Los Alamos
NATIONAL LABORATORY

Optimization for Carbon Transport & Storage

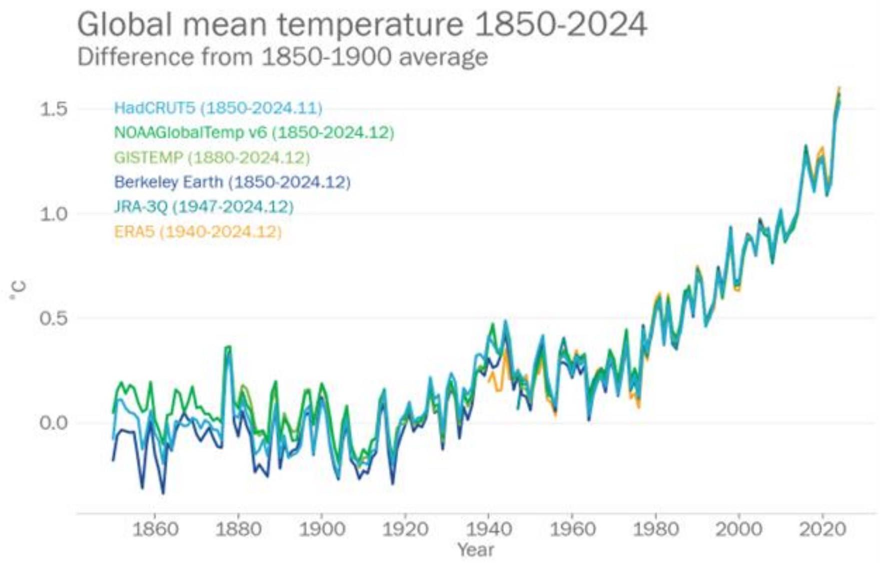
Bailian Chen

September 23, 2025

Golden, Colorado

LA-UR-25-29257

A Trip to Fairbanks



Source: World Meteorological Organization

WORLD METEOROLOGICAL ORGANIZATION
Weather Climate Water

Home / WMO confirms 2024 as warmest year on record at about 1.55°C above pre-industrial level

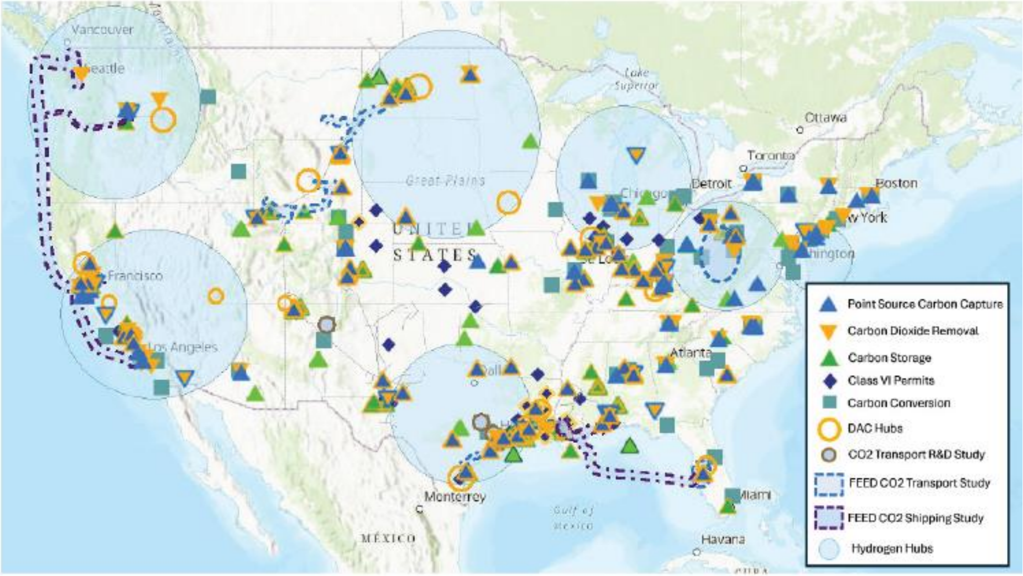
WMO confirms 2024 as warmest year on record at about 1.55°C above pre-industrial level

NEWS

10 January 2025

The World Meteorological Organization (WMO) has confirmed that 2024 is the warmest year on record, based on six international datasets. The past ten years have all been in the Top Ten, in an extraordinary streak of record-breaking temperatures.

Global warming is a reality we are facing today!



Source: DOE Carbon Management Strategy
DOE-funded carbon management projects as of
March 2024

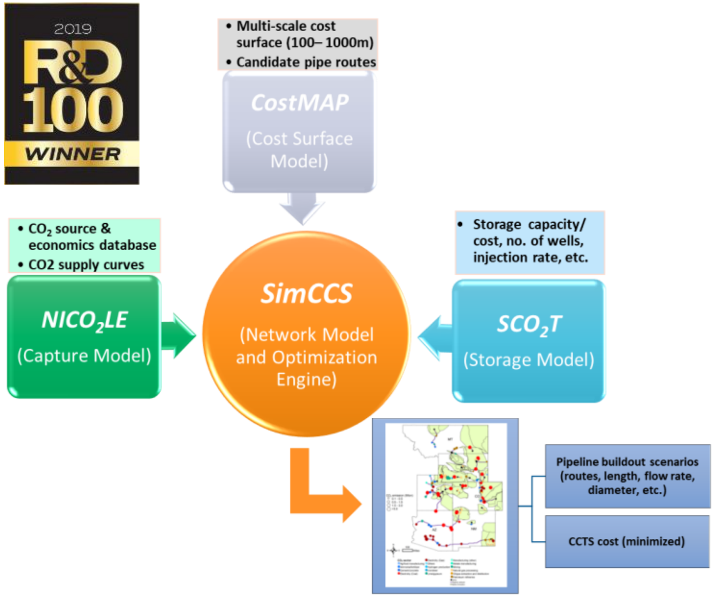
Should we maintain the momentum on carbon management?

Agenda

- Optimization of CO_2 Transport Network
- Optimization of CO_2 Storage under Geomechanical Risk

Transport Network Optimization

SimCCS: Determines Costs and Optimized Transport Routing by Integrating Factors Across the CCS Value Chain



Publicly available @ https://simccs.lanl.gov/

- ***NICO$_2$LE***
  - Understand commercial-scale capture opportunities
  - Geodatabase: Source locations, CO_2 streams, & capture costs
- ***SCO$_2$T***
  - Rapidly calculate realistic injection and storage costs
- ***CostMAP***
  - Identify likely corridors
  - Develop candidate pipeline routes for *SimCCS* optimization engine
- ***SimCCS***
  - Determine optimal regional/national network of CO_2 sources, CO_2 sinks, and CO_2 transport network that meet desired CCS goals

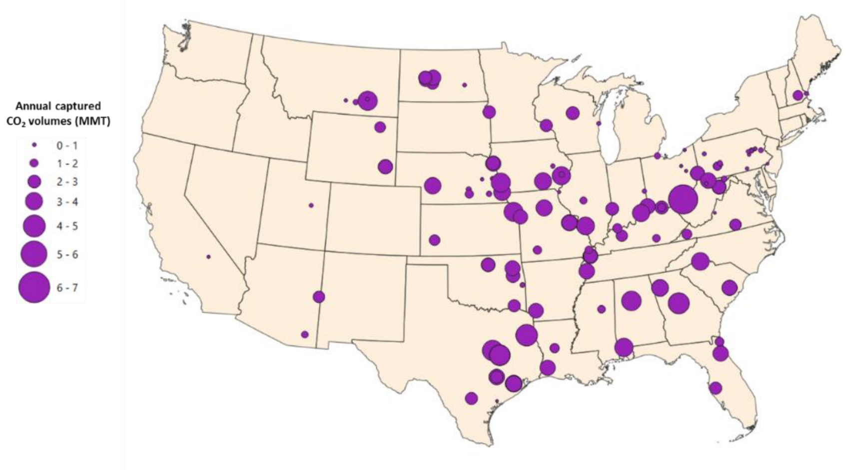
Example: Power Sector CO_2 Pipeline Analysis

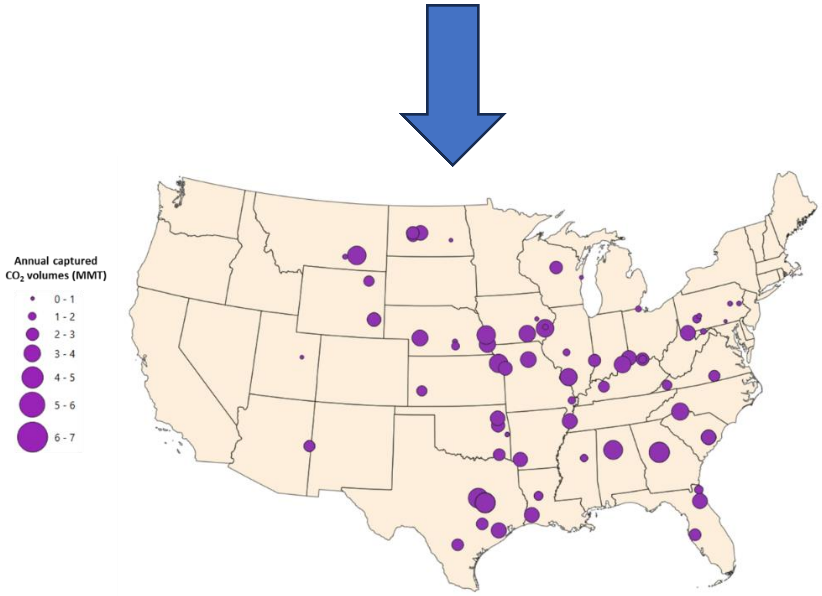
- **Background**: Policy makers need to understand the size of a CO_2 pipeline system needed to address significant portions of power sector emissions.

- **Objective**: Estimate the size and investment in the CO_2 pipeline network and storage sites necessary to meet proposed EPA power sector greenhouse gas emissions rules to inform feasibility assessment.

- **Sponsor**: DOE-Office of Policy

Coal Power Plant Fleets





Scenario 1: All Coal Units with No Retirement Dates

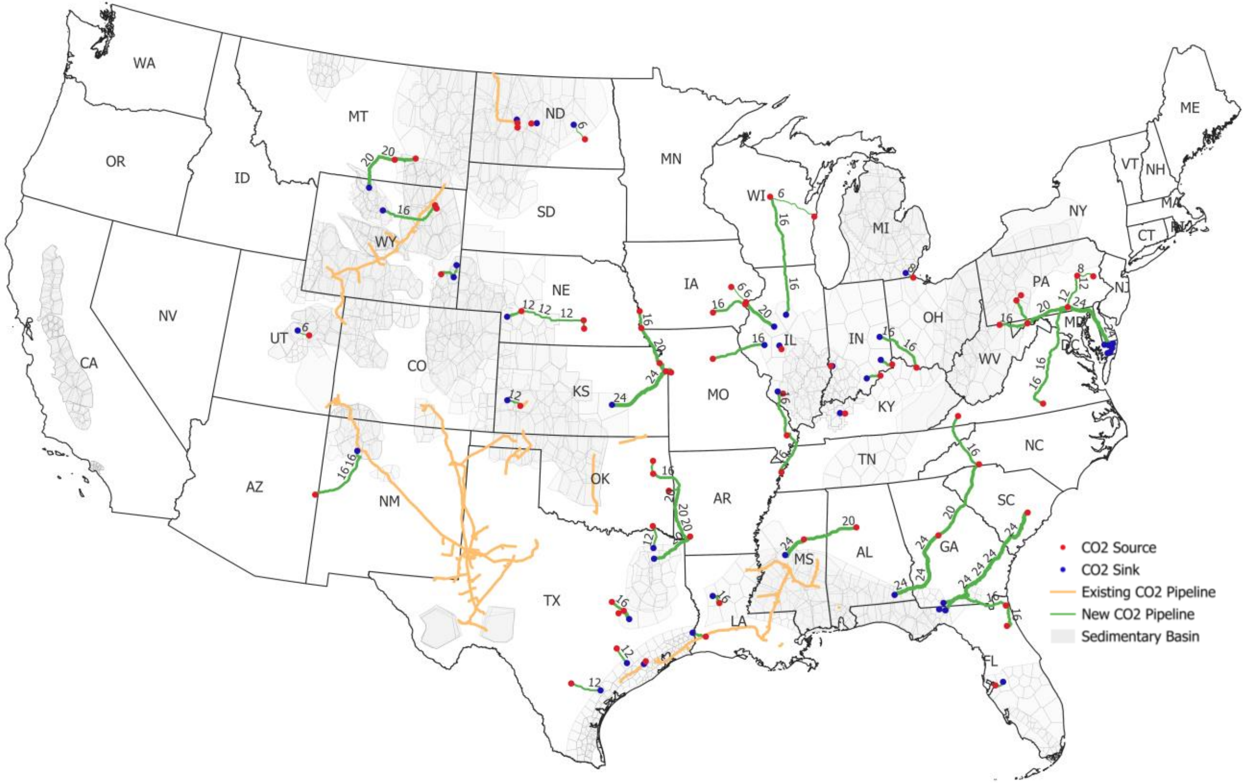
206 units
396 MMT/year

Scenario 2: Coal Units Unlikely to Retire by 2040

99 units
229 MMT/year

Chen, B., Sun, X., Ma, Z., Velasco Lozano, M., de Figueiredo, M., & Donohoo-Vallett, P. (2024). *CO_2 PIPELINE ANALYSIS FOR EXISTING COAL-FIRED POWER PLANTS* (No. LA-UR-24-23321). Los Alamos National Laboratory (LANL), Los Alamos, NM.

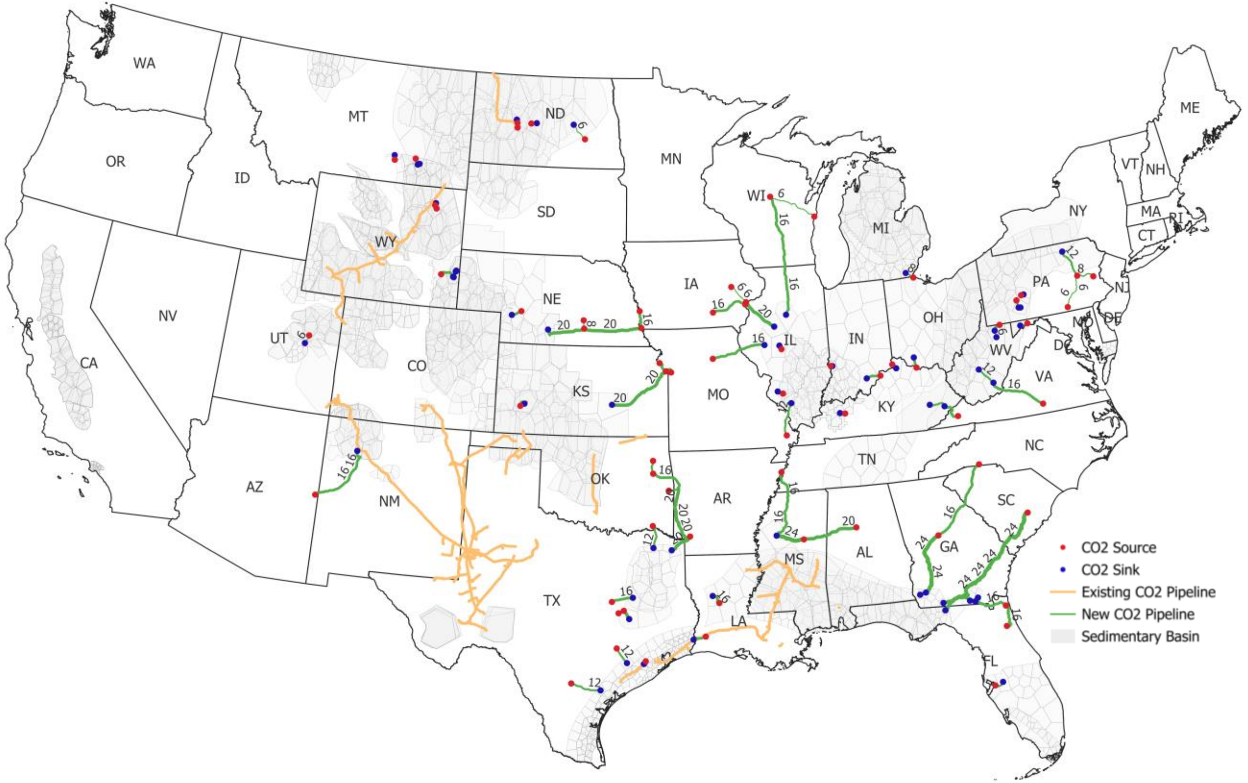
Scenario 2 – Case 1: Minimize Cost



- Existing CO_2 pipeline length in miles: 5,300

- Total new CO_2 pipeline length in miles: 5,661.3
- Total number of state crossing pipelines: 34

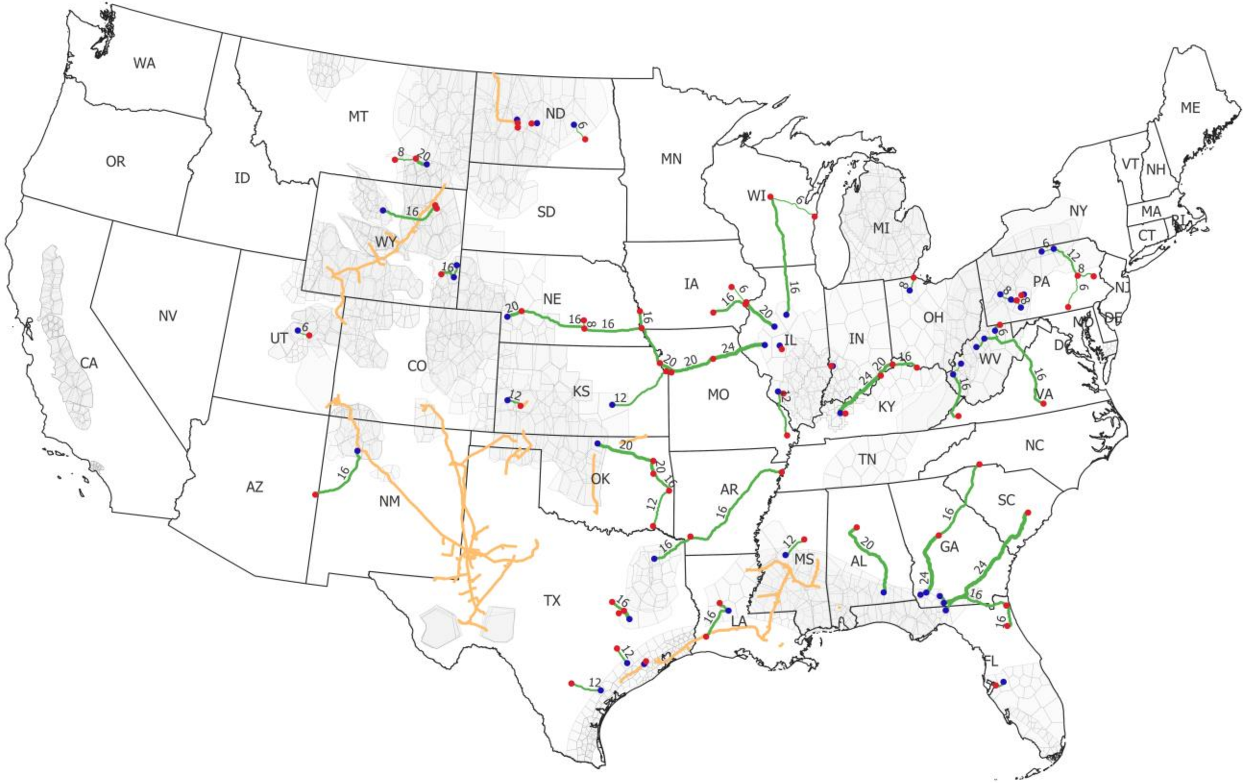
Scenario 2 – Case 2: Minimize Length



- Existing CO_2 pipeline length in miles: 5,300

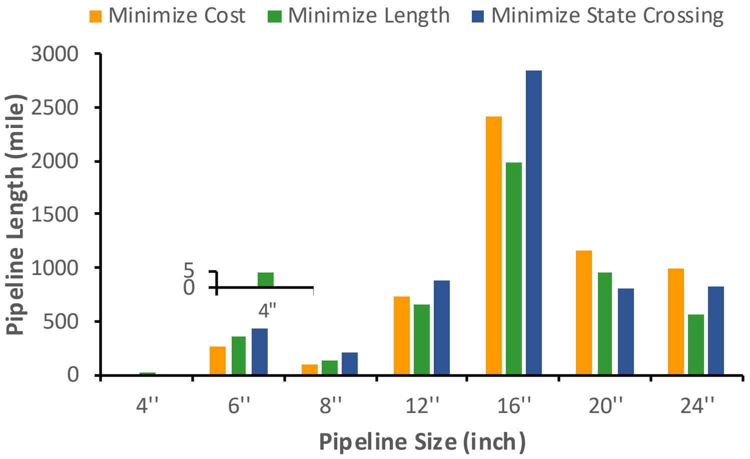
- Total new CO_2 pipeline length in miles: 4,658.0
- Total number of state crossing pipelines: 27

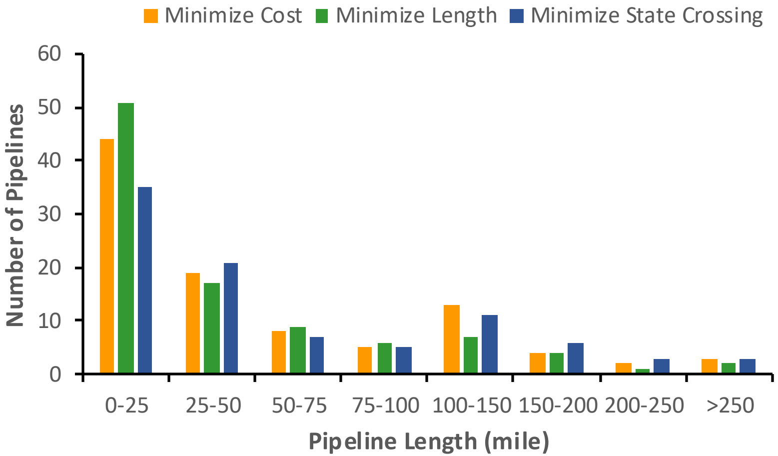
Scenario 2 – Case 3: Minimize State Crossing



- Existing CO_2 pipeline length in miles: 5,300
- Total new CO_2 pipeline length in miles: 5,990.0
- Total number of state crossing pipelines: 17

Scenario 2: Pipeline Size and Length





Scenario-Case	# of Coal Units	Total New Pipeline Length (miles)	% Segments < 25 miles	% Segments < 100 miles	# of State Crossings
S2C1 – Min cost	99	5,661.3	44.90%	77.55%	34
S2C2 – Min length	99	4,658.0	52.58%	85.57%	27
S2C3 – Min state crossing	99	5,990.0	38.46%	74.73%	17

- SimCCS demonstrates to be an effective toolset to support decision-making in the deployment of CCS transport infrastructure.

Optimization in Carbon Storage

- Science-informed Machine Learning to Accelerate Real Time (SMART) Decisions in Subsurface Applications

SMART

Real-Time Visualization
"CT" for the Subsurface

Rapid Prediction
Virtual Learning

Real-Time Forecasting
"Advanced Control Room"

Transforming decisions through **clear vision** of the present and future subsurface.

Technical Team

Carnegie Mellon University · Los Alamos National Laboratory · WV · National Energy Technology Laboratory · BATTELLE · EERC University of North Dakota · FACT

Lawrence Livermore National Laboratory · Colorado School of Mines · Oak Ridge National Laboratory · PennState · The University of Utah

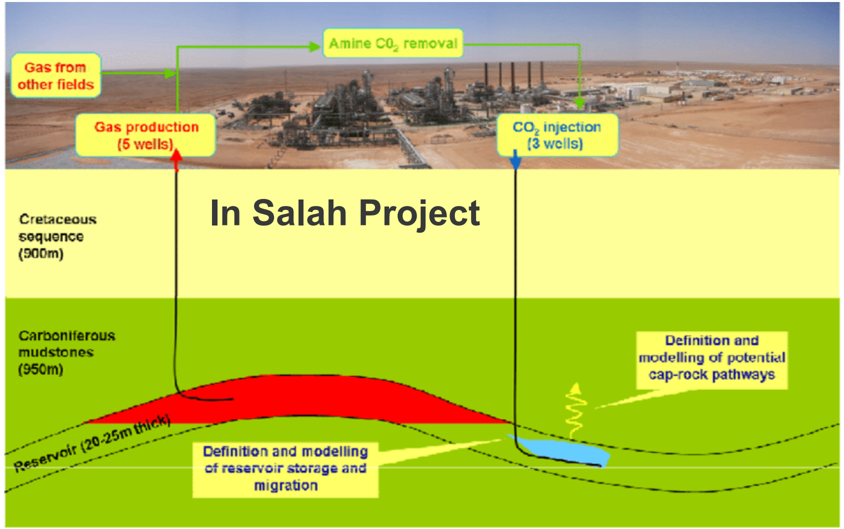
Pacific Northwest National Laboratory · Bureau of Economic Geology · ATM · Sandia National Laboratories · Berkeley Lab · Illinois

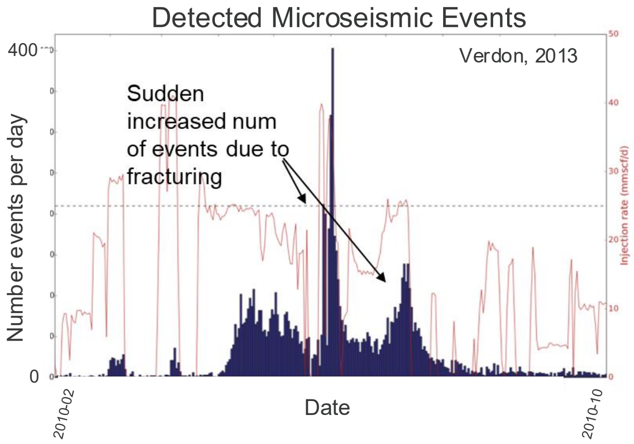
2020-Present

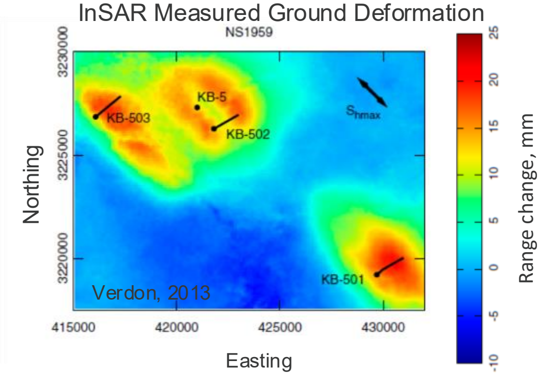
ML-based Optimization for CO_2 Injection under Geomechanical Risk

Zheng, F., Ma, M., Viswanathan, H., Pawar, R., Jha, B., & Chen, B. (2025). Deep Learning–Assisted Multiobjective Optimization of Geological CO_2 Storage Performance under Geomechanical Risks. *SPE Journal*, 30 (04):2073-2088.

Motivation

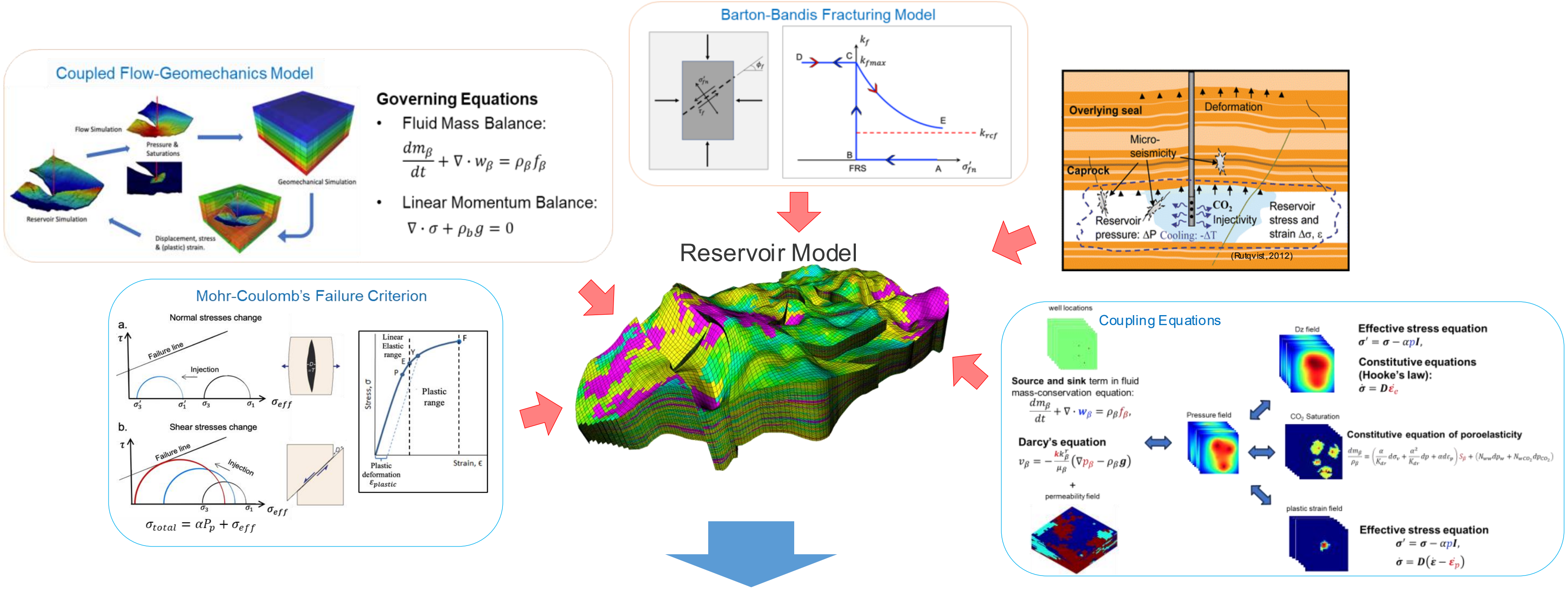






- A total of **3.8 mega-ton** of CO_2 were injected
- **9,506** micro-seismic events detected during injection
- Maximum of **25 millimeters uplift**

Motivation

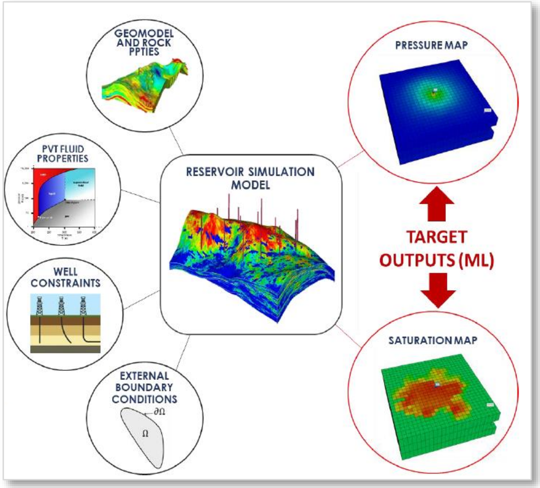


Computationally Demanding !!!

Introduction

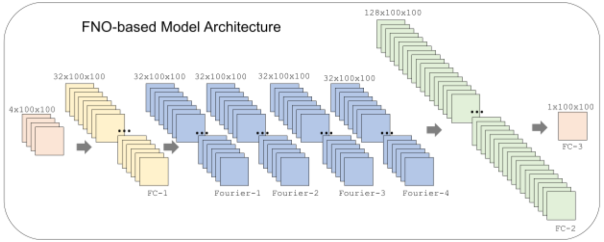
Main Objective:

Develop a ML-assisted optimization workflow to optimize CO_2 storage performance under Geomechanical risks.



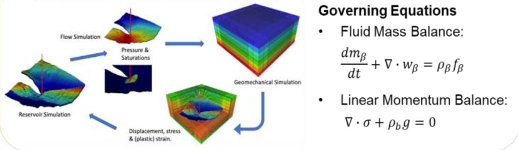
Major Components of Workflow:

1. Construct a physics-based CO_2 storage model and quantify the associated geomechanical risks, including ground displacement and safety factor.
2. Develop a ML-based surrogate model to output the quantified geomechanical risks.
3. Build an optimization workflow to optimization CO_2 storage while minimizing geomechanical risks.

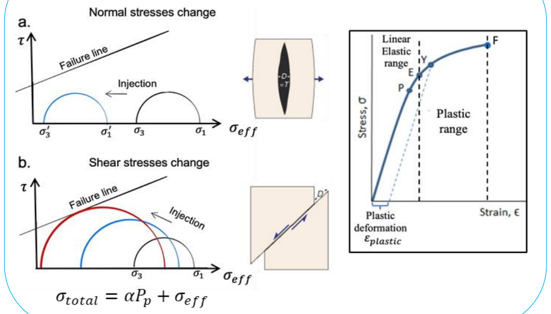


Methodology – Physics-based Model

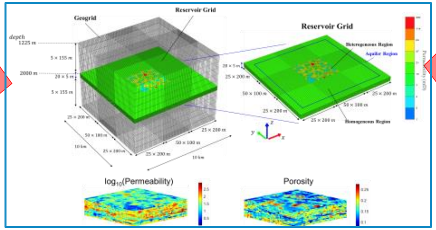
Build a coupled flow-geomechanics simulation model for CO_2 storage



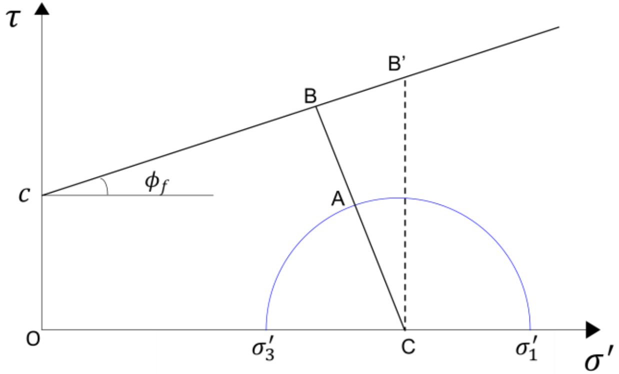
Mohr-Coulomb's Failure Criterion



Reservoir Model



Safety Factor (potential to trigger micro-seismicity)



$$SF = 1 - (\min(1, CA/CB))$$

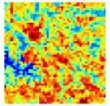
Large SF → safer injection
Small SF → dangerous
SF = 0 → Rock failure

Methodology – ML-based Model

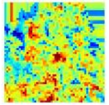
Construct an FNO-based surrogate model using synthetic dataset

Inputs:

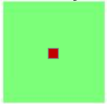
permeability



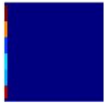
porosity

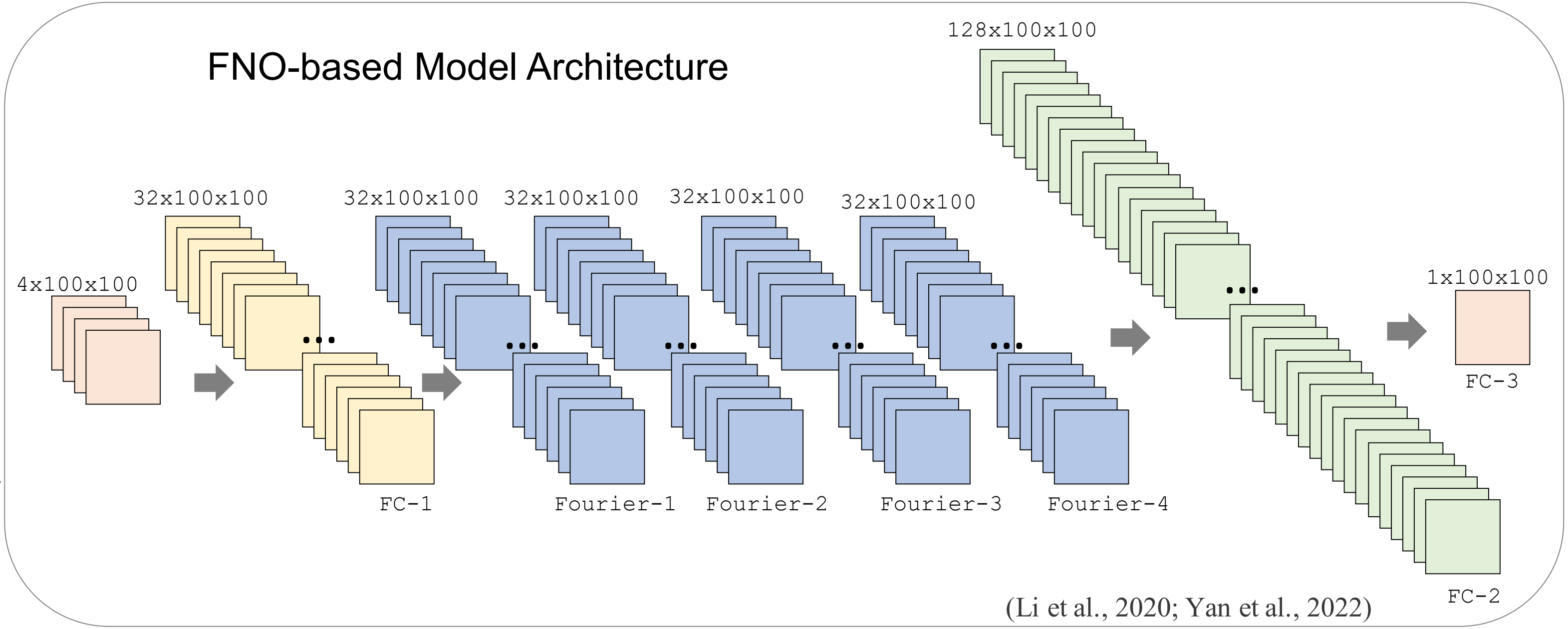


q_{inj}



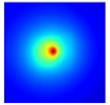
Injection history





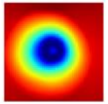
Outputs:

D_z

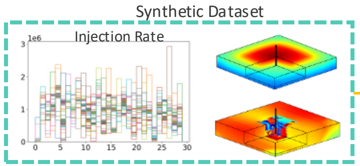


or

Safety factor



Methodology – General Optimization Workflow

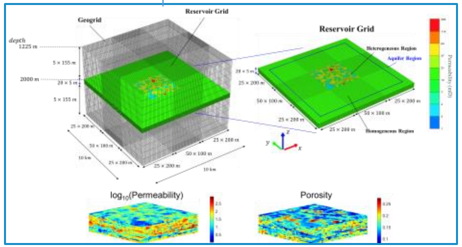


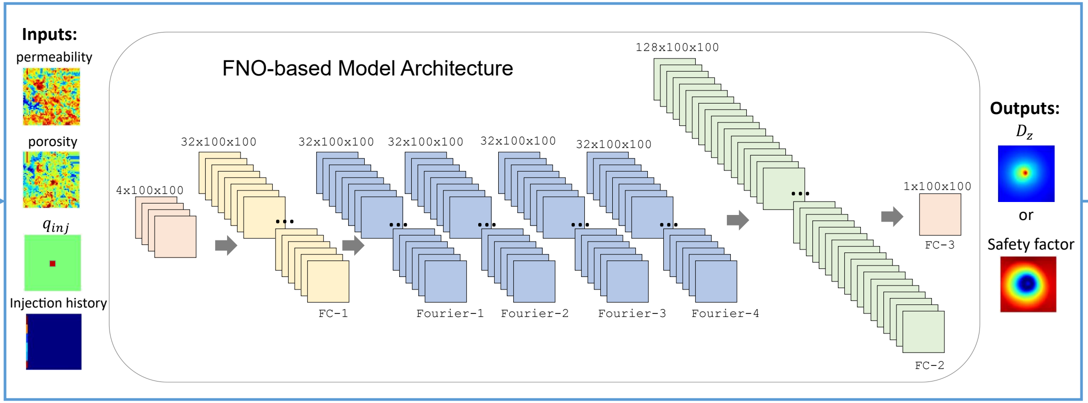
$$
f(\boldsymbol{u})\begin{cases} f_1 = \max(M_{CO_2}(\boldsymbol{u})), \\ f_2 = \min(\max(D_z)), \\ f_3 = \max(\min(safty\ factor)). \end{cases}
$$

$$
subject\ to\quad \begin{matrix} M_{CO_2\_min} \leq M_{CO_2}(\boldsymbol{u}), \\ M_{CO_2}(\boldsymbol{u}) \leq M_{CO_2\_max}. \end{matrix}
$$

Genetic Algorithm

Build physics-based model → Develop proxy model → Define decision variables and objective function → Select optimization algorithm → Determine the optimal control parameters





Result

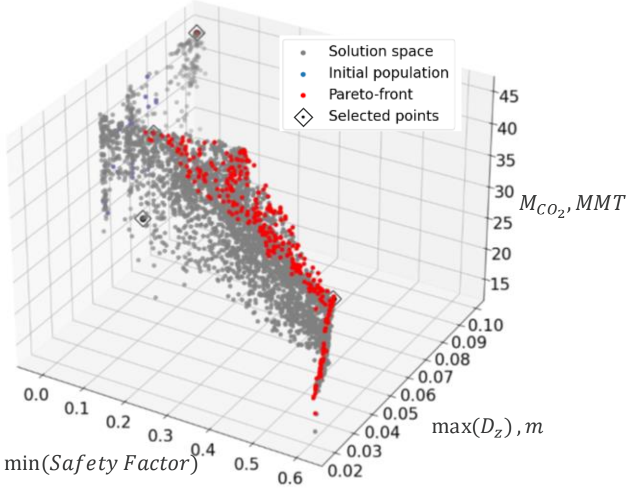
Optimization Formulation:

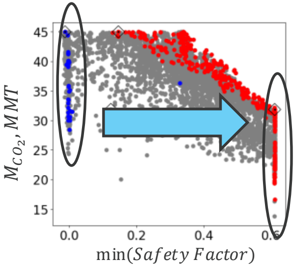
$$\boldsymbol{f}(\boldsymbol{u}) \begin{cases} f_1 = \max(M_{CO_2}(\boldsymbol{u})), \\ f_2 = \min(\max(D_z)), \\ f_3 = \max(\min(safty\ factor)). \end{cases}$$

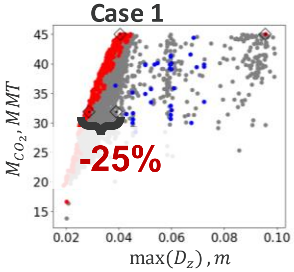
$$subject\ to \quad \begin{matrix} M_{CO_2\_min} \leq M_{CO_2}(\boldsymbol{u}), \\ M_{CO_2}(\boldsymbol{u}) \leq M_{CO_2\_max}. \end{matrix}$$

- The optimization algorithm successfully **improves** the initial population's minimum safety factor from **0** **(indicating rock fracturing)** to a Pareto population maximum value of **0.61** **(indicating safe injection)**.
- The optimal maximum vertical displacement also **decreased** from approximately **0.04 m** to about **0.03 m**, achieving **25% mitigation**.
- An **early maximum injection** allowed for **better pressure dissipation**, leading to **safer storage** (consistent with previous observation).

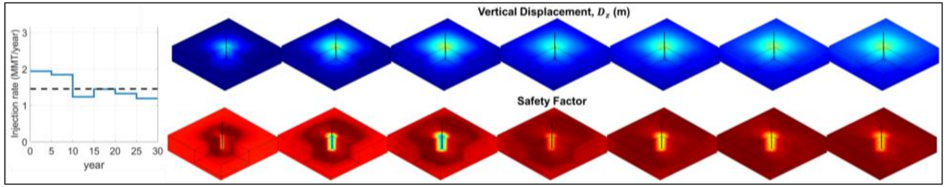
GA Optimization Results



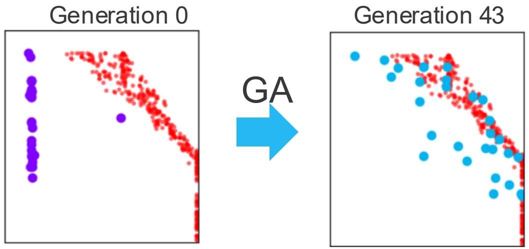




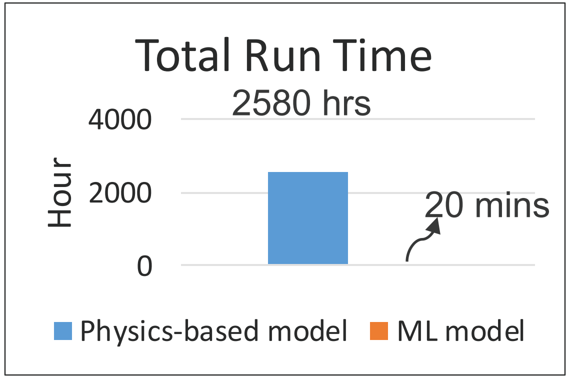
Case 1



Result – Computational Cost



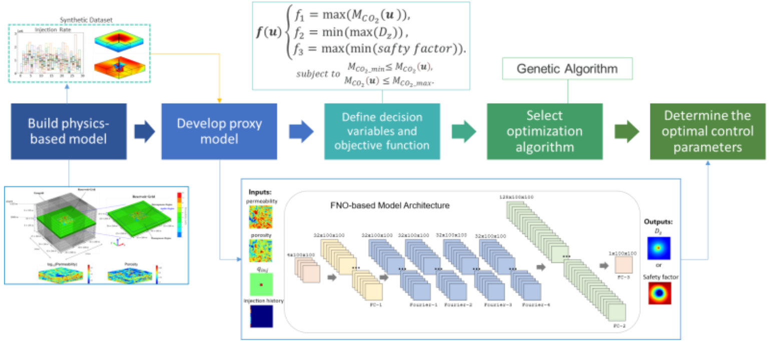
# of simulation evaluated: 1290



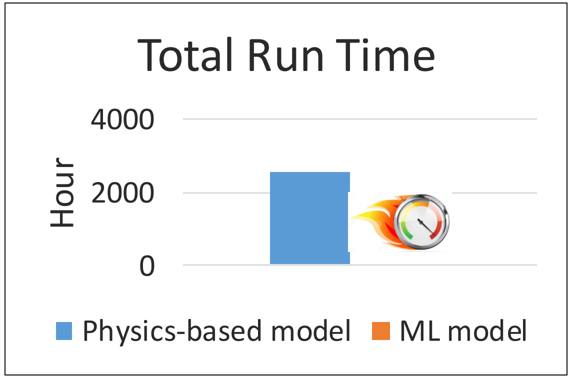
7,740 times faster!

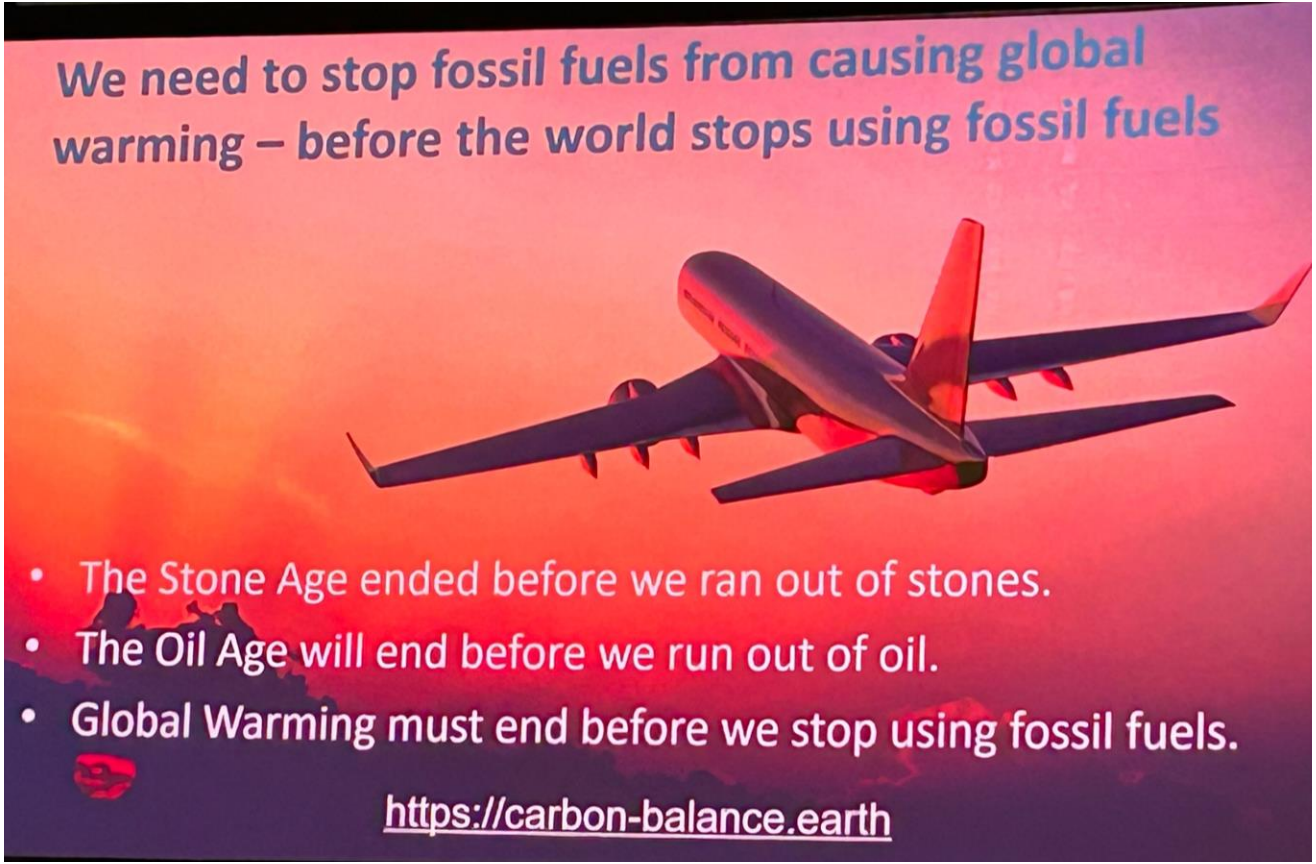
Summary

- Challenging problem – CO_2 Storage under Geomechanics:
  - Non-linear and Multiphysics Processes
  - Complex Rock's Failure/Fracturing Mechanisms
  - Non-convex, Global Optimization Formulation
  - High Computational Cost



- Demonstrated the effectiveness of using FNO-based ML-surrogate models and the NSGA-II Genetic Algorithm for optimizing CO_2 injection strategies under geomechanical risks.
- The Pareto-front indicates optimal **trade-offs** between CO_2 storage, safety (micro-seismicity), and vertical displacement.
- Achieved over **7,000-fold computational cost saving**.





Source: Myles Allen, Oxford University, GHGT-17 Keynote

Thank you!

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