Comparative Analysis of Compositional Two-Phase Flow Modeling in Heterogeneous Media Between the Discrete Event Simulation Method Coupled to a Split Node Formulation and Classical Timestep-Driven Approaches

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Outline

- Introduction to Discrete Event Simulations
- Discrete Event Simulations for Hybrid Finite Element Finite Volume Method
- Two Phase Flow Simulations: TDS vs. DES
- Material interfaces in Hybrid Finite Element Finite Volume Method
- Conclusions
Simulating multiphase flow imposes certain restrictions on the time step length due to the complexity of the reservoir and related emergent behaviour. The asynchronous time step methodology yields a speed up, particularly under the following conditions:

- High Mesh Resolution in specific regions (e.g. Small mesh near the wells, fractures, faults)
- High Permeability Contrasts (e.g. existence of high permeability zones such as fractures)
- Highly Non-linear Problems (e.g. non-linear two phase models such as Brooks Corey, two-phase gravitational effects)
Adaptime time-refinement approach

In adaptive time-refinement the solution updates locally in each cell by local time-increment. To simplify and to increase the efficient of synchronization procedure the time-steps usually taken as fractions of global time $\frac{\Delta t}{2^n}$. This approach is not increasing the accuracy of calculations, but in the same time it doesn't reduce the approximation order of numerical scheme. Thus the adaptive time-refinement will be more efficient than the general global-time stepping.

Let us consider the 1D heat equation and the numerical scheme of second order of approximation:

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( \kappa(t, x, T) \frac{\partial T}{\partial x} \right)$$  \hspace{1cm} (1)

$$\frac{T_{m+1}^{n+1} - T_m^n}{\tau} = \frac{\kappa}{\Delta x^2} \left( T_{m-1}^n - 2T_m^n + T_{m+1}^n \right)$$  \hspace{1cm} (2)
Adaptime time-refinement approach

Let us assume several regions $i = 1..m$, with different spatial sizes of cells, for instance as $\Delta x_i = 2^{i-1}\Delta x_1$, where $\Delta x_1$ the smallest size of cell. Each group of cells will be defined by numbers $n_i$ and $p_i = \frac{n_i}{N}$, where $n_i$ number of cells in each region, $p_i$ percent of cells from each group corresponding to the total number. Let us additionally assume that $\kappa = 1$. Then we will get $\Delta t_i = \frac{\Delta x_i^2}{2} = 2^{2(i-1)}\frac{\Delta x_1^2}{2} = 2^{2(i-1)}\Delta t_1$, where $\Delta t_1 = \Delta t_{\text{min}}$.

Let also $\tau_{\text{avg}}$ be the average time for calculation procedures for each cell during one time-step.
Adaptime time-refinement approach

We can estimate the time of calculations in global time-stepping and self-adaptive local time-stepping approaches and calculate the ratio.

\[
\frac{r}{t_{GTS}} = \frac{t_{LTS}}{t_{GTS}} = \frac{\tau_{avg} \frac{t_{end}}{\Delta t_{min}} N}{\tau_{avg} \frac{t_{end}}{\Delta t_{min}} \sum_{i=1}^{m} \frac{n_i}{2^{2(i-1)}}} = \frac{1}{\sum_{i=1}^{m} \frac{p_i}{2^{2(i-1)}}}
\]

So for instance if we will have the two groups of cells with corresponding percentages \( p_1 = 0.1, p_2 = 0.9 \) then the ration of GTS time to LTS time will be \( r \approx 3 \).
The way to distinguish Discrete Event Simulation (DES) from Timestep Driven Simulation (TDS) can be found in the nature of the state space.

**TDS :** \((X_d, T_d) \rightarrow Q\) — *is the mapping from discrete time – discrete space to continuous state space*

**DES :** \((X_d, T) \rightarrow Q_d\) — *is the mapping from continuous time – discrete space to discrete state space (Quantized State System)*
Taking the Cauchy ODE problem as an example, there will be a need to integrate right hand side:

\[ \dot{x}(t) = f(x(t), t), \quad x(t_0) = x_0 \]

\[ x(t_i + \Delta t_i) = x(t_i) + \int_{t_i}^{t_i + \Delta t_i} f(x(\tau), \tau) d\tau \]

DES and TDS approaches will view on these integrals differently:

\[ TDS : \int_{t_i}^{t_i + \Delta t_i} f(x(\tau), \tau) d\tau : \text{Riemann Integral} \]

\[ DES : \int_{t_i}^{t_i + \Delta t_i} f(x(\tau), \tau) d\tau : \text{Lebesgue Integral} \]
Bringing DES to the Finite Element-Finite Volume Framework

Discrete event simulations for solving partial differential equations were applied in conjunction with FD’s, FV’s and PIC approaches. But it can also be used together with other discretization methods. From the algorithmic point of view, to apply DES to the FEFV framework each Finite Volume must be associated with an Event Process, which will have the following main attributes:

- Scheduled Process Time
- Target Scalar Change (value constrained by a state change that is significant for corresponding Finite Volume)
Time Driven Simulation Cycle

Apply initial conditions
Find global minimum time step
\[ u = u_{\text{init}}, \Delta t = \min(\Delta t_i) \]

Find new global minimum time step
\[ \Delta t_{\text{new}} = \min(\Delta t_i) \]

Apply boundary conditions
\[ u|_{\Gamma} = u_{bc} \]

Update fluxes and sources
\[ F_{\text{new}}, q_{\text{new}} \]
Discrete Event Simulation Cycle

Apply initial conditions
Calculate time delays
Create Event List
Schedule Events

\[ u = u_{init}, \Delta t, list\{Event\} \]

Discret Event Driven Cycle

Pop event with the smallest time stamp \( t_{e,proc} \)
Set clock time:
\[ t_{clock} = t_{e,proc} \]

Reschedule Events:
- a) Calculate new time delays of event \( e \) and all dependent events
- b) Sort the Queue of Events

Update state \( e \)

Synchronize state \( e \):
- a) Either just Update or fully Process dependent Events
- b) Either Update fluxes and sources or apply Boundary Conditions
Thus the DES algorithm in general and also specifically in FEFV cell will consist on the following steps:

- Initialize all the events and schedule them (predict the delays of each event).

- Process the event with smallest process time (Update, Recalculate the Fluxes, Synchronize and Reschedule this Event).

  *Synchronization*: trigger the chain process of updating and processing the neighbour events until it will reach the ones which shouldn’t be process, because they didn’t reach the target scalar change.

  *Reschedule*: reschedule the event based on the new values of fluxes and process time, and resort the queue.

- Repeat the above steps until the queue is empty.
To increase the efficiency of the flux calculations in FEFV, we also introduce the Event attribute called *Rate Status*. Based on the current status of a nodal variable (associated with FEFV cell) the above algorithm can thus be applied to an *Element Centred Event*. This gives the possibility to visit the elements and provide the synchronization and calculation processes immediately for all the FV sectors of an FE cell, without repetition. Such approach can also extend application of DES to Finite Element Framework.
Rate of FV variable should be updated,
and FV process should be rescheduled
Rate of FV variable should be updated,
but FV process should not be rescheduled
Rate and status of FV variable stays the same
The standard DES approach can be improved by Preemptive-Event-Processing technique introduced by [Omelchenko2006]. It had the intention to bring DES into parallel world. The main idea of Preemptive-Event-Processing is to group all the events with small difference in expected time of processing $\delta t_{PEP}$ and to do the synchronization automatically for this group, without waiting for the call of confluent function from each of this events. For handling this group of events the additional construction PEP Stack is used in order to do the internal sorting process in small group instead of sorting the whole Event Queue. The control parameter $\delta t_{PEP}$ can be used either as a global or local condition on state variable change.
DES with Preemptive-Event-Processing

\[ \Delta t_{des} = \frac{\Delta f}{dt} \]

\[ \Delta t_{PEP} \]
Slightly compressible immiscible two phase flow

Pressure equation:

\[
\phi c_t \frac{\partial p_w}{\partial t} - \nabla \cdot \lambda_t K \nabla p_w + \nabla \cdot \left( \rho_w^{-1} v_w \nabla \rho_w + \rho_n^{-1} v_n \nabla \rho_n \right) = \\
= q_t + \nabla \cdot \lambda_n K \nabla p_c - \nabla \cdot K (\lambda_w \rho_w + \lambda_n \rho_n) g
\]

Saturation equation:

\[
\frac{\partial (\phi \rho_n S_n)}{\partial t} - \nabla \cdot (\rho_n \lambda_n K (\nabla p_w - \rho_n g)) - \nabla \cdot (\lambda_n \rho_n K \nabla p_c) = \rho_n q_n, \\
\text{or} \\
\frac{\partial (\phi \rho_n S_n)}{\partial t} + \nabla \cdot (\rho_n f_n (v_t - \lambda_w K \nabla p_c - \lambda_w (\rho_w - \rho_n) g))) = \rho_n q_n
\]
Incompressible immiscible two phase flow

Pressure equation:

\[ \int_{\Omega} \lambda_t K \nabla p \cdot \nabla N d\Omega = \int_{\Omega} q_t N d\Omega + \]
\[ + \int_{\Omega} K (\lambda_w \rho_w + \lambda_n \rho_n) g \cdot \nabla N d\Omega - \int_{\Omega} \lambda_n K \nabla p_c \cdot \nabla N d\Omega \]

Saturation equation:

\[ \int_{\Omega} W \frac{\partial}{\partial t} (\phi S_n) d\Omega - \int_{\Omega} W q_n d\Omega \]
\[ - \int_{\partial\Omega} W \cdot \left( \frac{k_{rn}}{\mu_n} K (\nabla p_w + \nabla p_c - \rho_n g) \right) \cdot n d\Gamma = 0 \]
Simulation characteristics:

- $K_m = 2.0 \times 10^{-14}$
- Incompressible two phase flow with gravity effects
- Brooks Corey rel. perm. model
- Injector(nw) well at low left corner, Producer at upper right corner
- $N_{elmts} = 5779$, $\frac{h_{min}}{h_{max}} = 0.04$
- Dimensions: $1.88 \times 1.25$ m
- Injection rate = $5.0 \cdot 10^{-5} m^3 s^{-1} (CO_2)$
- $\rho_w = 1045 kg \cdot m^{-3}$, $\rho_{nw} = 479 kg \cdot m^{-3}$
2D Kilve Bed 3 Fractured model (partial)
CPU Run Time Comparison ( $k_f / k_m = 4.165 \times 10^6$ )

All cases: $\Delta t_{\text{press}} = 10 \times \Delta t_{\text{CFL}}$

Fraction of Modelled Time (~800 [s])

CPU Run Time [hr]
Kilve Bed 3 2D results: DES vs IMPES, saturation plots

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[Images of saturation plots and CFL increment plot]
Kilve Bed 3 2D performance results: DES vs EXP, runtime plots

2D Kilve Bed 3 Fractured model
CPU Run Time Comparison

- DES PEP-EC $\Delta t_{\text{sat}} = \text{N/A}$
- TDS EXP $\Delta t_{\text{sat}} = 0.8^*\Delta t_{\text{CFL}}$

All cases: $\Delta t_{\text{press}} = 25^*\Delta t_{\text{CFL}}$

Fraction of Modelled Time (~125 [s])

CPU Run Time [hr]
For producing an accurate results on material interfaces with FEFV method one would require to apply special conditions and discontinuous solution (saturation) across the interface. Thus the extended capillary pressure condition was applied in this work on material interfaces [Duijn95]. What might be distinctive in our approach is that the explicit splitting of the nodes was enforced on the mesh level.
McWhorter Solution: Co-current and Counter-current flow
Three Zones of different materials
SplitNode approach
SplitNode approach
Conclusions and Future Work

- Discrete event simulation is a sufficiently general and flexible approach intended for multi scale type of problems, which have significant variations of characteristic times of different processes.
- The efficiency of DES is dependent on the amount of activity which occurs in the simulation with respect to the total amount of possible events. In general, the lower this ratio is, the better the performance of DES.
- Future work includes the implementation and study of the DES approach for compositional compressible flow in fractured media with application to \( CO_2 \) migration in saline aquifers.
