StrataTrapper Upscaling Toolkit

CCUS Innovation 2.0

Key Knowledge Deliverable 1.1 & 1.2

July 2024

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 contains two key knowledge deliverables. Key knowledge deliverable 1.1 is an open-source research codes for the characterisation of multiphase flow heterogeneity and conversion to flow functions for reservoir simulation. Key knowledge deliverable 1.2 is a report detailing the workflows for reservoir characterisation, and model creation and use.

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

KKD4.3 StrataTrapper Workshop to CCS project developers

KKD5.1 Annual reports

KKD5.2 Project final report

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KKD 1 — StrataTrapper software

KKD 1.1 — Research codes

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

A research software toolkit, written in MATLAB, was created to facilitate the conversion of information about the properties of a reservoir to be used in the StrataTrapper modelling approach. The purpose of the software is to accurately incorporate information about the heterogeneity of the reservoir, and particularly the capillary pressure heterogeneity, into an upscaled model used for reservoir simulation. The algorithm takes as input spatial statistical information about reservoir properties, including means, variances, and correlation lengths of flow properties. The output is a 3D reservoir model with upscaled flow properties, including relative permeability and capillary pressure, that may be used for dynamic reservoir simulation.

The upscaling approach closely follows the approach presented in Jackson & Krevor (2020) but includes a few key developments: The upscaling has been extended from 2D to 3D models; the calculation of upscaled relative permeability is now performed within the code and without calls to reservoir simulation software, significantly improving the computational performance.

The software toolkit is now publicly available via the GitHub repository https://github.com/ImperialCollegeLondon/StrataTrapper.

The `**main**` branch of this repository is a release branch. We recommend using and referring to the latest state of this branch. The repository has a `**README**` file which describes the purpose and the contents of the repository as well as our guidelines for users and potential contributors.

The StrataTrapper GitHub project has its own web page:

https://imperialcollegelondon.github.io/StrataTrapper/

This development was built on top of the work of Jackson and Krevor (2020) and the doctoral thesis of Wenck (2023). Within the project, the more efficient analytical approach was derived and implemented to evaluate upscaled relative permeabilities without any calls to external reservoir simulations. Those works in turn are developments of the upscaling approaches presented in Wolff et al., (2013) and Yang et al., (2013).

Key References

The upscaling approach implemented in this toolkit is described in detail in:

Samuel J. Jackson, Samuel Krevor
Small-Scale Capillary Heterogeneity Linked to Rapid Plume Migration During CO2 Storage
Geophysical Research Letters | 2020
https://doi.org/10.1029/2020GL088616

Nele Mareike Wenck
The Impact of Capillary Heterogeneity on Subsurface Carbon Dioxide Storage
PhD Thesis, Imperial College London, Department of Earth Science and Engineering | 2023

Those works developed this toolkit building on the upscaling approaches presented in:

Wolff, M., Flemisch, B., & Helmig, R. (2013). An adaptive multiscale approach for modeling two-phase flow in porous media including capillary pressure. Water Resources Research, 49(12), 8139-8159.

Yang, Z., Tian, L., Niemi, A., & Fagerlund, F. (2013). Upscaling of the constitutive relationships for CO2 migration in multimodal heterogeneous formations. International Journal of Greenhouse Gas Control, 19, 743-755.

KKD 1.2 — Reservoir characterisation workflow

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

Preamble

In StrataTrapper, we translate cutting edge research 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 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.

Reservoir simulations of injected CO2 plumes are central to the successful engineering and management of CO2 storage. Plume migration rates and direction determine the storage efficiency and significance of potential leakage pathways. The extent of residual and dissolution trapping are quantified through simulation-based history matching. Increasing simulation accuracy can de-risk and lower costs throughout the lifetime of a storage project including appraisal, project design, implementation, and abandonment.

Recent work at Imperial College London and University of Cambridge has identified that major inaccuracies in current modelling approaches are due to previously ignored impacts of small scale (cm-m) heterogeneities in multiphase flow properties. Plume migration rates, and the extent of residual and dissolution trapping in a field can all be enhanced by over 200% by these flow heterogeneities. The research has demonstrated the importance of these processes. There is now an opportunity to commercialise the research into simulation tools for site screening, appraisal, and forecast modelling of use by practitioners. We estimate that offshore storage costs may be reduced by 10% through this improved modelling approach, saving £10s of millions per project. The structure of StrataTrapper is designed to realise the commercial potential of the research advances in flow physics. Consortium partners BP, Storegga, and Drax are project developers of CCUS clusters in the UK and would like to make use of these tools. OpenGoSim provides the commercial platform necessary for these organisations and already works with BP and Storegga on the analysis of sites in the UK. The open publication of the research basis and engagement with additional practitioners will facilitate broader uptake. Demonstrations of the toolset with case studies within the UK will show the practicality and importance of this approach for modelling CO2 storage.

Upscaling Workflow

Description of the StrataTrapper's upscaling approach accompanied with visual examples of inputs and outputs.

The core of the StrataTrapper approach is in generating upscaled models preserving the effects imposed by fine-scale capillary pressure heterogeneities. Here, we demonstrate this core part supported with an example. At the same time, the research codes are shipped with an additional utility of generating heterogeneous fine-scale models, which can be used for synthesising numerous inputs for algorithm validation and testing.

Data availability

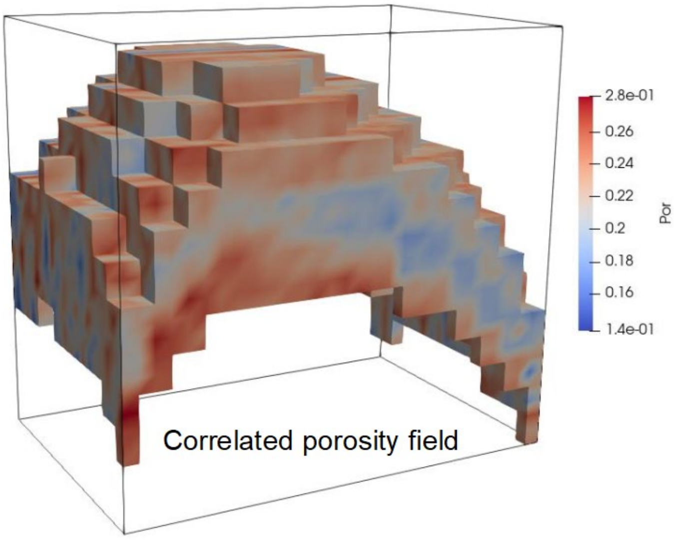
The input data and raw data of figures presented here
can be found in the Mendeley Data:

https://data.mendeley.com/datasets/5rcpb43g4w/1
DOI 10.17632/5rcpb43g4w.1

Inputs

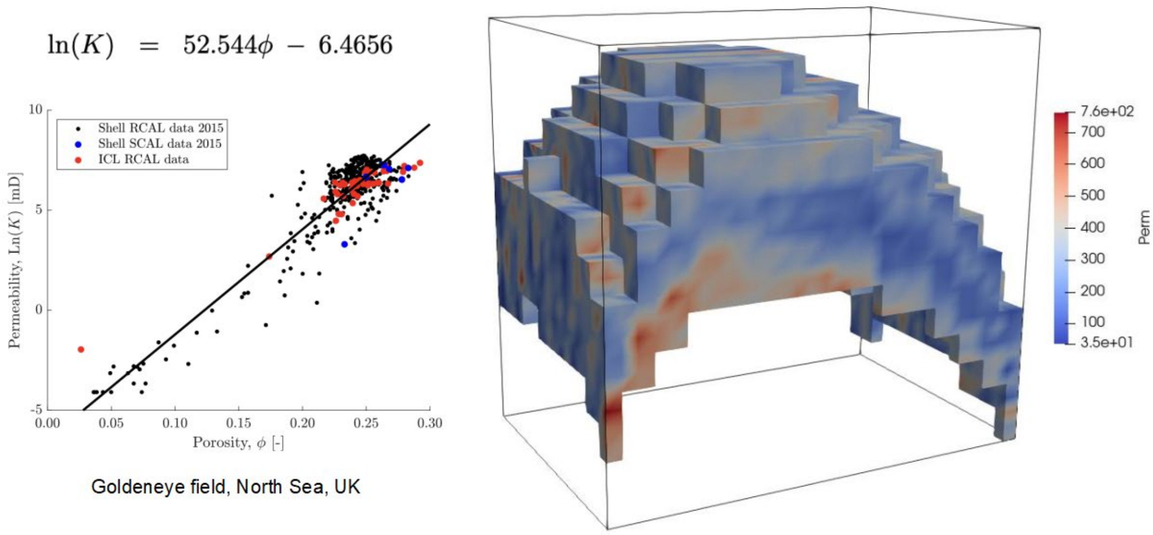
Initially, the workflow takes a fine-scale numerical model, focusing on the key properties of the porous medium itself and the rock-fluid interaction, e.g., porosity, permeability, fluid properties.

Figure 1: The correlated porosity field in fine-scale grid



In this example, the fine-scale porosity field was used to produce a correlated permeability field, but the permeability field may be input independently of the porosity field.

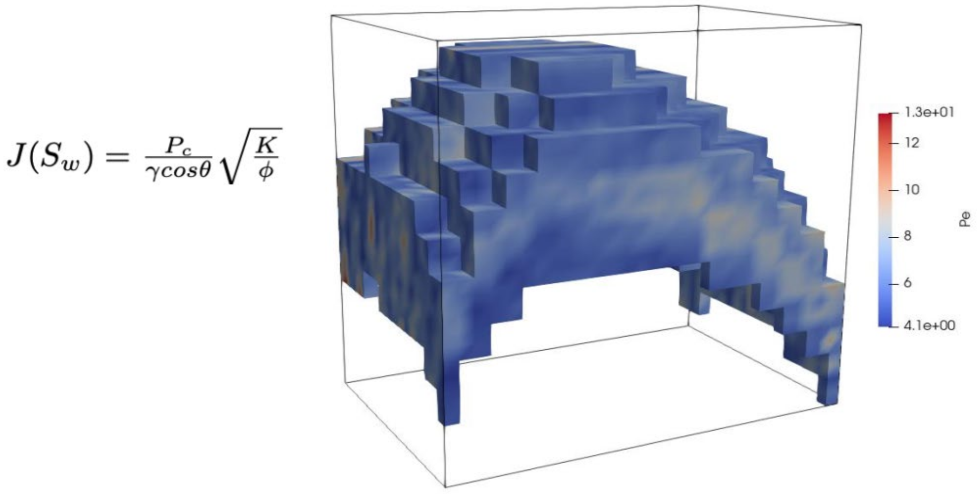
Figure 2: The correlated absolute permeability field in fine-scale grid



The essential part of the StrataTrapper upscaling approach is to account for small-scale heterogeneities in capillary pressure characteristics. Thus, input of heterogeneity in capillary pressure characteristics is also required.

As with the permeability and porosity relationship, it may be of interest to generate heterogeneity in the capillary pressure characteristics through a correlation. While this is not the required approach, it is supported in the toolkit and this is what we have done with this example. In this case, we use a J-Leverett scaling requiring information about the fluid-fluid interfacial tension. In the figure below, we demonstrate the corresponding fine-scale capillary entry pressure field.

Figure 3: The correlated capillary entry pressure field in fine-scale grid



Upscaling

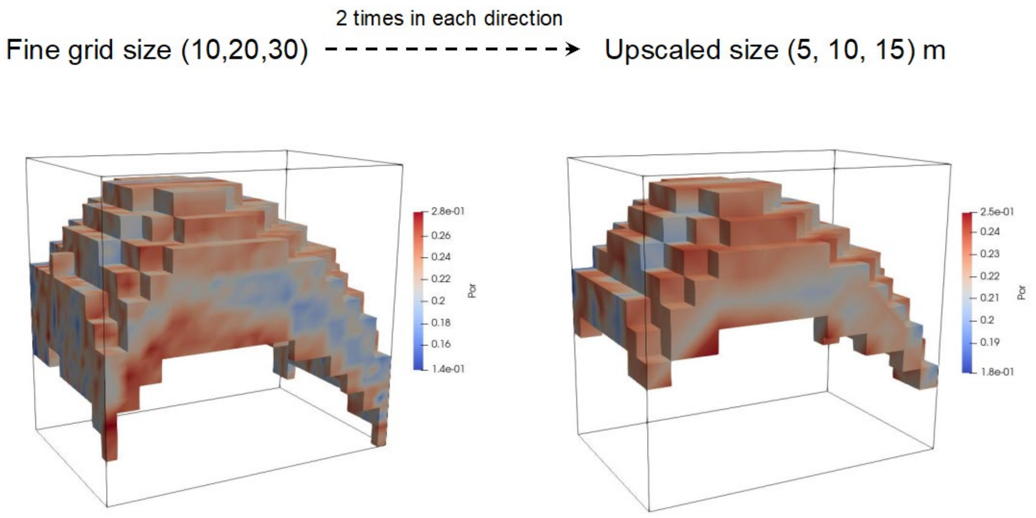
These inputs thus have created a fine scale model which is then ready for upscaling. Any alternative approach to generating a fine scale model is suitable, in which case the previous component of the toolkit may be ignored.

Once the fine scale model is produced, it is processed by the toolkit until the upscaled representation is produced. In this example, the linear size of each computational cell was doubled. So, the volumetric size of each gridblock became 8 times bigger.

Outputs

The first output of the workflow is the upscaled porosity field, which is also used to produce other upscaled properties. The upscaled porosity of each coarse grid block is calculated using volume averaging.

Figure 4: The upscaling of correlated porosity field



Along with the upscaled permeability field (**Figure 6**) and other values, the upscaled porosity field is used in evaluating the upscaled capillary pressure curves for each block of the upscaled grid of the model.

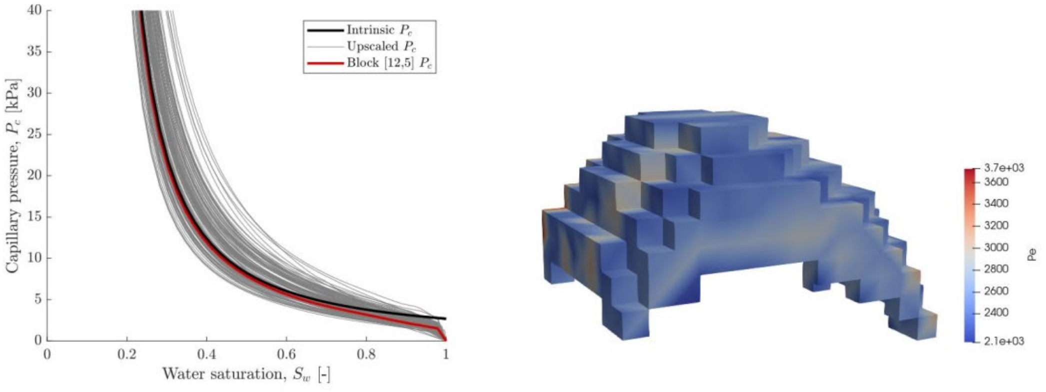
To capture the particular importance of capillary controls on the distribution of CO2 over small length scales (e.g., <10m), we adopt a macroscopic invasion percolation approach to obtain upscaled, drainage capillary pressures and relative permeabilities for each coarse grid block. The saturation range is split into equal increments. The increments represent the desired water saturations at which the upscaled macroscopic flow functions will be calculated. The domain is fully saturated with wetting phase. The initial, macroscopic boundary pressure is set to the average capillary pressure for the given water saturation. The local system is invaded with non-wetting phase starting from the boundary at which the macroscopic pressure is applied. A cell is invaded if it meets two criteria:

1. it is connected to the outlet or to a fine cell that is connected to the outlet,
2. the boundary pressure exceeds the local entry pressure.

Away from the block boundaries, two additional potential flow pathways are introduced into the percolation approach when considering a 3D, rather than 2D, domain. These are incorporated into the percolation algorithm.

Once all accessible and available cells are invaded, the fine-scale saturation distribution can be inverted from the fine-scale capillary pressure using the fine-scale ‘capillary pressure – saturation’ functional form. The upscaled saturation in each coarse grid block is calculated using volume averaging. If the difference between the obtained and the desired saturation is greater than the threshold, the boundary pressure is updated using a Newton-Raphson iteration, where the pressure gradient with respect to saturation is either determined from past iterations or from the functional form. After a new boundary pressure approximation has been determined, the macroscopic invasion percolation procedure is repeated, until the difference between the obtained upscaled saturation and the desired saturation is below the error threshold. Once achieved, the upscaled capillary pressure can be calculated using the intrinsic phase averages.

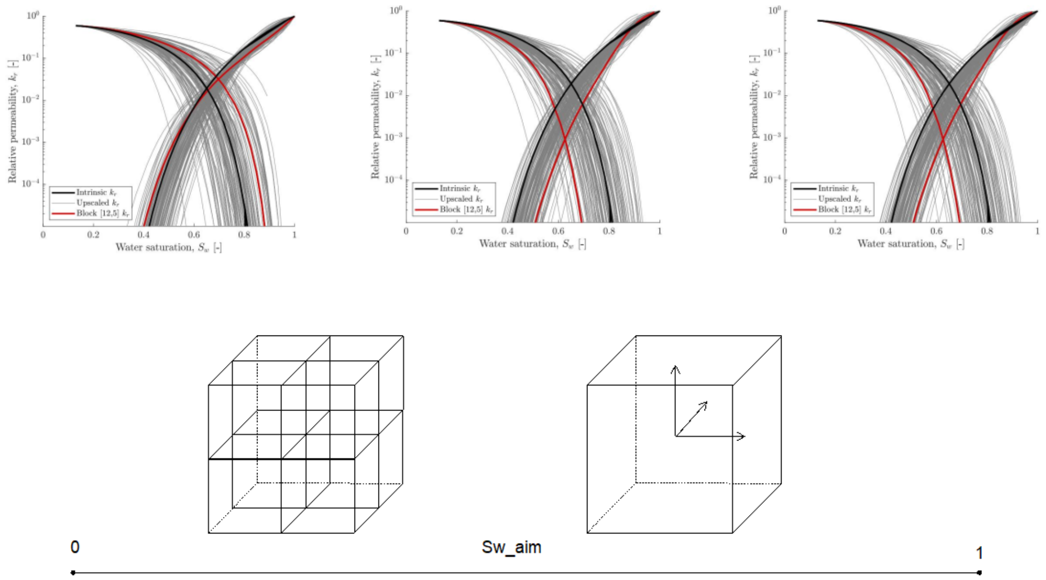
Figure 5: Upscaled capillary pressure curve in each block



For the relative permeability field, a pressure drop method is applied, whereby flow is imposed separately in each dimension for each coarse grid block. The fine-scale phase relative permeability distribution is inverted from the fine-scale saturation and permeability distribution. That fine-scale phase relative permeability distribution is used as the underlying permeability distribution, which changes for the wetting and non-wetting phase. Then, the effective permeability in each dimension is calculated using the average pressure drop across the subdomain using Darcy’s law.

Essentially, the heterogeneity of the fine-scale model turns into the anisotropy of the relative permeability field of the upscaled model. The figure below demonstrates resulting relative permeabilities in each direction.

Figure 6: Directionally upscaled relative permeability in coarsened cells



The above steps are repeated until all increments of the saturation range have been covered. Thereafter, the derived points are fitted with the LET and Brooks-Corey functional forms, respectively, to ensure the upscaled curves are smooth and monotonic.

The whole procedure is repeated for all coarse grid blocks until upscaled properties have been obtained for the entire domain.

Reference

Nele Mareike Wenck
The Impact of Capillary Heterogeneity on Subsurface Carbon Dioxide Storage
PhD Thesis, Imperial College London, Department of Earth Science and Engineering | 2023

Algorithm

The algorithmic representation of the upscaling workflow from a user's perspective. Each major step of the algorithm refers to a certain file of the StrataTrapper GitHub repository https://github.com/ImperialCollegeLondon/StrataTrapper . There are also references to the figures above.

Please refer to the GitHub repository's **README** for project structure.

Figure 7: Algorithmic representation of the upscaling workflow

```
Algorithm 1: Pore to Core to Field Scale Upscaling
Input  : The fluid properties in Fluid_transport_properties.mat
         The structure and petrophysical properties in A_input.txt
         The specific relations from report stored in A_input_report.m
Output : The upscalled model for simulation
Load reservoir & petrophysical properties. Define upscaling, and do the interpolation.
  A1_1_Generate_global_parameters .m
Generate the correlated porosity field (Figure. 1) in the fine-scale grid, which is utilized
  to calculate the permeability distribution (Figure. 2), as well as derive the entry capillary
  pressure field (Figure. 3) using the Leverett-J function. A2_1_Gene_data_stru_fine.m
Polygon transect fitting to reveal on-site geo-structure.
  A2_1_Gene_shift_structure_fine2.m
Construct the data structure and calculate the porosity distribution in the upscaled gid
  (Figure. 4). A2_2_Generate_data_structure_upscaled.m
for $k \in all\ coarse\ cells$ do
    for $i = 1 \cdots n$ (All aimed saturation points) do
        Calculate capillary pressure ($P_c$) at $S_{w,aim}$ using the Brooks-Corey equation with
          average entry pressure in the coarse cell. Set $P_c$ as the initial guess for the
          macroscopic boundary pressure, $P_b$. And define an initial $S_w$.
        while $(S^i_{w,aim} - S_w) > E_{thresh}$ do
            Perform Macroscopic Invasion Percolation (MIP): the local system is invaded
              with non-wetting phase at $P_b$ starting from the boundary cells and working
              inwards. A fine-scale cell is invaded if 1) it is connected to a cell which is
              connected to the boundary and 2) $P_b$ is greater than the cell's entry pressure.
            Once all accessible cells are invaded, calculate the upscaled $S_w$ (the fine-scale
              saturation distribution is inverted from the fine-scale capillary pressure
              distribution. The upscaled saturation is volume averaging one).
            Update $P_b$ based on the updated $S_w$.
        end
        The fine-scale relative permeability distribution is calculated using the known
          fine-scale saturation. A3_1_Perform_MIP_upscaling.m
    end
    Analytically calculate permeability in each direction using the fine-scale system at
      each saturation point. A4_1.m
    The macroscopic relative permeability at each phase saturation is calculated with
      Darcy's Law. The data points are subsequently fitted with a functional form.
      A4_3_Post_process_single_phase_files.m
end
```