GEOSX

An open-source multiphysics simulator for exascale carbon storage simulation

SCCS Annual Affiliates Meeting — November 16, 2021

Hervé Gross, Ph.D. on behalf of GEOSX contributors
https://github.com/GEOSX/GEOSX/graphs/contributors
herve.gross@totalenergies.com

Tools for CO_2 storage simulation

Challenges

Multiphysics

Large spatial extent

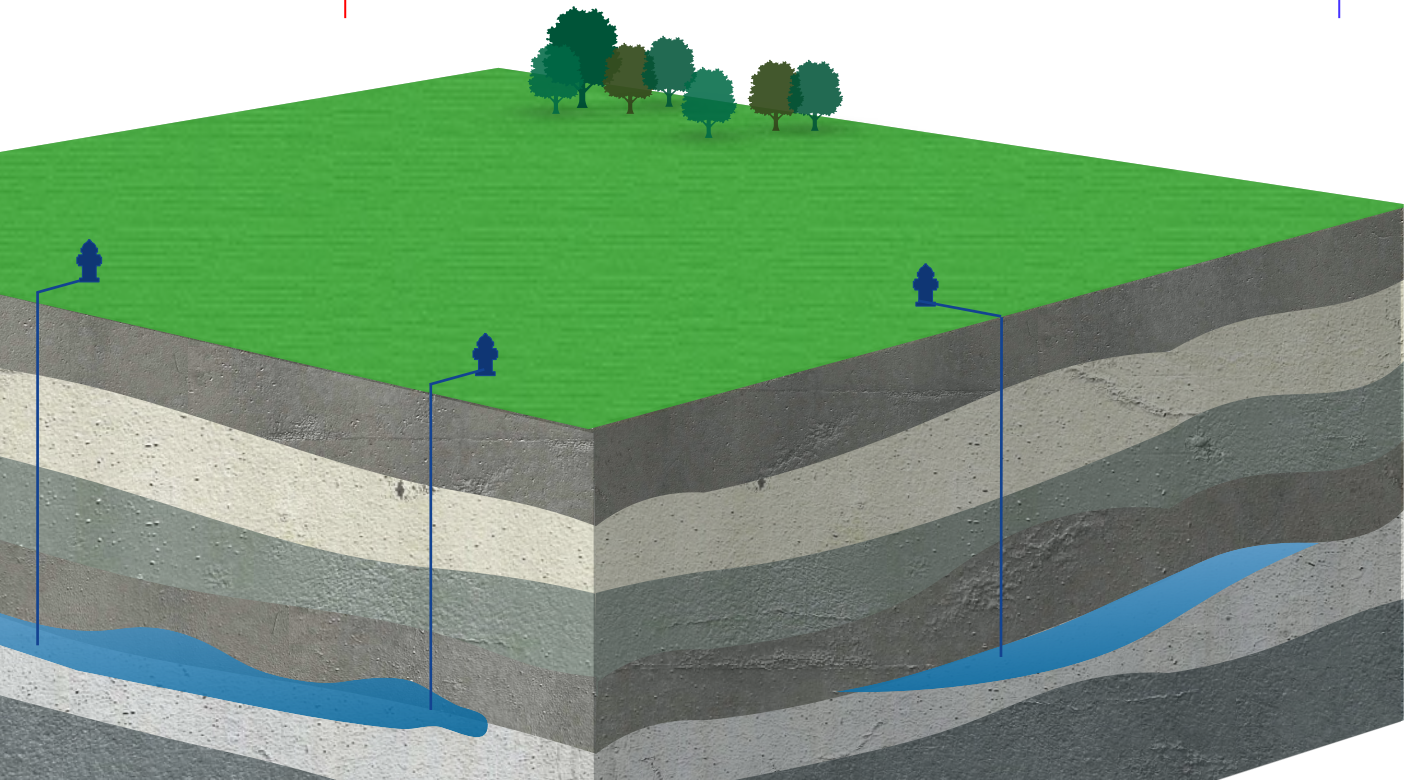
Long simulation periods

Solutions

Exascale computing

Advanced algorithms

Dedicated simulation tool



Well integrity and injectivity

Stress alterations

Migration, dissolution, mineralization

Fault activation risks

Surface expressions

Induced seismicity

State-of-the-art & open tools for CO_2 storage simulation needed

DIRECTIVE 2009/31/CE DU PARLEMENT EUROPÉEN ET DU CONSEIL

du 23 avril 2009

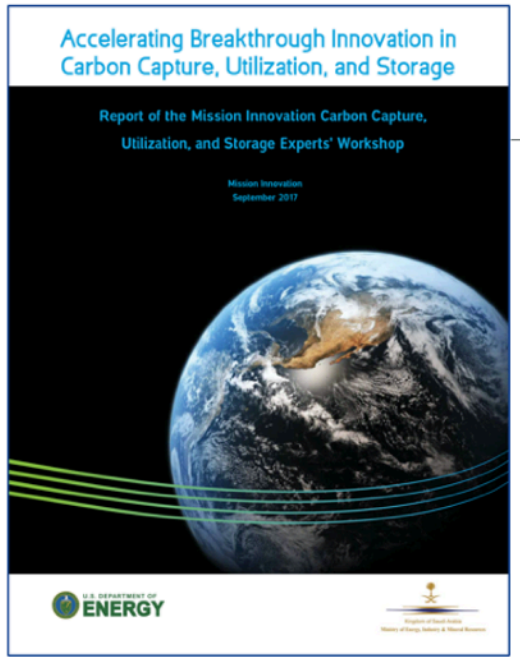
relative au stockage géologique du dioxyde de carbone et modifiant la directive 85/337/CEE du Conseil, les directives 2000/60/CE, 2001/80/CE, 2004/35/CE, 2006/12/CE et 2008/1/CE et le règlement (CE) n° 1013/2006 du Parlement européen et du Conseil

(Texte présentant de l'intérêt pour l'EEE)

June 2009

Directive européenne 2009/31/CE

La caractérisation et l'évaluation du complexe de stockage potentiel et des environs visées (…) s'effectuent en trois étapes selon les meilleures pratiques en vigueur au moment de l'évaluation



Sept 2017

Mission Innovation CCUS

HPC effort for CCS should expand beyond traditional reservoir simulation (…) to address the effects on regional hydrodynamics, pressure perturbations, modified stress fields, and deformation at the reservoir and basin scales.

June 2019

Mission Innovation CCUS

Establish[ing] one or more internationally recognized CO2 storage open-source software (…) would enable transparency, openness and wider collaboration.

World-class Partners

RESERVOIR SIMULATION

NUMERICAL METHODS

UNIVERSITÀ DEGLI STUDI DI PADOVA

USE CASES

SCIENTIFIC COMPUTING

CLIENT NEEDS

HPC R&D DEV

GEOMECHANICS

Dr. Josh White

Dr. Herve Gross

Prof. Hamdi Tchelepi

Randy Settgast

Chak Lee

Matteo Cusini

Julia Camargo

Shabnam Semnani

Madonna Yoder

Brian Han

Matthias Cremon

Quan Bui

Nicola Castelletto

Tao Jin

Yue Hao

Ben Corbett

Chris Sherman

Panayot Vassilevski

Daniel Osei-Kuffuor

François Hamon

Thomas Gazzola

Sergey Klevtsov

Andrea Franceschini

Mohammad Karimi Fard

Igor Shovkun

Antoine Mazuyer

Mamadou N'Diaye

Jacques Franc

Massimiliano Ferronato

Claudia Zoccarato

Laura Gazzola

Matteo Frigo

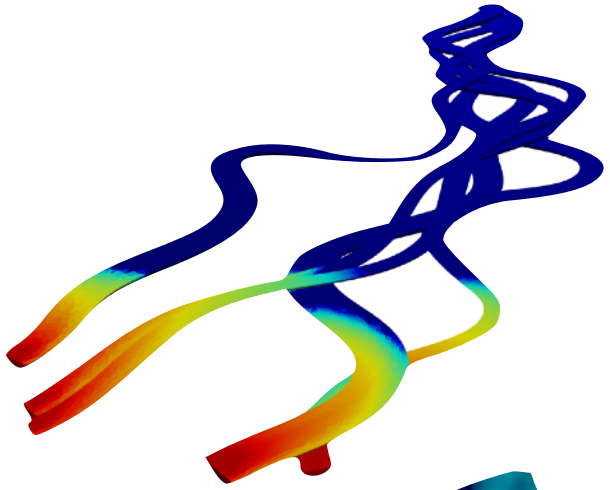
Yuan Tian

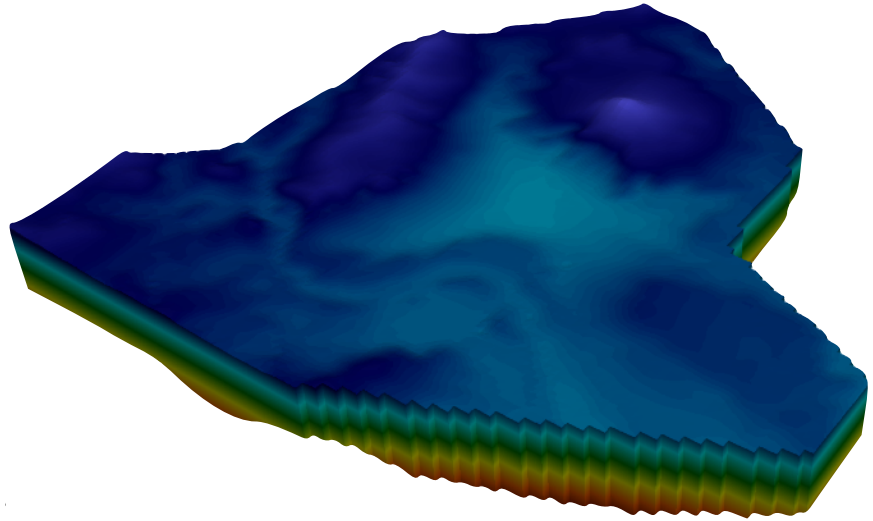
Jian Huang

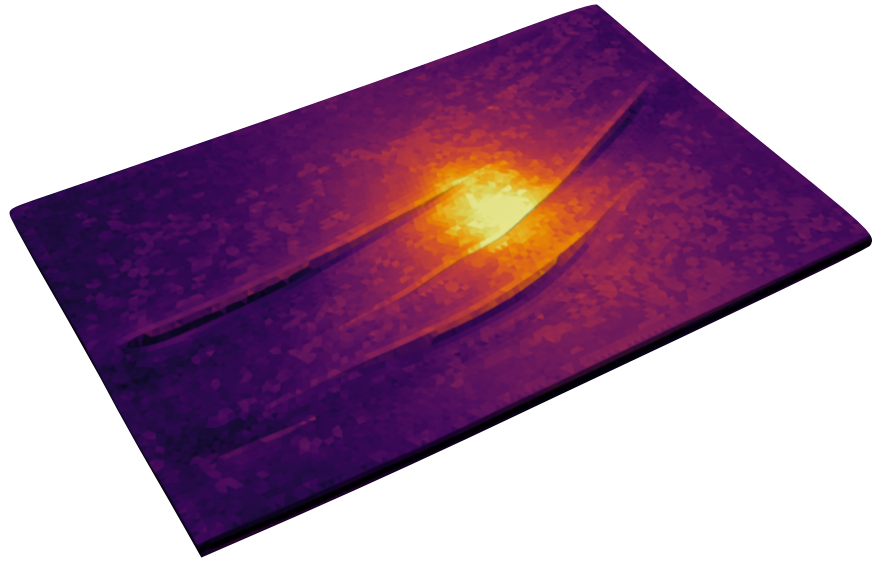
Andrea Borio

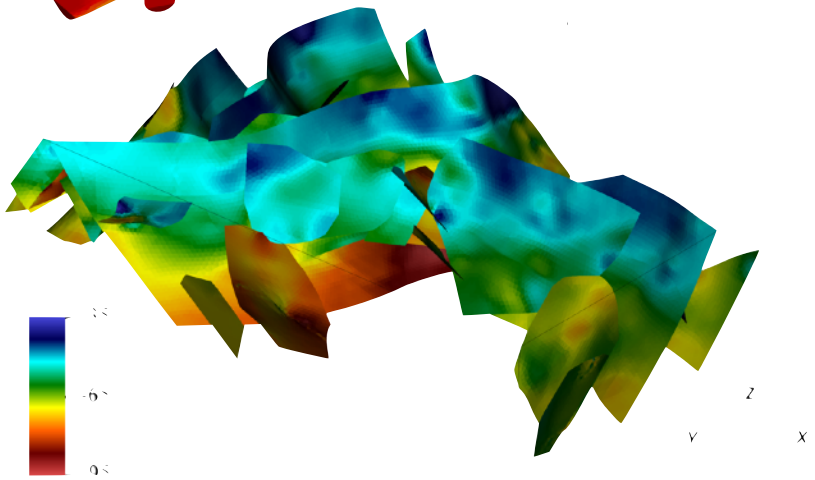
Year 3: Diversification of use cases and performance benchmarks

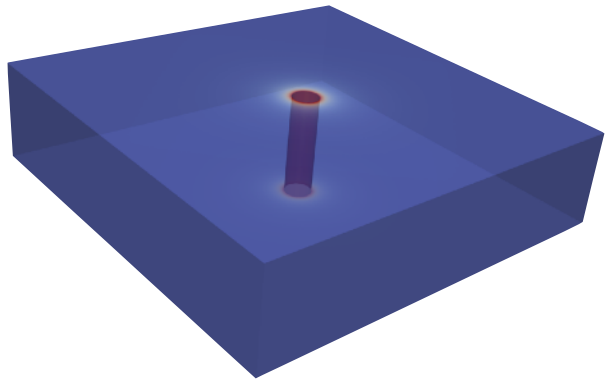
More advanced multiphysics, testing for performance

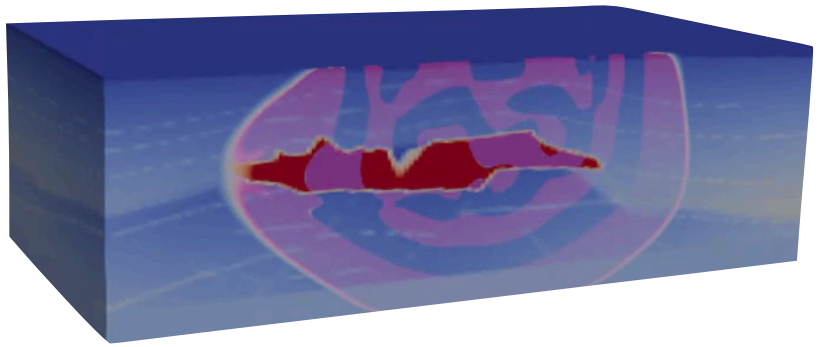












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Total and its Partners Release Next-Gene
Dioxide Stora

November 10, 2020 04:20 AM Eastern Standard Time

PARIS--(BUSINESS WIRE)--Regulatory News:

"We are proud of the development of GEOSX, the first tool able to simulate the geological storage of CO_2 at the gigaton scale. We are making its source code openly available to provide the scientific community the means to participate in the development of CCUS"

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(NYSE:TOT
University
carbon dio

GEOSX wa
computing
and safety
unmatched

The open-source nature of GEOSX aims to ensure a high level of tra
large-scale development of Carbon Capture, Utilization and Storage

"We are proud of the development of GEOSX, the first tool able to s
making its source code openly available to provide the scientific co
said Marie-Noëlle Semeria, Total's Chief Technology Officer. "G
Stanford as technological leaders in the simulation of CO_2 geologic

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CCUS: Total and its Partners Release Next-Gen CO2 Storage Simulator

11/26/2020

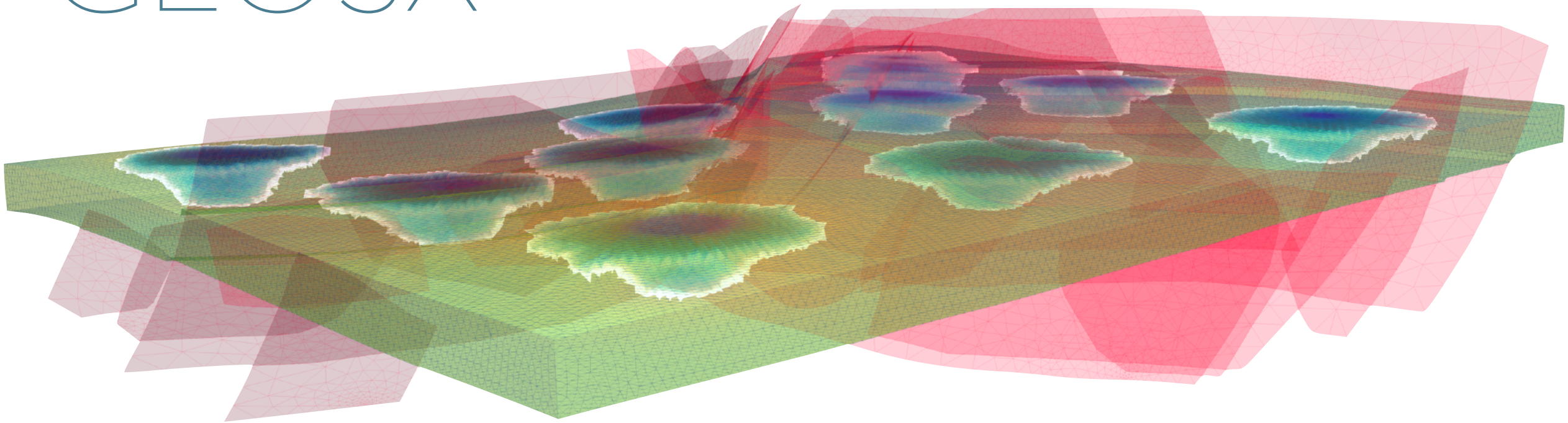
Total and its partners have just announced the first version of a high-performance simulator for large-scale geological CO_2 storage. The tool puts Total at the forefront of Carbon Capture, Utilization and Storage (CCUS) research. We met with Philippe Cordier, Head of the Scientific Computing and Artificial Intelligence research program at Total, who gave us an insight into how the Group's R&D digital programs are ramping up its energy transition and its transformation.

Total has announced the launch of a next-generation simulator designed to accurately predict the behavior over the long term of CO_2 stored in geological repositories and its environment. Developed using advanced new technologies in high-performance computing and applied mathematics, the GEOSX simulator aims to improve the management and safety of large-scale geological storage. It has been released as an open-source tool to support the entire industry in developing CCUS technologies, which are essential for achieving global carbon neutrality objectives.

The MAELSTROM research project at a glance

GEOSX is the first major milestone of the five-year FC-MAELSTROM research project launched in 2018 by Total, Stanford University School of Earth, Energy and Environmental Sciences, and the Lawrence Livermore National Laboratory of the United States Department of Energy. The project is led by a team based in California, working in collaboration with dozens of researchers from industry players, universities and institutions. It draws on each of its three partners' well-established and recognized expertise in reservoir simulation, geomechanics and high-performance computing.

GEOSX



MULTIPHYSICS

MULTILEVEL

EXASCALE

AUDITABLE

STRATEGIC

FLOW and TRANSPORT
Compositional Multiphase
Fully-implicit, isothermal formulation
Equations-of-state (cubic): PVT, flash
Three-phase extended black and dead oil
Two-phase CO2/brine
Assembled and solved on multi GPU

SOLID MECHANICS
Implicit and explicit time-stepping
Small and large-strain formulations
Advanced Rock models
Isotropic/Anisotropic elasticity
Poroelasticity, poroplasticity
Tightly-coupled & Fractional-step

DISCRETIZATION SCHEMES
Finite volume interface
Cell-centered method (TPFA)
Hybrid Mimetic Method TPFA
Quasi-TPFA inner products
Multi-segmented wells

LINEAR SOLVERS
Unified algebra interface
Hypre, Trilinos, Petsc
Krylov solvers (CG, GMRES, BiCGSTAB)
Preconditioners (AMG, ILU, MGR)
Block matrix and vector support
Serial and parallel direct solvers

CONTACT MECHANICS
Embedded Discrete Fractures
Enriched finite elements
Fault-contact using Lagrange multipliers
Conforming hydrofracture solver
Proppant: slurry, settling, bed build-up

FINITE ELEMENTS
First-order elements and quadrature
8-node hexahedron
6-node wedge
5-node pyramid
4-node tetrahedron

MESH AND DATA I/O
Unstructured 3D (reservoir)
Unstructured 2D (faults/fractures)
Importer for Gmsh, corner-point grids
Importer for LAS format wells
Output: Silo and VTK for VisIt and Paraview

Version 0.2.0
GitHub, Travis CI, Doxygen
LGPL 2.1
LLNL, Stanford, Total

GEOSX

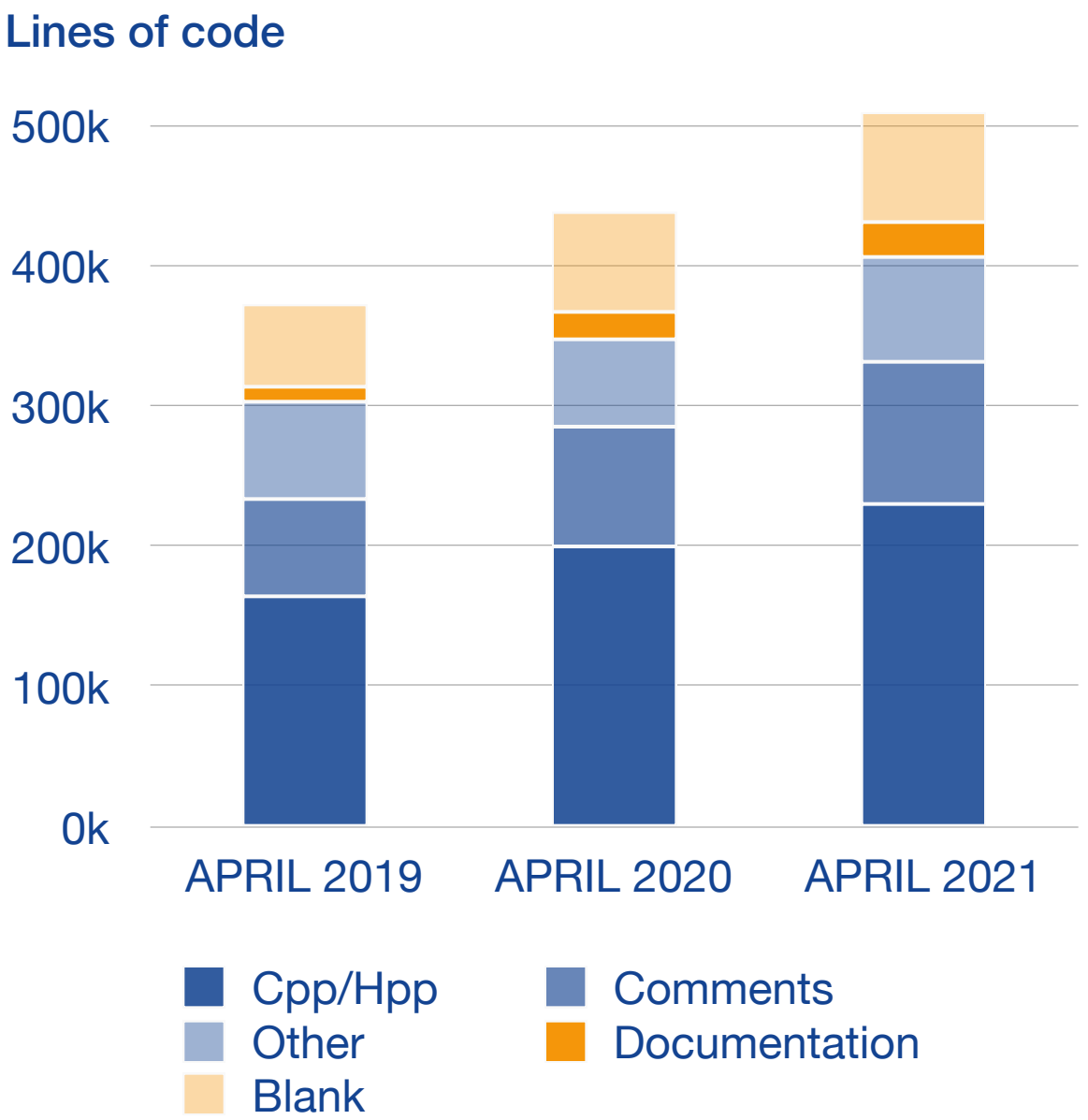
Multiphysics by design

Exascale-ready

Portable across Platforms

Open-source, certifiable

Technological Readiness Level 5



A support platform for R&D on GEOSX and with GEOSX

1. **Multigrid reduction preconditioning framework for coupled processes in porous and fractured media.** QM Bui, FP Hamon, N Castelletto, D Osei-Kuffuor, RR Settgast, JA White. arXiv:2101.11649

2. **Hybrid mimetic finite-difference and virtual element formulation for coupled poromechanics.** A Borio, FP Hamon, N Castelletto, JA White, RR Settgast. arXiv:2010.15470

3. **Preconditioners for multiphase poromechanics with strong capillarity.** JT Camargo, JA White, N Castelletto, RI Borja. International Journal for Numerical and Analytical Methods in Geomechanics. doi.org:10.1002/nag.3192

4. **An anisotropic viscoplasticity model for shale based on layered microstructure homogenization.** J Choo, SJ Semnani, JA White. International Journal for Numerical and Analytical Methods in Geomechanics. doi.org:10.1002/nag.3167

5. **Efficient solvers for hybridized three-field mixed finite element coupled poromechanics.** M Frigo, N Castelletto, M Ferronato, JA White. Computers and Mathematics with Applications. doi.org:10.1016/j.camwa.2020.07.010

6. **Simulation of coupled multiphase flow and geomechanics in porous media with embedded discrete fractures.** M Cusini, JA White, N Castelletto, RR Settgast. International Journal for Numerical and Analytical Methods in Geomechanics. doi:10.1002/nag.3168

7. **A macroelement stabilization for mixed finite element/finite volume discretizations of multiphase poromechanics.** JT Camargo, JA White, RI Borja. Computational Geosciences. doi:10.1007/s10596-020-09964-3

8. **Approximate inverse-based block preconditioners in poroelasticity.** A Franceschini, N Castelletto, M Ferronato. Computational Geosciences. doi:10.1007/s10596-020-09981-2

9. **Enhanced multiscale restriction-smoothed basis (MsRSB) preconditioning with applications to porous media flow and geomechanics.** SBM Bosma, S Klevtsov, O Møyner, N Castelletto, Journal of Computational Physics. doi.org:10.1016/j.jcp.2020.109934

10. **Nonlinear multigrid based on local spectral coarsening for heterogeneous diffusion problems.** CS Lee, F Hamon, N Castelletto, PS Vassilevski, JA White. Computer Methods in Applied Mechanics and Engineering. doi:10.1016/j.cma.2020.113432

11. **An inelastic homogenization framework for layered materials with planes of weakness.** SJ Semnani, JA White. Computer Methods in Applied Mechanics and Engineering. doi:10.1016/j.cma.2020.113221

12. **Algebraically stabilized Lagrange multiplier method for frictional contact mechanics with hydraulically active fractures.** A Franceschini, N Castelletto, JA White, HA Tchelepi. Computer Methods in Applied Mechanics and Engineering. doi:10.1016/j.cma.2020.113161

13. **Multi-stage preconditioners for thermal–compositional–reactive flow in porous media.** MA Cremon, N Castelletto, JA White. Journal of Computational Physics. doi:10.1016/j.jcp.2020.109607

14. **Scalable multigrid reduction framework for multiphase poromechanics of heterogeneous media.** QM Bui, D Osei-Kuffuor, N Castelletto, JA White. SIAM Journal on Scientific Computing. doi:10.1137/19M1256117

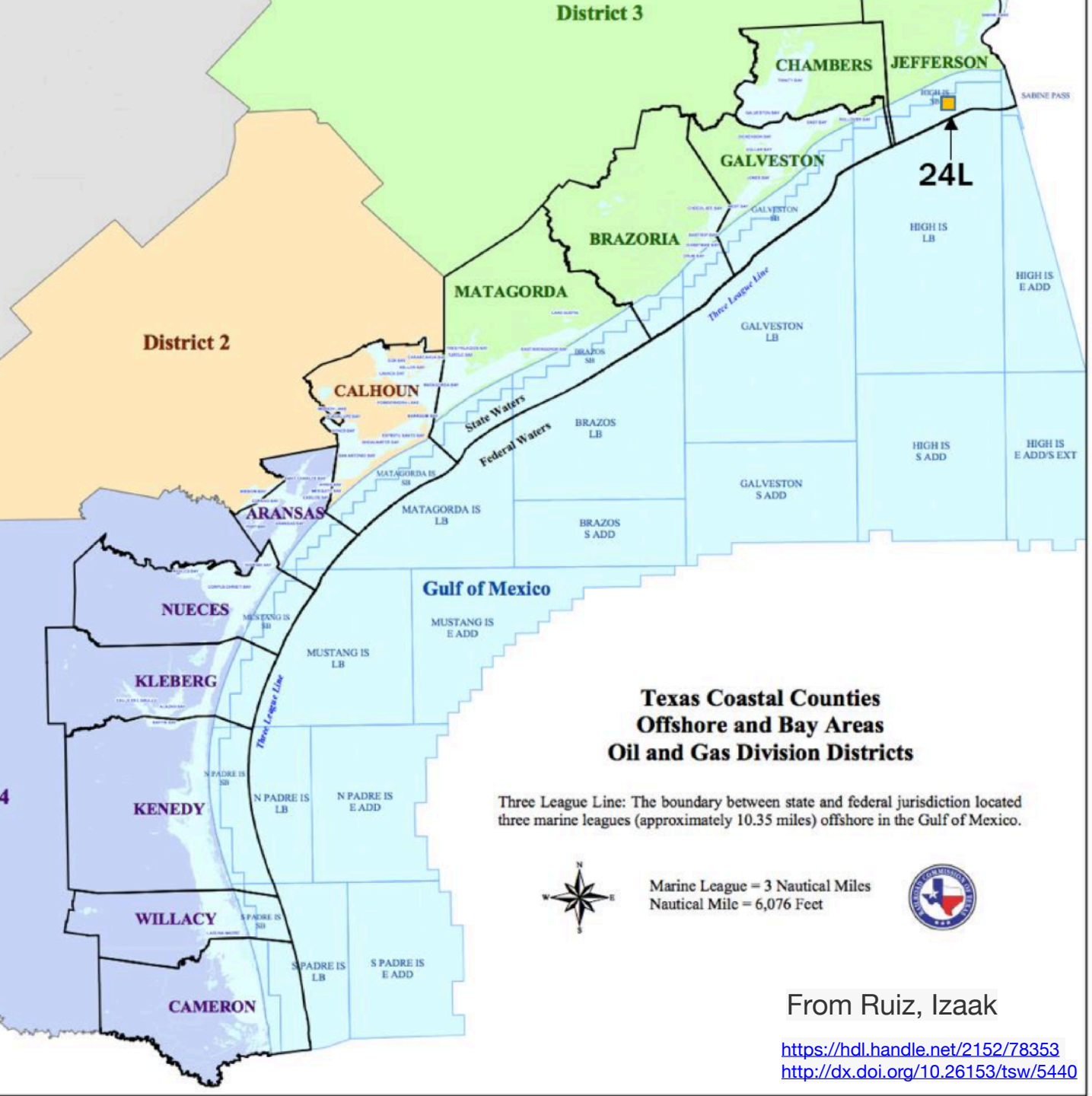
15. **Fully implicit multidimensional hybrid upwind scheme for coupled flow and transport.** F Hamon, B Mallison. Computer Methods in Applied Mechanics and Engineering. doi:10.1016/j.cma.2019.112606

16. **A two-stage preconditioner for multiphase poromechanics in reservoir simulation.** JA White, N Castelletto, S Klevtsov, QM Bui, D Osei-Kuffuor, HA Tchelepi. Computer Methods in Applied Mechanics and Engineering. doi:10.1016/j.cma.2019.112575

17. **Multiscale two-stage solver for Biot's poroelasticity equations in subsurface media.** Castelletto, S Klevtsov, H Hajibeygi, HA Tchelepi. Computational Geosciences. doi:10.1007/s10596-018-9791-z

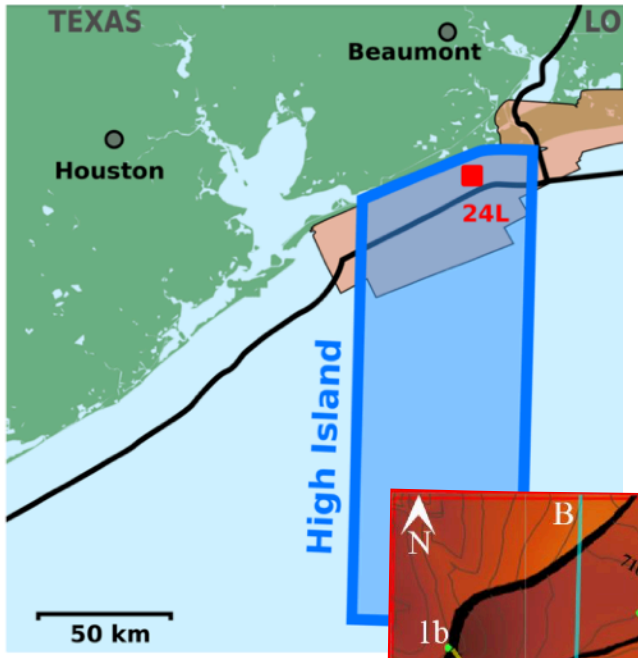
18. **Block preconditioning for fault/fracture mechanics saddle-point problems**. A Franceschini, N Castelletto, M Ferronato. Computer Methods in Applied Mechanics and Engineering. doi:10.1016/j.cma.2018.09.039.

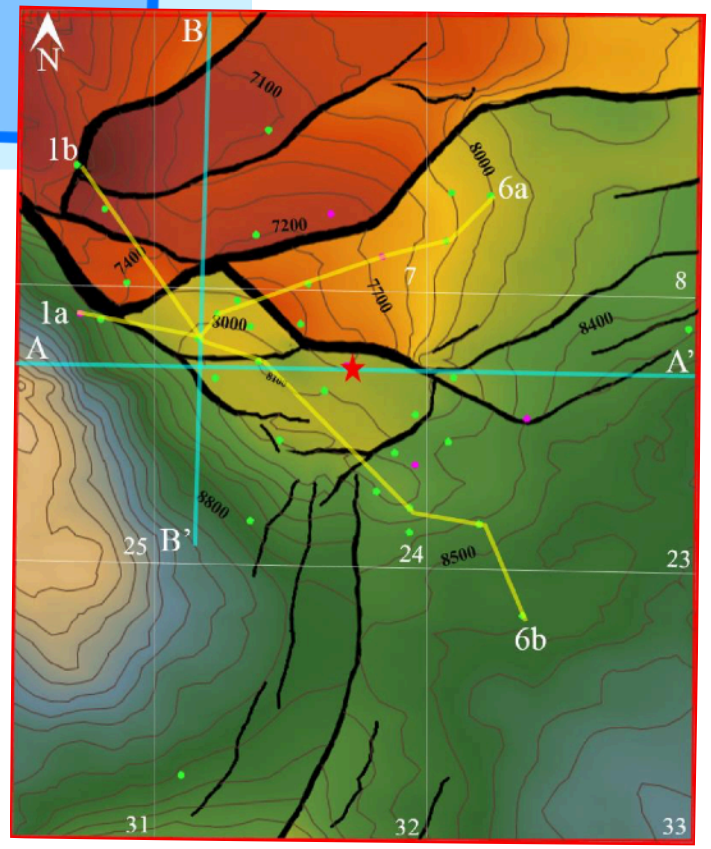
19. **A relaxed physical factorization preconditioner for mixed finite element coupled poromechanics.** M Frigo, N Castelletto, M Ferronato. SIAM Journal on Scientific Computing. doi:10.1137/18M120645X



From Ruiz, Izaak

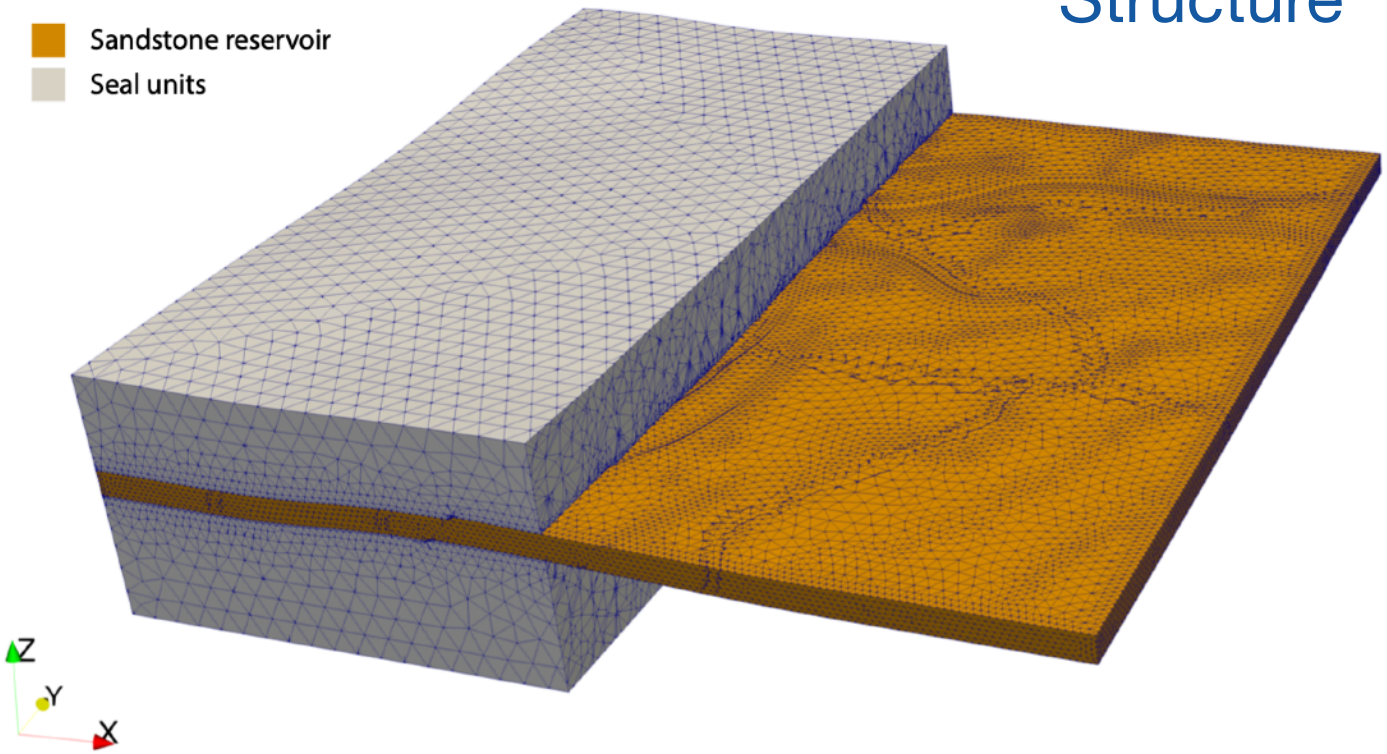
https://hdl.handle.net/2152/78353
http://dx.doi.org/10.26153/tsw/5440



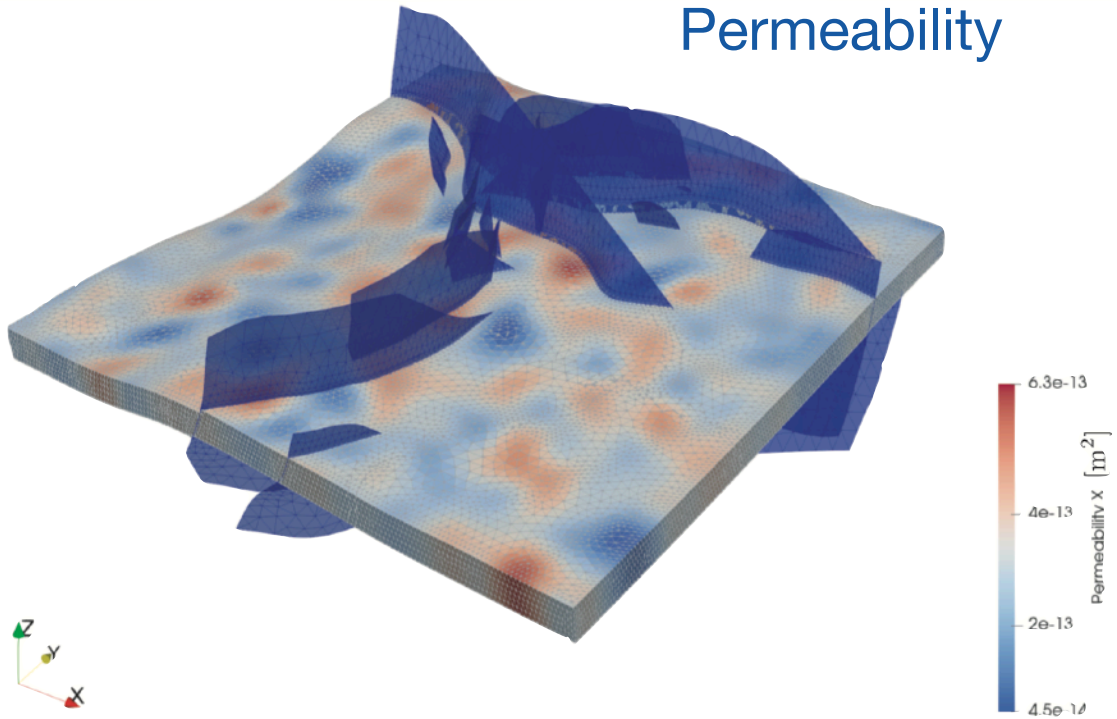


Poroelasticity at the Reservoir Scale

Structure



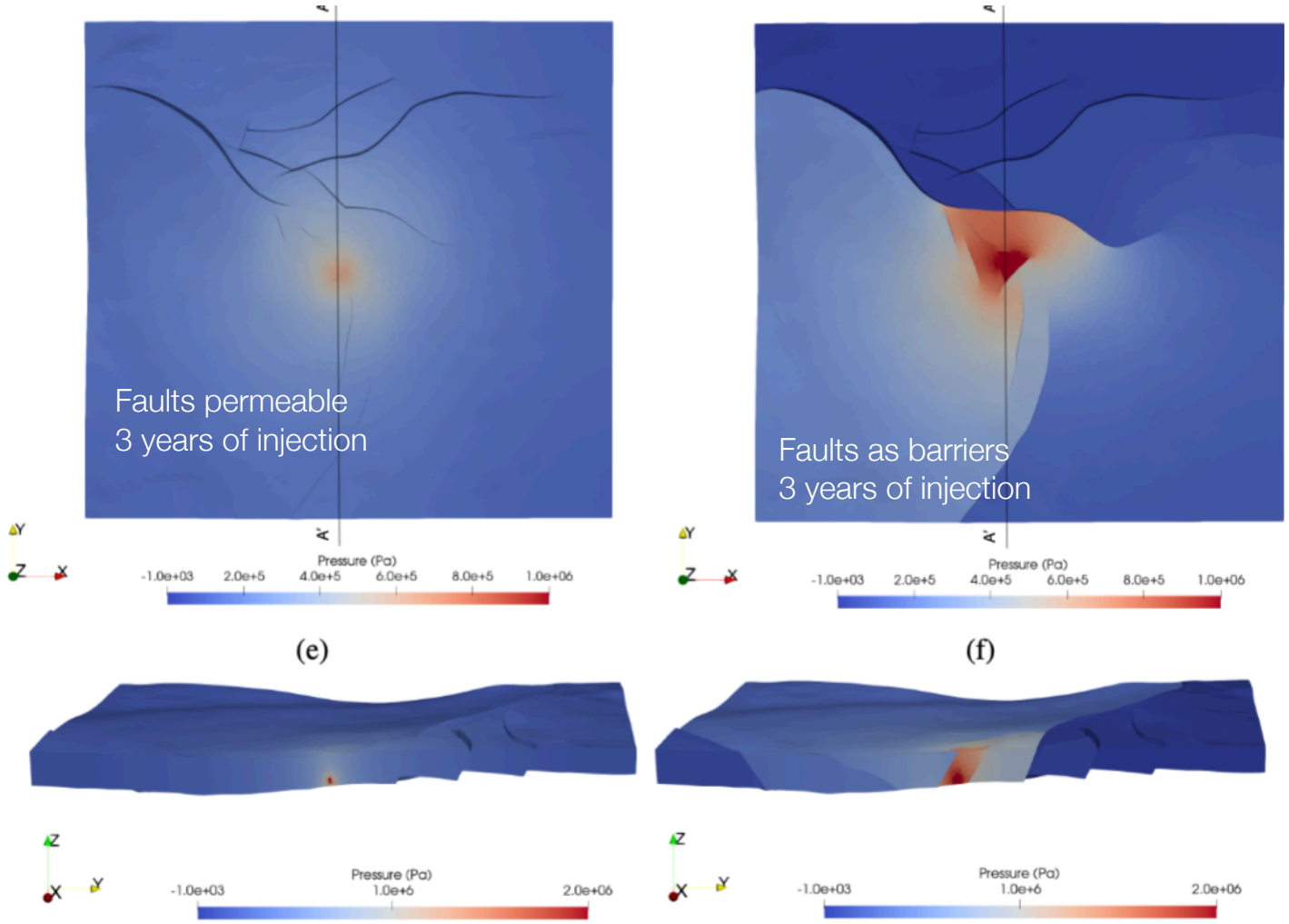
Permeability

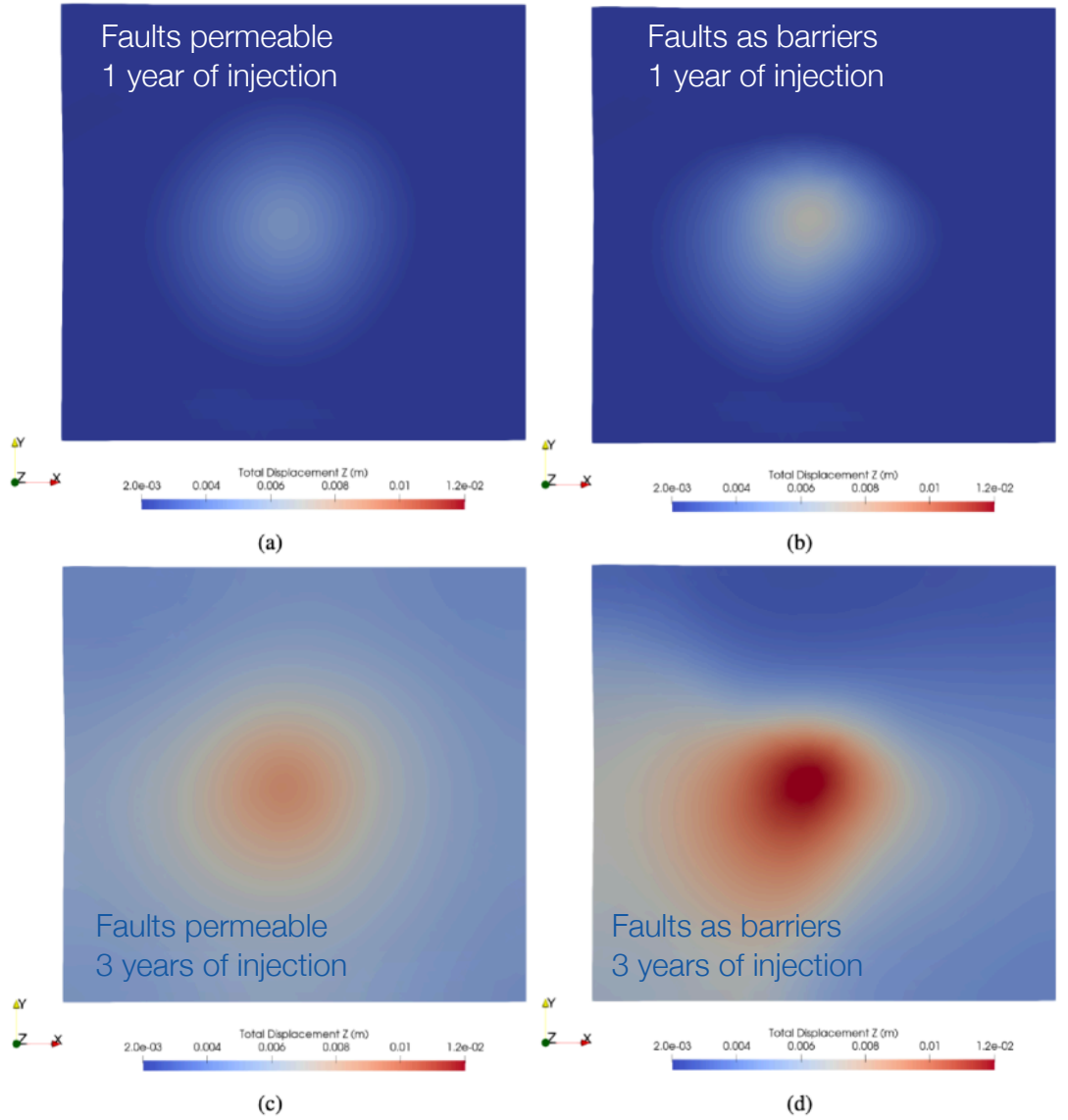


1.8 M tetrahedral cells, 50m in reservoir layers
300k nodes
2.7 M degrees of freedom
12 x 15 km

Deformation monitoring feasibility at an offshore carbon storage site
Interim progress report for GCCC, December 2020.
Julia T. Camargo & Joshua A. White

Are the faults permeable?



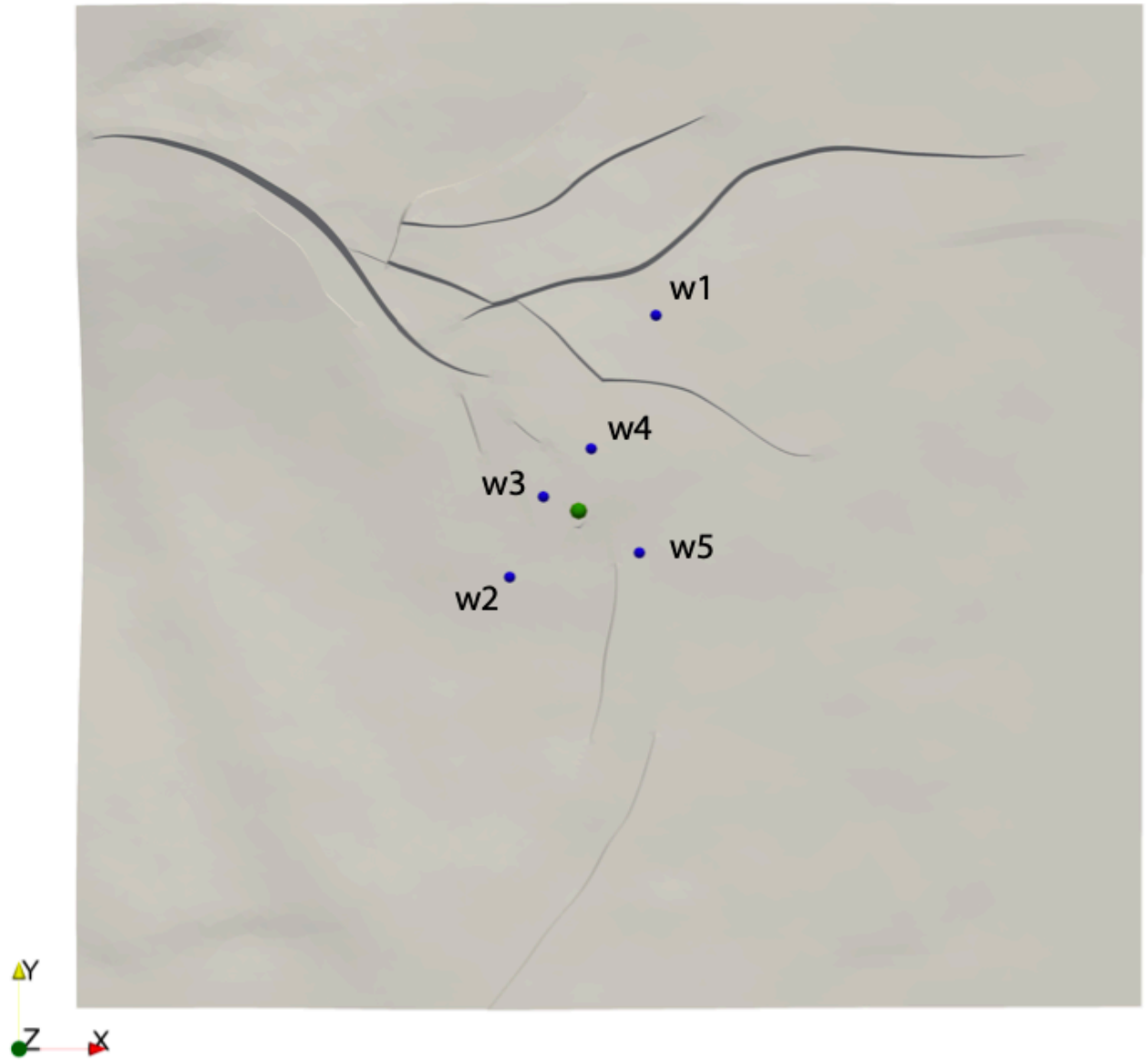


Pressure front
Faults are sealing

Deformation of the reservoir top
Faults are sealing

Is the injection detectable by fibre optic sensors?

After 3 years, faults acting as barriers



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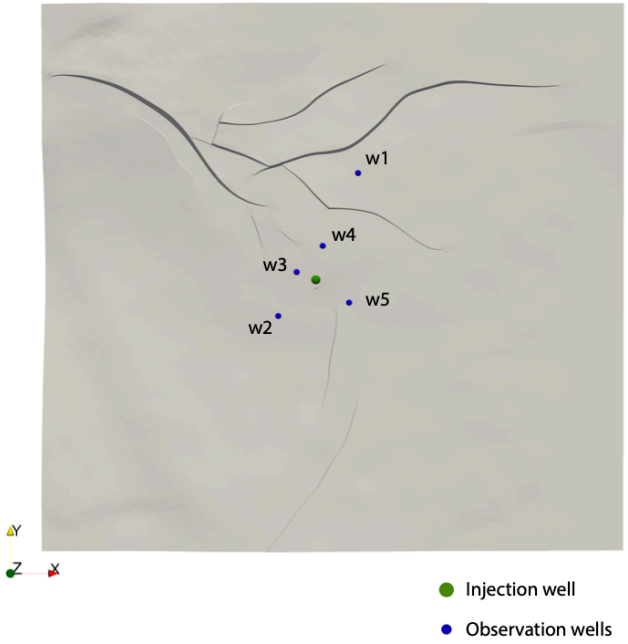
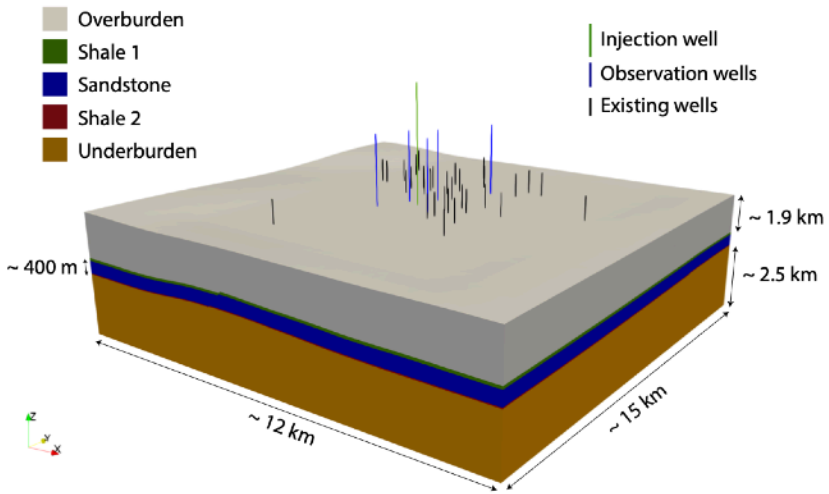
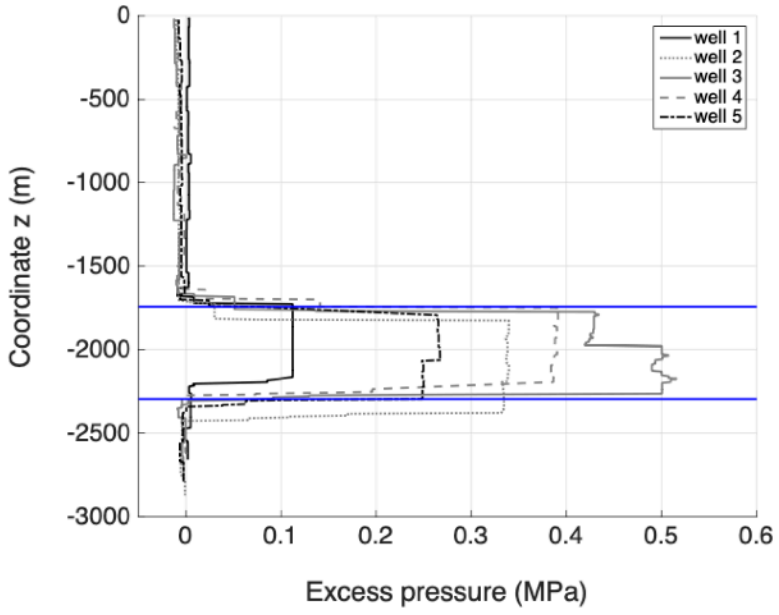
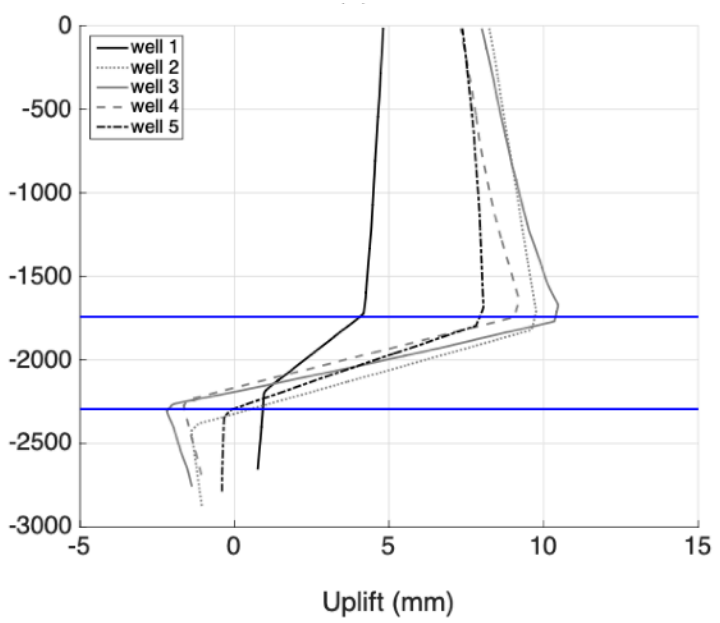
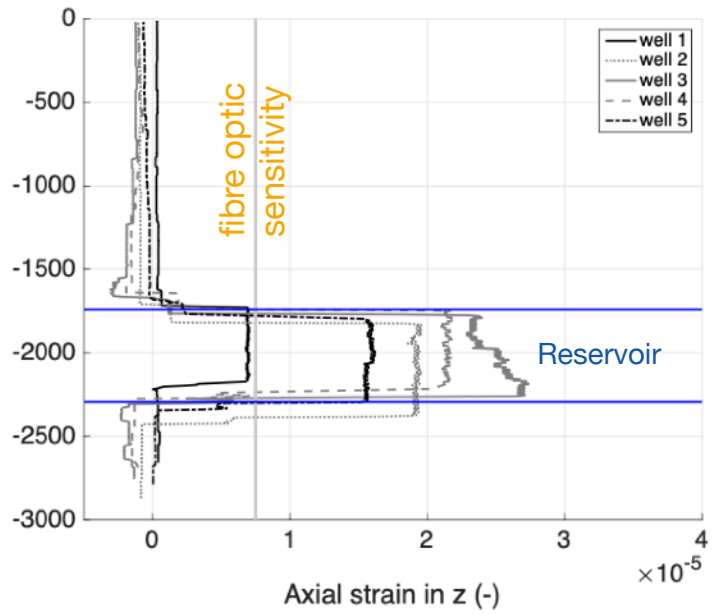




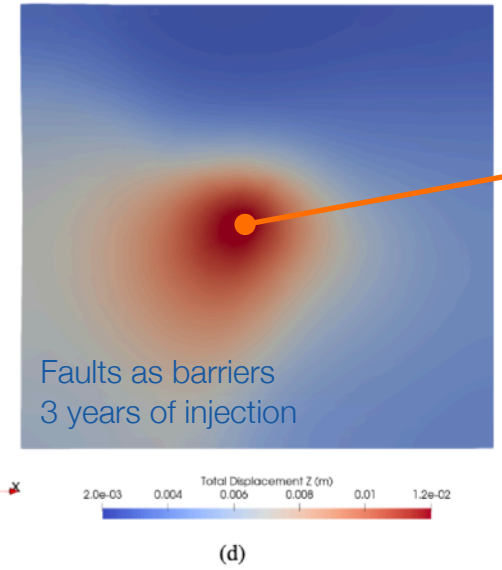


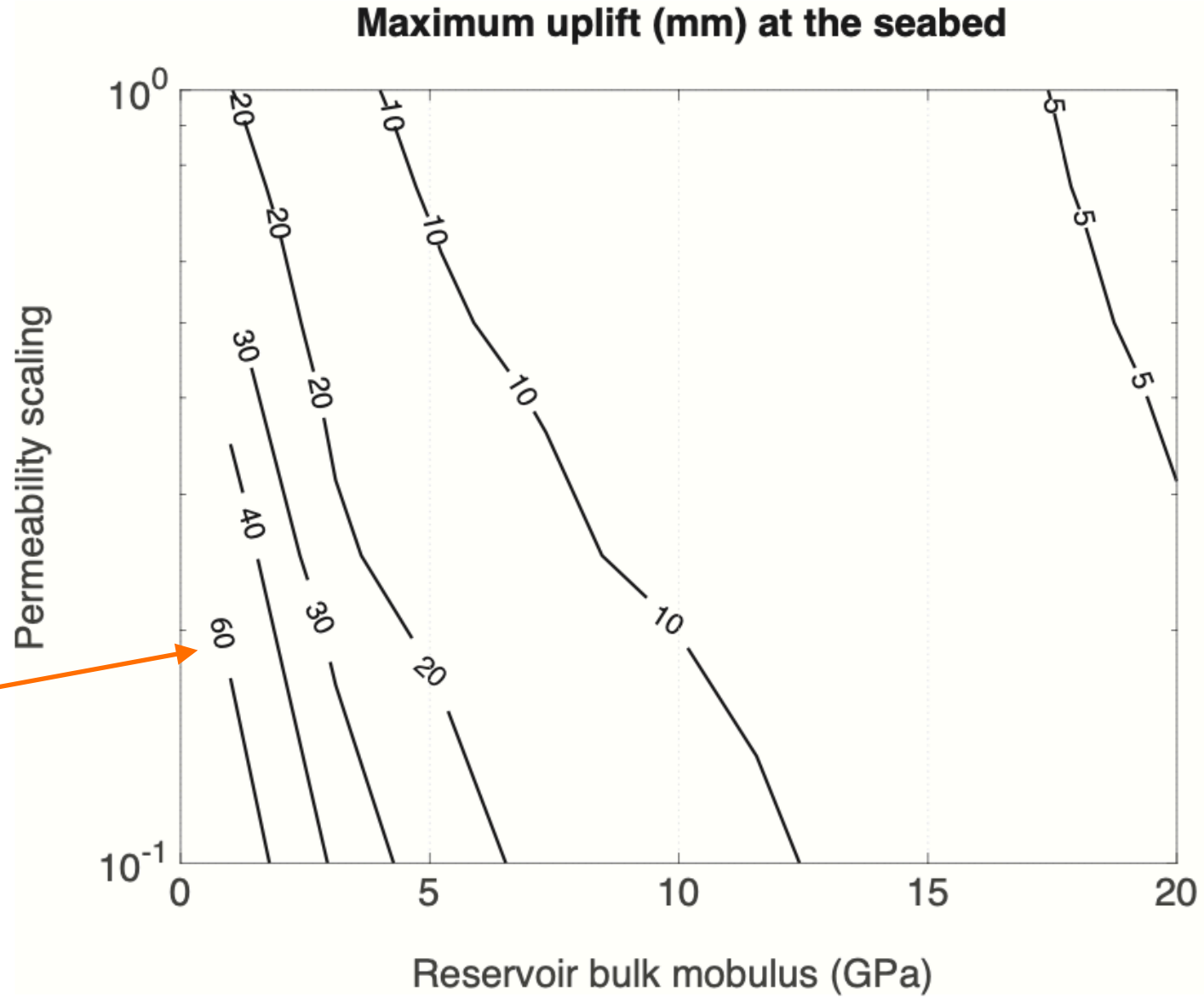




Uncertainty Quantification

What is the risk of uplift at the seabed, based on reservoir properties?





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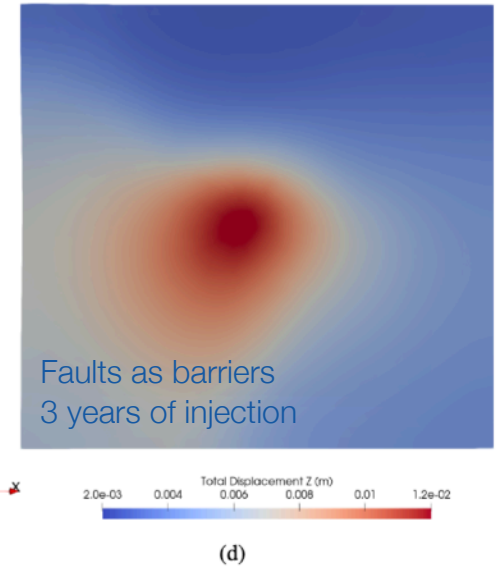
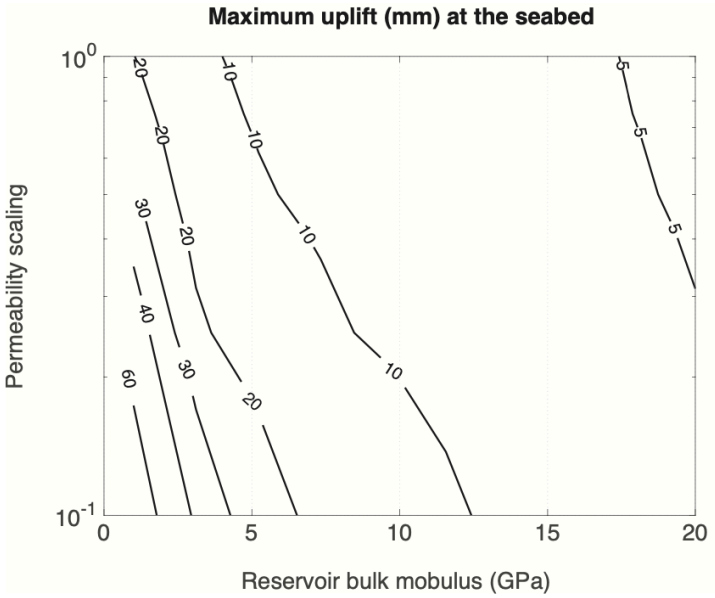
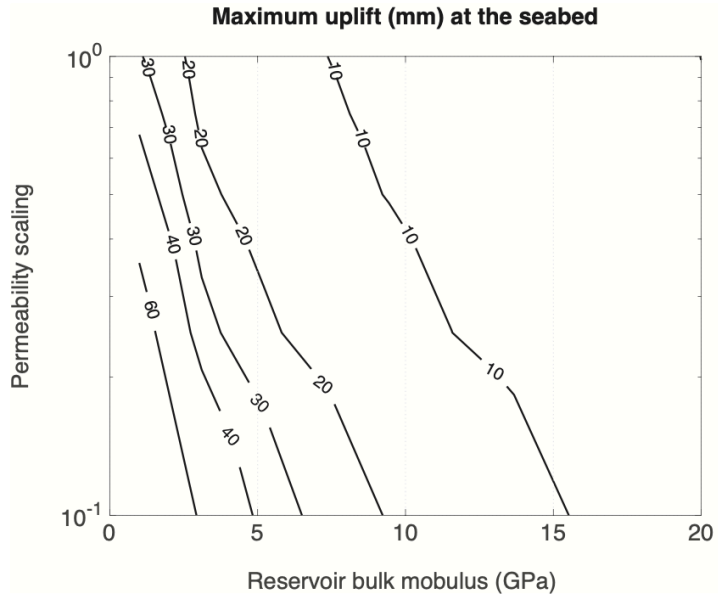
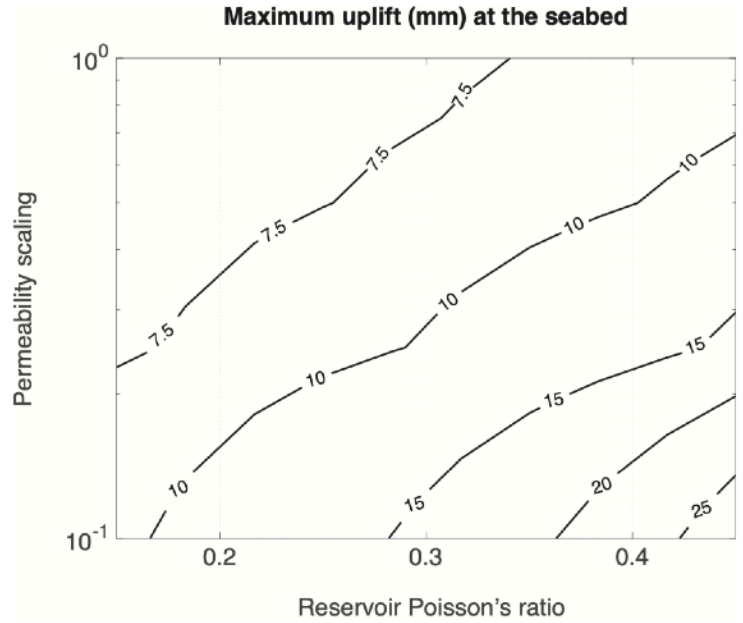
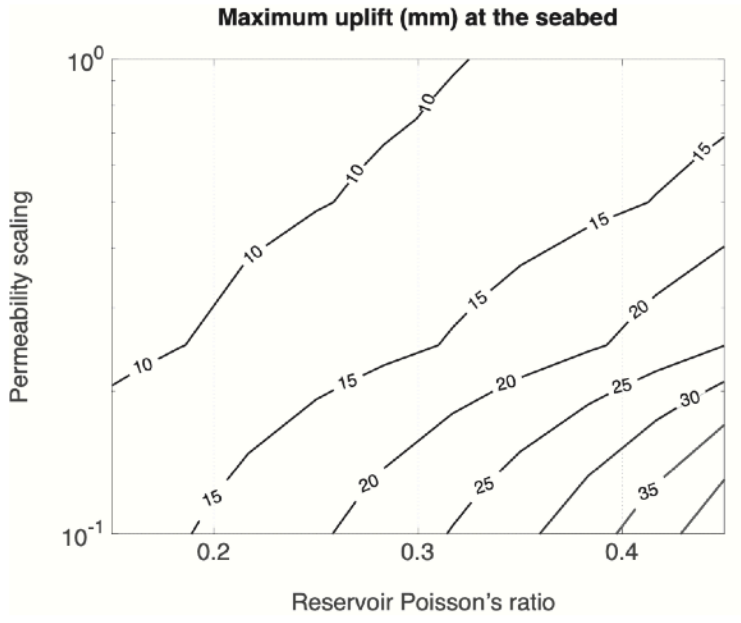


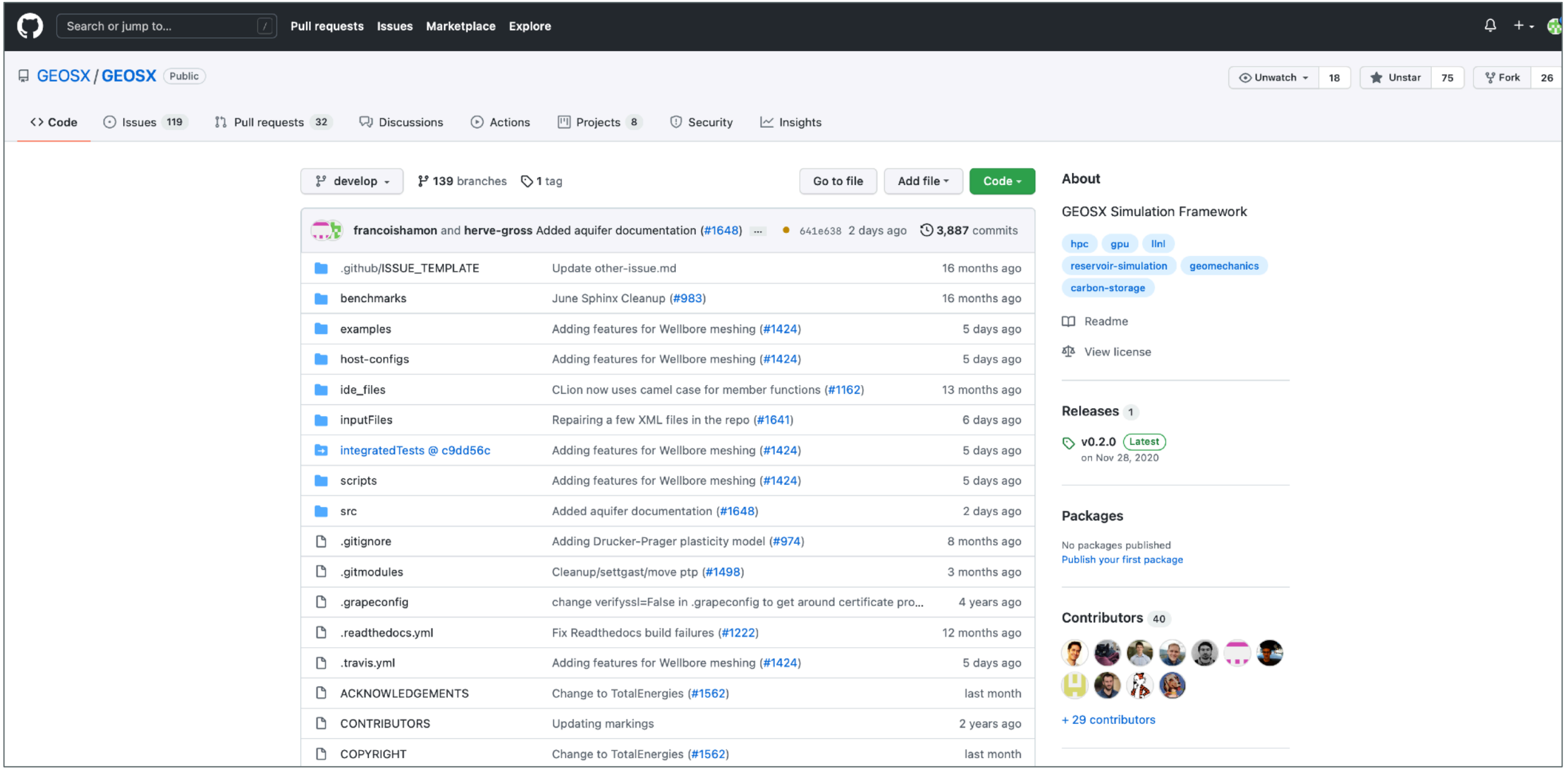




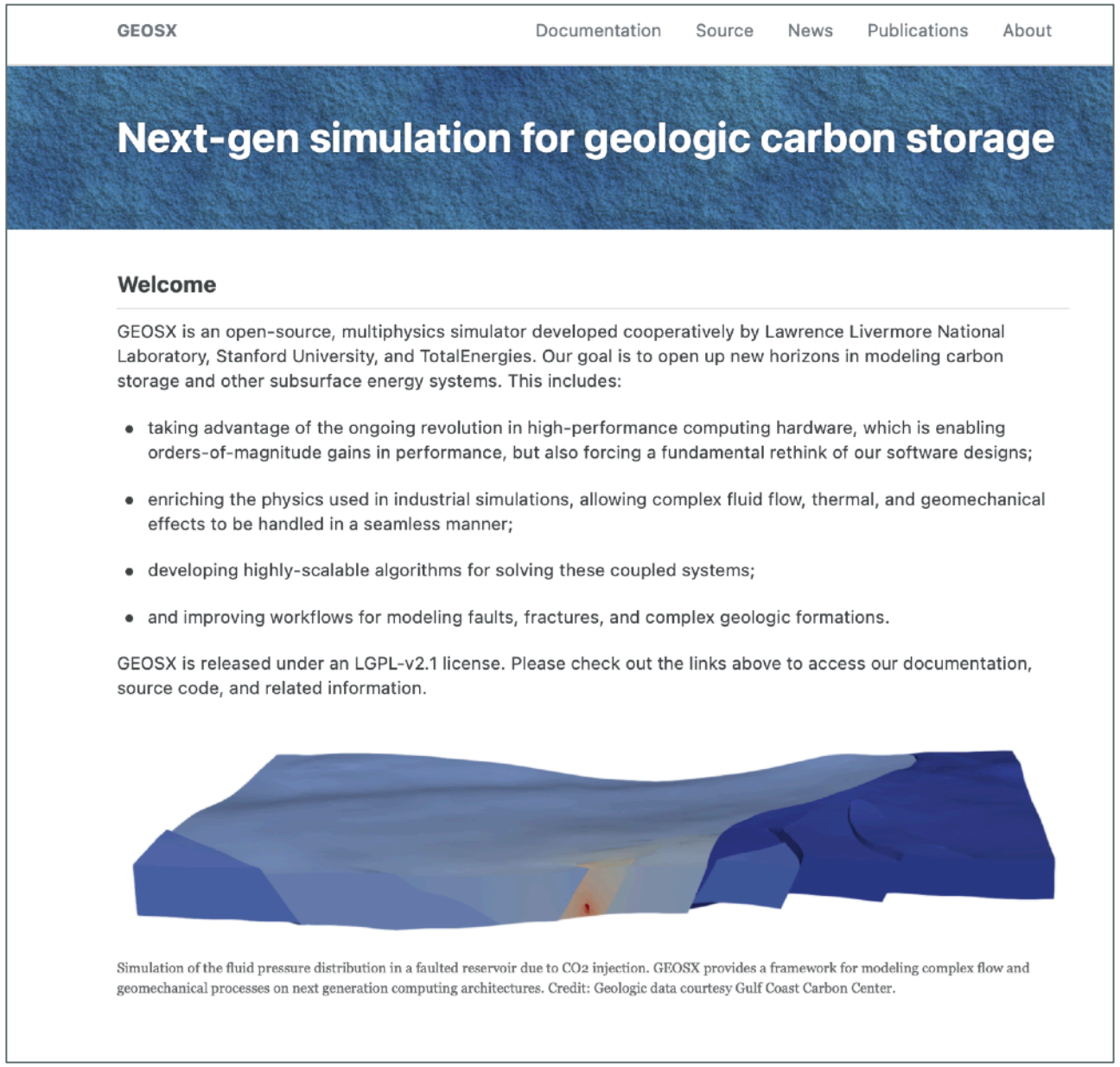




How can I try GEOSX? Can I just take a quick look?



How can I try GEOSX? Can I just take a quick look?



http://www.geosx.org

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Constitutive models
Defining properties
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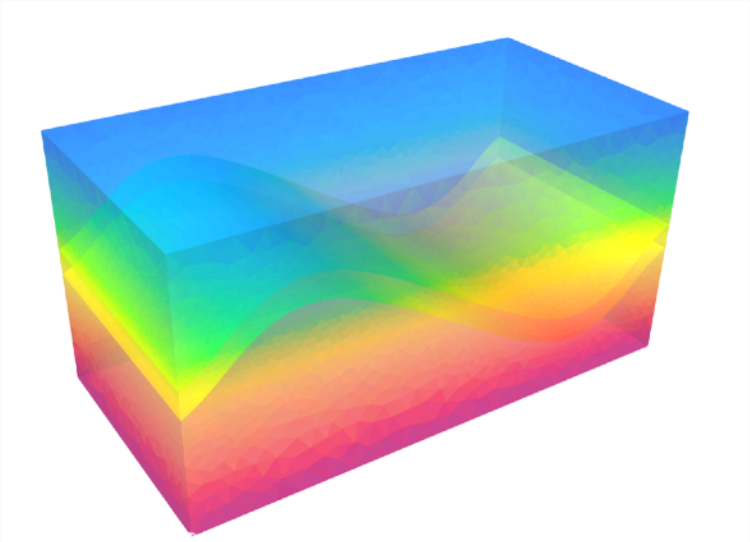

The mesh is defined using the GMSH file format (see Meshes for more information on the supported mesh file format). Each tetrahedron is associated to a unique tag.

The XML file considered here follows the typical structure of the GEOSX input files:

1. Solver
2. Mesh
3. Geometry
4. Events
5. NumericalMethods
6. ElementRegions
7. Constitutive
8. FieldSpecifications
9. Outputs
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Single-phase solver

Let us inspect the **Solver** XML tags.

This node gathers all the information previously defined. We use a classical `SinglePhaseFVM` Finite Volume Method, with the two-point flux approximation as will be defined in the **NumericalMethods** tag. The `targetRegions` refers only to the Reservoir region because we only solve for flow in this region. The `fluidNames` and `solidNames` refer the materials defined in the **Constitutive** tag.

The `NonlinearSolverParameters` and `LinearSolverParameters` are used to set usual numerical solver parameters such as the linear and nonlinear tolerances, the preconditioner and solver types or the maximum number of nonlinear iterations.

Is there a **documentation webpage** for GEOSX?

Call to Action

Find out more
www.geosx.org

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https://github.com/GEOSX/GEOSX

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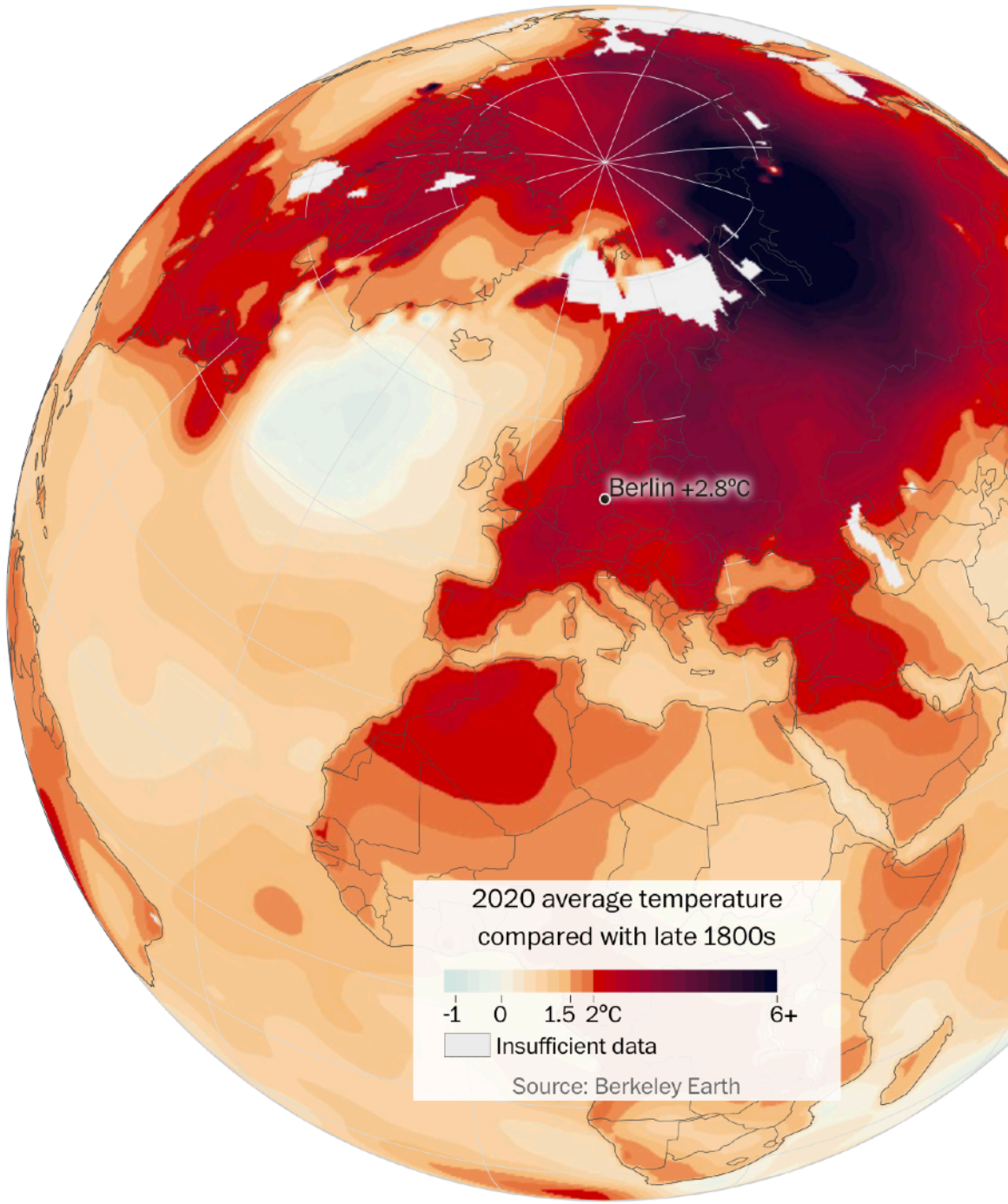

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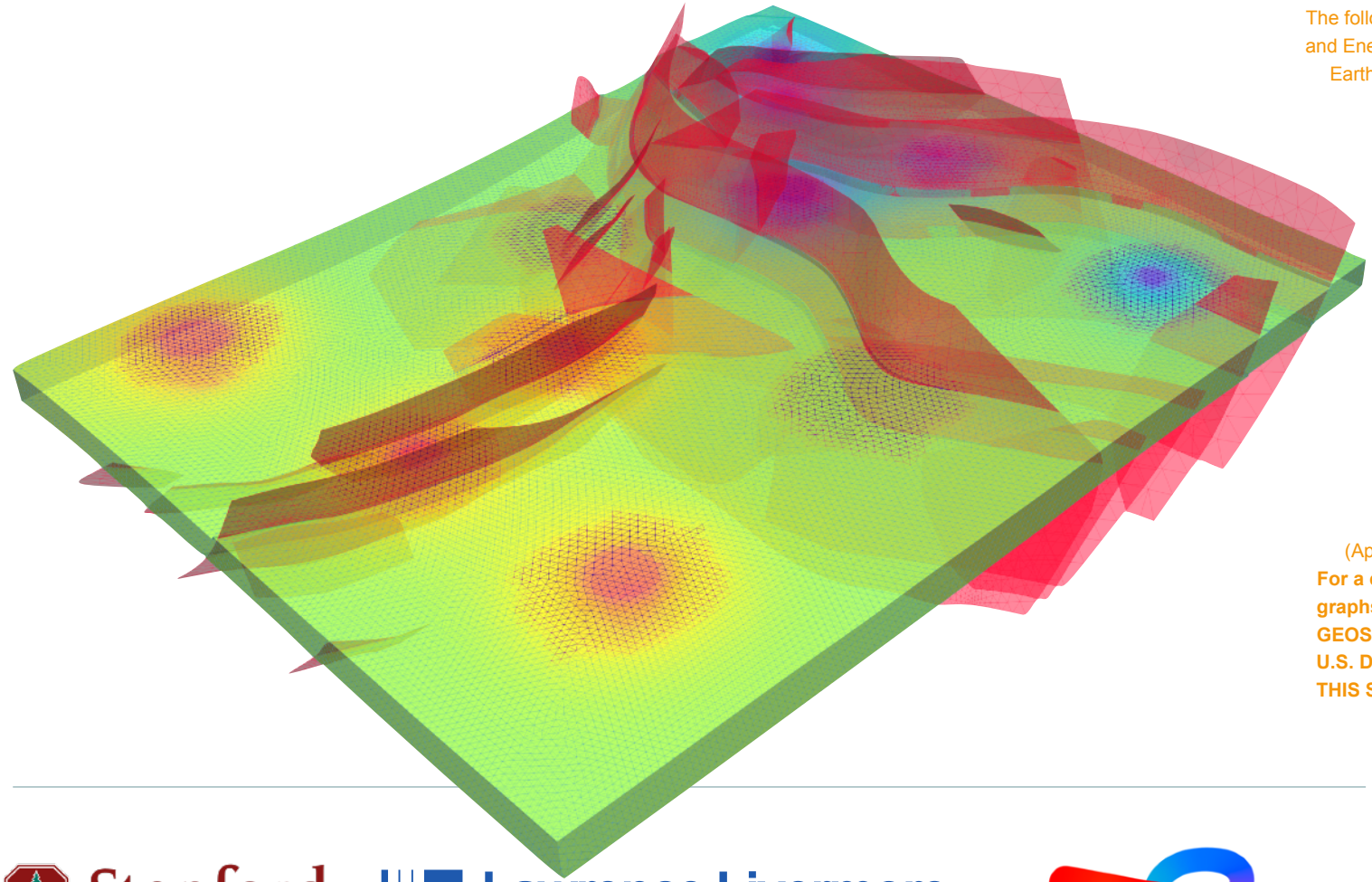

GEOSX is an open source project and is developed by a community of researchers at several institutions. The bulk of the code has been written by contributors from three main organizations: Lawrence Livermore National Laboratory, Stanford University, and Total, S.A..

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For a complete up-to-date list of contributors, see https://github.com/GEOSX/GEOSX/graphs/contributors

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