OPM Flow – overview and demonstration

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MSO4SC workshop
23rd May 2017

Overview of talk

Reservoir simulation

Mathematical formulation

Implementation with automatic differentiation

What next?

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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
  - CO_2storage

Reservoir simulators solve *systems of nonlinear PDEs* that are coupled to *well/facility models*.

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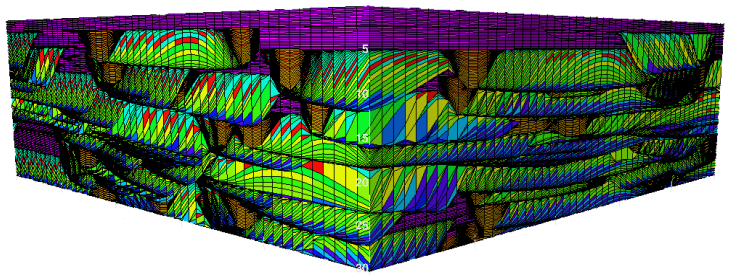

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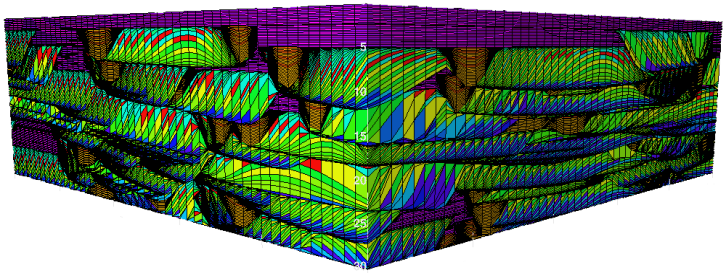
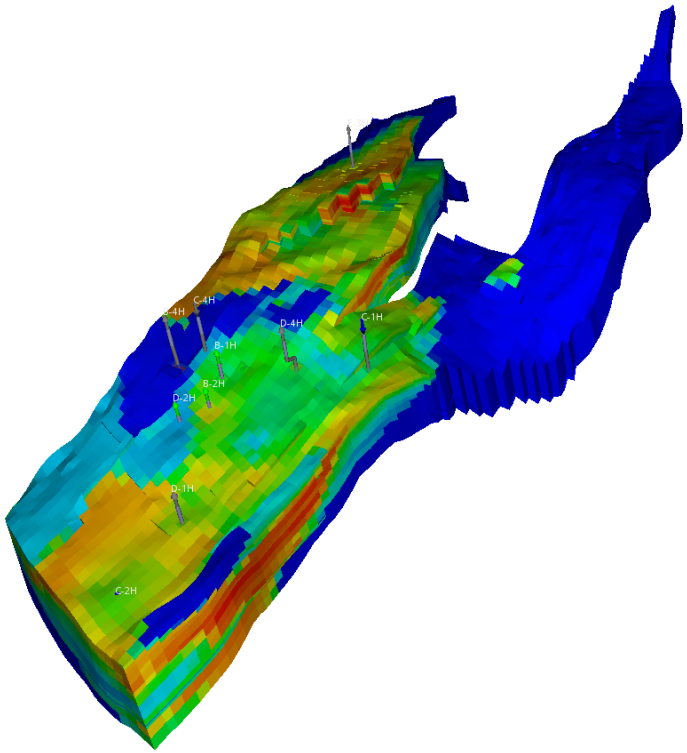




Why does it require HPC/Cloud

- 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):

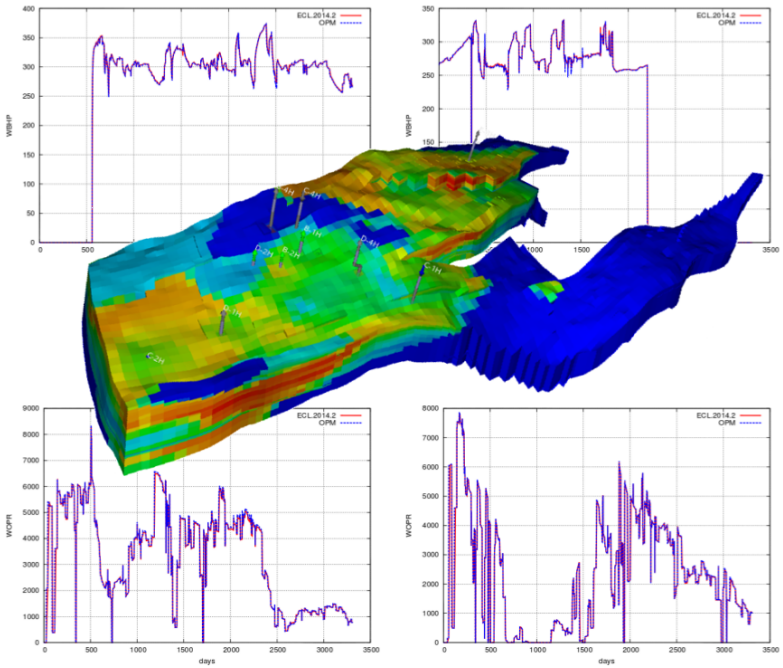
- (Tera)POWERS (Saudi-Aramco)
- MoReS (Shell)
- GPRS (Stanford University)
- ...

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

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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)
  - $\frac{\partial}{\partial t}\left(\phi A_\alpha\right) + \nabla \cdot \mathbf{u}_\alpha = Q_\alpha$

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  - $\mathbf{v} = -(1/\mu)\mathbf{K}(\nabla p - \rho \mathbf{g})$
- Multiphase flow: relative permeability and capillary pressure
  - flow rate reduced by k_r, function of fluid saturations
  - pressure difference between phases
  - $\mathbf{v}_\alpha = -(k_{r,\alpha}/\mu_\alpha)\mathbf{K}(\nabla p_\alpha - \rho_\alpha \mathbf{g})$

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*
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  - undersaturated oil (no gaseous phase)
  - undersaturated gas (no oleic phase)

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- (Subset of more general *compositional* model, must solve equation of state, such as Peng-Robinson)

System of equations

The continuous equations form a system of partial differential equations, one for each pseudo-component α:

$$\frac{\partial}{\partial t}\left(\phi A_\alpha\right) + \nabla \cdot \mathbf{u}_\alpha = Q_\alpha \tag{1}$$

where

$$A_w = m_\phi b_w s_w, \qquad \mathbf{u}_w = b_w \mathbf{v}_w, \tag{2}$$

$$A_o = m_\phi (b_o s_o + r_V b_g s_g), \qquad \mathbf{u}_o = b_o \mathbf{v}_o + r_V b_g \mathbf{v}_g, \tag{3}$$

$$A_g = m_\phi (b_g s_g + r_S b_o s_o), \qquad \mathbf{u}_g = b_g \mathbf{v}_g + r_S b_o \mathbf{v}_o. \tag{4}$$

and these additional relations should hold:

$$s_w + s_o + s_g = 1 \tag{5}$$

$$p_{cow} = p_o - p_w \tag{6}$$

$$p_{cog} = p_o - p_g. \tag{7}$$

The phase fluxes are given by Darcy's law:

$$\mathbf{v}_\alpha = -\lambda_\alpha \mathbf{K}(\nabla p_\alpha - \rho_\alpha \mathbf{g}). \tag{8}$$

Coupling to well model

What is the source term, anyway?

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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

Discrete equations (I)

The discretized equations and residuals are, for each pseudo-component α and cell i:

$$R_{\alpha,i} = \frac{\phi_{0,i} V_i}{\Delta t} \left(A_{\alpha,i} - A^0_{\alpha,i} \right) + \sum_{j \in C(i)} u_{\alpha,ij} + Q_{\alpha,i} = 0 \tag{9}$$

where

$$A_w = m_\phi b_w s_w, \qquad u_w = b_w v_w, \tag{10}$$

$$A_o = m_\phi (b_o s_o + r_{og} b_g s_g), \qquad u_o = b_o v_o + r_{og} b_g v_g, \tag{11}$$

$$A_g = m_\phi (b_g s_g + r_{go} b_o s_o), \qquad u_g = b_g v_g + r_{go} b_o v_o. \tag{12}$$

The relations (5), (6) and (7) hold for each cell i.

Discrete equations (II)

The fluxes are given for each connection ij by:

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

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

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

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

$$U(\alpha, ij) = \begin{cases} i & \Delta H_{\alpha,ij} \geq 0 \\ j & \Delta H_{\alpha,ij} < 0 \end{cases} \tag{17}$$

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 does AD provide

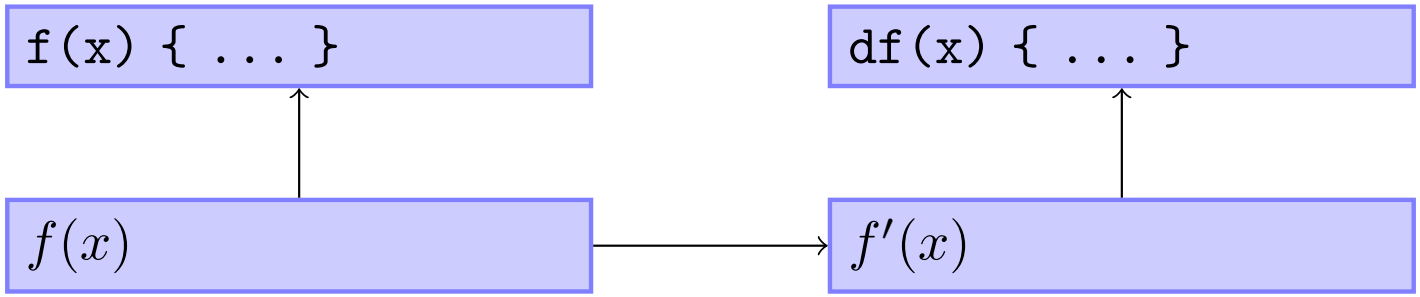
```
f(x) { ... }
```

```
df(x) { ... }
```

$f(x)$

$f'(x)$

What does AD provide



Traditional Process

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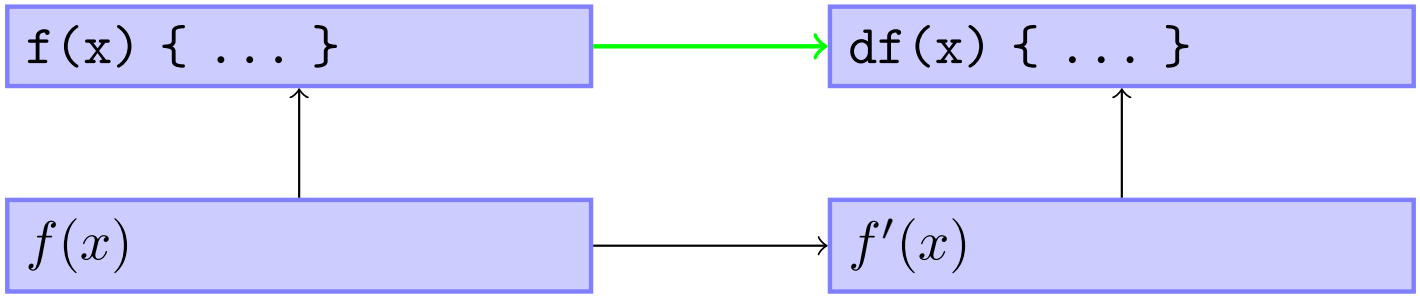

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Automatic Differentiation (AD)

- 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.

Basic idea

A numeric computation $y = f(x)$ can be written (D = derivative)

$$
\begin{aligned}
y_1 &= f_1(x) & \frac{dy_1}{dx}(x) &= Df_1(x) \\
y_2 &= f_2(y_1) & \frac{dy_2}{dx}(x) &= Df_2(y_1) \cdot Df_1(x) \\
&\vdots \\
y &= f_n(y_{n-1}) & \frac{dy}{dx}(x) &= Df_n(y_{n-1}) \cdot Df_{n-1}(y_{n-2}) \cdots Df_1(x)
\end{aligned}
$$

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:

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\begin{aligned}
f_1(u) &= u^2 & f_1'(u) &= 2uu' \\
f_2(u) &= \sin(u) & f_2'(u) &= \cos(u)u' \\
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f_4(u,v) &= u + v & f_4'(u,v) &= u' + v' \\
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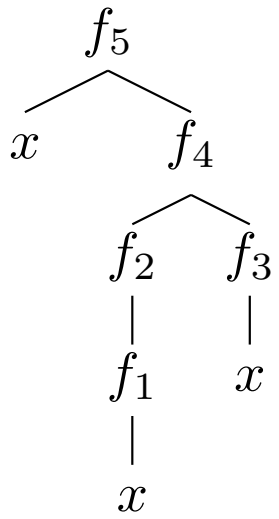
Rewritten:
$f(x) = f_5(x, f_4(f_2(f_1(x)), f_3(x)))$



Forward AD example (2)

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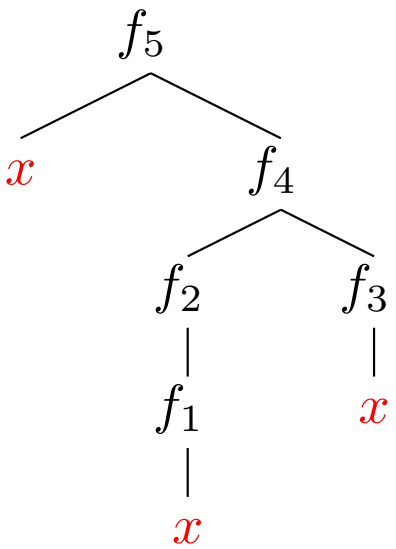

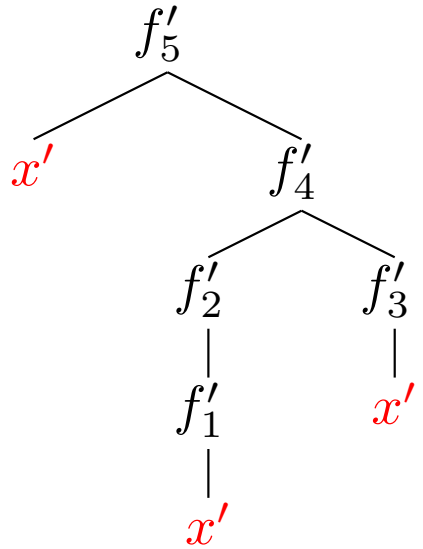

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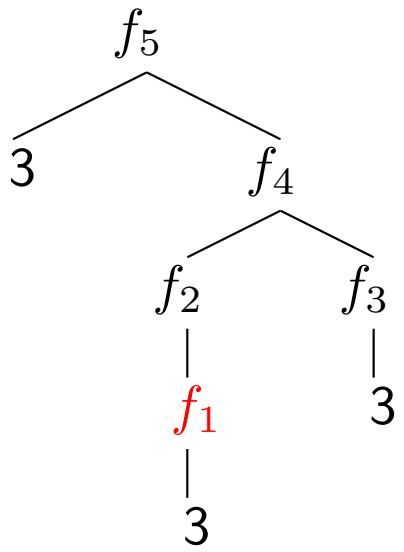

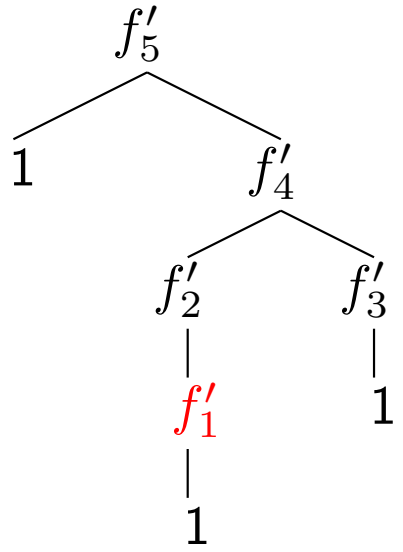

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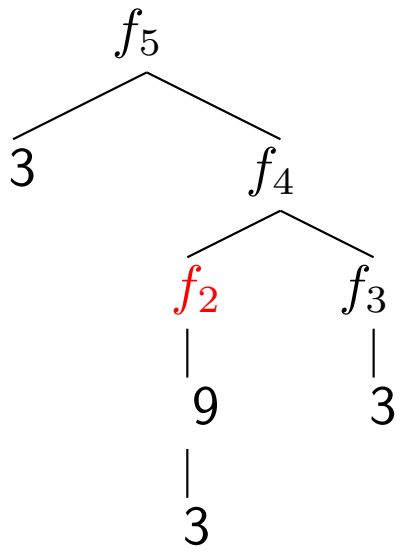

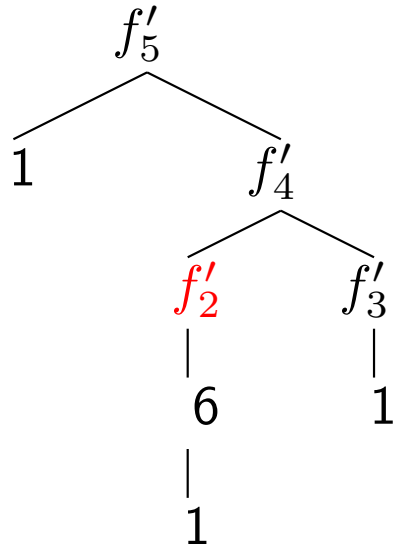

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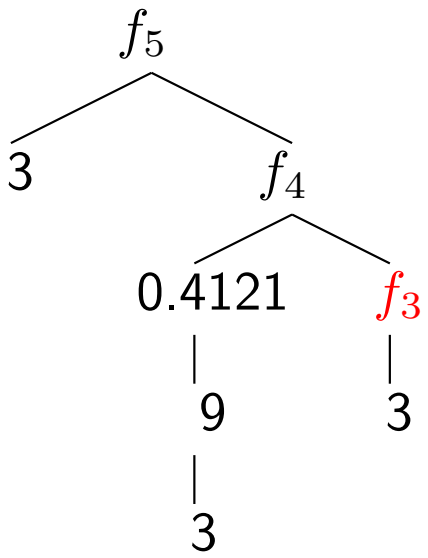

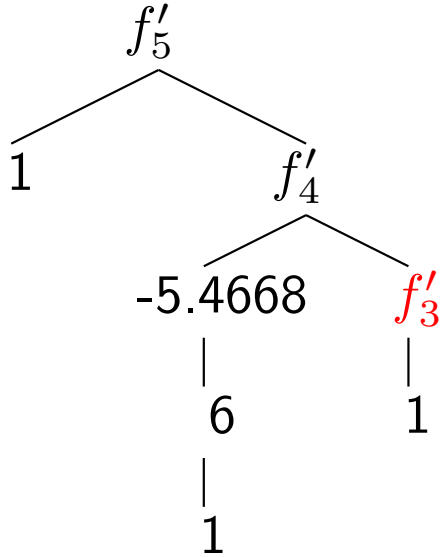

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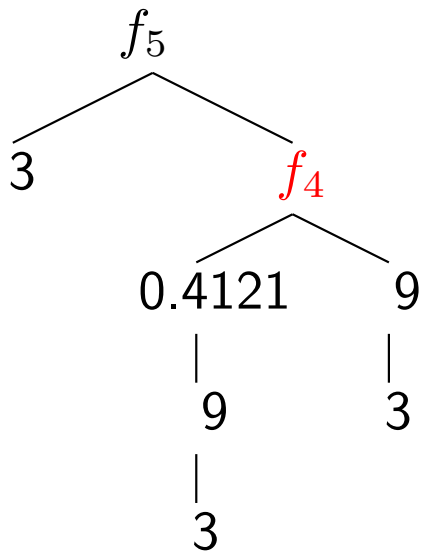

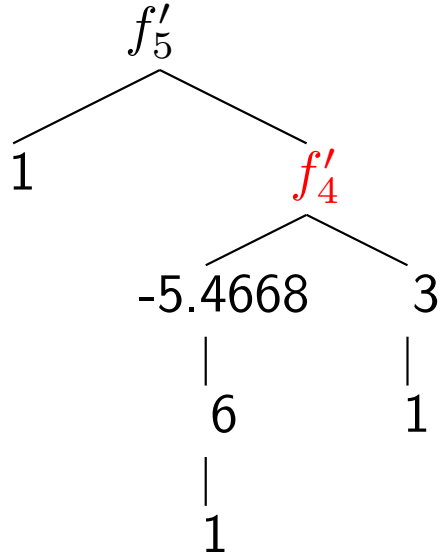

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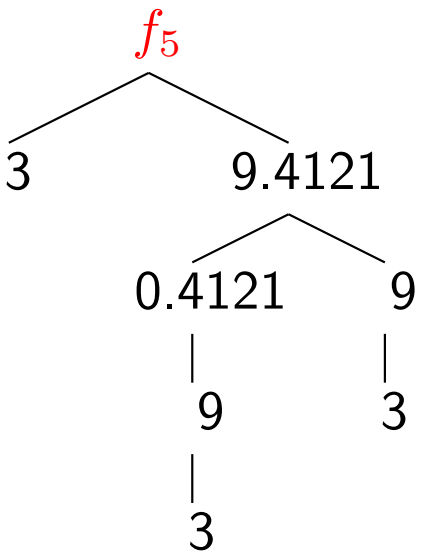

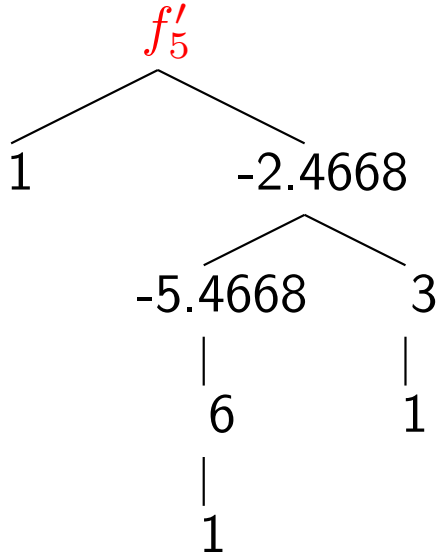

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f_1(u) &= u^2 & f_1'(u) &= 2uu' \\
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f_3(u) &= 3u & f_3'(u) &= 3u' \\
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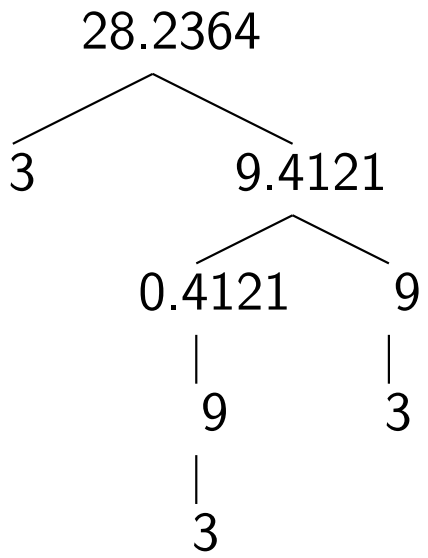

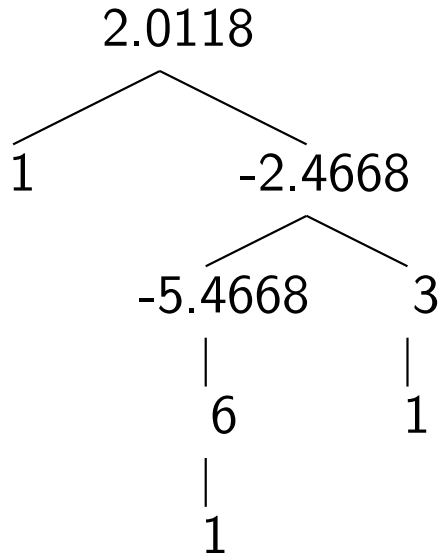

Properties of forward AD

- Easy to implement with operator overloading
- Storage required (scalar): $2\times$ normal (value, derivative).
- Storage required ($f : R^m \to R^n$): $(n+1)\times$ normal (value, derivative vector), unless sparse.

Reverse Mode AD

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:

$$\mathrm{adj}(u) = \mathrm{adj}(f_i)\frac{\partial f_i}{\partial u}.$$

Using $\mathrm{adj}(u)$ to mean the adjoint $\frac{df}{du}$.
(So $\mathrm{adj}(x)$ is our goal.)

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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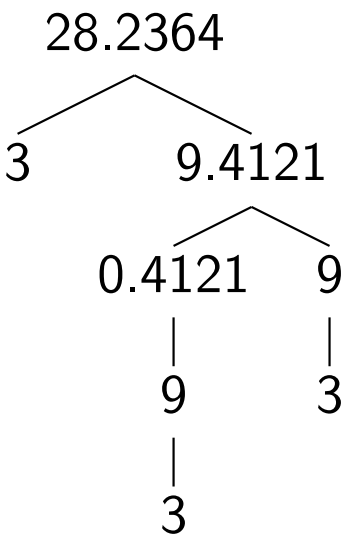

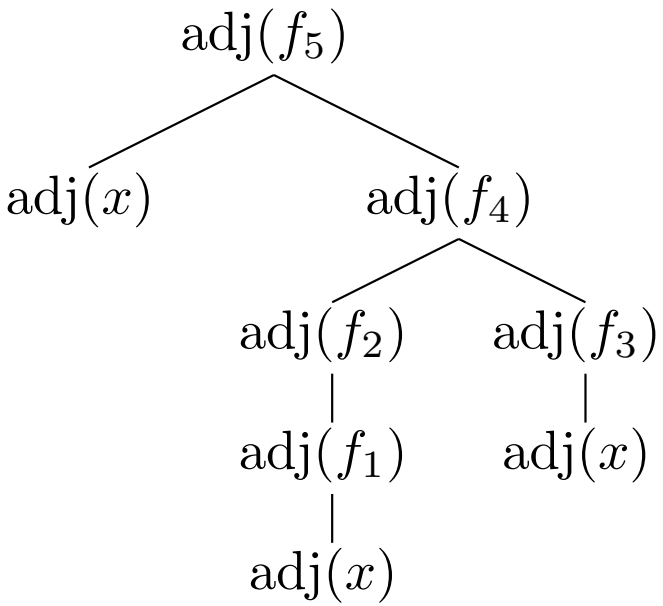

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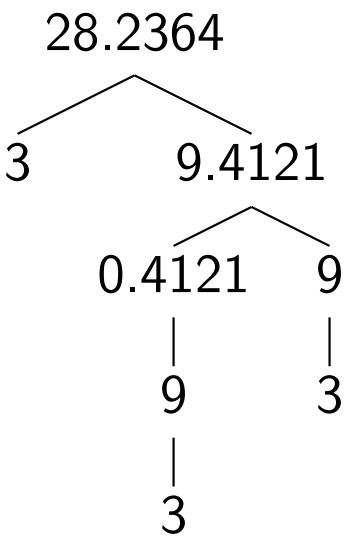

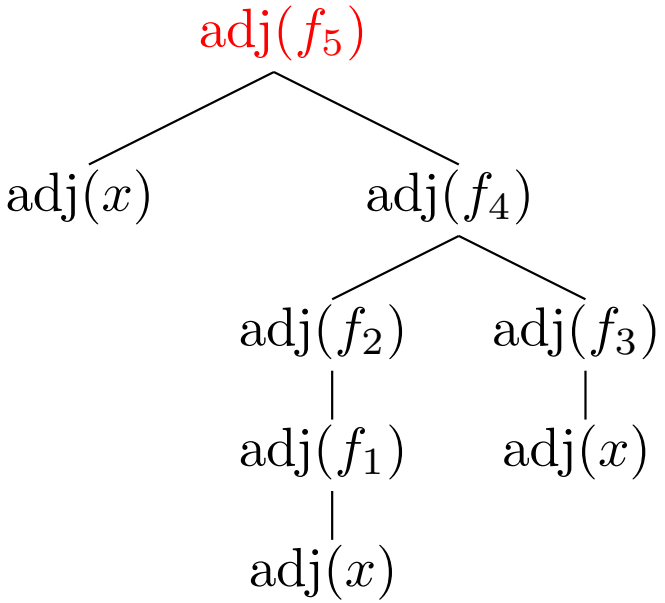

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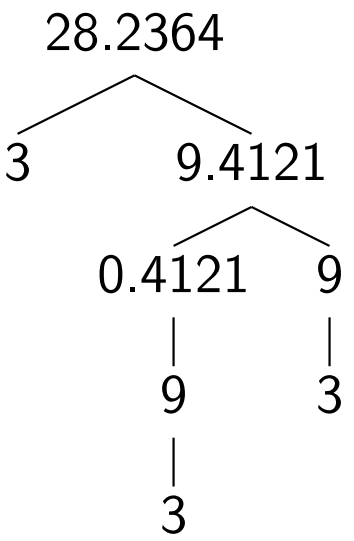

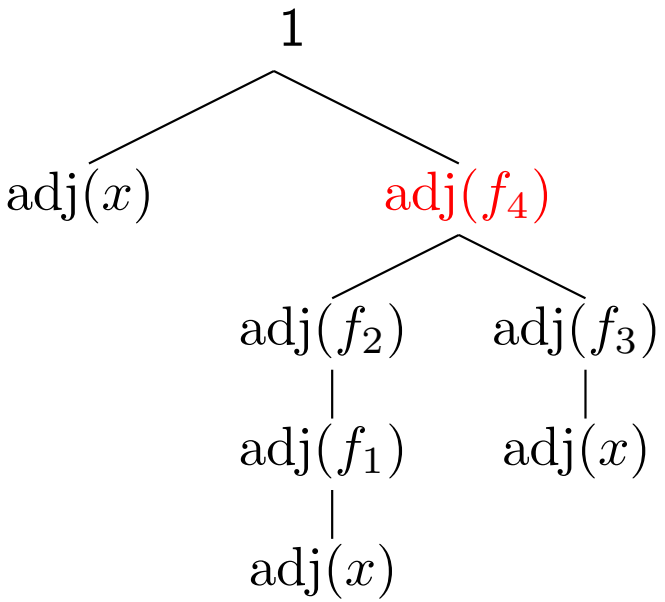

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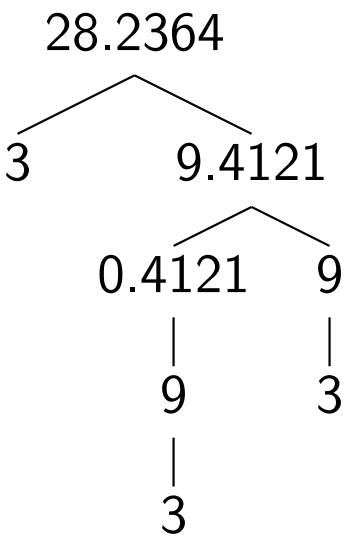

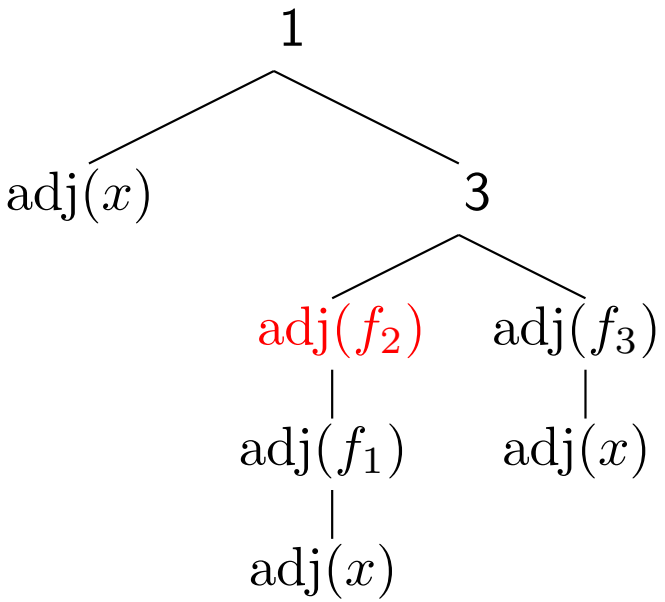

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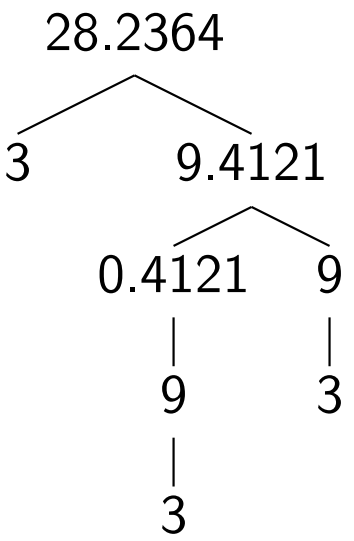

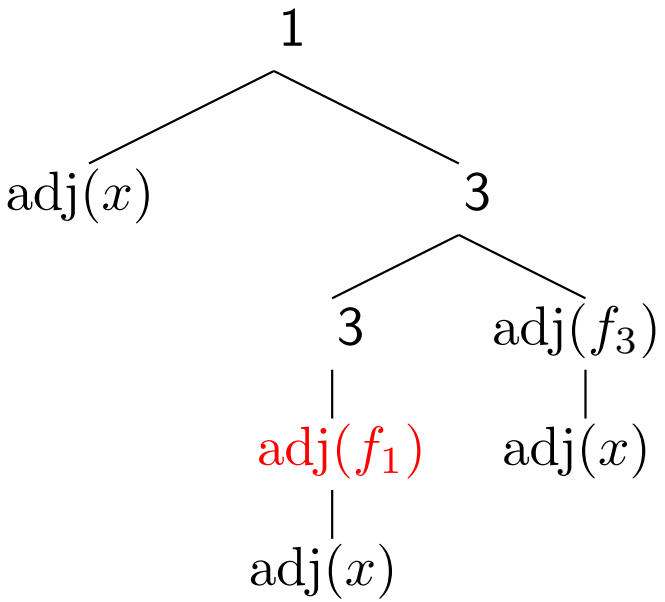

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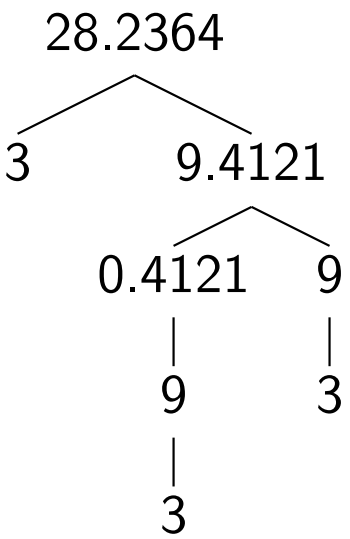

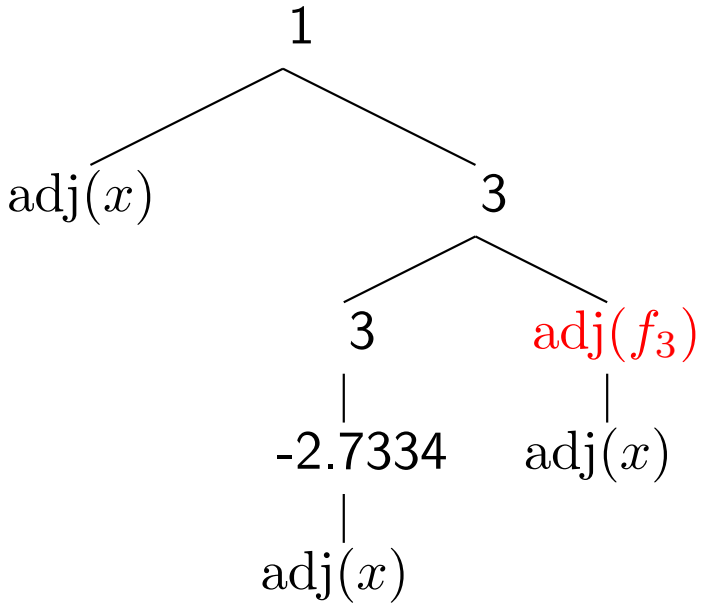

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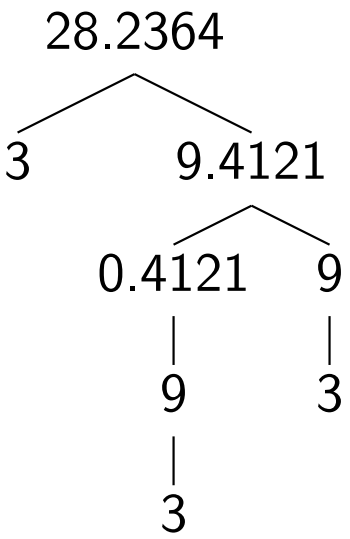

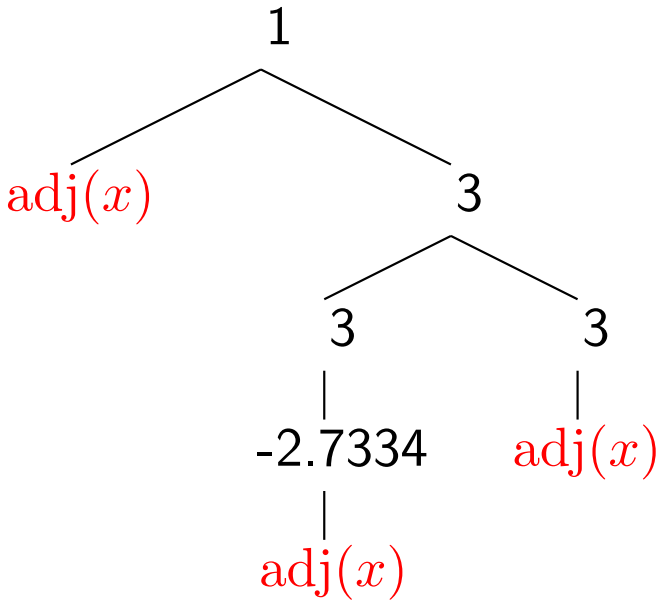

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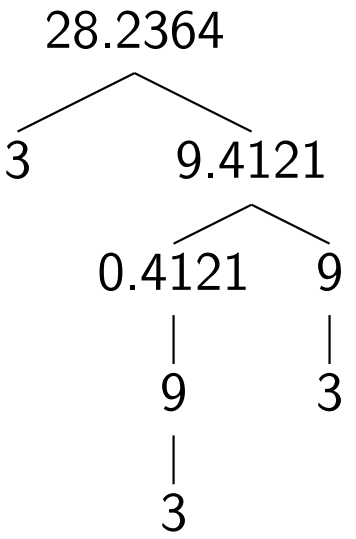

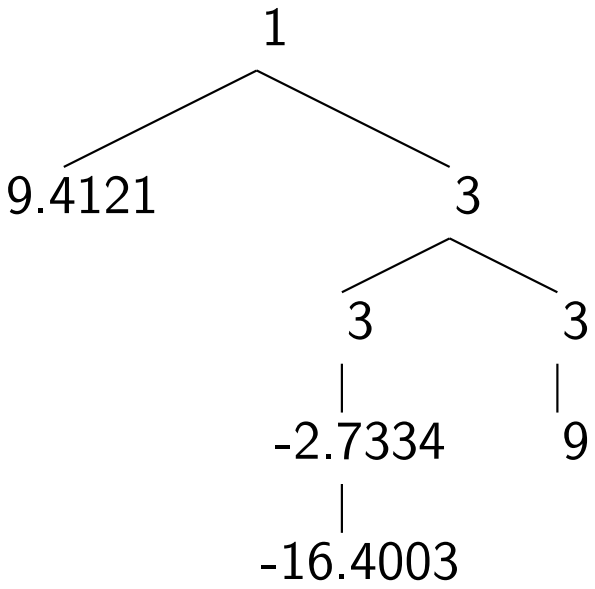

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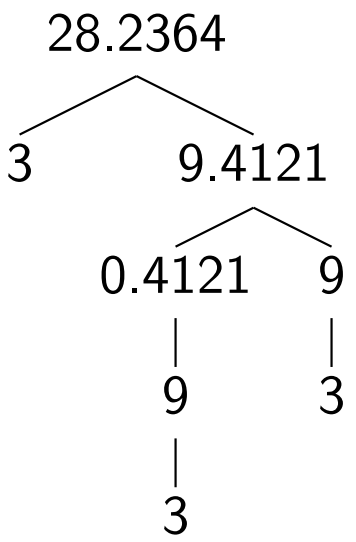

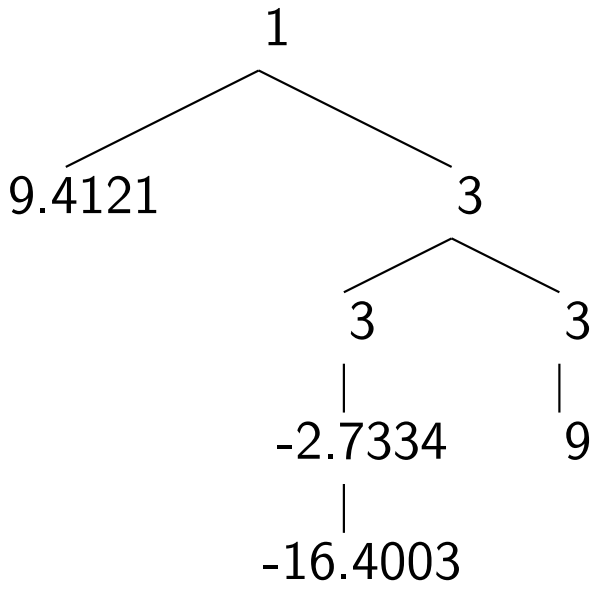

Must sum contributions:
$f'(3) = 9.4121 - 16.4003 + 9 = 2.0118.$

Automatic Differentiation: OPM implementations

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!