Efficient POD-Based deflation methods for the solution of ill-conditioned linear systems

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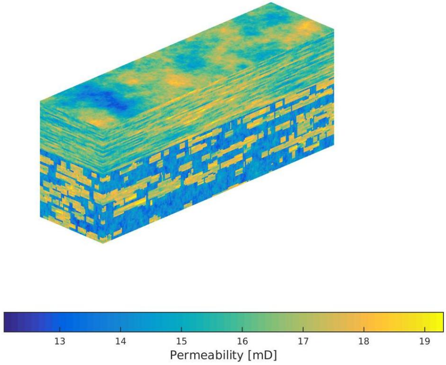
SPE 10 benchmark, 60 x 220 x 85 grid cells,
$\kappa(A) = 2.2 \times 10^6$.



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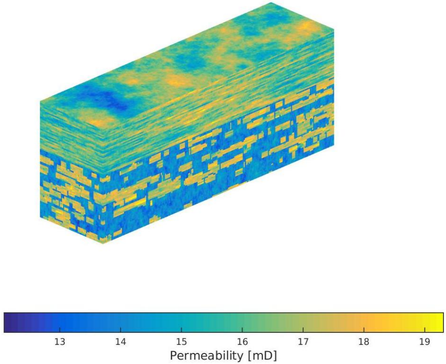

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ICCG, $\kappa(M^{-1}A) = 377$	1029

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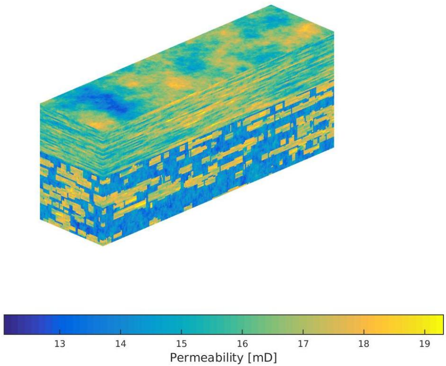

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ICCG, $\kappa(M^{-1}A) = 377$	1029
DICCG, $\kappa_{eff}(M^{-1}PA) = 82.7$	1

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Problem Definition

Reservoir Simulation

Governing equations [1]:

- Principle of mass conservation (for a fluid phase α);

$$\frac{\partial(\phi\rho_\alpha S_\alpha)}{\partial t} + \nabla\cdot(\rho_\alpha \mathbf{v}_\alpha) = \rho_\alpha q_\alpha. \quad (1)$$

- Darcy's law:

$$\mathbf{v}_\alpha = -\lambda_\alpha(\nabla p_\alpha - \rho_\alpha g \nabla d). \quad (2)$$

Fluid

S_α Saturation

$\lambda_\alpha(S_\alpha) = \frac{\vec{\mathbf{K}} k_{r\alpha}(S_\alpha)}{\mu_\alpha}$ Mobility

ρ_α Density

μ_α Viscosity

p_α Pressure

Rock

ϕ Porosity

$\vec{\mathbf{K}}$ Permeability

$k_{r\alpha}(S_\alpha)$ Relative permeability

Reservoir

d Depth

g Gravity

q_α Sources

Problem Definition

Single-phase flow (Incompressible)

$$-\nabla \cdot \frac{\vec{\mathbf{K}}}{\mu_\alpha}(\nabla p_\alpha - \rho_\alpha g \nabla d) = q_\alpha. \tag{3}$$

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Two-phase flow (Fractional flow formulation)

- Pressure

$$-\nabla \cdot (\lambda \nabla p_{nw}) = q - \nabla[\lambda_w \nabla p_c + (\lambda_{nw}\rho_{nw} + \lambda_w \rho_w) g \nabla d], \qquad (4)$$

- Total velocity $\mathbf{v} = \mathbf{v}_w + \mathbf{v}_{nw}$
- Saturation

$$\phi \frac{\partial S_w}{\partial t} + \nabla \cdot [f_w(\mathbf{v} + \lambda_{nw} \Delta\rho g \nabla d)] + \nabla \cdot (f_w \lambda_{nw} \nabla p_c) = q_w,$$

$\lambda = \lambda_{nw} + \lambda_w$

$p_c(S_w) = p_n - p_w$

$\Delta\rho = \rho_w - \rho_{nw}$

$f_w(S_w) = \frac{\lambda_w(S_w)}{\lambda_w(S_w) + \lambda_{nw}(S_{nw})}$

Problem Definition

Discretization, incompressible single-phase 2D problem

Combining Darcy's law and mass balance equation

$$-\nabla \cdot \lambda_\alpha(\nabla p_\alpha - \rho_\alpha g \nabla d) = q_\alpha.$$

No gravity terms

$$-\left(\nabla \cdot \lambda \nabla p\right)_x = -\frac{\partial}{\partial x}\left(\lambda_x \frac{\partial p}{\partial x}\right) =$$

$$= \frac{\lambda_{i+\frac{1}{2},j}(p_{i+1,j,l} - p_{i,j,l}) - \lambda_{i-\frac{1}{2},j,l}(p_{i,j,l} - p_{i-1,j,l})}{(\Delta x)^2}$$

$$-\nabla \cdot \lambda \nabla p = \mathbf{T}^1 \mathbf{p} = \mathbf{q} \qquad T_{i-\frac{1}{2},j,l} = \frac{\Delta y}{\Delta x}\lambda_{i-\frac{1}{2},j,l}.$$

[1] Transmissibility matrix [2].

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Two phases Incompressible problem

$$-\nabla \cdot (\mathbf{f}(\mathbf{S}^n)\lambda \nabla \mathbf{p}^n) = \mathbf{T}(\mathbf{S}^n)\mathbf{p}^n = \mathbf{q}^n.$$

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Conjugate Gradient Method (CG)

Linear system (SPD)

$\mathbf{Ax} = \mathbf{b}$	
Single phase	Two phases
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Successive approximations to obtain a more accurate solution $\mathbf{x}$ [3]

$$\mathbf{x}^0, \qquad \text{initial guess}$$

$$\vdots$$

$$\mathbf{x}^k = \mathbf{x}^{k-1} + \mathbf{M}^{-1}\mathbf{r}^{k-1}, \qquad \mathbf{r}^k = \mathbf{b} - \mathbf{A}\mathbf{x}^{k-1}.$$

$$min_{\mathbf{x}^k \in \mathcal{K}_k(\mathbf{A},\mathbf{r}^0)} ||\mathbf{x} - \mathbf{x}^k||_{\mathbf{A}}, \qquad ||\mathbf{x}||_{\mathbf{A}} = \sqrt{\mathbf{x}^T\mathbf{A}\mathbf{x}}.$$

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Convergence

$$||\mathbf{x} - \mathbf{x}^k||_{\mathbf{A}} \leq 2||\mathbf{x} - \mathbf{x}^0||_{\mathbf{A}} \left(\frac{\sqrt{\kappa(\mathbf{A})} - 1}{\sqrt{\kappa(\mathbf{A})} + 1} \right)^{k+1}.$$

PCG (ICCG)

Preconditioning

Improve the spectrum of **A**.

$$\mathbf{M}^{-1}\mathbf{A}\mathbf{x} = \mathbf{M}^{-1}\mathbf{b}.$$

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$$\kappa(\mathbf{M}^{-1}\mathbf{A}) \leq \kappa(\mathbf{A}).$$

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Cholesky Decomposition

If $\mathbf{A} \in \mathbf{R}^{n \times n}$ is *SPD*,

$$\mathbf{A} = \mathcal{L}\mathcal{L}^T$$

DPCG

Deflation

$$\mathbf{P} = \mathbf{I} - \mathbf{AQ}, \qquad \mathbf{P} \in \mathbb{R}^{n \times n}, \qquad \mathbf{Q} \in \mathbb{R}^{n \times n},$$
$$\mathbf{Q} = \mathbf{Z}\mathbf{E}^{-1}\mathbf{Z}^T, \qquad \mathbf{Z} \in \mathbb{R}^{n \times k}, \qquad \mathbf{E} \in \mathbb{R}^{k \times k},$$
$$\mathbf{E} = \mathbf{Z}^T\mathbf{A}\mathbf{Z} \text{ (Tang 2008, [4]).}$$

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Convergence

Deflated system

$$||\mathbf{x} - \mathbf{x}^k||_{\mathbf{A}} \leq 2||\mathbf{x} - \mathbf{x}^0||_{\mathbf{A}} \left(\frac{\sqrt{\kappa_{eff}(\mathbf{PA})} - 1}{\sqrt{\kappa_{eff}(\mathbf{PA})} + 1} \right)^{k+1}.$$

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Deflated and preconditioned system

$$||\mathbf{x} - \mathbf{x}^k||_{\mathbf{A}} \leq 2||\mathbf{x} - \mathbf{x}^0||_{\mathbf{A}} \left(\frac{\sqrt{\kappa_{eff}(\mathbf{M}^{-1}\mathbf{PA})} - 1}{\sqrt{\kappa_{eff}(\mathbf{M}^{-1}\mathbf{PA})} + 1} \right)^{k+1}.$$

$$\kappa_{eff}(\mathbf{M}^{-1}\mathbf{PA}) \leq \kappa(\mathbf{M}^{-1}\mathbf{A}) \leq \kappa(\mathbf{A}).$$

Deflation vectors

Recycling deflation (Clemens 2004, [5]).

$$\mathbf{Z} = [\mathbf{x}^1, \mathbf{x}^2, \mathbf{x}^{q-1}],$$

x^i's are solutions of the system.
Multigrid and multilevel (Tang 2009, [6]).
The matrices $\mathbf{Z}$ and $\mathbf{Z}^T$ are the restriction and prolongation matrices of multigrid methods.
Subdomain deflation (Vuik 1999,[7]).
* $\mathbf{Z}$ is obtained from a POD basis and used to construct a preconditioner (Pasetto et al. 2017 [8]).

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Proposal

Use solution of the system with diverse *rhs* as deflation vectors (Recycling deflation).

Use as deflation vectors the basis obtained from Proper Orthogonal Decomposition (POD).

Proper Orthogonal Decomposition (POD)

POD: find an 'optimal' basis for a given set of vectors (Markovinović 2009 [9], Astrid 2011 [10])

$$\Phi = [\phi_1, \phi_2, ...\phi_l] \in \mathbb{R}^{n\times l}$$

ϕ_i, basis functions.

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- Get the snapshots

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- Get the snapshots

$$\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, ...\mathbf{x}_m].$$

- Obtain l eigenvectors of $\mathbf{C}$ satisfying:
$\frac{\sum_{j=1}^{l} \lambda_j}{\sum_{j=1}^{m} \lambda_j} \leq \alpha, \qquad 0 < \alpha \leq 1.$

$$\mathbf{C} := \frac{1}{m}\mathbf{X}\mathbf{X}^T \equiv \frac{1}{m}\sum_{i=1}^{m} \mathbf{x}_i\mathbf{x}_i^T.$$

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Deflation vectors

Single-phase, $\mathbf{T}\mathbf{p}^n = \mathbf{q}^n$

- Recycling

Compute independent solutions with ICCG	Construct $\mathbf{Z}$	Use $\mathbf{Z}$ to solve
$\mathbf{T}\mathbf{p}_i = \mathbf{q}_i,$	$\mathbf{Z} = \begin{bmatrix} \mathbf{p}_1 & \cdots & \mathbf{p}_n \end{bmatrix},$	$\mathbf{T}\mathbf{p} = \mathbf{q}.$

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Two-phases, $\mathbf{T}^n\mathbf{p}^n = \mathbf{q}^n$

- Moving window, solving step t

Compute $t-1$ snapshots (ICCG)	Construct $\mathbf{Z}_m = POD(\mathbf{p}_i's)$	Use $\mathbf{Z}_m$ to solve
$\mathbf{T}^i\mathbf{p}^i = \mathbf{q}^i,$	$\mathbf{Z}_m = \begin{bmatrix} \phi^1 & \cdots & \phi^m \end{bmatrix},$	$\mathbf{T}^t\mathbf{p}^t = \mathbf{q}^t.$

Deflation vectors

Two-phases, $\mathbf{T}^n\mathbf{p}^n = \mathbf{q}^n$

- Training phase

Compute all solutions (ICCG) with rand *rhs*	Construct $\mathbf{C}_{(1:n)} = \frac{1}{n}\mathbf{X}\mathbf{X}^T$	Compute POD basis and use it as $\mathbf{Z}_m$
$\mathbf{T}^i\mathbf{p}^i = \mathbf{q}^i,$	$\mathbf{C}_{(1:n)} = \begin{bmatrix} \mathbf{c}^1 & \cdots & \mathbf{c}^n \end{bmatrix},$	$\mathbf{Z}_m = POD(\mathbf{C}_{(1:n)})$
$\mathbf{X} = [\mathbf{p}^1 \cdots \mathbf{p}^n]$		

Use $\mathbf{Z}_m$ to solve $\mathbf{T}\mathbf{p} = \mathbf{q}$ with diverse *rhs*.

Lemma 1. Let $\mathbf{A} \in \mathbb{R}^{n \times n}$ be a non-singular matrix, and $\mathbf{x}$ is the solution of

$$\mathbf{A}\mathbf{x} = \mathbf{b}. \tag{5}$$

Recycling deflation

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Let $\mathbf{b}_i \in \mathbb{R}^n$, $i = 1, ..., m$, be a set of linearly independent vectors, different *rhs*, such that $\mathbf{b} = \sum_{i=1}^{m} c_i \mathbf{b}_i$,

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Then, the following equivalence holds

$$\mathbf{b} = \sum_{i=1}^{m} c_i \mathbf{b}_i \quad \Leftrightarrow \quad \mathbf{x} = \sum_{i=1}^{m} c_i \mathbf{x}_i \quad \mathbf{x}_i \text{ l.i.,}$$ proof Diaz et al. 2018 [11].

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Lemma 2. If the the deflation matrix $\mathbf{Z}$ is constructed with a set of m vectors

$$\mathbf{Z} = \begin{bmatrix} \mathbf{x}_1 & \dots & \dots & \mathbf{x}_m \end{bmatrix},$$

such that $\mathbf{x} = \sum_{i=1}^{m} c_i\mathbf{x}_i$, with $\mathbf{x}_i$ *l.i.*, then the solution of system (5) is obtained with one iteration of DCG.

Recycling deflation

Lemma 2 (Proof).

$$\mathbf{x} = \mathbf{Q}\mathbf{b} + \mathbf{P}^T\hat{\mathbf{x}} \text{ (Diaz et al. 2018 [11]).}$$

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$$\mathbf{x} = \mathbf{Q}\mathbf{b} + \mathbf{P}^T\hat{\mathbf{x}} \text{ (Diaz et al. 2018 [11]).}$$

$$\mathbf{Q}\mathbf{b} = \mathbf{Z}\mathbf{E}^{-1}\mathbf{Z}^T\left(\sum_{i=1}^{m} c_i\mathbf{b}_i\right) = \mathbf{Z}(\mathbf{Z}^T\mathbf{A}\mathbf{Z})^{-1}\mathbf{Z}^T\left(\sum_{i=1}^{m} c_i\mathbf{A}\mathbf{x}_i\right)$$

Lemma 2 (Proof).

$$\mathbf{x} = \mathbf{Qb} + \mathbf{P}^T\hat{\mathbf{x}} \text{ (Diaz et al. 2018 [11]).}$$

$$\mathbf{Qb} = \mathbf{ZE}^{-1}\mathbf{Z}^T\left(\sum_{i=1}^{m} c_i\mathbf{b}_i\right) = \mathbf{Z}(\mathbf{Z}^T\mathbf{AZ})^{-1}\mathbf{Z}^T\left(\sum_{i=1}^{m} c_i\mathbf{Ax}_i\right)$$

$$= \mathbf{Z}(\mathbf{Z}^T\mathbf{AZ})^{-1}\mathbf{Z}^T(\mathbf{AZc}) = \mathbf{Zc}$$

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$$= c_1\mathbf{x}_1 + ... + c_m\mathbf{x}_m = \sum_{i=1}^{m} c_i\mathbf{x}_i = \mathbf{x}.$$

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$$\mathbf{A}(\mathbf{P}^T\hat{\mathbf{x}}) = \mathbf{P}\mathbf{A}\hat{\mathbf{x}} = \mathbf{P}\mathbf{b} = (\mathbf{I} - \mathbf{A}\mathbf{Q})\mathbf{b}$$

$$= \mathbf{b} - \mathbf{A}\mathbf{Q}\mathbf{b} = \mathbf{b} - \mathbf{A}\mathbf{x} = 0 \quad \Rightarrow \quad \mathbf{P}^T\hat{\mathbf{x}} = 0$$

Lemma 2 (Proof).

$$\mathbf{x} = \mathbf{Qb} + \mathbf{P}^T\hat{\mathbf{x}} \text{ (Diaz et al. 2018 [11]).}$$

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$$\mathbf{A}(\mathbf{P}^T\hat{\mathbf{x}}) = \mathbf{PA}\hat{\mathbf{x}} = \mathbf{Pb} = (\mathbf{I} - \mathbf{AQ})\mathbf{b}$$

$$= \mathbf{b} - \mathbf{AQb} = \mathbf{b} - \mathbf{Ax} = 0 \quad \Rightarrow \quad \mathbf{P}^T\hat{\mathbf{x}} = 0$$

$$\mathbf{x} = \mathbf{Qb} + \mathbf{P}^T\hat{\mathbf{x}} = \mathbf{Qb} = \mathbf{x}.$$

Accuracy of the snapshots

Error of an iterative method for an approximate solution $\mathbf{x}_i^k$

$$\mathbf{e}_r = \frac{||\mathbf{x}_i - \mathbf{x}_i^k||_2}{||\mathbf{x}_i||_2},$$

Accuracy of the snapshots

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$$\mathbf{e}_r = \frac{||\mathbf{x}_i - \mathbf{x}_i^k||_2}{||\mathbf{x}_i||_2}, \qquad \mathbf{r}_i = \frac{||\mathbf{r}_i^k||_2}{||\mathbf{b}||_2} = \frac{||\mathbf{b}_i - \mathbf{A}\mathbf{x}_i^k||_2}{||\mathbf{b}||_2} \leq \epsilon,$$

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where, using as stopping criterion $\epsilon = 10^{-\eta}$

$$\frac{||\mathbf{x}_i - \mathbf{x}_i^k||_2}{||\mathbf{x}_i||_2} \leq \kappa_2(\mathbf{A})\mathbf{r}_i = \kappa_2(\mathbf{A})\epsilon = \kappa_2(\mathbf{A}) \times 10^{-\eta}.$$

Accuracy of the snapshots

Error of an iterative method for an approximate solution $\mathbf{x}_i^k$

$$\mathbf{e}_r = \frac{||\mathbf{x}_i - \mathbf{x}_i^k||_2}{||\mathbf{x}_i||_2}, \qquad \mathbf{r}_i = \frac{||\mathbf{r}_i^k||_2}{||\mathbf{b}||_2} = \frac{||\mathbf{b}_i - \mathbf{A}\mathbf{x}_i^k||_2}{||\mathbf{b}||_2} \leq \epsilon,$$

where, using as stopping criterion $\epsilon = 10^{-\eta}$

$$\frac{||\mathbf{x}_i - \mathbf{x}_i^k||_2}{||\mathbf{x}_i||_2} \leq \kappa_2(\mathbf{A})\mathbf{r}_i = \kappa_2(\mathbf{A})\epsilon = \kappa_2(\mathbf{A}) \times 10^{-\eta}.$$

After one iteration of DCG we obtain

$$\mathbf{x}^1 = \sum_{i=1}^{m} c_i \mathbf{x}_i^{1(i)}, \text{ and,}$$

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Error DCG: $\mathbf{e}_r = \kappa_2(\mathbf{A}) \times 10^{-\eta}$.

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Single-phase flow (Recycling Deflation vectors).

System configuration					
Well pressures [bars]					
	$P1$	$P2$	$P3$	$P4$	I
	-275	-275	-275	-275	1100
Snapshots (4 linearly independent)					
	$P1$	$P2$	$P3$	$P4$	I
$\mathbf{z}_1$	0	-275	-275	-275	825
$\mathbf{z}_2$	-275	0	-275	-275	825
$\mathbf{z}_3$	-275	-275	0	-275	825
$\mathbf{z}_4$	-275	-275	-275	0	825

Table: Well configurations.

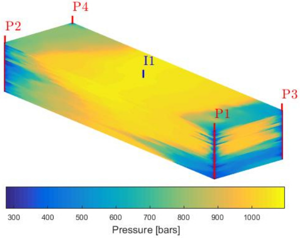


Figure: Pressure field.

Layers	ICCG	DICCG
1	251	1
35	536	1
85	1029	1

Table: Number of iterations, $tol = 10^{-7}$.

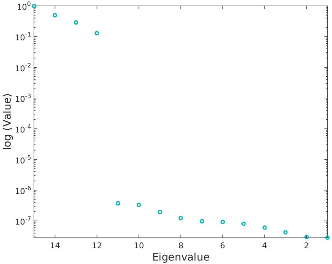
Single-phase flow (Recycling Deflation vectors).

Snapshots					
	$P1$	$P2$	$P3$	$P4$	I
$\mathbf{z}_5$	-275	-275	-275	-275	1100
$\mathbf{z}_6$	0	0	-275	-275	550
$\mathbf{z}_7$	-275	0	0	-275	550
$\mathbf{z}_8$	-275	-275	0	0	550
$\mathbf{z}_9$	-275	0	-275	0	550
$\mathbf{z}_{10}$	0	-275	0	-275	550
$\mathbf{z}_{11}$	0	-275	-275	0	550
$\mathbf{z}_{12}$	-275	0	0	0	275
$\mathbf{z}_{13}$	0	-275	0	0	275
$\mathbf{z}_{14}$	0	0	-275	0	275
$\mathbf{z}_{15}$	0	0	0	-275	275

Numerical experiments

Single-phase flow (Recycling Deflation vectors).

Snapshots					
	$P1$	$P2$	$P3$	$P4$	I
$\mathbf{z}_5$	-275	-275	-275	-275	1100
$\mathbf{z}_6$	0	0	-275	-275	550
$\mathbf{z}_7$	-275	0	0	-275	550
$\mathbf{z}_8$	-275	-275	0	0	550
$\mathbf{z}_9$	-275	0	-275	0	550
$\mathbf{z}_{10}$	0	-275	0	-275	550
$\mathbf{z}_{11}$	0	-275	-275	0	550
$\mathbf{z}_{12}$	-275	0	0	0	275
$\mathbf{z}_{13}$	0	-275	0	0	275
$\mathbf{z}_{14}$	0	0	-275	0	275
$\mathbf{z}_{15}$	0	0	0	-275	275



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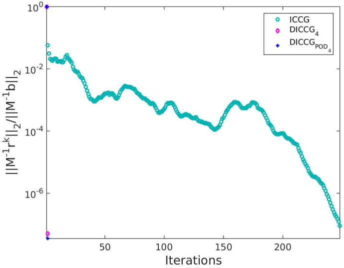
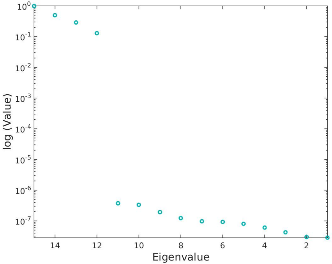
$\mathbf{z}_{12}$	-275	0	0	0	275
$\mathbf{z}_{13}$	0	-275	0	0	275
$\mathbf{z}_{14}$	0	0	-275	0	275
$\mathbf{z}_{15}$	0	0	0	-275	275





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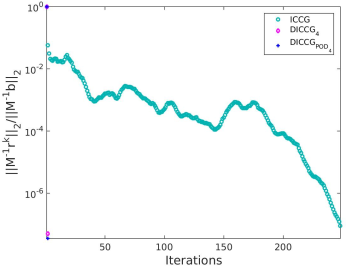
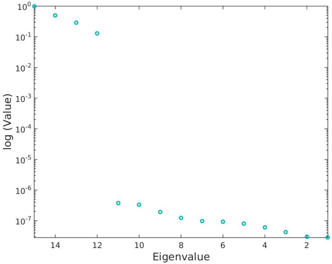
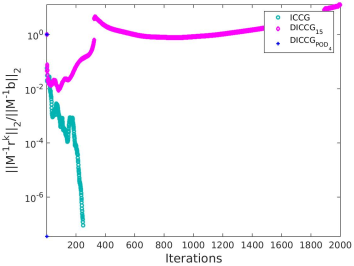
$\mathbf{z}_{13}$	0	-275	0	0	275
$\mathbf{z}_{14}$	0	0	-275	0	275
$\mathbf{z}_{15}$	0	0	0	-275	275







Two-phase flow, injection through left boundary
(Moving window approach)

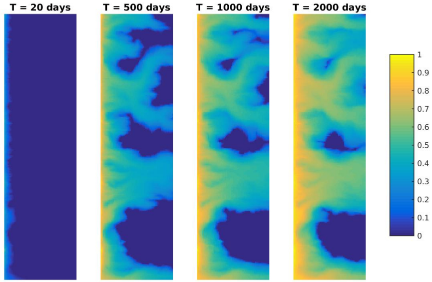


Figure: Water Saturation, 1 layer.

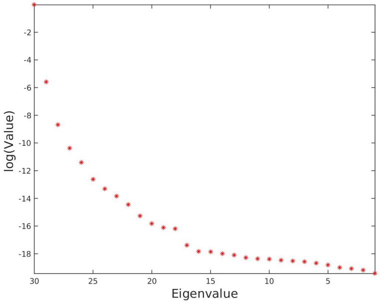


Figure: Eigenvalues of $\mathbf{C} = \frac{1}{m}\mathbf{X}\mathbf{X}^T$.

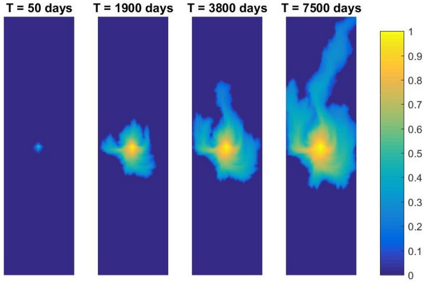
Two-phase flow, injection through left boundary
(Moving window approach)

Total ICCG Iterations	DICCG Method	ICCG Iterations (snapshots)	DICCG Iterations	Total ICCG + DICCG Iterations	% of Total ICCG Iterations
1 layer					
42062	$DICCG_{10}$	2309	8153	10462	25
42062	$DICCG_{30}$	6923	4035	10958	26
35 layers					
66728	$DICCG_{10}$	2759	17190	19949	30
66728	$DICCG_{30}$	8535	11798	20333	30

Table: Number of iterations of the ICCC and DICCG methods.

Numerical experiments

Two-phase flow, injection through wells
(Training phase approach)



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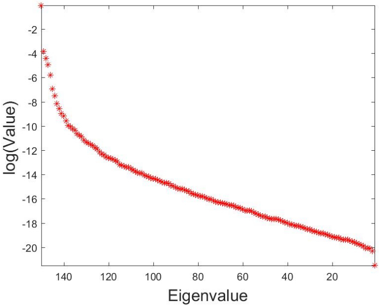

Figure: Eigenvalues of $\mathbf{C} = \frac{1}{m}\mathbf{X}\mathbf{X}^T$.

Numerical experiments

Two-phase flow, injection through wells
(Training phase approach)

1 layer			
Total ICCG	DICCG Method	Iter	% ICCG Iter
P_{bhp} = 275 [bars]			
32237	$DICCG_{30}$	5503	17
32237	$DICCG_{10}$	8811	27
P_{bhp} = 200 [bars]			
32237	$DICCG_{30}$	5794	18
32237	$DICCG_{10}$	9207	29
P_{bhp} = 400 [bars]			
32237	$DICCG_{30}$	4818	15
32237	$DICCG_{10}$	8094	25

35 layers			
Total ICCG	DICCG Method	Iter	% ICCG Iter
P_{bhp} = 275 [bars]			
59806	$DICCG_{30}$	13093	22
59806	$DICCG_{10}$	22577	38
P_{bhp} = 200 [bars]			
59806	$DICCG_{30}$	13256	22
59806	$DICCG_{10}$	23529	39
P_{bhp} = 400 [bars]			
59806	$DICCG_{30}$	12959	22
59806	$DICCG_{10}$	21526	36

Table: number of iterations of the ICCC and DICCG methods.

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Conclusions

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- We tested these methodologies for reservoir simulation examples. However, they are not exclusively applicable to these problems, but to any transient problem and other linear solvers.

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