Level set methods for simulating multiphase displacements on the pore scale

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Level Set Methods

› **Reference textbooks:**
  
  
Level set method

A method to describe evolution of interfaces between fluids (or materials) that may change shape and topology (e.g., merge, split, deform)

Some applications:

• Computational fluid dynamics
• Fracture mechanics
• Crystal growth, grain rearrangement
• Visualization
• Image analysis (e.g., for medical use)
  — Segmentation, Noise removal, Extraction of objects etc..
Some interesting links...

  
  • 2 times Oscar winner for developing techniques for better visual effects in movies (Harry Potter, Star Wars, Terminator, Pirates of the Carribean, etc...), Examples: simulation of hair, water splash, fire, wind, cloth, destruction etc...

› James Sethian: [https://math.berkeley.edu/~sethian/](https://math.berkeley.edu/~sethian/)
  
  • Award-winning soap bubble animation using VIIM (Saye & Sethian JCP 2012, Science 2013):
    
Contents

› Level set methods and related techniques
  • Reinitialization (Sussman et al., JCP 1994, Peng et al., 1999)
  • Extension velocities (Peng et al., 1999; Adalsteinsson and Sethian, 1999)

› Application example within «Digital Rock Physics»:
  • Level set methods for simulating capillary-controlled multiphase displacements on the pore scale:
    – Capillary pressure
    – Hysteresis
    – Trapping and remobilization
An interface tracking method where the interface is given as the zero contour of an implicit function $\phi: \phi(\vec{x}, t) = 0$

The LS function $\phi$ is one dimension higher than the interface.

Regions inside/outside of the interface are defined through the sign of $\phi$:

$\Omega^+ = \{\vec{x}: \phi(\vec{x}, t) > 0\}$

$\Omega^- = \{\vec{x}: \phi(\vec{x}, t) < 0\}$

Normally $\phi$ is given by the signed distance function (SDF):

$\phi(\vec{x}, t) = \pm|\vec{x} - \vec{x}_0|$, where $\vec{x}_0$ is located on the interface.

SDF has the property $|\nabla \phi| = 1$ which ensures numerical stability.
Level Set Method (LSM)  
(Sethian & Osher, 1988)

› Interfaces are described by $\phi(\tilde{x}(t), t) = 0$:

$\phi_t + \nabla \phi \cdot \frac{d\tilde{x}}{dt} = 0$, $\vec{V} = \frac{d\tilde{x}}{dt}$ (velocity).

Assume $\vec{V} = V_n \vec{N} + V_T \vec{T}$, $\vec{T}$ = tangential vector.

$\vec{N} \cdot \nabla \phi = |\nabla \phi|$ and $\vec{T} \cdot \nabla \phi = 0$.

$\Rightarrow \phi_t + V_N |\nabla \phi| = 0$

› The method handles topological changes, such as interface merging and splitting, in a natural manner.

› Surface normal $\vec{N}$ and curvature $\kappa = \nabla \cdot \vec{N}$ are directly related to $\phi$

› The surface evolves by specifying a surface velocity which could include a normal and advective component:

$$\phi_t + V_N |\nabla \phi| + \vec{V}_{adv} \cdot \nabla \phi = 0$$
During iterations with the evolution equation, steep gradients $\nabla \phi$ may develop and $\phi$ will lose its SDF property ($|\nabla \phi| = 1$).
Therefore, to maintain numerical stability, the LS function $\phi$ must be reinitialized to SDF occasionally. This is done by solving
\[
\phi_t + S(\phi)(|\nabla \phi| - 1) = 0, \quad S(\phi) = \text{sign function}
\]
An example of void/solid SDF calculation:

\[
\psi = 0 \quad \text{(void/solid LS function)}
\]
1. Initialize LS-function $\phi$ to a signed distance function by solving:
   $$ \phi_t + S(\phi)(|\nabla \phi| - 1) = 0 \quad (*) $$

2. Iterate $\phi$ forward in time with LS evolution equation
   $$ \phi_t + \nu_N |\nabla \phi| + \vec{v}_{adv} \cdot \nabla \phi = 0, \quad (**) $$

   - $\phi_t$: Time iteration with Runge-Kutta Methods (e.g., 3rd order)
   - $\nu_N |\nabla \phi|$: Central differences for curvature ($\kappa = \nabla \phi / |\nabla \phi|$)
   - $\vec{v}_{adv} \cdot \nabla \phi$: WENO & advective upwinding scheme

   WENO = Weighted Essentially Non-Oscillatory

   [1st order RK: Forward Euler step: $\phi^{n+1} = \phi^n - \Delta t(\nu_N^n |\nabla \phi^n| + \vec{v}_{adv}^n \cdot \nabla \phi^n)$]

3. Repeat from step 1.

4. Reinitialize $\phi$ by solving (*) after specified time iterations. Similar techniques are used for solving (*) and (**).
Extension Velocity

> WHAT: Velocity (given on the interface) extended (extrapolated) in the normal direction OFF the interface such that:

\[ \nabla v_{ext} \cdot \nabla \phi = 0 \]

> WHY: Extension velocity provides a meaningful velocity for problems it is not known away from the interface regions

> Advantages:

- Extension velocity preserves \( \phi \) as an SDF (\(|\nabla \phi| = 1\)), allowing less frequent reinitializations in numerical implementations
- Allows for larger time steps (based on CFL conditions)

> HOW: Construct extension velocity by solving PDE:

\[ v_t + S(\phi) \vec{N} \cdot \nabla v = 0, \quad v = \text{velocity component} \]

\[ \vec{N} = \frac{\nabla \phi}{|\nabla \phi|} \]
We shall show that, for an LS evolution equation,
\[ \phi_t + v_N |\nabla \phi| + \mathbf{v}_{\text{adv}} \cdot \nabla \phi = 0, \quad \mathbf{v}_{\text{adv}} = (v_1, v_2, v_3), \]
we can construct extension velocities satisfying
\[ \nabla v_N \cdot \nabla \phi = 0 \]
\[ \nabla v_1 \cdot \nabla \phi = 0 \]
\[ \nabla v_2 \cdot \nabla \phi = 0 \]
\[ \nabla v_3 \cdot \nabla \phi = 0, \]
such that \(|\nabla \phi| = 1\) for all time (in theory).
Extension Velocity (Proof)

1. Normal velocity, $v_N$:
\[
\frac{d}{dt} |\nabla \phi|^2 = 2 \nabla \phi \frac{d}{dt} \nabla \phi \\
= -2 \nabla \phi \cdot \nabla (v_n |\nabla \phi|) \\
= -2 \nabla \phi \cdot \nabla v_n |\nabla \phi| - 2 \nabla \phi \cdot v_n \nabla |\nabla \phi| \\
= 0.
\]

$\Rightarrow \nabla \phi_t = -\nabla (v_n |\nabla \phi|)$

2. Advective velocity components, $v_i$:
\[
\phi_t + v_1 \phi_x = 0 \\
\frac{d}{dt} |\nabla \phi|^2 = 2 \nabla \phi \frac{d}{dt} \nabla \phi \\
= -2 \nabla \phi \cdot \nabla (v_1 \phi_x) \\
= -2 (\nabla \phi \cdot \nabla v_1) \phi_x - 2 v_1 \nabla \phi \cdot \nabla \phi_x \\
= 0.
\]

$\Rightarrow \nabla \phi_t = -\nabla (v_1 \phi_x)$

\[\Rightarrow \text{Similar for } y- \text{and } z-\text{components}.\]

$\frac{1}{2} \frac{d}{dx} |\nabla \phi|^2 = 0$
Extension Velocity

Simulation procedure:
1. Construct extension velocities by solving
   \[ v_t + S(\phi) \vec{N} \cdot \nabla v = 0, \quad \text{for each velocity component } v. \]
2. Iterate \( \phi \) one time step forward with LS evolution equation
   \[ \phi_t + v_N |\nabla \phi| + \vec{v}_{adv} \cdot \nabla \phi = 0, \]
   using extension velocities from step 1.
3. Repeat from step 1.
4. Perform reinitialization periodically.
Applications - Objective

› Develop pore-scale models for simulating capillary-controlled motion of two & three fluids directly on 3D rock geometries

› At equilibrium:
  • Young-Laplace equation satisfied in pore space:
    \[ P_{ci} = \sigma_{ij} C_{ij}, \ ij = go, ow, gw \ . \]
  • Young’s equation satisfied on pore walls:
    \[ \sigma_{ij} \cos \theta_{ij} = \sigma_s - \sigma_s, \ ij = go, ow, gw. \]
    This yields a constraint on \( \sigma_{ij} \) and \( \theta_{ij} \):
    \[ \sigma_{gw} \cos \theta_{gw} = \sigma_{go} \cos \theta_{go} + \sigma_{ow} \cos \theta_{ow} \]
    \[ C_{ij} = \text{Interface curvature} \]
    \[ \sigma_{ij} = \text{Interfacial tension} \]
    \[ \theta_{ij} = \text{Contact angle} \]
    (Bartell-Osterhof Eq.).

› Two fluids: Level set method

› Three fluids: Variational (or Multiple) level set method
Rock imaging: Micro-CT at LBNL

Reconstructed and segmented Bentheim sandstone sample

- Size of subset: 750x750x750 voxels
- Resolution 4.5 microns
- Total sample size 5x5x5 mm³

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Synchrotrons

Advanced Light Source (ALS) at LBNL, Berkeley:

Advanced Photon Source (APS) in Argonne, Illinois (used by Oregon State University):
For each capillary pressure, evolve $\phi$ until equilibrium using

$$\phi_t + (C - \kappa) |\nabla \phi| = 0,$$

where $V_n = C - \kappa$ and $C = P_c/\sigma =$ Input interface curvature.

The solution $V_N = 0$ yields surfaces of constant mean curvature.

$\psi =$ Static pore/solid LS function

- $\psi = 0$
- $\phi = 0$

A constraint prevents $\phi = 0$ from invading solid ($\theta = 0^\circ$).
3D Simulation: Castlegate Sandstone

- Void-solid surface described by $\psi = 0$:
- Porosity 20.6 %
- Voxel size 5.6 $\mu$m
- Small subset 100x100x70 voxels

Data set available on the internet (Network Generation Comparison Forum):
http://xct.anu.edu.au/network_comparison/
$C = 0.30$

= Non-wetting phase
($\phi_{nw} < 0$)
Castlegate Sandstone

\[ C = 0.50 \]

= Non-wetting phase
Castlegate Sandstone

\[ C = 0.60 \]

= Non-wetting phase
$C = 0.75$

= Non-wetting phase
$C = 0.80$

= Non-wetting phase
Castlegate Sandstone

\[ C = 0.85 \]

= Non-wetting phase
Castlegate Sandstone

\[ C = 0.95 \]

\textcolor{red}{= \text{Non-wetting phase}}
Castlegate Sandstone

\[ C = 1.05 \]

- Non-wetting phase
Castlegate Sandstone

\[ C = 1.15 \]

= Non-wetting phase
Castlegate Sandstone

\[ C = 1.35 \]

\( \text{red} = \text{Non-wetting phase} \)
3D LSM simulation: Castlegate sandstone

$C = 1.6$

Structure of the wetting phase:

Isolated wetting phase is located in narrow pore throats and constrictions
Castlegate sandstone

Capillary pressure curve:
Simulation in fractured rock

- Computer-generated fractured sample from LBNL
- The non-wetting phase invades the diagonal micro-fracture and some of the large pores first

\[ C = 0.25 \]
Simulation in fractured rock

- Computer-generated fractured sample from LBNL
- The non-wetting phase invades the diagonal micro-fracture and some of the large pores first

\[ C = 0.55 \]

\[ \kappa_0 = 1 / \Delta x \]

\[ S_w \]

\[ \text{red} = \text{Non-wetting phase} \]

\[ \text{gray} = \text{Grains} \]
LS Method with Contact Angle (CA-LSM) (Jettestuen, et al., WRR 2013)

formation of the contact angle in the solid at steady state:

$$\cos \beta = \mathbf{n}_\psi \cdot \mathbf{n}_\phi = \frac{\nabla \psi}{|\nabla \psi|} \cdot \frac{\nabla \phi}{|\nabla \phi|} = - \cos \theta$$

Contact angle:
$$\theta = 180^\circ - \beta$$
Formation of the contact angle in the solid at steady state:

\[ \nabla \psi \cdot \nabla \phi - \cos \beta |\nabla \psi| |\nabla \phi| = 0 \]

Contact angle:
\[ \theta = 180^\circ - \beta \]
LS Method with Contact Angle (CA-LSM)

Resulting evolution equation:

\[ \phi_t + H(\psi)(C - \kappa) |\nabla \phi| + H(-\psi)S(\psi)B(\nabla \psi \cdot \nabla \phi - \cos \beta |\nabla \psi||\nabla \phi|) = 0 \]

- **Pore space**: \( \psi > 0 \)
  - Balance between capillary and interfacial forces in the pore space

- **Solid phase**: \( \psi < 0 \)
  - Formation of the contact angle in the solid phase

\[ B = O(1/\Delta x) \text{ constant} \]
\[ \theta = 180^\circ - \beta = \text{Contact angle} \]
\[ \psi = \text{LS function describing the pore walls} \]
\[ H = \text{Heaviside step function} \]
\[ S = \text{Sign function} \]

(Jettestuen, et al., WRR 2013)

Heaviside \( H(\phi) \) and delta \( \delta(\phi) \) functions facilitates phase volume and interfacial area calculation.
Castlegate sandstone - Drainage

$\theta = 0^\circ$

(standard level set model)

$\theta = 20^\circ$

$\theta = 40^\circ$

$C = 0.50$

Red = Non-wetting phase

Gray = Grains
Castlegate sandstone - Drainage

$\theta = 0^\circ$
(standard level set model)

$\theta = 20^\circ$

$\theta = 40^\circ$

$C = 0.60$

= Non-wetting phase
= Grains
Castlegate sandstone - Drainage

\[ \theta = 0^\circ \]
(standard level set model)

\[ \theta = 20^\circ \]

\[ \theta = 40^\circ \]

\[ C = 0.70 \]

- \( \text{red} = \text{Non-wetting phase} \)
- \( \text{gray} = \text{Grains} \)
Castlegate sandstone - Drainage

\( \theta = 0^\circ \)
(standard level set model)

\( \theta = 20^\circ \)

\( \theta = 40^\circ \)

\( C = 1.0 \)

- \( \text{red} = \text{Non-wetting phase} \)
- \( \text{gray} = \text{Grains} \)
Castlegate sandstone - Imbibition

\[ C = 0.40 \quad C = 0.30 \quad C = 0.25 \]

\[ \theta = 20^\circ \]

Non-wetting phase retracts to larger pore openings after growth of wetting-phase films has led to snap-off in pore-throat constrictions.

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Castlegate sandstone – Capillary pressure curves

Drainage:

Drainage & imbibition ($\theta = 20^\circ$):

Hysteresis
Summary

A 3D level set based pore-scale model has been developed to simulate capillary-controlled displacements in rock images.

- A method to include arbitrary contact angles has been developed and implemented.
- Simulations in 3D pore geometries demonstrate that the model accounts for well-known pore-scale mechanisms:
  - Piston-like invasion
  - Haines jumps (drainage)
  - Wetting-phase film growth and snap-off (imbibition)
  - Interface coalescence and retraction
  - Hysteresis occurs between drainage and imbibition due to different displacement mechanisms
Variational Level Set (VLS) Method

- Developed for motion of triple junctions
- We add solid phase and contact angle to existing method

For each fluid:
\( \phi_i \) (LS function)
\( p_i \) (phase pressure)
\( \gamma_i \) (surface tension)
\( \beta_i \) (solid/pore intersection angle)

\[ \gamma_s - \gamma_i \cos \beta_i \] (solid/fluid interfacial tension)
Variational Level Set Method

Total energy:
\[ E = E_1 + E_2 + E_3 \]

Bulk energy:
\[ E_1 = \sum_{i=g,o,w} p_i \int_{\Omega} H(-\phi_i)H(\psi) d\Omega \]

Fluid/fluid interfacial energy:
\[ E_2 = \sum_{i=g,o,w} \gamma_i \int_{\Omega} \delta(\phi_i)|\nabla \phi_i|H(\psi) d\Omega \]

Solid/fluid interfacial energy:
\[ E_3 = \sum_{i=g,o,w} (\gamma_s - \gamma_i \cos \beta_i) \times \int_{\Omega} H(-\phi_i)\delta(\psi)|\nabla \psi| d\Omega \]
Variational Level Set Method

Overlap/vacuum regions occur if $\phi_i$ moves with independent velocities.
Variational Level Set Method

Constraint prevents overlap/vacuum regions:
\[
\frac{1}{2} \int_{\Omega} \left( \sum_{i=g,o,w} H(-\phi_i) - 1 \right)^2 \, dV = 0
\]

Interfacial tensions \( (\sigma_{ij}) \), capillary pressures \( (P_{cij}) \) and contact angles \( (\theta_{ij}) \) are defined at the interfaces.
Variational Level Set Method

Stable interface configurations:

**Pore space:**

\[ P_{cij} = (\gamma_i + \gamma_j)\kappa_i \]  
(Young-Laplace Equation)

**Pore walls (\& solid):**

\[
\cos \theta_{ij} = \frac{\gamma_j \cos \beta_j - \gamma_i \cos \beta_i}{\gamma_i + \gamma_j}
\]  
(Young Equation)

\[
\sigma_{gw} \cos \theta_{gw} = \sigma_{go} \cos \theta_{go} + \sigma_{ow} \cos \theta_{ow}
\]
Variational Level Set Method

Putting it all together:

\[ f(\phi_g, \phi_o, \phi_w) = \int_\Omega \left( \sum_{i=g,o,w} p_i H(-\phi_i) H(\psi) + \sum_{i=g,o,w} \gamma_i \delta(\phi_i) |\nabla \phi_i| H(\psi) \right. \]

\[ + \left. \frac{\lambda}{2} \left( \sum_{i=g,o,w} H(-\phi_i) - 1 \right)^2 \right) \]

\[ - \sum_{i=g,o,w} \gamma_i \left( \frac{\nabla \phi_i}{|\nabla \phi_i|} \cdot \frac{\nabla \psi}{|\nabla \psi|} - \cos \beta_i \right) \delta(\psi) |\nabla \psi| H(-\phi_i) \right) dV \]

(Young-Laplace in pore space)

(No overlap/vacuum constraint)

(Formation of contact angle on pore/solid surface)

\[ \lambda = \text{Lagrange multiplier} \]
Variational Level Set Method

Minimizing $f$ with respect to $\phi_i, i = g, o, w$ gives three evolution equations:

$$(\phi_i)_t + \lambda \left( \sum_{j=g,o,w} H(-\phi_j) - 1 \right) |\nabla \phi_i| + H(\psi)(p_i - \gamma_i \kappa_i)|\nabla \phi_i|$$

$$+ \frac{H(-\psi)}{\Delta x} S(\psi) \gamma_i (\nabla \phi_i \cdot \nabla \psi - \cos \beta_i |\nabla \phi_i| |\nabla \psi|) = 0, \quad i = g, o, w$$

$H(-\psi)/\Delta x$ has replaced $\delta(\psi)$ to extend contact angle into solid, which is more accurate numerically.

The solution $\phi_i$ must satisfy the constraint at all times:

$$\frac{d}{dt} \frac{1}{2} \int_\Omega \left( \sum_{i=g,o,w} H(-\phi_i) - 1 \right)^2 dV = - \sum_{i=g,o,w} \int_\Omega \left( \sum_{j=g,o,w} H(-\phi_j) - 1 \right) \delta(\phi_i)(\phi_i)_t dV = 0$$

This gives an expression for the Lagrange multiplier $\lambda$. 

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Relation between $\beta$, $\gamma$ and $\theta$

› At equilibrium, the zero contours of $\phi$ in solid satisfy:

$$\gamma_i (\nabla \psi \cdot \nabla \phi_i - \cos \beta_i |\nabla \psi||\nabla \phi_i|) = \gamma_j (\nabla \psi \cdot \nabla \phi_j - \cos \beta_j |\nabla \psi||\nabla \phi_j|)$$

› The intersection angles between the zero contours of $\psi$ and $\phi$ form the contact angles at the interfaces:

$$\cos \theta_{ij} = \hat{n}_\psi \cdot \hat{n}_\phi_j = \frac{\nabla \psi}{|\nabla \psi|} \cdot \frac{\nabla \phi_j}{|\nabla \phi_j|} \quad (\nabla \phi_j = -\nabla \phi_i)$$

› This yields the following contact angle expressions:

$$\cos \theta_{ij} = \frac{\gamma_j \cos \beta_j - \gamma_i \cos \beta_i}{\gamma_j + \gamma_i}, \quad ij = go, ow, gw.$$  

› These relations satisfy the Bartell-Osterhof equation:

$$\sigma_{gw} \cos \theta_{gw} = \sigma_{go} \cos \theta_{go} + \sigma_{ow} \cos \theta_{ow}$$
Alternative Approach: Multiphase Level Set Method with «Projection Step»

› Alternative technique for removing overlap/vacuum regions

› Uncoupled evolution equations:

\[
(\phi_i)_t + H(\psi)(p_i - \gamma_i \kappa_i) |\nabla \phi_i| \\
+ \frac{H(-\psi)}{\Delta x} S(\psi) \gamma_i (\nabla \phi_i \cdot \nabla \psi - \cos \beta_i |\nabla \phi_i| |\nabla \psi|) = 0, \quad i = g, o, w
\]

› After each time iteration, perform a projection step:
  • Subtract the average of the two smallest \(\phi_i\) from all \(\phi_i\) in each point

› Example when \(\phi_g > \phi_o, \phi_w\):

\[
\phi_g = \phi_g - (\phi_o + \phi_w)/2, \\
\phi_o = \phi_o - (\phi_o + \phi_w)/2, \\
\phi_w = \phi_w - (\phi_o + \phi_w)/2.
\]

(Losasso, Fedkiw et al., 2006)
Multiphase Level Set Method – «Projection Step»

› So, what is the role of the «projection step»?
› Illustrating 1D example – Initial configuration:

![Diagram showing the initial configuration with phases water, oil, and gas]
Multiphase Level Set Method – «Projection Step»

› Illustrating 1D example:

› Configuration after some time using uncoupled equations without projection step (dashed curves):

\[ \phi = 0 \]

= Overlap regions
Illustrating 1D example:

Configuration after projection step:

The projection step moves the intersections between $\phi_i$ to level $\phi = 0$. 
Multiphase Level Set Method – «Projection Step»

 › Illustrating 1D example:

 › Configuration after projection step & reinitialization:

![Diagram showing phase distribution](Image)
Implementation

› Input parameters: $p_i, \gamma_i$ and $\beta_i, i = g, o, w$.
› Quasi-static three-phase VLS simulation by changing phase pressures stepwise
› In each pressure step, evolve $\phi_i, i = g, o, w$ until equilibrium is reached (i.e., solve the 3 evolution equations) and calculate fluid saturations
› Standard explicit numerical techniques for LS methods are used
› For invasion of non-wetting phase: Add a layer of pore space with invading phase at the inlet
› For invasion of wetting or intermediate-wetting phase: Add a porous plate wetted and saturated by the invading phase at inlet
› Boundary conditions:
  • Inlet: Linear extrapolation
  • All other boundaries: $\vec{n} \cdot \nabla \phi_i = 0, i = g, o, w$
› We simulate two-phase saturation history with contact-angle LS method (Jettestuen et al., WRR 2013)
Simulation on sandstone: Simultaneous Water-Alternate-Gas (SWAG) invasion
(Helland & Jettestuen, SCA 2014)

Interfacial tensions:
\[ \sigma_{ow} = 0.02, \sigma_{go} = 0.0101, \]
\[ \sigma_{gw} = 0.03 \text{ N/m} \]

Contact angles:
\[ \theta_{ow} = 20^\circ, \theta_{go} = 7.9^\circ, \]
\[ \theta_{gw} = 16.3^\circ \]

Water cusps at gas/oil/water triple lines

\[ P_{cow} = 1.25 \text{ kPa} \]
\[ P_{cgo} = 0.67 \text{ kPa} \]

\[ S_{wi} = 0.13 \]

(Stable)
SWAG invasion

Water snap-off due to water-cusp growth at gas/oil/solid contact lines

Oil and gas retract to larger Pore openings after water invaded throat

(unsable)

\[ P_{cow} = 1.07 \text{ kPa} \]
\[ P_{cgo} = 0.76 \text{ kPa} \]

\[ S_{wi} = 0.13 \]
SWAG invasion

Oil retracts to larger pore openings after water occupied throat due to 2-phase snap-off event

\(P_{cow} = 1.07 \text{ kPa}\)
\(P_{cgo} = 0.76 \text{ kPa}\)

\(S_{wi} = 0.13\)
**SWAG invasion**

Oil isolated between water and gas

(unstable)

\[ P_{cow} = 1.07 \text{ kPa} \]
\[ P_{cg_o} = 0.76 \text{ kPa} \]

\[ S_{wi} = 0.13 \]
SWAG invasion

\[ P_{\text{cow}} = 1.07 \text{ kPa} \]
\[ P_{\text{cgo}} = 0.76 \text{ kPa} \]

\[ S_{\text{wi}} = 0.13 \]

(Stable)
SWAG invasion

Thickness of water layer increases

(unstable)

\[ P_{cow} = 0.89 \text{ kPa} \]
\[ P_{cgo} = 0.85 \text{ kPa} \]

\[ S_{wi} = 0.13 \]
SWAG invasion

Gas/oil/water triple lines form

(unstable)

\[ P_{cow} = 0.89 \text{ kPa} \]
\[ P_{cgo} = 0.85 \text{ kPa} \]

\[ S_{wi} = 0.13 \]
SWAG invasion

«3-phase snap-off» occurs as a result of water-cusp growth at the gas/oil/water triple lines

(unstable)

\[ P_{cow} = 0.89 \text{ kPa} \]
\[ P_{cgo} = 0.85 \text{ kPa} \]

\[ S_{wi} = 0.13 \]
SWAG invasion

Gas and oil retract to larger pore openings

\[ P_{cow} = 0.89 \text{ kPa} \]
\[ P_{cg\alpha} = 0.85 \text{ kPa} \]

\[ S_{wi} = 0.13 \] (Stable)
Two-phase simulations with $\theta_{ow} = 20^\circ$ (Jettestuen et al., WRR 2013)

- Primary drainage:
  - $C_{ow} = 0.50$
  - $C_{ow} = 0.60$
  - $C_{ow} = 0.70$

- Imbibition:
  - $C_{ow} = 0.40$
  - $C_{ow} = 0.30$
  - $C_{ow} = 0.25$

- Non-wetting phase retracts to larger pore openings after growth of wetting-phase films has led to snap-off in pore-throat constrictions
3-Phase Gas and Water Invasion

› **Gas invasion:**

- Water
- Oil
- Gas

Trapped water

\[ S_{wi} = 0.13 \]

**Simultaneous Gas & Water (SWAG) invasion:**

- Water cusp growth at gas/oil interface
- Water snap-off on gas/oil interface
- 2-phase snap-off
- Disconnected oil

\[ S_{wi} = 0.06 \]
3-Phase vs. 2-phase Capillary Pressure Curves (Water-wet case)

Gas/Oil capillary pressure:

\[ P_{cgo} \] increases with \( S_{wi} \):
- Gas prefer to displace oil
- Water blocks pathways for gas/oil displacement

Oil/water capillary pressure:

\[ P_{cow} \] can be higher in presence of gas:
- Water snap-off on gas/oil interfaces occurs at higher \( P_{cow} \) than water snap-off of oil (2-phase).
Mixed Wettability

› **2-phase water invasion:**

Water-filled, water-wet «porous plate» at water inlet (blue dots).

› **3-phase SWAG invasion:**

Oil cusps at gas/water interfaces

Trapped gas in big pores surrounded by oil cusps & water
3-Phase vs. 2-phase Capillary Pressure Curves
(«Mixed- to Oil-wet» case)

$P_{cgo}$-curves:

$P_{cow}$-curves:

$P_{cgw}$-curves:

Water displaces gas, with oil cusps/films present.

2- and 3-phase curves are similar for high oil saturations.

$P_{cgw}$(3-phase) → $P_{cgw}$(2-phase) as $P_{cgo}$ increases and $P_{cow}$ decreases (oil saturation decreases)
Gas invasion into a water-wet sphere-pack pore throat
Simulated entry pressure agree with analytic solution (MS-P/Purcell)
Need for Adaptive Grid Refinement

Oil layers vanish and triple lines form during gas invasion.
Error (MS-P/Purcell) < 2 %.

Oil layers exist after gas invasion
Error (MS-P/Purcell) < 3.9 %.
Thickness of water ring depends on which fluid it contacts.
Volume-preserving motion of isolated ganglia

- Capillary trapping (2- and 3-phase flow)
- Double and multiple displacement events (3-phase flow)
  - Example: Gas $\rightarrow$ disconnected oil $\rightarrow$ water
- The pressure of the preserved phase volume is calculated as

$$p_i = \frac{V_i^{target} - V_i^n}{\Delta t A_i^n}$$

where:

- $V_i^{target}$ = Initial or desired volume of phase $i$
- $V_i^n$ = Volume of phase $i$ in time iteration $n$
- $A_i^n$ = Surface area of phase $i$ in time iteration $n$
- $\Delta t$ = Time step

- The $p_i$-term grows or shrinks phase $i$ equally around its boundary

(Saye & Sethian, PNAS, 2011)
Volume-preserving motion - Validation

Tests of «oil-volume targeting» in right-angled triangle

- Analytic solutions (dashed curves)
- Error scales linearly with grid spacing,
  \[ \delta A \sim \Delta x: \]
  \[
  \delta A = \frac{1}{2} \sum_{i=g,o,w} \int_{\Omega} \frac{H(\psi)|H(\phi_{i,\text{true}}) - H(\phi_i)|}{L_i} \, dV
  \]

\[ \theta_{go} > \theta_{ow} \]

\[ \theta_{go} < \theta_{ow} \]
Volume-preserving motion – Sinusoidal Pore

› Double displacement (Gas $\rightarrow$ isolated oil $\rightarrow$ water):
› Oil-wet condition
› Behavior between 2 stable configurations
Volume-preserving motion – Sinusoidal Pore

Triple lines & gas/water interface form
Volume-preserving motion – Sinusoidal Pore

![Diagram showing sinusoidal pore with labeled phases: Gas, Oil, Water.](image-url)
Volume-preserving motion – Sinusoidal Pore

Gas retracts in corners behind the front.
Volume-preserving motion – Sinusoidal Pore
Volume-preserving motion – Sinusoidal Pore

Gas invades corners behind the front.

Diagram showing the movement of gas, oil, and water in a sinusoidal pore.
Volume-preserving motion – Sinusoidal Pore

Gas retracts in corners behind the front.

Oil snap-off on gas/water interface
Volume-preserving motion – Sinusoidal Pore
Volume-preserving motion – Sinusoidal Pore

Gas invades the corners when the front is at narrow constriction.
Volume-preserving motion – Sinusoidal Pore
Volume-preserving motion – Sinusoidal Pore
Volume-preserving motion – Sinusoidal Pore

Gas

Water

Oil
Volume-preserving motion – Sinusoidal Pore
Volume-preserving motion – Sinusoidal Pore

Stable configuration
Volume-preserving motion – Sinusoidal Pore

› 4 simulations (oil-wet and water-wet cases with two different oil volumes)
› Relative volume error is less than 0.2% during the processes
Volume-preserving motion – Sinusoidal Pore

› Significant oil pressure fluctuations as oil moves through narrow and wide regions

› Assuming $\Delta x = 1 \mu m$, $P_{cgo}$ and $P_{cow}$ varies with up to 2 kPa during displacement for water-wet case, and a little bit less for the oil-wet case.
Volume-preserving motion – Sinusoidal Pore

Gas/water capillary pressure is smaller with disconnected oil present between gas and water:

\[ P_{\text{water}} \text{ (Pa)} \]

\[ S_o \to 0 \]

Water-wet case

\[ P_{\text{gas-water}} \text{ (Pa)} \]

\[ S_o \to 0 \]

Oil-wet case
Volume-preserving motion in 3D rocks

› Mechanism for mobilizing isolated oil in water-wet rock
› Onset of double displacement (water $\rightarrow$ isolated oil $\rightarrow$ gas) by water snap-off at gas/oil interface. Oil volume error < 2%.
Volume-preserving motion in 3D rocks

› Oil invasion in oil-wet rock and preservation of the gas phase

› Oil surrounds gas due to oil snap-off on gas/water interfaces and gas becomes capillary trapped. Gas volume error < 1.5%.
2-phase pore-scale experiments in literature

(Andrew, Blunt et al., TIPM 2015)

› Drainage in Limestone at reservoir conditions (50°C & 10MPa), imaged by x-ray μ-CT
› Water withdrawn at low, constant rate
› Capillary number $\sim 10^{-11}$

Observations in drainage:
• Haines jumps with co-operative behavior
• Capillary pressure before Haines jump (time $t_1$) is higher than after (time $t_2$)
• Snap-off events can lead to temporarily isolated NWP droplets
• Interfaces vibrate when they are close to critical events

Imbibition:
• Ganglion dynamics, etc...

Do we need to include viscous forces to describe this multiphase behavior at the pore scale?
Are these observations just a consequence of constant rate?
Can «Volume-Targeting» simulation describe this multiphase behaviour? Yes (at least qualitatively)!

› Approach: Take saturations as input and calculate phase pressures (instead of specifying pressure and calculate saturation)

We assume $\Delta S_o = 0.05$

- NWP at $S_o$
- NWP at $S_o + \Delta S_o$

For drainage, we observe:
- Haines jumps with co-operative behavior (local imbibition) that results in temporarily smaller capillary pressure
- Interfaces vibrate until target volume is reached accurately
Adaptive Mesh Refinement (AMR) & Parallelization

› Needed for accurate calculations on big domains (heterogeneous chalk)

› We will implement AMR & parallelism by coupling our codes to R&D AMR library SAMRAI (developed at LLNL)

› Parallel computations on Notur HPC facilities
Status and Capabilities Multiphase LS Method

- Quasi-static capillary-dominated displacement at uniform or mixed wettability (for 2 and 3 phases)
- Drainage & imbibition processes (invasion of gas, water or oil)
- Transition from 3- to 2-phase flow
- Motion of wetting-phase cusps and triple lines are captured very well
- Oil layers are modelled accurately if grid resolution is sufficiently fine
- Continuous validation by comparing simulations with analytic solutions on idealized pore geometries.
- Global phase volume preservation
The work plans

First priority:
› Finish AMR & parallelization
› Finish implementation of local volume preservation:
  • Volume preservation of individual drops that can merge or break

Then:
› Start simulations on big domains
  • Priority: 1. chalk; 2. bead pack; 3. sandstone
  • 2-phase motion first, 3-phase motion afterwards
  • Relative permeability
› Add compressibility (gas) to volume preservation approach, using EoS
› Introduce gas by depressurization (model gas bubble nucleation)
› Relate water chemistry to changes in wettability

2 December 2015
Conclusions

› Multiphase Level Set simulations give increased insight into the pore-scale mechanisms that explain differences and similarities between 2- and 3-phase capillary pressure curves.

› Water-wet conditions:
  • Gas/oil capillary pressure increases with Swi, as water blocks gas/oil displacement paths.
  • Imbibition oil/water capillary pressure curves differ because «3-phase water snap-off» on gas/oil interfaces occurs at a higher oil/water capillary pressure than standard 2-phase snap-off events.

› «Mixed- to oil-wet» conditions:
  • Similar 2- & 3-phase capillary pressure curves for small gas & water saturations.
  • Gas is trapped by oil cusps and water in big pores (not narrow throats), but the amount of trapped gas and its location seems to depend on Swi.
Conclusions

Multiphase Level Set simulations with volume preservation (3 phases) or «volume targeting» (2 phases) show «dynamic» behavior:

- Haines jumps with co-operative behavior due to limited phase availability
- Non-monotonic capillary pressure changes

Double displacements must be viewed together with snap-off mechanisms:

- Snap-off can represent the onset of double displacements (for mobilizing oil)
- Snap-off can also trap the disconnected fluid permanently
- Pressure oscillations and temporary snap-off events can occur as the disconnected fluid moves through narrow and wide pore regions
- Presence of disconnected oil decreases the gas/water capillary pressure during gas invasion
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