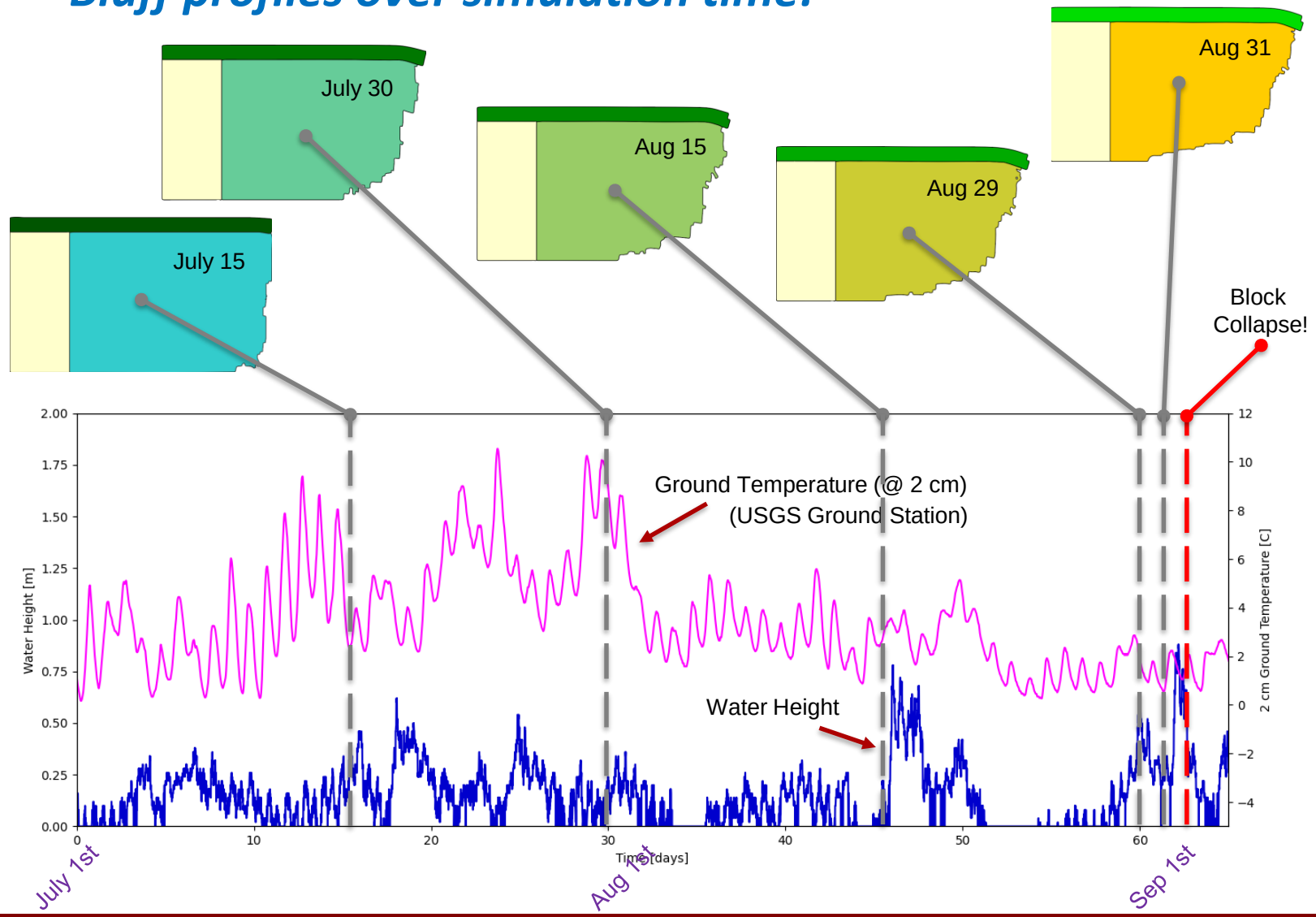
- **Increasing value** → less deformation/unit stress
- **Decreasing value** → more deformation/unit stress → material more likely to fail in strain
- Plays strong role in **rate of denudation**

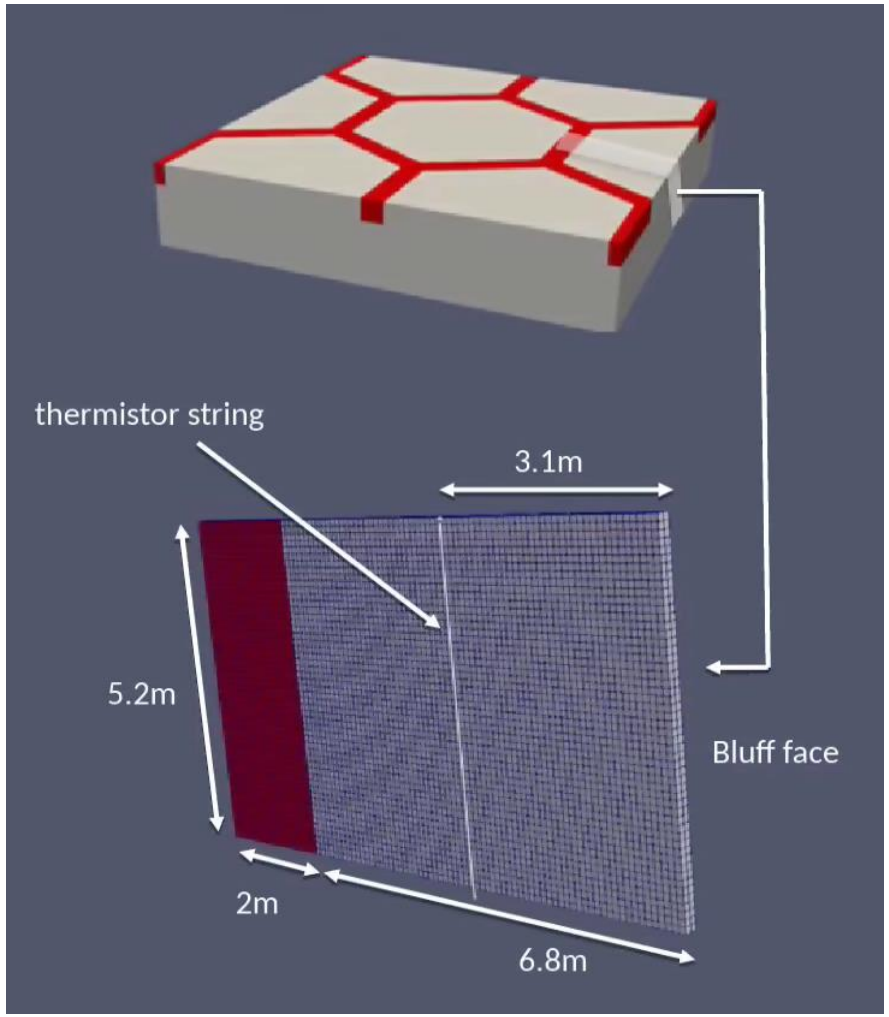
E Weakening Factor: factor by which the residual elastic modulus is divided at locations where the ocean is in contact with the bluff

- Reflects **localized adjustment** in material properties from material dissolution due to ocean-bluff contact
- **Increasing value** → more deformation/unit stress → material more likely to fail in strain
- Plays strong role in **niche formation**

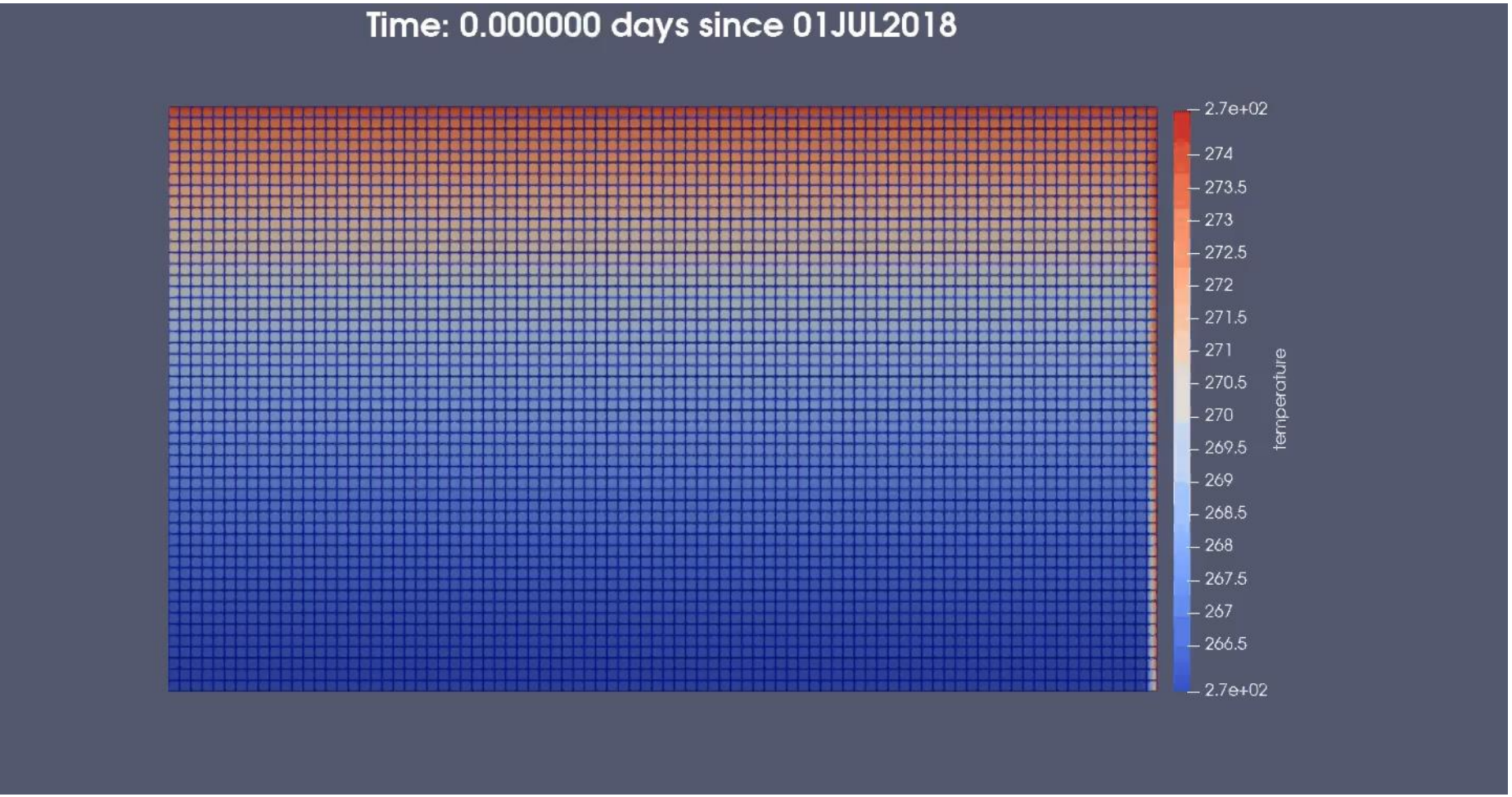
Thermo-mechanical coupling: 2.5D slice

Bluff profiles over simulation time:



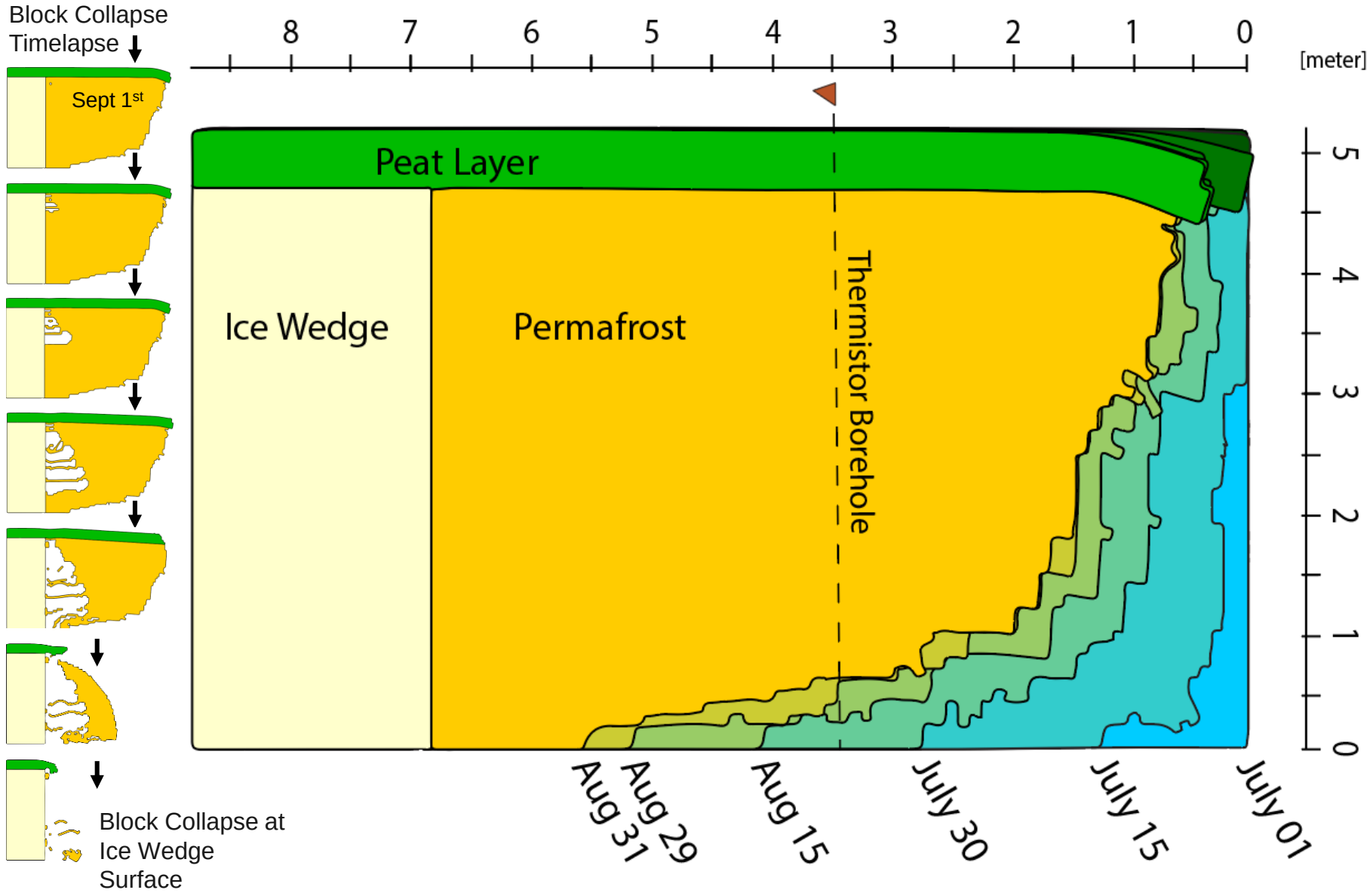


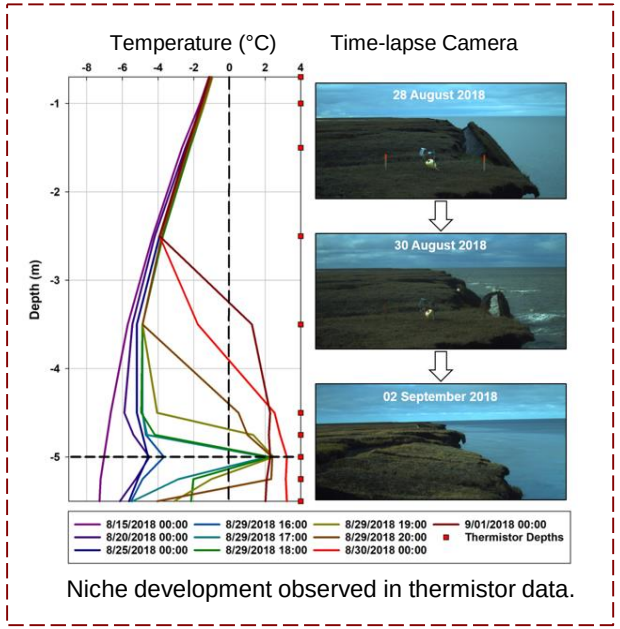
Thermo-mechanical coupling: 2.5D slice



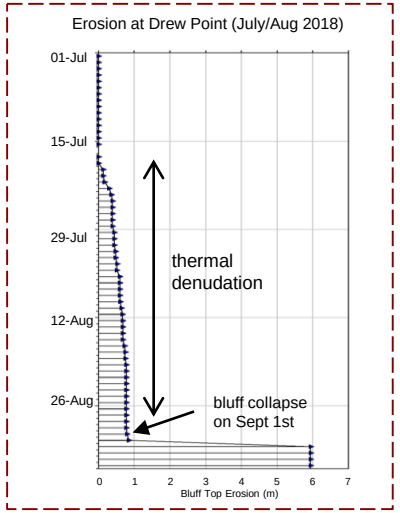
Calibrated ACE model ***capable of simulating*** Sept. 1, 2018 ***block collapse event*** observed at Drew Point, AK!

Thermo-mechanical coupling: 2.5D slice



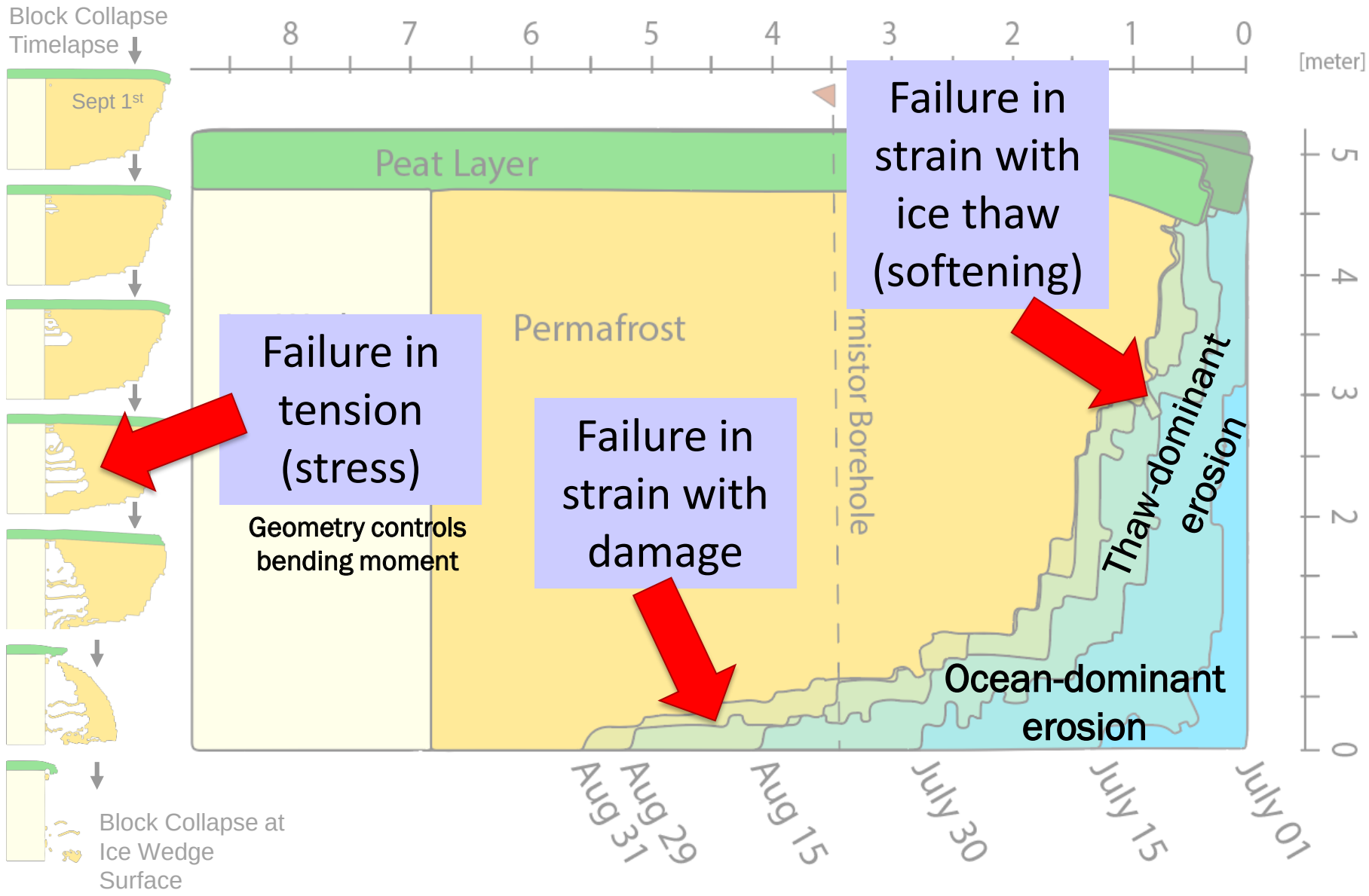


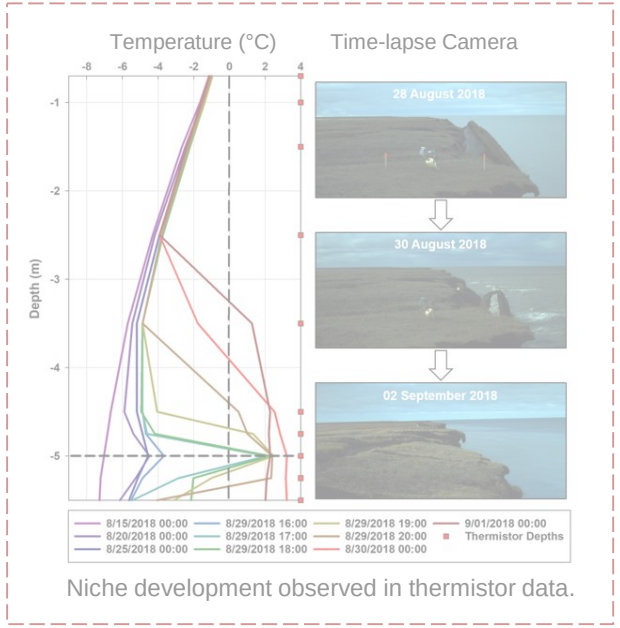
Niche development observed in thermistor data.



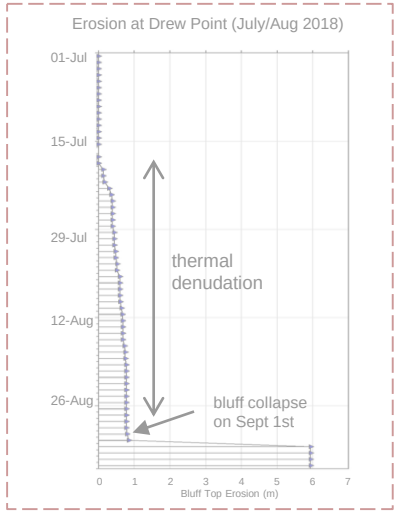
Field Data Used for Calibration

Thermo-mechanical coupling: 2.5D slice





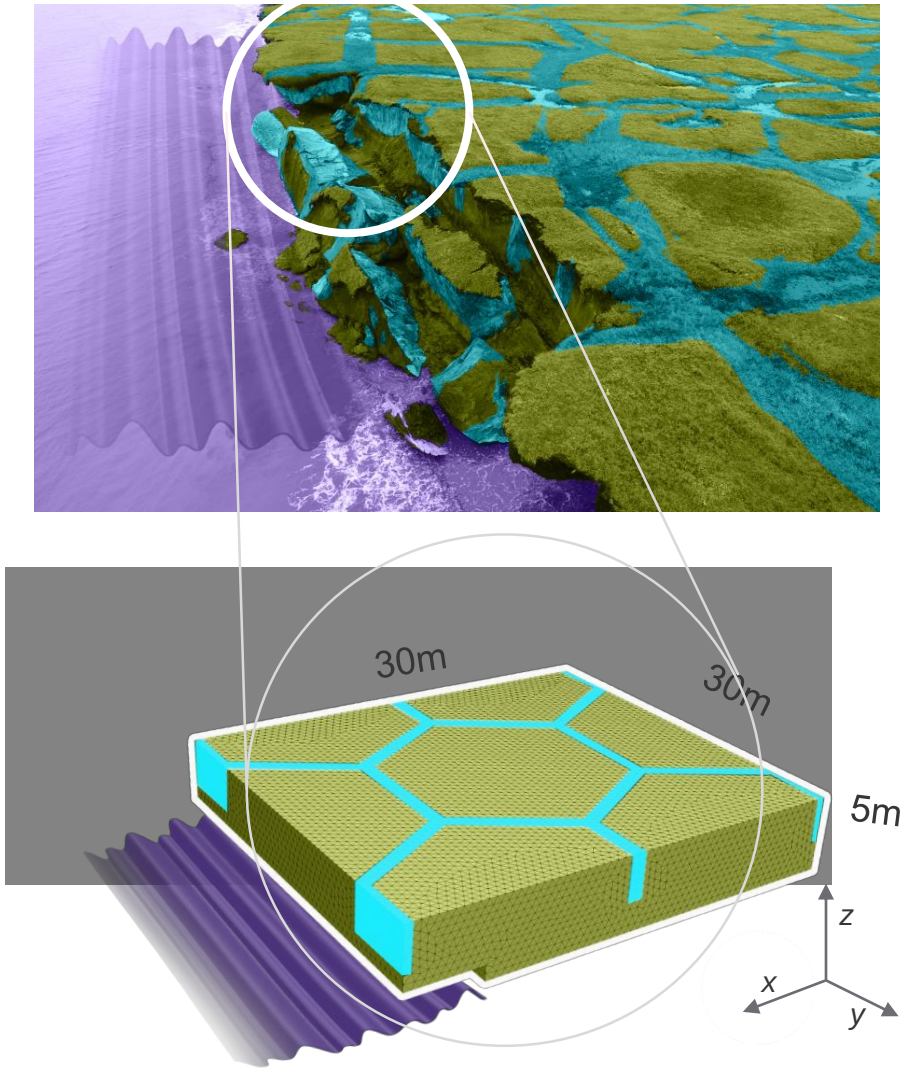
Niche development observed in thermistor data.



Field Data Used for Calibration

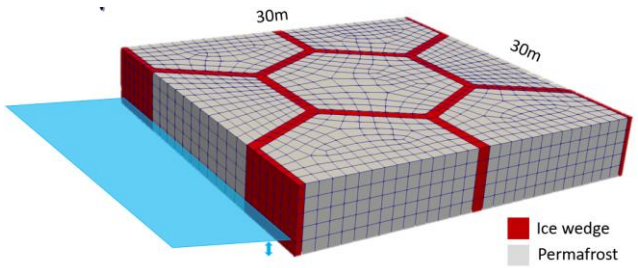
Summary

- We have developed a ***thermo-mechanical*** coupled FEM model, ***ACE***, that can simulate ***transient niche development*** and ***permafrost erosion*** within Albany-LCM.
- The model was ***calibrated*** using data from a series of ***experiments*** on frozen soil samples from Drew Point, Alaska that were performed at Sandia's Geomechanics Laboratory, as well as ***observational data*** collected at the same location.
- The model incorporates ***boundary conditions*** from the ***WW3+SWAN+Delft3D*** wave models and observational data from field campaigns at Drew Point, Alaska.
- ***Sensitivity studies*** can provide ***insight*** into which parameters are most important to ***permafrost demise,*** and assist with ***model calibration***.



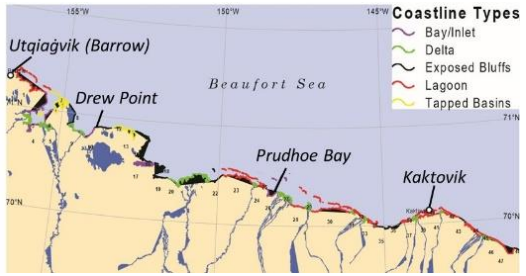
Current and future work

- **<u>Interface project:</u> upscale** ACE terrestrial model to meso/macro scales for integration into E3SM
  - ➢ Upscaling will be performed from **"catalog"** of 6-7 ACE runs for different terrestrial configurations/locations in northern Alaska



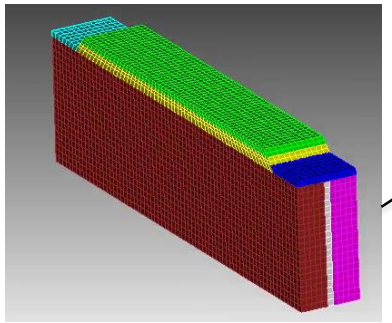
Micro-scale (ACE) model
10s of m, storm duration

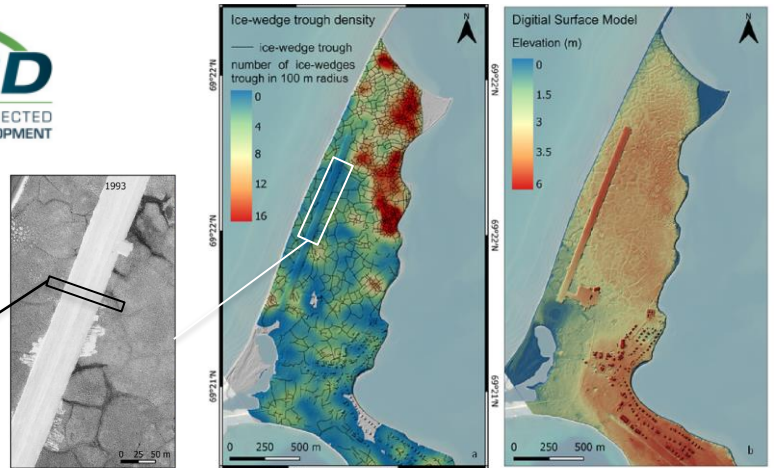
Meso-scale model
10s of km, monthly duration



Macro-scale model
100s of km, annual+ duration

- **<u>Arctic Critical Infrastructure (ACI) project</u>**: aims to develop a computational model capable of analyzing various permafrost-infrastructure **scenarios**, **failure modes**, and **risk-mitigation strategies**
  - ➢ **UQ** is **critical** to this project/problem!
  - ➢ ***Initial exemplar***: Paulatuk airstrip in northern Canada (right).





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Drew Point calibration/validation paper in preparation!

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[9] J. Frederick, A. Mota, D. Bull, I. Tezaur. "Thermo-chemo-mechanical coupling for Arctic Coastal Erosion", J. Comput. Appl. Math. 397 113533, 2021.

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