Disclaimer and copyright reservation

Definition - TotalEnergies / Company

The entities in which TotalEnergies SE directly or indirectly holds an interest are separate and independent legal entities. The terms "TotalEnergies", "TotalEnergies company" and "Company" used in this document are used to refer to TotalEnergies SE and its affiliates included in the scope of consolidation. Similarly, the terms "we", "us", "our" may also be used to refer to these entities or their employees.
It cannot be inferred from the use of these expressions that TotalEnergies SE or any of its affiliates is involved in the business or management of any other company of the TotalEnergies company.

Disclaimer

This presentation may include forward-looking statement within the meaning of the Private Securities Litigation Reform Act of 1995 with respect to the financial condition, results of operations, business, strategy and plans of TotalEnergies that are subject to risk factors and uncertainties caused by changes in, without limitation, technological development and innovation, supply sources, legal framework, market conditions, political or economic events.
TotalEnergies does not assume any obligation to update publicly any forward-looking statement, whether as a result of new information, future events or otherwise.
Further information on factors which could affect the company's financial results is provided in documents filed by TotalEnergies with the French *Autorité des Marchés Financiers* and the US Securities and Exchange Commission.
Accordingly, no reliance may be placed on the accuracy or correctness of any such statements.

Copyright

TotalEnergies

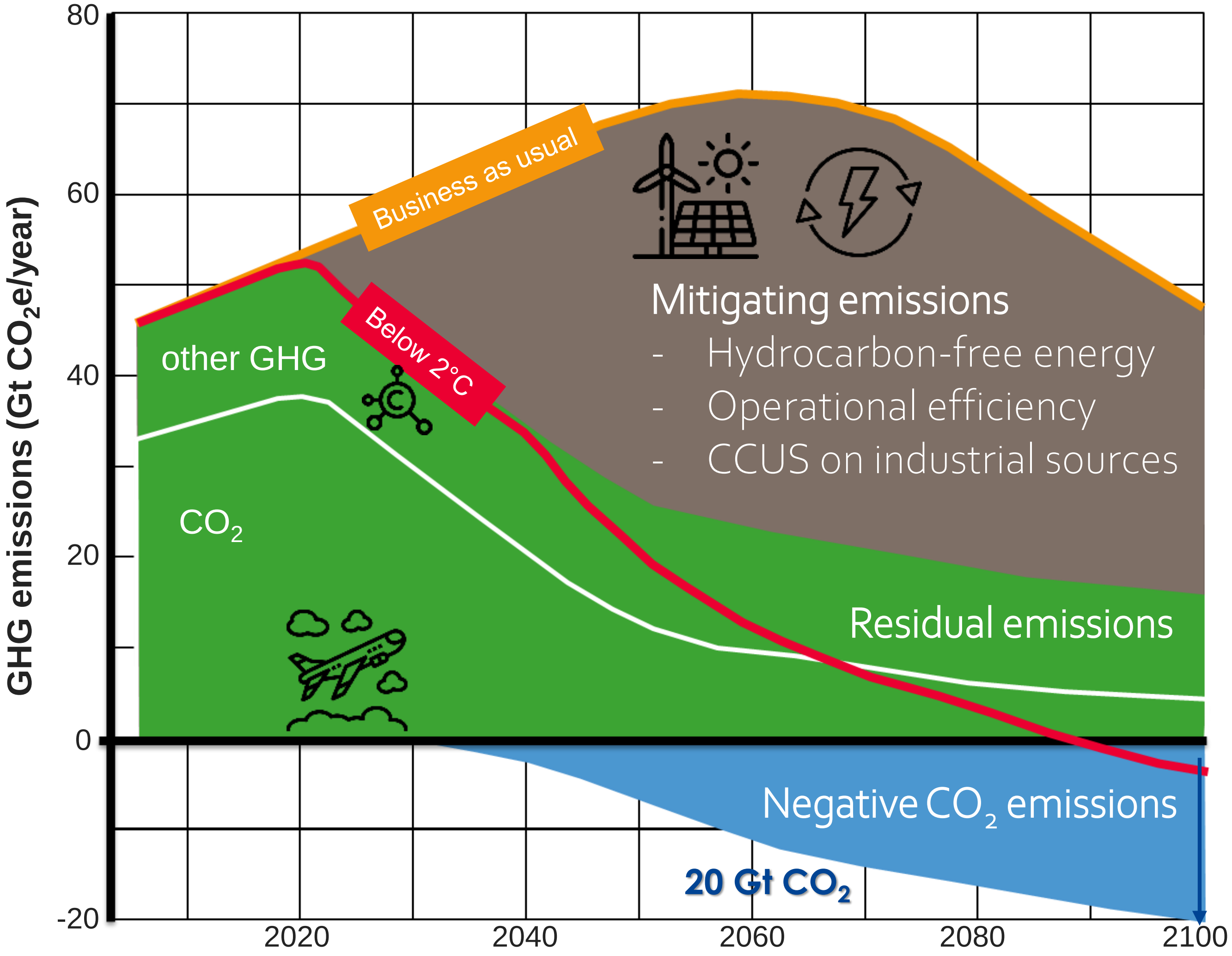
Exascale multiphysics simulator platform for CO2 sequestration and monitoring

1/ Context

2/ Challenges

3/ Algorithm motifs related to the project

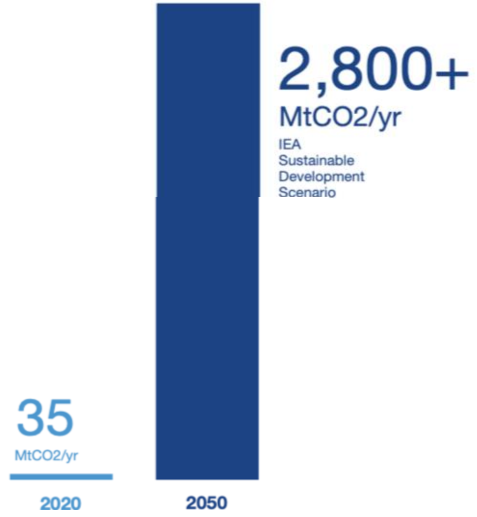
The role of CCUS in climate change mitigation

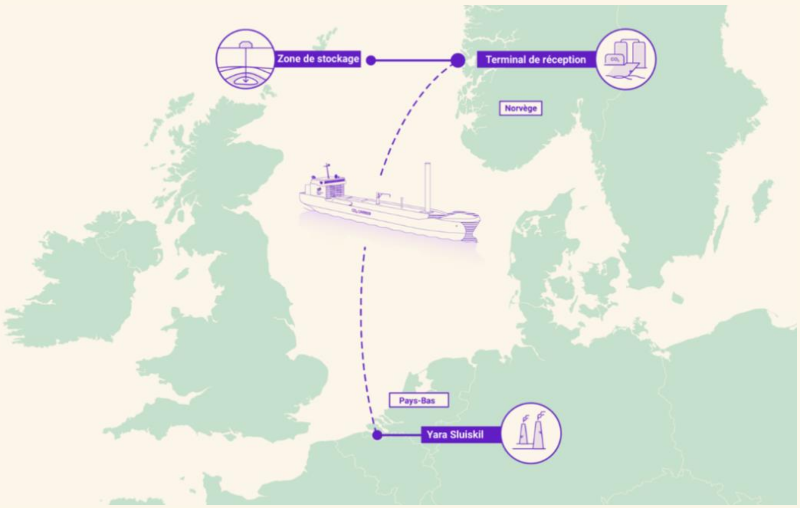


Source: The Emissions Gap Report 2017. United Nations Environment Programme (UNEP)

TotalEnergies

Inria

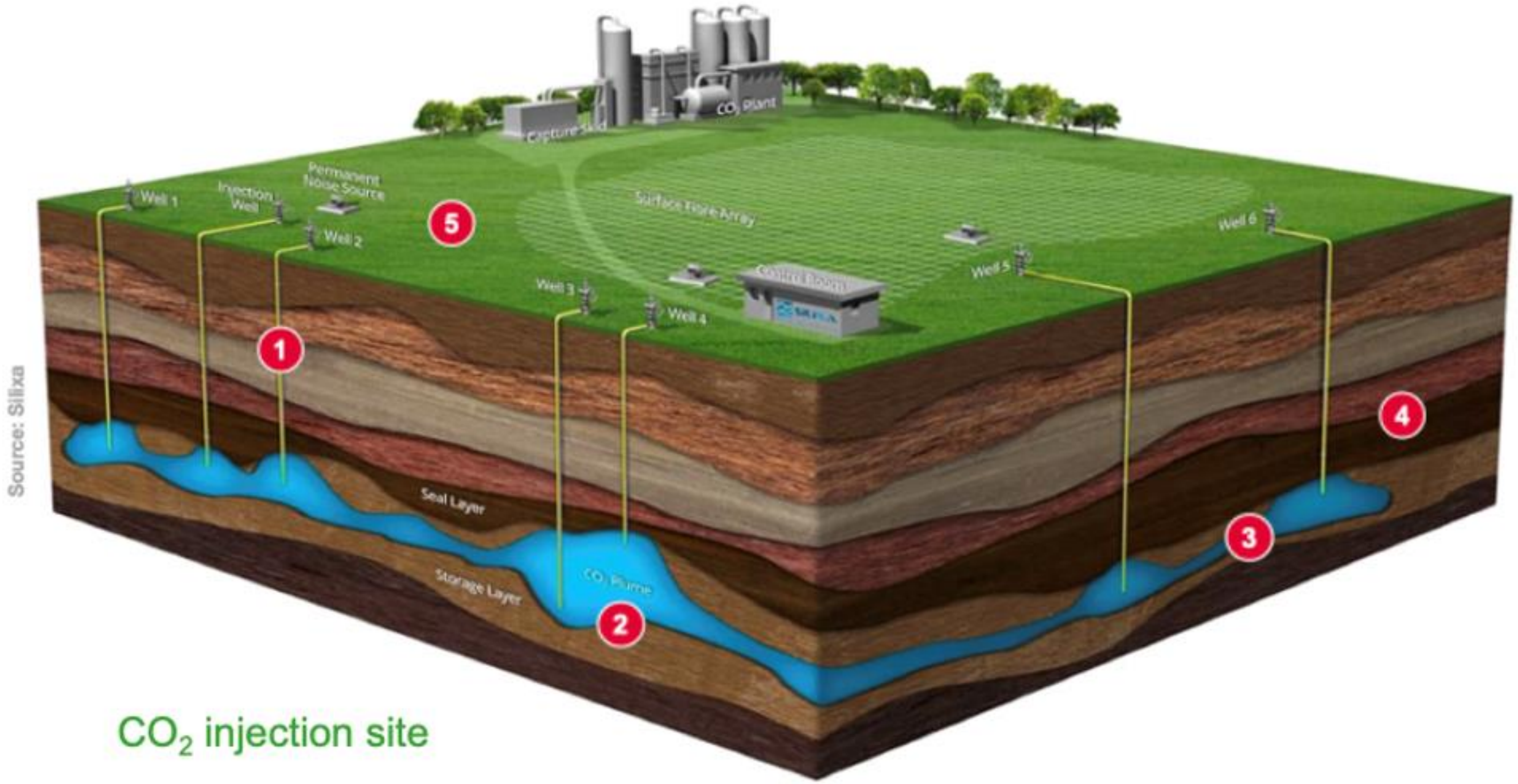




Northern Lights enters into cross-border transport and storage agreement with Ørsted

May 15, 2023

Preserving the integrity of the injection site is a priority issue



CO_2 injection site

1. Well integrity/injectivity
2. Pressure/Stress change
Fault Activation
3. CO_2 transport & trapping
4. Seal integrity
5. Surface deformation
Seismicity

TotalEnergies Inria

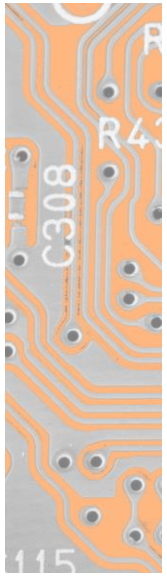
Modeling and simulation challenges

Flow, geo-mechanics, gravimetry, …

…and **seismic** modelling/inverse problem

Essential for demonstrating **safety** and **perennity**

Monitoring acquisition technology is evolving (**DAS**)

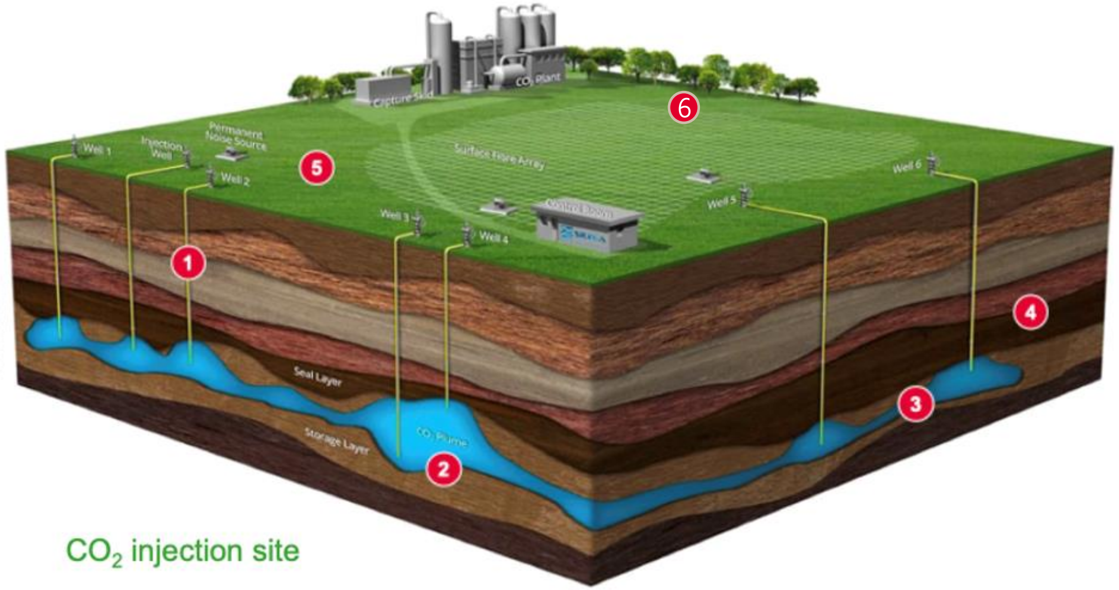


Large Scale: 98% storage in Aquifer

Long Term Simulation: post injection matters

Solutions:

- ✓ **Scalable** algorithms (exascale)
- ✓ Seismic methods **coupled** w/ CO2 injection simulation.
- ✓ Perennial: **portability**



1 Well integrity/injectivity

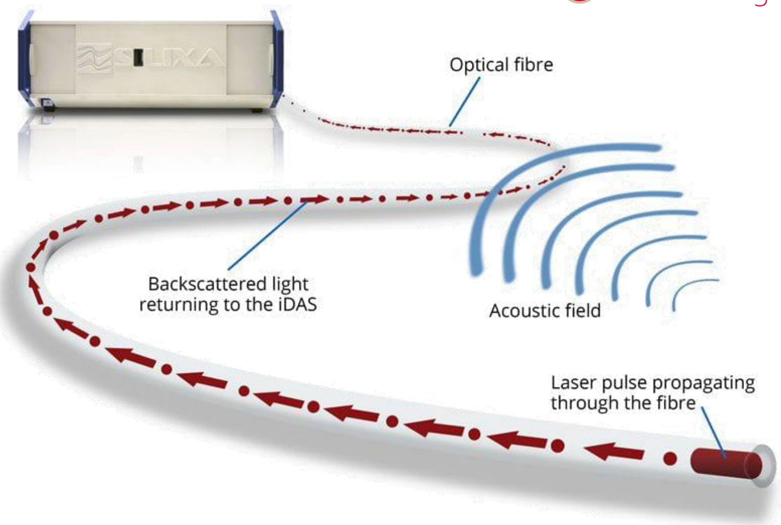
2 Pressure/Stress change
Fault Activation

3 CO_2 transport & trapping

4 Seal integrity

5 Surface deformation
Seismicity

6 Monitoring system (DAS)



TotalEnergies

Inria

GEOS:Next-gen simulation for geologic carbon storage

GEOS
Multiphysics Simulator on HPC

Stanford University

Lawrence Livermore National Laboratory

TotalEnergies

Chevron

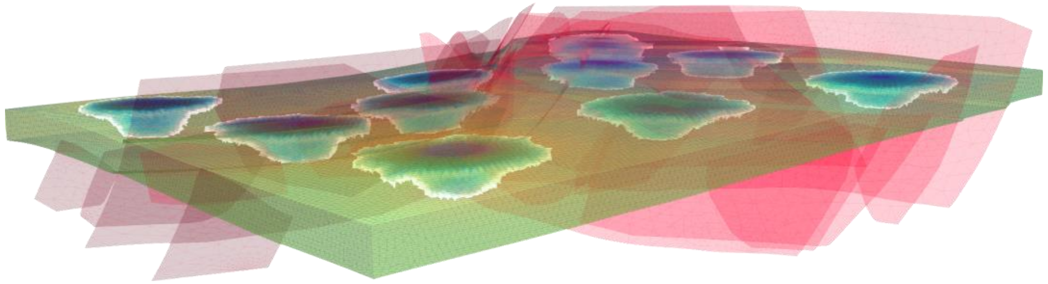
Key dates:

2018: FC-MAELSTROM: a 5 years project in collaboration with Lawrence Livermore National Laboratory, Stanford University, and TotalEnergies.

2020: GEOS is released as an open-source Multiphysics simulation platform

2022: a 4 years TotalEnergies and Inria joint team to extend GEOS Multiphysics to geophysics monitoring: **MAKUTU** project

Feb 2022: FC-MAELSTROM2 a 5 years extension of FC-MAELSTROM project with Chevron as new member.



MULTIPHYSICS

EXASCALE

AUDITABLE

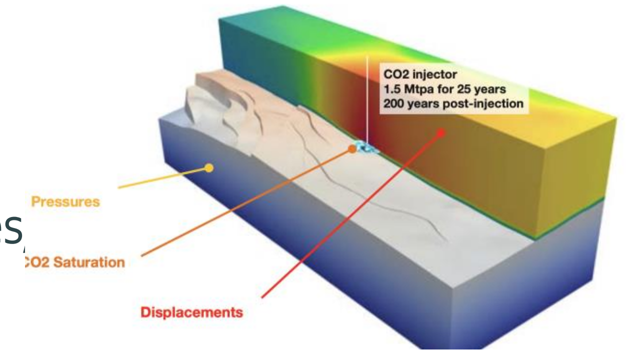
STRATEGIC

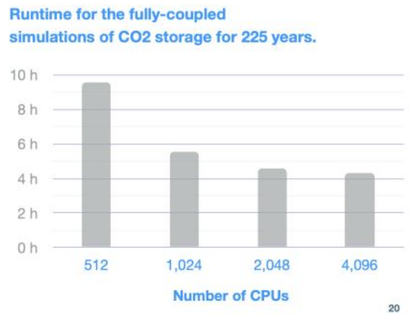
TotalEnergies Inria

GEOS:Next-gen simulation for geologic carbon storage

- Multi-physics, multi-scale (Flow, geomechanics, fractures)
- Open-source and auditable
- Flexibility to develop workflows via PyGEOS
- State-of-the-art programming model

✓ Targets exascale platforms





fully-coupled simulations of CO_2 storage

RAJA → NVIDIA CUDA, AMD HIP RT, SYCL, OpenMP

C-style for-loop

```
double* x ; double* y ;
double a, sum = 0;

for ( int i = beg; i < end; ++i ) {
    y[i] += a * x[i] ;
    sum += y[i] ;
}
```

RAJA-style loop

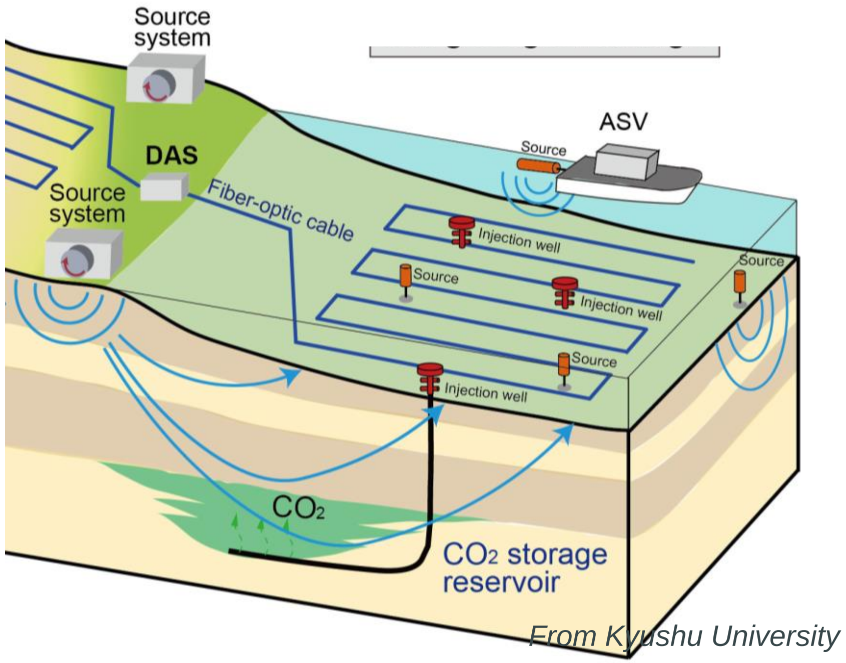
```
double* x ; double* y ;
double a ;
RAJA::SumReduction< reduce_policy, double > sum(0);
RAJA::RangeSegment range(beg, end);

RAJA::forall< exec_policy > ( range, [=] (int i) {
    y[i] += a * x[i] ;
    sum += y[i];
} );
```

TotalEnergies Inria

Makutu: Extend GEOS to seismic for CO_2 monitoring

- Take advantage of long partnership with Inria in the development
  Numerical methods for **waves** in complex media
- Take advantage of GEOS software architecture and programming model

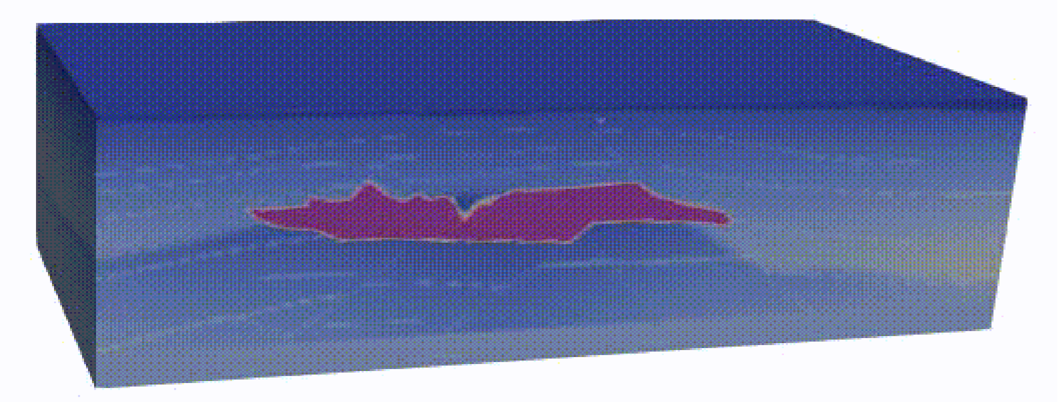


Develop highly optimized wave equations kernels

Develop **workflows** for CO_2 monitoring

De-risk CO_2 injection: monitor **plumes/leaks**

Modelize monitoring of **long-term integrity** of CO_2 reservoir/seal

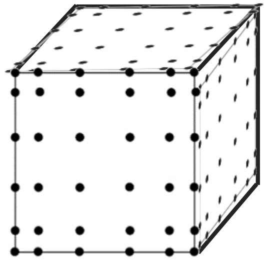


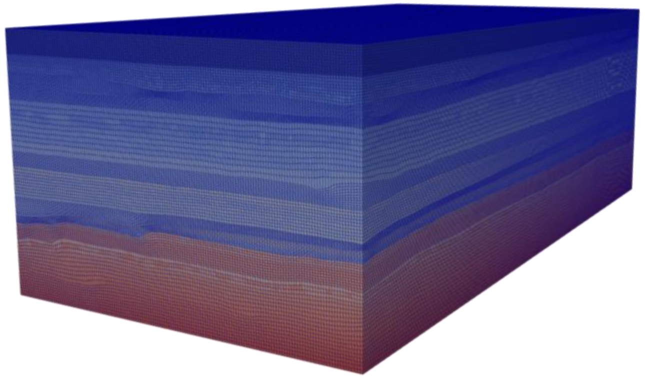
TotalEnergies Inria

Enriching GEOS kernels with elastodynamics

Base wave propagation kernels:

- ✓ Acoustic /elastic, 1st and 2nd order
- ✓ Gauss-Lobatto Spectral Element approach
- ✓ DAS acquisition

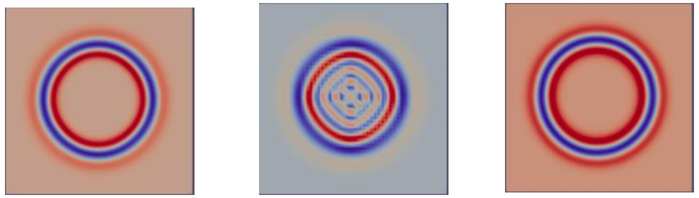




Up to 5th order in space:

- ✓ Full use of GEOS solver kernel structure

Take Advantage of in house GPUs cluster (thanks to RAJA)



Q1: 1M cells | Q1: 125k cells | Q3: 125k cells

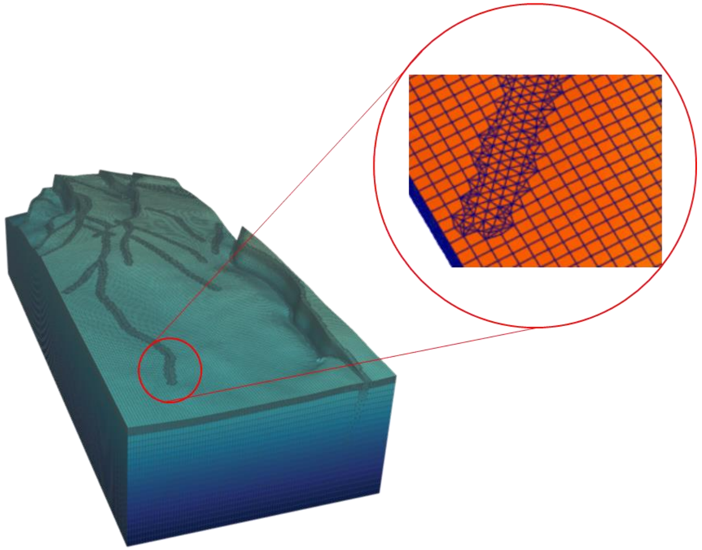
Init. time	Run time	Total time
187s	1430s	1617s
4s	26s	32s

Short-term:

- ✓ SEM VTI Anisotropic
- ✓ SEM Elastico-Acoustic

Mid-term:

- ✓ Discontinuous Galerkin and mixed formulations
- ✓ Pure SEM CG/DG
- ✓ Hex-dominant SEM + DG



TotalEnergies Inria

Performance optimization

Initialization

- ✓ Mesh pre-processing & parallel mesh loading
- ✓ Optimization of geometric map construction

Kernel

- ✓ Single precision (32 bits)
- ✓ Remove unnecessary precalcs on GPU
- ✓ Optimized SEM formulation $O(p^9) \rightarrow O(p^5)$

GPU Memory footprint reduction

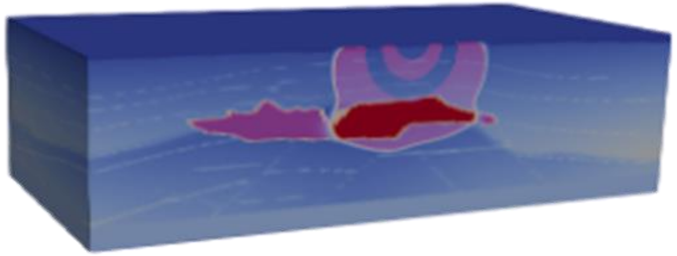
- ✓ Precalcs on CPU
- ✓ Optimized storage / on the fly computation

I/O

- ✓ LIFO asynchronous implementation

MPI

- ✓ Low-level optimization of pack/unpack (MPI)



SEG3D: 95M mesh elements

Time

Init. time	Run time	Total time
697s	79s	778s
78s	37s	116s

Q1, 18MPI/18GPUs, total speedup: 7

Memory

host	device	Run time	Total time
15.8GB	3.4GB	46.5s	147s
15.8GB	0.58GB	46.5s	154s

GPU memory reduction factor: 6

TotalEnergies Inria

Develop advanced workflows PyGEOS

Appeal to practitioners

- ✓ Unlock powerful, complex, domain-specific workflows
- ✓ Flexibility to integrate different libraries:
- ✓ Optimization, ML,….

Status

- ✓ Extension of PyGEOS wrappers
- ✓ Makutu library with utility python classes
- ✓ Basic applications
  - ✓ acquisition management, propagation, FWI
- ✓ Developing more complex workflows
  - ✓ Coupled reservoir + 4D seismic

```python
from pygeosx import initialize,apply_initial_conditions,_finalize
from seismicUtilities.sepUtils import create_dict, write_sep
from seismicUtilities.segy import exportToSegy
from timeit import default_timer as timer

comm = MPI.COMM_WORLD
nRank= comm.Get_size()
rank = comm.Get_rank()
```

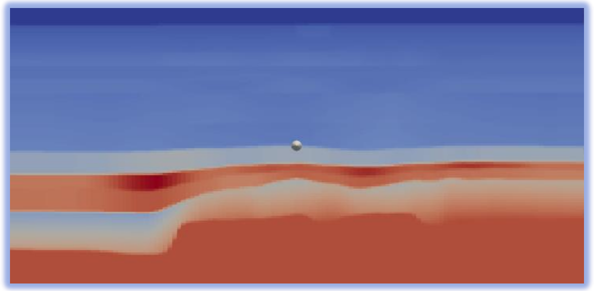
Init & import

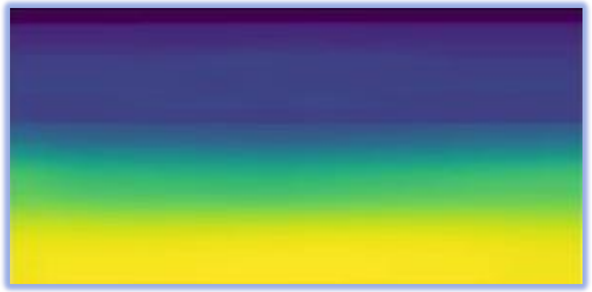
```python
    # get parameters form XML file
    solver=geosx.get_group("/Solvers/acousticSolver")
    srcPos=solver.get_wrapper("sourceCoordinates").value()
    recvPos=solver.get_wrapper("receiverCoordinates").value()
    event=geosx.get_group("/Events")
    maxTime=event.get_wrapper("maxTime").value()
    eventSolver=geosx.get_group("/Events/solverApplications")
    dt=eventSolver.get_wrapper("forceDt").value()
    execOneStep=solver.execute
```

Wrap & access

```python
    time=0
    cycle=0
    startExecuteTimeLoop=timer()
    while time<maxTime:
        if rank == 0 and cycle%100 == 0:
            print("time = %.3fs," % time, "dt = %.4f," % dt, "iter =", cycle
        execOneStep(time,dt)
        time+=dt
        cycle+=1
    comm.Barrier()
    endExecuteTimeLoop=timer()
```

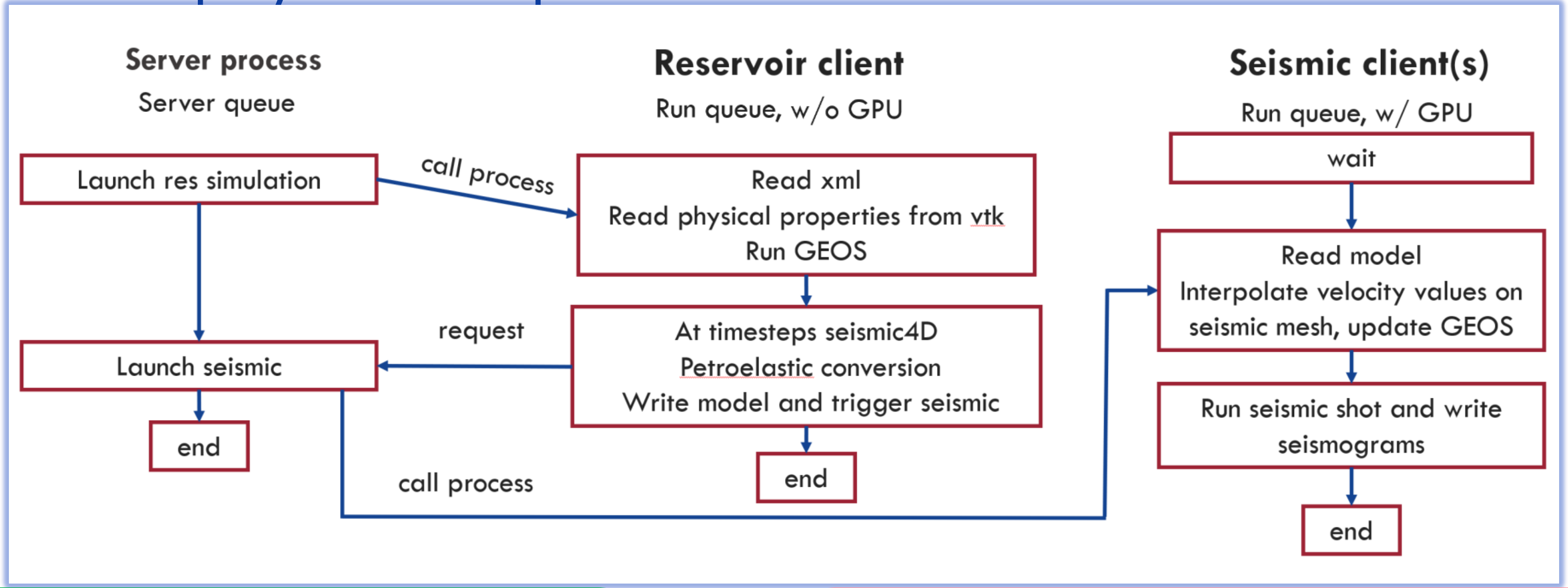
Mix Python & GEOS





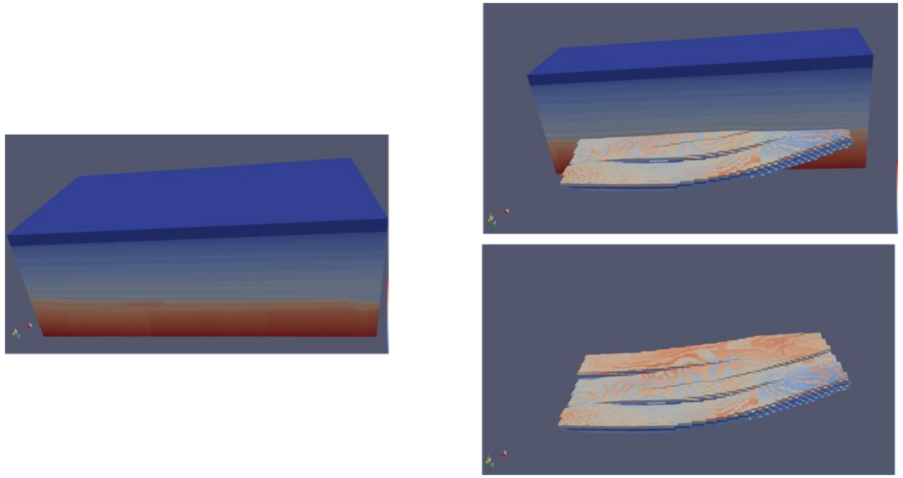
TotalEnergies Inria

Develop Multiphysics coupled workflows

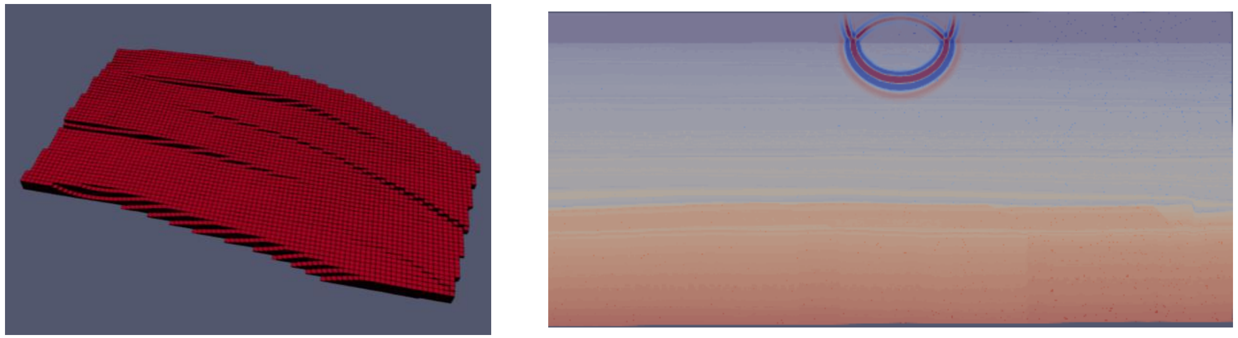


Using in-house RPC client-server library

Common model



Single python script, GEOS



Algorithm motifs related to the project

- Mesh generation
  - Optimized hex-meshes, and hex-dominant meshes for wave propagation,
  - Adaptive Mesh refinement (AMR) for fluid simulation (optional).

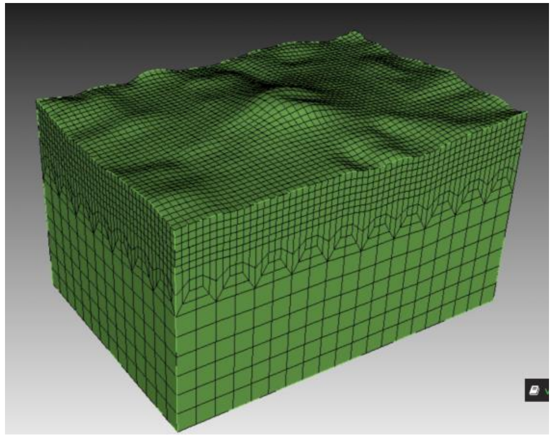
- Performance optimization:
  - Optimized tensor operations for SEM-CG, SEM-CD-DG,
  - Parallel programming model including task programming, explicit data distribution, multithreading and SIMT,
  - Sub-domain decomposition,
  - Efficient asynchronous IO including data compression capabilities for store/read wavefields used for Full Wave Inversion (FWI).

- Improve workflows with Machine learning:
  - Non repeatability of seismic acquisition,
  - Direct inversion of CO_2 plume from 4D effects,
  - Improving FWI convergence…

Part of Makutu work program

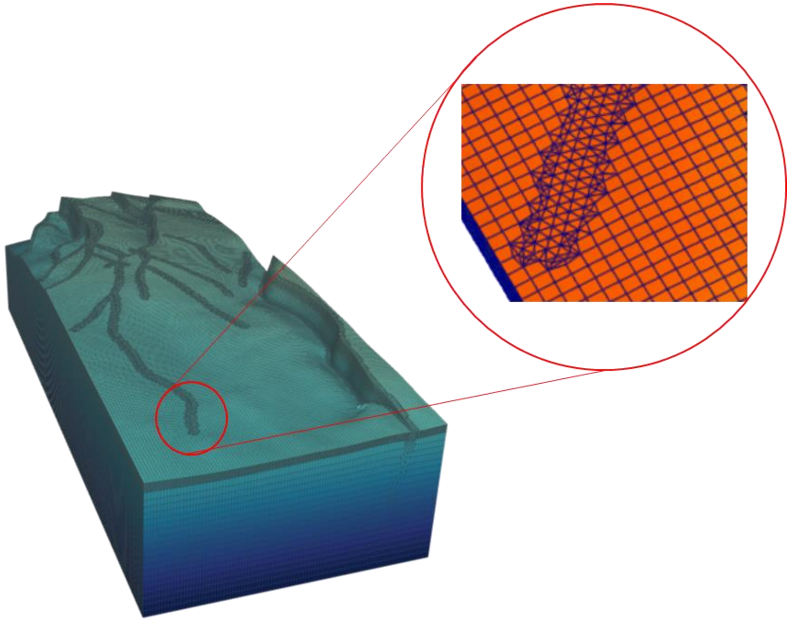
TotalEnergies

Mesh optimization



Discretization methods rely on fully unstructured meshes:

- Hexahedra: SEM wave equation, Geomechanics
- Tetrahedra: compositional flows
- Hex-dominant :
  - A mix of hexahedra, tetrahedra, prisms, pyramids,
  - Compositional flows-Geomechanics, SEM-DG wave equation



Mesh optimization for wave propagation:

- Respects seismic source wavelength, medium velocity properties for a given numerical approximation accuracy,
- Mesh extraction to take care of limited aperture,
- Automatic remeshing (FWI workflow).

Adaptive Mesh refinement for compositional flows

TotalEnergies Inria

Performance optimization

Development of advanced numerical approximation for solving wave equation:

- Hex-SEM-CG, Hex-SEM-CG-DG, HexDom-SEM-CG-DG,
- Optimized tensor operators to speed up performances of WE solvers,

➔ Development of highly optimized low level discretization function would contribute to improve performances.

Parallel programming:

- Several level of parallelism:
  - Explicit data distribution: MPI, sub-domain decomposition.
  - Multithread @ host level: RAJA
  - SIMT @device level: RAJA
- Task parallelism: solvers scheduling and shot profile distribution

➔ Explore task programming model @ all levels.

Efficient IO:

- LIFO implementation and HDF5 format already implemented

➔ Explore different IO strategies taking into account different storage hierarchies andvery large number of IO requests

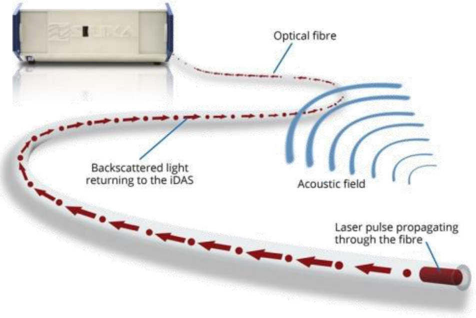
TotalEnergies Inria

Improve workflows with Machine learning

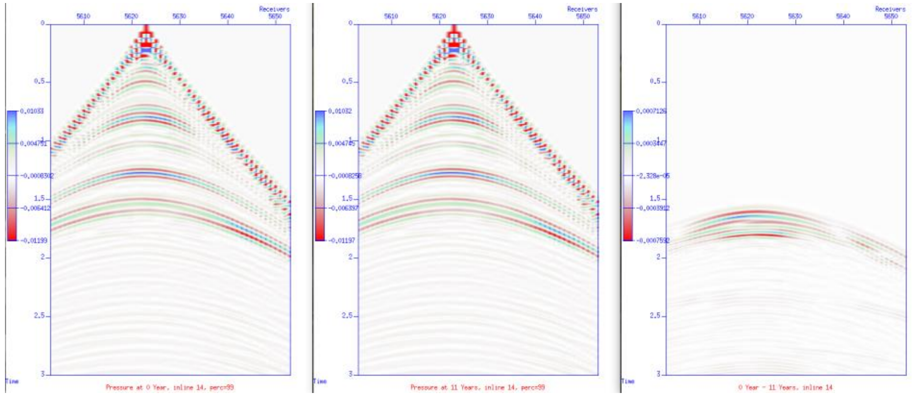
Machine learning, easily accessible through the natural python interface.

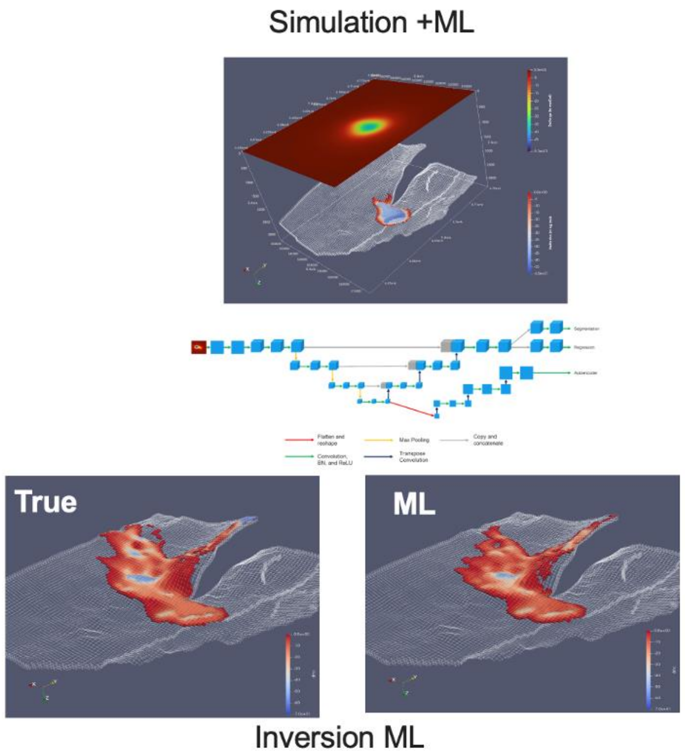
Implement advanced workflows:

- Acquisition repetability



- Direct CO2 plume Inversion
- Improve reservoir properties
- Improve FWI process
- Reduce order modeling
- Speedup performances….



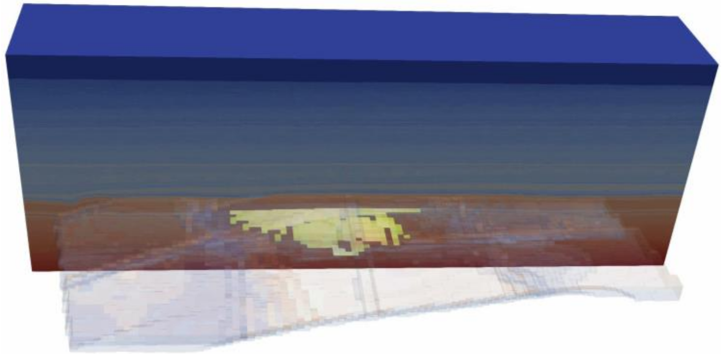


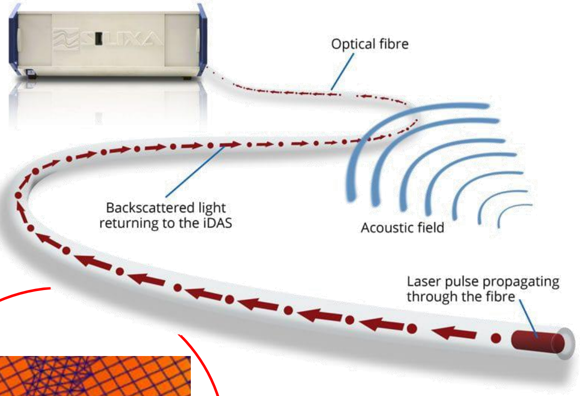
Example: Time lapse gravimetry coupled with simulation and machine learning applied to the prediction of the evolution of the CO_2 plume

From Bertrand Denel, bertrand.denel@totalenergies.com

Conclusions and perspectives

- CCUS scale by 2050
- Multiphysics modeling/simulation **beyond traditional**
- **GEOS**: Next-gen simulation for geologic carbon storage and
  … **geophysical monitoring**
- **Makutu**: bridge between reservoir simulation and seismic imaging



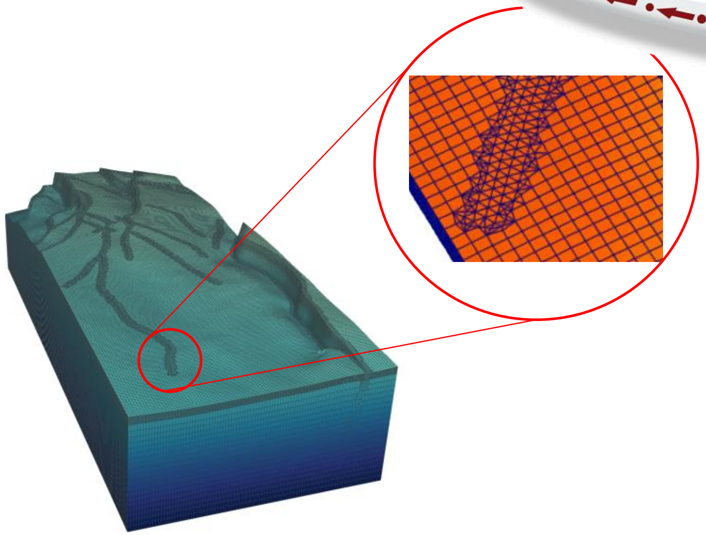


Perspectives

- **Discontinuous Galerkin** approaches in GEOS
  - Objective: **shared multi-physics model**

- **DAS** seismic inversion
- Validation on real/representative **applications**
  - Coupled simulations, (reservoir, geomechanics, gravity)
- **Machine Learning** workflows
  - Reduced order modeling , direct plume inversion

- GEOS infrastructure contributions



https://github.com/GEOS-DEV/GEOS/

https://github.com/GEOS-DEV/makutu/

TotalEnergies