A Julia-based Parallel Simulator for the Description of the Coupled Flow, Thermal and Geological Processes in Hydrate-bearing Geologic Media

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Outline

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Background

What is Gas Hydrate?
- Solid crystalline compounds in which gas molecules are encaged inside the lattices of ice crystals.
- The worldwide quantity of gas hydrate range between $10^{15}$ to $10^{18} \text{ m}^3$.
- Formed at high pressure and low temperature conditions.
- The three main suggested methods of gas production from CH$_4$-hydrate deposits are depressurization, thermal stimulation and inhibitor injection.
- Simulators for gas hydrate production are inevitably complicated because of the need to fully consider the coupled flow, thermal, thermo-dynamic and geochemical processes.
Objective

- To develop the Julia flow and transport simulator (JFTS), a Message Passing Interface (MPI)-based parallel simulator.
- To develop a module describing all phase coexistence combinations of the phase diagram of the $\text{H}_2\text{O} - \text{CH}_4$ system that are possible in geologic media.
- To develop the associated hydrate module describing the coupled flow, thermal and chemical processes.
- To evaluate the computational performance of the parallel simulator through comparisons to the performance of well-established serial simulators that solve the hydrate problem.
Methodology

- The JFTS+H simulator is a fully implicit compositional simulator that describes heat and up to four mass components (H$_2$O, CH$_4$, CH$_4$-hydrate, water-soluble inhibitor) distributed among four phases (Aqueous, Gas, Hydrate, and Ice).
- There are 13 possible combinations in geologic media and check phase transition at every Newton-Raphson iterations.
- Implementing the MPI interface in all components.
- Using the METIS library for domain decomposition and the LIS library to solve the matrix system of linear equations.
Field scale problem

- The reservoir model is composed of three hydrate-bearing layers and two hydrate-free interlayers.
- The reservoir region are overlain and underlain by very-low-permeable muds.
- Gas production is based on depressurization-induced dissociation of the CH$_4$-hydrates.
- The system is 2-dimensional grid includes $170 \times 149 = 25,330$ grid blocks.
- The Jacobian matrix comprises a total of $170 \times 149 \times 4 = 101,320$ simultaneous linear equations.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Description</th>
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<tbody>
<tr>
<td>Overburden</td>
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<tr>
<td>Hydrate layer 1</td>
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<td>Hydrate layer 2</td>
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<tr>
<td>Interlayer 2</td>
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<td>Hydrate layer 3</td>
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<tr>
<td>Underburden</td>
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</tbody>
</table>

- Typical job size
  - HPRC Cluster: Ada
  - Software: Julia, MPI, LIS, and METIS
  - Cores: 128
  - Memory: 2560 MB per processors
  - Run time: 2 hours
Simulation Results and Validation

**CH₄-hydrate dissociation Mass Rate**

![Graph showing CH₄-hydrate dissociation mass rate](image)

Mass rate of the CH₄ gas release from hydrate dissociation in the 2D field scale problem

**Cumulative Mass of released methane gas**

![Graph showing cumulative mass of released methane gas](image)

Cumulative mass of the CH₄ gas released from hydrate dissociation in the 2D field scale problem

Reference: TOUGH_HYDRATE v1.5, Moridis (2014)
Simulation Results

Spatial Distribution of Pressure

Pressure distribution in the well vicinity at the end of simulation in the 2D field scale problem

Spatial Distribution of Gas Phase Saturation

Gas saturation distribution in the well vicinity at the end of simulation in the 2D field scale problem

Depressurization works and gas is evolved around the well

Reference: TOUGH_HYDRATE v1.5, Moridis (2014)
Computational Performance

The relationship between total elapsed time and number of processors in the study of field scale problem

The relationship between speed up, efficiency and number of processors in the study of field scale problem
Summary

• The JFTS+H simulator was developed to model the coupled flow, thermal/thermo-dynamics and chemical processes associated with the formation and dissociation of hydrate in geologic media.

• The JFTS+H code has been validated against the TOUGH+HYDRATE v1.5 simulator.

• The JFTS+H simulator can simulate field-scale problems of gas production from hydrate deposits.

• Analysis and evaluation of the computational performance of JFTS+H shows conclusively that the MPI-based parallel version of the code delivers a significant and scalable speed-up.
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Reference

• The Julia Programming Language(https://julialang.org/)


• NATIONAL ENERGY TECHNOLOGY LABORATORY (https://netl.doe.gov/oil-gas/gas-hydrates)