High Fidelity Computational Analysis of CO2 Trappings at Pore-scales

Project Number: DE-FE0002407

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U.S. Department of Energy

National Energy Technology Laboratory
Carbon Storage R&D Project Review Meeting
Developing the Technologies and Building the
Infrastructure for CO_2 Storage

August 21-23, 2012

Presentation Outline

- Benefit to the Program
- Project Overview
- Technical Status
  - Pore-network modeling
  - Conductance derivation for irregular geom.
  - Pore-to-CFD Computations
  - Paul M. Delgado's presentation "Stochastic Multiscale Modeling of Fluid Flow in Porous Media for CO2 Storage Applications"
- Accomplishments
- Summary

Benefit to the Program

- Identify the Program goals being addressed.
  - CO_2 capacity assessments, simulation, and risk assessments
- Project benefits statement:

Increasing CO_2 emissions to the atmosphere from the anthropogenic sources is expected to be the major cause undesirable Climate Change and Global warming trends of our planet. One method to mitigate this threat is to capture CO_2 before releasing to the atmosphere and store it in the subterranean reservoirs (e.g., exhausted coal seams or oil fields) or utilize it for Enhanced Oil Recovery (EOR) or Methane Gas Recovery. However, the overall storage, leakage, and migration potential of CO_2 within these reservoirs is not well understood. Due to the expense and risk involved with testing Carbon Capture Utilization & Storage (CCUS) technologies, it is crucial to simulate the flow of CO_2 at the high fidelity. **This is achieved by computational investigation using semi-empirical variational calculus methods for computing flow conductance rule in single- and multi-phase systems and multi-scale framework for coupling the micro- and macro- scales.**

Project Overview:
Goals and Objectives

- Develop a computational technique to estimate fluid conductance.

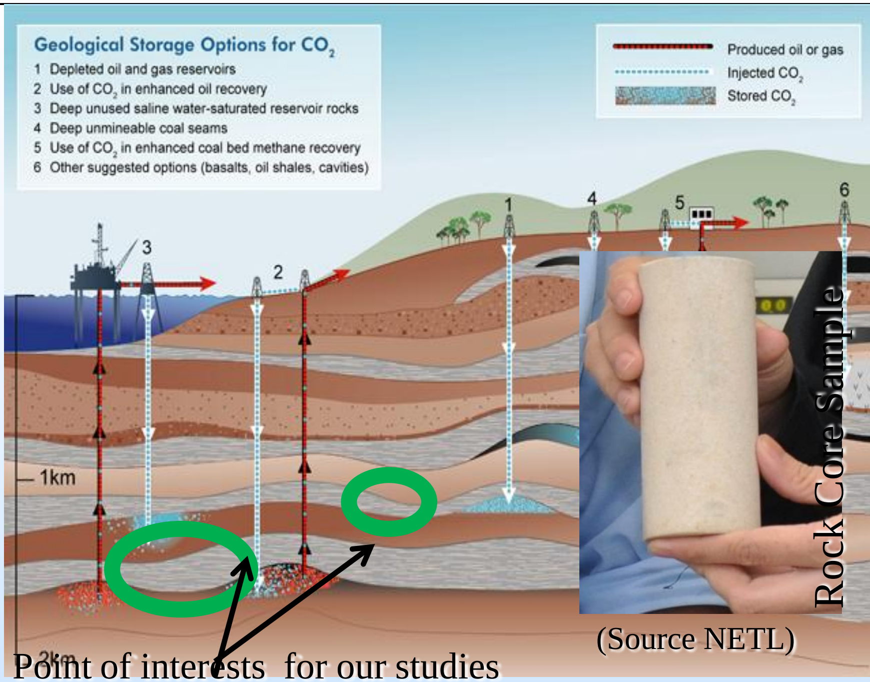
- Investigate the capillary effects at pore-scale to determine the on CO2 sequestration kinetics and storage capacity.

- Develop a framework for coupled system of micro-scale (pore-scale) physics with macro-scale (a reservoir scale) physics.

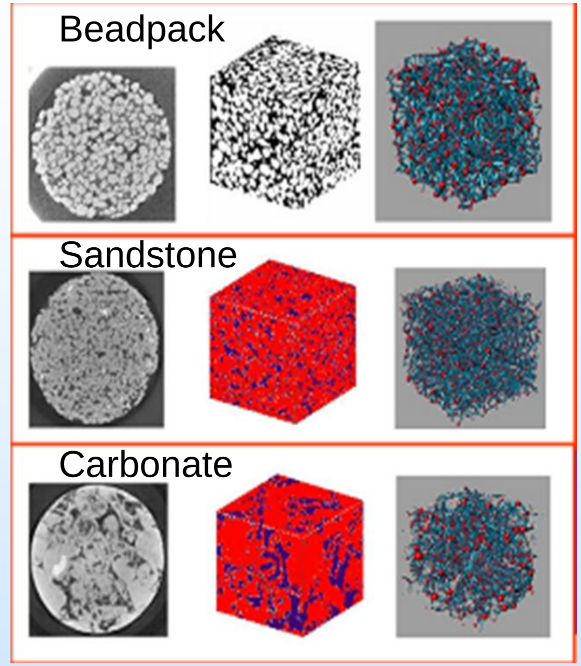
Technical Status

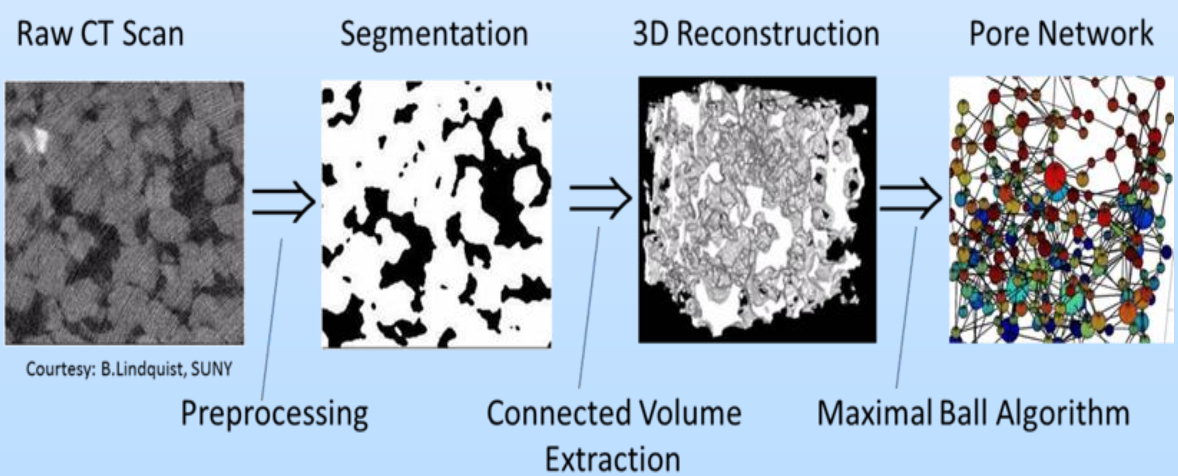
- Pore-network modeling
- Conductance derivation for irregular geometry
- Pore-to-CFD Computations
- Paul M. Delgado’s presentation “*Stochastic Multiscale Modeling of Fluid Flow in Porous Media for CO2 Storage Applications*”

Pore-network construction



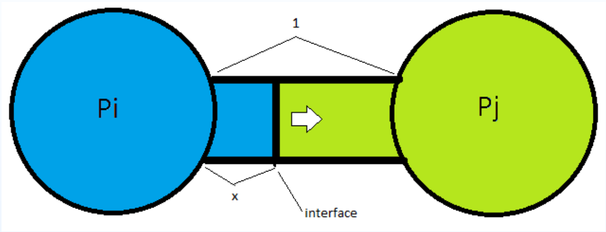
(Source NETL)





Pore network construction

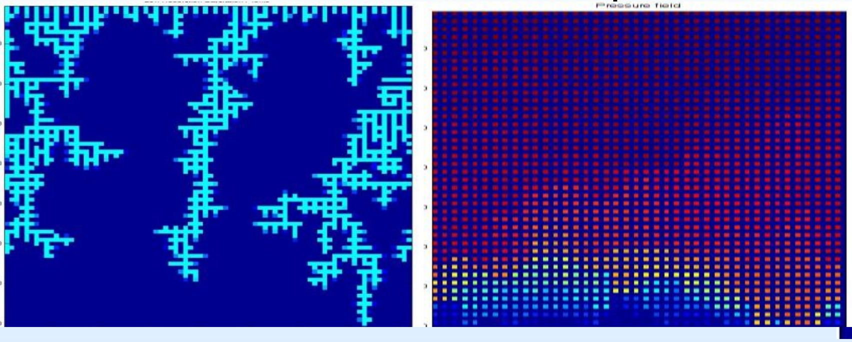
Pore-network modeling



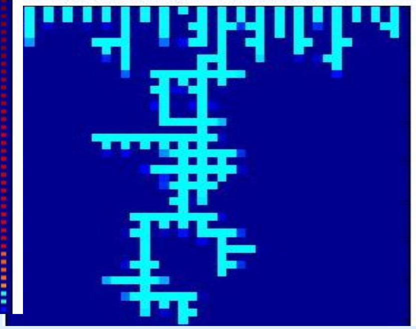
$$q_{ij} = g_{ij} \nabla P_{ij} \qquad \sum_{j \in K_i} q_{ij} = 0$$

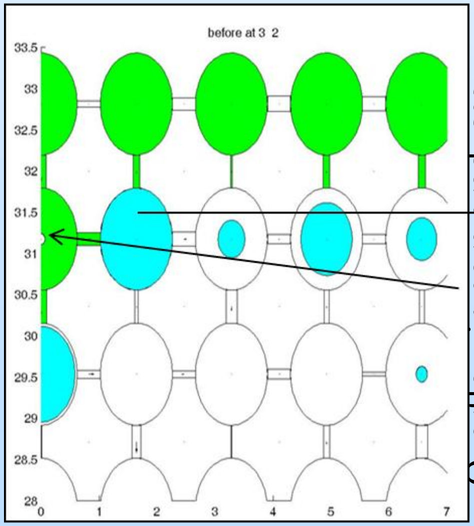
$$g = \frac{\pi \times r^4}{8\left(x\mu_{inv} + (1-x)\mu_{def}\right)L}$$

Saturation and Pressure profiles

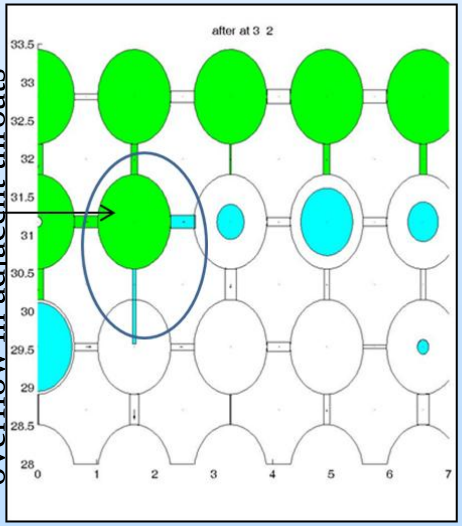


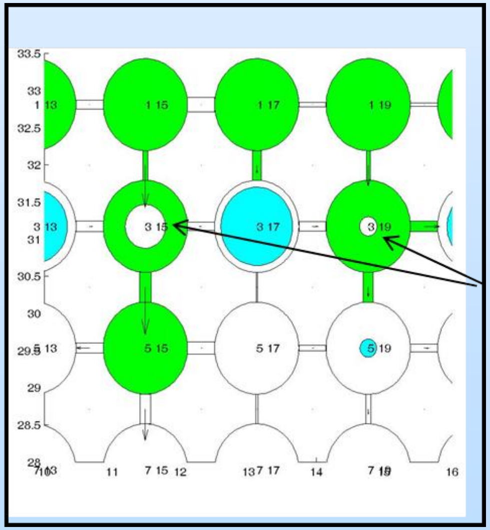
Constant injection





Overflow in pore produces overflow in adjacent throats





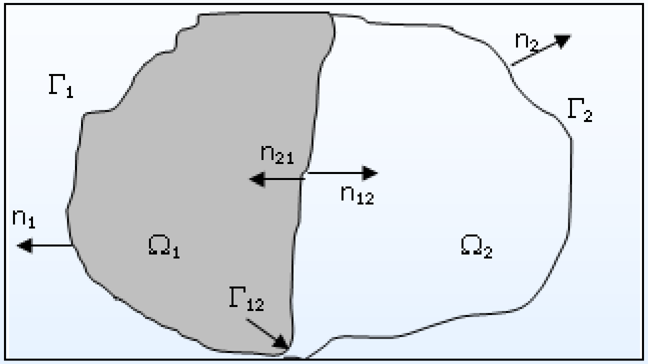
Address backflow with Artificial reservoir

Pore-network modeling

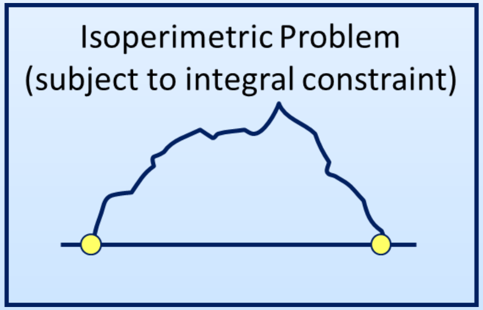
Video 1

Video 2

Variational Formulations



Express solution of Stokes equation in terms of the minimization of a functional I[f] (meaning just an integral of a function of f and its derivatives over the flow domain). Most treatments start by considering the one-dimensional case



The fluid velocities $w_1(x,y)$ and $w_2(x,y)$ satisfy

$$\nabla^2 w_i = -\frac{G_i}{\mu_i} \quad on\ (x,y) \epsilon\ \Omega_i$$

BCs: $w_i(x,y) = 0\ on (x,y) \epsilon\ \Gamma_i = 0$

$$w_1(x,y) = w_2(x,y), \&$$

$$\mu_1 \boldsymbol{n}_{12} \,.\, \boldsymbol{\nabla} w_1(x,y) = \mu_2 \boldsymbol{n}_{21} \,.\, \boldsymbol{\nabla} w_2(x,y) = 0 \quad on(x,y) \epsilon \Gamma_{12}$$

Introduce a functional $I[f_1, f_2]$ such that f_i is any C_2-regular function vanishing on Γ_i and $f_1 = f_2$ on Γ_{12}.

Variational Formulations

Fluxes: $q_i = \int_{\Omega_i} w_i dx\, dy$

Minimization of the functional results in

$$I[f_1, f_2] = \tfrac{1}{2}\int_{R_1} dxdy\, \{\mu_1 \underline{\nabla} f_1 . \underline{\nabla} f_1 - 2G_1 f_1\} + \tfrac{1}{2}\int_{R_{21}} dxdy\, \{\mu_2 \underline{\nabla} f_2 . \underline{\nabla} f_2 - 2G_2 f_2\}$$

$I[f_1,f_2] \geq I[w_1,w_2]$ with equality if and only if $f_1 = w_1$ and $f_2 = w_2$

In fact, we show

$$I[f_1, f_2] - I[w_1, w_2] =$$

$$\tfrac{1}{2}\int_{R_2} dxdy\, \mu_1 \underline{\nabla}(f_1 - w_1).\underline{\nabla}(f_1 - w_1) + \tfrac{1}{2}\int_{R_2} dxdy\, \mu_2 \underline{\nabla}(f_2 - w_2).\underline{\nabla}(f_2 - w_2)$$

Now

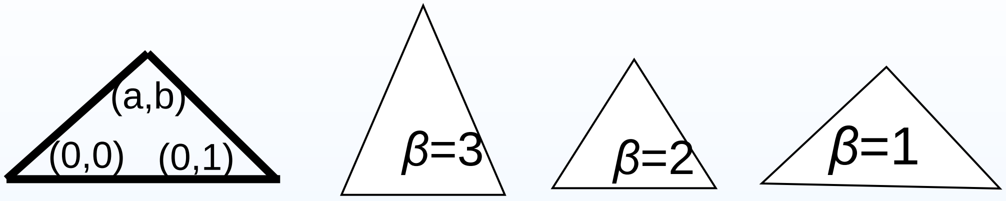
$$\mu_i \underline{\nabla}(f_i - w_i).\underline{\nabla}(f_i - w_i) = \mu_i \{\underline{\nabla} f_i . \underline{\nabla} f_i - 2\underline{\nabla} w_i . \underline{\nabla} f_i + \underline{\nabla} w_i . \underline{\nabla} w_i\}$$

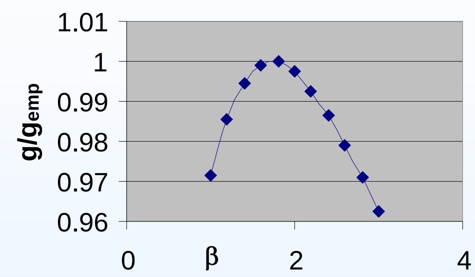
$$= \mu_i \{\underline{\nabla} f_i . \underline{\nabla} f_i - \underline{\nabla} w_i . \underline{\nabla} w_i - 2\underline{\nabla} w_i . \underline{\nabla}(f_i - w_i)\}$$

$$= \mu_i \{\underline{\nabla} f_i . \underline{\nabla} f_i - \underline{\nabla} w_i . \underline{\nabla} w_i - 2\underline{\nabla} . \{\underline{\nabla} w_i (f_i - w_i)\} + 2\nabla^2 w_i (f_i - w_i)\}$$

$$= \mu_i \{\underline{\nabla} f_i . \underline{\nabla} f_i - 2(G_i/\mu_i) f_i - \{\underline{\nabla} w_i . \underline{\nabla} w_i - 2(G_i/\mu_i) w_i\} - 2\underline{\nabla} . \{\underline{\nabla} w_i (f_i - w_i)\}\}$$

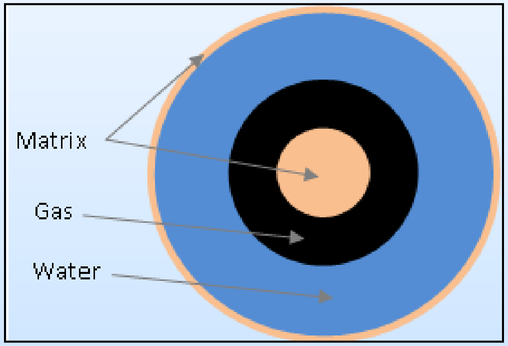
Flow Conductance Derivation





$$a = \tfrac{1}{2}, \beta' = \beta, \Rightarrow g = \frac{\beta^3}{160(3+\beta^2)}$$

$$g_{emp} = 0.6\frac{(area)^3}{(perimeter)^2} = \frac{3\beta^3}{320(1+\sqrt{1+\beta^2})^2}$$



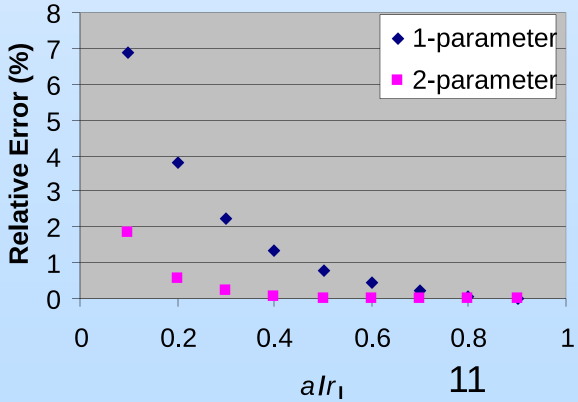
Annular flow: $a < r < 1$, $G/\mu = 1$

Exact solution: $w = \frac{1}{4}\left(1 - r^2\right) - \frac{\left(1-a^2\right)}{\ln\left(\frac{1}{a}\right)}\ln\left(\frac{1}{r}\right)$

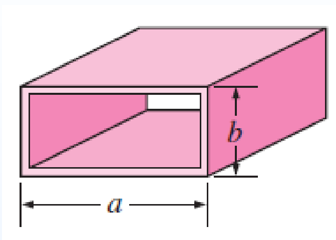
1&2 parameter choices for f:

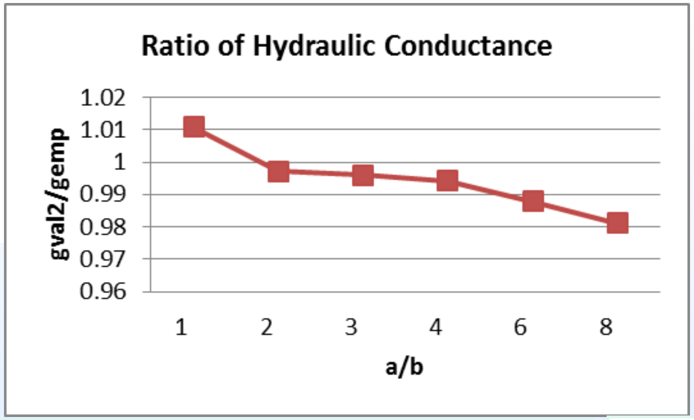
$$f = \alpha(1-r)(r-a)$$

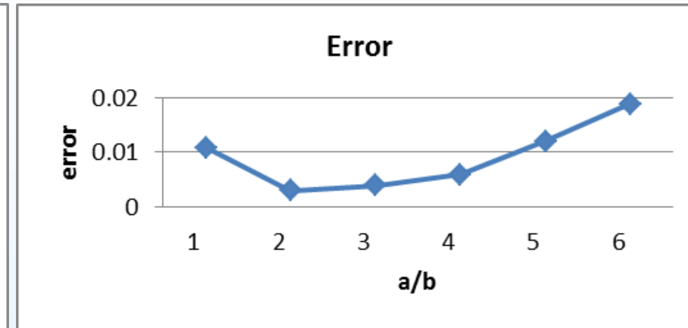
$$f = (1-r)\{\alpha(r-a) + \beta(1-a^2)\}$$



Flow Conductance Derivation



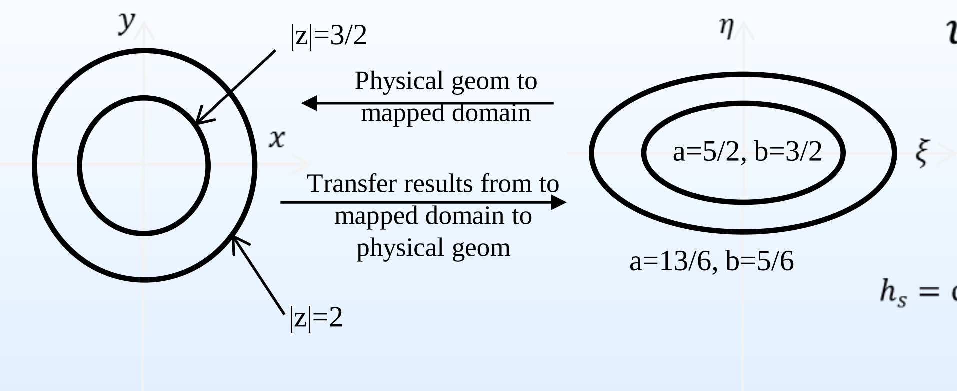




r	Flow resistance factor		
	f	f_{val1}	f_{val2}
1	56.92/Re	57.6/Re	56.9829/Re
1.5	N/A	59.904/Re	58.9759/Re
2	62.20/Re	64.0/Re	62.3823/Re
2.5	N/A	68.1796/Re	65.7029/Re
3	68.36/Re	72.0/Re	68.6318/Re
4	72.92/Re	78.336/Re	73.3537/Re
5	N/A	83.2/Re	76.9438/Re
6	78.80/Re	86.9878/Re	79.7622/Re
7	N/A	90/Re	82.035/Re
8	82.32/Re	92.4444/Re	83.9067/Re
10	N/A	96.1587/Re	86.8061/Re
15	N/A	101.7/Re	91.2704/Re
20	N/A	104.751/Re	93.8025/Re

r	Hydraulic Conductance, g		$\frac{g_{val2}}{g_{emp}}$	Er
	g_{emp}	g_{val2}		
1	0.0347222	0.0350983	1.0108	0.01083
1.5	N/A	0.0732503	N/A	N/A
2	0.114327	0.113992	0.997078	0.00292
2.5	N/A	0.155306	N/A	N/A
3	0.197484	0.196702	0.99604	0.00396
4	0.280856	0.279195	0.994088	0.00591
5	N/A	0.361014	N/A	N/A
6	0.447529	0.44213	0.987936	0.01206
7	N/A	0.522643	N/A	N/A
8	0.614285	0.602668	0.98109	0.01891
10	N/A	0.761648	N/A	N/A
15	N/A	1.15556	N/A	N/A
20	N/A	1.54713	N/A	N/A

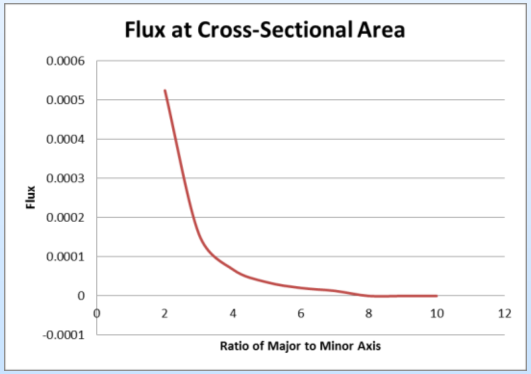
Flow Conductance – Conformal Mapping



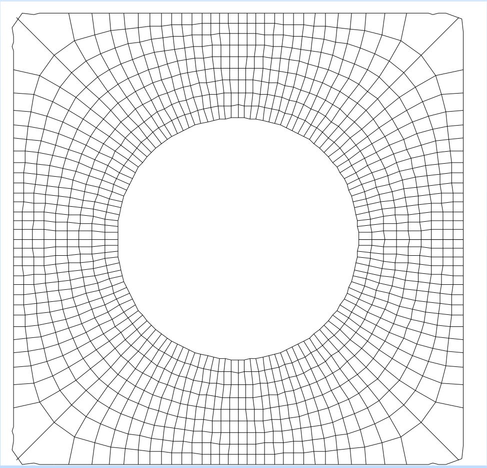
$$u + iv = w = f(z) = z + \frac{1}{z}$$

$$f^{'}(z) = 1 - \frac{1}{z^2} = \frac{(z+1)(z-1)}{z^2}$$

$$h_s = \det\left(\begin{pmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} \\ \frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta} \end{pmatrix}^{-1}\right)$$



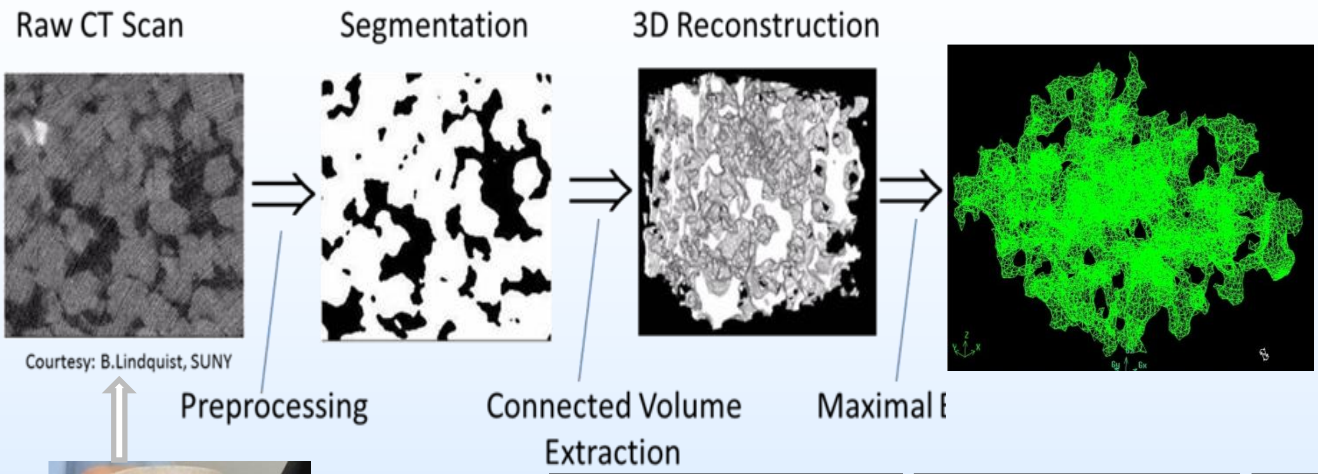
$$q = \int f dA = \int f(\xi,\eta) h_s d\xi d\eta,$$



Modified Schwarz-Christoffel Transformations

$$f(z) = A\int^{z} \prod_{j=1}^{n} (z^{'} - z_j)^{(\alpha_j - 1)} dz' + B$$

Pore-to-CFD



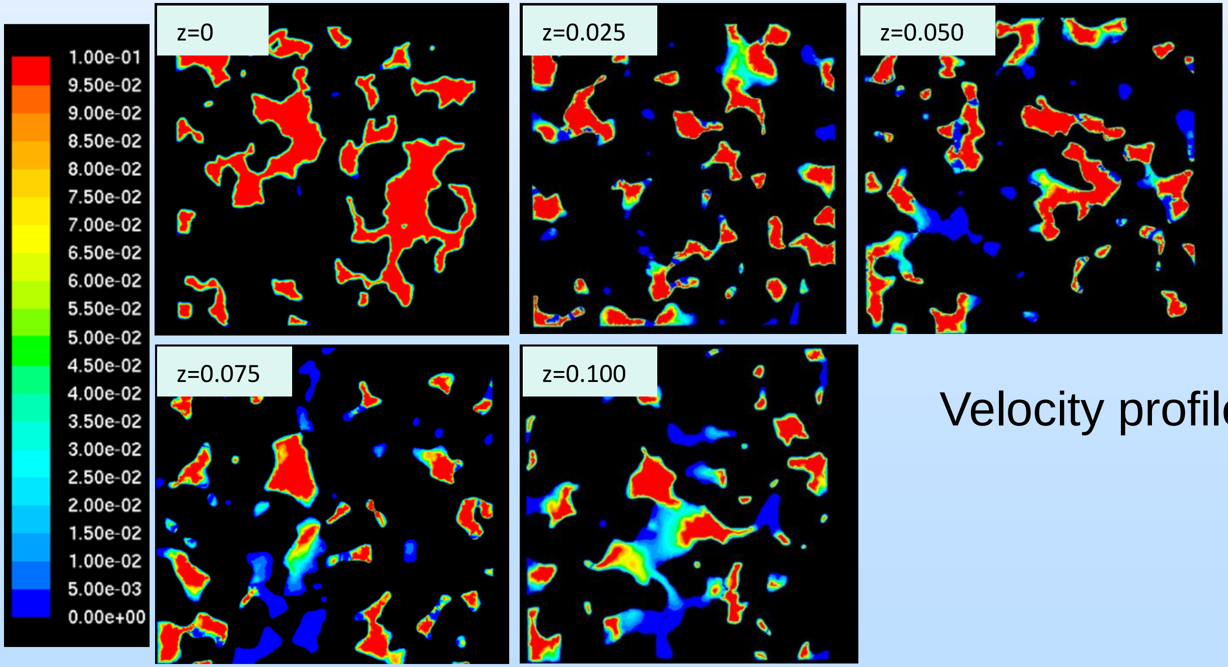
CFD Mesh:

4,321,166 elements

924,426 nodes

Duration for meshing 24-48 hrs

Software used: Gambit



Velocity profile

Accomplishments to Date

- Developed conductance model for irregular pore-cross section using conformal mapping
- Created pore-network reconstruction for CT-scanned images from NETL and Examined the flow kinetics of flow using CFD
- Addressed the convergence issues associated with the backflow in the pore-network model obtained from the NETL
- Devised a framework for coupling micro-scale with macro-scale
- Developed non-Newtonian flow models using variational calculus approach

Summary

- Key Findings
  - Variational methods seem a promising way of obtaining approximate analytical expressions for hydraulic conductance of pore elements for input into pore network models
  - Resolved backflow issues using virtual storage
- Lessons Learned
  - Micro- to macro-scale coupling is not so straightforward due to significant orders of scale differences
  - Pore network has numerical convergence issues
- Future Plans
  - Micro-scale (pore-scale) to macro-scale (Reservoir scale)
  - Develop advance linear algebra-solver
  - High Performance Computing

Appendix

– Organization Chart

– Gantt Chart

– Bibliography

Organization Chart

Principal Investigator: Dr. Vinod Kumar

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Organization Chart

Students participants:
- Mr. P. Delgado, Doctoral, Computational Science & Engineering
- Ms. Fan Chen, Doctoral, Computational Science & Engineering
- Mr. Todd Dorethy, M.S., Computational Science & Engineering
- Mr. N. Kavoori, M.S., Mechanical Engineering (Graduated, 2010)
- Other students who partially supported us on this project:

  Dr. K. Katta (Computational Science),
  Mr. Enrique Busquestes (BS, Mechanical)
  Mr. R. Chacon (BS, Mechanical)
  Mr. E. Cordero (BS, Mechanical),
  Mr. J. Ortega (BS, Mechanical),
  Ms. S. Afrin (MS, Mechanical),
  Mr. D. Llauhas (BS, Mechanical),
  Mr. D. Landis (Computational Science),
  Mr. G. Aceves (Mechanical)

Note: This project also enabled Mr. P. Delgado to get the NSF's LSAMP Scholarship for his continuation of doctoral studies and helped the PI to acquire funding from Student Employment Program (provided by the university from a funding from the state of Texas

Gantt Chart

Task Title	Project Tasks	Budget Period: 1st half						Budget Period: 2nd half					
		Q1	Q2	Q3	Q4	Q5	Q6	Q7	Q8	Q9	Q10	Q11	Q12
Program Management	Task 1												
Simple model	Task 2												
External Resources	Task2.1												
Build simple model	Task2.2												
Single phase flow model	Task2.3												
Verification of the Model	Task2.4												
Multiphase system	Task 3												
Build multiphase model	Task3.1												
W/ Complex Geometries	Task3.2												
Verification of the Model	Task3.3												
Reservoir simulations	Task4												
Choose the reservoir	Task4.1												
Lab-Scale System	Taskt4.2												
Conductance derivation	Taks4.3												
Experimental Data	Task4.5												
Coupled Model	Task5												
Code Integration	Task5.1												
Simulations & verification	Taks5.2												

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