How to use recent developments of the MATLAB Reservoir Simulation Toolbox for fast prototyping of complex fluid models

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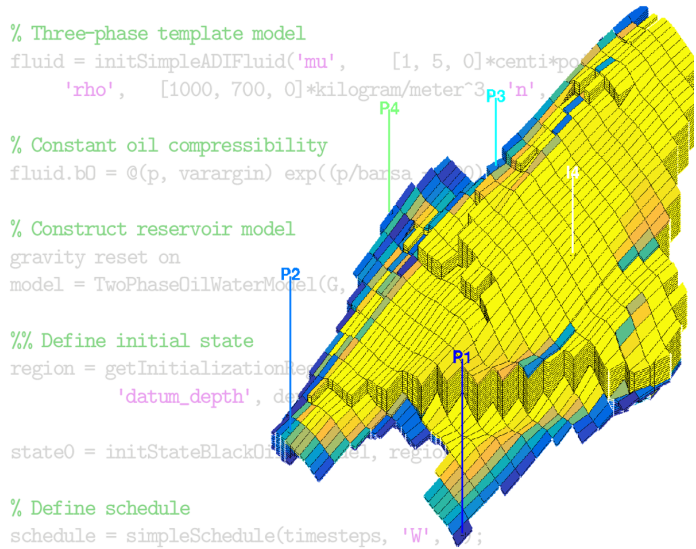
MATLAB Reservoir Simulation Toolbox (MRST)

Transforming research on reservoir modelling

Unique prototyping platform:

- Standard data formats
- Data structures/library routines
- Fully unstructured grids
- Rapid prototyping:
  - Differentiation operators
  - Automatic differentiation
  - Object-oriented framework
  - State functions
- Industry-standard simulation



http://www.mrst.no

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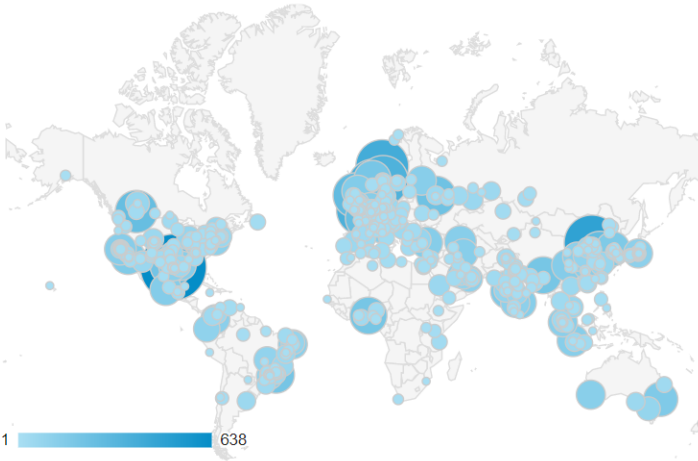
Large international user base:

- downloads from the whole world
- 124 master theses
- 56 PhD theses
- 226 journal papers (not by us)
- 144 proceedings papers

Numbers are from Google Scholar notifications

Used both by academia and industry



Google Analytics: access pattern for `www.mrst.no`
Period: 1 July 2018 to 31 December 2019
Unique downloads: 5 516 (103 countries and 838 cities)

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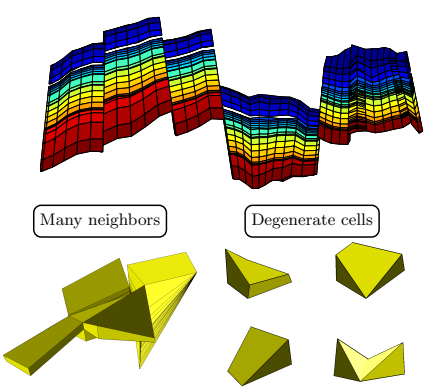
Word cloud generated from titles of journal papers

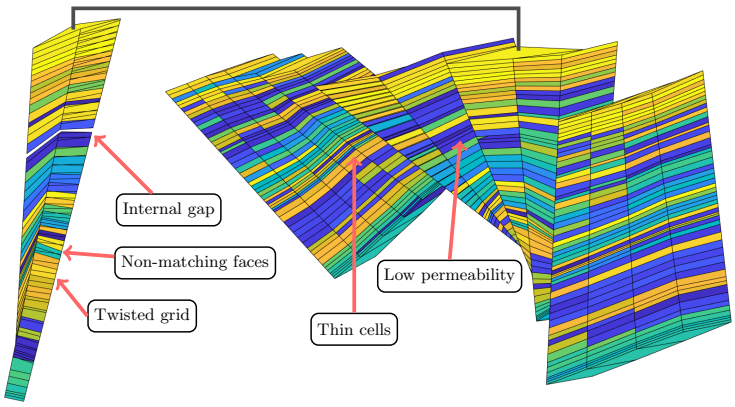
Reservoir simulation in MATLAB...?

- Use abstractions to express your ideas in a form close to the **underlying mathematics**
- Build your program using an **interactive** environment:
  - try out each operation and build program as you go
  - extensive and flexible **debugging** capabilities
- Dynamic type checking lets you **prototype** while you test an existing program:
  - run code **line by line**, inspect and change variables at any point
  - step back and rerun parts of code with changed parameters
  - add new behavior and data members while executing program

- MATLAB is fairly efficient using vectorization, logical indexing, external iterative solvers, etc.
- Avoids build process, linking libraries, cross-platform problems
- Builtin mathematical abstractions, numerics, data analysis, visualization, debugging/profiling,
- Use scripting language as a wrapper when you develop solvers in compiled languages
- We considered Python, but found it to be less mature (same with Julia a few years ago)

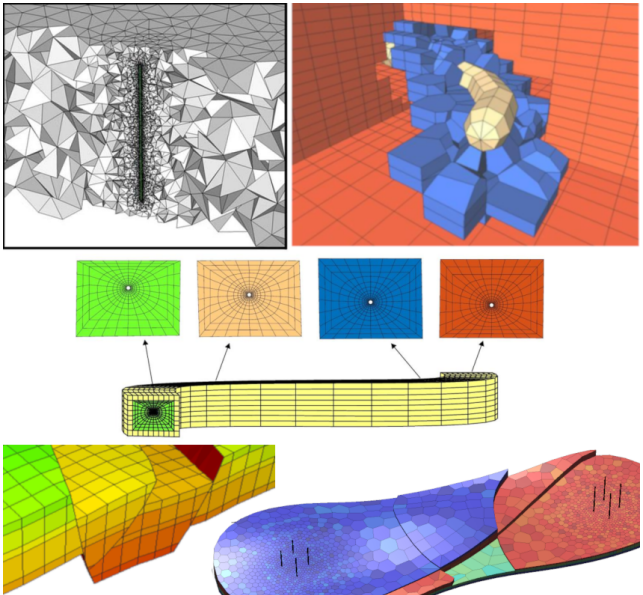
Corner-point grids (the most widespread format in industry):





Many special cases and tricks to be (re)invented

Complex, unstructured grids



A wide variety of grid formats:

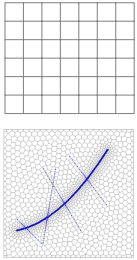
- Tetrahedral, prismatic
- PEBI
- General polyhedral/polytopal
- Hybrid, cut-cell, or depogrids
- Local refinements ...

MRST grids are chosen to always be **fully unstructured**
$\longrightarrow$ can implement algorithms without knowing the specifics of the grid

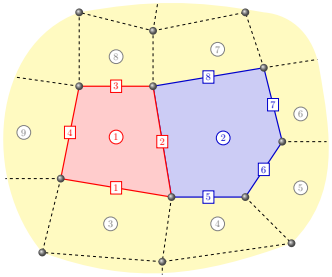
Also: coarse grids made as static or dynamic partitions of fine grid

Discrete differentiation operators

Idealized models



Grid structure in MRST



c	F(c)
1	1
1	2
1	3
1	4
2	5
2	6
2	7
2	8
2	2
3	1
⋮	⋮
⋮	⋮

Map: cell → faces

f	C_1	C_2
1	3	1
2	1	2
3	1	8
4	9	1
5	4	2
6	2	5
7	2	6
8	2	7
⋮	⋮	⋮
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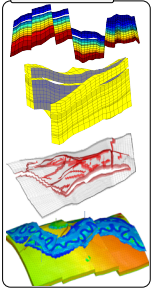
Map: face → cells

Industry models



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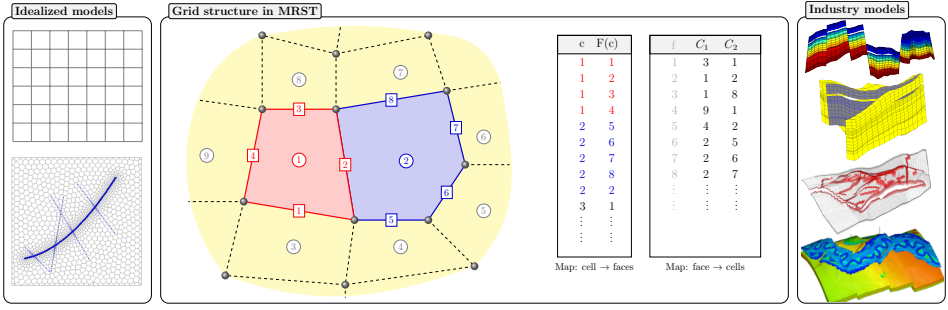

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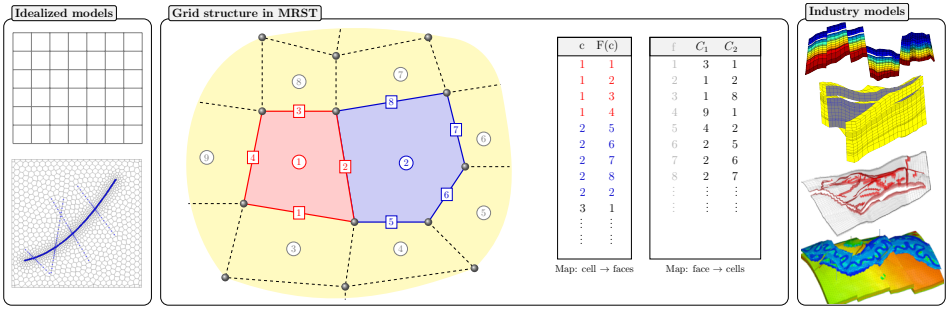
For finite volumes, the discrete `div` operator is a linear mapping from faces to cells:

$$\texttt{div}(\boldsymbol{v})[c] = \sum_{f \in F(c)} \operatorname{sgn}(f)\boldsymbol{v}[f], \qquad \operatorname{sgn}(f) = \begin{cases} 1, & \text{if } c = C_1(f), \\ -1, & \text{if } c = C_2(f). \end{cases}$$

Here, $\boldsymbol{v}[f]$ denotes a discrete flux over face f with orientation from cell $C_1(f)$ to cell $C_2(f)$

Discrete differentiation operators



The discrete `grad` operator maps from cell pair $C_1(f), C_2(f)$ to face f:

$$\texttt{grad}(\boldsymbol{p})[f] = \boldsymbol{p}[C_2(f)] - \boldsymbol{p}[C_1(f)],$$

where $\boldsymbol{p}[c]$ is a scalar quantity associated with cell c

Both are linear operators and can be represented as sparse matrix multiplications

Close correspondence with mathematics

Continuous

Incompressible flow:

$$\nabla \cdot (\mathbf{K}\nabla p) + q = 0$$

Compressible flow:

$$\frac{\partial(\phi\rho)}{\partial t} + \nabla \cdot (\rho\mathbf{K}\nabla p) + q = 0$$

Discrete in MATLAB

Incompressible flow:

```
eq = div(T .* grad(p)) + q;
```

Compressible flow:

```
eq = (pv(p).*rho(p)-pv(p0).*rho(p0))/dt ...
    + div(avg(rho(p)).*T.*grad(p))+q;
```

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Discretization of flow models leads to large systems of nonlinear equations. Can be linearized and solved with Newton's method

$$\boldsymbol{F}(\boldsymbol{u}) = \boldsymbol{0} \qquad \Rightarrow \qquad \frac{\partial \boldsymbol{F}}{\partial \boldsymbol{u}}(\boldsymbol{u}^i)(\boldsymbol{u}^{i+1} - \boldsymbol{u}^i) = -\boldsymbol{F}(\boldsymbol{u}^i)$$

Coding necessary Jacobians is **time-consuming** and **error prone**

$$\boldsymbol{F}(\boldsymbol{u}) = \boldsymbol{0} \qquad \Rightarrow \qquad \frac{\partial \boldsymbol{F}}{\partial \boldsymbol{u}}(\boldsymbol{u}^i)(\boldsymbol{u}^{i+1} - \boldsymbol{u}^i) = -\boldsymbol{F}(\boldsymbol{u}^i)$$

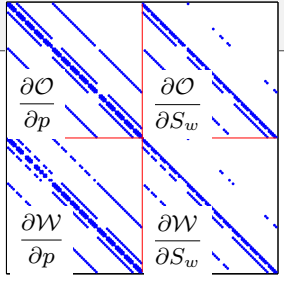
Automatic differentiation: Combine chain rule and elementary differentiation rules by means of operator overloading to efficiently evaluate all derivatives to machine precision

$\rightarrow$ Computing Jacobians amounts to writing down residual equations.

$$\frac{(\phi \boldsymbol{S}_\alpha \boldsymbol{\rho}_\alpha)^{n+1} - (\phi \boldsymbol{S}_\alpha \boldsymbol{\rho}_\alpha)^n}{\Delta t^n} + \mathtt{div}(\boldsymbol{\rho v})_\alpha^{n+1} = (\boldsymbol{\rho q})_\alpha^{n+1}$$

Residual equations are computed as for single-phase flow‡

```
water = (1/dt).*(vol.*rW.*sW - vol0.*rW0.*sW0) + div(vW);
oil   = (1/dt).*(vol.*rO.*(1-sW) - vol0.*rO0.*(1-sW0)) + div(vO);
eqs   = {oil, water};
eq    = cat(eqs{:});
```



‡ **Darcy's law:**
upstream operator is a combination of vector product and logical indexing

In sum: excellent approach for fast prototyping of simple simulators

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However, things soon start piling up

- complex rock-fluid/PVT models + hysteretic behavior
- advanced well models and simulation schedules
- time-step control, iteration control, line search, preconditioning, iterative solvers, ...

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Cure: the object-oriented AD-OO framework to separate:

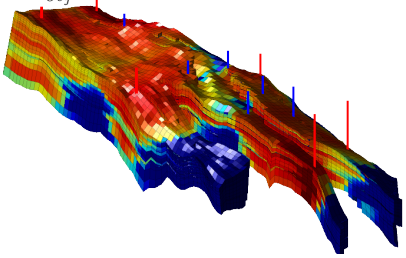
- physical models
- discretizations and discrete operators
- nonlinear solver and time-stepping
- assembly and solution of the linear system

Only expose needed details and increase reuse of developed functionality

Simulator: differentiable graph

1) Define continuous residual equations
$r_i = \frac{\partial m_i}{\partial t} + \nabla \cdot \vec{v} - q_i = 0$

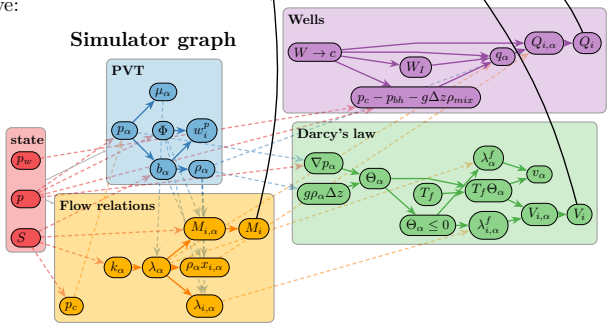
3) Differentiate discrete residual with AD and solve:
$J_{ij} = \frac{\partial R_i}{\partial v_j}, \quad x^{k+1} = x^k - J^{-1}R, \ldots$



4) Post: Make decisions, compute sensitivites, ...

2) Create *simulator graph* to discretize equations

$$R_i = \frac{1}{\Delta t}\left(M_i^{n+1} + M_i^{n} \right) + \nabla \cdot V_i - Q_i$$



Simulation on graphs	Graph of functions for multiphysics problems Easy to modify, extend and understand Smart automatic differentiation for high performance

State functions: modularity and computational cache

Similar quantities appear in multiple flow models, but can have different functional relationships

It would be convenient to have:

- Dependency management: keep track of dependency graph, ensure all input quantities have been evaluated before evaluating a function
- Generic interfaces: avoid defining functional dependencies explicitly, e.g., $G(S)$, and $G(p, S)$.
- Lazy evaluation with caching
- Enable spatial dependence in parameters while preserving vectorization potential
- Implementation independent of the choice of primary variables

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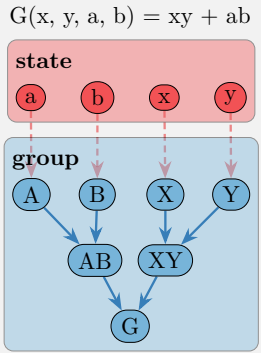

Worked example: CO_2 injection with mobility control

$$\frac{1}{\Delta t}(\boldsymbol{M}_\alpha^{n+1} - \boldsymbol{M}_\alpha^n) + \mathtt{div}(\boldsymbol{V}_\alpha) - \boldsymbol{Q}_\alpha = \boldsymbol{0}, \quad \alpha = w, g$$

$$\boldsymbol{V}_g = -\boldsymbol{\rho}_g \boldsymbol{\lambda}_g \boldsymbol{K} \mathtt{grad}(\boldsymbol{p}_g), \quad \boldsymbol{\lambda}_g = \frac{\boldsymbol{k}_{r,g}}{\boldsymbol{\mu}_g}$$

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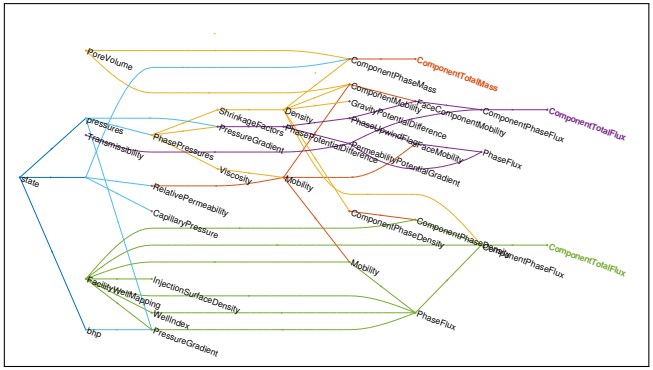

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Mobility control: increase mobility of injected gas by adding surfactant
$\rightarrow$ foam formation

Modelled through mobility multiplier F[1]
$\rightarrow$ we only have to change the relevant part (`Mobility`) in the simulator graph

[1] Grimstad et al (2018)

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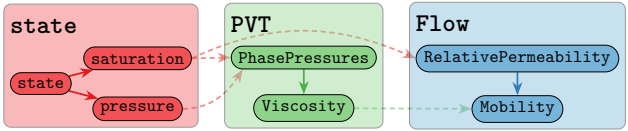
Standard mobility




```
classdef MultipliedMobility < StateFunction
    function mob = evaluateOnDomain(prop, model, state)
        kr  = prop.getEvaluatedDependencies(state, 'RelativePermeability');
        mu  = model.getProp(state, 'Viscosity');
        mob = cellfun(@(x, y) x./y, kr, mu, 'UniformOutput', false);
    end
end
```

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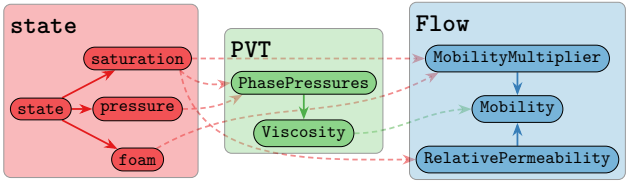


```
classdef MultipliedMobility < Mobility
    function mob = evaluateOnDomain(prop, model, state)
        mob = evaluateOnDomain@Mobility(prop, model, state);
        F   = prop.getEvaluatedDependencies(state, 'MobilityMultiplier');
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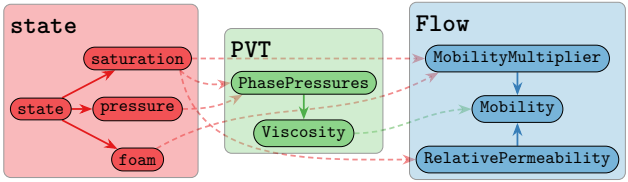


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Dependencies on other properties are defined in the implementation
→ evaluated in the correct order, and **only once** per nonlinear iteration

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What about computational performance?

Total time of a program consists of several parts:

programming + debugging
+ documenting + testing + executing

MRST is designed to prioritize the first four over the last

Does this mean that MRST is slow and not scalable?

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Total time of a program consists of several parts:

programming + debugging
+ documenting + testing + executing

MRST is designed to prioritize the first four over the last

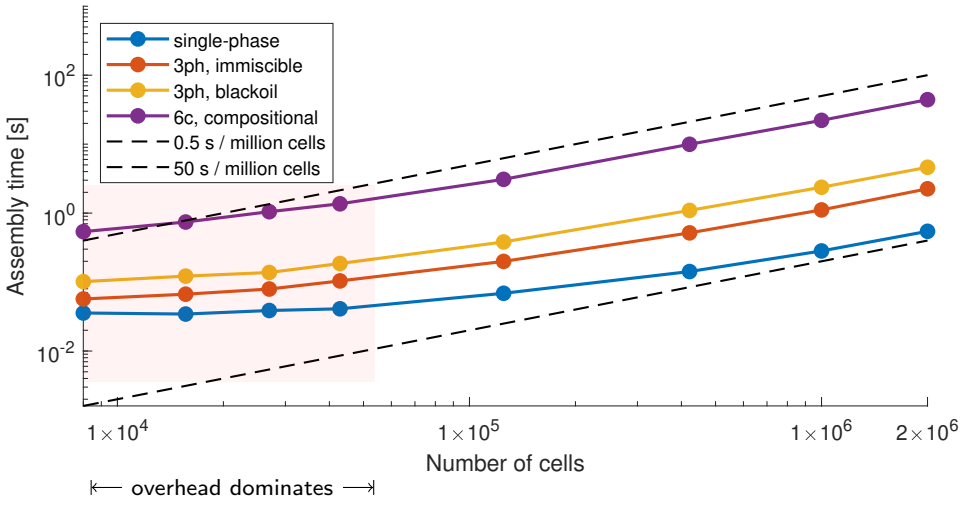
Does this mean that MRST is slow and not scalable?

No, I would say its is surprisingly efficient

Potential concerns:

- MATLAB is interpreted
  cure: JIT, vectorization, logical indexing, pre-allocation, highly-efficient libraries
- Redundant computations
  cure: state functions = dependency graph + computational cache
- Computational overhead
  cure: new auto diff backends
- Scalability/performance
  cure: external high-end iterative solvers

New backends for automatic differentiation



New AD backends: storage optimized wrt access pattern, MEX-accelerated operations

Efficient linear solvers

Interface to external linear algebra packages implemented as classes in AD-OO framework

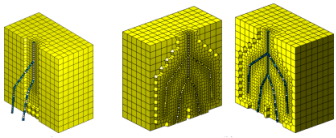
Example: compressible three-phase, black-oil problem

Solver	Req.	8,000 cells	125,000 cells	421,875 cells	1,000,000 cells
LU	–	2.49 s	576.58 s	–	–
CPR*	–	0.90 s	137.30 s	–	–
CPR*	AGMG	0.18 s	3.60 s	13.78 s	43.39 s
CPR*	AMGCL	0.21 s	3.44 s	16.20 s	51.35 s
CPR	AMGCL	0.07 s	0.43 s	3.38 s	10.20 s
CPR	AMGCL†	0.05 s	0.86 s	1.97 s	5.60 s
CPR	AMGCL‡	0.05 s	0.38 s	1.33 s	3.82 s

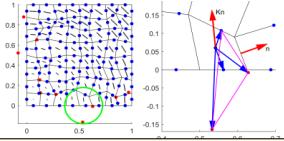
$*$ – in MATLAB, † – block AMGCL (block ILU + AMG/CPR), ‡ – block AMGCL with tweaks

Performance is approaching commercial and compiled academic codes

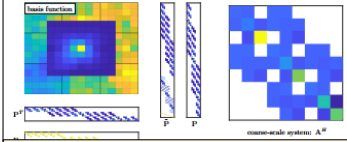
New book: Advanced modelling with MRST



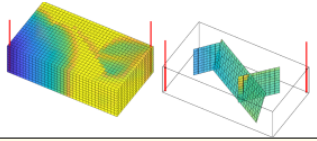
Berge et al.: Constrained Voronoi grids



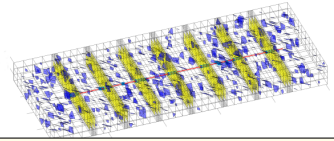
Al Kobaisi & Zhang: nonlinear FVM



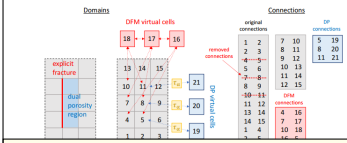
Lie & Møyner: multiscale methods



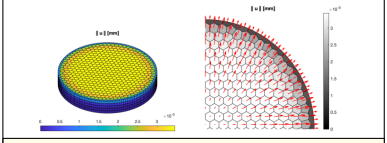
Wong et al.: embedded discrete fractures



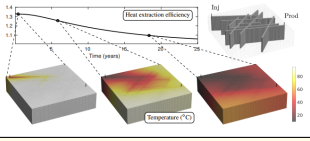
Olorode et al.; fractured unconventionals



March et al.: unified framework, fractures



Varela et al.: unsaturated poroelasticity



Collignon et al.: geothermal systems

Klemetsdal & Lie: discontinuous Galerkin

Møyner: state functions, AD backends

Sun et al.: chemical EOR

Møyner: compositional

Andersen: coupled flow & geomechanics

MRST Textbook
Knut-Andreas Lie. *An Introduction to Reservoir Simulation Using Matlab/GNU octave*. Cambridge University Press, 2019 (Open access). DOI: 10.1017/9781108591416

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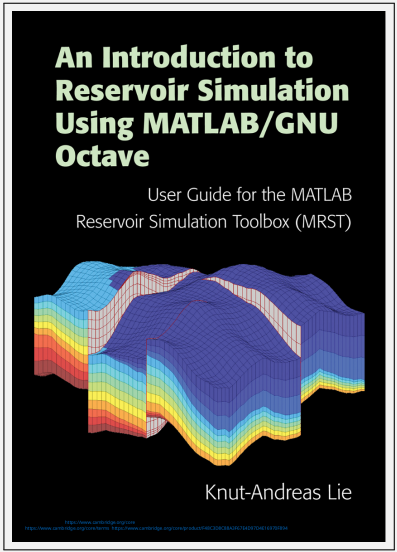

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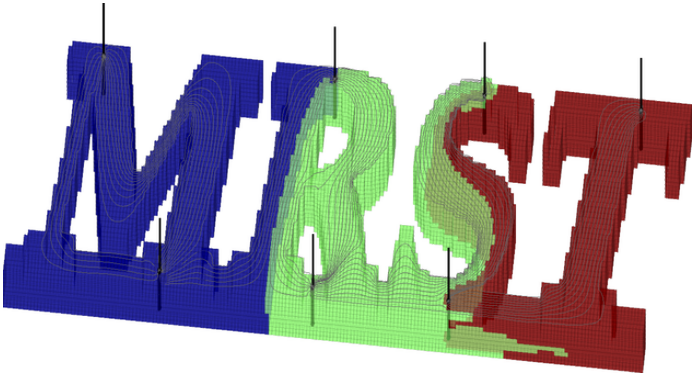

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