

Stochastic Particle Method (SPM): A Lagrangian Modeling Framework to Study CO₂ Sequestration in Subsurface Formations

ABSTRACT

Computational Method

- A Lagrangian approach to solve phase transport in porous media
- A particle represents a phase (physical particles)
- Particles can carry various properties such as composition
- It is different from deterministic particle methods such as SPH
- Saturation is a local statistical property
- Physical particle evolution is approximated by a stochastic process
- Motivation: natural modeling framework for complex processes

Applications

Numerical simulation framework for CO₂ sequestration in subsurface formations. The problem involves complex non-equilibrium processes:

- Dissolution of CO₂ in brine
- Chemical reactions
- Trapping of CO₂

SPM is a rigorous frame-work that can deal with non-equilibrium phenomena based on

- Statistical information from pore scale physics
- Joint PDFs, correlation time and length scales

MATHEMATICAL MODEL AND SOLUTION ALGORITHM

Validation for 2-Phase Darcy Flow: An Example of a Stochastic Model

Phase indicator (particle property) $s^* = \begin{cases} 0 & \text{if particle is of phase 0} \\ 1 & \text{if particle is of phase 1} \end{cases}$ **Saturation of phase 0: a statistical quantity** $S = 1 - \langle s^* \rangle$

Phase transport equation $\frac{\partial S}{\partial t} + v_{tot} \cdot \nabla f(S) = \nabla C \nabla S + \nabla D \nabla S$ v_{tot} -total velocity

$C(S)$ -capillary dispersion coefficient $D(v_{tot})$ -pore scale dispersion coefficient

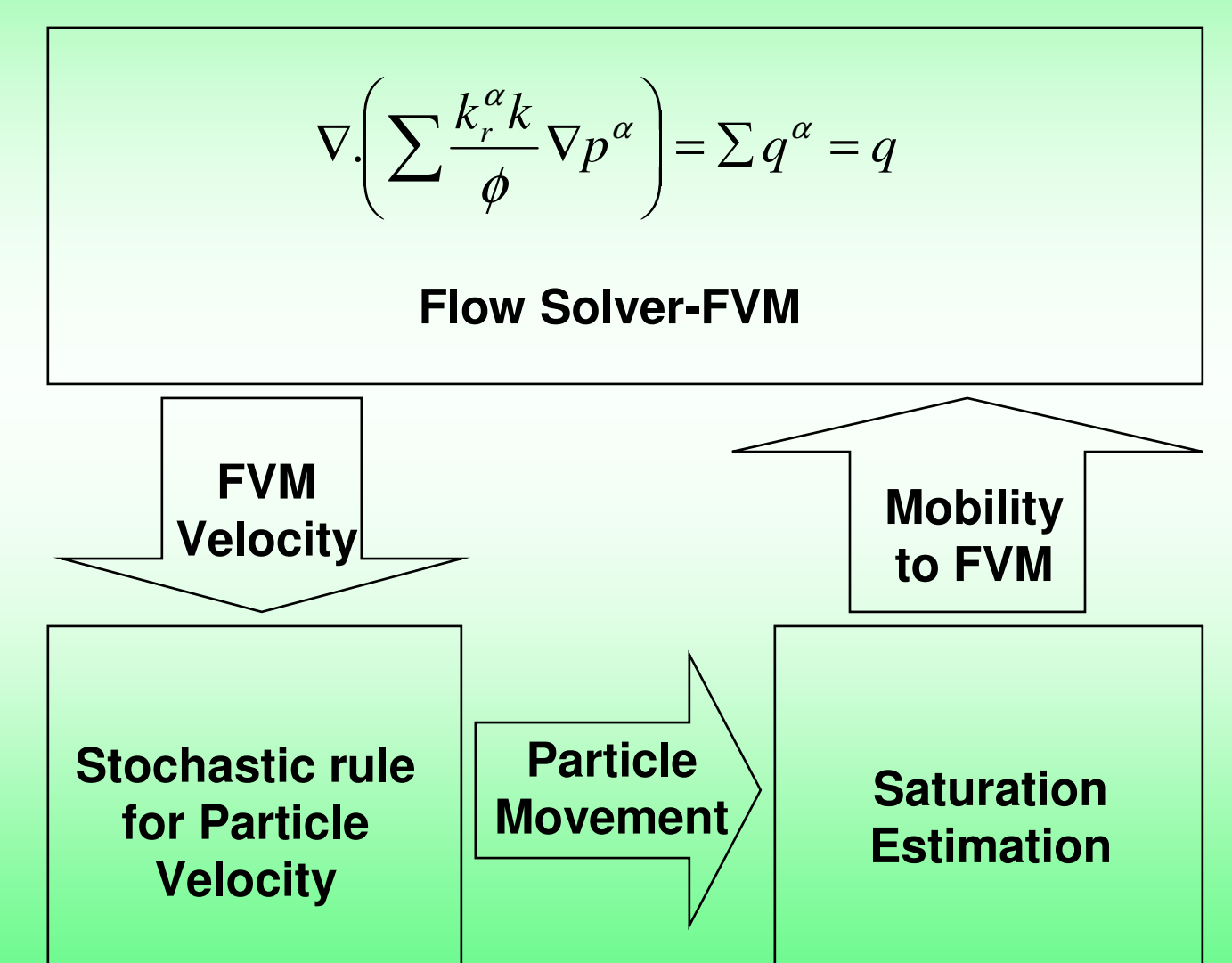
Consistent stochastic rule for particle displacement

$$dx^* = \begin{cases} v_{tot} \frac{f(S)}{S} dt + \frac{C(S)}{S} \nabla S dt + \sqrt{2D(v_{tot})} dt \xi + D'(v_{tot}) \nabla S dt & s^* = 0 \\ v_{tot} \frac{f(1-S)}{1-S} dt - \frac{C(S)}{1-S} \nabla S dt + \sqrt{2D(v_{tot})} dt \xi + D'(v_{tot}) \nabla S dt & s^* = 1 \end{cases}$$

ξ -random variable with normal distribution

NOTE: same concept can be generalized for more complex physics; e.g., non-equilibrium processes

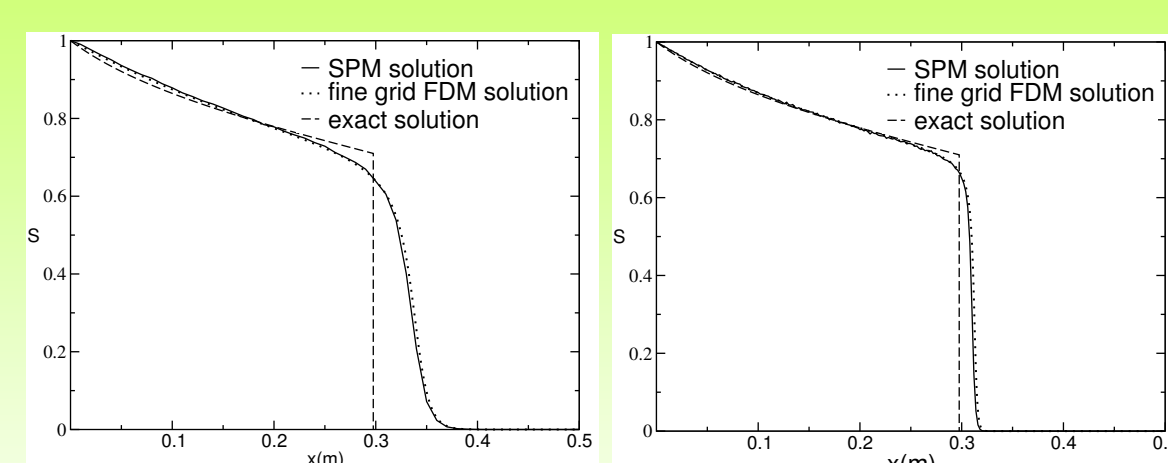
Algorithm



VALIDATION

1D Test Case: Buckley-Leverett Problem

Saturation of injected phase after $t=0.25s$ for two grid spacings
 $v_{tot}=1m/s, C=0.$



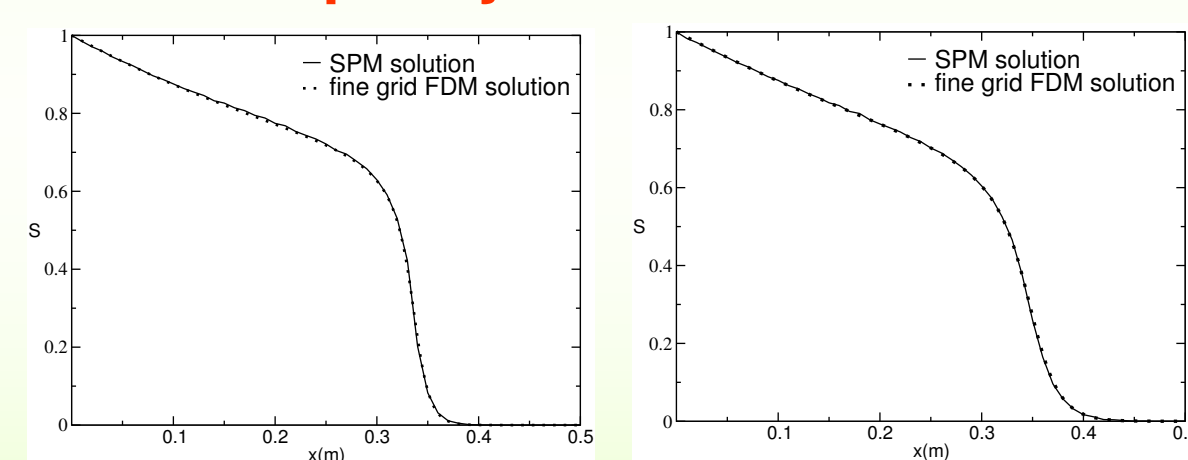
$D=0.01, dx=0.01$

$D=0.002, dx=0.002$

1D Test Case: Buckley-Leverett Problem with Capillary Pressure

Constant C

Saturation of injected phase after $t=0.25s, D=0.001, dx=0.01.$

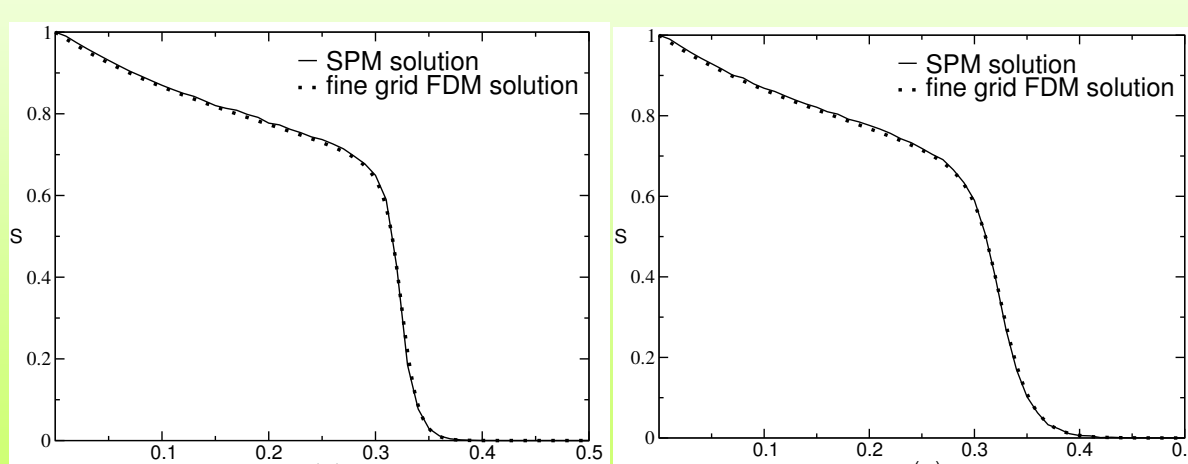


$C=0.01$

$C=0.02$

Non-constant C, $C(S) = \frac{C_0(1-S)^2}{S^2 + (1-S)^2}$

Saturation of injected phase after $t=0.25s, D=0.001, dx=0.01.$



$C_0=0.01$

$C_0=0.02$

2D Test Case: Quarter-Five Spot Configuration

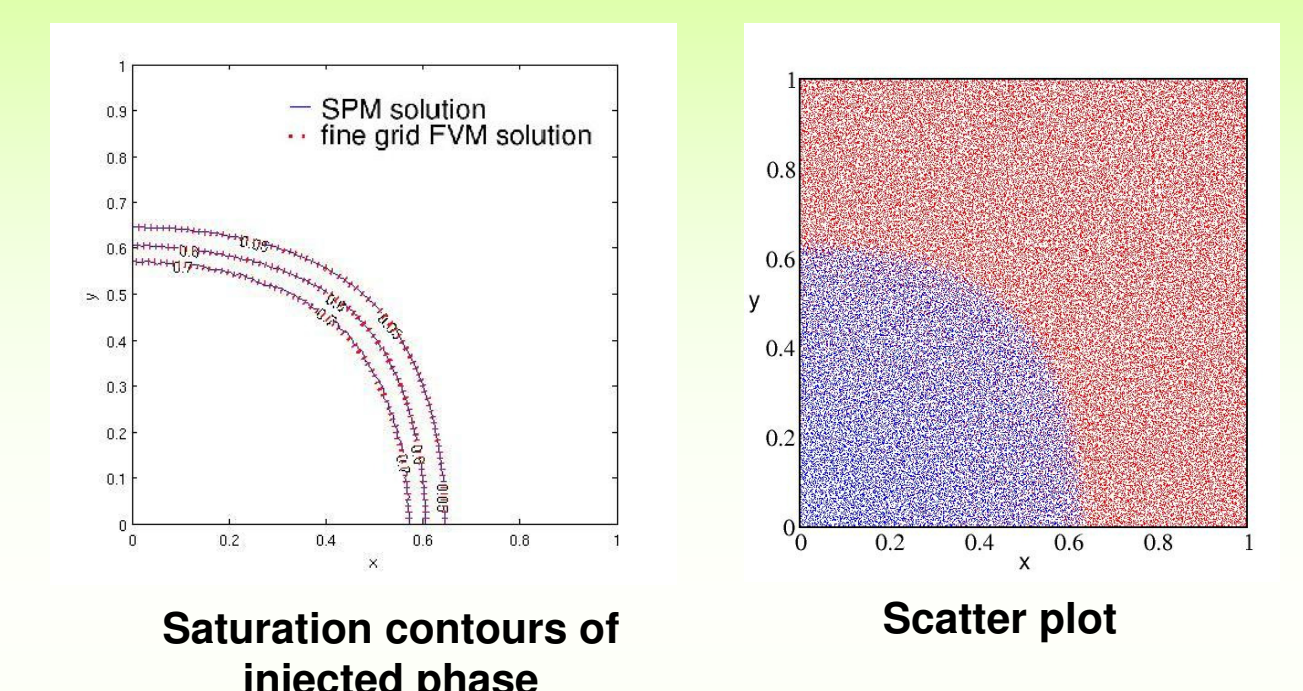
Homogeneous Permeability Field

Simulation results after 0.25 PVI

Grid = 100*100

In the scatter plot, blue particles are injected in the domain initially filled with red particles.

$D=0.01 v_{tot}, C=0$



Saturation contours of injected phase

Scatter plot

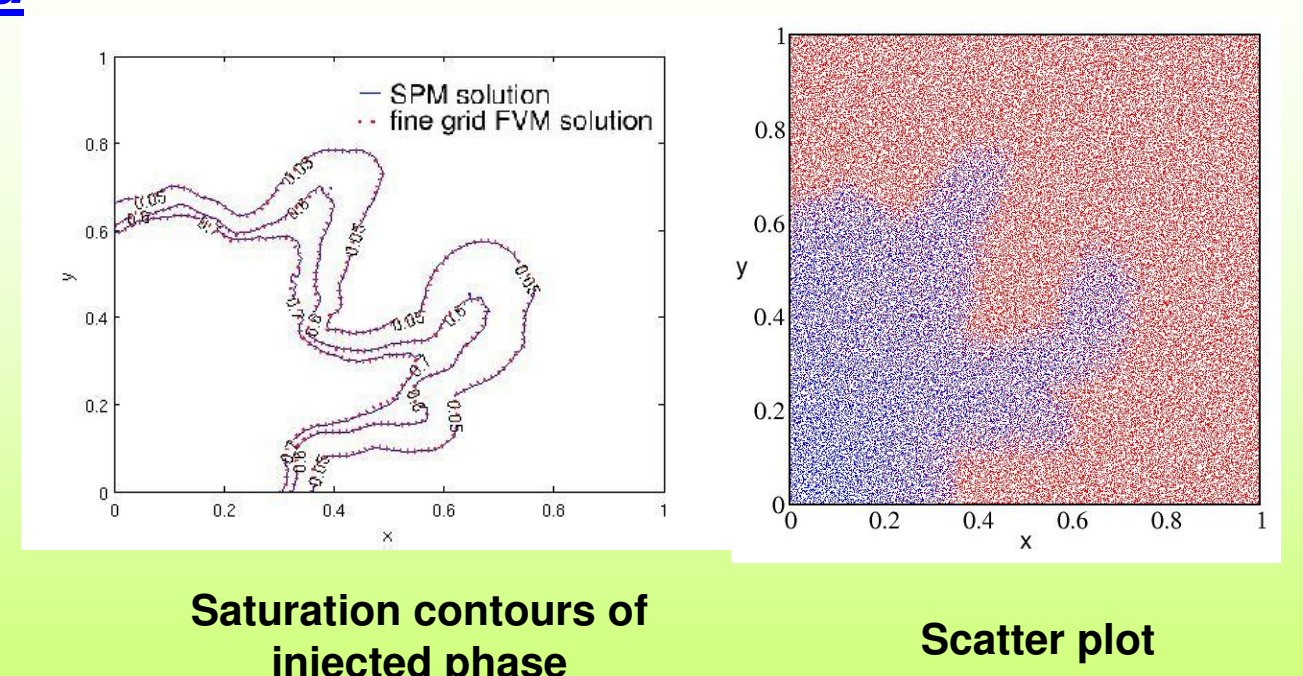
Heterogeneous Permeability Field

Simulation results after 0.25 PVI

Grid = 100*100

In the scatter plot, blue particles are injected in the domain initially filled with red particles.

$D=0.01 v_{tot}, C=0$



Saturation contours of injected phase

Scatter plot

OUTLOOK

- Transporting particles with more complex rules that are consistent with the pore scale dynamics. The rules for particle movement can be provided by pore network simulations
- Using SPM for the problem of CO₂ sequestration in subsurface formations: A numerical tool to study complex processes; dissolution of CO₂ in brine, reaction, trapping etc.
- Extract effective models for finite volume simulator