Modelling CO2 storage in large-scale aquifer systems

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Why do we need carbon capture and storage (CCS)?

Most IEA/IPCC scenarios require *widespread use of CCS* to reach the 2° target, latest scenario requires storing 3800 Mt/yr

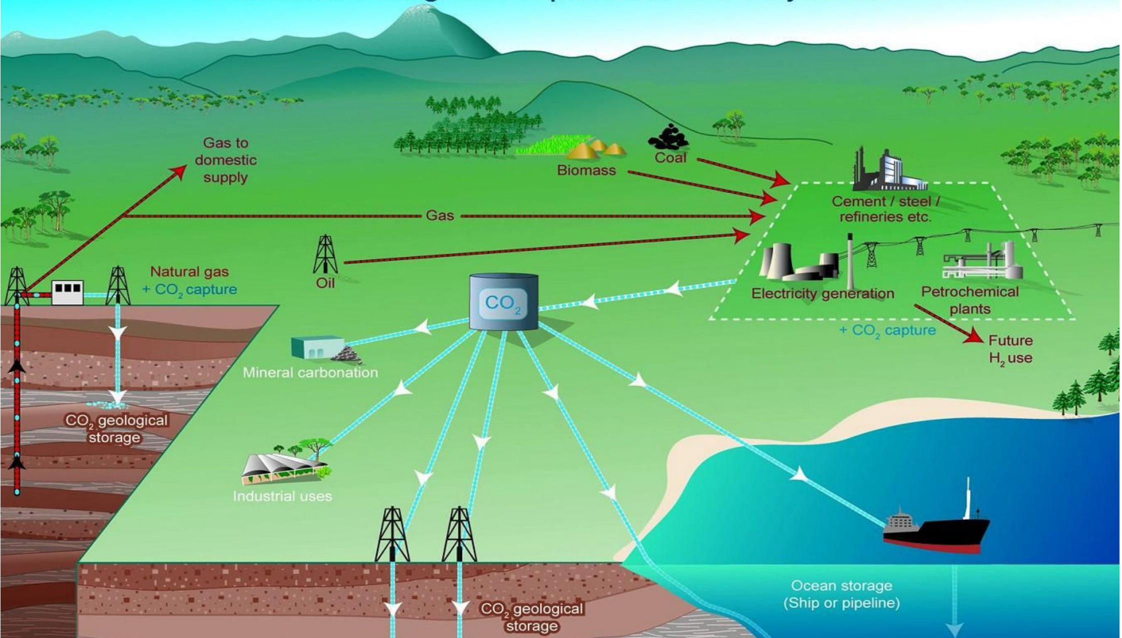
Even if renewable energy grows 5% annually

- continuing current situation will give 3.2° warming
- large-scale CCS will be largely responsible to pick up the slack (through negative emissions)

"Three years to safeguard our climate" (Nature, June 2017)

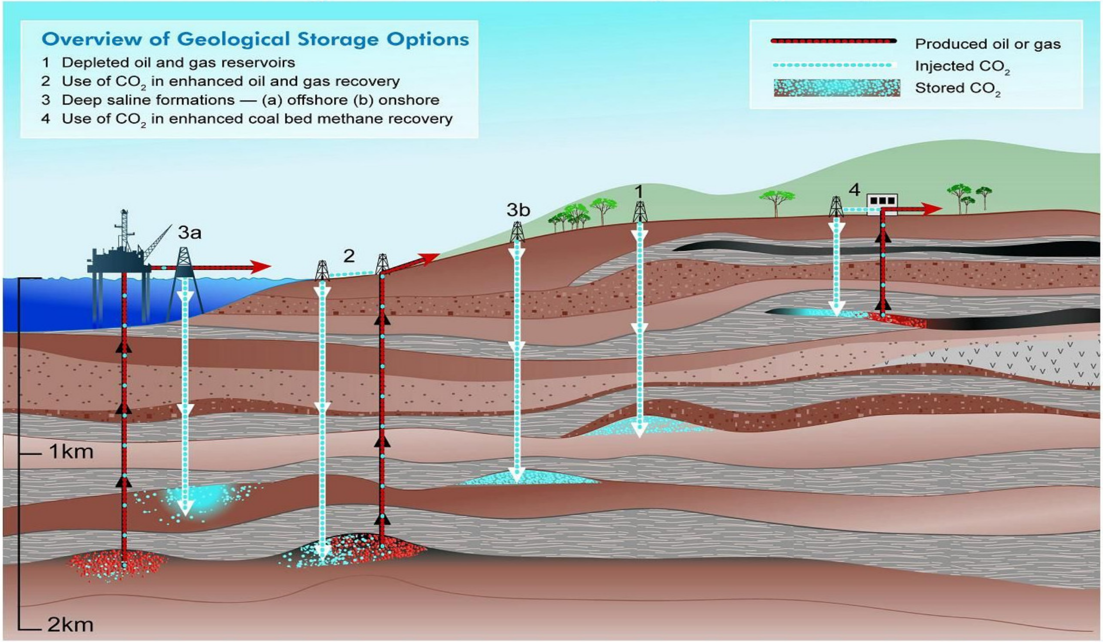
- the *entire* carbon budget might be spent in just 4 years, or 15 years on average

Schematic diagram of possible CCS systems



Adapted from: Special Report on Carbon Dioxide Capture and Storage, IPCC (2005)

Methods for storing CO2 in deep underground geological formations



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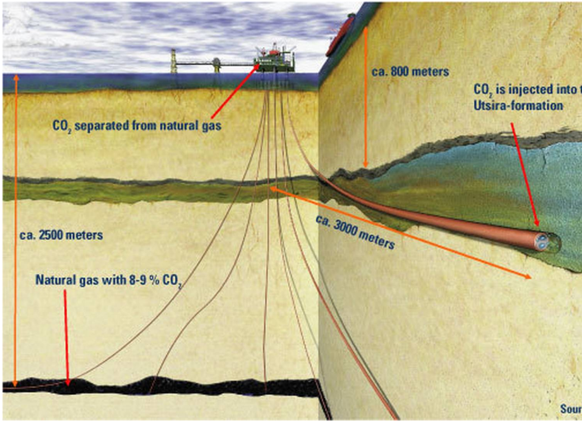
Thinking big

Sleipner: first offshore CO_2 storage project. Injected 1Mt/yr into the Utsira formation since 1996



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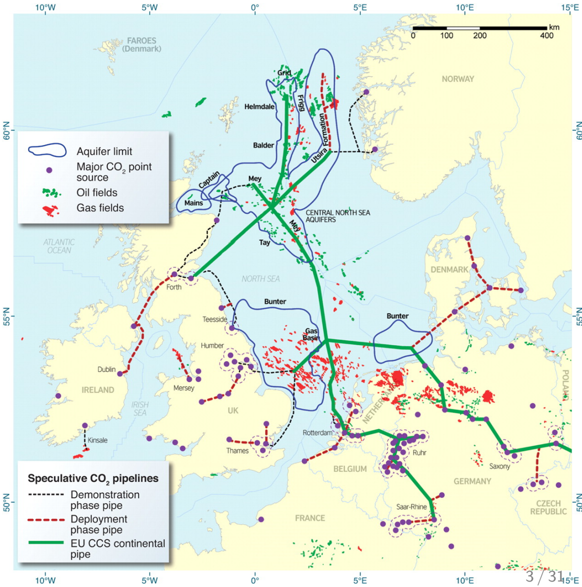
From Sleipner to central storage hub in the North Sea.

Need to store several gigatonnes per year to significantly affect European point emissions

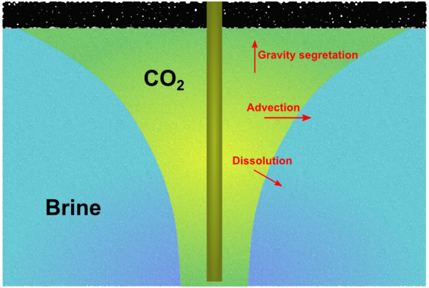
This is more than 1000 times the magnitude of ongoing operations

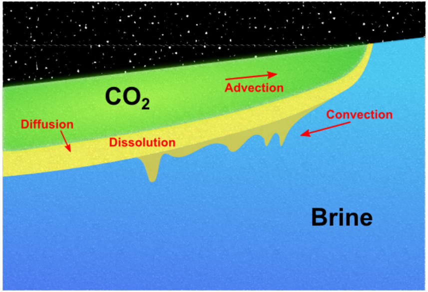


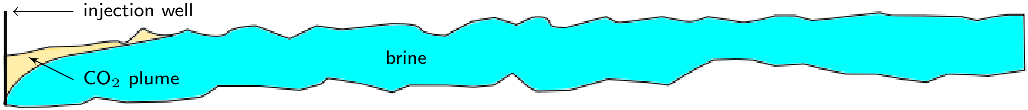
Primary physical processes of CO_2 storage

- Injection driven by viscous pressure drop
- CO_2 forms a supercritical phase that is lighter and weakly soluble in water

- Buoyant plume will migrate upward in the formation, displacing brine
- Upward movement limited by the caprock







Three key modelling questions

To evaluate feasibility of possible injections, one must assess:

- capacity: how much?
- injectivity: how fast?
- safety: will it leak?

Challenging task because site characteristics vary a lot and data are scarce

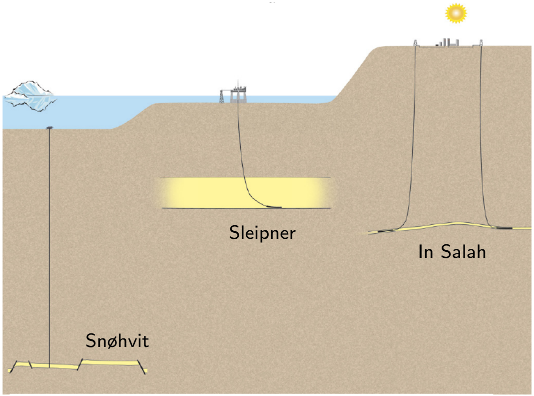
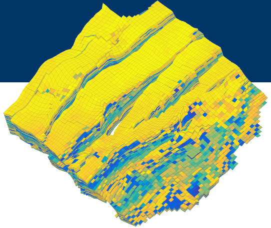


Illustration: Eiken et al, Lessons Learned from 14 years of CCS Operations: Sleipner, In Salah and Snøhvit, Energy Procedia (2011)

Simulation models

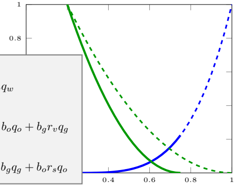


Somewhat simplified, consist of three parts:

1. a **geological model** – volumetric grid with cell/face properties describing the porous rock formation

2. a **flow model** – describes how fluids flow in a porous medium (conservation laws + appropriate closure relations)

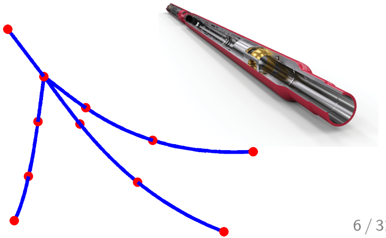
3. a **well model** – describes flow in and out of the reservoir, in the wellbore, flow control devices, surface facilities



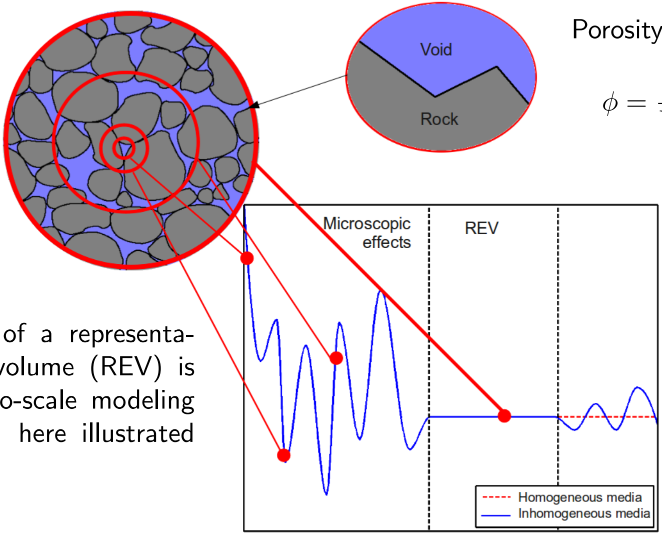
$$\partial_t(\phi b_w S_w) + \nabla\cdot(b_w \vec{u}_w) = b_w q_w$$

$$\partial_t[\phi(b_w S_o + b_g r_v S_g)] + \nabla\cdot(b_o\vec{u}_o + b_g r_v \vec{u}_g) = b_o q_o + b_g r_v q_g$$

$$\partial_t[\phi(b_g S_g + b_o r_s S_o)] + \nabla\cdot(b_g\vec{u}_g + b_o r_s \vec{u}_o) = b_g q_g + b_o r_s q_o$$



Geologic model: representative elementary volume



Porosity:

$$\phi = \frac{V_v}{V_v + V_r}$$

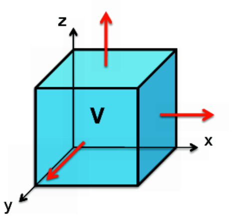
The assumption of a representative elementary volume (REV) is essential in macro-scale modeling of porous media, here illustrated for porosity.

Flow model: governing equations for fluid flow

1. Conservation of mass

$$\frac{\partial}{\partial t}\int_V m\,dx + \oint_{\partial V} \vec{F}\cdot\vec{n}\,ds = \int_V r\,dx$$

m=mass, $\vec{F}$=flow rate, r=fluid sources



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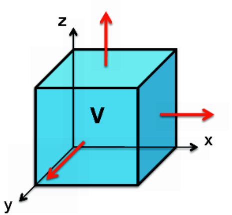
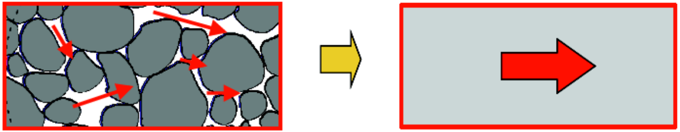


2. Darcy's law – empirical law for processes on unresolved scale

$$\vec{u} = -\mathbf{K}(\nabla p - \rho g \nabla z)/\mu$$



Similar to Fourier's law (heat) [1822], Ohm's law (electric current) [1827], Fick's law (concentration) [1855], except that we now have *two driving forces*

Flow model: single-phase flow

$$\frac{\partial(\phi\rho)}{\partial t} + \nabla\cdot(\rho\vec{u}) = q, \qquad \vec{u} = -\frac{\mathbf{K}}{\mu}(\nabla p - \rho g \nabla z)$$

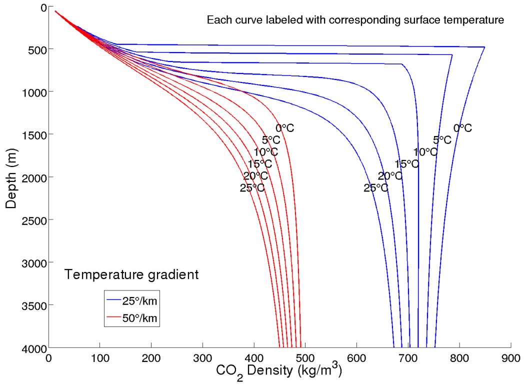
Special cases:

- incompressible flow:

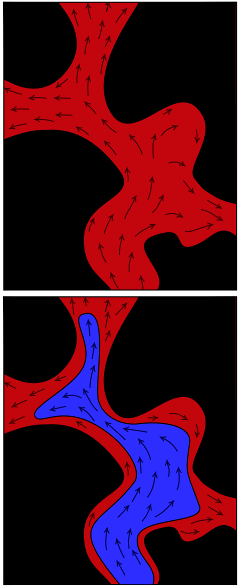
$$-\nabla\cdot(\mathbf{K}\nabla p) = q$$

- weakly compressible flow:

$$\frac{\partial p}{\partial t} = \frac{1}{\mu\phi c}\nabla\cdot(\mathbf{K}\nabla p)$$



Flow model: multiphase flow



Multiphase extension of Darcy's law (Muskat, 1936):

$$\vec{u}_\alpha = -\frac{\mathbf{K}_\alpha(S_\alpha)}{\mu_\alpha}\big(\nabla p_\alpha - \rho_\alpha g \nabla z\big),$$

Effective permeability experienced by one phase is reduced by the presence of other phases, $\mathbf{K}_\alpha = \mathbf{K} k_{r\alpha}(S_{\alpha_1}, \ldots, S_{\alpha_m}), \quad 0 \leq k_{r\alpha} \leq 1$

Mass-balance equations for each phase (Muskat, 1945):

$$\frac{\partial(\phi \rho_\alpha S_\alpha)}{\partial t} + \nabla \cdot \big(\rho_\alpha \vec{u}_\alpha\big) = q_\alpha$$

Flow model: incompressible two-phase flow

Elliptic pressure equation

$$\nabla \cdot \vec{u} = q, \qquad \vec{u} + \lambda \mathbf{K}\big[\ \nabla p\ -\ (f_w\rho_w + f_n\rho_n)\vec{g}\ -\ f_w \nabla P_c\ \big] = 0$$

Hyperbolic transport equation (saturation equation)

$$\phi \frac{\partial S_w}{\partial t} + \nabla\big[\ f_w\vec{u}\ +\ f_w\lambda_n(\rho_w - \rho_n)\mathbf{K}\vec{g}\ +\ f_w\lambda_n P_c' \nabla S_w\ \big] = q_w.$$

Notation used above:

$$\lambda_\alpha = k_{k\alpha}/\mu_\alpha$$
$$f_\alpha = \lambda_\alpha / \textstyle\sum_\alpha \lambda_\alpha$$

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Four different physical effects

- advection
- convection
- segregation
- capillarity

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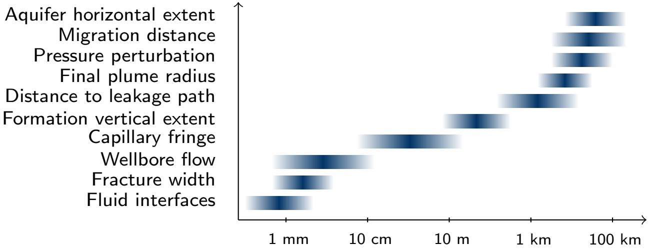
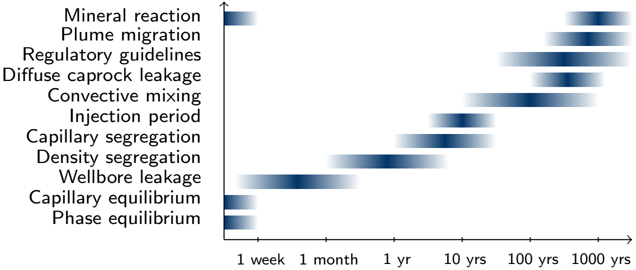
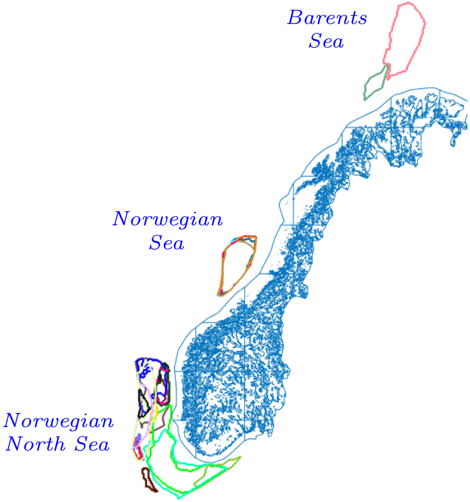
A true multiscale problem





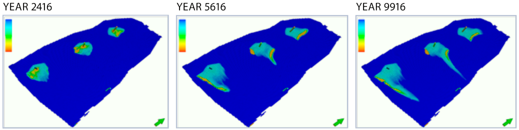


Estimating storage capacity

Site-specific estimates

Dynamic estimates: direct numerical simulations of specific site

Can incorporate technical, economical and regulatory constraints



Volume of CO_2 injected vs. migration time

From: "CO_2 Storage Atlas, Norwegian North Sea" (NPD, 2011)

Computationally challenging to incorporate necessary geological uncertainty in 3D simulations

Regional estimates

Static estimates: $M_{CO_2} = E \times A_{\text{av}} H_{\text{av}} \phi_{\text{av}} \times \rho_{CO_2}$

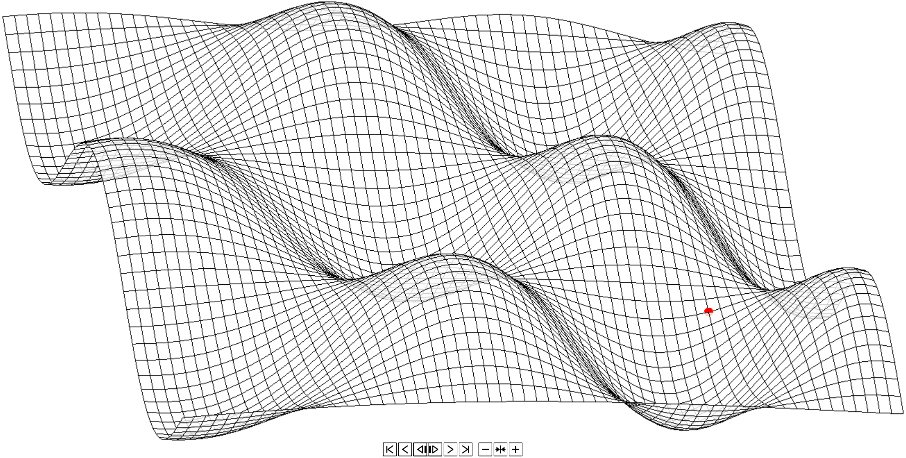
- $A_{\text{av}} H_{\text{av}} \phi_{\text{av}}$ - estimated total pore space
- E - *efficiency factor*

Statistical/analytical approach; no simulation

From: "Carbon Utilization and storage Atlas 2012" (USDOE, NETL)'

Computationally intractable at necessary 3D resolution

Simplest possible analysis: structural trapping



Model reduction: eliminate time and only consider infinitesimal, buoyant trickle of CO_2

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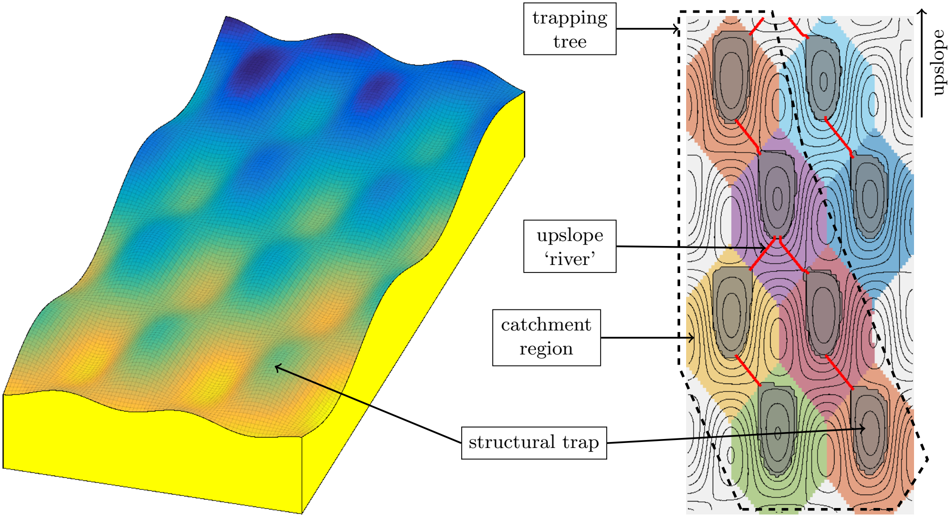
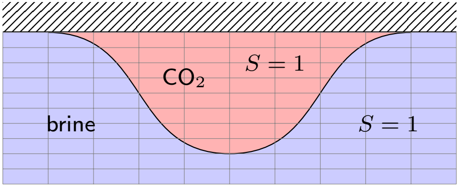


Model reduction: eliminate time and only consider infinitesimal, buoyant trickle of CO_2

Analogy with hydrology

- traps $\rightarrow$ lakes
- spill paths $\rightarrow$ rivers
- spill points $\rightarrow$ lake outlets
- catchment areas $\rightarrow$ catchment areas
- watersheds $\rightarrow$ watersheds

Model reduction of dynamic equations



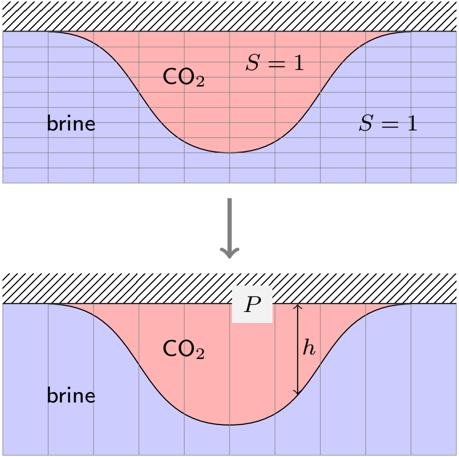
Observations:

- very large aspect ratios
- large difference in fluid densities, which means buoyancy effects are strong
- gravity segregation is almost instantaneous compared with lateral flow
- CO_2 plume is very thin and hence high vertical resolution is required

Two natural simplifications:

- depth-integrate the equations
- assume vertical equilibrium

Model reduction of dynamic equations



Incompressible flow:

$$\phi \frac{\partial s}{\partial t} + \nabla \cdot \left[\lambda \boldsymbol{K} \left(\nabla p - \rho \vec{g}\right)\right] = 0$$

Depth integration:

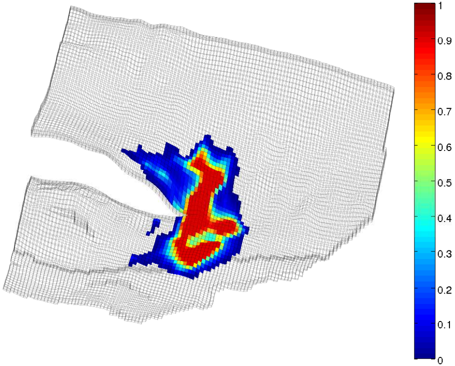
$$\int_{top}^{bottom} \left[\phi \frac{\partial s}{\partial t} + \nabla \cdot \left[\lambda \boldsymbol{K} \left(\nabla p - \rho \vec{g}\right)\right]\right] = 0$$

Assuming sharp interface:

$$\phi \frac{\partial h}{\partial t} + \nabla_{\parallel} \cdot \left[\lambda \boldsymbol{K} \left(\nabla_{\parallel} P - \rho \vec{g}\right)\right] = 0$$

Model reduction of dynamic equations

Example: Johansen formation



CO_2 saturation 500 yrs after start of injection (110 year injection period)

Numerical efficiency for VE:

- vertical equilibrium $\longrightarrow$ only one cell in the vertical direction $\longrightarrow$ much fewer grid cells
- weaker dynamic coupling $\longrightarrow$ fewer time steps

Time-step restrictions for *explicit* scheme

Time	Advection	Convection	Segregation
injection	1 yr	201 yr	8 yr
migration	—	164 yr	8 yr
injection	0.1 yr	10 yr	0.04 yr
migration	—	12 yr	0.04 yr

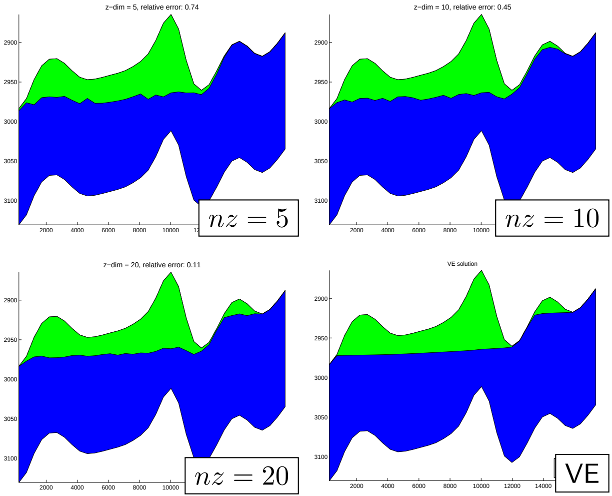
VE model 3D model

Model reduction of dynamic equations

Example: Johansen formation

Analytical expression for vertical fluid distribution $\longrightarrow$ 'infinite' vertical resolution

In particular, more accurate than under-resolved 3D simulation

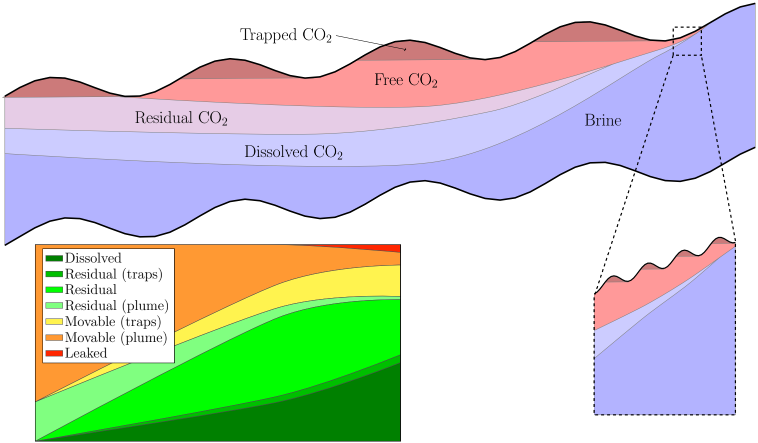


General VE formulation

Formulated as industry-standard black-oil type model†:

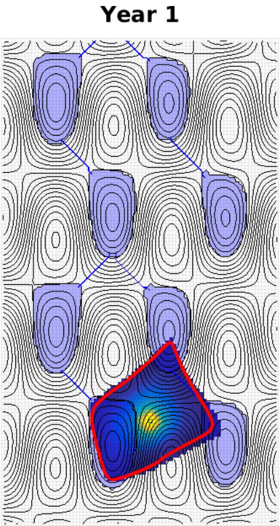
- capillary fringe
- compressibility
- dissolution and convective mixing
- geological heterogeneity
- hysteretic effects
- subscale trapping effects
- geomechanical, thermal,

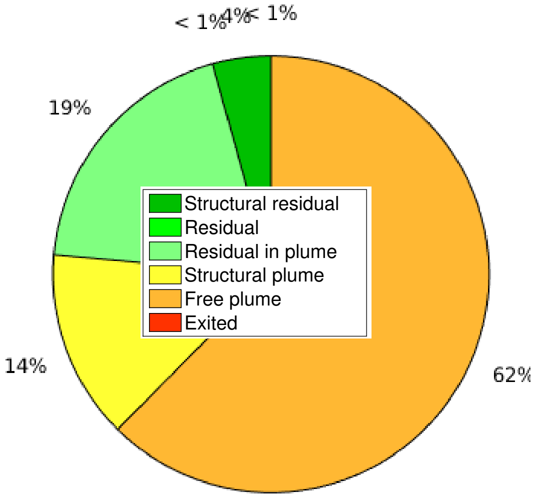
Robust and fully implicit discretization



† Using relative permeability $k_{r\alpha}(S,p)$ upscaled (homogenized) to match behavior on subscale grid

Example: 10 years injection, 3000 years migration





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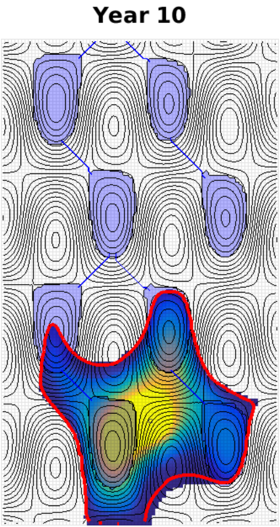

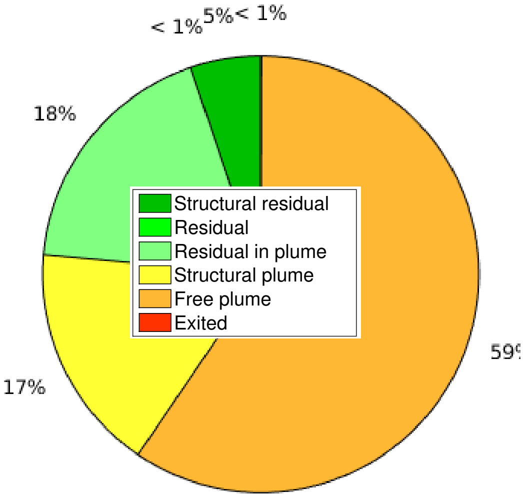

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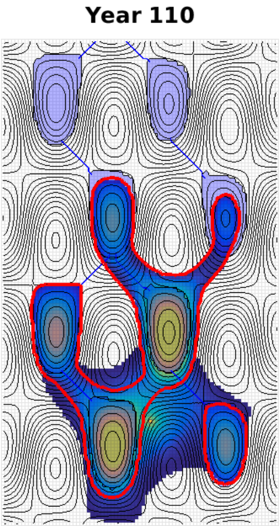

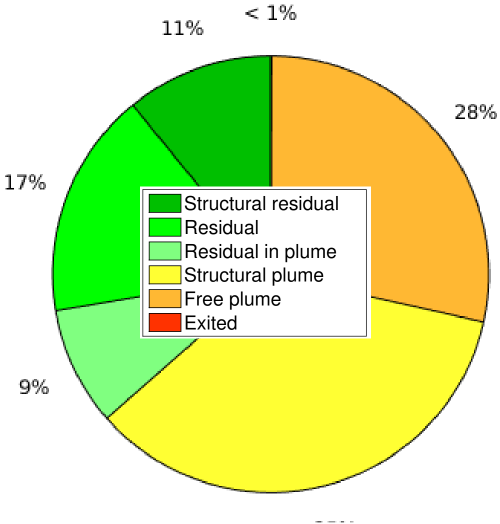

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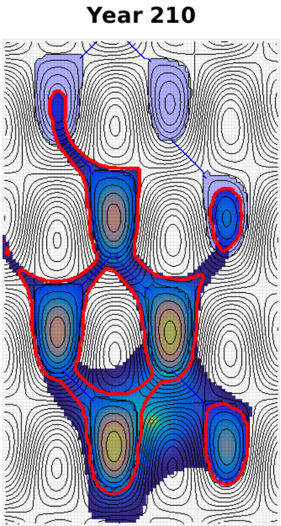

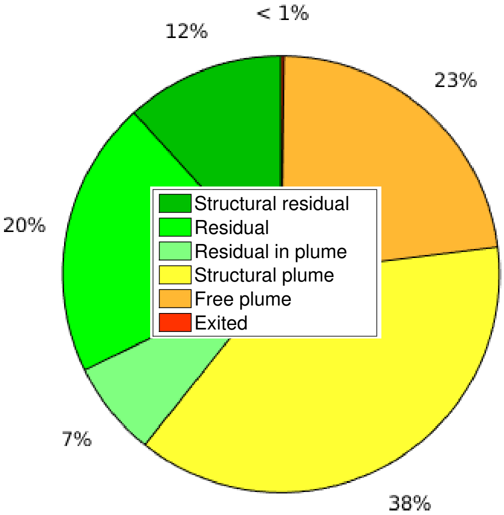

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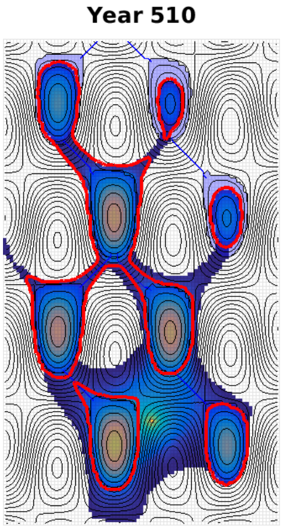

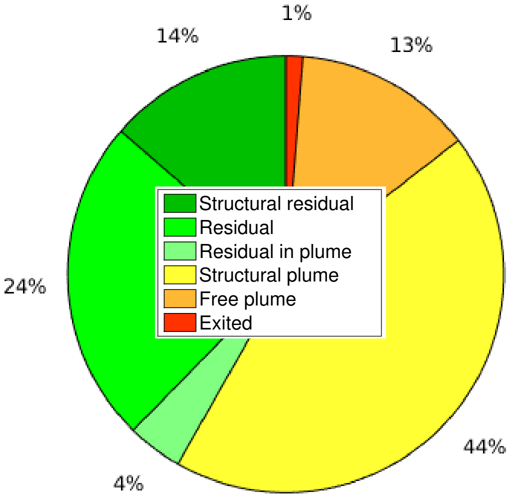

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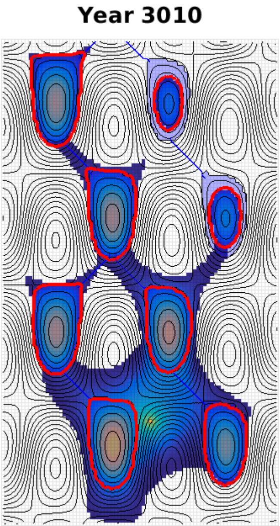
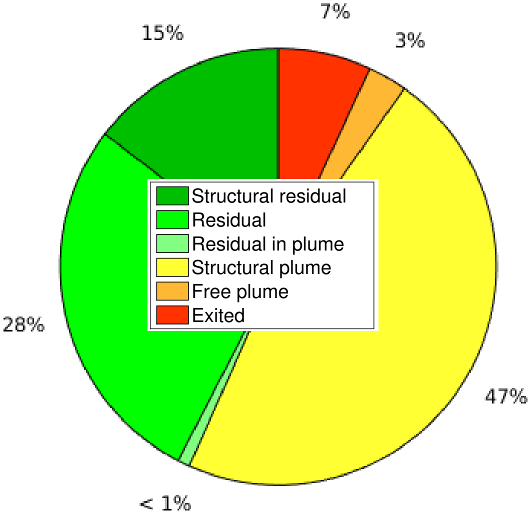
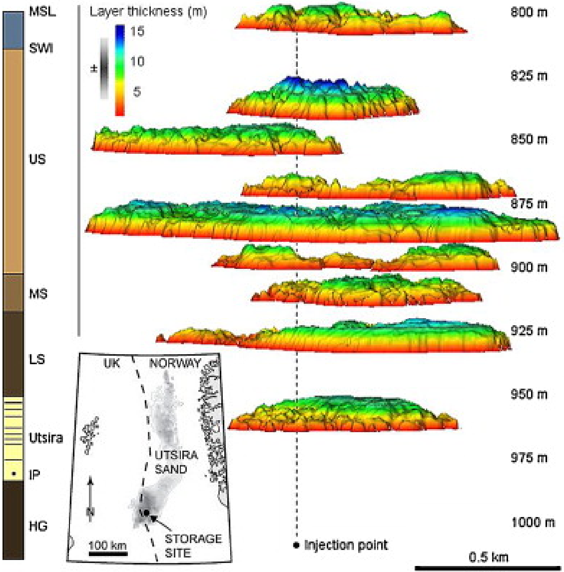
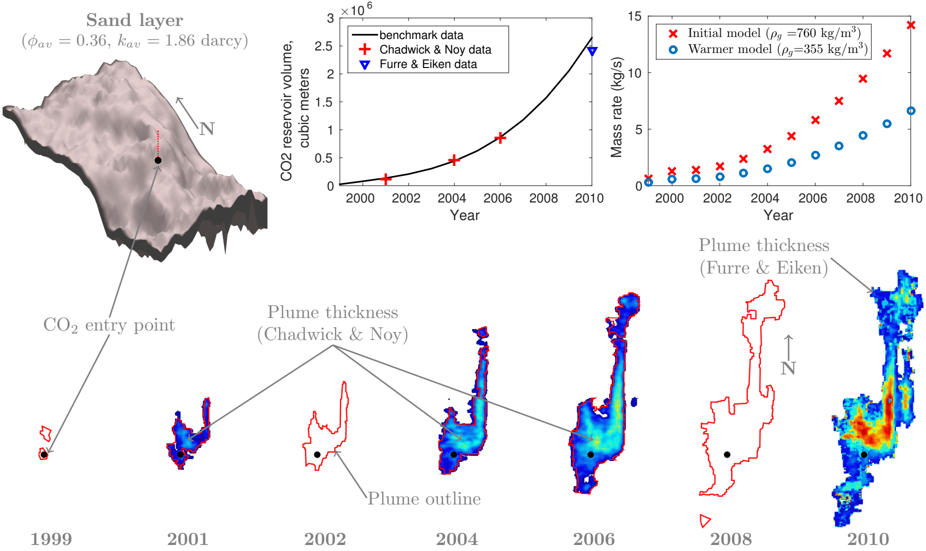


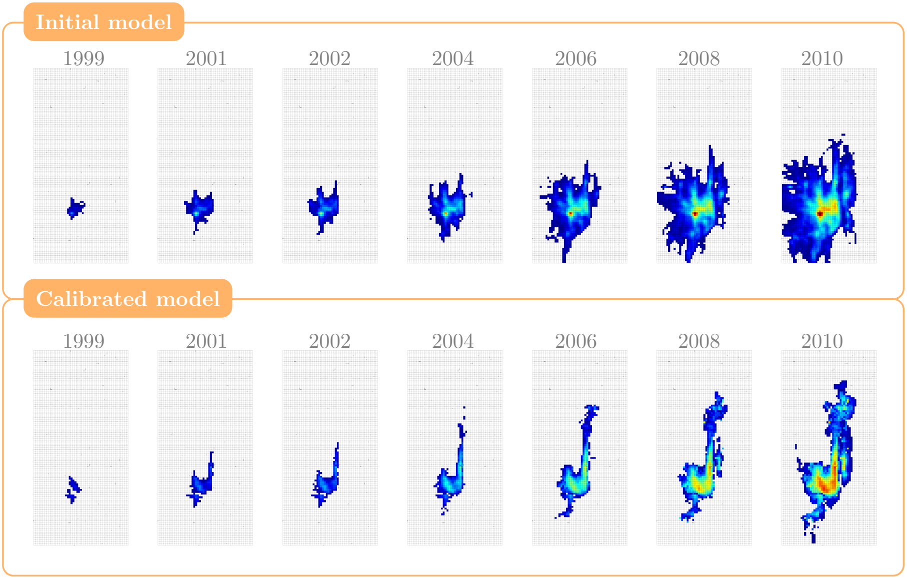


Calibrating the Sleipner model



Calibrating the Sleipner model



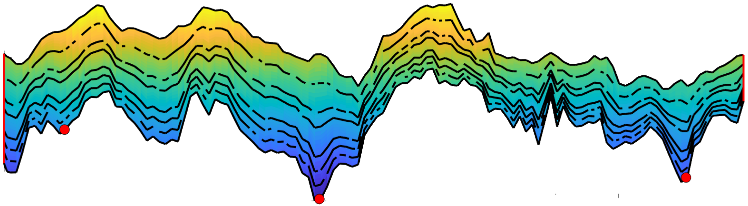


CO_2 density change: $760 \rightarrow 478$ kg/m^3
Injection rate change: $0.92 \times$ benchmark rates

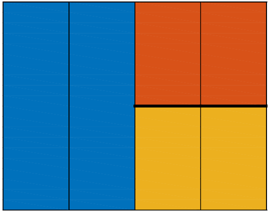
Grid elevation change: $+/-$ 5 meters
Permeability change: $1.85 \rightarrow 12$ darcy
Porosity change: $0.36 \rightarrow 0.37$

More complex geology ⟶ hybrid 3D–VE simulation

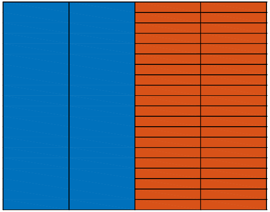
- Fully automated coarsening for models with many (near) impermeable horizons
- Regions automatically detected and discretized
- Near-well regions: 3D grid with coupling wells and surface facilities
- Transition between VE-zones, diffuse leakage, fine-scale are all included



Coupling types:

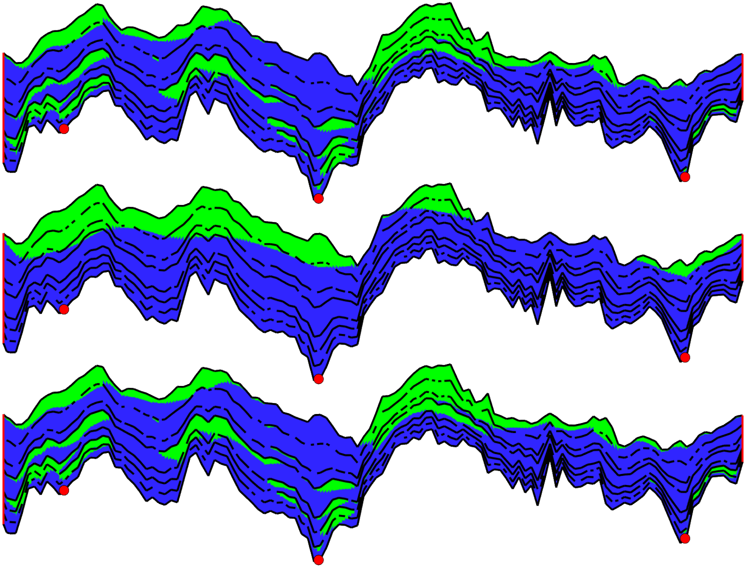


VE to VE

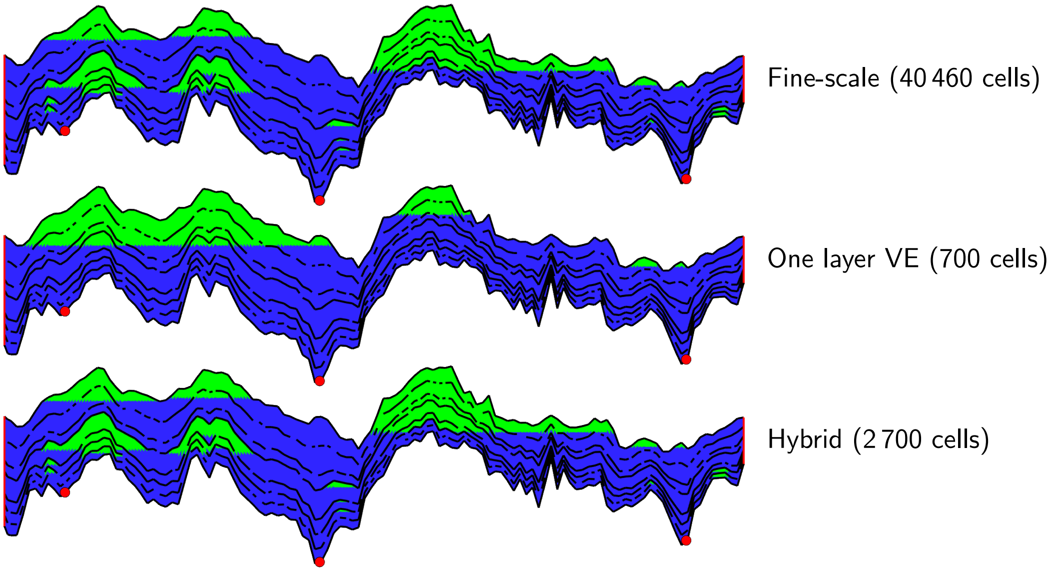


Fine-scale to VE

Example: Sleipner-type scenario (injection)



Example: Sleipner-type scenario (migration)



Optimization of injection points and rates

$$O(q) = \int_0^T \sum_i q_i \, dt - C \cdot L(q) - C_p \sum_j \left[\max(0, p_j - p_j^{\mathsf{max}})\right]^2$$

Three contributions to objective function

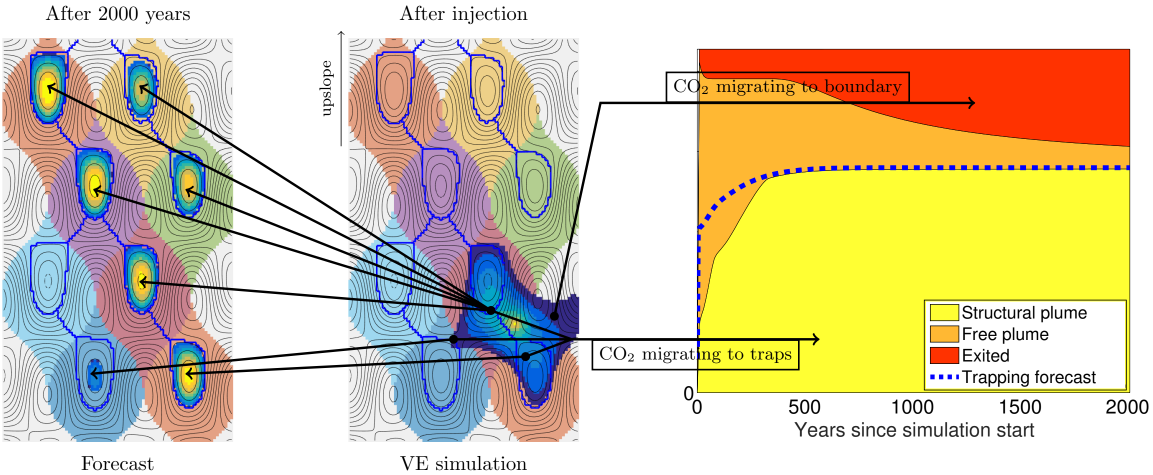
- Injected amount of CO_2
- Amount of CO_2 leaked at end of simulation, penalized by factor C
- Cells with pressure p_j exceeding safety limit p_j^{max}, penalized by factor C_p

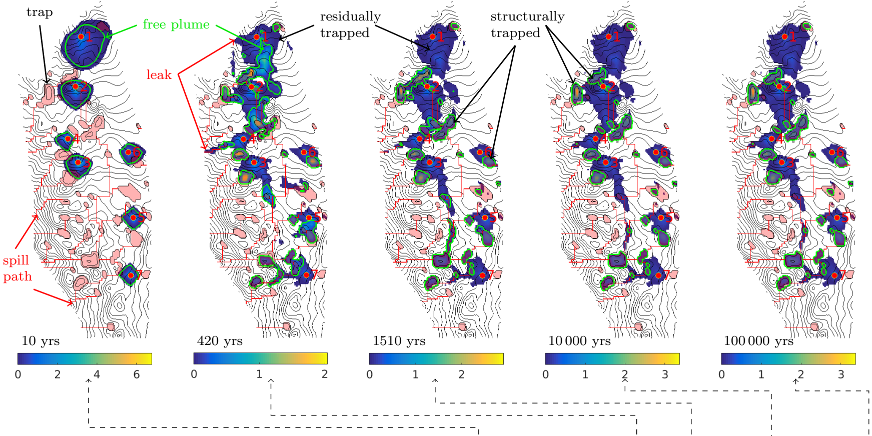
Remarks:

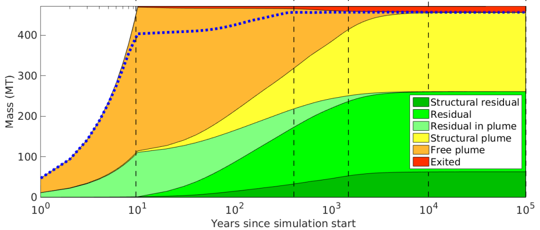
- Each evaluation of O requires a *full* simulation acellerate
- Our framework enables ∇O to be computed by an adjoint approach[†]
- For brevity, no constraints are specified here

† J.D. Jansen, Adjoint-based optimization of multi-phase flow through porous media - a review, Computers & Fluids 46 (2011)

Accelerated simulation: early exit by forecast algorithm



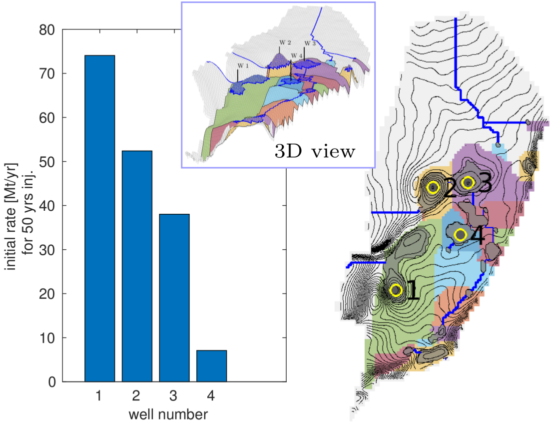




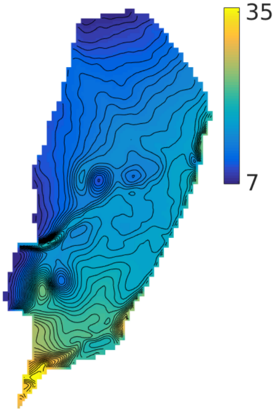
Forecast converges after 450 years. No need to simulate 10 000 yrs

Optimization with multiple constraints

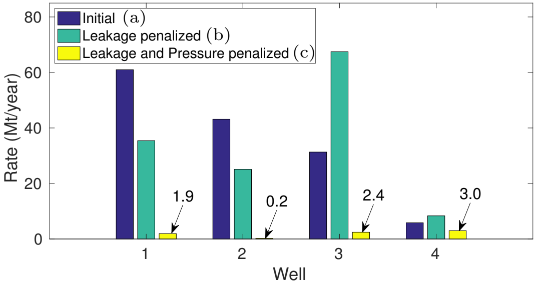
How much can we safely inject into this formation to maximize storage while maintaining the integrity of the caprock?

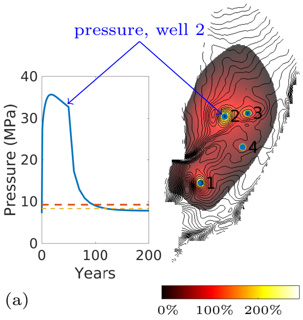


Well placement, initial rates, and trapping structure

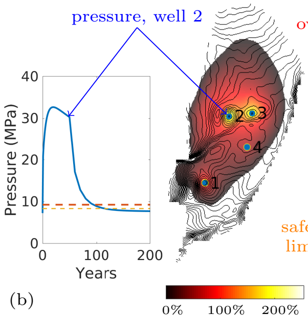


Overburden pressure (MPa)

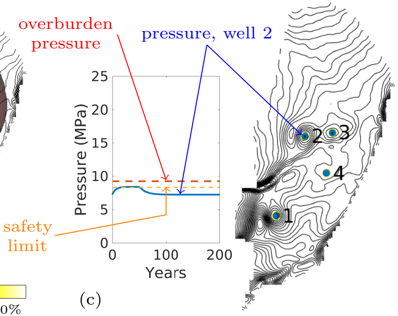




Initial rates,
overburden pressure exceeded



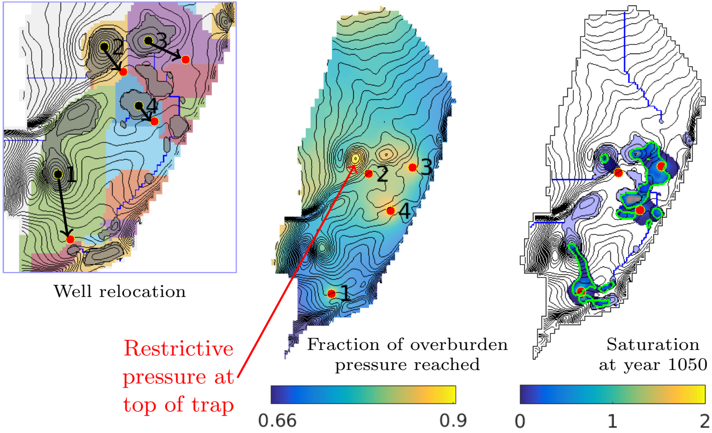
Leakage penalized,
overburden pressure exceeded

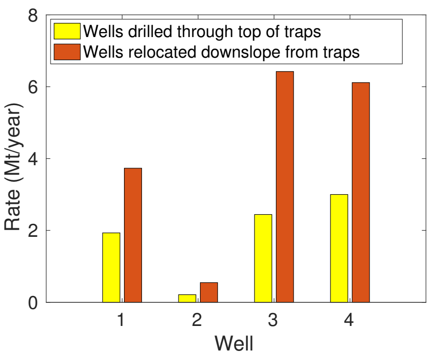


Leakage and pressure penalized,
no violations

Strategies to enchance storage

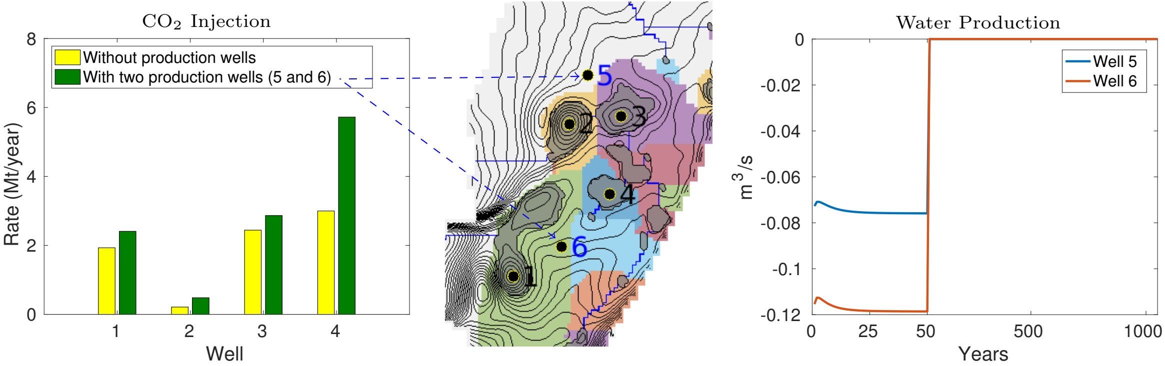
Relocating wells downslope from trap increases storage from 380 to 850 Mt





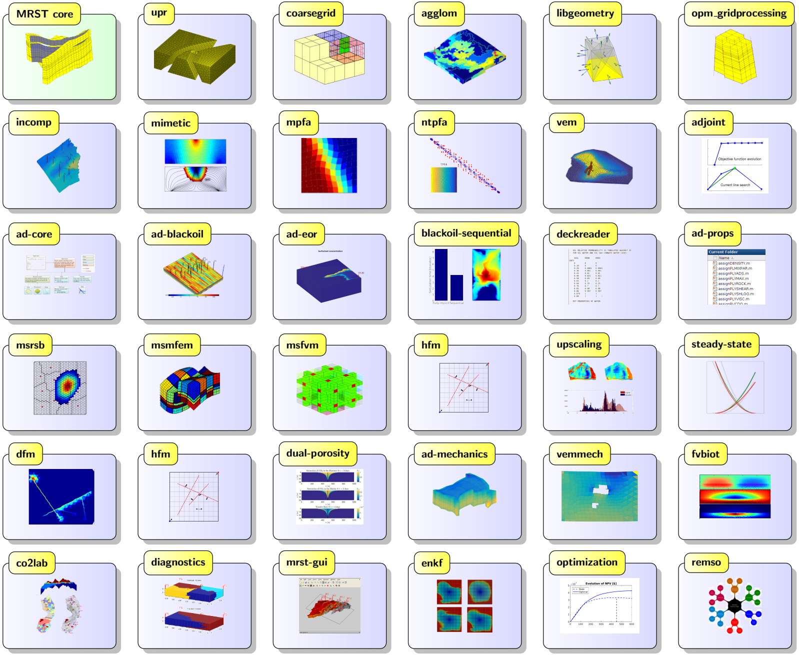
Strategies to enchance storage

Adding two water producers increases storage from 380 to 574 Mt



Summary

- Discussed modelling of long-term CO_2 storage in large-scale aquifer systems
- Multiscale problem, computationally intractable with standard 3D simulation
- Presented various model reductions:
  - Spill-point/trapping analysis – static capacity estimates
  - Vertical equilibrium: reduce dimension and improve dynamic couplings
- Discussed various optimization methods: initial guess from trapping analysis, acceleration by VE simulation, use of adjoints, ...
- Only a few simple examples presented herein
- Implemented as free open-source software: MRST-co2lab



Grid generation and coarsening

Discretization and solvers for incompressible flow

Discretization and solvers for compressible flow

Upscaling and multiscale methods

Fractured media and geomechanics

Workflow tools

http://www.sintef.no/MRST