OPM Flow – overview and demonstration

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MSO4SC workshop
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Overview of talk

Reservoir simulation

Mathematical formulation

Implementation with automatic differentiation

What next?
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What next?
What is reservoir simulation

Simulation of *porous medium* flow in *subsurface reservoirs*.

Examples of use:
- **Energy industry**
  - Forecasting and optimizing oil and gas production.
  - Forecasting and optimizing geothermal energy production.
- **Environmental management**
  - Groundwater flows and pollutants
  - \( \text{CO}_2 \) storage

Reservoir simulators solve *systems of nonlinear PDEs* that are coupled to *well/facility models*. 
Why is it hard?

- Porous medium is strongly heterogeneous and anisotropic.
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- Grids with high aspect ratio, fully unstructured, polygonal cells.
- Nontrivial phase behaviour. Phases can appear and disappear as fluid components dissolve or vaporize.
- Coupling to wells can connect regions that are far away from each other.
- The models are highly nonlinear.
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Why does it require HPC/Cloud

- Model sizes increasing (Saudi-Aramco record: 1e12 cells)
- Model complexity increasing (well/facility models, fluid models)
- New mechanisms (polymer, CO$_2$) require better resolved fronts
- Large ensembles for history matching, optimization, uncertainty quantification
The market situation

Commercial reservoir simulators (expensive but comprehensive):

- ECLIPSE, Intersect (Schlumberger)
- IMEX, GEM, STARS (CMG)
- Nexus (Landmark)
- tNavigator (Rock Flow Dynamics)

In-house simulators (unavailable to outsiders):

- (Tera)POWERS (Saudi-Aramco)
- MoReS (Shell)
- GPRS (Stanford University)

Open source simulators:

- OPM Flow
- MRST (Sintef)
OPM Flow at a glance

- Open source
- Handling cases of full industrial complexity (wells, properties)
- Competitive performance
- Currently used to study (for example):
  - Oil production: history matching and prediction of field performance
  - Enhanced oil recovery: CO2, polymer
  - CO2 sequestration
- Automatic differentiation enables rapid development of fluid models.

**Ambition: to be a strong base for both industrial development and academic research**
Overview of talk

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What next?
Physical laws and behaviours

- Conservation of mass
  - for each fluid pseudocomponent (oil, gas, water)
  - for injected EOR fluids (polymer, CO$_2$, surfactants)
  - (for ion species)

\[
\frac{\partial}{\partial t} (\phi A_\alpha) + \nabla \cdot \mathbf{u}_\alpha = Q_\alpha
\]
Physical laws and behaviours

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  - for injected EOR fluids (polymer, CO\(_2\), surfactants)
  - (for ion species)
  - \( \frac{\partial}{\partial t}(\phi A_\alpha) + \nabla \cdot u_\alpha = Q_\alpha \)

- Darcy’s law (single phase)
  - \( v = -(1/\mu)K(\nabla p - \rho g) \)
Physical laws and behaviours

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- Darcy’s law (single phase)
  - $v = -(1/\mu)K(\nabla p - \rho g)$

- Multiphase flow: relative permeability and capillary pressure
  - flow rate reduced by $k_r$, function of fluid saturations
  - pressure difference between phases
  - $v_\alpha = -(k_{r,\alpha}/\mu_\alpha)K(\nabla p_\alpha - \rho_\alpha g)$
The black-oil model

- “Black-oil” model assumptions
  - Lump HC species into two (pseudo)components (oil, gas)
  - Allow oleic *phase* to contain both oil and gas *components*
    - Dissolved gas ratio, $r_S$
  - Allow gaseous *phase* to contain both oil and gas *components*
    - Vaporized oil ratio, $r_V$
  - Assumed always at thermodynamic equilibrium
  - Simple enough PVT relations to use table lookup
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- Consequence: phase and component confusion!
- Consequence: can have three different states:
  - fully saturated (all three phases present)
  - undersaturated oil (no gaseous phase)
  - undersaturated gas (no oleic phase)
The black-oil model

▶ “Black-oil” model assumptions
  ▶ Lump HC species into two (pseudo)components (oil, gas)
  ▶ Allow oleic phase to contain both oil and gas components
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▶ Consequence: can have three different states:
  ▶ fully saturated (all three phases present)
  ▶ undersaturated oil (no gaseous phase)
  ▶ undersaturated gas (no oleic phase)

▶ (Subset of more general compositional model, must solve equation of state, such as Peng-Robinson)
The continuous equations form a system of partial differential equations, one for each pseudo-component $\alpha$:

$$\frac{\partial}{\partial t} (\phi A_\alpha) + \nabla \cdot u_\alpha = Q_\alpha$$

where

$$A_w = m_\phi b_w s_w, \quad u_w = b_w v_w,$$

$$A_o = m_\phi (b_o s_o + r_V b_g s_g), \quad u_o = b_o v_o + r_V b_g v_g,$$

$$A_g = m_\phi (b_g s_g + r_S b_o s_o), \quad u_g = b_g v_g + r_S b_o v_o.$$  

and these additional relations should hold:

$$s_w + s_o + s_g = 1$$

$$p_{cow} = p_o - p_w$$

$$p_{cog} = p_o - p_g.$$  

The phase fluxes are given by Darcy’s law:

$$v_\alpha = -\lambda_\alpha K (\nabla p_\alpha - \rho_\alpha g).$$
What is the source term, anyway?

\[ \frac{\partial}{\partial t} (\phi A_\alpha) + \nabla \cdot u_\alpha = Q_\alpha \]
Coupling to well model

What is the source term, anyway?

\[
\frac{\partial}{\partial t} (\phi A_{\alpha}) + \nabla \cdot u_{\alpha} = Q_{\alpha}
\]

Well rates!

- Computed using separate well model(s).
- Must be solved *simultaneously* with reservoir equations.
Discretization

The system is discretized using:

- First-order implicit Euler in time
- First-order finite volumes in space
  - two-point flux approximation (!)
  - phase-based upwinding of properties

Why such “primitive methods” (low order, inconsistent)?

- Historically, finite difference methods
- Need systems that linear solvers can deal with well
- Sufficient for practical purposes
- Discretization errors not significant compared to inherent uncertainty

Quite a bit has been done by various groups (not mainstream yet):

- Consistent discretizations (MPFA, mimetic)
- Higher-order FV or DG methods
- Higher-order time discretizations
The discretized equations and residuals are, for each pseudo-component \( \alpha \) and cell \( i \):

\[
R_{\alpha,i} = \frac{\phi_{0,i} V_i}{\Delta t} (A_{\alpha,i} - A_{\alpha,i}^0) + \sum_{j \in C(i)} u_{\alpha,ij} + Q_{\alpha,i} = 0
\] (9)

where

\[
A_w = m_\phi b_w s_w, \quad u_w = b_w v_w, \tag{10}
\]
\[
A_o = m_\phi (b_o s_o + r_{og} b_g s_g), \quad u_o = b_o v_o + r_{og} b_g v_g, \tag{11}
\]
\[
A_g = m_\phi (b_g s_g + r_{go} b_o s_o), \quad u_g = b_g v_g + r_{go} b_o v_o. \tag{12}
\]

The relations (5), (6) and (7) hold for each cell \( i \).
The fluxes are given for each connection $ij$ by:

$$ (b_\alpha v_\alpha)_{ij} = (b_\alpha \lambda_\alpha m_T) U(\alpha, ij) T_{ij} \Delta H_{\alpha,ij} $$  \hspace{1cm} (13)

$$ (r_\beta b_\alpha v_\alpha)_{ij} = (r_\beta \lambda_\alpha m_T) U(\alpha, ij) T_{ij} \Delta H_{\alpha,ij} $$  \hspace{1cm} (14)

$$ \Delta H_{\alpha,ij} = p_{\alpha,i} - p_{\alpha,j} - g \rho_{\alpha,ij} (z_i - z_j) $$  \hspace{1cm} (15)

$$ \rho_{\alpha,ij} = (\rho_{\alpha,i} + \rho_{\alpha,j})/2 $$  \hspace{1cm} (16)

$$ U(\alpha, ij) = \begin{cases} i & \Delta H_{\alpha,ij} \geq 0 \\ j & \Delta H_{\alpha,ij} < 0 \end{cases} $$  \hspace{1cm} (17)
Solving the discrete equations

Main method: Newton-Raphson

- solve large heterogenous linear systems
- challenging to precondition (CPR + AMG best?)
- must modify updates for phase changes
- must handle convergence failures (timestep cuts)
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What next?
What does AD provide

\[ f(x) \{ \ldots \} \quad \text{df}(x) \{ \ldots \} \]

\[ f(x) \quad f'(x) \]
What does AD provide

Traditional Process

- Human implements code to evaluate \( f(x) \)
- Manual or symbolic calculation to derive \( f'(x) \)
- Human implements code to evaluate \( f'(x) \)
What does AD provide

Traditional Process
- Human implements code to evaluate $f(x)$
- Manual or symbolic calculation to derive $f'(x)$
- Human implements code to evaluate $f'(x)$

Automatic Differentiation (AD)
- Human implements code to evaluate $f(x)$
- Computer code to evaluate $f'(x)$ is automatically generated
Benefits of using AD

AD makes it easier to create simulators:
- only specify nonlinear residual equation
- automatically evaluates Jacobian
- sparsity structure of Jacobian automatically generated

Note that AD is *not* the same as finite differencing!
- no need to define a 'small' epsilon
- as precise as hand-made Jacobian
- ... but much less work!

Performance (of equation assembly) will usually be somewhat slower than a *good* hand-made Jacobian implementation.
A numeric computation $y = f(x)$ can be written ($D = \text{derivative}$)

$$y_1 = f_1(x) \quad \frac{dy_1}{dx}(x) = Df_1(x)$$

$$y_2 = f_2(y_1) \quad \frac{dy_2}{dx}(x) = Df_2(y_1) \cdot Df_1(x)$$

$$\vdots$$

$$y = f_n(y_{n-1}) \quad \frac{dy}{dx}(x) = Df_n(y_{n-1}) \cdot Df_{n-1}(y_{n-2}) \cdots Df_1(x)$$

Automatic Differentiation:

- make each line an elementary operation
- compute right derivative values as we go using chain rule
Implementation approaches

Two main methods:

Operator overloading

- requires operator overloading in programming language
- syntax (more or less) like before (non-AD)
- efficiency can vary a lot, depends on usage scenario
- easy to implement and experiment with
- Examples: OPM, Sacado (Trilinos), ADOL-C

Source transformation with AD tool

- can be implemented for almost any language
- may restrict language syntax or features used
- efficiency can be high (depends on AD tool)
- Examples: TAPENADE, OpenAD
Types of AD

Two different approaches.
(We compute $f(x)$, $u$ is some intermediate variable.)

Forward Mode
Carry derivatives with respect to independent variables:

$$(u, \frac{du}{dx})$$

Reverse Mode
Carry derivatives with respect to dependent variables (adjoints):

$$(u, \frac{df}{du})$$
Forward AD example (1)

Example function: \( f(x) = x(sin(x^2) + 3x) \).

Sequence of elementary functions:

\[
\begin{align*}
  f_1(u) &= u^2 & f'_1(u) &= 2uu' \\
  f_2(u) &= \sin(u) & f'_2(u) &= \cos(u)u' \\
  f_3(u) &= 3u & f'_3(u) &= 3u' \\
  f_4(u, v) &= u + v & f'_4(u, v) &= u' + v' \\
  f_5(u, v) &= u \cdot v & f'_5(u, v) &= u'v + uv'
\end{align*}
\]

Rewritten:
\[
f(x) = f_5(x, f_4(f_2(f_1(x)), f_3(x)))
\]
Forward AD example (2)

Example function: \( f(x) = x(sin(x^2) + 3x) \). Computing \( f(3), f'(3) \).

Sequence of elementary functions:

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\begin{align*}
  f_1(u) &= u^2 & f_1'(u) &= 2uu' \\
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  f_3(u) &= 3u & f_3'(u) &= 3u' \\
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\]

\[
\begin{array}{c}
    f_5 \\
    3 \\
    f_4 \\
    0.4121 \\
    f_3 \\
    9 \\
    3 \\
    3 \\
\end{array} \quad \begin{array}{c}
    f'_5 \\
    1 \\
    f'_4 \\
    -5.4668 \\
    f'_3 \\
    6 \\
    1 \\
    1 \\
\end{array}
\]
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\end{align*}
$$

\[
\begin{array}{c}
28.2364 \\
3 \quad 9.4121
\end{array}
\]

\[
\begin{array}{c}
0.4121 \\
9 \quad 3
\end{array}
\]

\[
\begin{array}{c}
9 \\
3
\end{array}
\]

\[
\begin{array}{c}
2.0118 \\
1 \quad -2.4668
\end{array}
\]

\[
\begin{array}{c}
-5.4668 \\
6 \quad 1
\end{array}
\]

\[
\begin{array}{c}
1
\end{array}
\]
Properties of forward AD

- Easy to implement with operator overloading
- Storage required (scalar): $2 \times$ normal (value, derivative).
- Storage required ($f : \mathbb{R}^m \rightarrow \mathbb{R}^n$): $(n + 1) \times$ normal (value, derivative vector), unless sparse.
Recall: Reverse Mode
Carry derivatives with respect to dependent variables (adjoints):

\[(u, \frac{df}{du})\]

We will use the chain rule again, but in the opposite direction:

\[\text{adj}(u) = \text{adj}(f_i) \frac{\partial f_i}{\partial u}.\]

Using \(\text{adj}(u)\) to mean the adjoint \(\frac{df}{du}\).
(So \(\text{adj}(x)\) is our goal.)
Example function: \( f(x) = x\sin(x^2) + 3x \). Computing \( f(3) \), \( f'(3) \).

Sequence of elementary functions:

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\[28.2364\]
\[\begin{array}{c}
  3 \\
  0.4121 \\
  \ \ | \\
  \ \ | \\
  \ \ 9 \\
  \ \ | \\
  \ \ 3 \\
  \ \ | \\
  \ \ 3
\end{array}\]

\[\begin{array}{c}
  \text{adj}(f_5) \\
  \text{adj}(x) \\
  \text{adj}(f_4) \\
  \text{adj}(f_2) \\
  \text{adj}(f_3) \\
  \text{adj}(f_1) \\
  \text{adj}(x) \\
  \text{adj}(x)
\end{array}\]
Reverse AD example

Example function: \( f(x) = x(sin(x^2) + 3x) \). Computing \( f(3) \), \( f'(3) \).

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\text{adj}(f_2) & \text{adj}(f_3) \\
\text{adj}(f_1) & \text{adj}(x) \\
\text{adj}(x) &
\end{array}\]

Must sum contributions:

\[f'(3) = 9.4121 - 16.4003 + 9 = 2.0118\]
Example function: \( f(x) = x(sinx^2 + 3x) \). Computing \( f(3), f'(3) \).

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    f_4(u, v) &= u + v & \text{adj}(u) &= \text{adj}(f_4), & \text{adj}(v) &= \text{adj}(f_4) \\
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    3 & \quad 9.4121 \\
    0.4121 & \quad 9 \\
    & \quad 9 \\
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    & \quad \text{adj}(f_2) \quad \text{adj}(f_3) \\
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\]
Reverse AD example

Example function: \( f(x) = x(s\sin(x^2) + 3x) \). Computing \( f(3), f'(3) \).

Sequence of elementary functions:

\[
\begin{align*}
f_1(u) &= u^2 & \text{adj}(u) &= \text{adj}(f_1) \cdot 2u \\
f_2(u) &= \sin(u) & \text{adj}(u) &= \text{adj}(f_2) \cdot \cos(u) \\
f_3(u) &= 3u & \text{adj}(u) &= \text{adj}(f_3) \cdot 3 \\
f_4(u,v) &= u + v & \text{adj}(u) &= \text{adj}(f_4), \quad \text{adj}(v) &= \text{adj}(f_4) \\
f_5(u,v) &= u \cdot v & \text{adj}(u) &= \text{adj}(f_5) \cdot v, \quad \text{adj}(v) &= \text{adj}(f_5) \cdot u
\end{align*}
\]

\[
\begin{align*}
28.2364 \\
3 & \\
3 & 9.4121 \\
0.4121 & 9 \\
9 & 3 \\
3 & 3 \\
\text{adj}(f_1) & \text{adj}(x) \\
\text{adj}(x) & \text{adj}(x)
\end{align*}
\]
Example function: $f(x) = x(sin(x^2) + 3x)$. Computing $f(3), f'(3)$.

Sequence of elementary functions:

- $f_1(u) = u^2$, $\text{adj}(u) = \text{adj}(f_1) \cdot 2u$
- $f_2(u) = \sin(u)$, $\text{adj}(u) = \text{adj}(f_2) \cdot \cos(u)$
- $f_3(u) = 3u$, $\text{adj}(u) = \text{adj}(f_3) \cdot 3$
- $f_4(u, v) = u + v$, $\text{adj}(u) = \text{adj}(f_4)$, $\text{adj}(v) = \text{adj}(f_4)$
- $f_5(u, v) = u \cdot v$, $\text{adj}(u) = \text{adj}(f_5) \cdot v$, $\text{adj}(v) = \text{adj}(f_5) \cdot u$

Must sum contributions: $f'(3) = 9.4121 - 16.4003 + 9 = 2.0118$
Reverse AD example

Example function: $f(x) = x(sin(x^2) + 3x)$. Computing $f(3)$, $f'(3)$.

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- $f_5(u, v) = u \cdot v$ \quad \text{adj}(u) = \text{adj}(f_5) \cdot v$, \quad \text{adj}(v) = \text{adj}(f_5) \cdot u$

Must sum contributions: $f'(3) = 9.4121 - 16.4003 + 9 = 2.0118$. 

Diagram:

```
28.2364
3 9.4121
 0.4121 9
   9 3
    9 3
     -2.734 adj(x)
      3 adj(x)
       adj(x)
```
Reverse AD example

Example function: \( f(x) = x(sin(x^2) + 3x) \). Computing \( f(3), f'(3) \).

Sequence of elementary functions:

\[
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  f_5(u, v) &= u \cdot v & \text{adj}(u) &= \text{adj}(f_5) \cdot v, & \text{adj}(v) &= \text{adj}(f_5) \cdot u
\end{align*}
\]

Must sum contributions:

\[
\begin{align*}
  f'(3) &= 9.4121 - 16.4003 + 9 = 2.0118
\end{align*}
\]
Reverse AD example

Example function: $f(x) = x(sin(x^2) + 3x)$. Computing $f(3)$, $f'(3)$.

Sequence of elementary functions:

- $f_1(u) = u^2 \quad \text{adj}(u) = \text{adj}(f_1) \cdot 2u$
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- $f_4(u, v) = u + v \quad \text{adj}(u) = \text{adj}(f_4), \quad \text{adj}(v) = \text{adj}(f_4)$
- $f_5(u, v) = u \cdot v \quad \text{adj}(u) = \text{adj}(f_5) \cdot v, \quad \text{adj}(v) = \text{adj}(f_5) \cdot u$

\[
\begin{align*}
28.2364 & = 3 \cdot 9.4121 \\
9.4121 & = 0.4121 \cdot 9 \\
0.4121 & = 0.3 \cdot 3 \\
9.4121 & = 3 \cdot 3 \\
-2.7334 & = -2.7334 \cdot 9 \\
-16.4003 & = -16.4003 \cdot 3 \\
1 & = 1 \cdot 1 \\
3 & = 3 \cdot 3 \\
9 & = 9 \cdot 1
\end{align*}
\]

Must sum contributions:

\[
f'(3) = 9.4121 - 16.4003 + 9 = 2.0118.
\]
AutoDiffBlock (legacy)

- class implementing *forward AD*
- deals with *vectors of values* at a time
- derivatives are *sparse matrices*
- implemented with operator overloading
- based on Eigen library for basic types and operands
- helper library provides discrete div, grad etc.

Evaluation (new effort)

- class implementing *forward AD*
- deals with *a single scalar value* at a time
- derivatives are *compile-time-size vectors*
- implemented with operator overloading
- discrete div, grad must be implemented “manually”
Overview of talk

Reservoir simulation

Mathematical formulation

Implementation with automatic differentiation

What next?
We keep pursuing...

- **Performance**
  - Improving preconditioners and linear solvers
  - New discretizations, nonlinear preconditioning
  - Parallel scaling

- **Usability**
  - Reference manual started!
  - More output/logging options
  - Better error messages

- **Deployability**
  - Container usage
  - MSO4SC Portal and web integration
  - Better error messages
Further ahead: some possibilities

- New fluid models for CO$_2$, EOR options.
- Scriptable? Python? Cling-able?
- More flexible boundary conditions
- Higher order DG methods?
- Consistent discretizations?
- Fully compositional fluid model?
- New I/O system for parallel scalability?
- Preprocessing tools?
Thank you for listening!