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UNIVERSITY OF CAMBRIDGE

OpenGoSim

# StrataTrapper Implementation in OpenGoSim

CCUS Innovation 2.0

Key Knowledge Deliverable 4.1 & 4.2

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**Key Knowledge Deliverable Cover Sheet**

This Key Knowledge Deliverable (KKD) has been produced by Imperial College London as part of the DESNZ CCUS Innovation 2.0 programme. The document is reflective of the status of the project at the time of writing. The material presented could have been subject to change as the project matured. These documents should not be considered a full representation of the final project.

Description of the project: In StrataTrapper we translate cutting edge research carried out at Imperial College London and the University of Cambridge on the geological fluid dynamics and trapping of CO2 into innovative characterisation and modelling software tools that will be used by industry to reduce risks and costs of CO2 storage projects. The tools will be commercialised through incorporation into the CO2 reservoir simulation platform OpenGoSim, in addition to being made open-source. We will work with industry partners bp, Storegga, and Drax power to demonstrate the applicability of these tools to the Endurance field in the Southern North Sea and the East Mey Site in the Central and Northern North Sea. The result of the work will be the commercialisation of the StrataTrapper reservoir simulation tools for the rapid screening, risking, project design, and management of CO2 storage.

This report describes two key knowledge deliverables. Key knowledge deliverable 4.1 is the implementation of the StrataTrapper user interface in the OpenGoSim software Stratus. Key knowledge deliverable 4.2 describes the accelerated OpenGoSimSimulator.

The following is the full list of KKD's to be published under StrataTrapper:

KKD1.1 Open-source research codes for the characterisation of multiphase flow heterogeneity and conversion to flow functions for reservoir simulation

KKD1.2 A report detailing the workflows for reservoir characterisation, and model creation and use

KKD2.1 Open-source research codes for the rapid estimate of the impacts of heterogeneity on lateral plume migration, residual and dissolution trapping

KKD2.2 A report detailing the use and limitations of reduced physics models for various applications, including screening and probabilistic analysis

KKD3.1 Publicly available models of the Endurance and East Mey sites

KKD3.2 A report analysing the impacts of multiphase flow heterogeneity on CO2 migration and trapping in the case study sites

KKD4.1 StrataTrapper user interface in Stratus

KKD4.2 Accelerated OGS simulator

KKD4.3 StrataTrapper Workshop to CCS project developers

KKD5.1 Annual reports

KKD5.2 Project final report

Any enquiries regarding this publication should be sent to us at:
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# Contents

# KKD 4 — StrataTrapper Implementation in OpenGoSim

## KKD 4.1 — StrataTrapper user interface in Stratus

*A report detailing the status of the implementation of the StrataTrapper upscaling technique into the OpenGoSim simulation platform.*

### Preamble

OpenGoSim (OGS) is integrating the StrataTrapper upscaling technique developed by Imperial college (ref. 1, 2) into the workflow commonly used by reservoir engineers when modelling CO2 injection into saline aquifers. The core of this method, referred to as Macroscopic Invasion Percolation (MIP), is to include the effects of sub-grid level heterogeneity, particularly capillary pressure heterogeneity, for the flow in dynamic models that use a practical resolution. Practical in the sense that simulation time is reasonable to do the studies required in the assessment of a CO2 storage site.

Starting from data on a finer computational grid, too expensive to simulate, the MIP method produces a set of directional relative permeability functions (pseudo), which include the geological detail from the original model into a new coarsened model. These functions are loaded and used by a reservoir simulator for each grid block of the coarser model.

### Implementation of StrataTrapper user interface

#### Status

During the first phase of the project, we implemented in the OGS reservoir simulator (PFLOTRAN-OGS) the capability to read and use directional relative permeability functions. As PFLOTRAN-OGS is open-source software, the implementation of this interface is now open to the public, with the code available in the following repository:

https://bitbucket.org/opengosim/pflotran_ogs_1.8/src/pflotran_ogs_1.8/

And the documentation of such capability is also available in the OGS public wiki:

https://docs.opengosim.com/theory/dir_relperms/

https://docs.opengosim.com/manual/input_deck/grid/grdecl/#krnumx-krnumy-krnumz

In 2024 the attention has switched to the implementation of the MIP algorithm that generates the pseudo functions. The initial plan was to use an open-source implementation provided by Imperial College. However, as most of the code available was written in Matlab, we decided to rewrite the software in C++, for efficiency reasons and to avoid the need for future clients to purchase a Matlab licence.

The new program, called Focus, provides a keyword file reader, grid construction, initialisation and output infrastructure around the basic MIP pseudo function calculation.

The input is the one of a reservoir simulation case, including a grid description, PVT and saturation function data, and an initial equilibrated solution. In many ways, this is a standard reservoir simulation input deck, but with no time-dependent data such as wells.

Focus has two modes of running. In REFINE mode it takes a single dataset, performs a synthetic refinement on each grid block of that dataset, applies a degree of heterogeneity to each of the resulting fine grid cells, and then calculates MIP pseudo function for each the cells in the original dataset. In COARSEN mode it takes an existing dataset and produces a new coarsened version of that dataset. The MIP pseudoisation is used to construct new pseudo functions which include the geological detail from the original model into the new coarsened model.

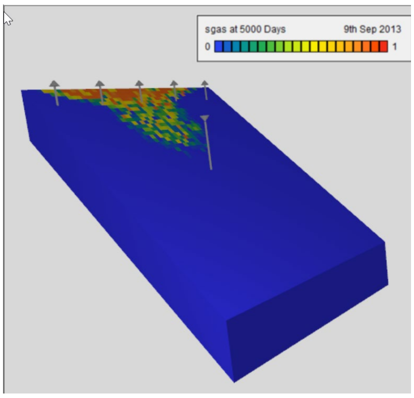
Focus can handle non-trivial grids supplied in an industry standard format, an important feature to integrate this new StrataTrapper modelling technique in the workflow of reservoir engineers.

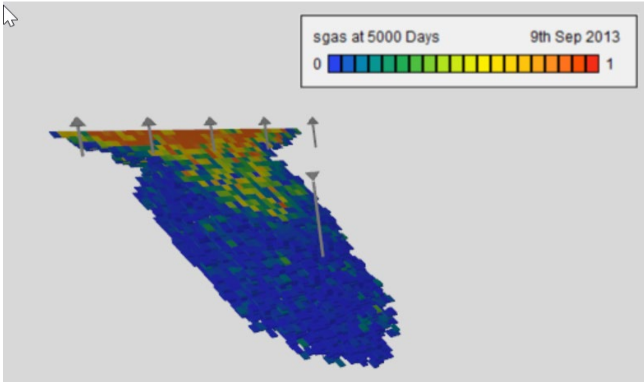
Following a validation versus the Imperial College Matlab implementation, we run a few cases to start the testing of the software. Below the description and results of one of the models used in this initial testing phase.

## Sloping reservoir case study

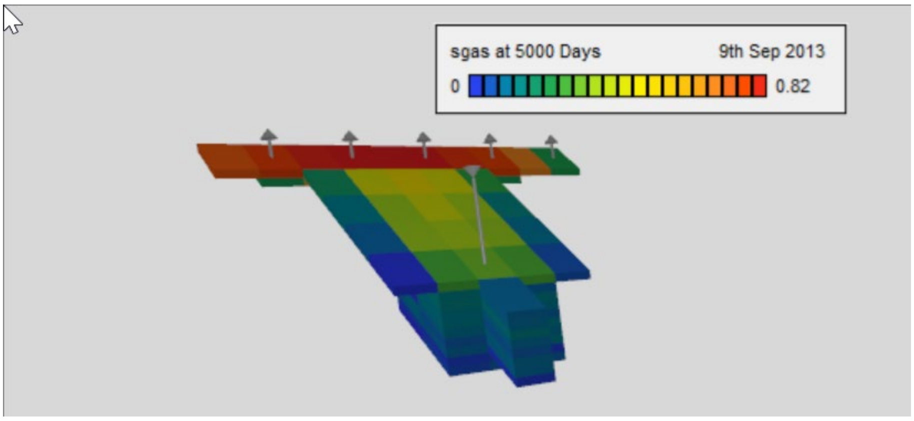
In this case we construct a small sloping reservoir, injecting at the bottom of the structure for 500 days, then shutting the wells and allowing the gas to migrate upwards towards the crest of the reservoir for another 4500 days. The fine grid run is 50x50x50, and takes 69.7 mins to run on a 4-core workstation. The coarsened grids are 10x10x10, and each takes less than 15 secs to run. Focus generated 3000 sets of pseudo saturation functions – one for each direction on the coarse grid.

The plots below exaggerate the vertical direction by a factor of 4. Looking at top of the fine grid case we see that gas has reached the top of the reservoir at 5000 days. However, in the second picture we remove the cells with zero gas saturation and we can see considerable gas trapping in the structure:

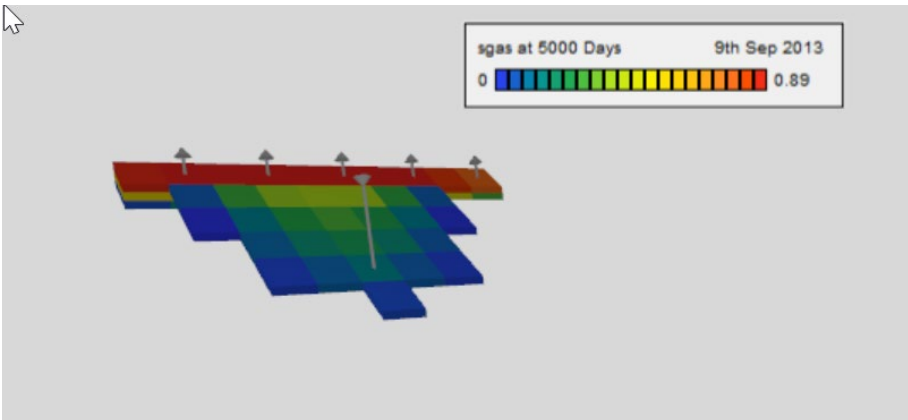



Looking at the coarse grid case with the MIP pseudos, we can see a similar trapped zone, although at a lower resolution:




However, without the pseudos, but instead with the original single rock curve, we see:




In this case the gas has mainly simply risen into the top layer of cells. As previously, the improved match with the pseudos is encouraging.

## Stratus interface and future work

Focus has been designed to become a library of Stratus, and will be installed by Stratus alongside PFLOTRAN-OGS that loads the output of the Focus upscaling. We have used Stratus to visualise the simulation results above for the coarse and fine grids, as a data interface between Focus and PFLOTRAN-OGS already exists, and Stratus post- process PFLOTRAN-OGS results. However, in the final phase of the project we will consider a closer integration (e.g. running Focus from Stratus) and to add more visualisation functionalities to help analysing the input and output of Focus. At the same time, we will also work on some more realistic model, to improve robustness and efficiency.

## References

1. Samuel J. Jackson and Samuel Krevor, “Small-Scale Capillary Heterogeneity Linked to Rapid Plume Migration During CO2 Storage”, Geophysical Research Letters, Aug 2020.

2. ‘Supporting information for "Small-scale capillary heterogeneity linked to rapid plume migration during CO2 storage"’, S. J. Jackson and S. Krevor.

# KKD 4.2 — Accelerated OGS Simulator

*A report detailing the new OGS high-performance reservoir simulation technology for high-resolution CCS studies.*

## Preamble

Within the StrataTrapper project, OpenGoSim (OGS) has developed Nimbus, a new-technology high-performance reservoir simulation code, to target modern computer architectures, by supporting parallel processing on both CPU and GPU hardware. A major objective of Nimbus is that it will be future-proof against new high performance computing developments. Its architecture implements techniques to make coding for both CPU and GPU simpler.

Nimbus is capable of thermal simulation of gas-water and oil-gas-water cases, and will be the OGS next generation simulator to model CO2 injection in both saline aquifers and depleted hydrocarbon fields.

## Latest progress and current performance of Nimbus

The core of a reservoir simulator, and the part that takes the majority of the run-time, is the linear equation solver, therefore this is the part of the software we have worked on to improve performance. The solver used in Nimbus is a two-stage CPR (constrained pressure residual). First a single pressure equation is formed and solved using an AMG (algebraic multigrid) method; and then all the equations (pressure, temperature and composition are solved together in a second stage, normally some sort of ILU (incomplete lower-upper decomposition) method. This is all combined into an acceleration method such as ORTHOMIN or GMRES.

The objective is to produce at an optimized CPR solver for GPUs, and we are perusing two approaches to achieve this goal, each with advantages and trade-offs. 1) An in-house Nimbus CPR solver, which we are able to develop and optimize for our needs, directly using the internal Nimbus matrix format. 2) An open-source linear solver, HYPRE (ref. 1), which has been developed for a wider range of applications and requires an interface to the Nimbus matrix, but can enjoy more manpower from a team of specialists in linear solvers.

We achieved significant gains optimising the in-house CPR solver, improving both the GPU implementation of second stage and the AMG solver.

We then tested the HYPRE Multigrid Reduction (MGR) linear solver (refs 2,3), which includes a GPU implementation, and can be seen as a generalisation of the CPR. We confirmed that we are able to use the MGR in a way that has similar performance to our in-house CPR implementation. However, when testing large models we encountered efficiency issues with the HYPRE interface, which we are still working on to resolve.

We tested Nimbus performance on the SPE10 industry benchmark (ref. 4). Nimbus runs on the Nvidia A30 GPU outperforms PFLOTRAN-OGS simulations on top-end CPUs. The A30 is a mid-range GPU, therefore more gain are expected from more powerful models (e.g. A100 or H100).

In the final phase of the project, we will focus on adding essential capabilities to Nimbus to be able to simulate more realistic saline aquifer models, and make the software more robust. In parallel we will finish the testing of HYPRE.

## References

[1] https://hypre.readthedocs.io/en/latest/solvers-mgr.html

[2] Bui, Quan M., et al. "A scalable multigrid reduction framework for multiphase poromechanics of heterogeneous media." SIAM Journal on Scientific Computing 42.2 (2020): B379-B396.

[3] Wang, Lu, et al. "Multigrid reduction for coupled flow problems with application to reservoir simulation." SPE Reservoir Simulation Conference?. SPE, 2017.

[4] Christie, M.A., and Blunt, M.J.: “Tenth SPE Comparison Problem: A Comparison of Upscaling Techniques”, SPE 72469, Aug 2001.