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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

- **Mitigating emissions**
  - Hydrocarbon-free energy
  - Operational efficiency
  - CCUS on industrial sources


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.

1. Well integrity/injectivity
2. Pressure/Stress change Fault Activation
3. CO₂ transport & trapping
4. Seal integrity
5. Surface deformation
6. Seismicity
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
GEOS: Next-gen simulation for geologic carbon storage

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.
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
- Targets exascale platforms
Makutu: Extend GEOS to seismic for CO$_2$ monitoring

- Take advantage of long partnership with Inria in the development of 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.

[Image of CO$_2$ storage reservoir schematic]
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)

Short-term:
- SEM VTI Anisotropic
- SEM Elastico-Acoustic

Mid-term:
- Discontinuous Galerkin and mixed formulations
- Pure SEM CG/DG
- Hex-dominant SEM + DG
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 $O(p^3) \rightarrow O(p^5)$

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

<table>
<thead>
<tr>
<th></th>
<th>Init. time</th>
<th>Run time</th>
<th>Total time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q1, 18MPI/18GPUs, total speedup: 7</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td></td>
<td>697s</td>
<td>79s</td>
<td>778s</td>
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<td>37s</td>
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Memory

<table>
<thead>
<tr>
<th></th>
<th>host</th>
<th>device</th>
<th>Run time</th>
<th>Total time</th>
</tr>
</thead>
<tbody>
<tr>
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<td>15.8GB</td>
<td>3.4GB</td>
<td>46.5s</td>
<td>147s</td>
</tr>
<tr>
<td></td>
<td>15.8GB</td>
<td>0.58GB</td>
<td>46.5s</td>
<td>154.5s</td>
</tr>
</tbody>
</table>

GPU memory reduction factor: 6
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

from pygeosx import initialize, apply_initial_conditions, finalize
from seismicUtilities.segy import create_dct, write_segy
from seismicUtilities.segy import export_tosegy
from timelt import default_timer as timer

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

# get parameters from 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

time = 0
cycle = 0
startExecuteTimeLoop = timer()
while time < maxTime:
    if rank == 0 and cycle % 100 == 0:
        print("time = %3.3fs, % time, " % dt, "% dt, " % time)
        execOneStep(time, dt)
        time = dt
cycle = cycle + 1
comm.Barrier()
endExecuteTimeLoop = timer()
Develop Multiphysics coupled workflows

- **Server process**
  - Server queue
  - Launch res simulation
  - Launch seismic
  - Common model

- **Reservoir client**
  - Run queue, w/o GPU
  - Read xml
  - Read physical properties from vtk
  - Run GEOS
  - At timesteps seismic4D
  - Petroelastic conversion
  - Write model and trigger seismic

- **Seismic client(s)**
  - Run queue, w/ GPU
  - Wait
  - Read model
  - Interpolate velocity values on seismic mesh, update GEOS
  - Run seismic shot and write seismograms

Using in-house RPC client-server library

- 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 CO2 plume from 4D effects,
  - Improving FWI convergence...

Part of Makutu work program
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
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 and very large number of IO requests
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 CO2 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

[GitHub Link]  
https://github.com/GEOS-DEV/GEOS/  
https://github.com/GEOS-DEV/makutu/