



SOCIETY OF
CORE ANALYSTS

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Short Course

Interpretation of Pore Scale Experiments - Alternative Descriptions of Porous Media Flow by Topological Means

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Imperial College
London

With key contributions from

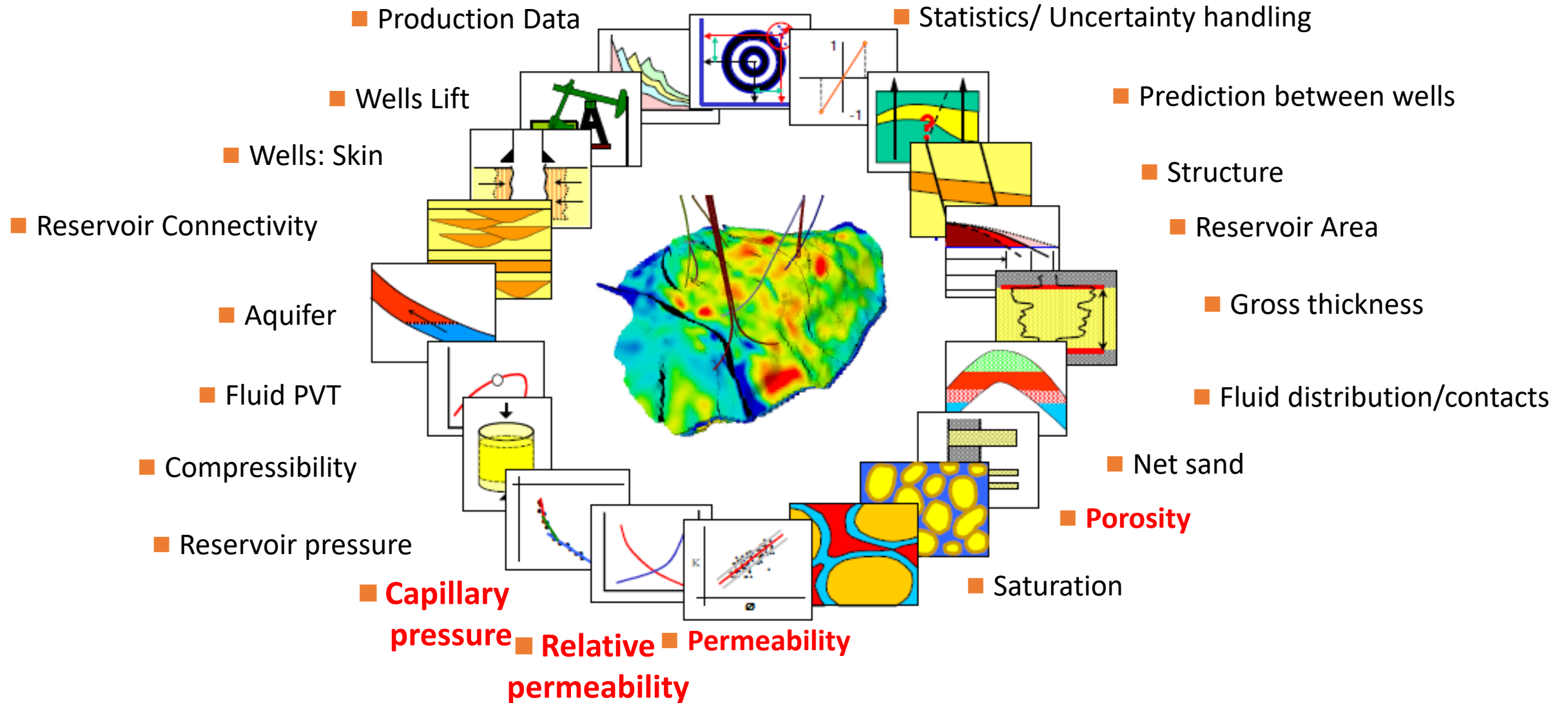
James McClure (Virginia Tech), **Steffen Schlüter** (UFZ Potsdam), **Anna Herring** (ANU), **Christoph Arns** (UNSW)



Outline

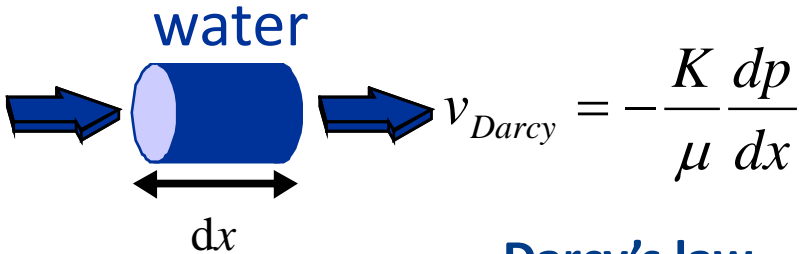
1. Motivation / necessity for and advantages of a geometric state function
 - 2-phase Darcy = phenomenological extension from 1-phase to 2-phase flow
 - example of having incomplete state variables: ideal gas equation of state
2. Introduction:
 - introducing Minkowski functionals
 - Hadwiger's theorem, Gauss-Bonnet Theorem, Steiner's formula
3. Description how we found it
 - general background: ganglion dynamics → topological changes
 - beamline data of 2013 experiment: → Hysteresis in Euler characteristic χ
 - proof: (1) Hadwiger's theorem, (2) 220000 LBM simulations
4. Software: Avizo, FIJI (BoneJ plugin), Matlab, Python, Dragonfly/DeepRocks
5. Applications,
 - hysteresis model for relative permeability
 - new route to pc and relative permeability
 - Digital Rock: validation of pore scale simulation techniques
 - wettability: description of contact angle as deficit curvature

Integrated Subsurface Workflow



Multiphase Flow in Porous Media at Darcy Scale

Single-Phase

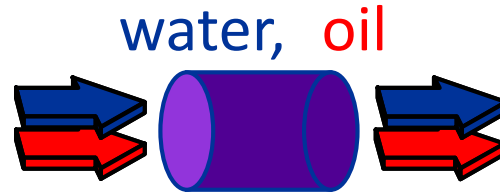


Darcy's law

μ viscosity
 P pressure
 K (K_{abs}) absolute permeability

Viscous law (similar to pipe flow) can be derived from upscaling Stokes flow at pore scale by homogenization

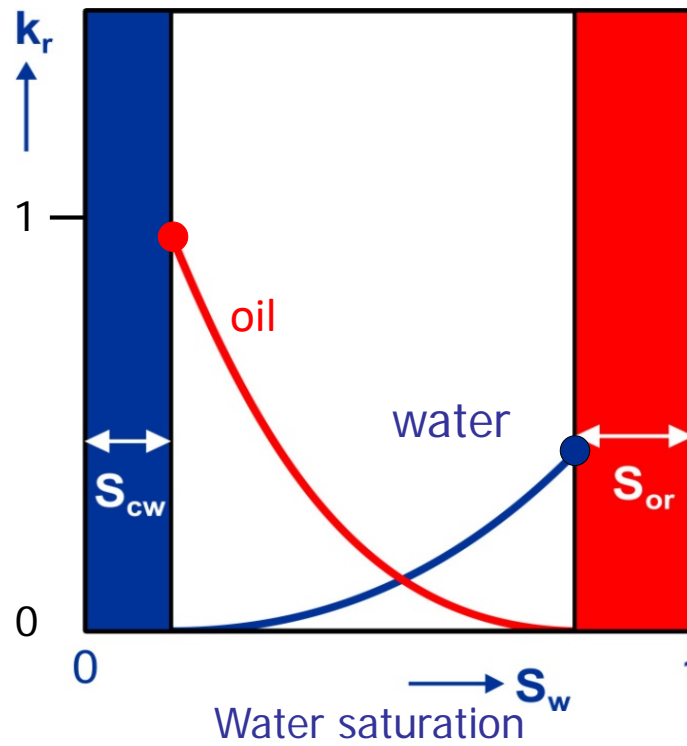
Two-Phase



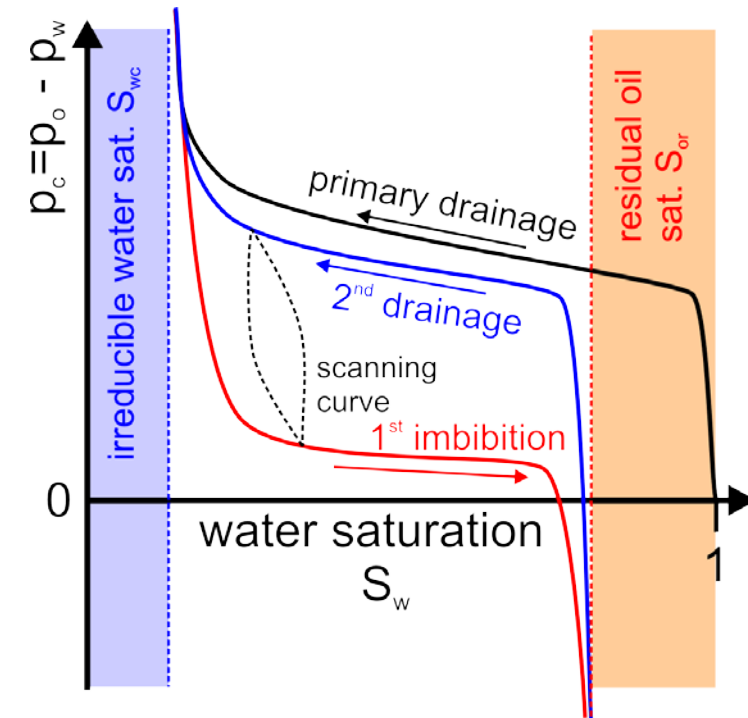
$i=W,O$

Phenomenological extension of Darcy's law

relative permeability $k_{r,i} = k_{r,i}(S_w)$

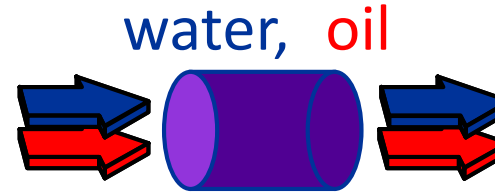


Capillary pressure $p_c = p_o - p_w$



Historical Overview – Classification of the Problem

- 1930s: **flow problem**: mass & momentum balance
(Wykoff & Botset, Muskat & Meres, Leverett)

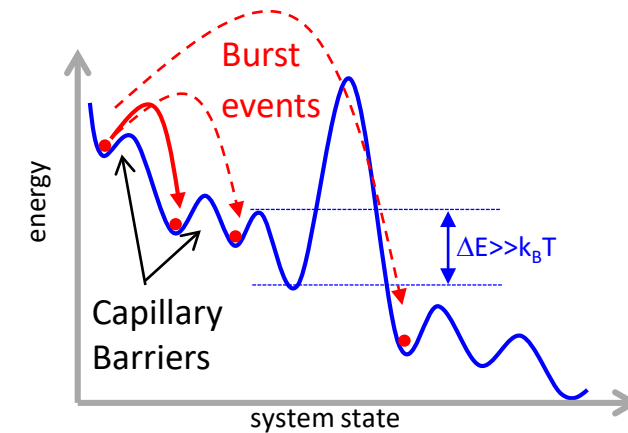


- 1970s: thermodynamics of pore scale displacements
(Morrow, Swanson & Yuan)

$$\Delta F = -S\Delta T - \sum_{\alpha=1}^2 p_{\alpha} \Delta V_{\alpha} + \sigma_{1,2} \Delta A_{1,2}$$

Morrow 1970

- 1990s: **equilibrium thermodynamics problem**:
mass, momentum & energy balance (Hassanizadeh & Gray)
ganglion dynamics in 2D micromodels (Avraam & Payatakes)



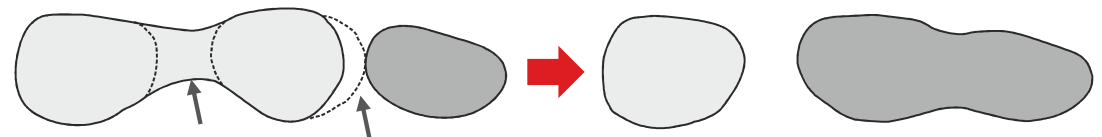
- 2000s: **non-equilibrium thermodynamic problem** – no global energy minimum
TCAT (Gray & Miller)

- 2010s: **non-local dynamics**, ganglion dynamics in 3D

$S_w + A_{nw}$ does not close pc hysteresis

Armstrong, McClure et al. 2018

- 2018: **state variables**: S_w, A_{nw}, p_c, χ

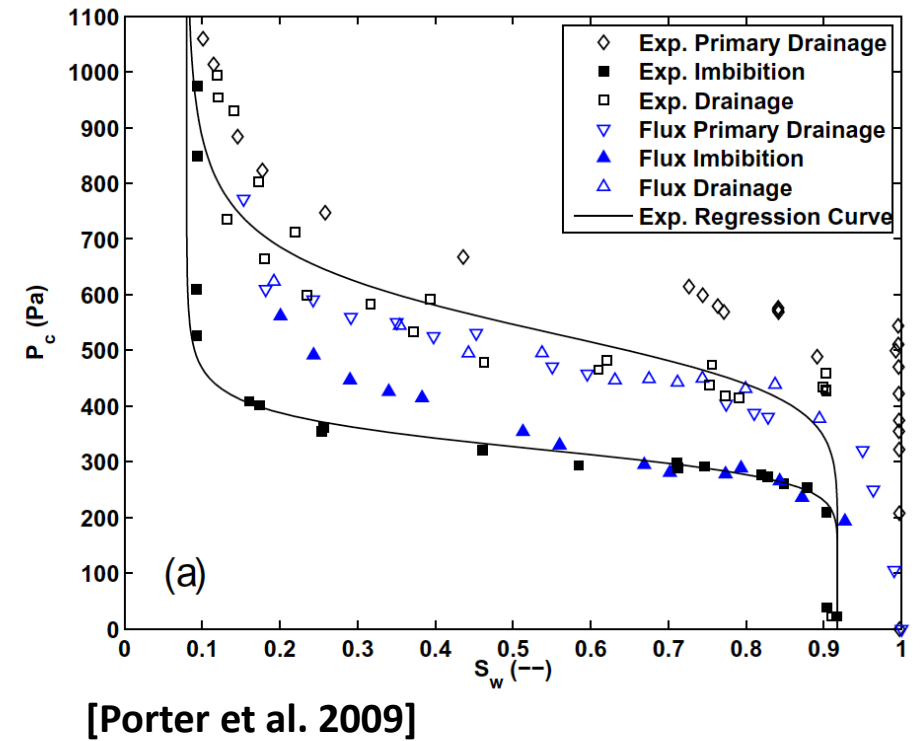
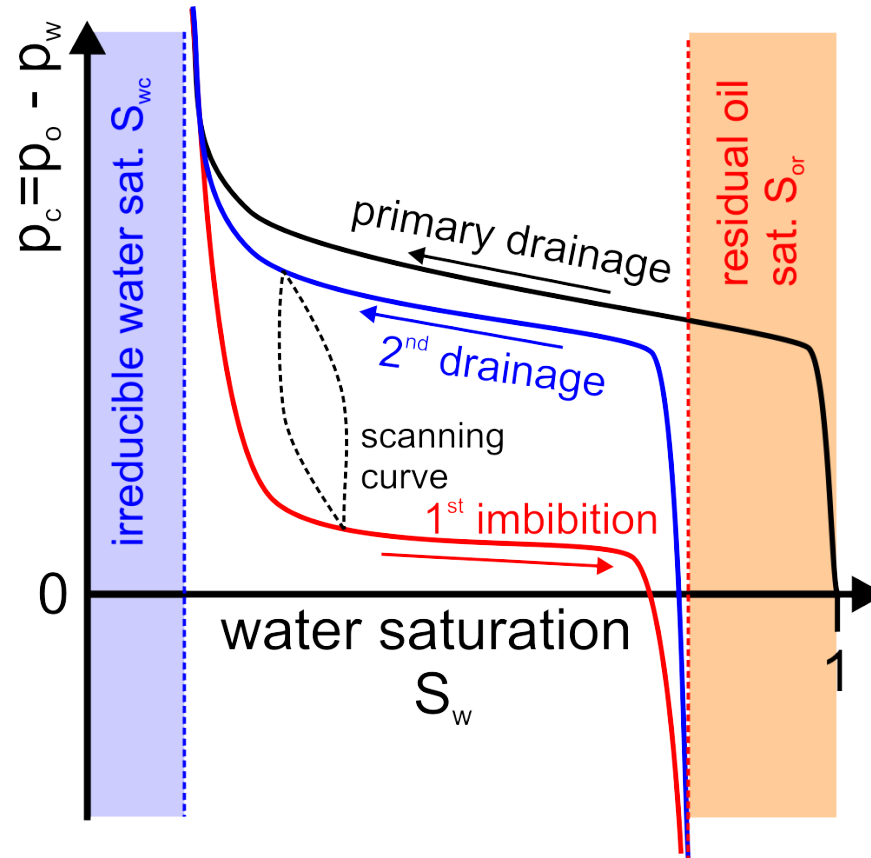


- 2019: **wettability** (upscaled contact angle as deficit Gaussian curvature)

Unresolved Issue: Capillary Pressure - Hysteresis

Capillary pressure function of saturation only $P_{nw} - P_w = P_c = f(S_w)$

But: hysteresis



Hysteresis challenges the validity of 2-phase Darcy. But is it really hysteresis ?

What constitutive relationships properly represent multiphase flow?

Consequence of Insufficient Number of State Variables

Example: ideal gas, equation of state

$$p \cdot V = nRT$$

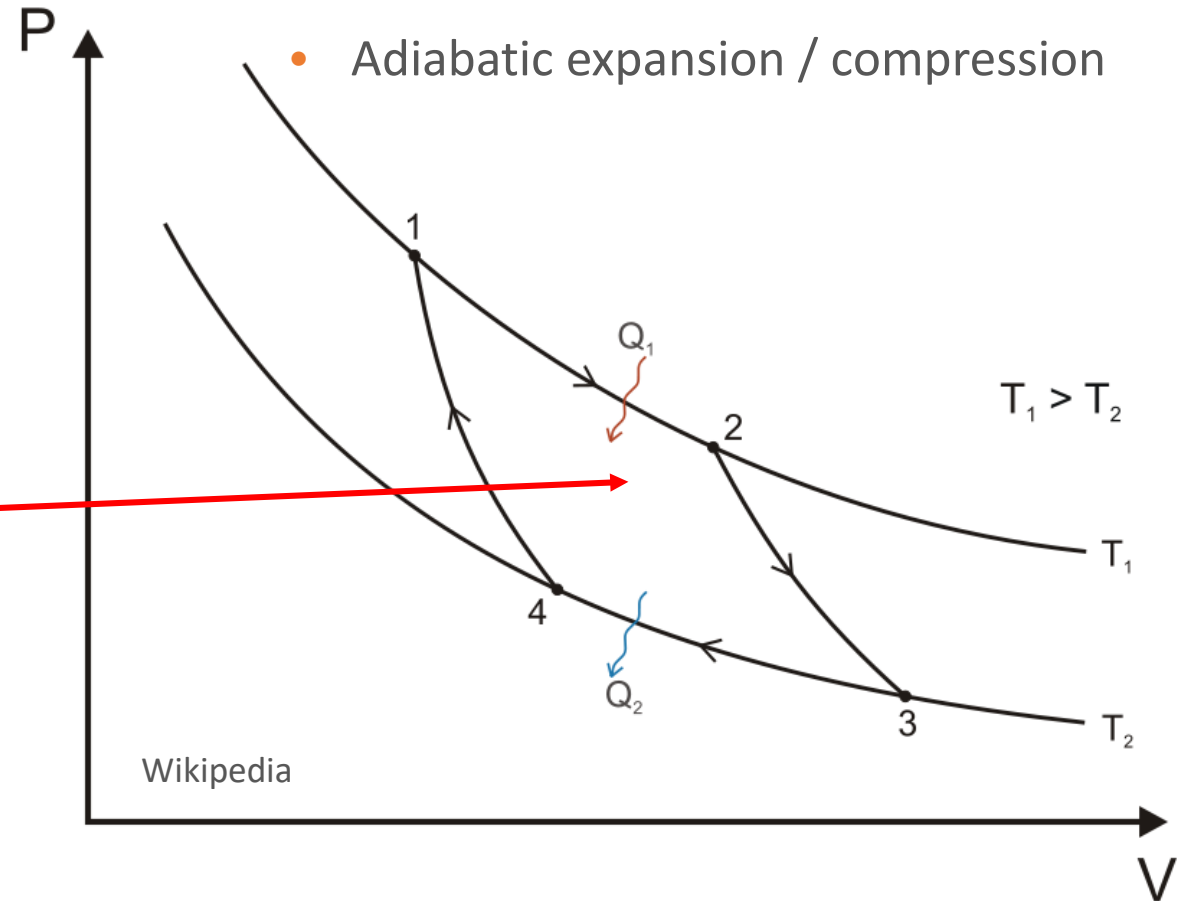
Imagine we did not know about Temperature ...
and only do P – V experiments,
without measuring or controlling T ...

Apparent
hysteresis

But with correct number of state variables, p , V , T ,
there is no hysteresis (for an ideal gas).

Carnot cycle

- Isothermal expansion / compression
- Adiabatic expansion / compression



Saturation S_w and Interfacial Area A_{nw} are State Variables of P_c

Pressure-
volume
work Interfacial
Energy
term

$$\Delta F = -S\Delta T - \sum_{\alpha=1}^2 p_{\alpha} \Delta V_{\alpha} + \sigma_{1,2} \Delta A_{1,2}$$

Thermodynamics: free energy

Morrow, 1970

4 Minkowski Functionals

m_0 = volume (saturation

m_1 = interfacial area

m_2 = mean curvature

m_3 = Gauss curvature = $2\pi\chi$

$$M_0^n = \lambda(\Omega_n) = \int_{\Omega_n} dr$$

$$M_1^n = \lambda(\Gamma_n) = \int_{\Gamma_n} dr$$

$$M_2^n = \int_{\Gamma_n} \left(\frac{1}{R_1} + \frac{1}{R_2} \right) dr$$

$$M_3^n = \int_{\Gamma_n} \frac{1}{R_1 R_2} dr$$

But that did not close
the capillary hysteresis
(McClure, Gray, Miller ...)

This term was not included in the traditional theories

The Source of Capillary Pressure Hysteresis

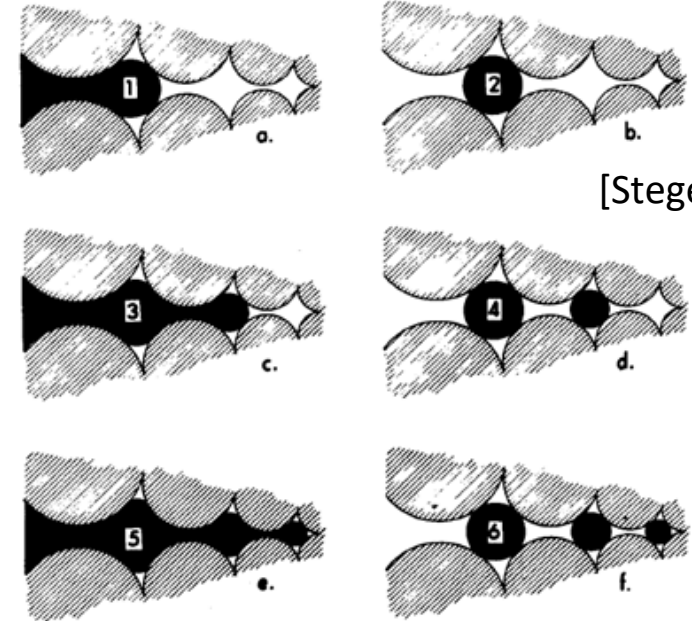
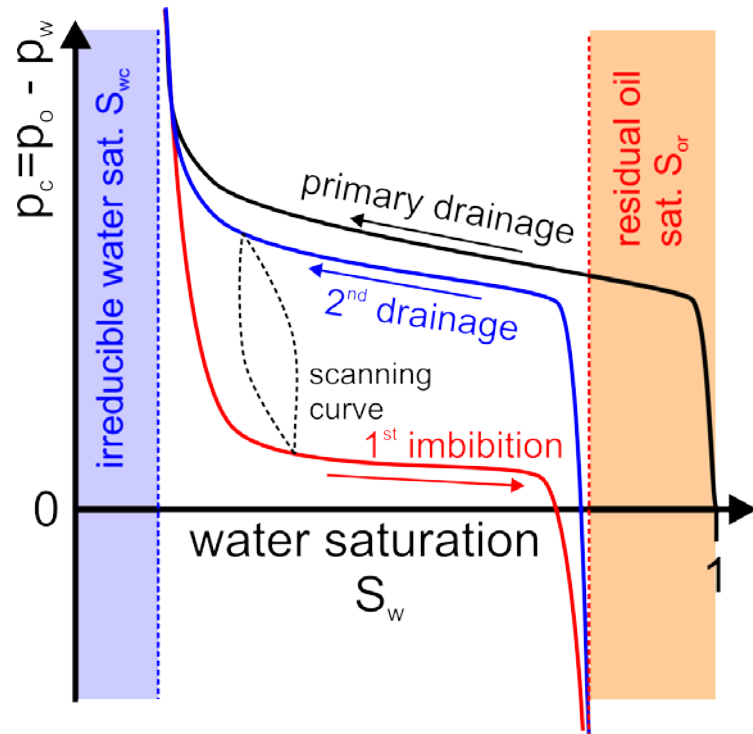
Darcy Scale

Pore Scale

Macroscopic Darcy-scale
"saturation functions"

=

f(pore scale fluid distribution)



[Stegemeier 1977]

= geometrical shape in 3D

The Source of Capillary Pressure Hysteresis

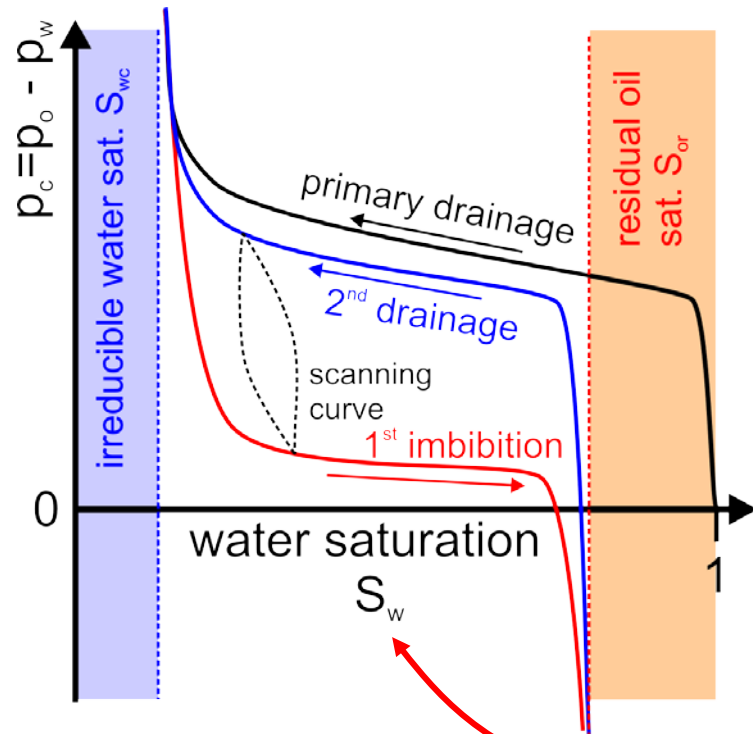
Darcy Scale

Pore Scale

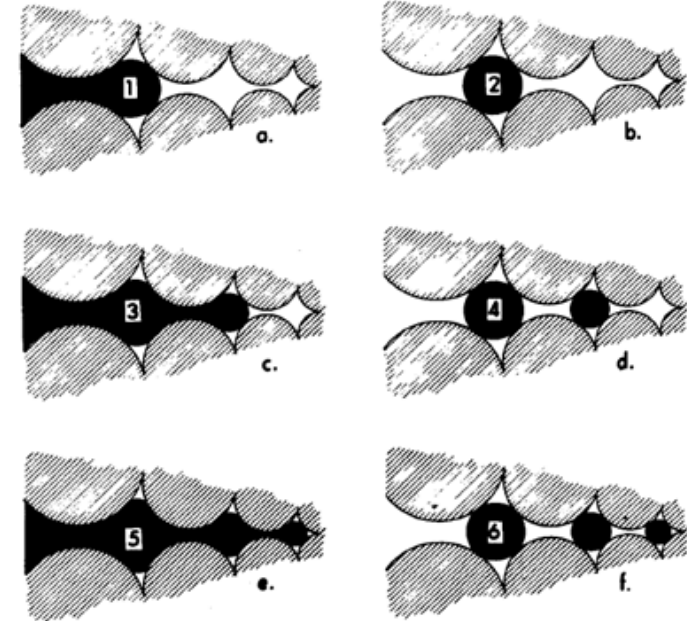
Macroscopic Darcy-scale
"saturation functions"

=

f(pore scale fluid distribution)



state
variables



= geometrical shape in 3D

Hadwiger's Theorem:
Uniquely parameterized by 4 Minkowski Functionals

The Minkowski Functionals

→ Apply to Multiphase Flow

Named after **Hermann Minkowski**, Mathematician (1864-1909)

Herring et al. Advances in Water Resources 62, 47-58, 2013.

McClure et al. Phys. Rev. Fluids, 2018

Integral Geometry

Hadwiger's theorem: unique characterization of 3D objects by 4 Minkowski functionals

m_0 = volume (saturation)

m_1 = interfacial area

m_2 = mean curvature (cap. pressure)

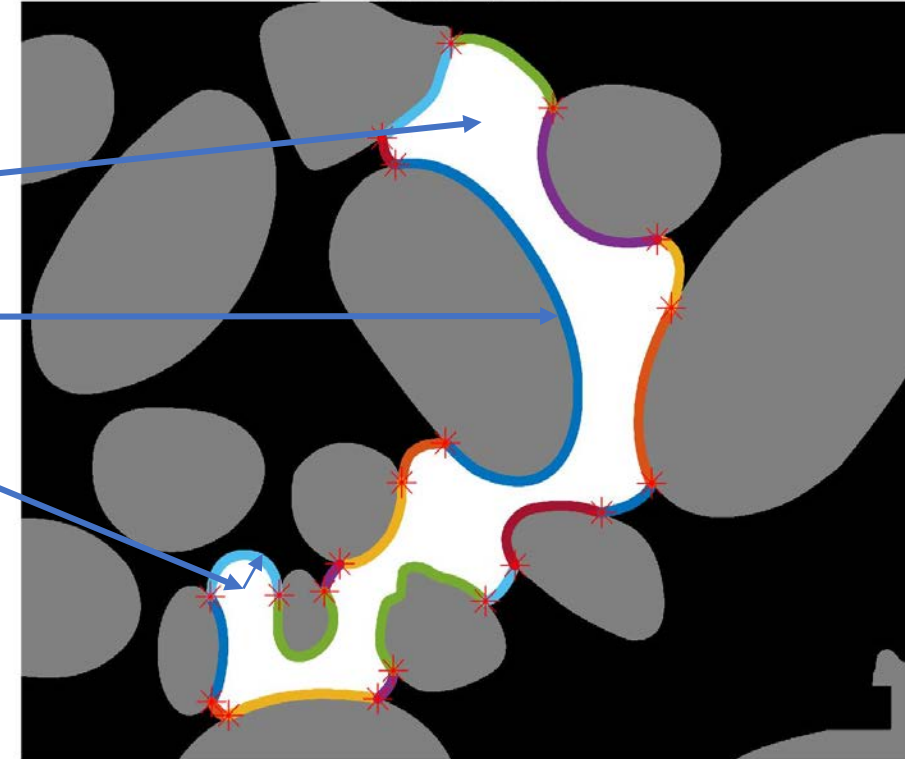
m_3 = integral curvature = $2\pi\chi$

$$M_0^n = \lambda(\Omega_n) = \int_{\Omega_n} dr$$

$$M_1^n = \lambda(\Gamma_n) = \int_{\Gamma_n} dr$$

$$M_2^n = \int_{\Gamma_n} \left(\frac{1}{R_1} + \frac{1}{R_2} \right) dr$$

$$M_3^n = \int_{\Gamma_n} \frac{1}{R_1 R_2} dr .$$



Klaus R. Mecke, Dietrich Stoyan, Statistical Physics and Spatial Statistics. The Art of Analyzing and Modeling Spatial Structures and Pattern Formation, Lecture Notes in Physics, Springer, 2000.

C. H. Arns, M. A. Knackstedt, K. Mecke, 3D Structural Analysis: Sensitivity of Minkowski Functionals. Journal of Microscopy 240, 181-196, 2010.

H.J. Vogel, U. Weller, S. Schlüter, Quantification of Soil Structure Based on Minkowski Functions, Computers & Geosciences 36, 126-1251, 2010.

The Euler Characteristic

Named after **Leonhard Euler**, German Mathematician (1707-1783)

$$M_3(X) = \int_{\delta X} \underbrace{[1/(r_1 r_2)]}_{\text{Gaussian curvature}} ds = 2\pi \chi(\delta X) = 4\pi \chi(X)$$

$$\frac{1}{r_1} + \frac{1}{r_2} \quad \text{mean curvature}$$

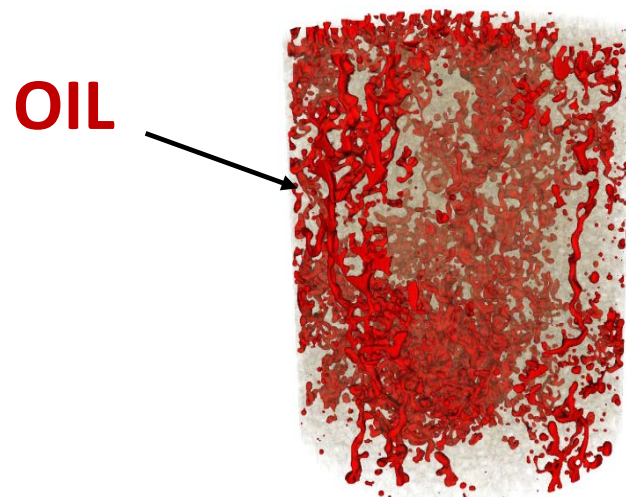
$$\frac{1}{r_1} \cdot \frac{1}{r_2} \quad \text{Gaussian curvature}$$

- Euler Characteristic measures the **bulk connectivity** of an object

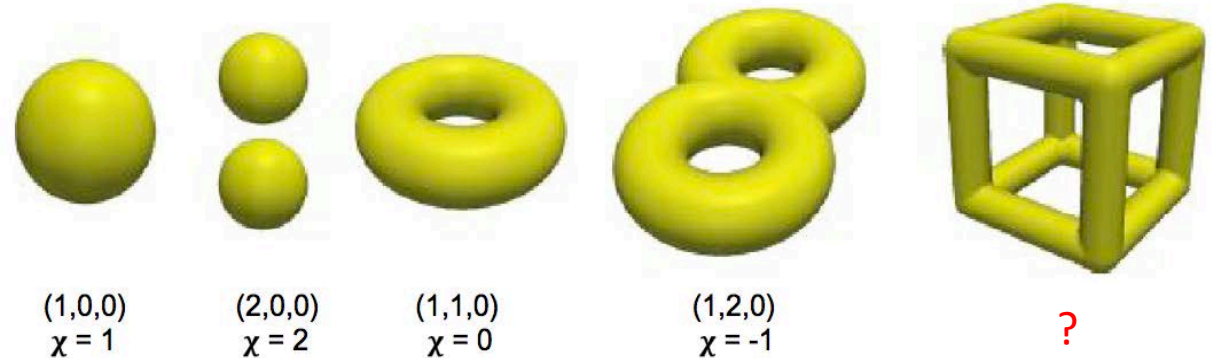
$$X = \text{Objects} - \text{Loops} + \text{Voids}$$

[Herring et al. 2012]

Or a collection of objects:

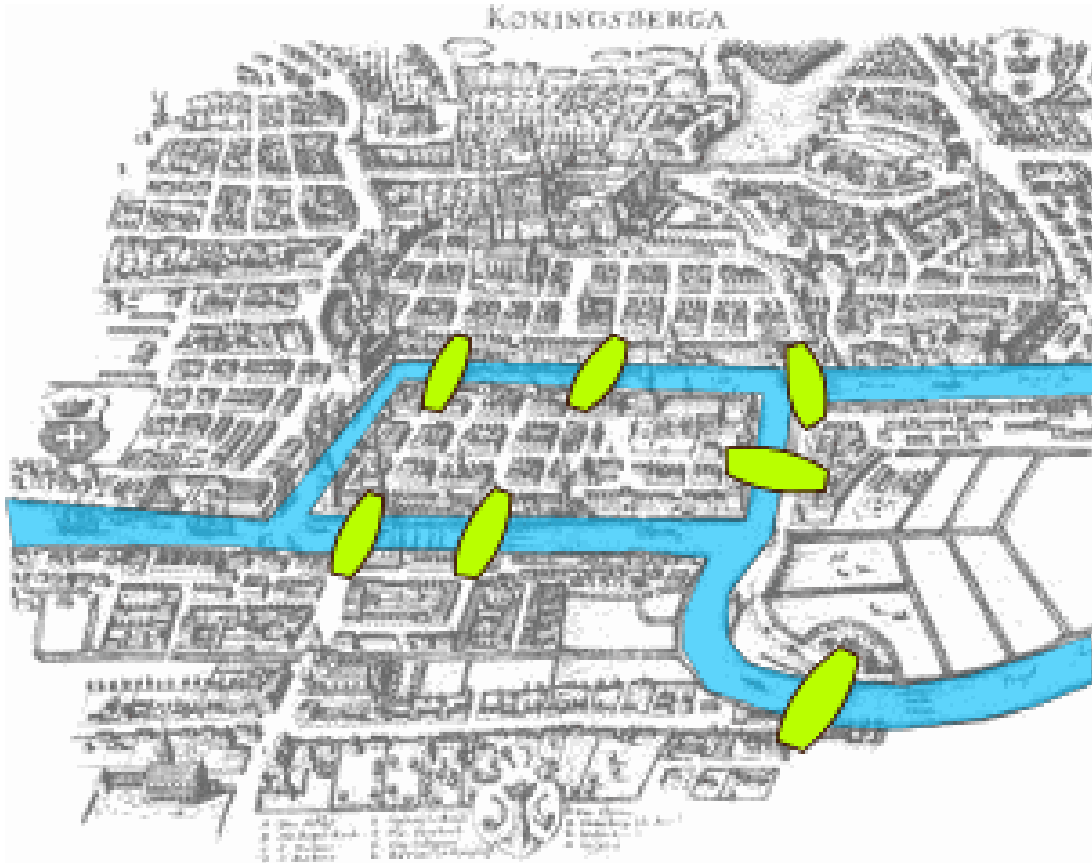


$$X(\text{OIL}) = -40$$



... a cube has 6 faces

Leonhard Euler and the Seven Bridges of Königsberg



2 islands
separated by a river
7 bridges

Walk to cross each bridge only once ?

L. Euler: not possible + proof

The city of [Königsberg](#) in [Prussia](#) (now [Kaliningrad](#), [Russia](#)) was set on both sides of the [Pregel River](#), and included two large islands - [Kneiphof](#) and [Lomse](#) - which were connected to each other, or to the two mainland portions of the city, by seven bridges. The problem was to devise a walk through the city that would cross each of those bridges once and only once (Source: Wikipedia)

https://en.wikipedia.org/wiki/Seven_Bridges_of_K%C3%B6nigsberg

The Euler Characteristic

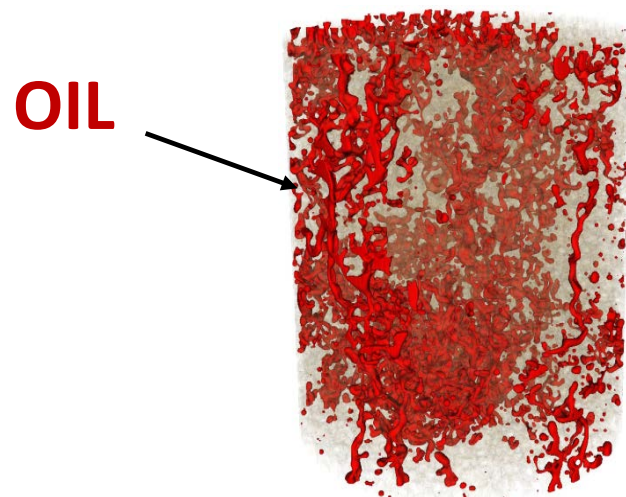
$$M_3(X) = \int_{\delta X} [1/(r_1 r_2)] ds = 2\pi\chi(\delta X) = 4\pi\chi(X)$$

- Euler Characteristic measures the **bulk connectivity** of an object

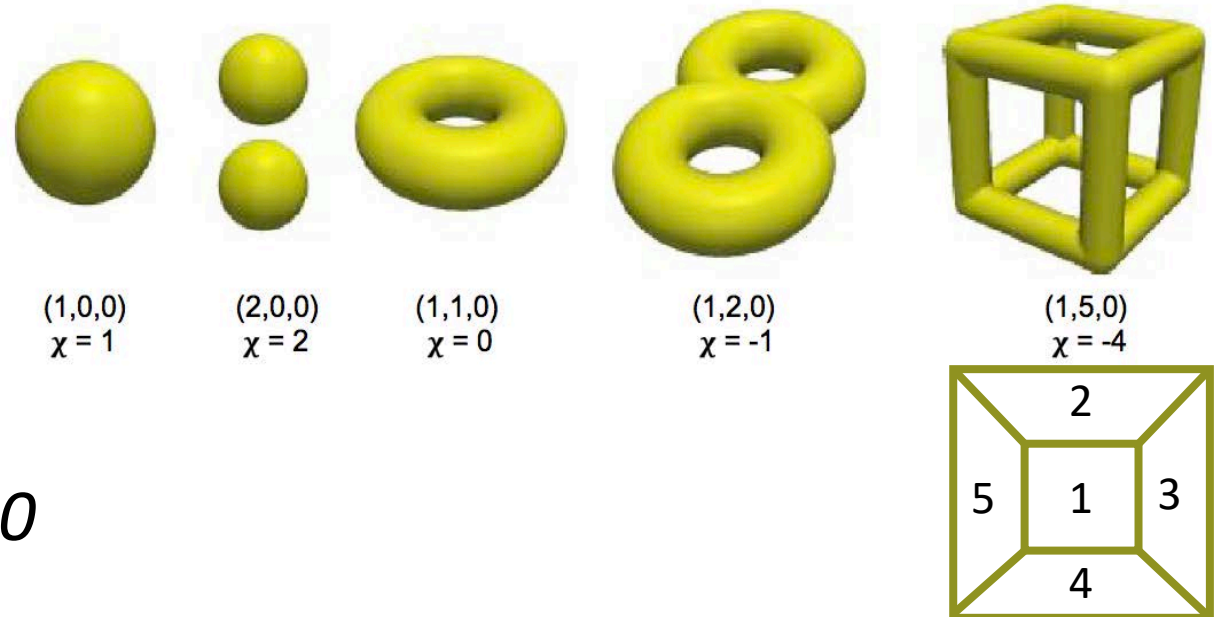
$$\chi = \text{Objects} - \text{Loops} + \text{Voids}$$

[Herring et al. 2012]

Or a collection of objects:



$$\chi(\text{OIL}) = -40$$



(1) Hadwiger's Theorem

A remarkable theorem is the ‘completeness’ of the Minkowski functionals proven 1957 by H. Hadwiger [21]. This *characterization theorem* asserts that any additive, motion-invariant and conditionally continuous functional \mathcal{M} is a linear combination of the $d + 1$ Minkowski functionals M_ν ,

$$\mathcal{M}(A) = \sum_{\nu=0}^d c_\nu M_\nu(A) \quad , \quad (7)$$

with real coefficients c_ν independent of A . Motion-invariance of the functional means that the functional \mathcal{M} does not depend on the location and orientation of the grain A . Since quite often the assumption of a homogeneous and isotropic system is made in physics, motion-invariance is not a very restrictive constraint on the functional. Nevertheless, in the case where external fields are applied

(2) Gauss-Bonnet Theorem

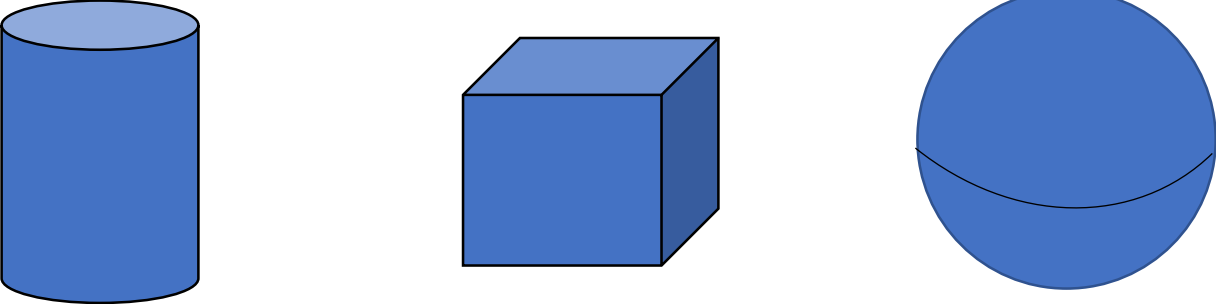
Explains the relationship between Gaussian curvature and topology.

Gaussian curvature

$$k_f = \left(\frac{1}{r_1} \cdot \frac{1}{r_2} \right)$$
$$\int_S [1/(r_1 r_2)] ds + \int_B k_g dl = 2\pi \chi(S)$$

$\chi(S) = 2$ $\chi(S) = 2$ $\chi(S) = 2$

$p_c(S_w) = \gamma \cdot \left(\frac{1}{r_1} + \frac{1}{r_2} \right)$
Mean curvature



The curvature is either on the **surface** (Gaussian Curvature) or at the **edges** (Geodesic Curvature)

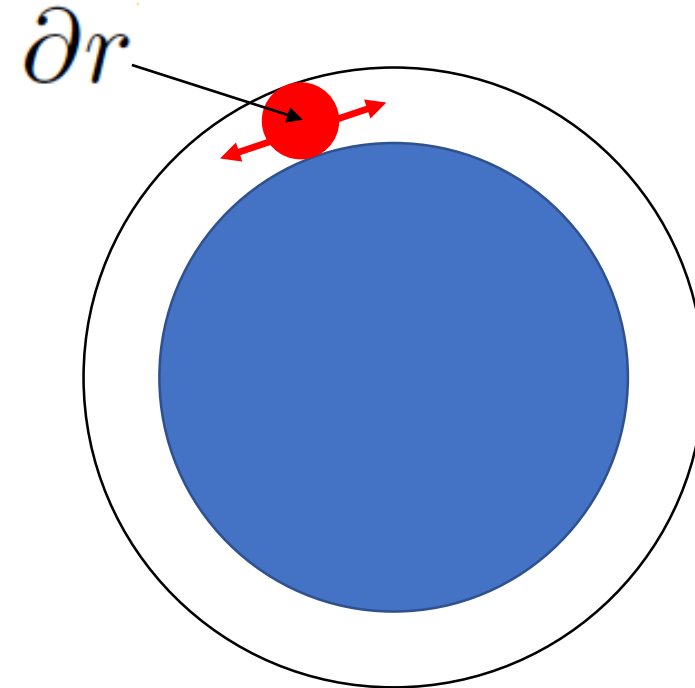
(3) Steiner's Formula

Provides a means to identify relationships between the Minkowski functionals

Volume

$$\lambda(X \oplus \partial r) - \lambda(X) = \sum_{i=1}^3 a_i M_i r^i$$

Explains how the volume (dependent) of an object changes depending on the objects morphology (independent)



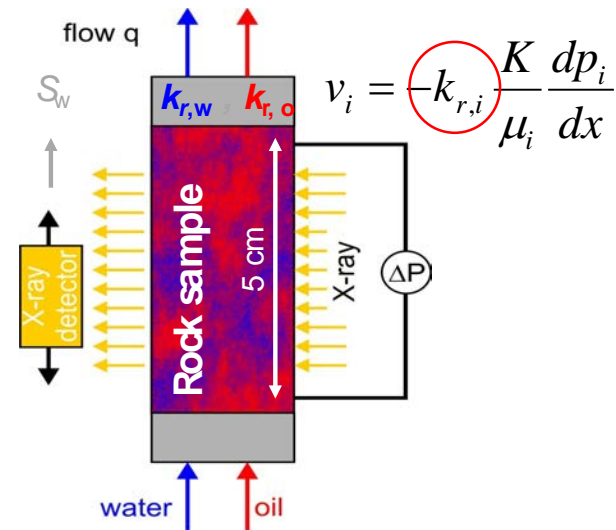
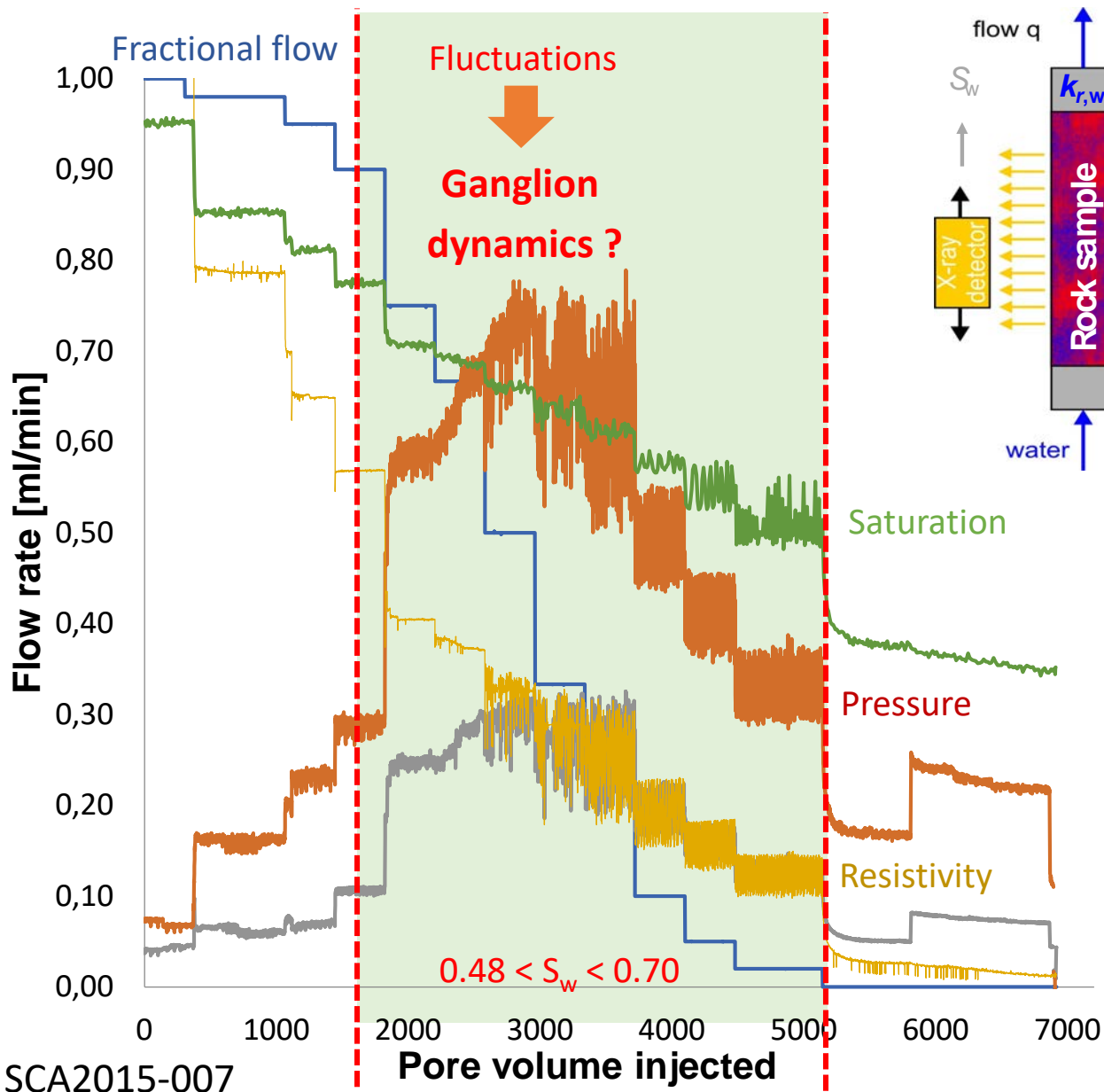
Example: sphere ...

$$V(\Omega_i \oplus \delta \zeta) - V(\Omega_i) = \frac{4}{3} \pi (r + \delta r)^2 - \frac{4}{3} \pi (r)^2 = A_i \delta r + H_i (\delta r)^2 + \frac{4}{3} \pi \chi_i (\delta r)^3$$

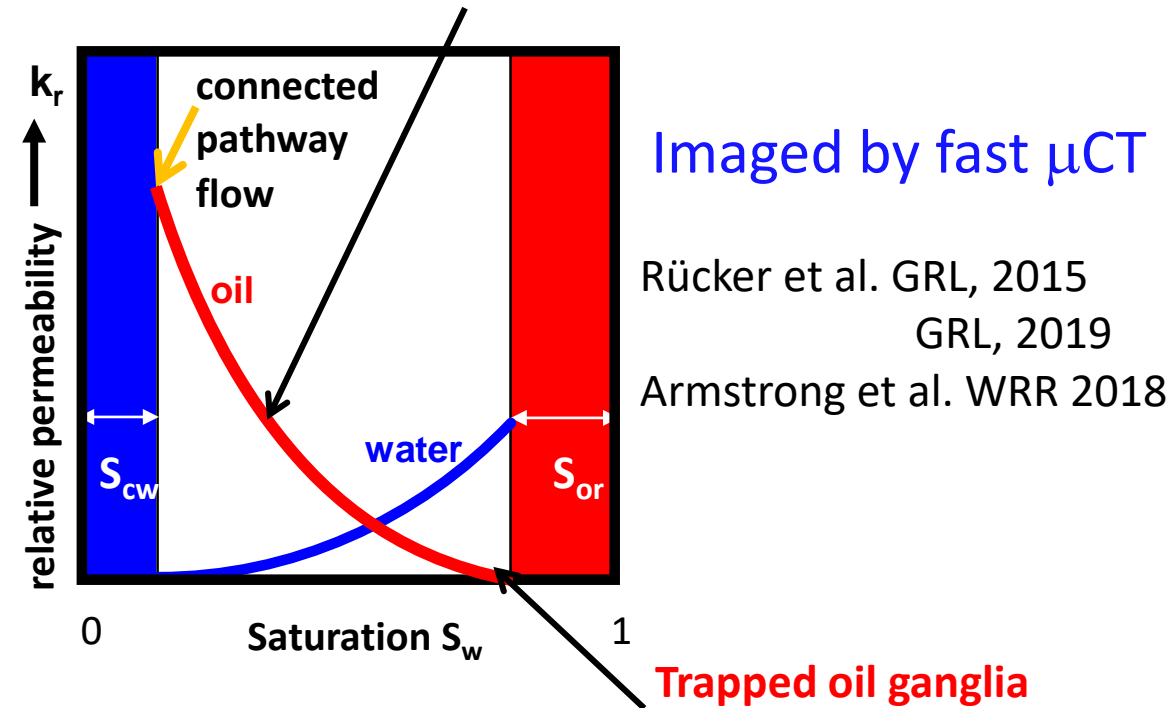
Mean width $H_i = \int_{\Gamma_i} \frac{\kappa_1 + \kappa_2}{2} dS$

$$\begin{aligned} A_i &= 4\pi r^2 \\ H_i &= 4\pi r \\ \chi_i &= 1 \end{aligned}$$

Background: Cluster Dynamics in SCAL Experiments

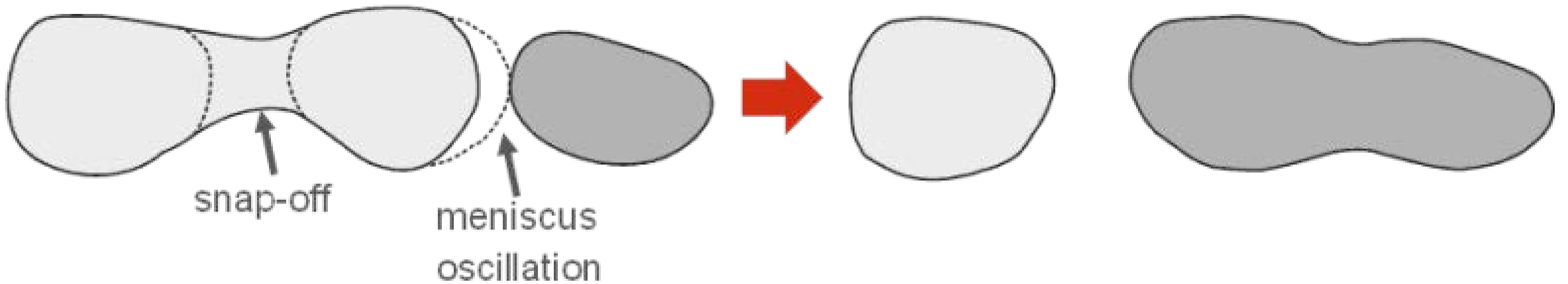


ganglion dynamics



Cluster Dynamics Introduces Topological Changes

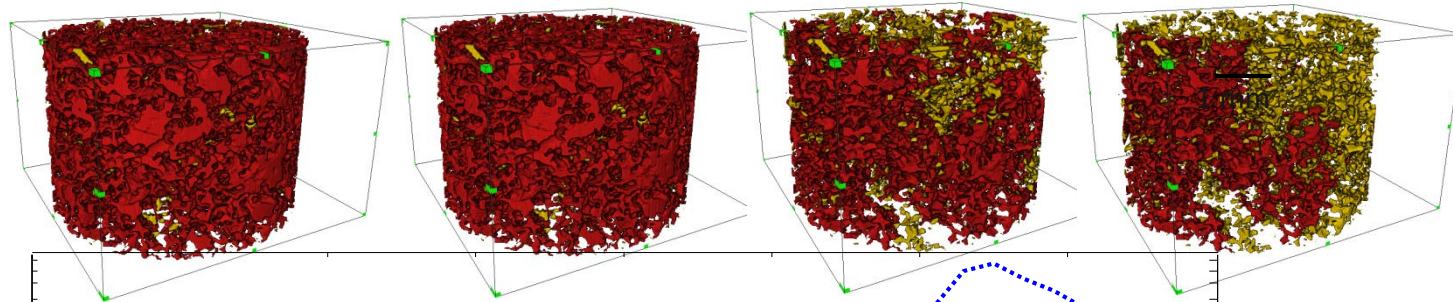
Strongly water-wet



Introduces Topological Changes

Cluster Dynamics Introduces Topological Changes

Rücker et al. GRL, 2015



$$\chi = \text{Objects} - \text{Loops} + \text{Voids}$$

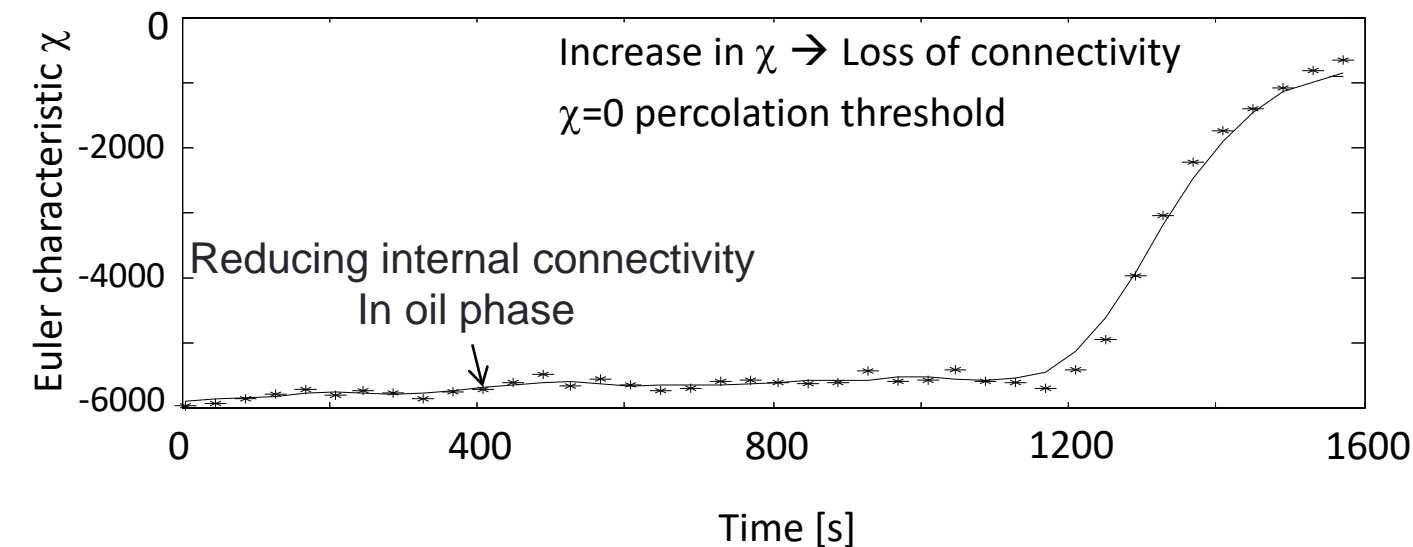
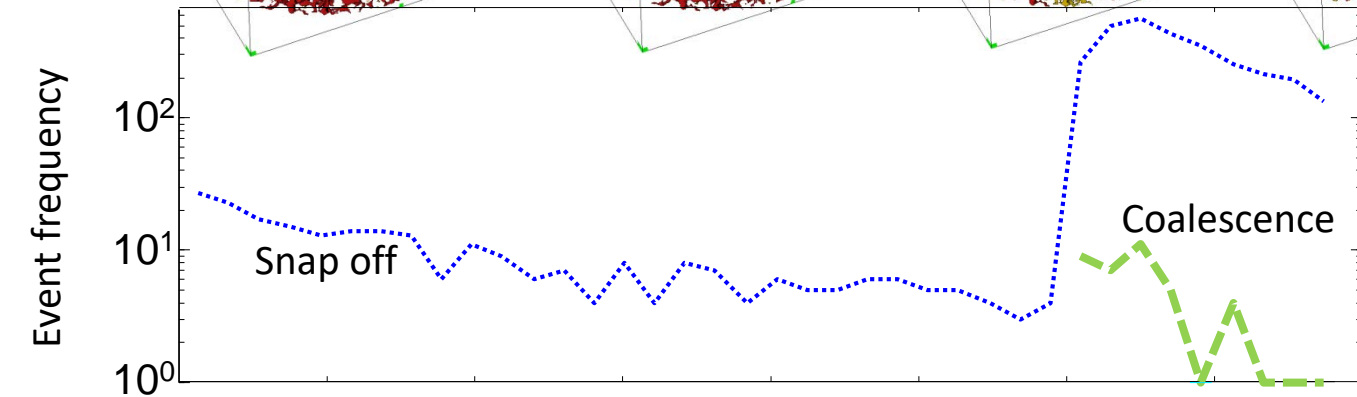
Snap-off

- disconnection
- #objects increases
- χ increases

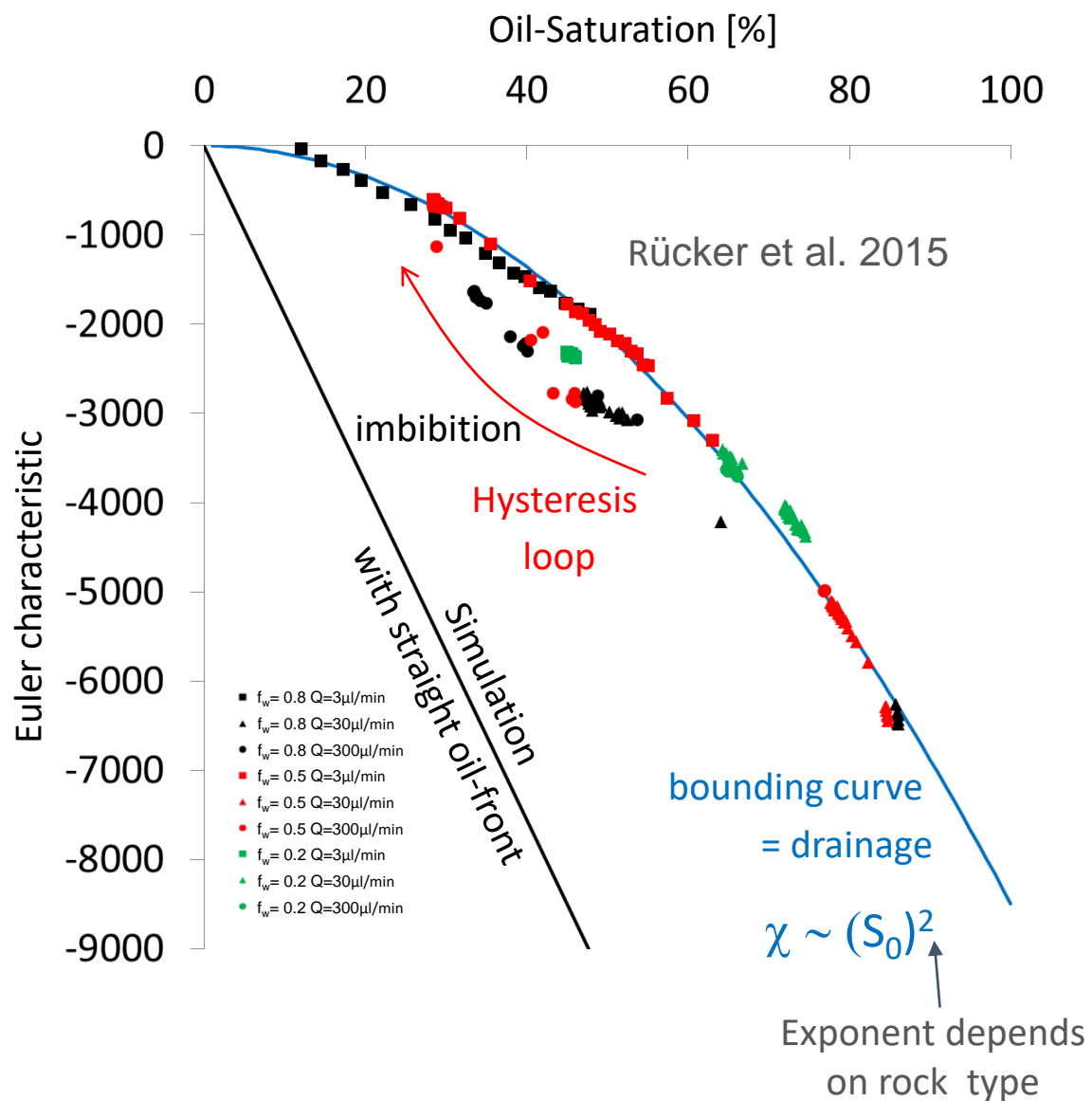
Coalescence

- connection
- #objects decreases
- χ decreases

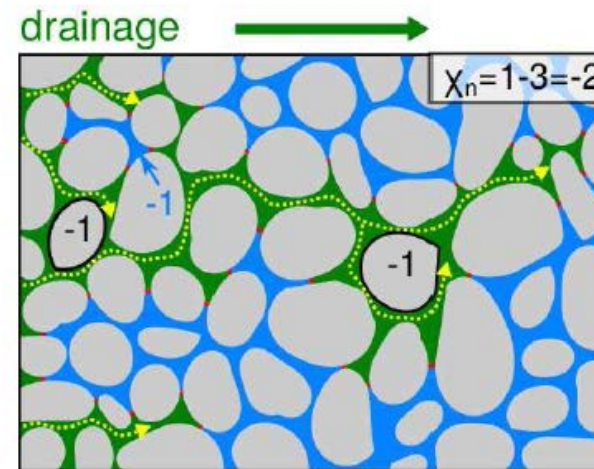
Here: #snap-off > #coalescence
→ net χ increase



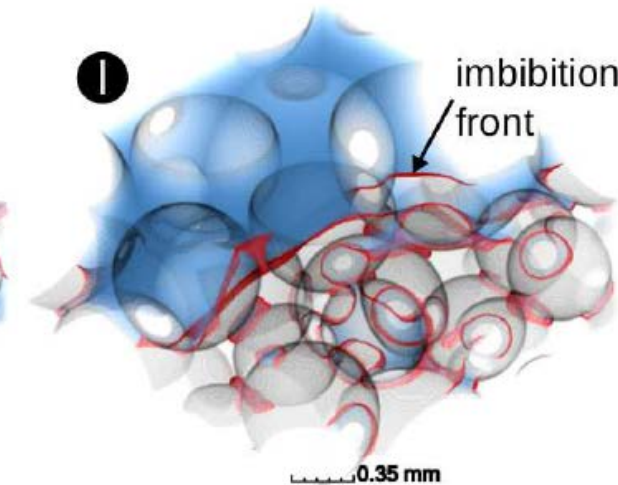
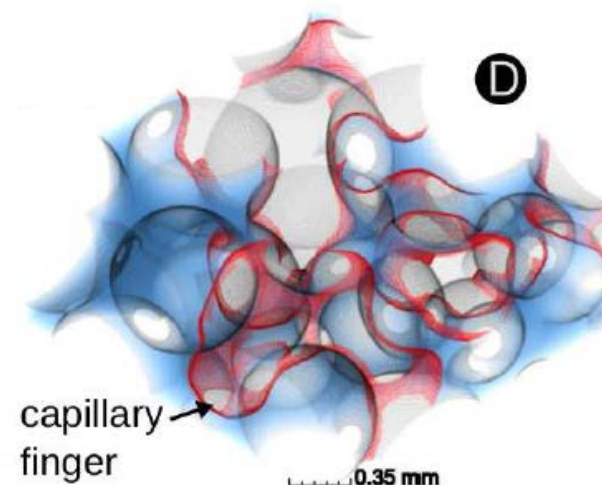
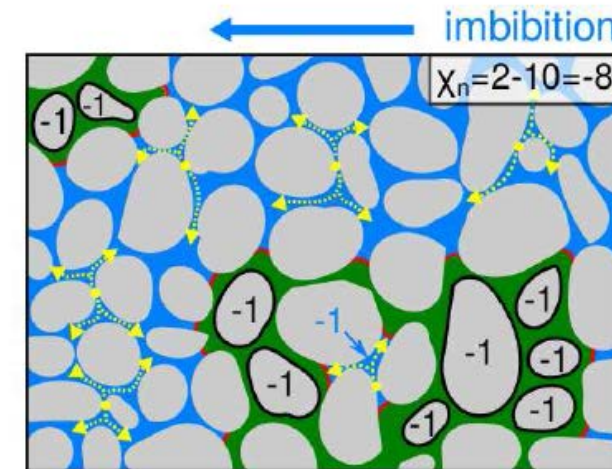
The Discovery of the 4th State Variable



Drainage =
maintaining connectivity
(avoid forming loops)



Imbibition =
Snap-off \rightarrow formation of
clusters and loops



Proof by Direct Numerical Simulation

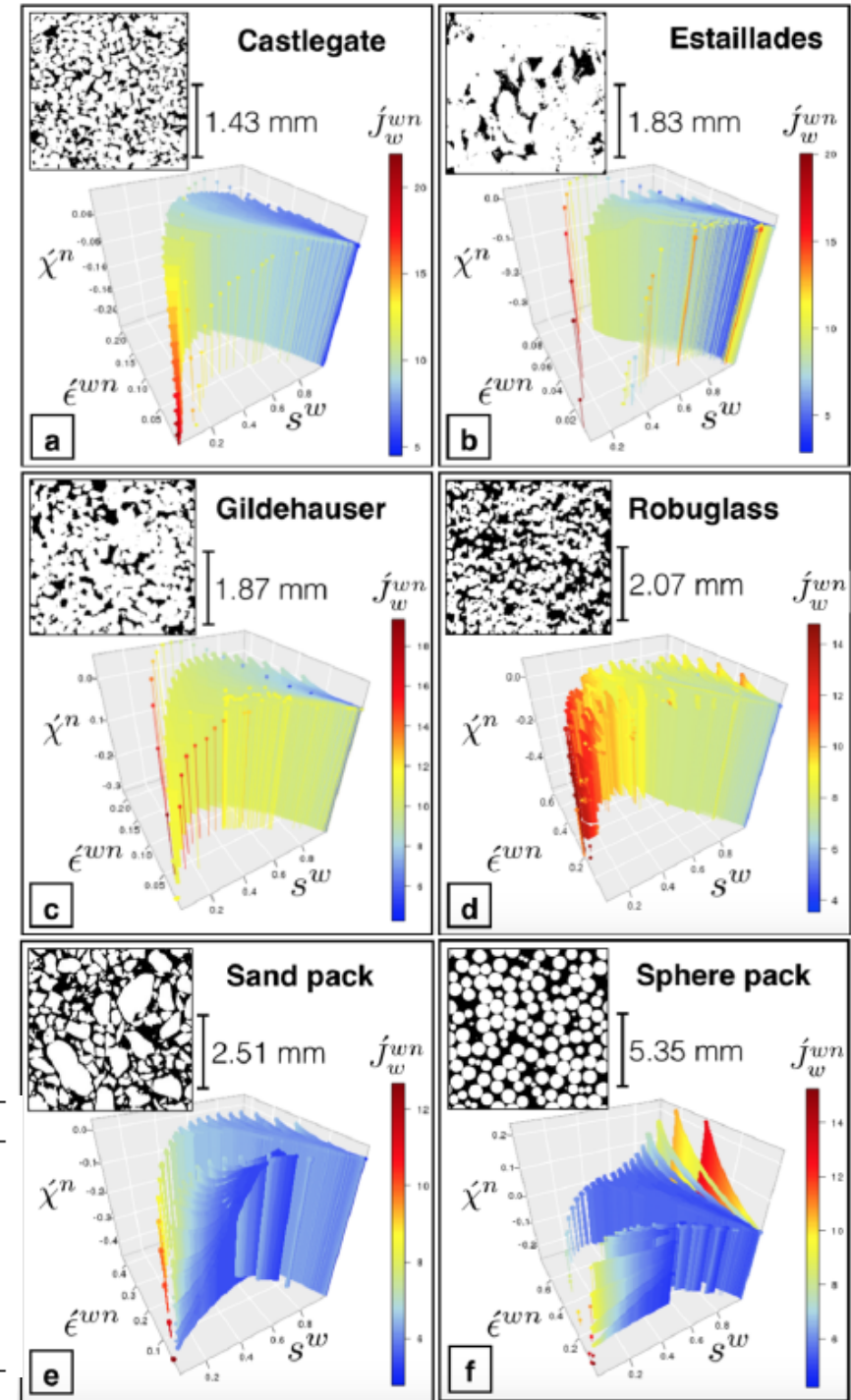
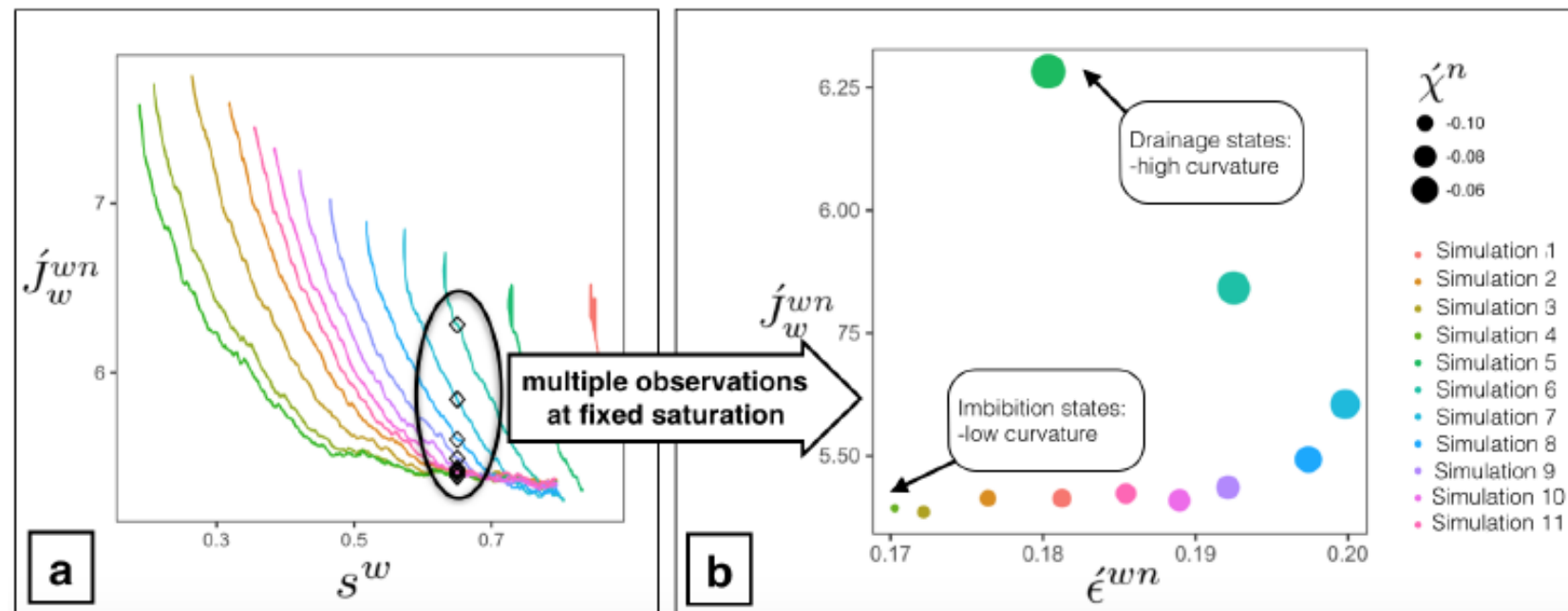
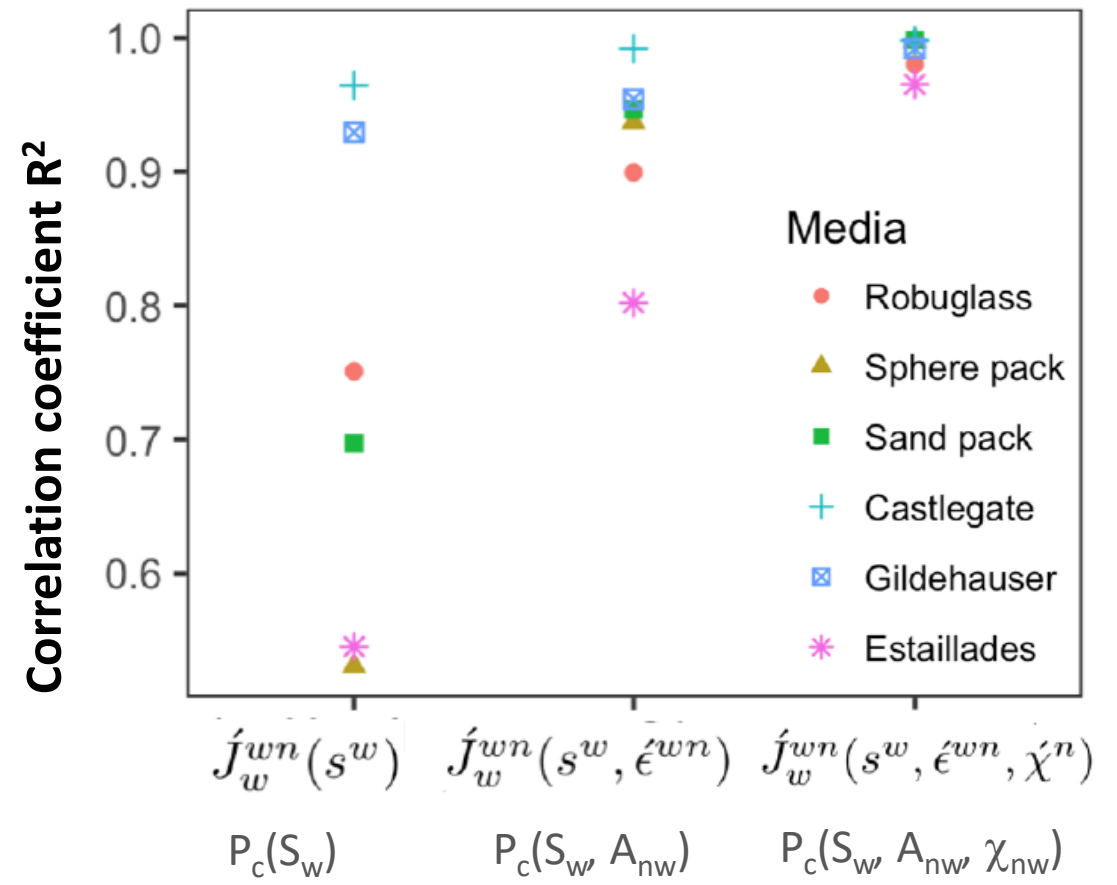
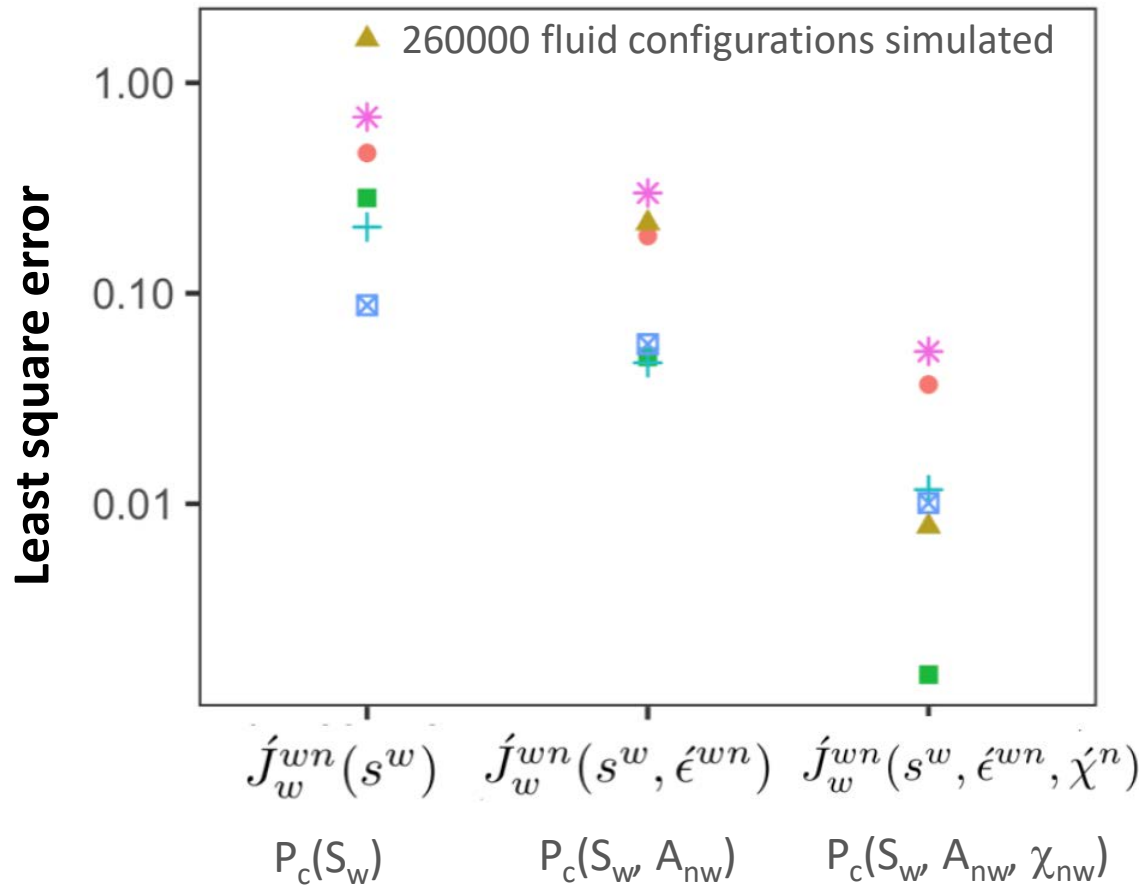


FIG. 6. Traditional models assume that the macroscale capillary pressure is a function only of the saturation of the wetting fluid. Two-fluid displacement simulations within a sand pack show that: (a) At fixed saturation, s^w , the relative mean curvature j_w^{wn} can attain many possible values depending on the system history; (b) $j_w^{wn}(s^w, \epsilon^{wn})$ is non-unique for $s^w = 0.65$.

| Media | ϵ | $D(\text{mm})$ | Size (voxels) | Sim. | Config. |
|-------------|------------|----------------|-----------------------------|-------|---------|
| Castlegate | 0.205 | 0.111 | $512 \times 512 \times 512$ | A,D | 23,123 |
| Estailades | 0.111 | 0.124 | $834 \times 834 \times 556$ | A,B,D | 23,599 |
| Gildehauser | 0.188 | 0.133 | $852 \times 852 \times 569$ | A,B,D | 38,788 |
| Robuglass | 0.345 | 0.173 | $988 \times 988 \times 598$ | A,B,D | 49,515 |
| Sand pack | 0.376 | 0.368 | $512 \times 512 \times 512$ | A,C,D | 64,650 |
| Sphere pack | 0.369 | 1.00 | $900 \times 900 \times 900$ | A,C,D | 59,341 |

Proof by Direct Numerical Simulation

McClure et al. Phys. Rev. Fluids, 2018

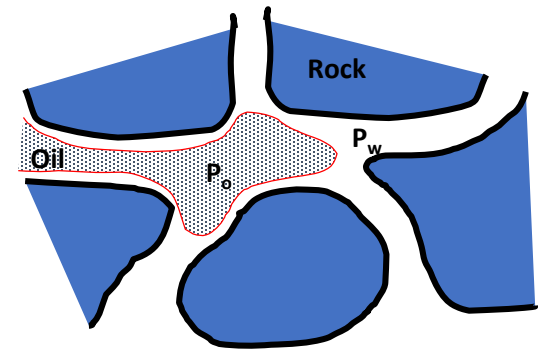


Saturation and Saturation + Interfacial Area are not sufficient to fully parameterize hysteresis (error > 10%)
 → Saturation + Interfacial Area + Euler Characteristic: error < 10% → full set of state variables

Upscaling from Pore to the Darcy Scale

“Pore scale”

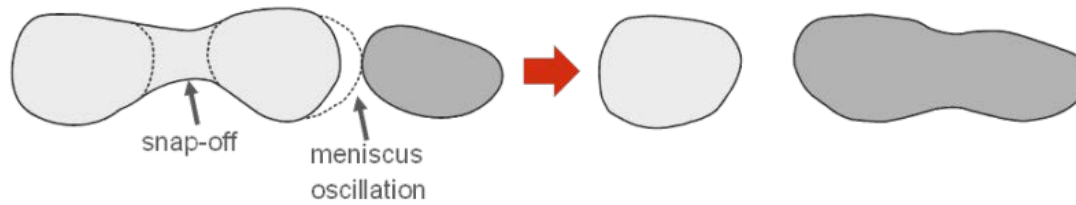
Single pores
continuum oil & water phases
Single interfaces



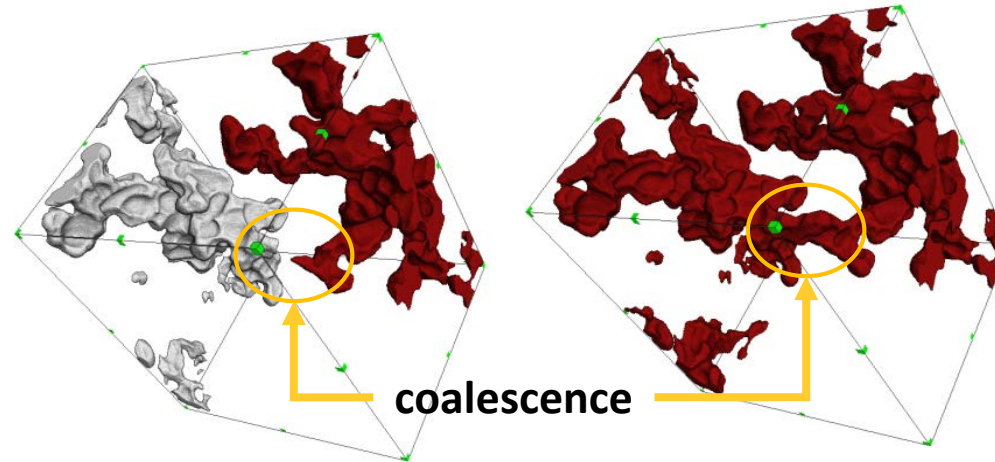
Capillary

“Cluster scale”

Non-wetting phase clusters,
Cooperative dynamics



Coalescence & breakup
→ **Changing topology**

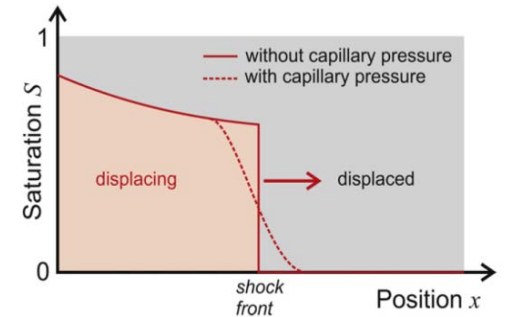


State variables:
Minkowski functionals

“Darcy scale”

Continuum mechanics:
porosity, permeability, saturation
phenomenological description

$$v_i = -k_{r,i} \frac{K}{\mu_i} \frac{dp_i}{dx}$$



Multiphase REV?

Viscous

μm

mm

cm

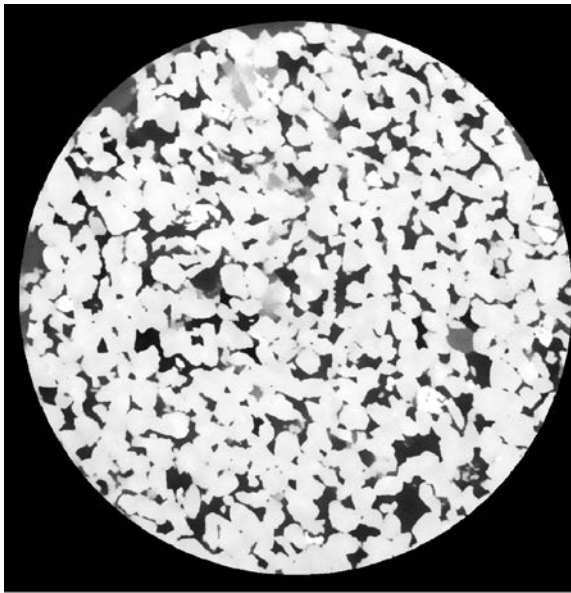
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How to Compute - Software Packages

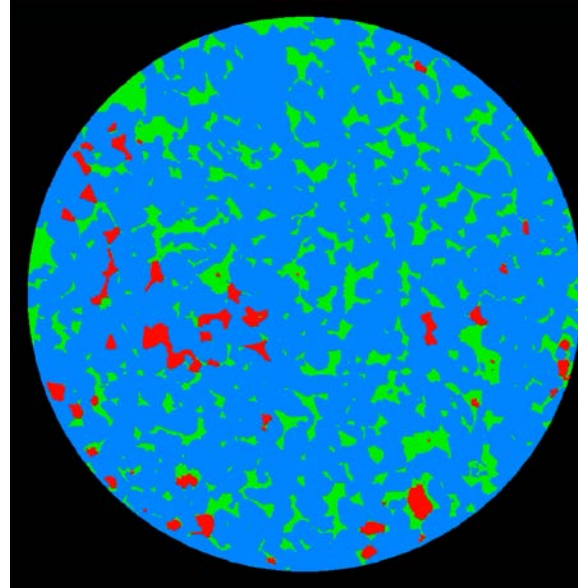
0. Image processing
 1. Avizo
 2. ImageJ and FIJI: BoneJ plugin
 3. Python – scikit-image (currently only 2D)
 4. Matlab
 5. Quantim (https://www.ufz.de/export/data/2/94413_quantim4_ref_manual.pdf)
 6. Boundary and connectivity issues
 7. Dragonfly/DeepRocks – compute χ on network

Image Processing

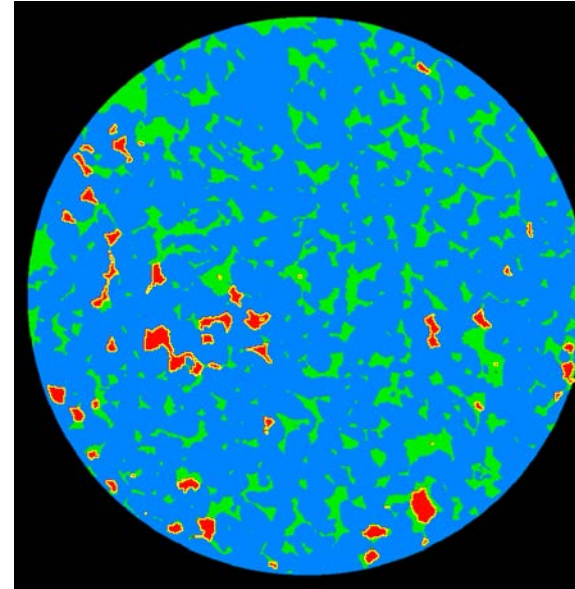
μ CT image $\xrightarrow{\text{segmentation}}$ Segmented $\xrightarrow{\text{select phase}}$ Oil Phase $\xrightarrow{\text{object analysis}}$ Oil clusters



16 bit grey level
(potentially filter)

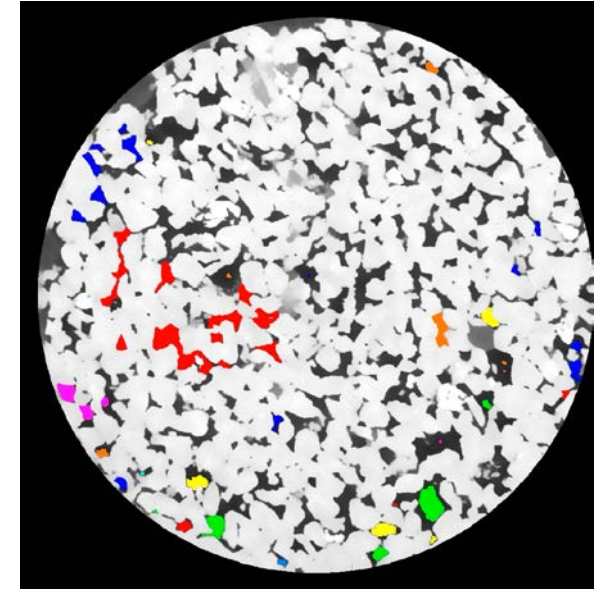


Segmented image
Blue = rock
Red = oil
Green = gas



For each **phase** compute

- Volume
- Interfacial area
- Mean curvature
- Euler characteristic



For each **cluster** compute

Avizo: Mean Curvature

segmentation

Label analysis

- Volume
- Area
- Euler char.

Generate surface
(spline interpolation)

- Mean curvature
- Gaussian curvature

Avizo - topologycourse.hx

File Edit Project View Window Help

START PROJECT RECIPES SEGMENTATION ANIMATION

Project View

Open Data... Create Plot Image Plot in Viewer Caption Snapshot

Sphere.tif.am Ortho Slice

Interactive Thresholding Bounding Box

Sphere.thresholded* Volume Rendering Settings Volume Rendering

Label Analysis Sphere.label* Sphere.Label-Analysis*

Generate Surface Sphere.surf* Surface View

Curvature

MaxCurvatureInv* MeanCurvature* Histogram

2Spheres.tif*

Properties

Histogram

Data: MeanCurvature

Overall: mean=0.496786 deviation=2.52344 rms=2.57155

In Range: mean=0.142703 deviation=0.115986 rms=0.183884

Range: min 0.019465 max 1 Reset

Max Num Bins: 256

Histogram Options: absolute relative ln % + cumulative

Plot Options: line drawing logarithmic

Threshold: >= 0.019465 : 100. %

Tindex: T 90 :

auto-refresh Apply

Ready

Tables

Sphere.Label-Analysis

| Area3d | BaryCenterX | BaryCenterY | BaryCenterZ | Euler3D | index |
|---------|-------------|-------------|-------------|---------|-------|
| 1262.52 | 50.0 | 50.0 | 50.0 | 1.0 | 1.0 |
| 1262.52 | 50.0 | 50.0 | 50.0 | 1.0 | 1.0 |
| 1262.52 | 50.0 | 50.0 | 50.0 | 1.0 | 1.0 |
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| -inf | -- | -- | -- | -- | -- |
| inf | -- | -- | -- | -- | -- |

| Area3d | BaryCenterX | BaryCenterY | BaryCenterZ | Euler3D | index |
|---------|-------------|-------------|-------------|---------|-------|
| 1262.52 | 50.0 | 50.0 | 50.0 | 1.0 | 1 |

Histogram-Plot

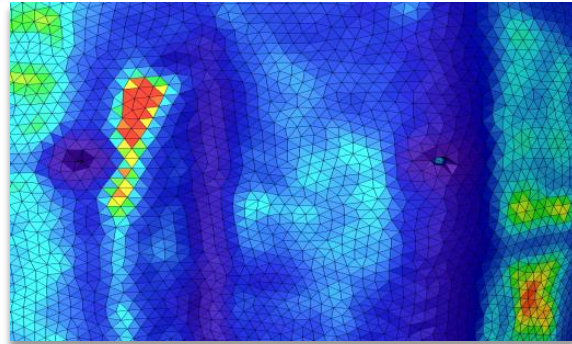
File Edit Axis Help

MEMORY USAGE 39%

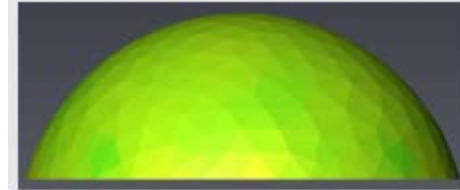
Avizo : Surface meshes

- Surface property calculation

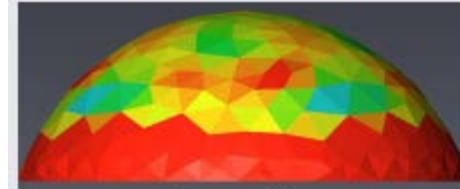
- **Curvature**
- Distance
- Roughness
- Thickness



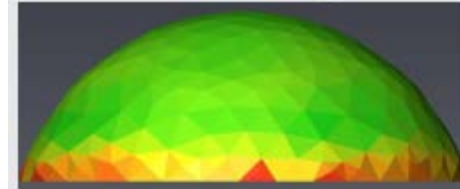
Surface-based Approach:



Imported Surface

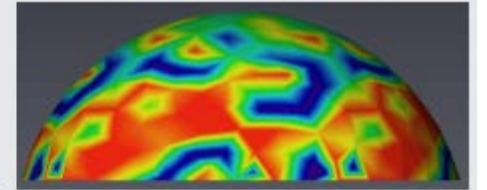


Smoothing

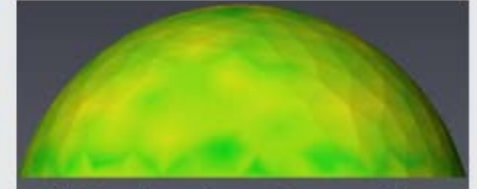


Neighborhood Averaging

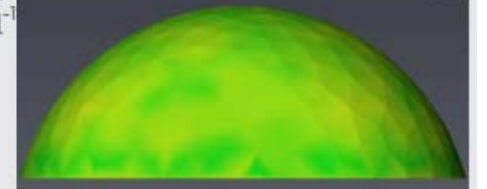
Voxel-based Approach:



Imported Surface



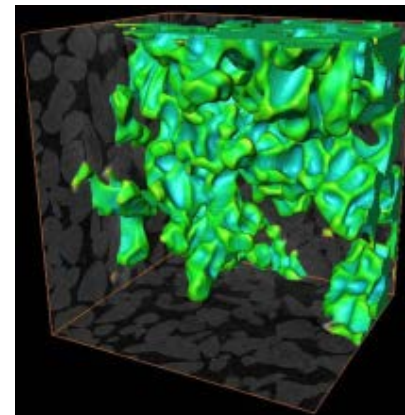
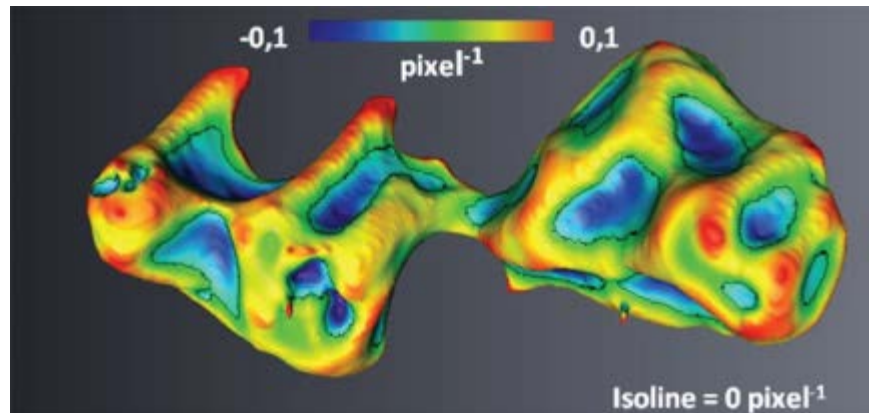
1st Derivative Smoothing



2^d Derivative Smoothing



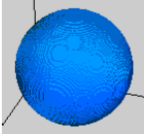
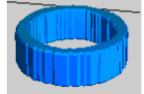
SCA2012-55








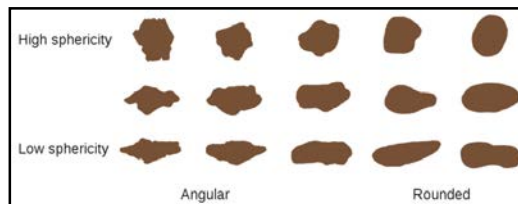
Avizo : Object Analysis

- Analysis

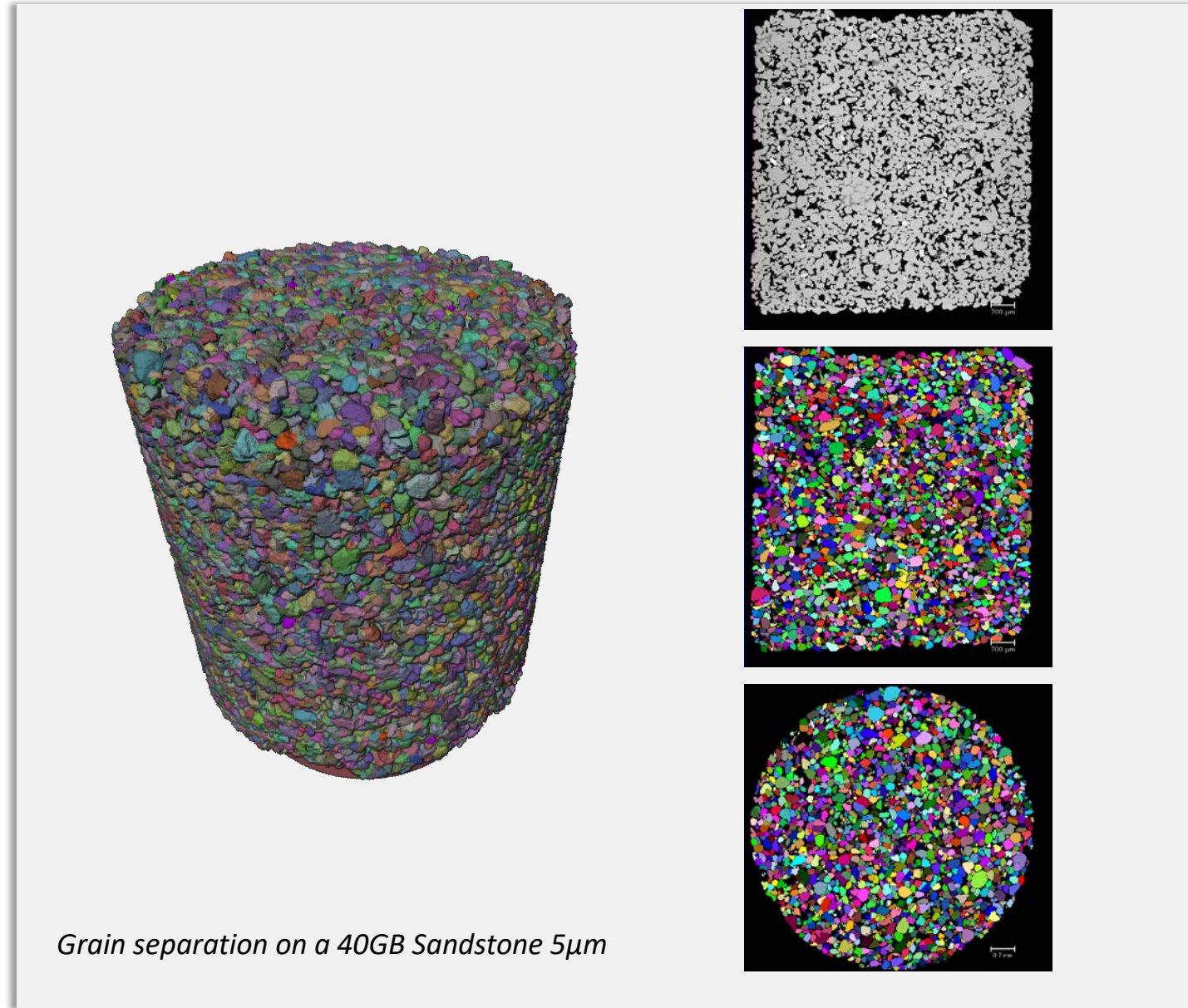
- Shape factor
- Equivalent diameter
- **Volume, area**
- **Euler**
- Orientation
- Roundness
- Sphericity
- Rugosity
- Crofton

| | | |
|-----------------------------------------------------------------------------------|------------------------------|-------------|
|  | Solid sphere | Euler3D = 1 |
| | Empty sphere | Euler3D = 2 |
|  | Rectangular section Torus | Euler3D = 0 |

| Name | Picture | Volume | Area | Sphericity |
|------------------------|------------------------------------------------------------------------------------|-----------------------------------|-------------------------------|-------------------------------------------------------------------------------------------------|
| Platonic Solids | | | | |
| tetrahedron |  | $\frac{\sqrt{2}}{12} s^3$ | $\sqrt{3} s^2$ | $\left(\frac{\pi}{6\sqrt{3}}\right)^{\frac{1}{3}} \approx 0.671$ |
| cube (hexahedron) |  | s^3 | $6 s^2$ | $\left(\frac{\pi}{6}\right)^{\frac{1}{3}} \approx 0.806$ |
| octahedron |  | $\frac{1}{3}\sqrt{2} s^3$ | $2\sqrt{3} s^2$ | $\left(\frac{\pi}{3\sqrt{3}}\right)^{\frac{1}{3}} \approx 0.846$ |
| dodecahedron |  | $\frac{1}{4}(15 + 7\sqrt{5}) s^3$ | $3\sqrt{25 + 10\sqrt{5}} s^2$ | $\left(\frac{(15 + 7\sqrt{5})^2 \pi}{12(25 + 10\sqrt{5})^2}\right)^{\frac{1}{3}} \approx 0.910$ |
| icosahedron |  | $\frac{5}{12}(3 + \sqrt{5}) s^3$ | $5\sqrt{3} s^2$ | $\left(\frac{(3 + \sqrt{5})^2 \pi}{60\sqrt{3}}\right)^{\frac{1}{3}} \approx 0.939$ |

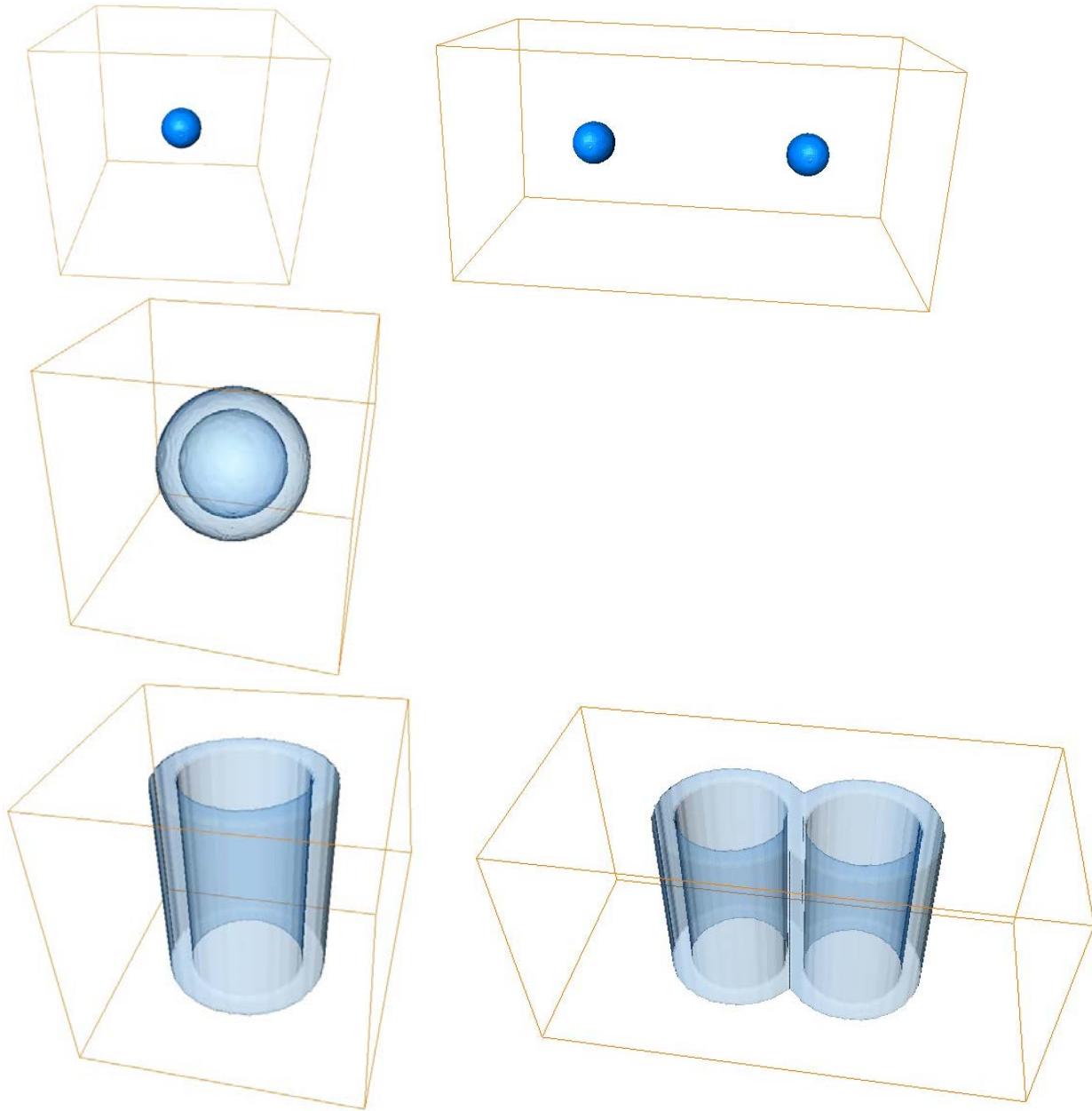


- Classification



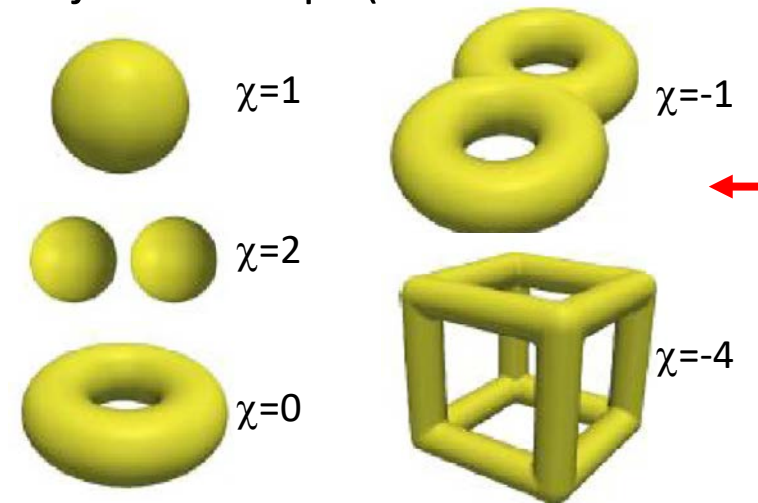
Grain separation on a 40GB Sandstone 5µm

Avizo: Euler Characteristic



| | Volume | Area | BarX | Bary | Barz | Euler |
|---------------|--------|---------|---------|------|------|-------|
| Sphere | 4169 | 1262.52 | 50 | 50 | 50 | 1 |
| 2spheres | 4169 | 1262.52 | 50 | 50 | 50 | 1 |
| | 4169 | 1262.52 | 150 | 50 | 50 | 1 |
| sum | 4170 | 1263.52 | | | | 2 |
| hollow sphere | 72982 | 16953.9 | 50 | 50 | 50 | 2 |
| ring | 110284 | 27631.2 | 50 | 50 | 50 | 0 |
| doughnut | 203899 | 49396.3 | 99.9872 | 50 | 50 | -1 |

Euler Characteristic $\chi =$
Objects – Loops (+ Inclusions)

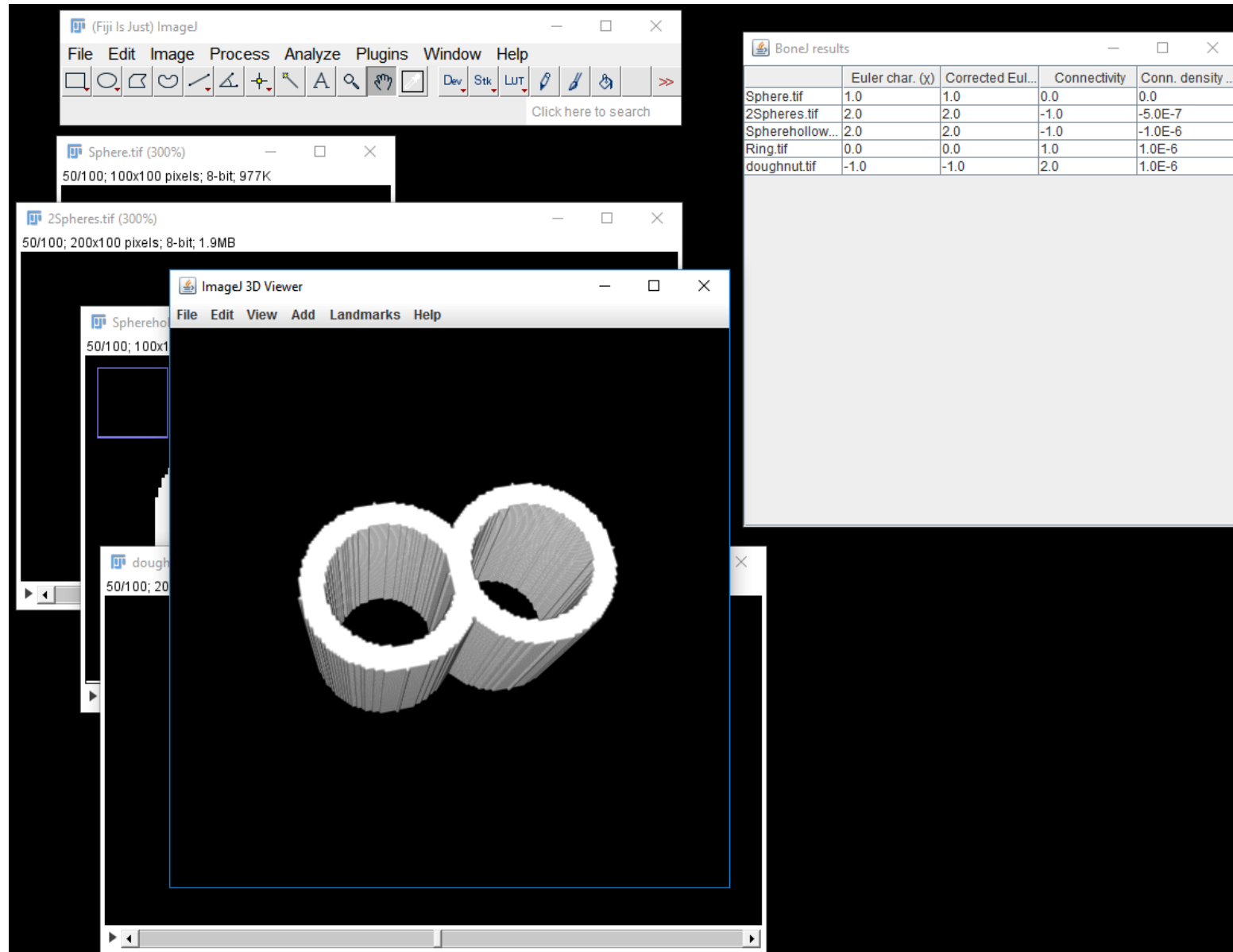


ImageJ and FIJI: BoneJ plugin (OpenSource)

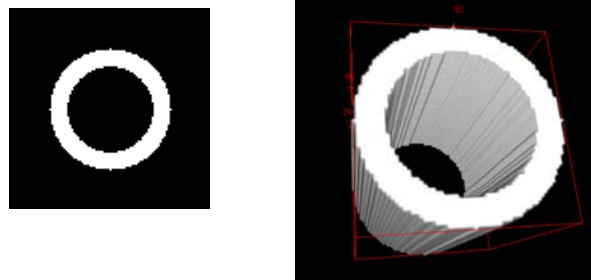
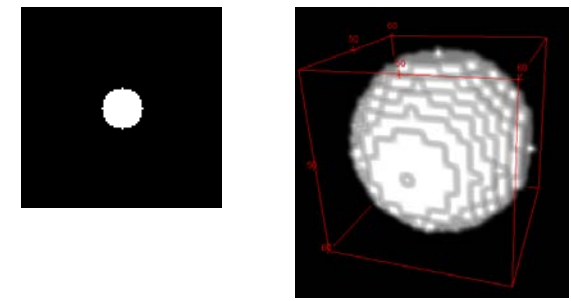
ImageJ - <https://imagej.nih.gov/ij/>

FIJI - <https://fiji.sc/>

BoneJ - <http://bonej.org/>

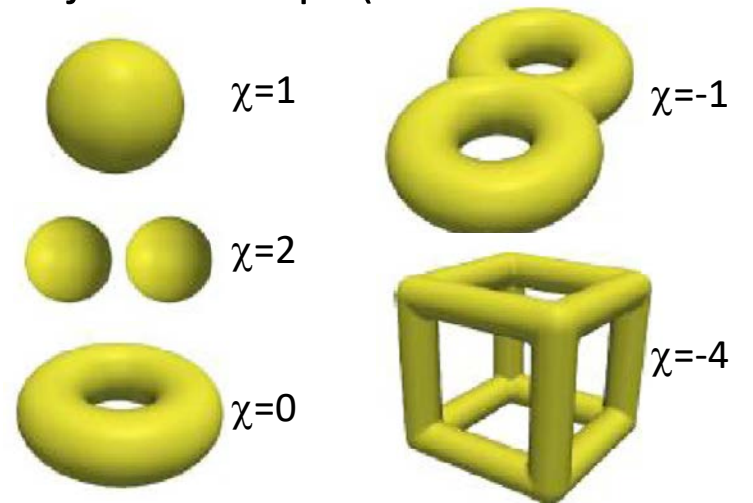


ImageJ and FIJI: BoneJ plugin (OpenSource)



| | Euler char. (χ) | Corrected Euler ($\chi + \dots$) | Connectivity | Conn. density (pixel ³) | Surface area (pixel ²) |
|------------------|------------------------|------------------------------------|--------------|-------------------------------------|------------------------------------|
| Sphere.tif | 1.0 | 1.0 | 0.0 | 0.0 | 1263.9727775132994 |
| 2Spheres.tif | 2.0 | 2.0 | -1.0 | -5.0E-7 | 2527.9455550266375 |
| Spherehollow.tif | 2.0 | 2.0 | -1.0 | -1.0E-6 | 18358.24357045593 |
| Ring.tif | 0.0 | 0.0 | 1.0 | 1.0E-6 | 29282.273575259434 |
| doughnut.tif | -1.0 | -1.0 | 2.0 | 1.0E-6 | 52570.373993201676 |

Euler Characteristic $\chi =$
Objects – Loops (+ Inclusions)

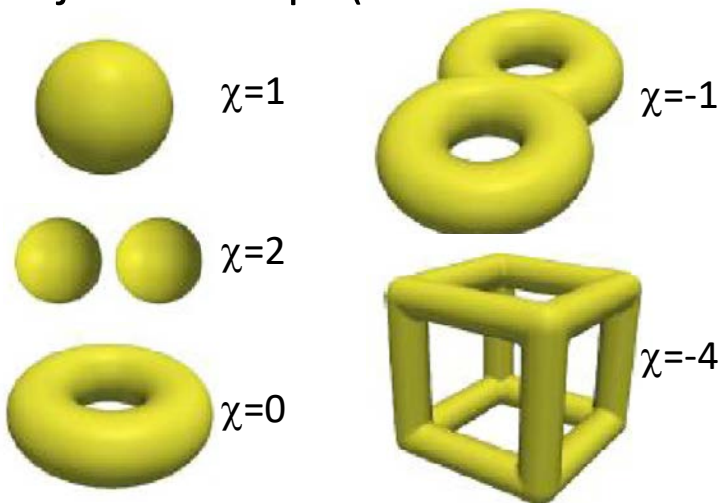




Many functions unfortunately currently only in 2D !



Euler Characteristic $\chi =$
Objects – Loops (+ Inclusions)



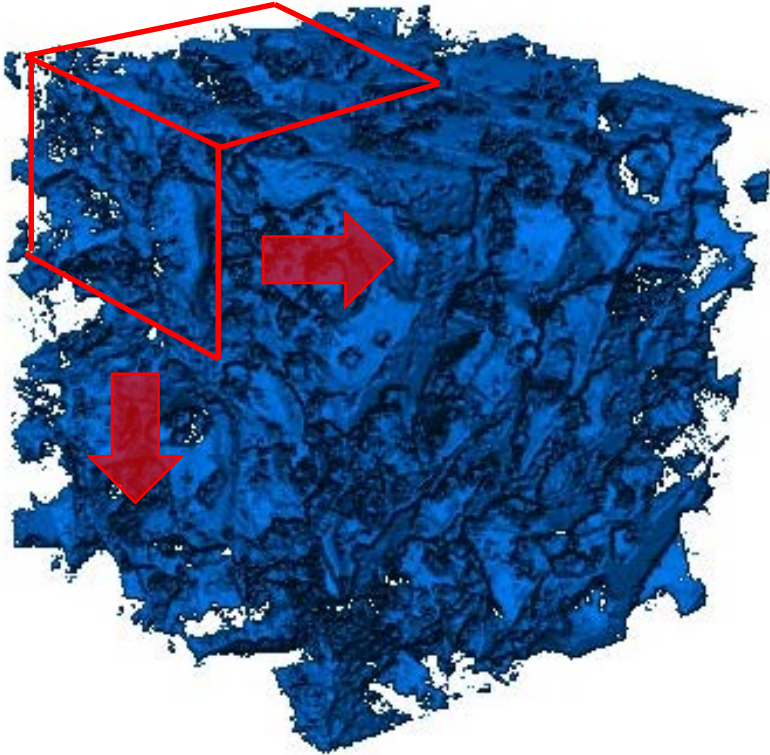
Herring, AWR 2013

```

17 import matplotlib.pyplot as plt
18 from skimage import io
19 from skimage.measure import label, regionprops
20
21 filenamelist=['Sphere.tif', 'Ring.tif', 'doughnut.tif']
22
23
24 fig = plt.figure()
25 i=1
26 for imagename in filenamelist:
27     image = io.imread(imagename)
28     xdim, ydim, zdim = image.shape
29     label_img = label(image[int(xdim/2), :, :])
30     regions = regionprops(label_img)
31     for props in regions:
32         el = props.euler_number
33     #     ar = props.area
34     ax = fig.add_subplot(1,3,i)
35     ax.imshow(image[int(xdim/2), :, :], cmap=plt.cm.gray)
36     ax.set_title('Euler = '+str(el), loc="left")
37     ax.set_xticks(())
38     ax.set_yticks(())
39     ax.axis('off')
40     i=i+1
41
42 plt.show()

```

MATLAB



<https://github.com/mattools/matImage>

Legland, D.; Kiêu, K. & Devaux, M.-F. Computation of Minkowski measures on 2D and 3D binary images. Image Anal. Stereol., 2007, 26, 83-92

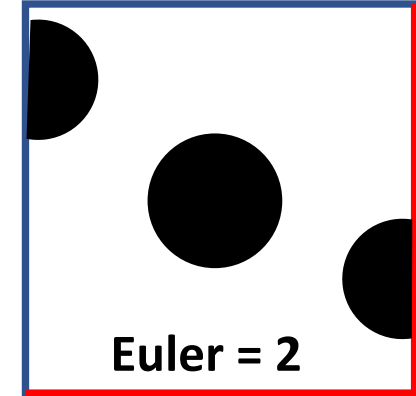
```
for w_idx = [900] % ROI size
    w_surface = [];
    w_labels = [];
    i_loc = ((mask_x - w_idx)/2)+1;
    j_loc = ((mask_y - w_idx)/2)+1;
    k_loc = ((mask_z - w_idx)/2)+1;
    roi = FinalImage(i_loc:i_loc+w_idx-1, j_loc:j_loc+w_idx-1,
k_loc:k_loc+w_idx-1);
    [Euler_roi, Euler_labels]= imEuler3d(roi);
% Implements Euler number codes
    w_Euler = vertcat(w_Euler, Euler_roi);
    w_labels = vertcat(w_labels, Euler_labels);
    file_name = [num2str(w_idx), 'Filename_900.mat'];
    save(file_name, 'w_Euler', 'w_labels')
end
```

Boundary and Connectivity Issues

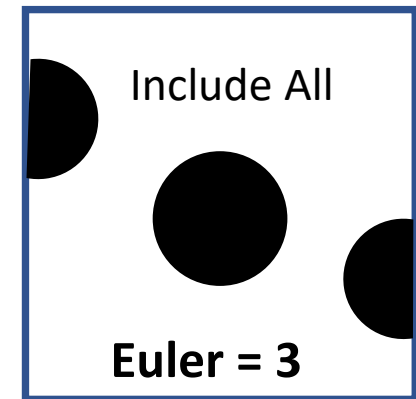
| ROI size | Euler3D calculated by Avizo | Euler3D calculated with MATLAB codes |
|----------|-----------------------------|--------------------------------------|
| 200 | -5.07E+02 | -5.62E+02 |
| 300 | -2.70E+03 | -2.69E+03 |
| 400 | -6.76E+03 | -6.80E+03 |

Boundary Issues

Include



Exclude

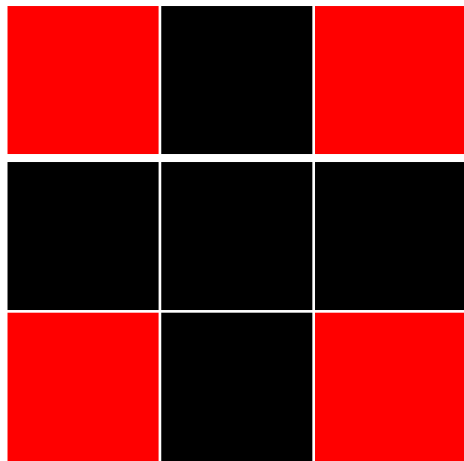


Do these two objects connect?

YES → Euler = 1

No → Euler = 2

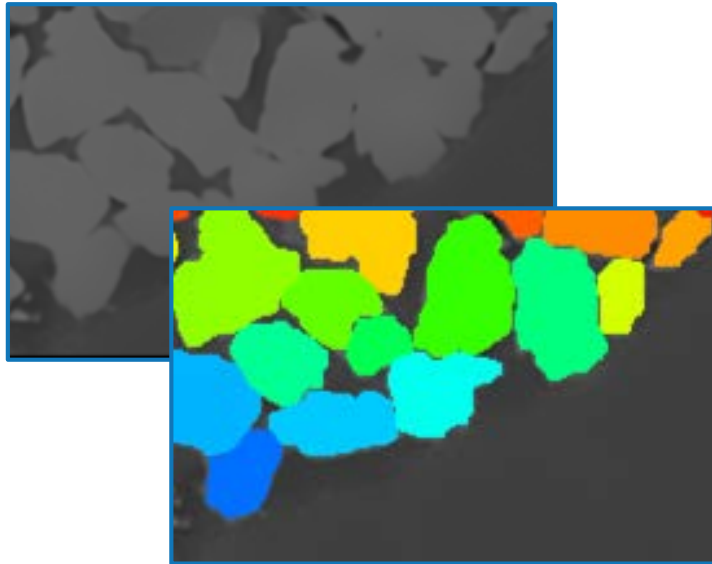
Pixel Connectivity



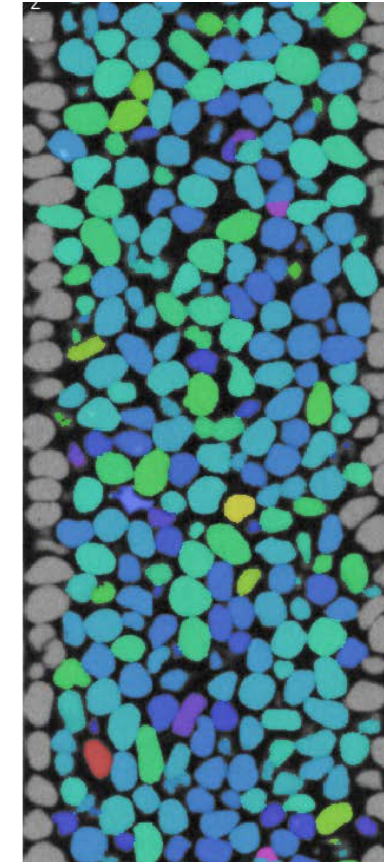
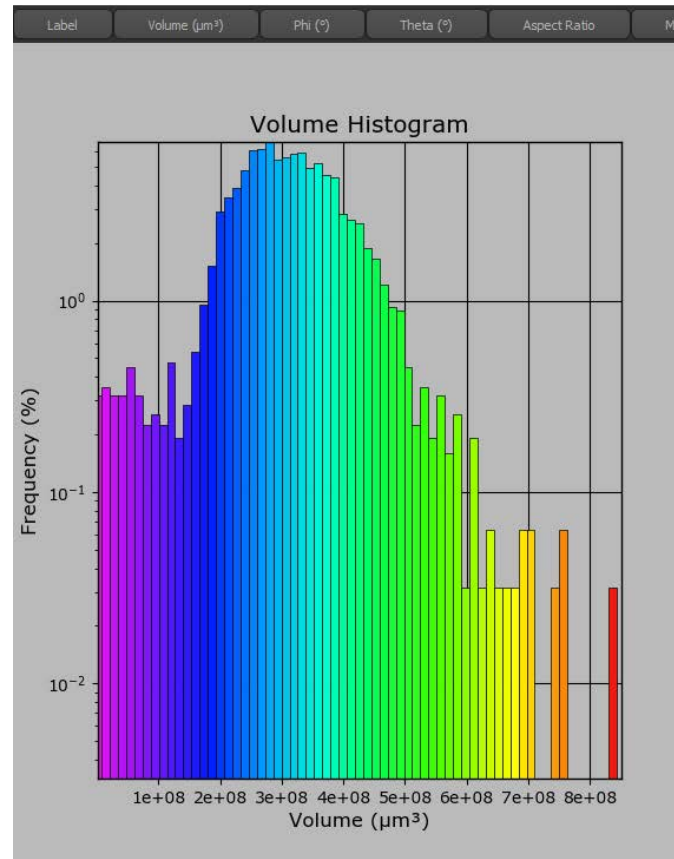


Color and Sort by measurement

- Volume
- Surface area
- Aspect Ratio
- Phi
- Theta
- Position (x,y,z)
- Intensity (mean, min, max, stdev)



Grain separation and labeling by Deep Watershed



Whole Core

Medical CT, Core photography

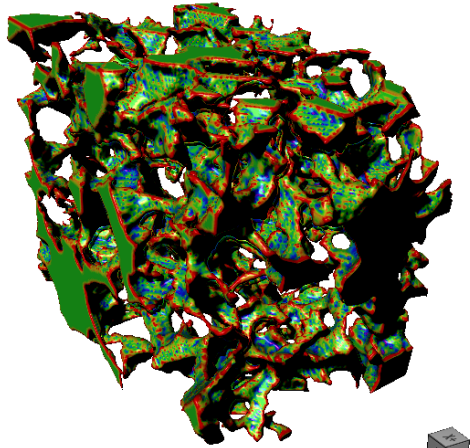
Plugs and Cuttings

Micro-CT, Nano-CT, FIB-SEM

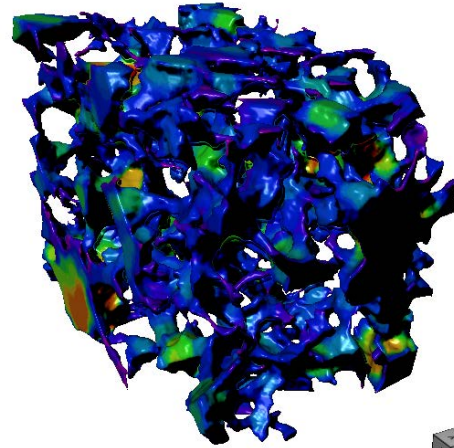
Thin Section

LM, SEM, TEM, CL, Mineralogy

Courtesy of
TheObjects



Curvature Mesh

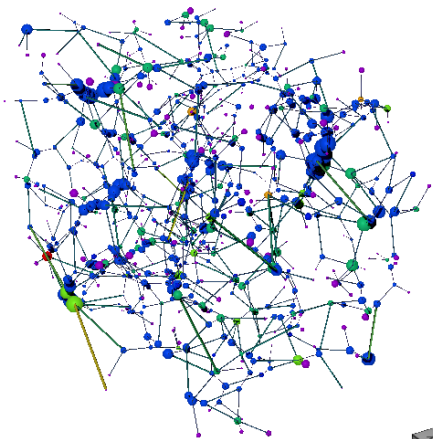


Thickness Mesh



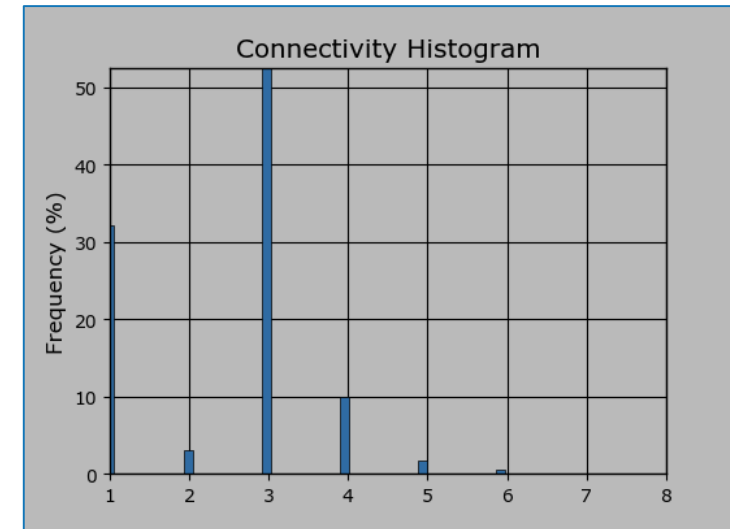
Mesh operations

- Smoothing
- Decimation
- Thickness
- **Mean Curvature**
- **Gaussian Curvature**



Pore network

- Nodes scaled by pore body radius
- Nodes colored by connectivity index
- Edges colored by edge length
- **$\chi = -212$ (Euler characteristic)**

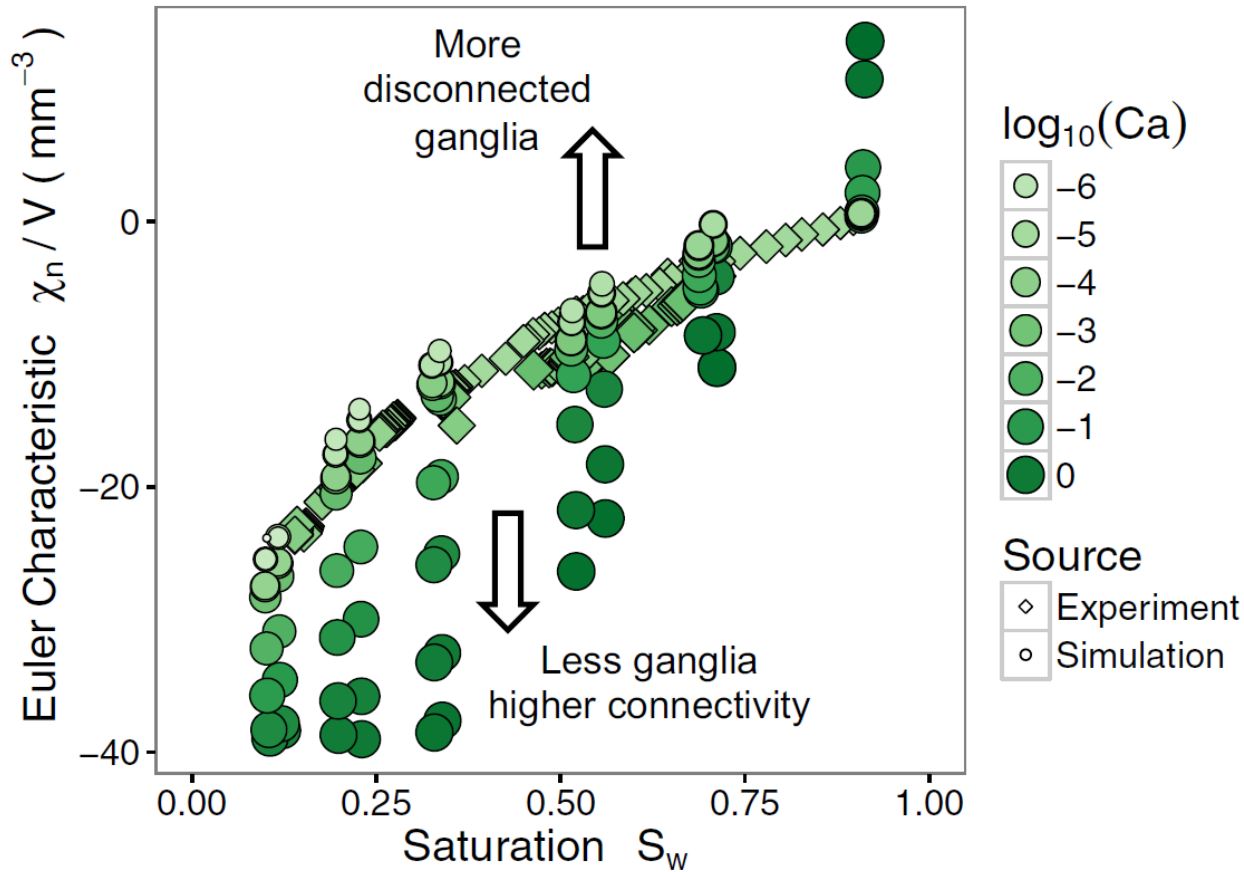


Applications

1. Digital Rock: Validation of pore scale simulators: relative permeability
2. new route to relative permeability
3. Phase connectivity inferred from resistivity measurements
4. Phase connectivity in critical gas saturation
5. Hysteresis models for Darcy-scale flow
6. Wettability: Description of contact angle as deficit curvature
7. Wettability: bi-continuous interfaces in intermediate/mixed-wet rock
8. Petrology mineral analysis for interpreting relative permeability
9. Permeability in fracture networks

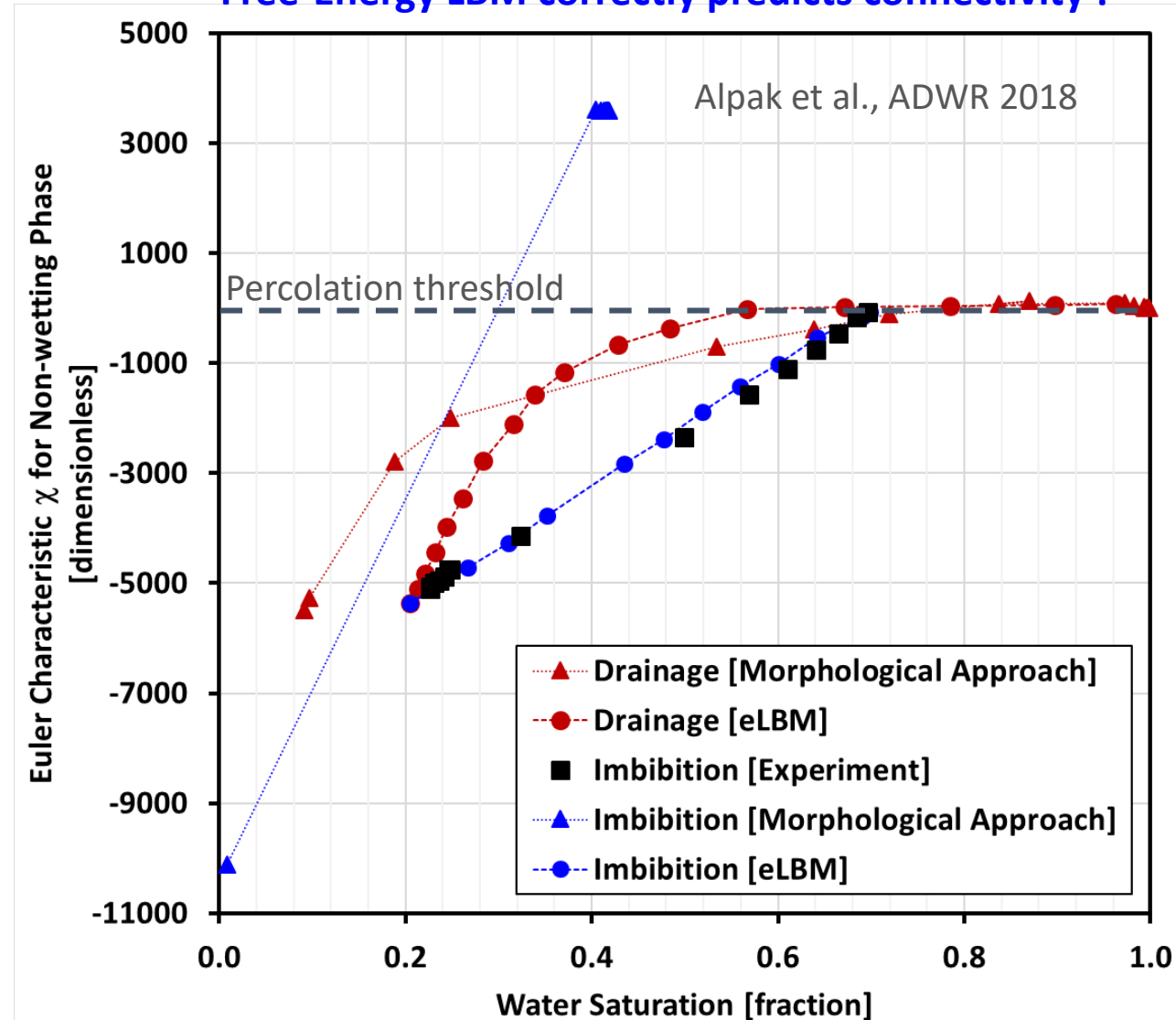
Application: Validation of Pore Scale Simulation

LBM fractional flow simulation: match with exp. data



McClure et al, PRE, 2016

Free-Energy LBM correctly predicts connectivity !

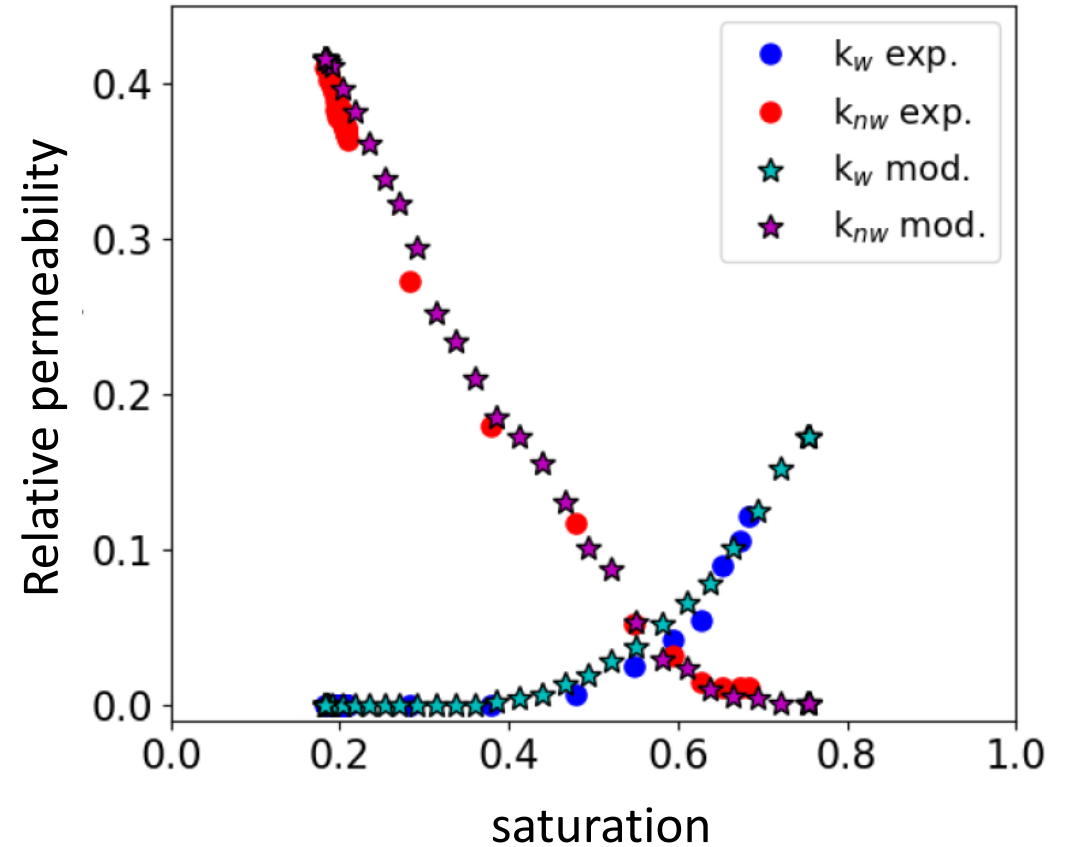
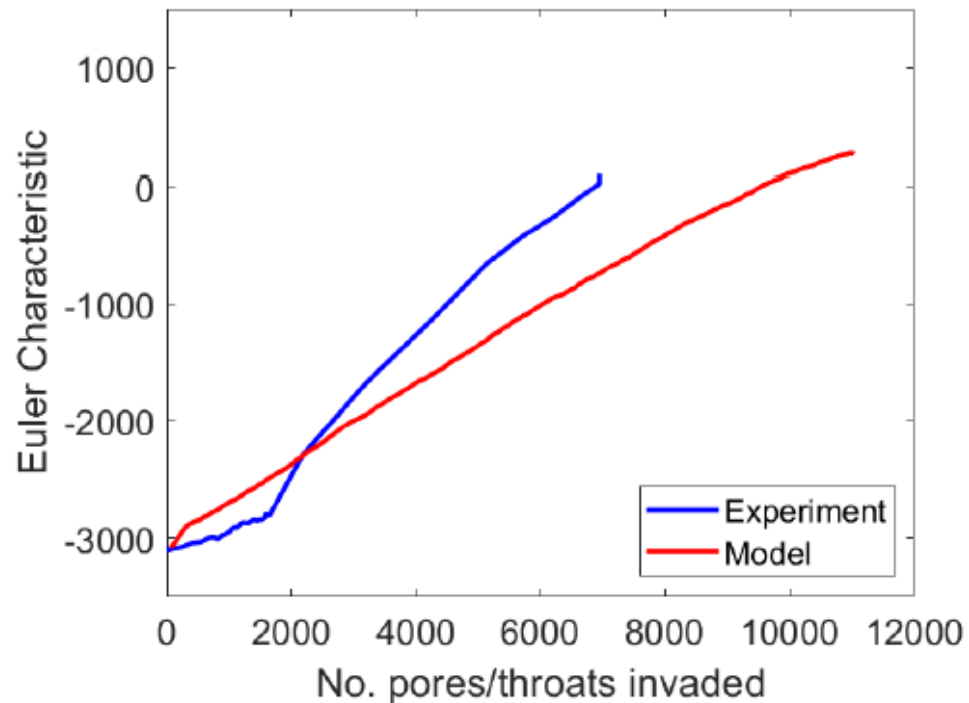


Application: Validation of Pore Scale Simulation

Model: quasi-static Pore Network Model (Ruspini et al. 2018)

Rock: Gildehauser sandstone (similar to Bentheimer)

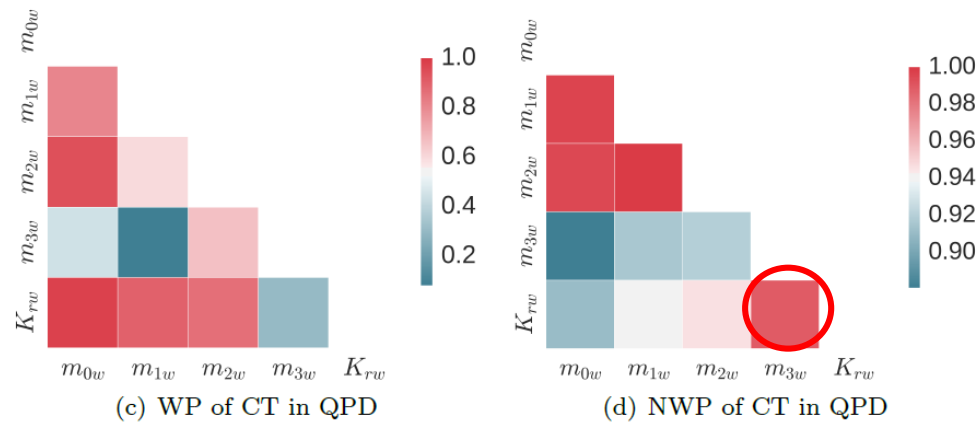
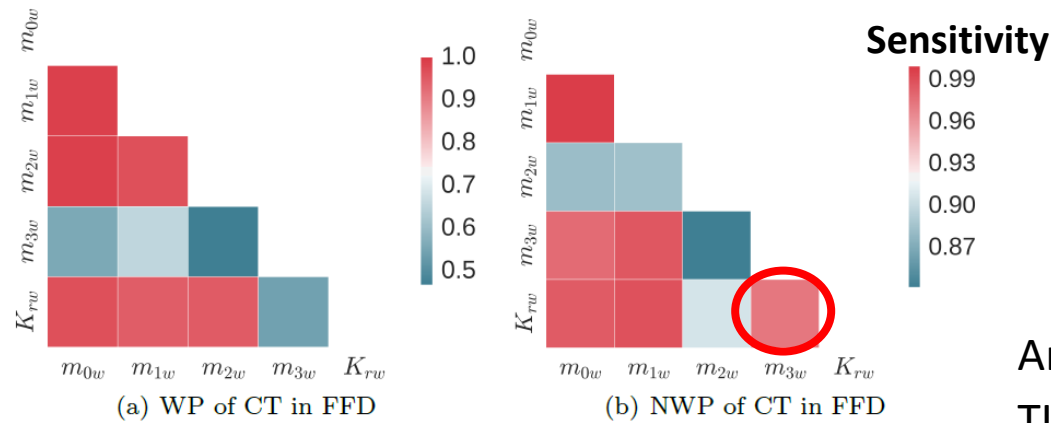
Imbibition



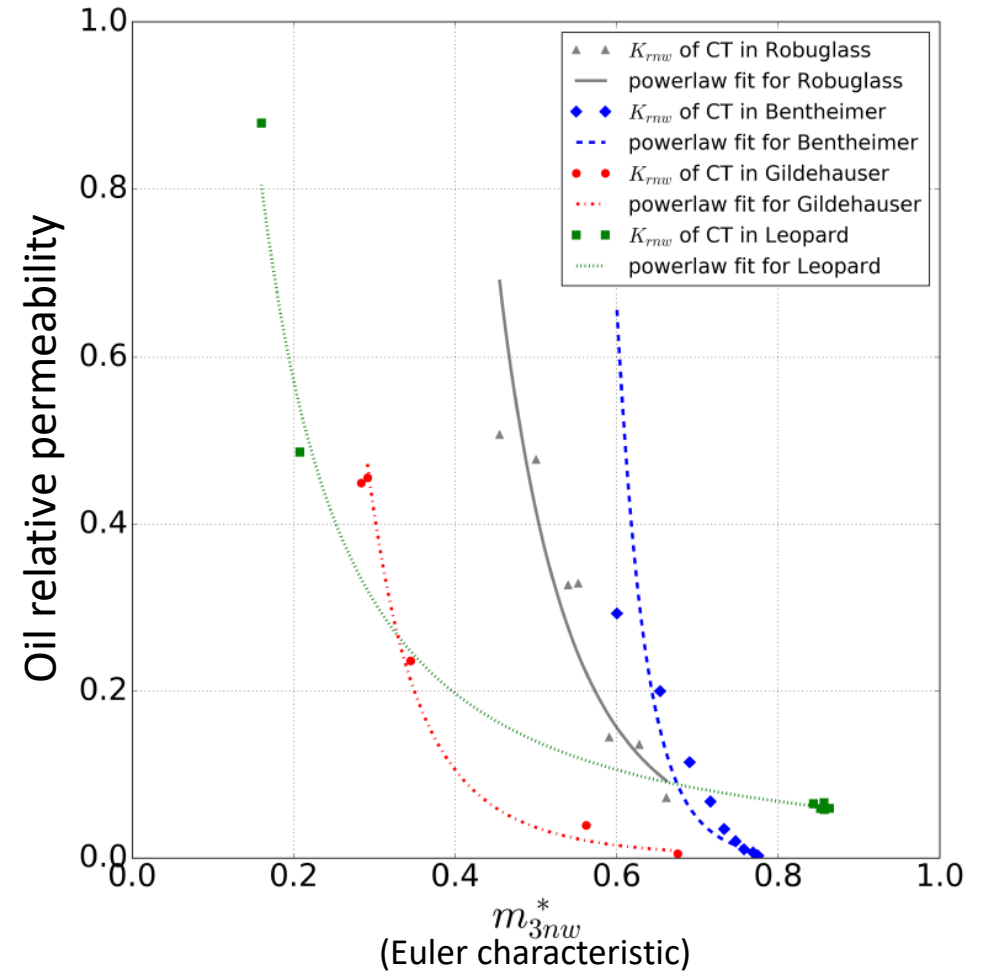
Application: new route to relative permeability

Non-wetting phase relative permeability has high sensitivity with Euler characteristic

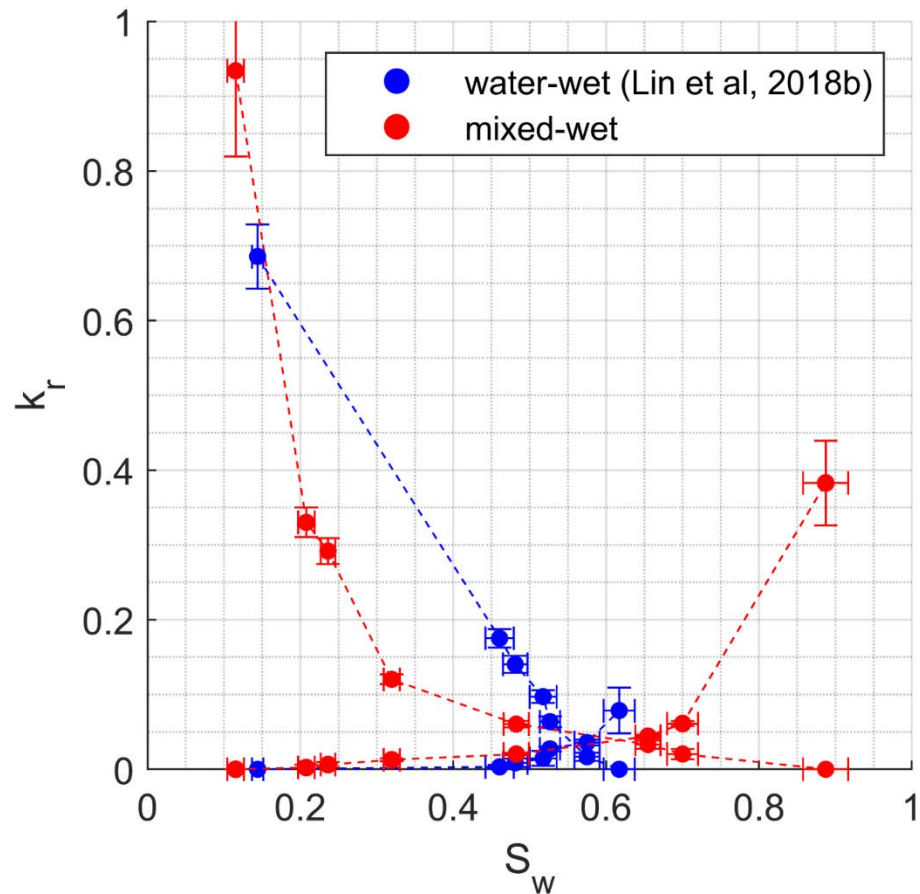
Non-wetting phase relative permeability is simple Power law function of Euler characteristic



Armstrong et al.
TIPM 2017



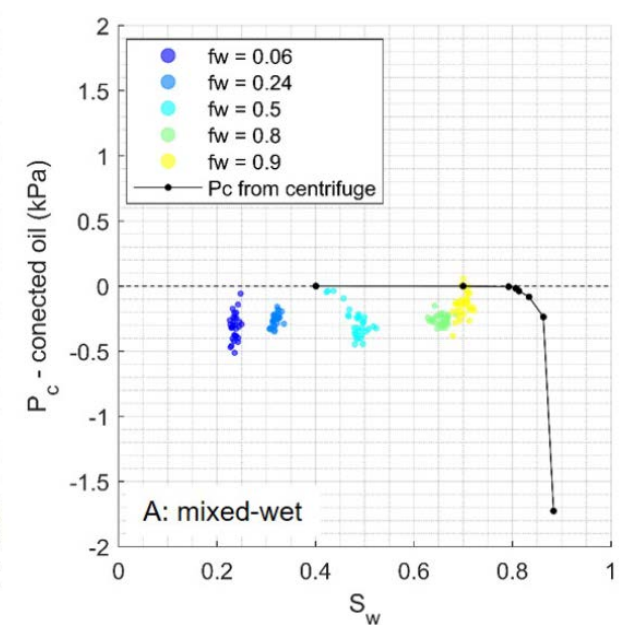
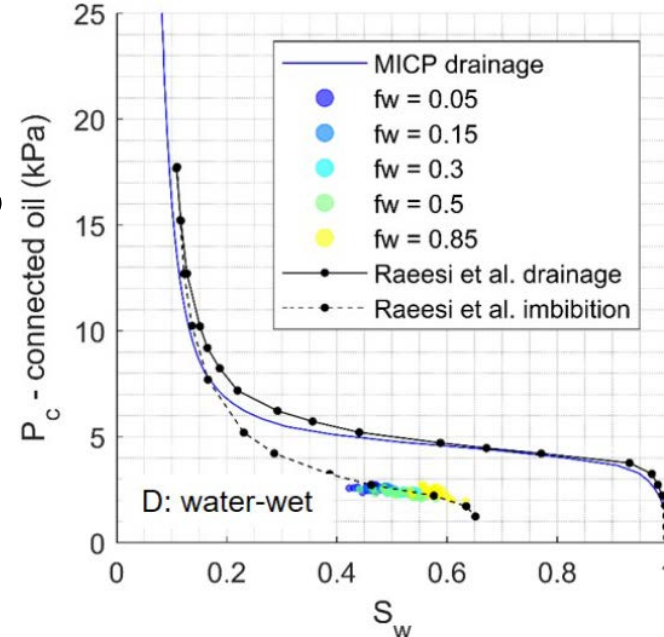
Bi-Continuous Interfaces



■ Mean curvature ~ 0

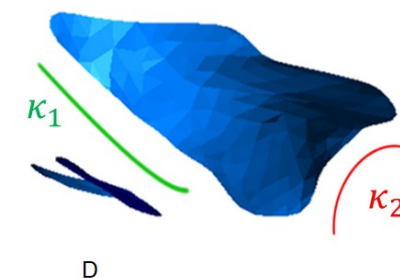
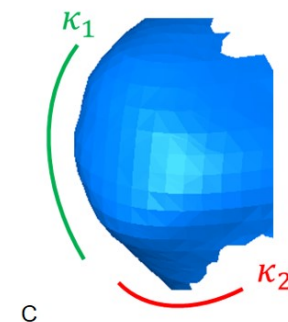
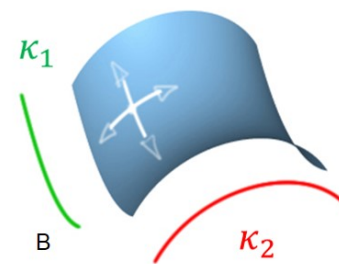
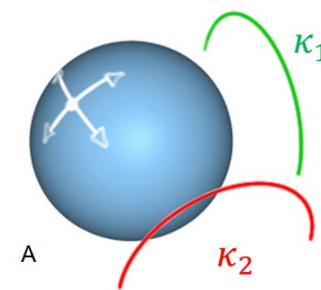
■ Gaussian curvature < 0

→ bi-continuous interfaces with high connectivity



Water-wet

Mixed-wet



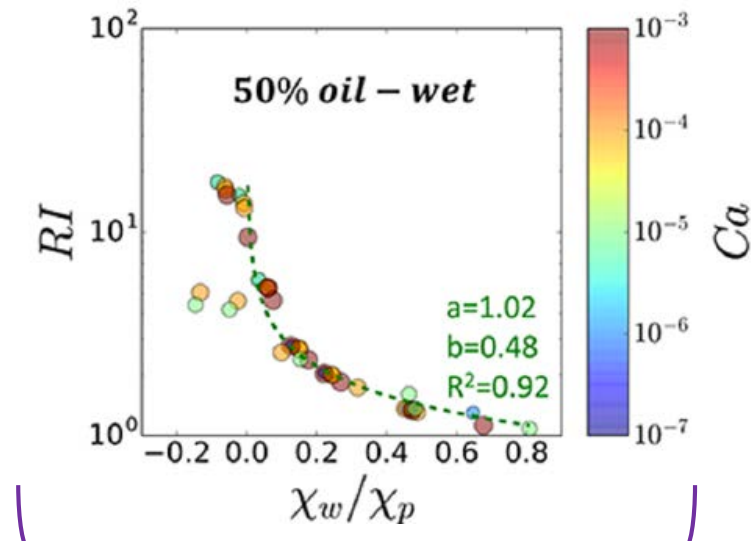
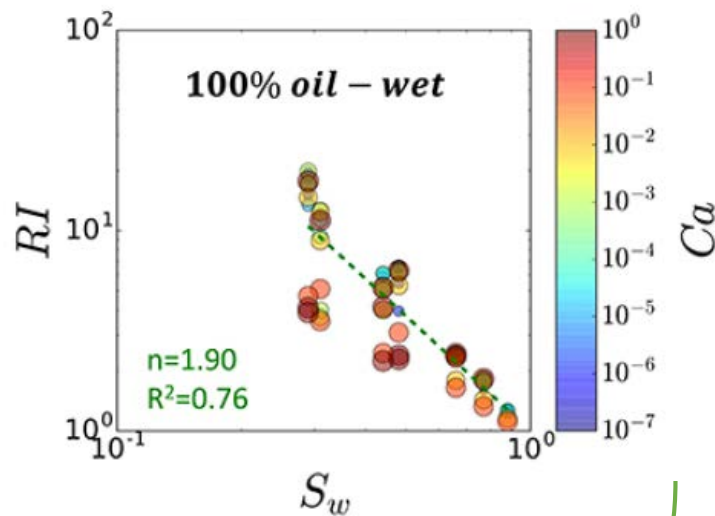
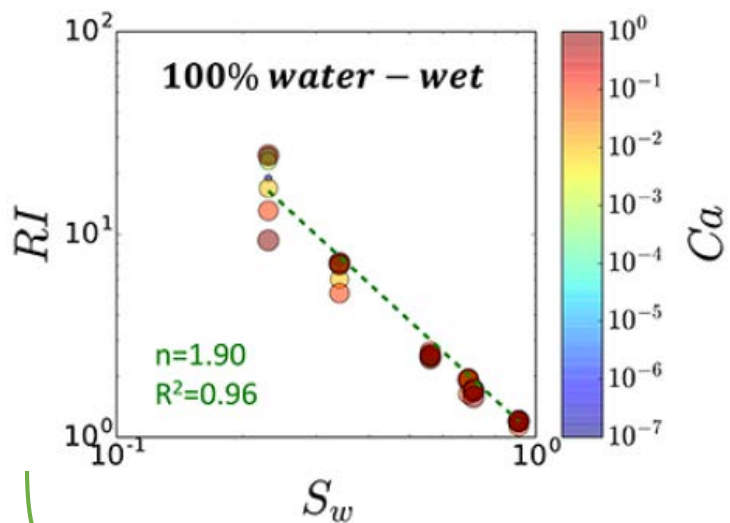
$$K = \kappa_1 \kappa_2 > 0$$

$$K = \kappa_1 \kappa_2 \leq 0$$

Resistivity Index and Topology

Percolation Theory:

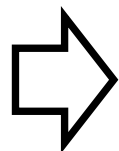
$$\xi \sim (p - p_c)^\beta$$



Percolation parameter = **Saturation**

Percolation parameter = **Topology**

Models comparing percolation parameters for various wetting conditions.

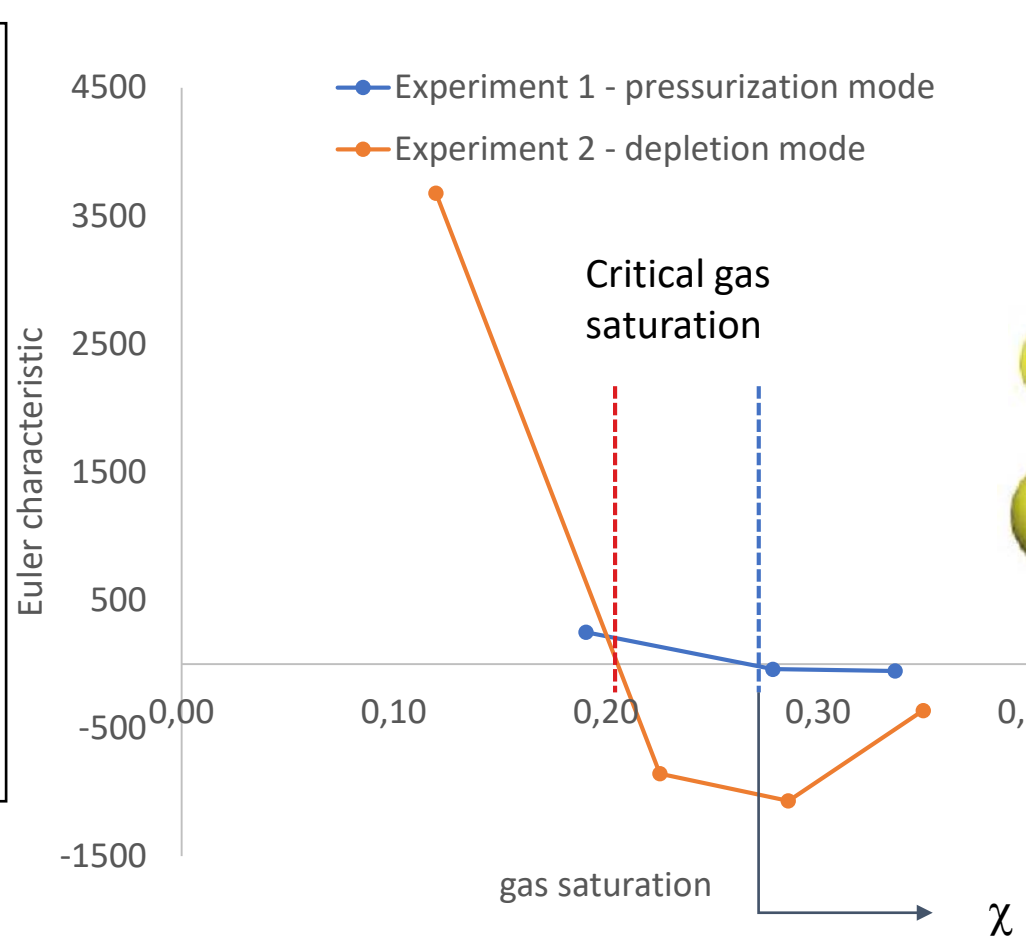
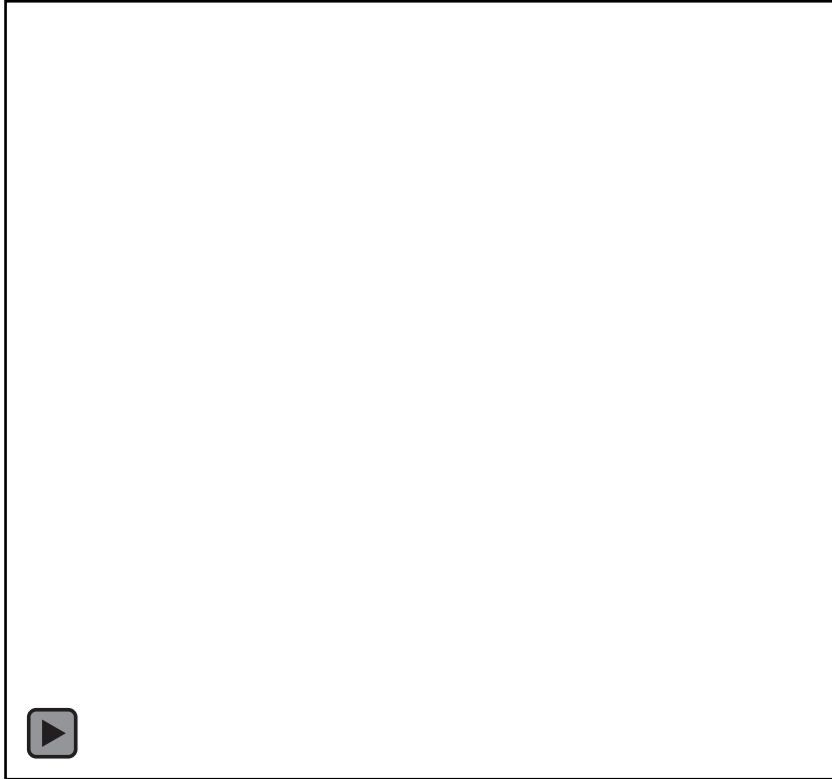


| Wettability | $lg(RI) \sim lg(S_w)$ | $lg(RI) \sim lg(\chi_w/\chi_p)$ |
|----------------|-----------------------|---------------------------------|
| 100% water-wet | 0.98 | 0.22 |
| 50% water-wet | 0.97 | 0.97 |
| 50% oil-wet | 0.88 | 0.96 |
| 100% oil-wet | 0.82 | 0.90 |

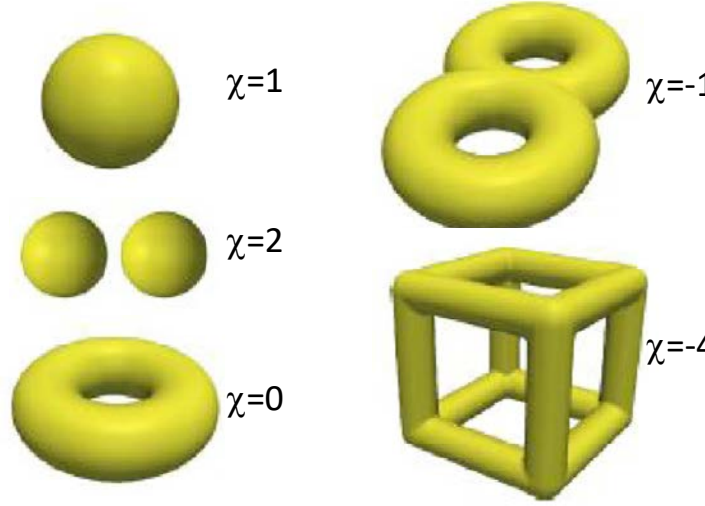


Euler characteristic inferred from RI

Phase Connectivity in Critical Gas Saturation



Euler Characteristic $\chi =$
Objects – Loops (+ Inclusions)



$\chi = 0 \rightarrow$ percolation threshold

→ See SCA021 on Wednesday, 11:30

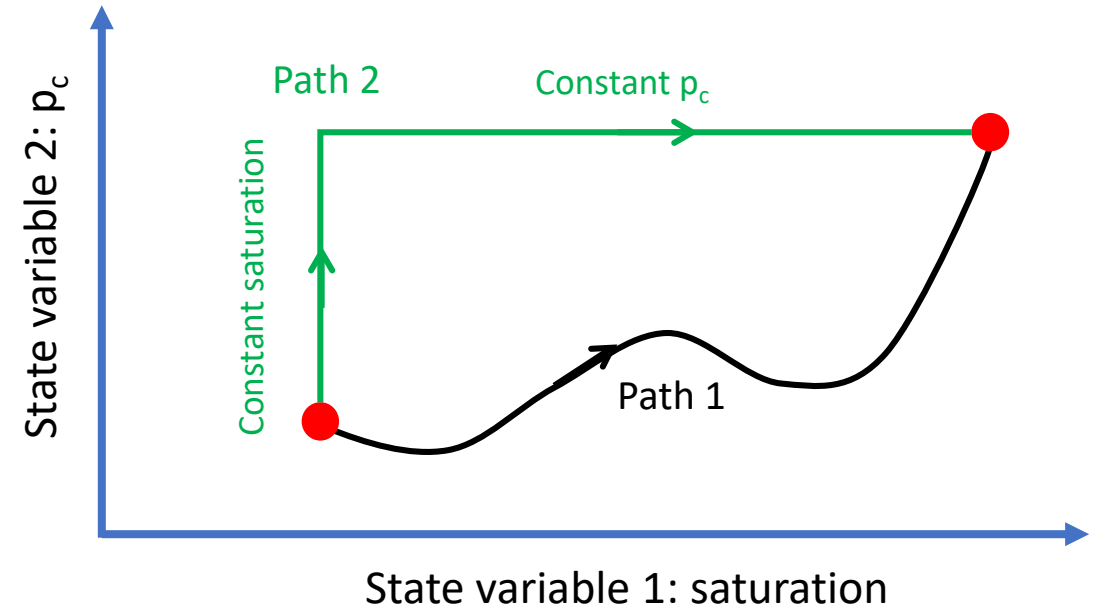
Application: Relative Permeability Hysteresis Modelling

Advantage of state-variable description: path-independence

1. Can express any parameter, e.g. k_r as total differential of state variables

$$dk_r = \underbrace{\frac{\partial k_r}{\partial S} dS + \frac{\partial k_r}{\partial \hat{\chi}} d\hat{\chi}}_{\text{Phase distribution}} + \underbrace{\frac{\partial k_r}{\partial I} dI}_{\text{Wettability}} + \underbrace{\frac{\partial k_r}{\partial N_{CA}} dN_{CA}}_{\text{Capillary number}} + \underbrace{\frac{\partial k_r}{\partial \lambda} d\lambda}_{\text{Rock structure}}$$

SPE-182655 (Penn State group)



2. Can choose different paths to measure k_r

- e.g. branch 1: constant saturation (steady-state, constant fractional flow F_w)
- branch 2: constant p_c (porous plate)

Application: Relative Permeability Hysteresis Modelling

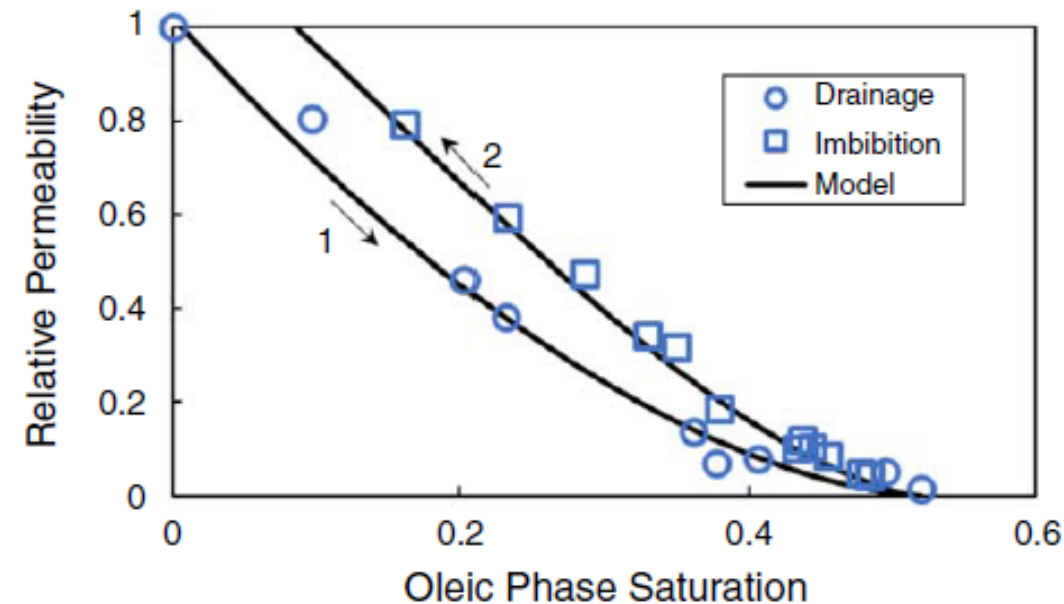
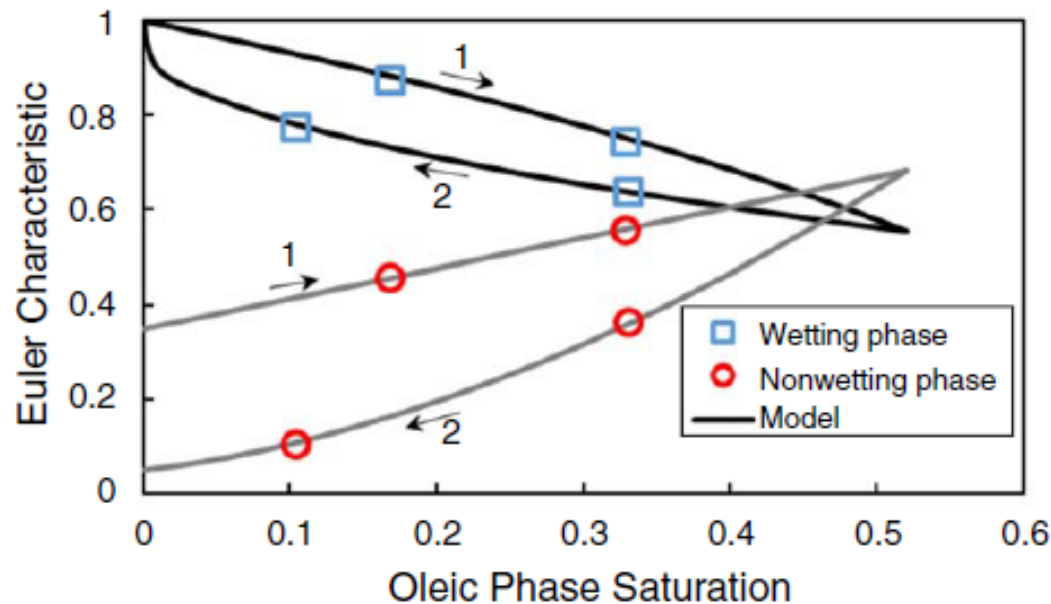
Relative permeability as an

Equation of State (EOS)

SPE-182655 (R. T. Johns)

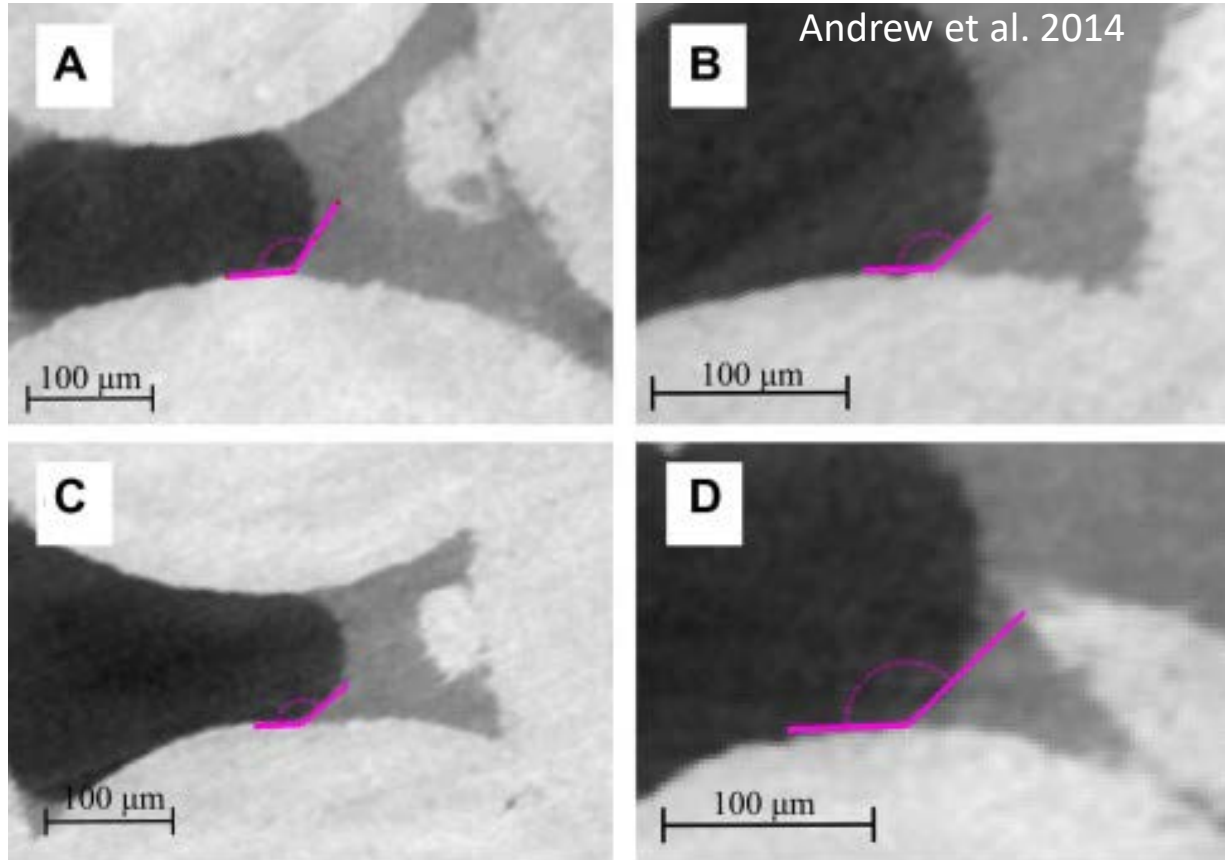
$$dk_r = \underbrace{\frac{\partial k_r}{\partial S} dS + \frac{\partial k_r}{\partial \hat{\chi}} d\hat{\chi}}_{\text{Phase distribution}} + \underbrace{\frac{\partial k_r}{\partial I} dI}_{\text{Wettability}} + \underbrace{\frac{\partial k_r}{\partial N_{CA}} dN_{CA}}_{\text{Capillary number}} + \underbrace{\frac{\partial k_r}{\partial \lambda} d\lambda}_{\text{Rock structure}}$$

| | | |
|------------------------------------------|--------------------------------------------------------|--------------------------------------|
| | $\frac{\partial S}{\partial t} > 0$ | $\frac{\partial S}{\partial t} < 0$ |
| $\frac{\partial \hat{\chi}}{\partial S}$ | $\alpha_z \left(\frac{\hat{\chi} - 1}{S - 1} \right)$ | $\frac{1}{C_z (\hat{\chi} S)^{n_z}}$ |



Application: Wettability

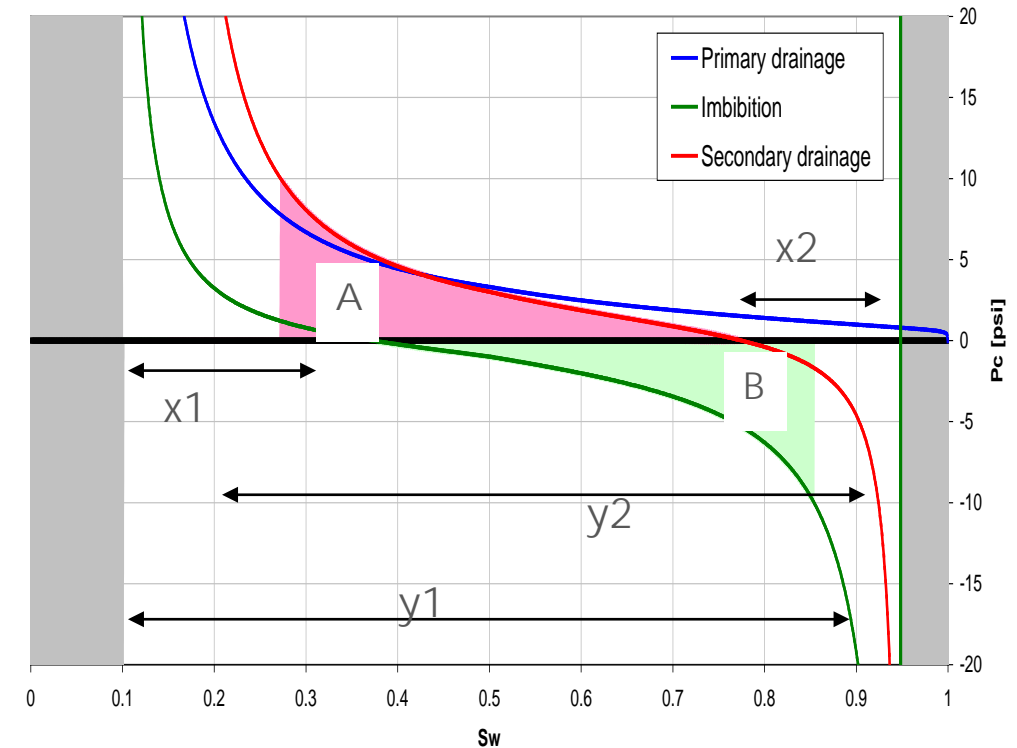
Pore scale



Effective contact angle \neq intrinsic contact angle
(Intrinsic contact angle \sim surface energy)

Darcy-SCAL scale

via capillary pressure curve



Contact Angle from Deficit Curvature

Gauss-Bonnet Theorem

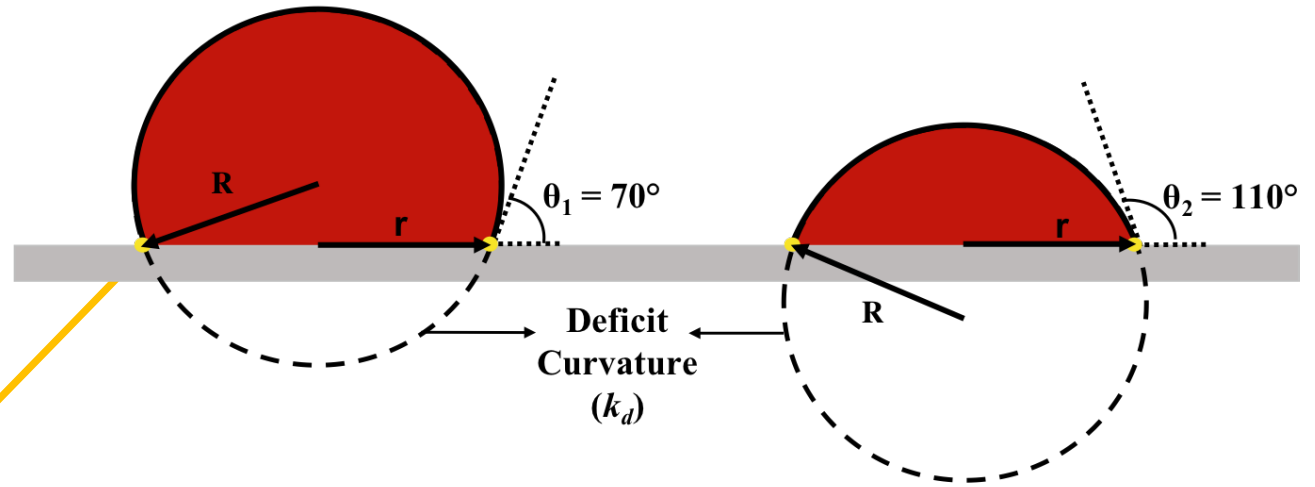
$$\int_S [1/(r_1 r_2)] ds + \int_B k_g dl = 2\pi\chi(S)$$

Total geodesic curvature
along the **contact line**

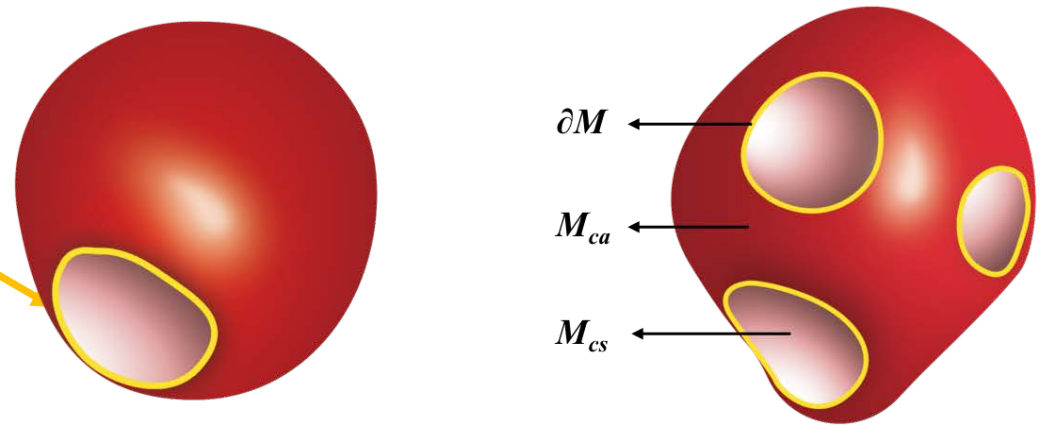
Deficit Curvature, k_d

Macroscopic contact angle $\theta_{macro} = \frac{\kappa_d}{4N_c}$

Sessile Drop



3D Oil Cluster



Contact Angle = Deficit Curvature

Gauss Bonnet Theorem

$$2\pi\chi(M) = \int_M \overset{\text{Gaussian curvature}}{\kappa_T} dS + \int_{\partial M} \overset{\text{Geodesic curvature}}{\kappa_g} dC$$

For each region:

Fluid-Fluid

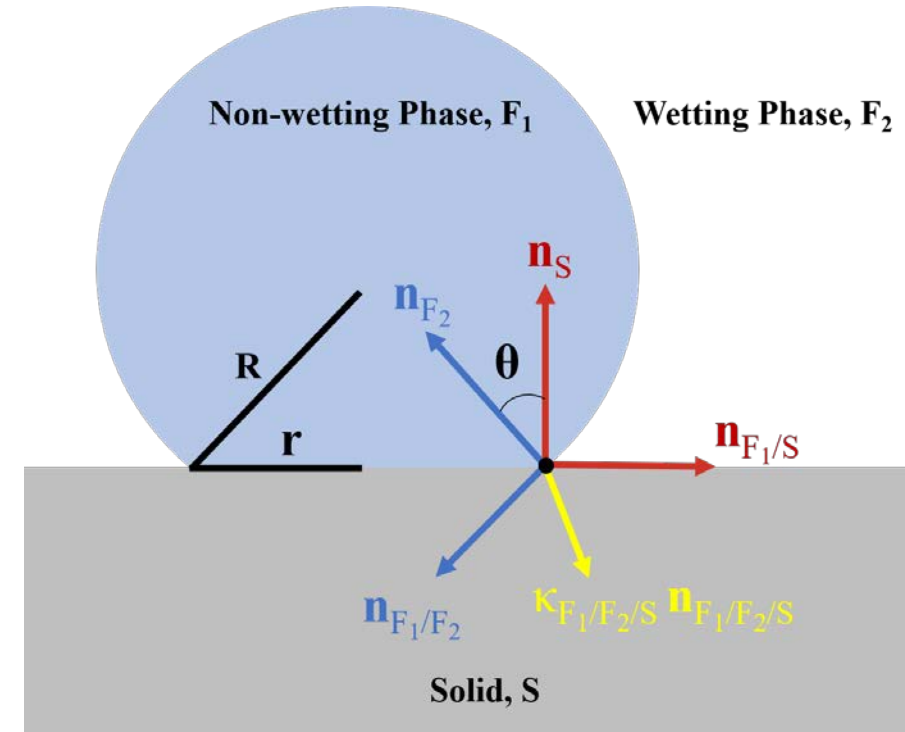
$$2\pi\chi(M_{ab}) = \int_{M_{ab}} \kappa_T dS + \int_{\partial M_{ab}} \kappa_g dC,$$

Fluid-solid

$$2\pi\chi(M_{bs}) = \int_{M_{bs}} \kappa_T dS + \int_{\partial M_{bs}} \kappa_g dC.$$

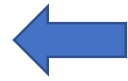
$$4\pi\chi(C) = 2\pi\chi(M_{ab}) + 2\pi\chi(M_{bs})$$

$$= \int_{M_{ab}} \kappa_T dS + \int_{M_{bs}} \kappa_T dS + \int_{\partial M} (\kappa_{gab} + \kappa_{gbs}) dC$$



Contact Angle = Deficit Curvature

$$k_d = 4\pi\chi(C) - \kappa_{ab}A_{ab} - \kappa_{bs}A_{bs}$$



$$4\pi\chi(C) = 2\pi\chi(M_{ab}) + 2\pi\chi(M_{bs})$$

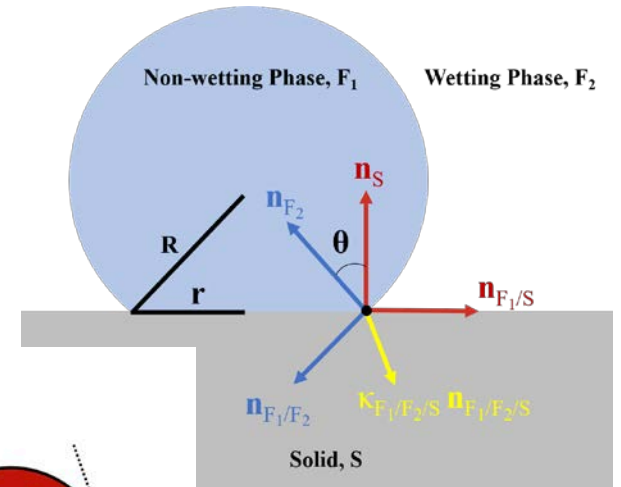
$$= \int_{M_{ab}} \kappa_T dS + \int_{M_{bs}} \kappa_T dS + \int_{\partial M} (\kappa_{gab} + \kappa_{gbs}) dC$$

with

$$\kappa_{ab} = \frac{1}{A_{ab}} \int_{M_{ab}} \kappa_T dS,$$

$$\kappa_{bs} = \frac{1}{A_{bs}} \int_{M_{bs}} \kappa_T dS,$$

$$k_d = \int_{\partial M} (\kappa_{gab} + \kappa_{gbs}) dC = \int_{\partial M} \kappa_{abs} \mathbf{n}_{abs} \cdot [\mathbf{n}_S \sin \theta + \mathbf{n}_{bs}(1 - \cos \theta)] dC$$



For N_c contacts with solid

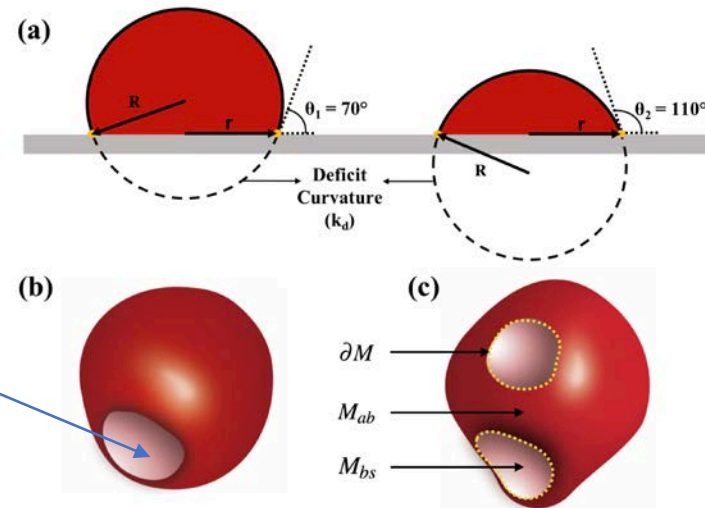
$$k_d = \sum_{j=1}^{N_c} \int_{\partial M_j} \kappa_{abs} \mathbf{n}_{abs} \cdot [\mathbf{n}_S \sin \theta + \mathbf{n}_{bs}(1 - \cos \theta)] dC$$



Macroscopic contact angle

$$\theta^{macro} = \frac{k_d}{4N_c}$$

Number of contacts N_c



Contact Angle = Deficit Curvature

Macroscopic contact angle $\theta^{macro} = \frac{k_d}{4N_c}$

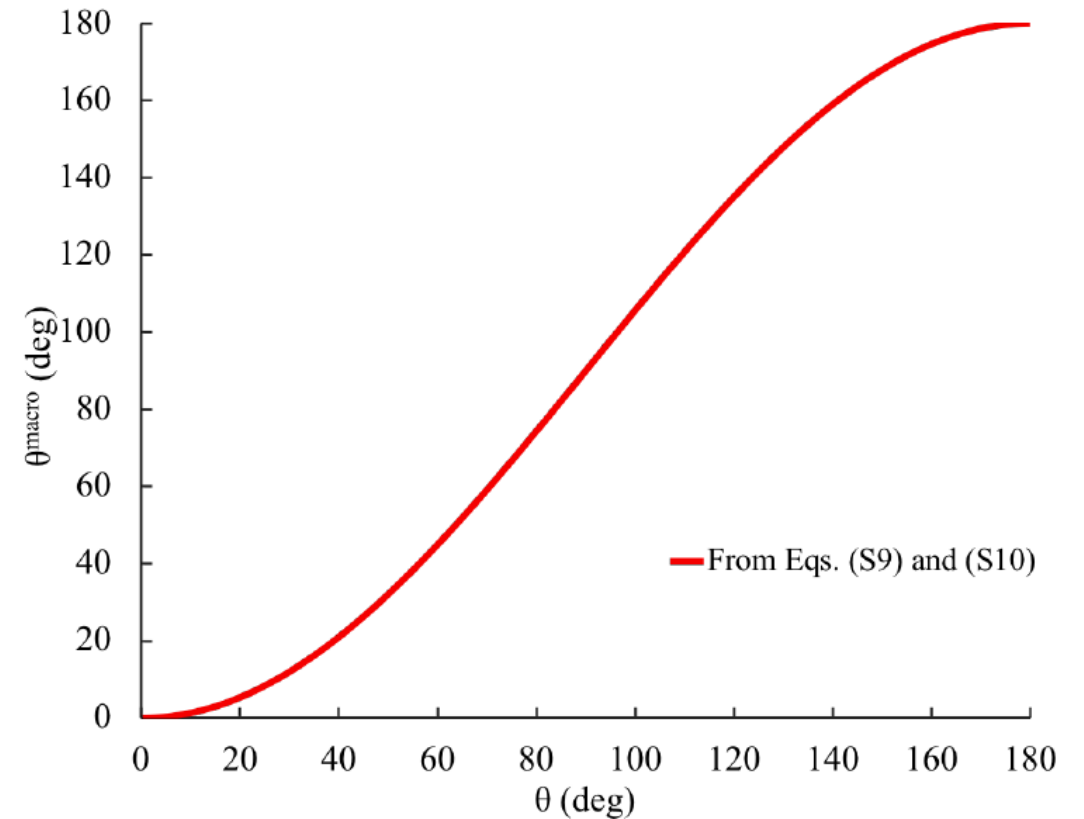
For 1 sessile droplet:

$$\kappa_{gab} = -\sqrt{1 - (r/R)^2}/r \quad \kappa_{gbs} = 1/r.$$

$$r = R \sin \theta.$$

$$\begin{aligned} k_d &= \int_{\partial M} \frac{1}{r} \left(1 - \sqrt{1 - (r/R)^2}\right) dC \\ &= 2\pi \left(1 - \sqrt{1 - (R \sin \theta / R)^2}\right) \\ &= 2\pi(1 - \cos \theta). \end{aligned}$$

$$\theta^{macro} = \frac{\pi(1 - \cos \theta)}{2}$$



Contact Angle = Deficit Curvature

Macroscopic contact angle $\theta^{macro} = \frac{k_d}{4N_c}$

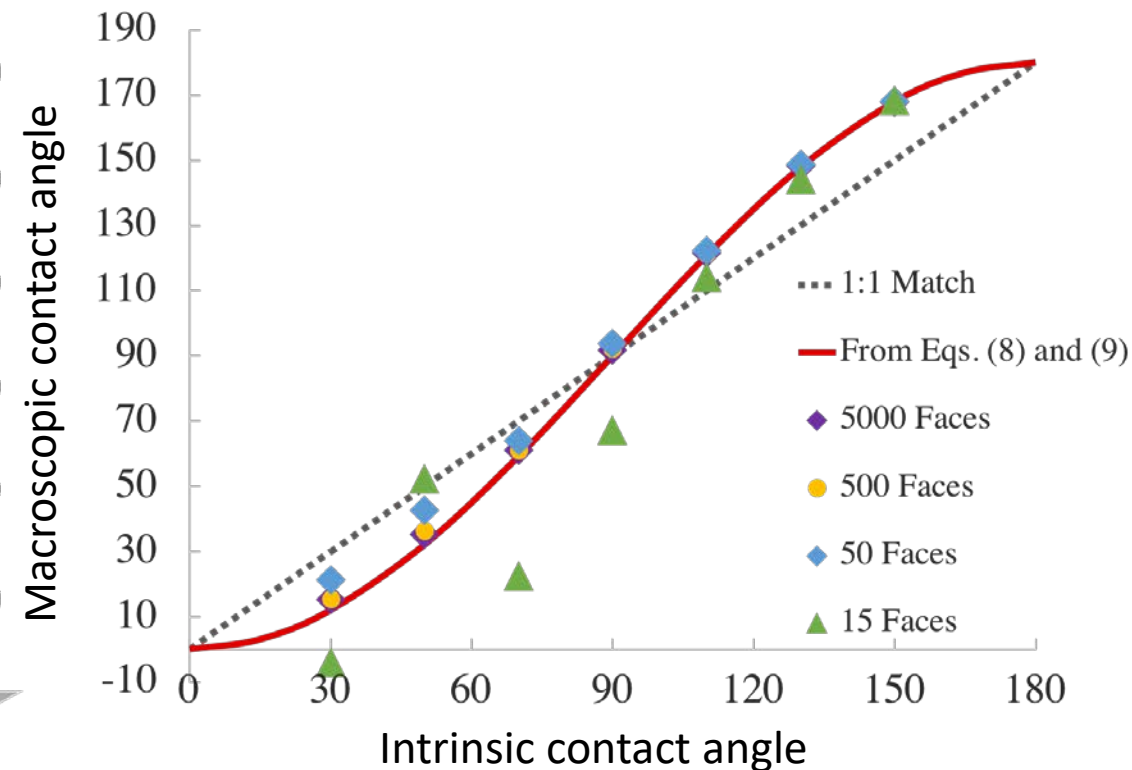
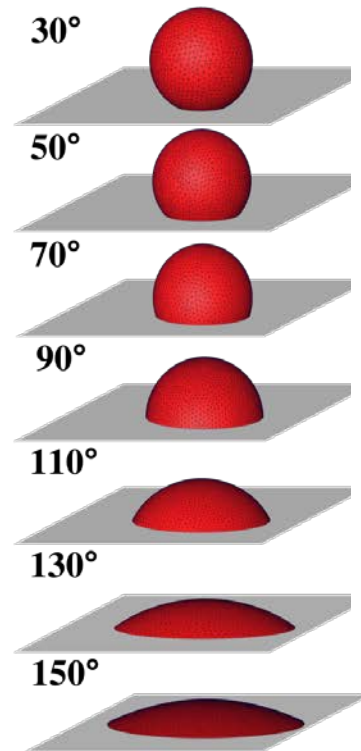
For 1 sessile droplet:

$$\kappa_{gab} = -\sqrt{1 - (r/R)^2}/r \quad \kappa_{gbs} = 1/r.$$

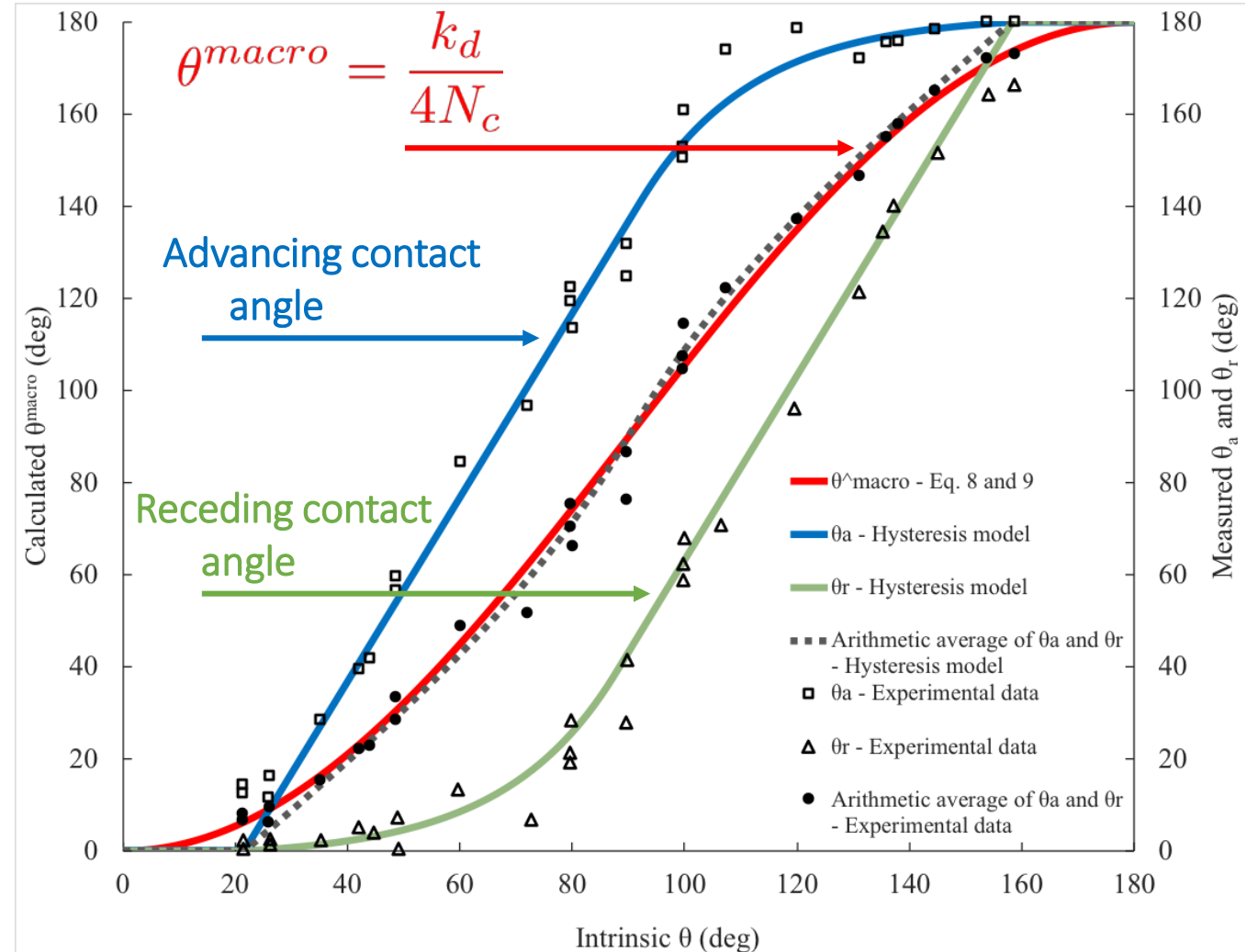
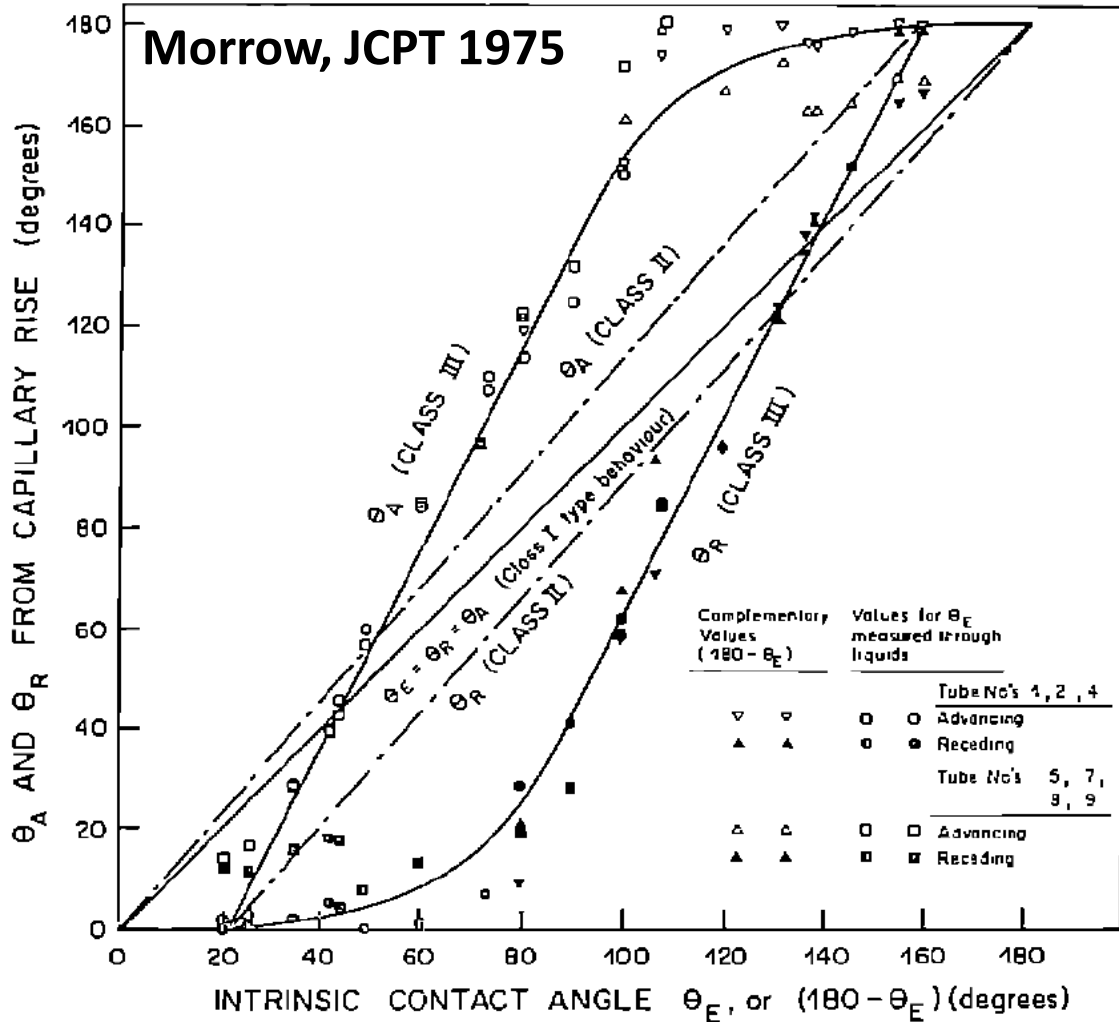
$$\begin{aligned} k_d &= \int_{\partial M} \frac{1}{r} \left(1 - \sqrt{1 - (r/R)^2}\right) dC \\ &= 2\pi \left(1 - \sqrt{1 - (R \sin \theta / R)^2}\right) \\ &= 2\pi(1 - \cos \theta). \end{aligned}$$

$$\theta^{macro} = \frac{\pi(1 - \cos \theta)}{2}$$

$$r = R \sin \theta.$$

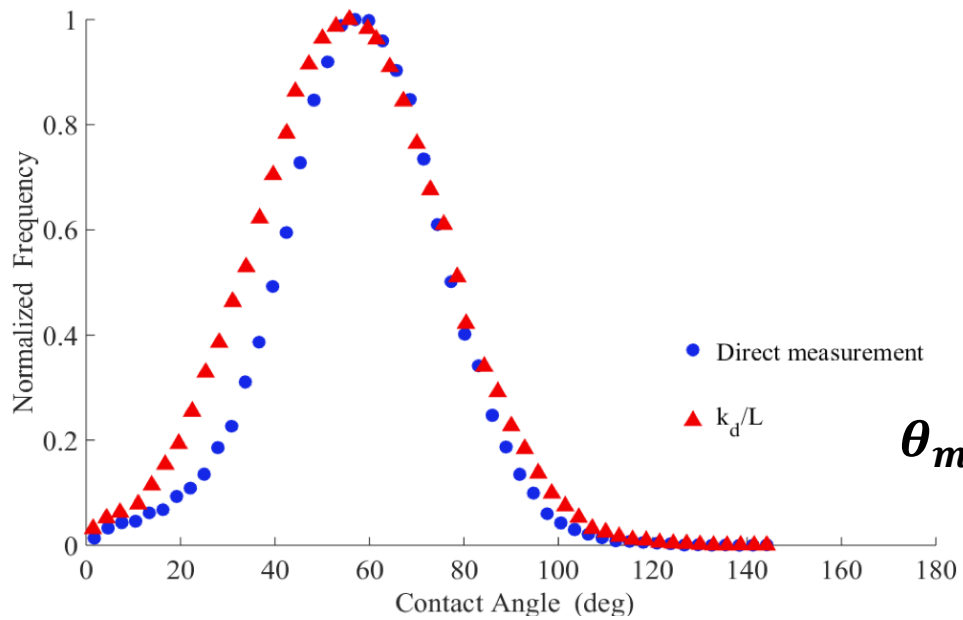


Validation: Advancing and Receding Contact angle

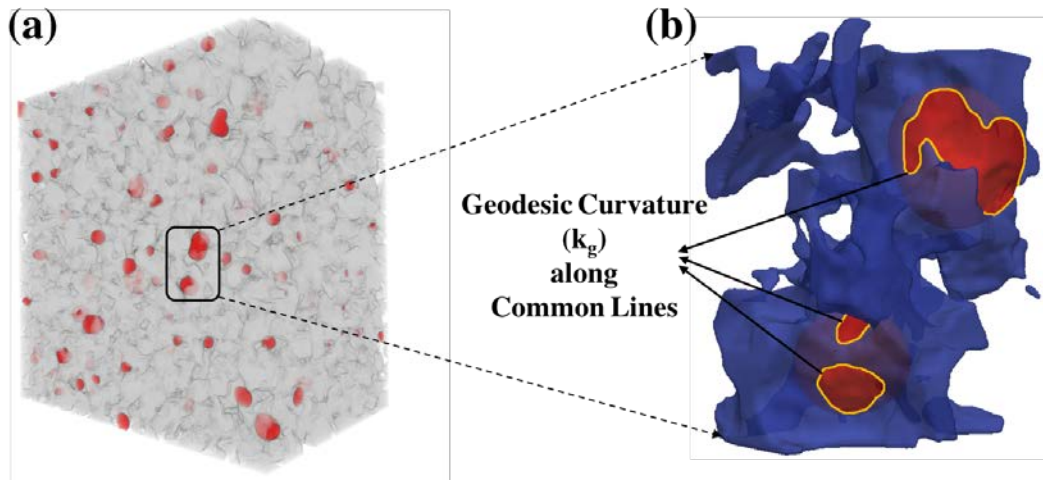


Predicting Contact Angle from oil cluster distribution & $p_c(S_w)$

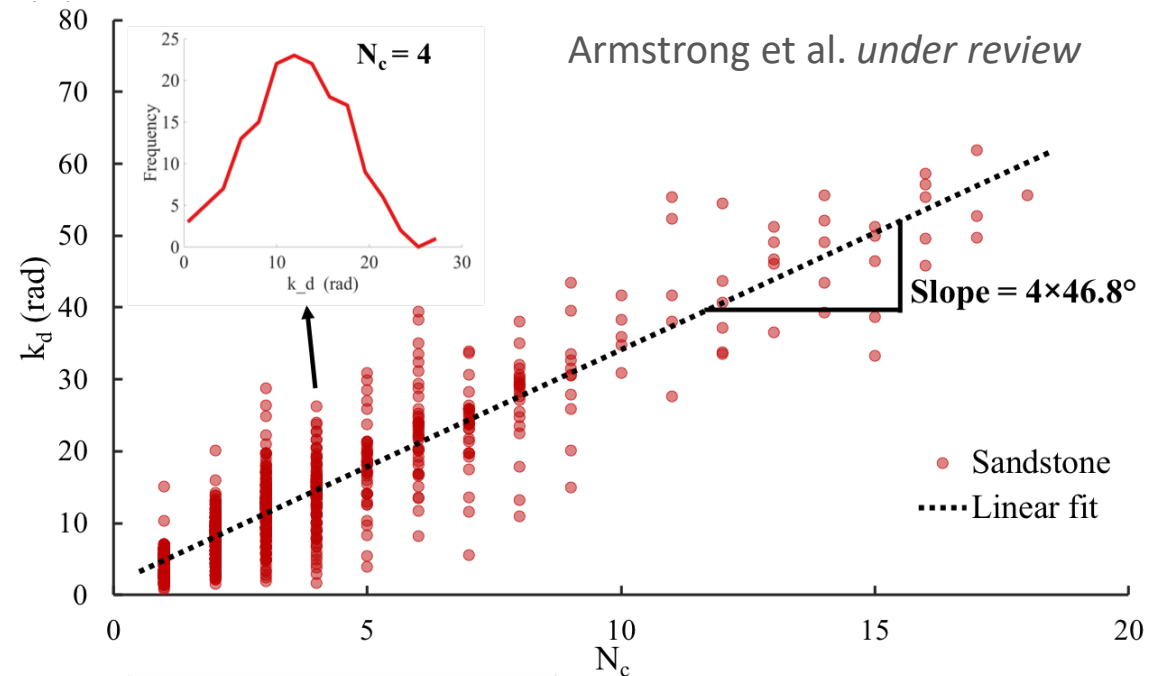
→ SCA009 (Tuesday, 9:30)



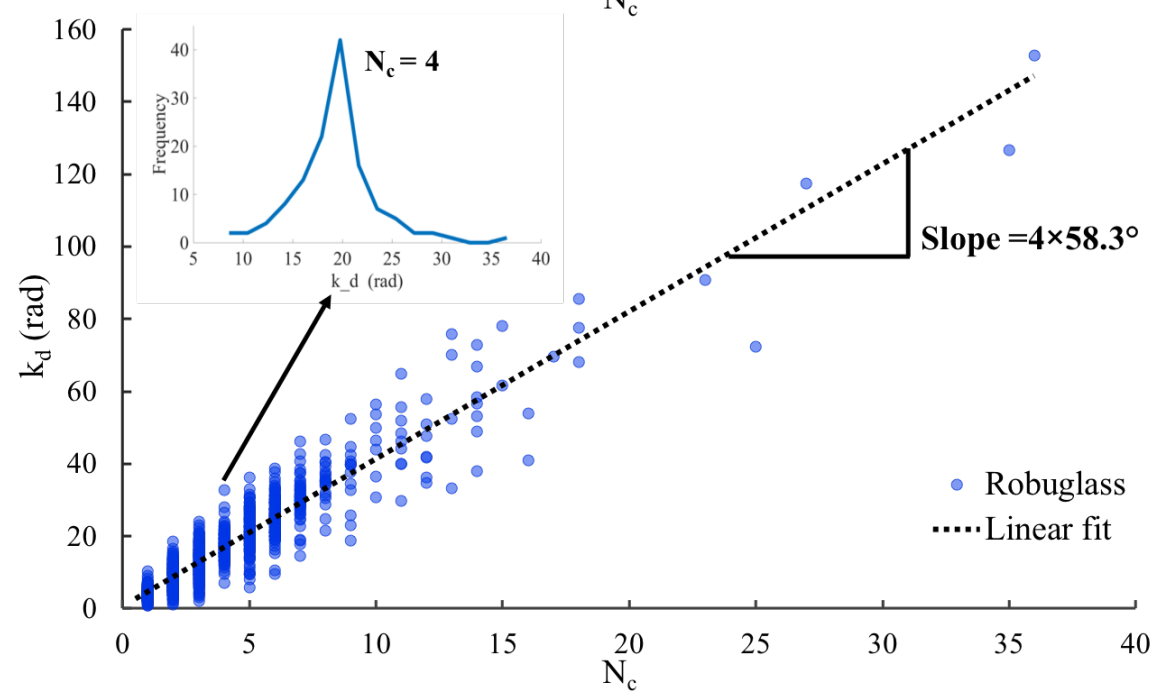
$$\theta_{macro} = \frac{\kappa_d}{4N_c}$$



Sandstone rock

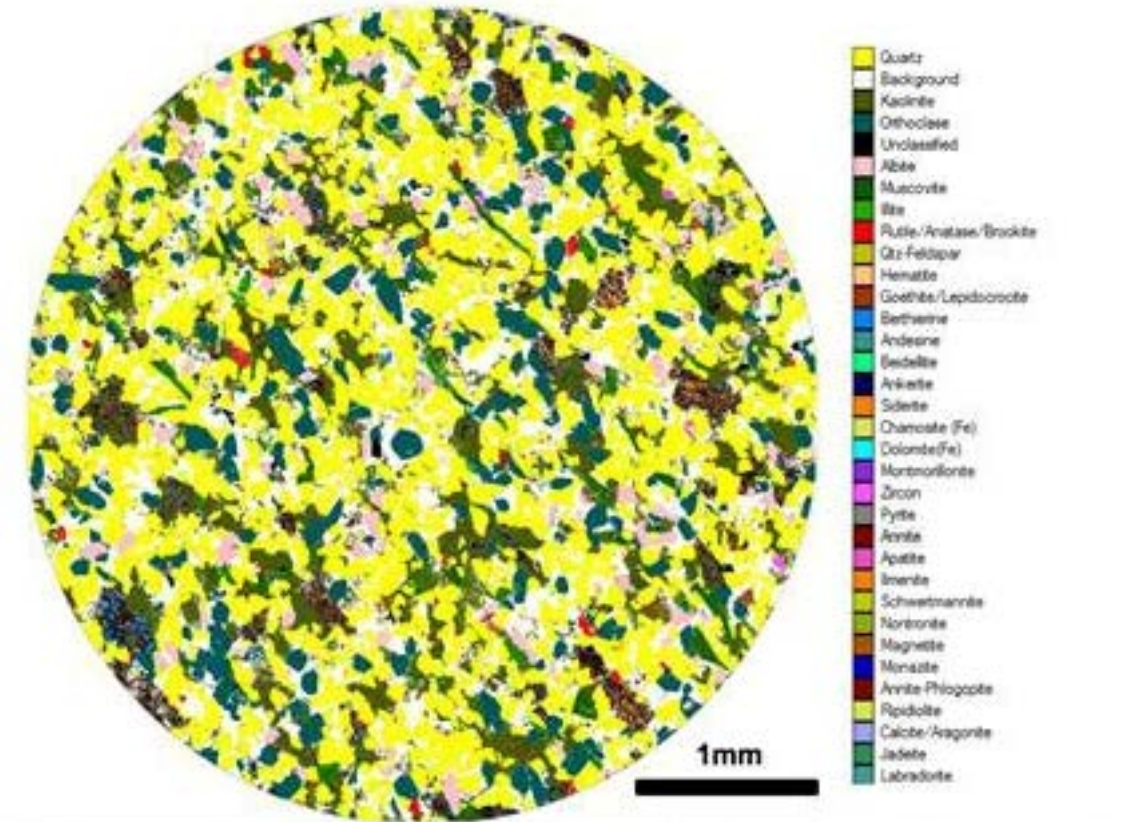


Sintered glass

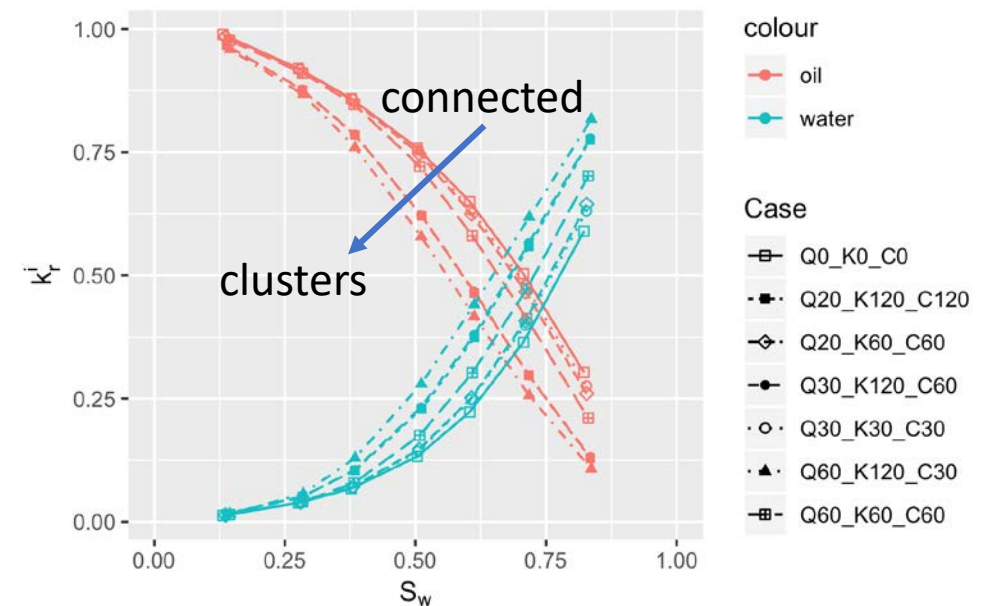
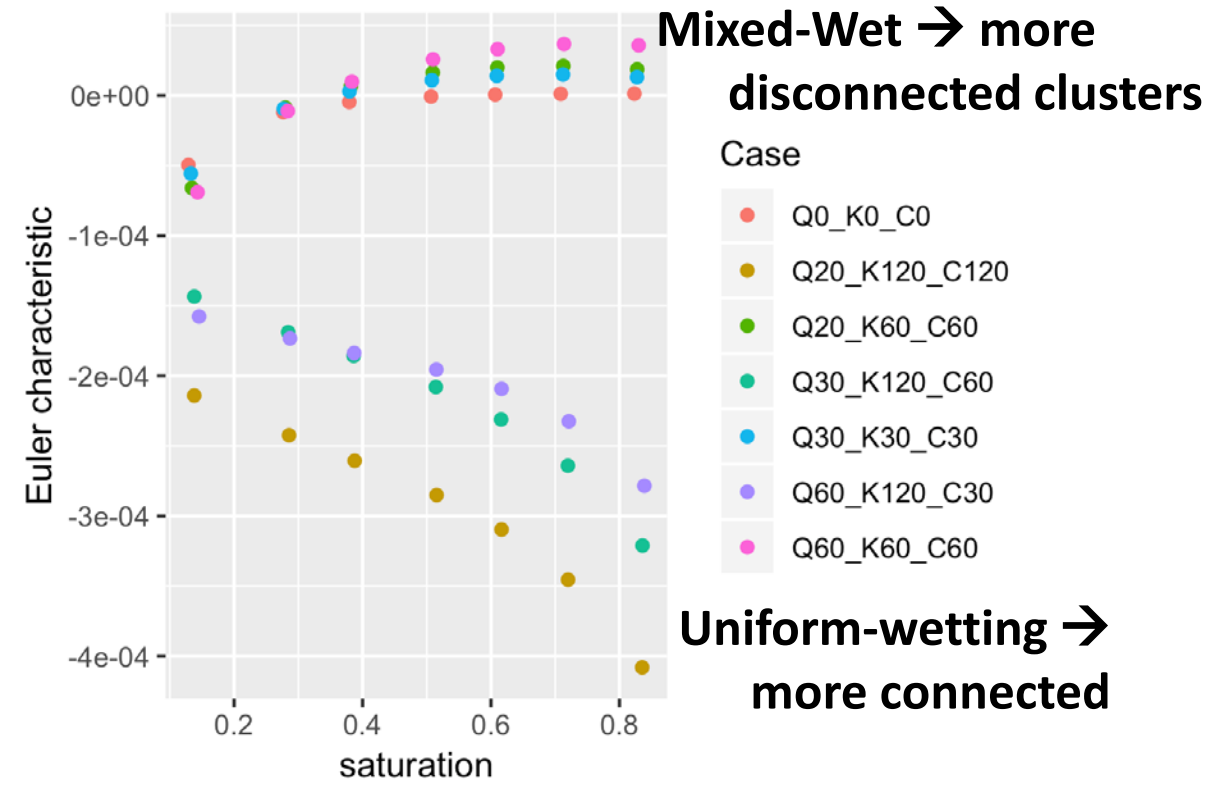


Minerology, Wettability and Topology

QEMSCAN DATA, Pore-Scale Minerology



Euler characteristic quantifies impact of wettability on the connectivity of the oil phase



Fractured Porous Media

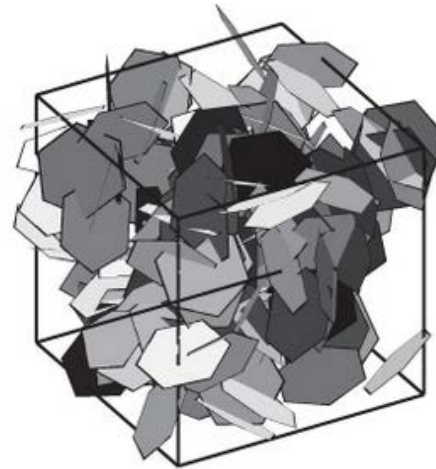
Original works of Adler (Fractured Porous Media)

PRL, Scholz et al. 2012

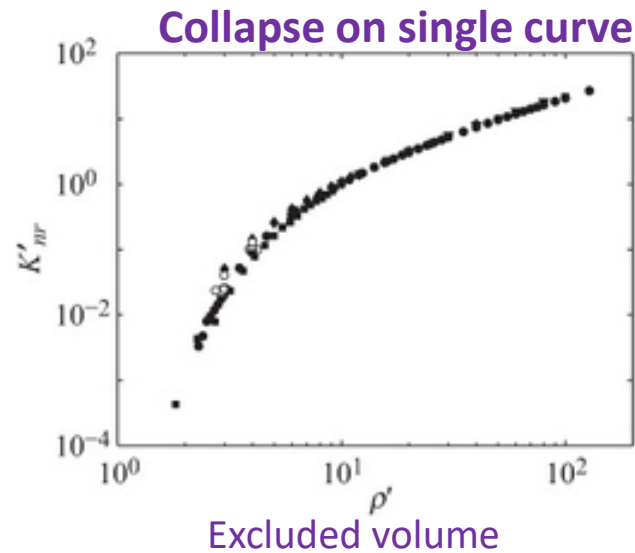
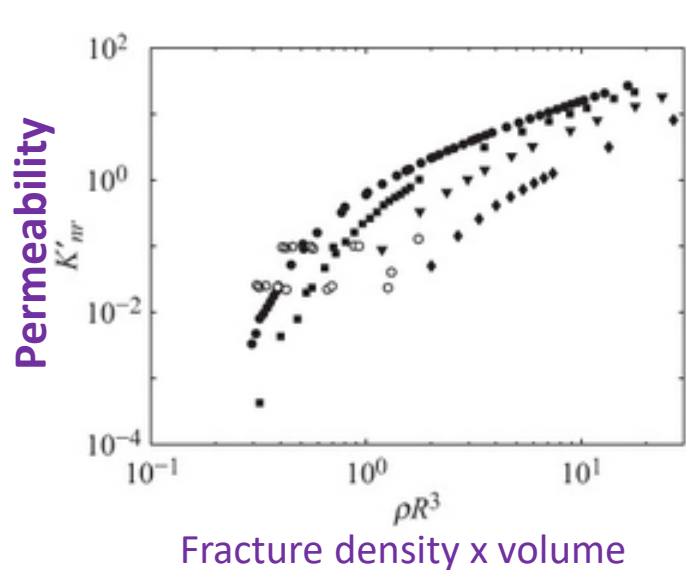
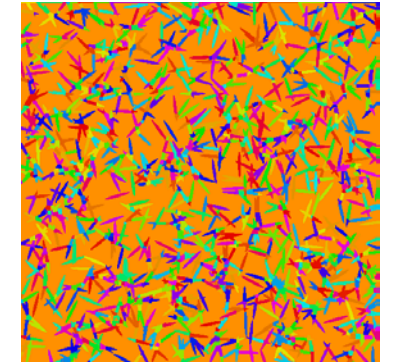
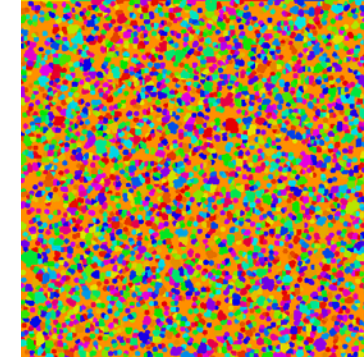
Dimensionless Density, ρ'

A measure of the connectivity of the fracture network

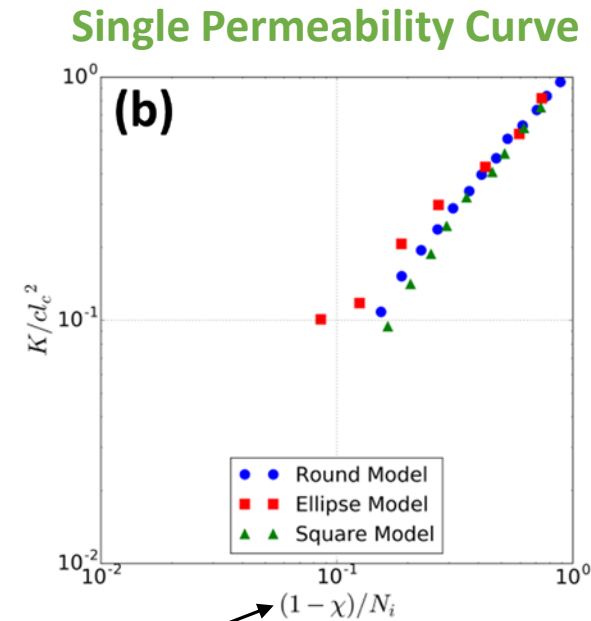
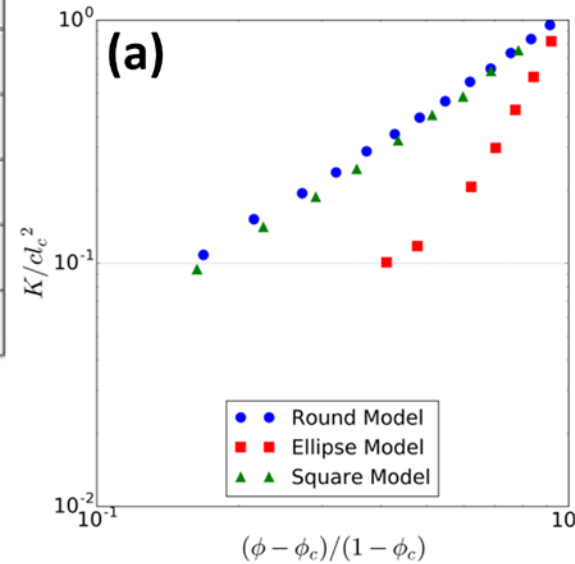
Fracture Network



2D Porous Structures



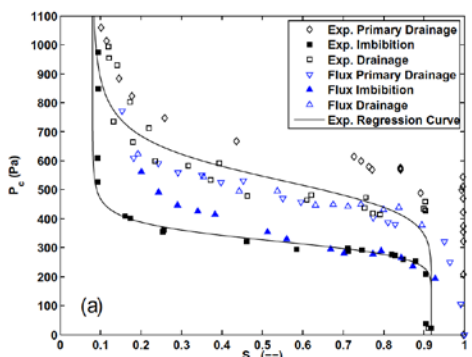
Number of Loops, $B_1 = [(\rho'/2) - 1]\rho'$



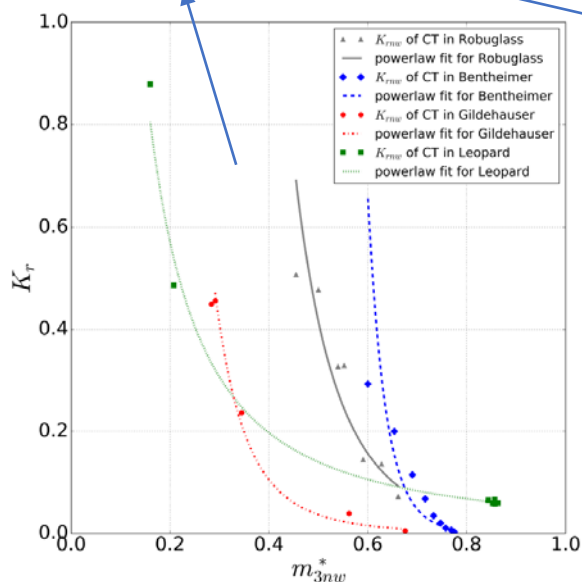
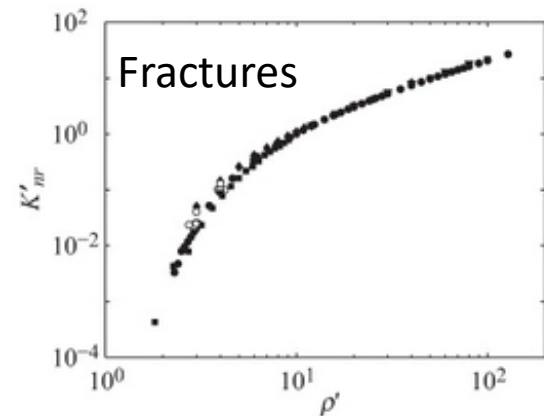
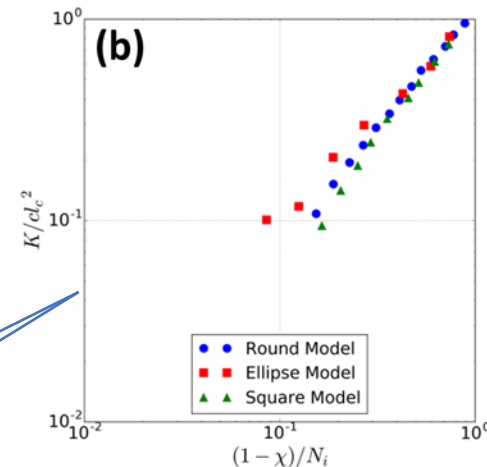
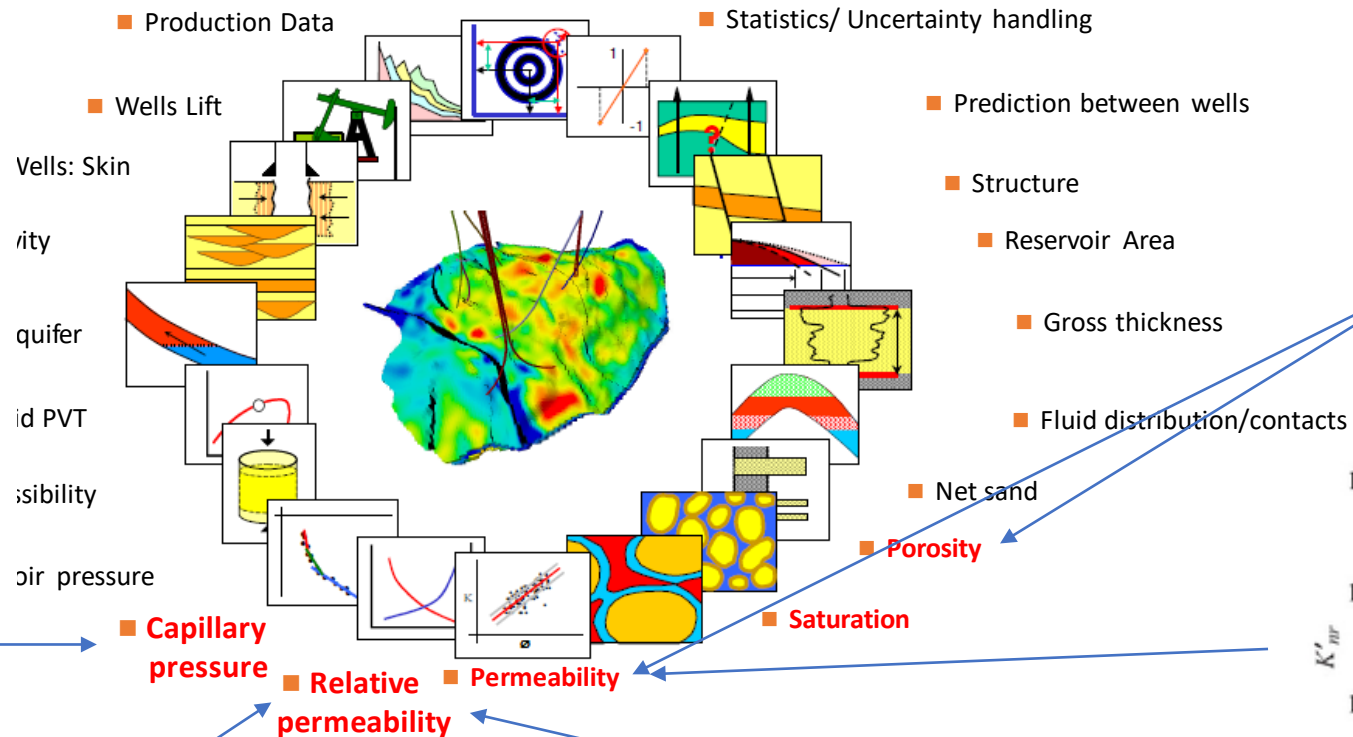
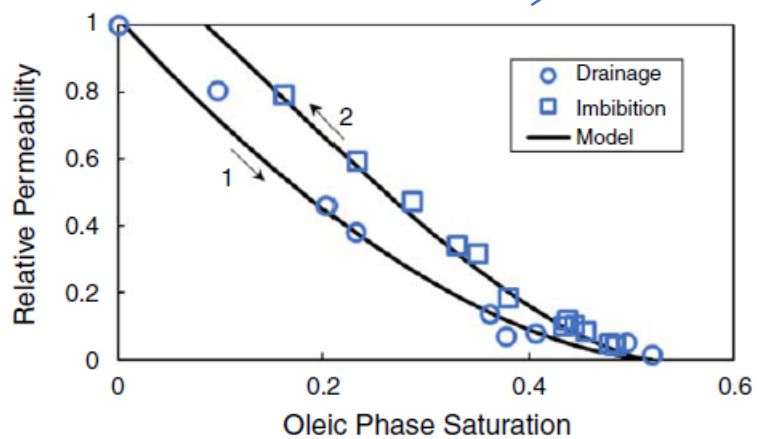
[LOOPS + OBJECTS] / OBJECTS

Conclusions

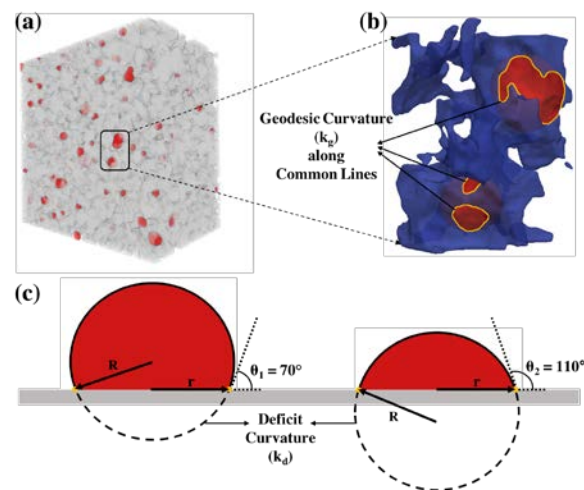
Pc hysteresis



Relperm hysteresis



wettability



Key Literature

Review Papers and Textbooks

- Porous Media Characterization Using Minkowski Functionals: Theories, Applications and Future Directions
Transport in Porous Media, 2018 *in press* doi:10.1007/s11242-018-1201-4
- J. Ohser, F. Mücklich, Statistical analysis of microstructures in materials science, Wiley, 2000.
- Klaus R. Mecke, Dietrich Stoyan, Statistical Physics and Spatial Statistics. The Art of Analyzing and Modeling Spatial Structures and Pattern Formation, Lecture Notes in Physics, Springer, 2000.

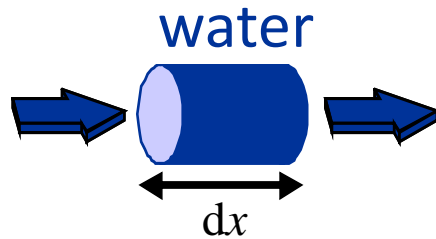
Research Papers

- C. H. Arns, M. A. Knackstedt, K. Mecke, 3D Structural Analysis: Sensitivity of Minkowski Functionals.
Journal of Microscopy 240, 181-196, 2010.
- H.J. Vogel, U. Weller, S. Schlüter, Quantification of Soil Structure Based on Minkowski Functions,
Computers & Geosciences 36, 126-1251, 2010.
- Herring et al. Advances in Water Resources 62, 47-58, 2013.
- S. Schlüter, S. Berg, M. Rücker, R. T. Armstrong, H.-J. Vogel, R. Hilfer and D. Wildenschild,
Pore scale displacement mechanisms as a source of hysteresis for two-phase flow in porous media
Water Resources Research 52(3), 2194-2205 2016.
- J. E. McClure, R. T. Armstrong, M. A. Berrill, S. Schlüter, S. Berg, W. G. Gray, C. T. Miller
A geometric state function for two-fluid flow in porous media, Phys. Rev. Fluids 3(8), 084306, 2018.
- Z. Liu, A. Herring, A. Sheppard, C. Arns, S. Berg, R. T. Armstrong, Morphological characterization of two-phase flow using
X-ray microcomputed tomography flow-experiments, Transport in Porous Media 118(1), 99-117, 2017.

Backup

2-Phase Flow in Porous Media

Single-phase

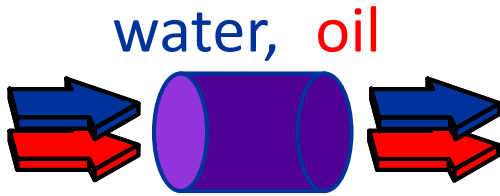


Darcy's law

$$v_{Darcy} = -\frac{K}{\mu} \frac{dp}{dx}$$

Phenomenological extension of Darcy's law
i.e. not a law anymore

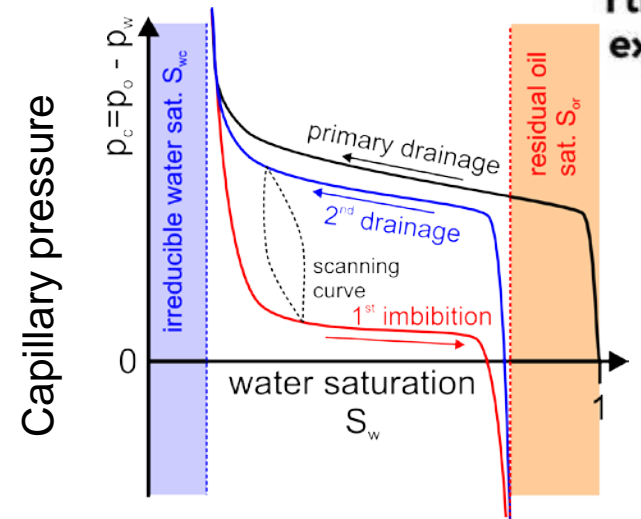
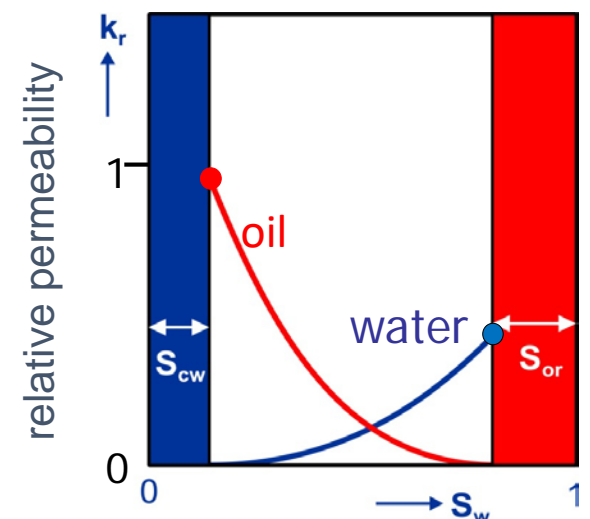
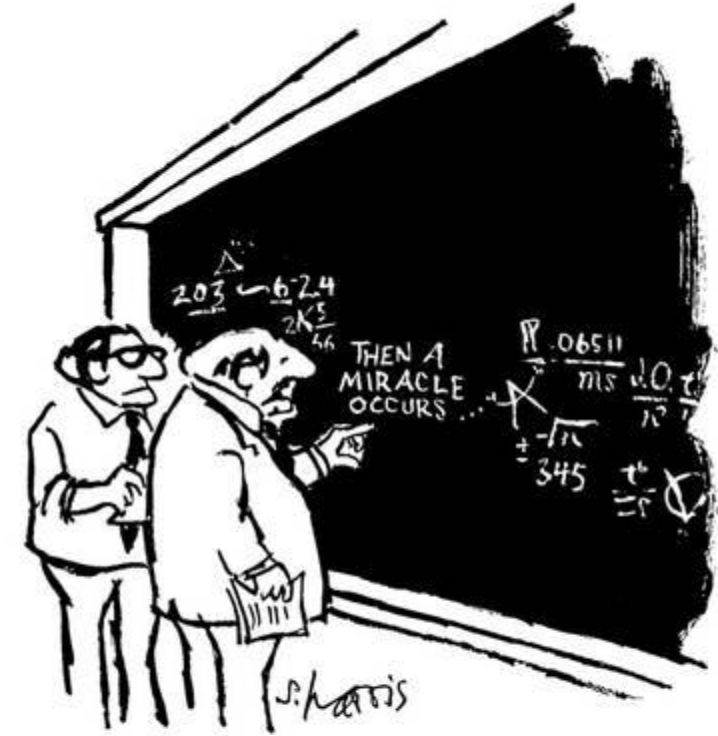
Multi-phase



$$v_i = -k_{r,i} \frac{K}{\mu_i} \frac{dp_i}{dx}$$

$$k_{r,i} = k_{r,i}(S_w)$$

$$p_c = p_o - p_w = p_c(S_w)$$



"I think you should be more explicit here in step two."

So far this has been sufficient, but

When trying to augment SCAL by Digital Rock, it is important to

- correctly classify the problem

And it becomes inevitable to understand what relative permeability actually is, i.e. face the

- Upscaling from Pore to Darcy Scale challenge

More conceptually.

The State Variables of Capillarity

Hadwiger's theorem: unique characterization of 3D objects by 4 Minkowski functionals

m_0 = volume (saturation)

m_1 = interfacial area

m_2 = mean curvature (cap. pressure)

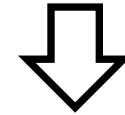
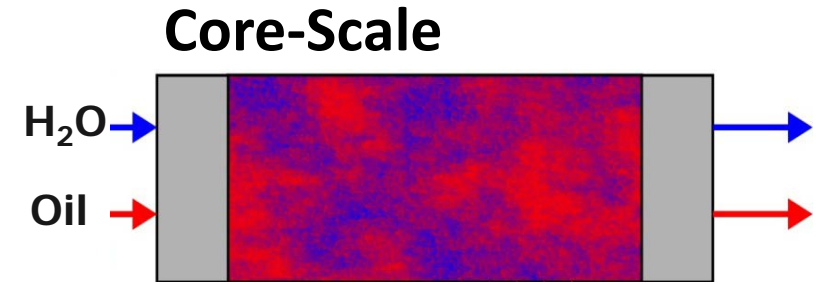
m_3 = integral curvature = $2\pi\chi$

$$M_0^n = \lambda(\Omega_n) = \int_{\Omega_n} dr$$

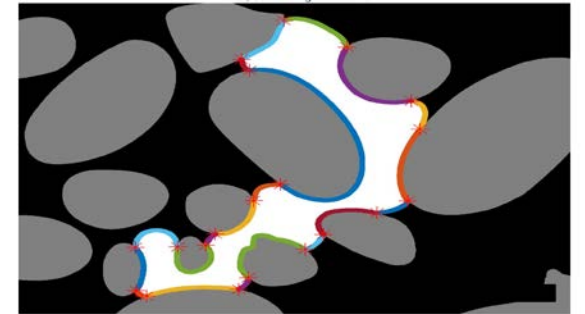
$$M_1^n = \lambda(\Gamma_n) = \int_{\Gamma_n} dr$$

$$M_2^n = \int_{\Gamma_n} \left(\frac{1}{R_1} + \frac{1}{R_2} \right) dr$$

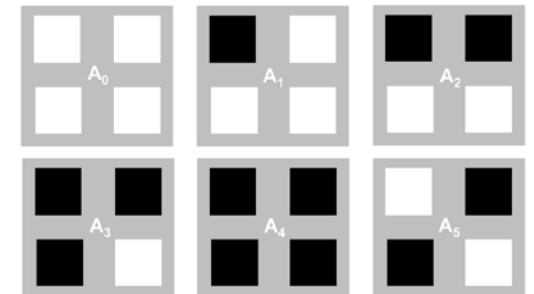
$$M_3^n = \int_{\Gamma_n} \frac{1}{R_1 R_2} dr .$$



Pore-Scale



Voxel-Scale



Capillary Pressure vs. Saturation

Capillary Pressure

$$P^c = \gamma J_w^{wn}$$

- P_c - S_w is essentially a geometric definition (or statement)
- Saturation does not uniquely define the geometrical state
- Steiner's formula suggests that all four MF are required for a unique definition

MF in terms of macro-scale parameters

$$M_0^n = \epsilon^n V$$

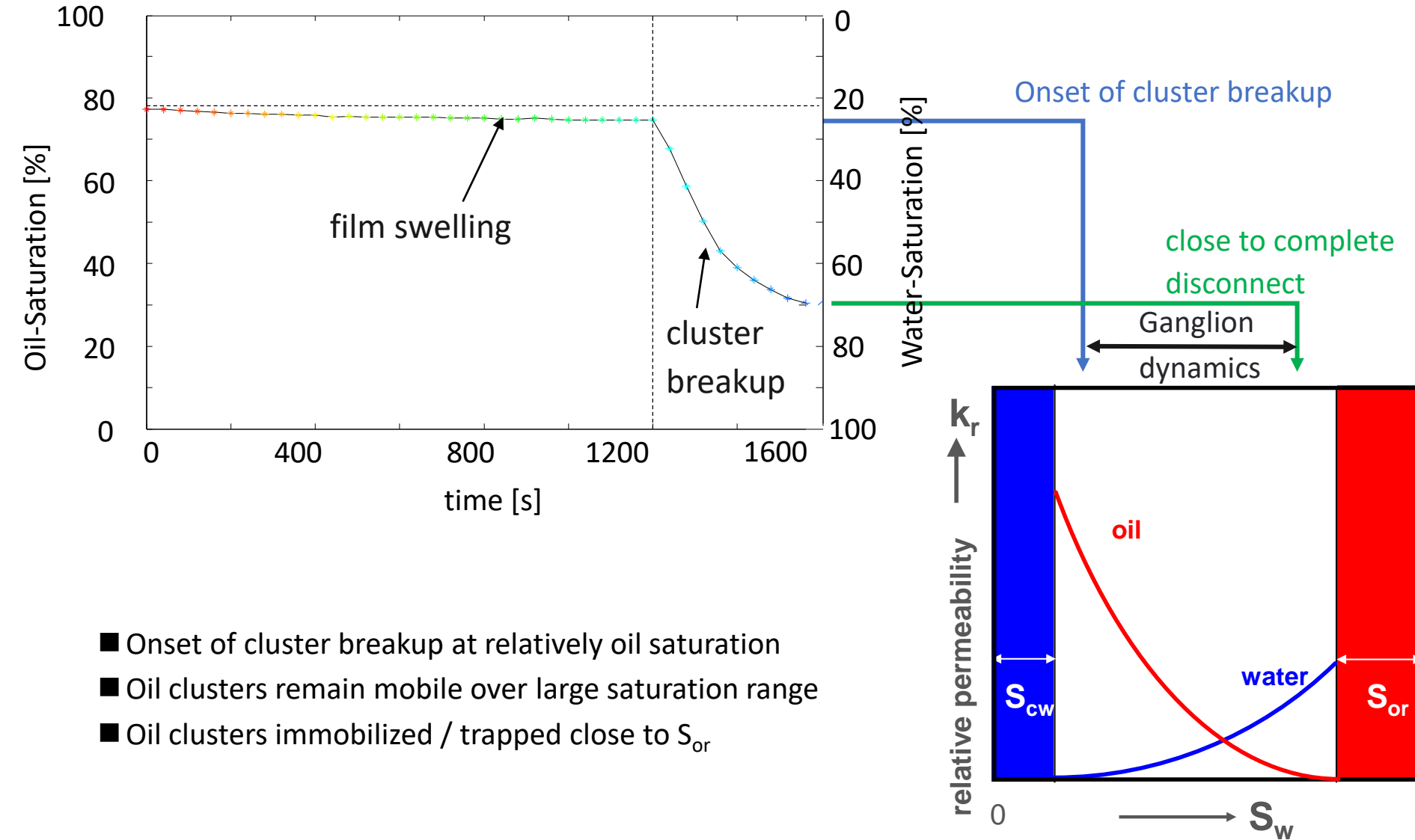
$$M_1^n = (\epsilon^{wn} + \epsilon^{ns}) V$$

$$M_2^n = (J_w^{wn} \epsilon^{wn} + J_s^{ns} \epsilon^{ns}) V$$

$$M_3^n = \chi^n$$

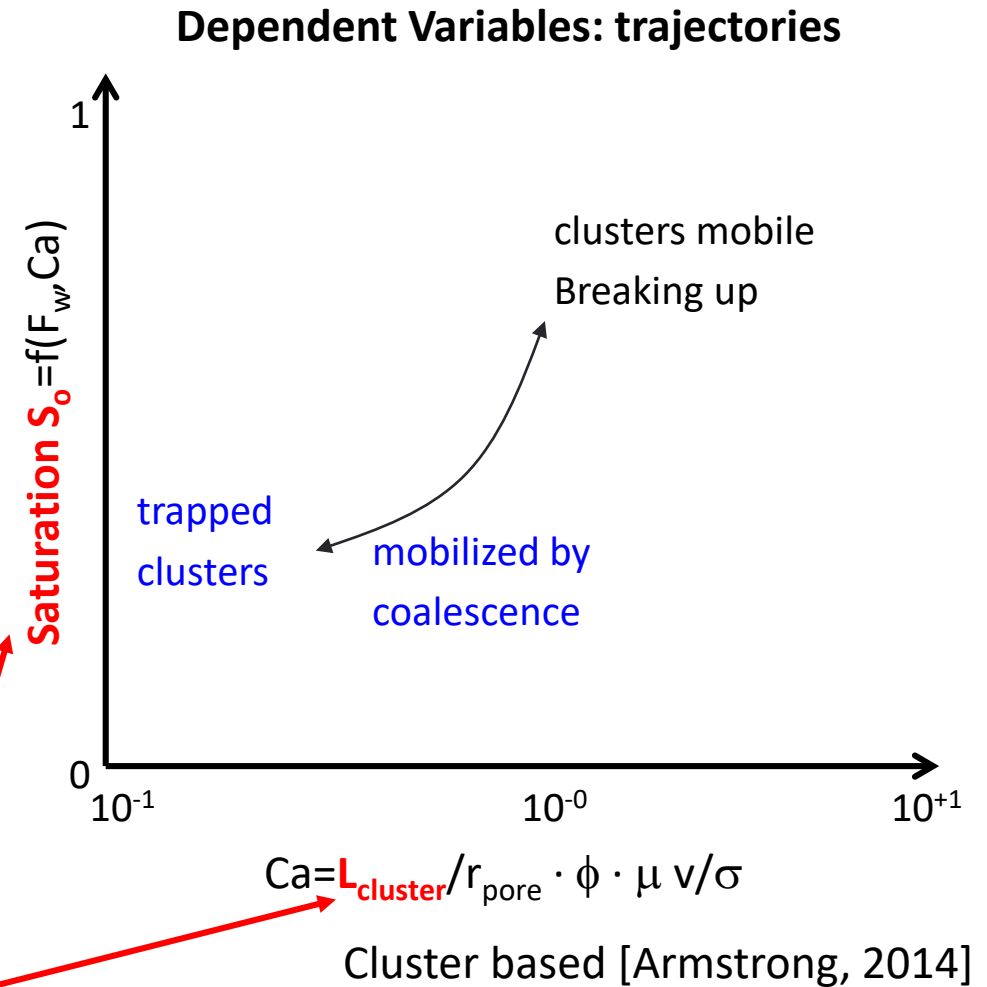
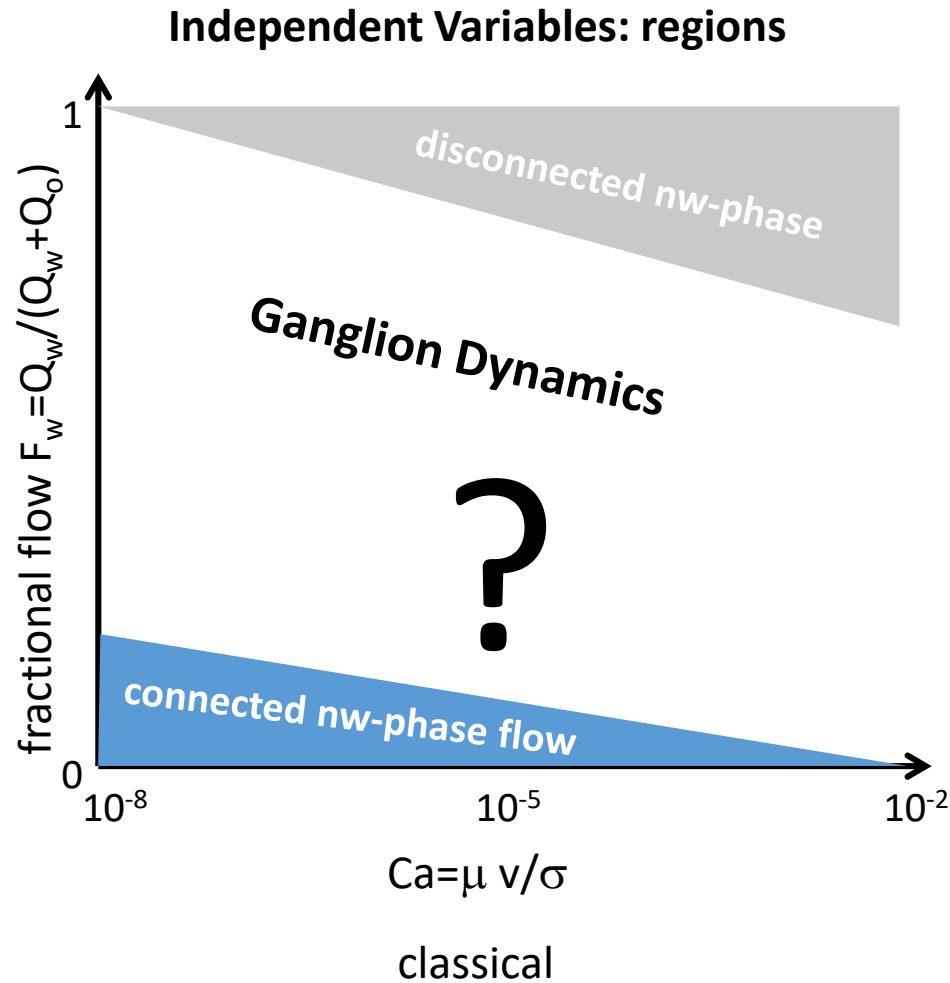
Cluster Dynamics Introduces Topological Changes

[Rücker et al., GRL, 2015]



Co-existence of connected pathway flow and ganglion dynamics over most of the mobile saturation range

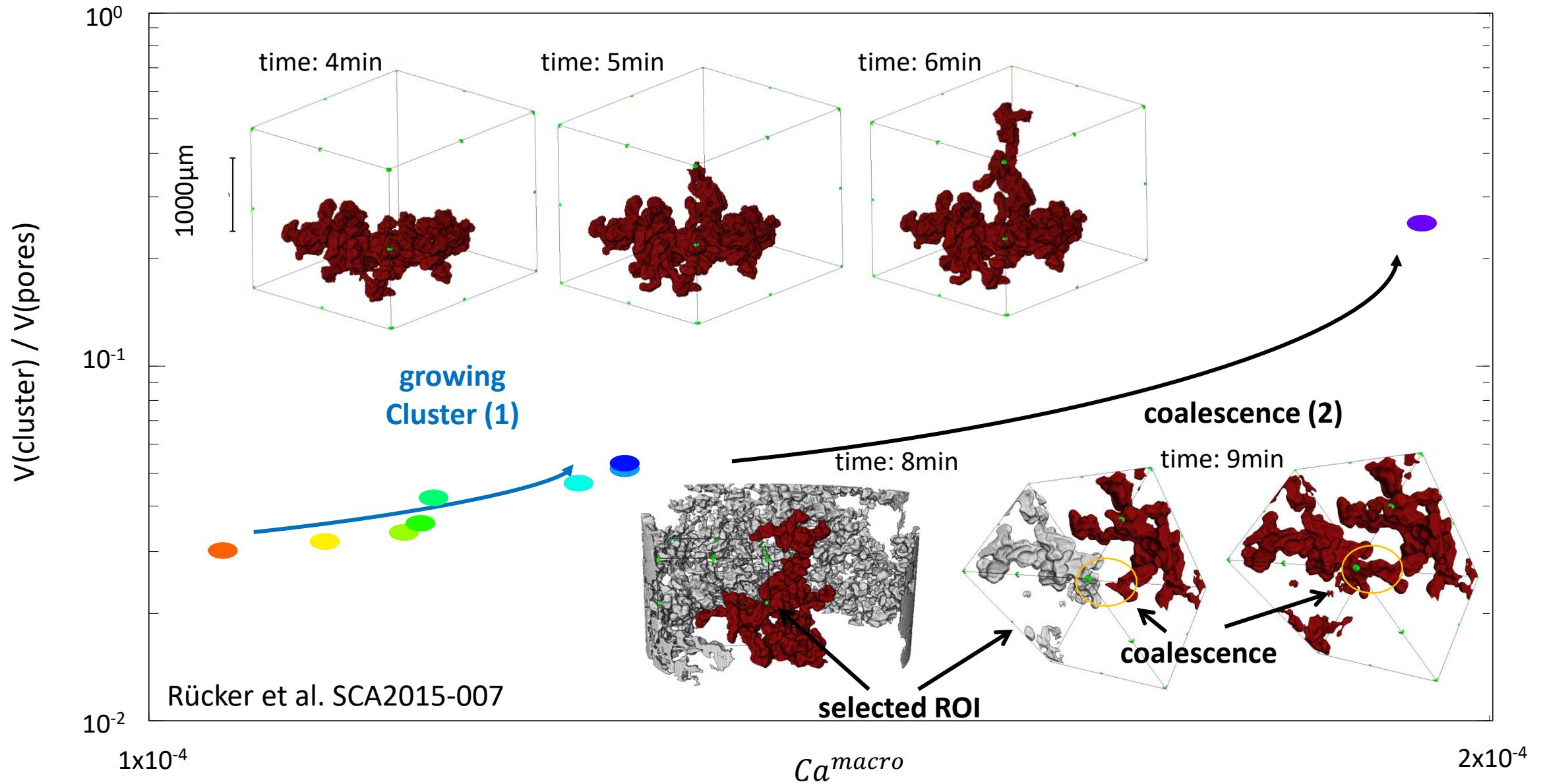
Characterization of Flow Regimes: Phase Diagrams ...



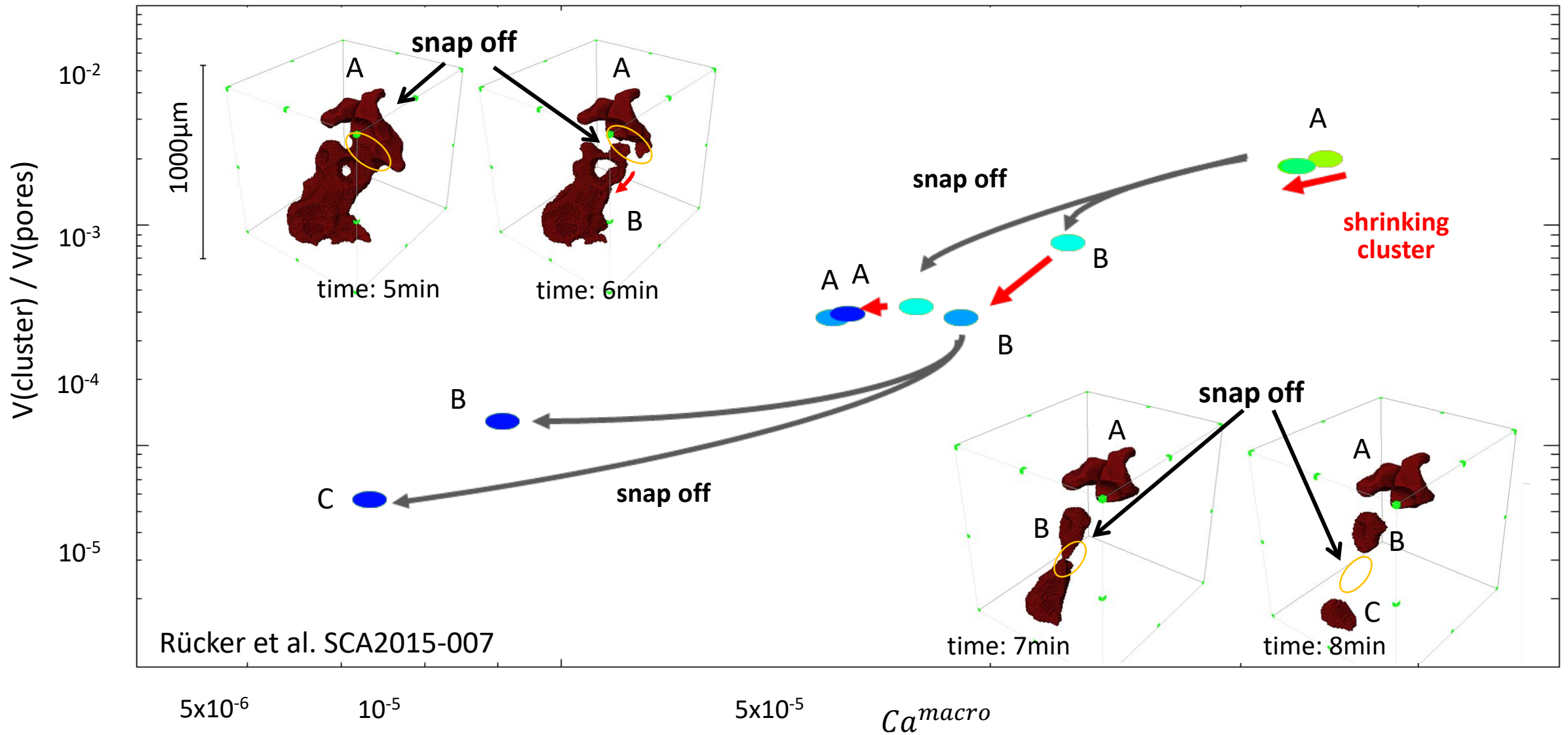
State variables

(at the time we did not know yet that we should have used A_{nw})

Clusters: Growing and Coalescence $\rightarrow \chi$ decreases



Clusters: Break-up by Snap-off $\rightarrow \chi$ increases

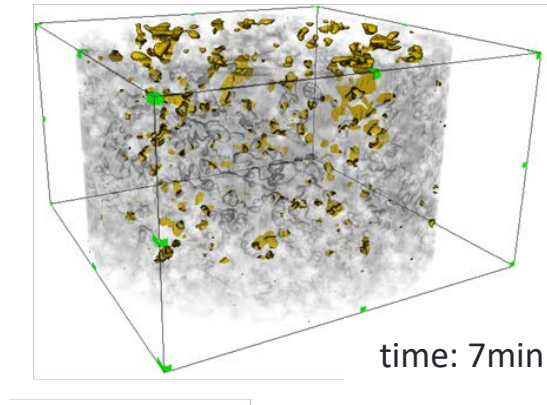


Characterization of Flow Regimes: Phase Diagrams ...

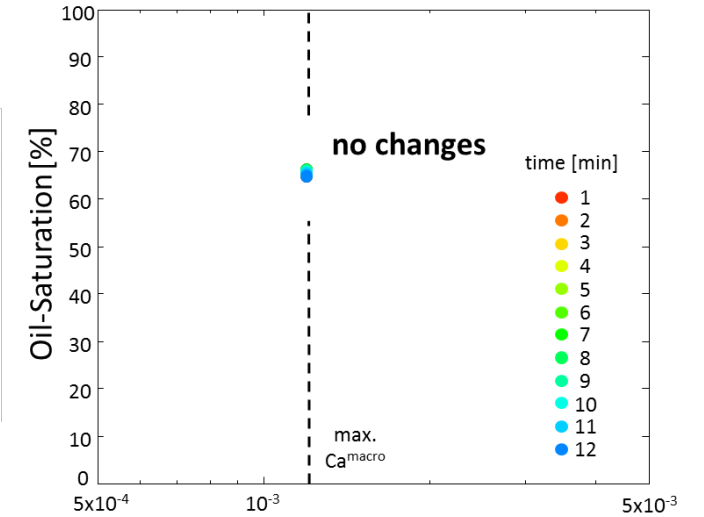
Connected pathway flow

time: 3min

time: 5min

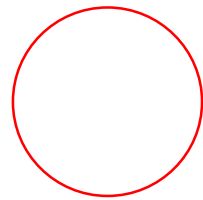


time: 7min

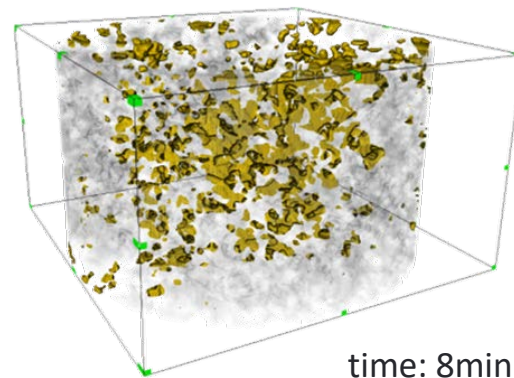


Ganglion dynamics

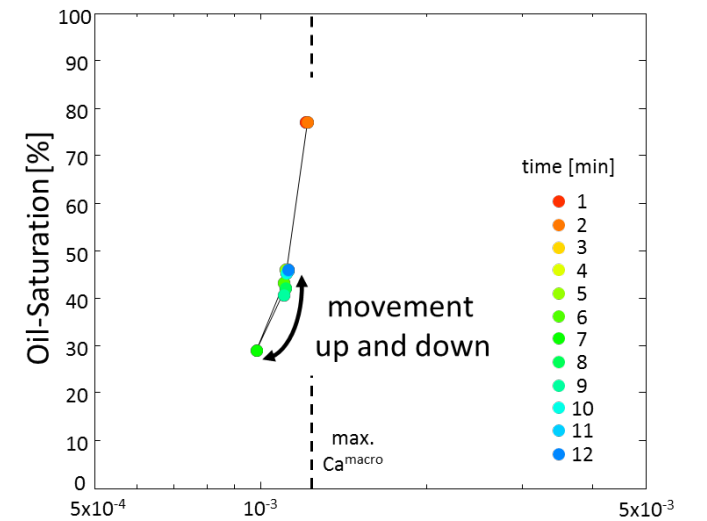
time: 6min



time: 7min



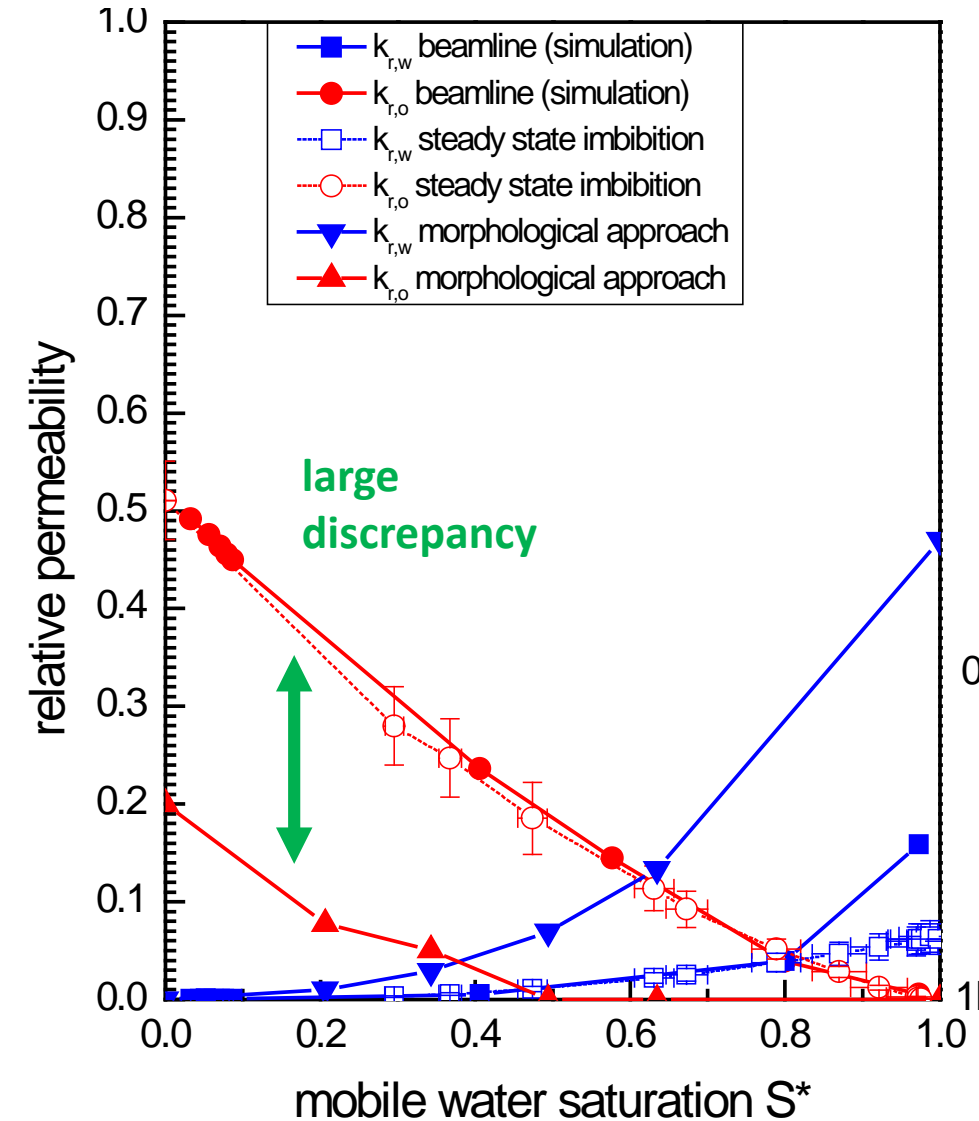
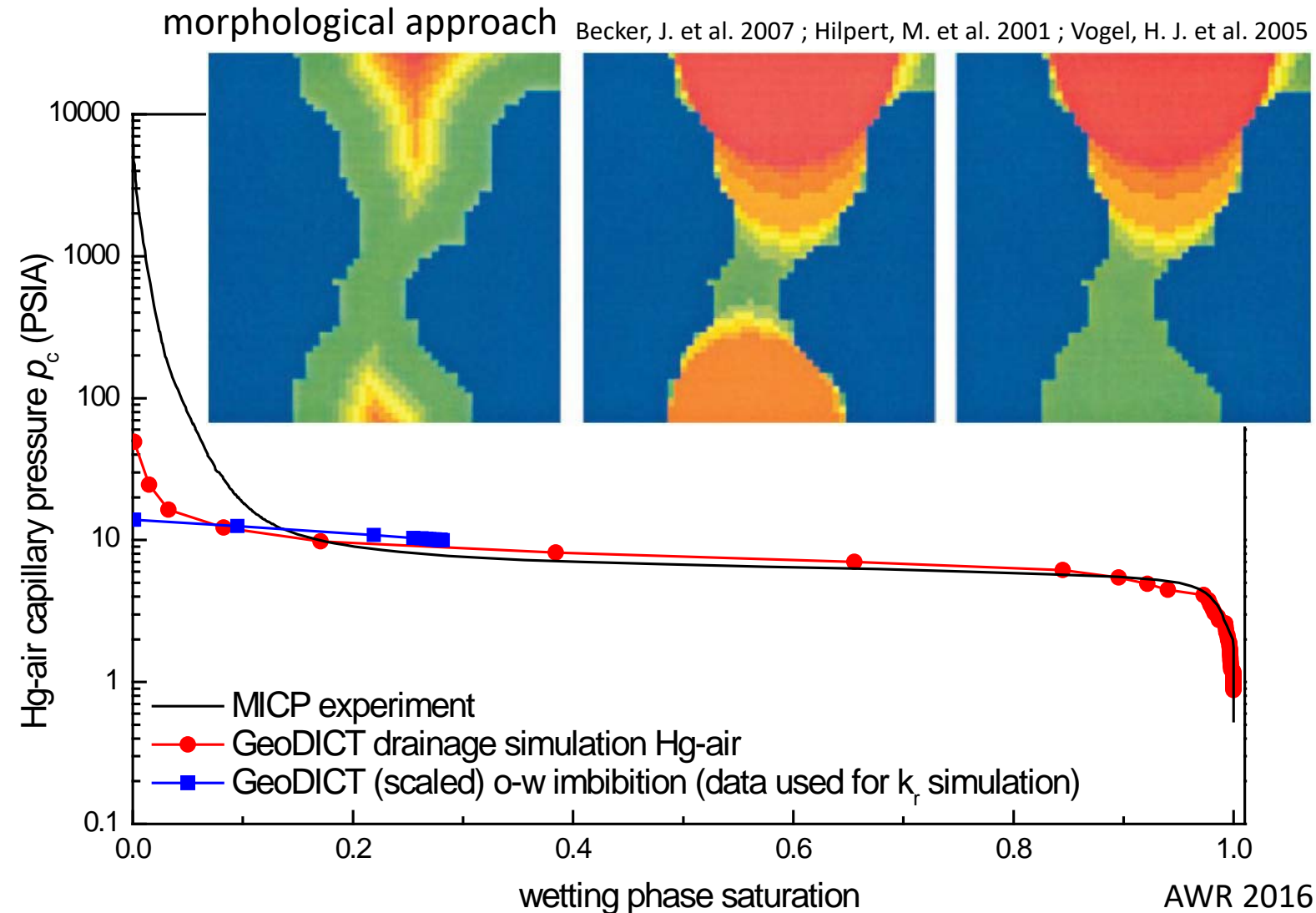
time: 8min



$$Ca_o^{macro} = \frac{l^{cl}}{r^p} \varphi \frac{\mu_w v}{\gamma_{wnw}}$$

Application: Validation of Pore Scale Simulation

Can we obtain imbibition relative permeability from a quasi-static approach ?



Influence of Wettability on Topology

Dynamic Connectivity → [PNAS, Reynolds et al. 2017]



Power Associated with Flow

$$\mathcal{P}_i = \frac{dW}{dt} = -\mathbf{q}_i \cdot \nabla p \approx \frac{\mu_i q_i^2}{K_i}$$

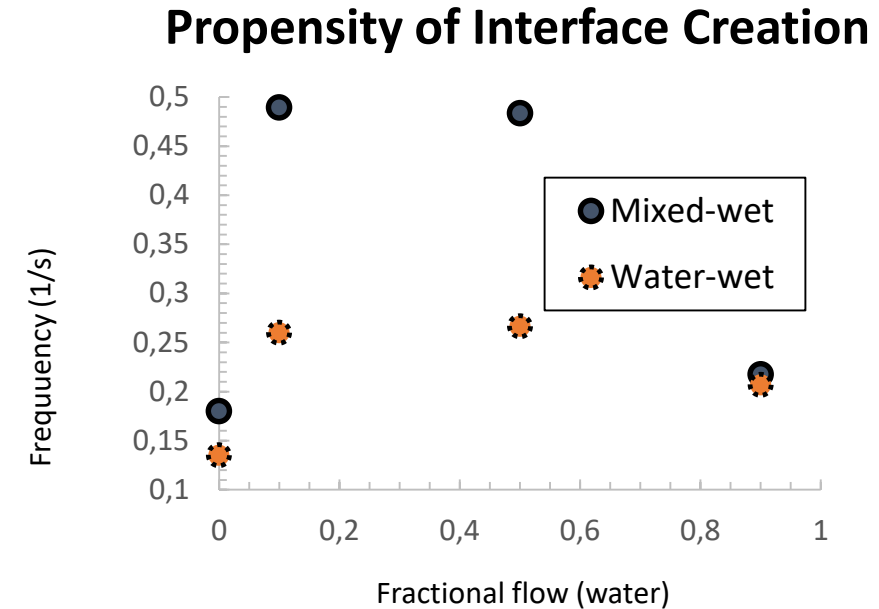
Surface Energy of WP/NWP Interface

$$(\text{Surface energy}) E = \frac{\sigma}{l}$$

Tested Two Different Wettabilities

Water Wet: $l = 0.72$

Mixed-Wet = -0.11



Generation of Unknown Phase

