

Two-scale computational modelling of unsaturated water flow in soils exhibiting small-scale heterogeneity

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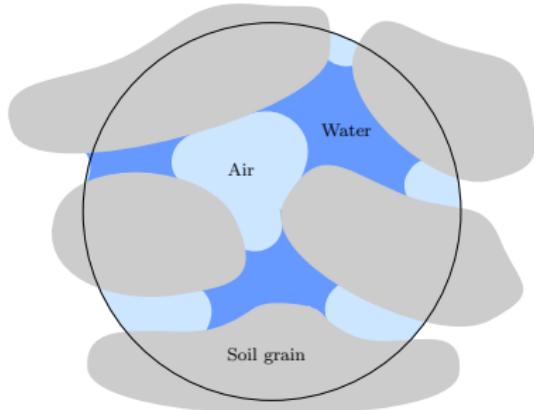


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Unsaturated water flow

- ▶ Immiscible two-phase (air and water) flow
- ▶ Darcy's Law (phase α):

$$\mathbf{q}_\alpha = -\frac{k_{r,\alpha}}{\mu_\alpha} K (\nabla p_\alpha - \rho_\alpha \mathbf{g})$$



- ▶ Capillary pressure $p_c = p_a - p_w$
- ▶ Mass conservation (phase α):

$$\frac{\partial (\rho_\alpha \phi S_\alpha)}{\partial t} + \nabla \cdot (\rho_\alpha \mathbf{q}_\alpha) = 0$$

where $S_w + S_a = 1$

Richards' equation

- ▶ Assumptions:
 - (a) air phase is at a constant and atmospheric pressure
 - (b) water phase is incompressible and of constant density
- ▶ Single equation for the water saturation:

$$\frac{\partial \theta(h)}{\partial t} + \nabla \cdot (-K(h)\nabla(h+y)) = 0$$

where $h = p_c/(\rho_w g)$ is the capillary pressure head, $\theta = \phi S_w$ is the moisture content and K is the hydraulic conductivity.

- ▶ Closure relationships [van Genuchten (1980)]:

$$\theta(h) = \theta_r + (\theta_s - \theta_r)S_e(h)$$

$$K(h) = K_{\text{sat}} \sqrt{S_e} \left(1 - \left(1 - S_e^{1/m}\right)^m\right)^2$$

$$S_e(h) = (1 + (-\alpha h)^n)^{-m}$$

Problem statement

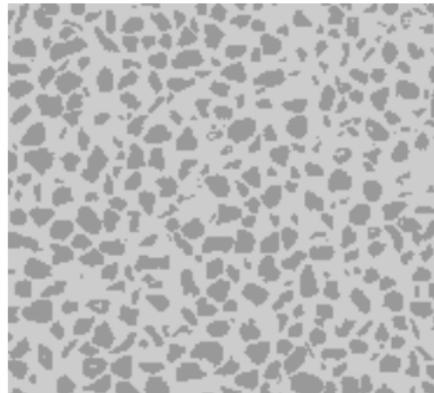
- ▶ Richards' equation in two-dimensions

$$\frac{\partial \theta(h)}{\partial t} + \nabla \cdot [-K(h) \nabla (h + y)] = 0$$

- ▶ Domain comprised of two sub-domains Ω_a (connected) and Ω_b (disconnected) with different hydraulic properties:

$$\theta(h) = \begin{cases} \theta_a(h) & \text{in } \Omega_a \\ \theta_b(h) & \text{in } \Omega_b \end{cases}$$

$$K(h) = \begin{cases} K_a(h) & \text{in } \Omega_a \\ K_b(h) & \text{in } \Omega_b \end{cases}$$



Heterogeneous domain

Ω_a ■ Ω_b ■

- ▶ Computational cost of direct numerical simulation is prohibitively expensive when the domain exhibits small-scale heterogeneity.

Two-scale model for unsaturated flow

- ▶ Macroscopic equation ($x \in \Omega$)

$$\frac{\partial}{\partial t} \theta_{\text{eff}}(h_a) + \nabla_x \cdot [-\mathbf{K}_{\text{eff}}(h_a) \nabla_x (h_a + x_2)] = Q$$

- ▶ Microscopic equation ($y \in \Omega_{x,b}$)

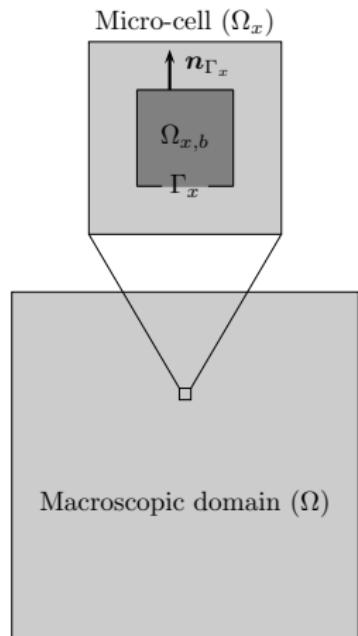
$$\frac{\partial}{\partial t} \theta_b(h_b) + \nabla_y \cdot [-K_b(h_b) \nabla_y (h_b + y_2)] = 0$$

- ▶ Microscopic boundary condition ($y \in \Gamma_x$)

$$h_a = h_b$$

- ▶ Source term

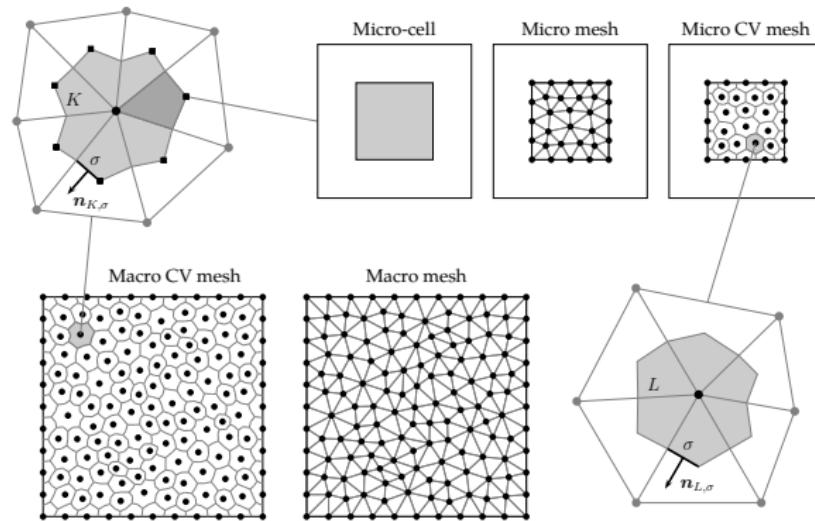
$$Q = \frac{1}{|\Omega_x|} \int_{\Gamma_x} -K_b(h) \nabla_y (h_b + y_2) \cdot \mathbf{n}_{\Gamma_x} ds$$



[Szymkiewicz and Lewandowska (2006)]

Unstructured CV spatial discretisation

- Unstructured vertex-centered CV method [Carr and Turner (2014)]



- Existing numerical strategies (e.g., Szymkiewicz and Lewandowska (2008)) only applicable to simple inclusion geometries

Meshing of micro-cells

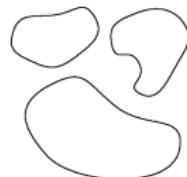
Image-based meshing code built on GMSH [Guezaine and Remacle (2009)]



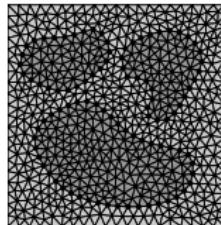
Bitmap image



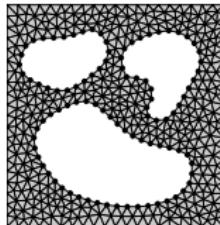
Binary image



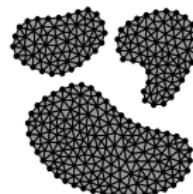
Edge detection



Full micro-cell



Ω_a only



Ω_b only

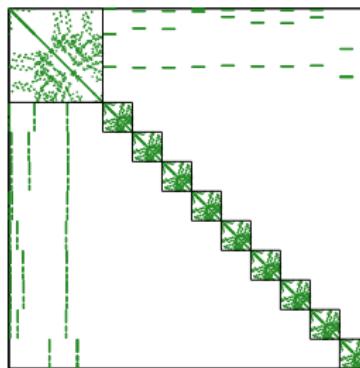
Spatially-discrete system

- ▶ Spatial discretisation can be expressed in the form

$$\frac{d\mathbf{u}}{dt} = \mathbf{g}(\mathbf{u}), \quad \mathbf{u}(0) = \mathbf{u}_0 \in \mathbb{R}^N,$$

where $N = \text{num_macro_nodes} + \text{num_macro_elements} \times \text{num_micro_nodes}$.

- ▶ Example sparsity structure of Jacobian matrix (zoomed in)



Time stepping: exponential integrator

EEM: A Jacobian-free variable-stepsize Krylov-subspace ODE solver based on the exponential Euler method [Carr et al. (2011, 2013)]:

$$\frac{d\mathbf{u}}{dt} = \mathbf{g}(\mathbf{u}) \quad \xrightarrow{\text{Linearise}} \quad \frac{d\mathbf{u}}{dt} = \mathbf{g}_n + \mathbf{J}_n(\mathbf{u} - \mathbf{u}_n)$$

where $\mathbf{g}_n = \mathbf{g}(\mathbf{u}_n)$ and $\mathbf{J}_n = \mathbf{J}(\mathbf{u}_n)$, and solve exactly over a single time step:

$$\mathbf{u}_{n+1} = \mathbf{u}_n + \tau_n \varphi(\tau_n \mathbf{J}_n) \mathbf{g}_n$$

where $\varphi(\mathbf{A}) = \mathbf{A}^{-1}(e^{\mathbf{A}} - \mathbf{I})$.

- ▶ Explicit scheme
- ▶ Krylov subspace methods for computing $\varphi(\tau_n \mathbf{J}_n) \mathbf{g}_n$ converge rapidly without preconditioning, and require only matrix-vector products with \mathbf{J}_n :

$$\mathbf{J}_n \mathbf{v} \approx [\mathbf{g}(\mathbf{u}_n + \varepsilon \mathbf{v}) - \mathbf{g}(\mathbf{u}_n)] / \varepsilon$$

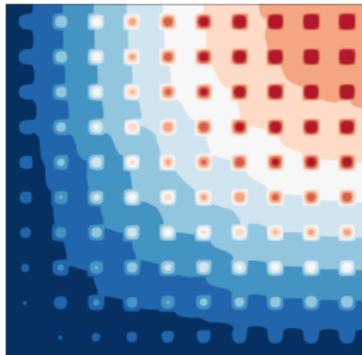
Code implementation details

- ▶ Code developed in C++
- ▶ Linear algebra operations performed using BLAS and LAPACK libraries:
 - (a) Intel MKL (HPC Platform)
 - (b) Accelerate framework (Macbook Pro)
- ▶ ODE right-hand side function $\mathbf{g}(\mathbf{u})$ implemented in parallel using OpenMP

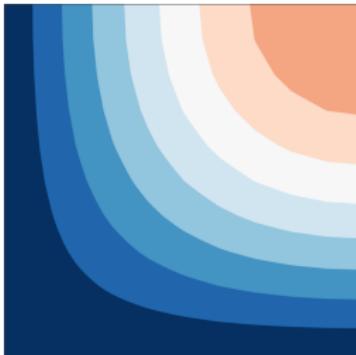
```
#include <omp.h>
omp_set_num_threads(NUM_THREADS);
#pragma omp parallel for
for (k=0; k<num_macro_elements; k++)
{
    ...
}
```

- ▶ Code accommodates both triangular and quad elements at both scales

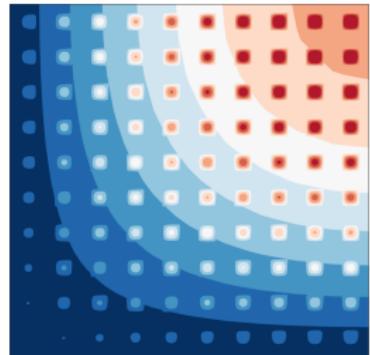
Test case: simple diffusion problem



Full (fine-scale) model
(15 mins)



Macroscopic model
(1 sec)

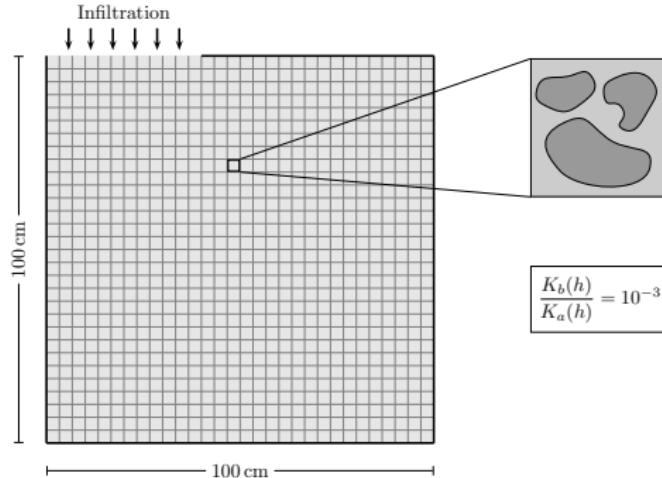


Two-scale model
(20 secs)

Mesh details:

- ▶ Full (fine-scale) model: 400×400 grid, $N = 160,801$
- ▶ Macroscopic model: 20×20 grid, $N = 441$
- ▶ Two-scale model: 20×20 grid (macro), 10×10 grid (micro), $N = 48,841$

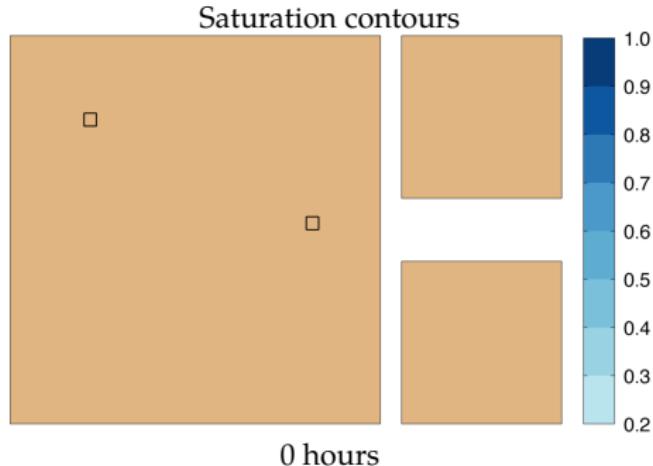
Simulation: unsaturated water flow



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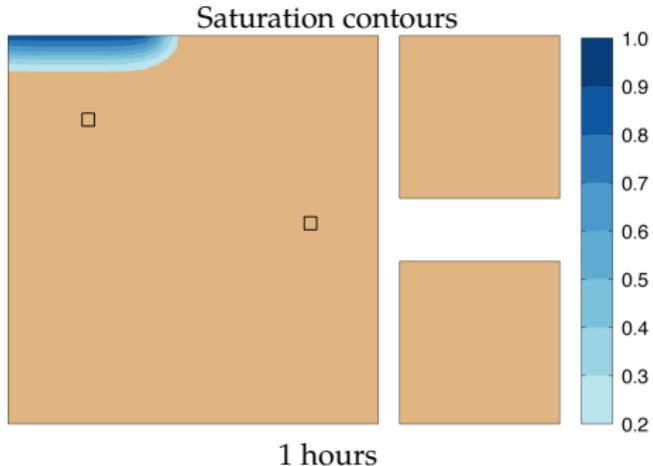
- ▶ Macroscopic mesh (structured): 30×30 grid, 961 nodes
- ▶ Microscopic mesh (unstructured): 532 elements, 316 nodes
- ▶ Total number of unknowns: $N = 961 + 900 \times 316 = 285,361$

Simulation: unsaturated water flow



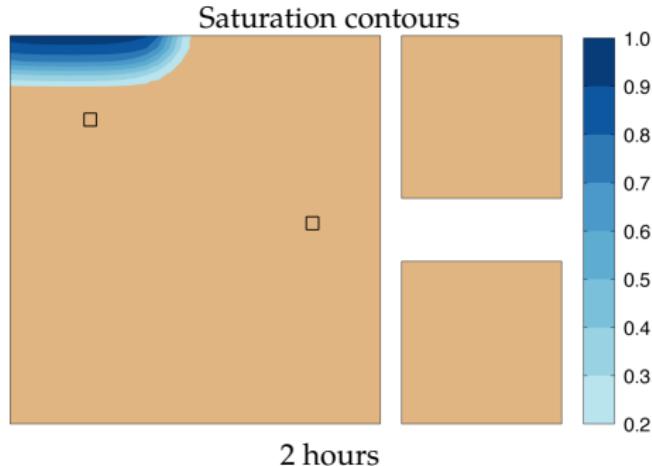
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Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



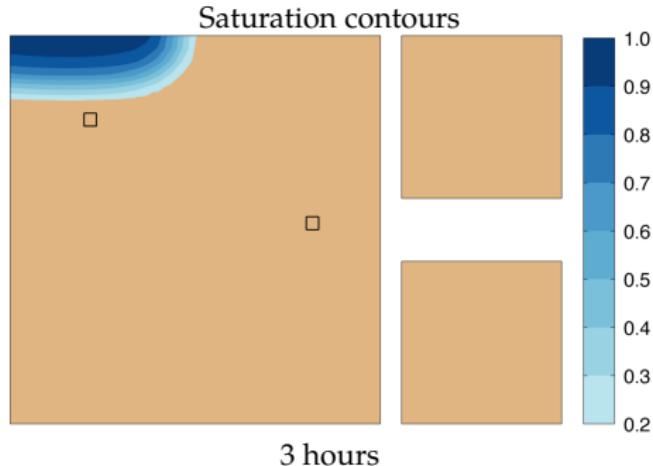
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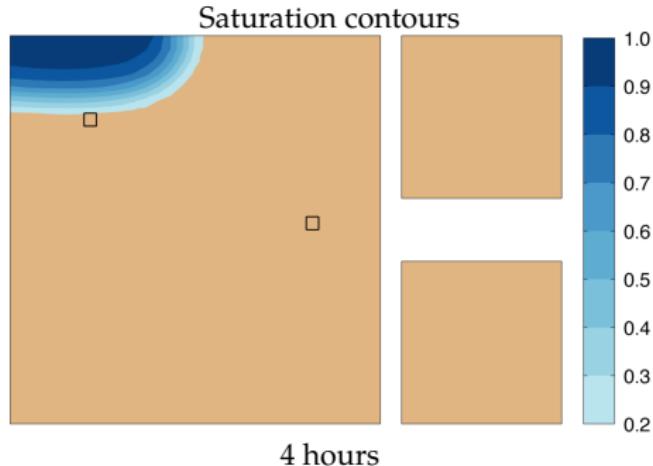
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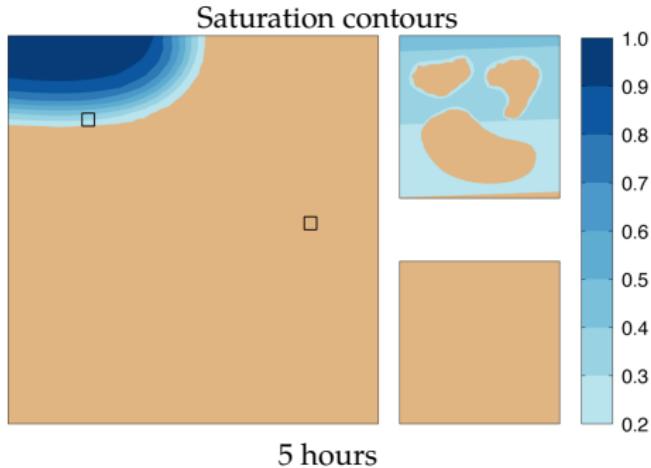
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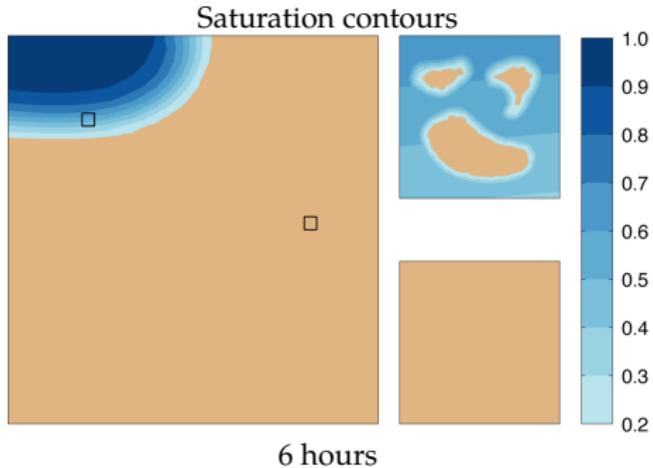
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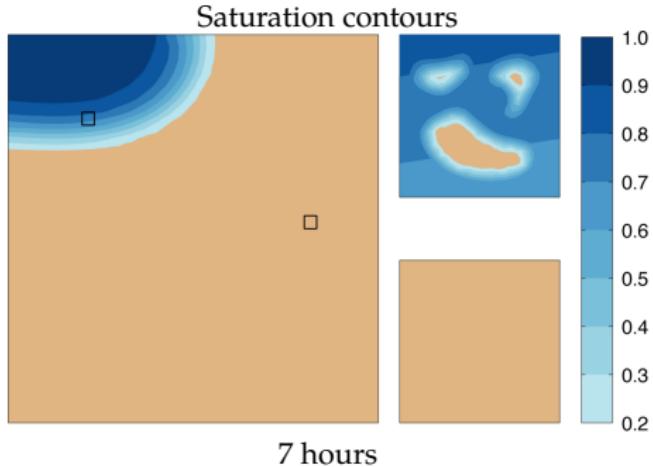
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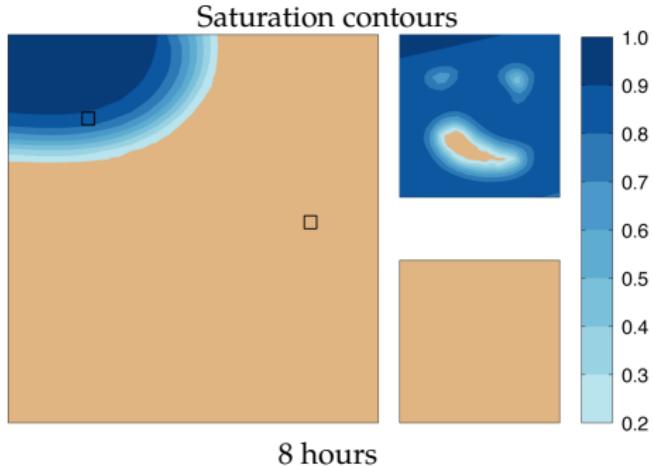
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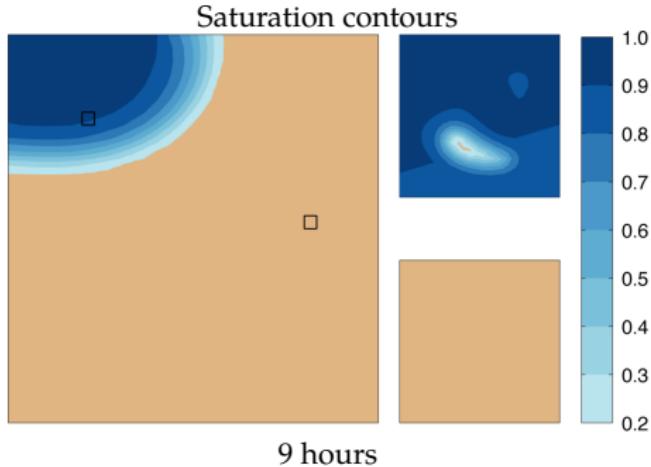
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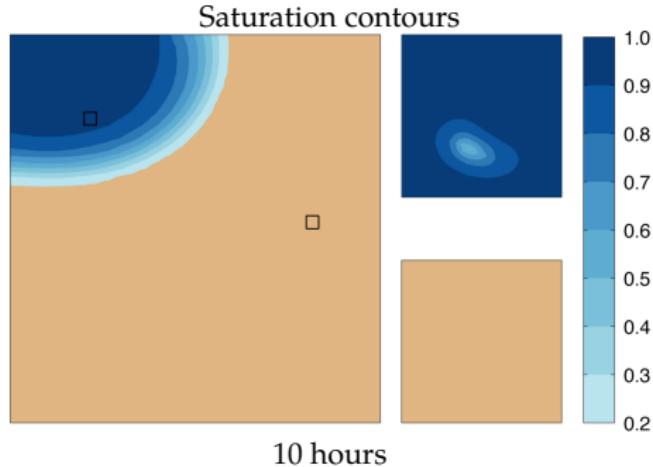
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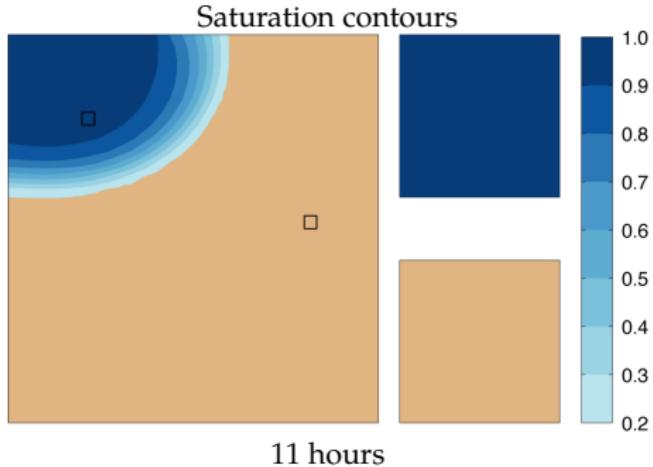
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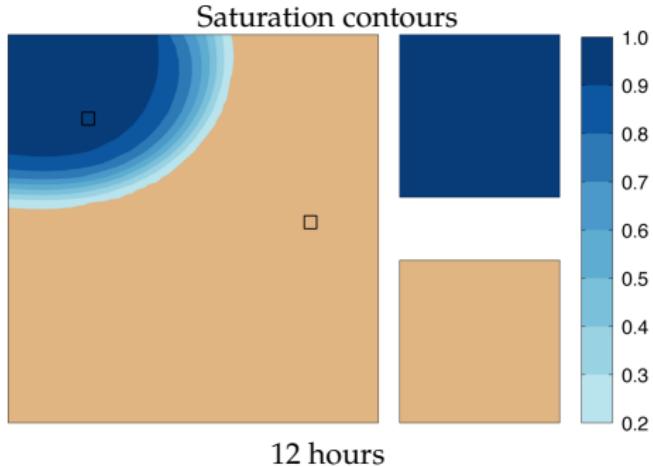
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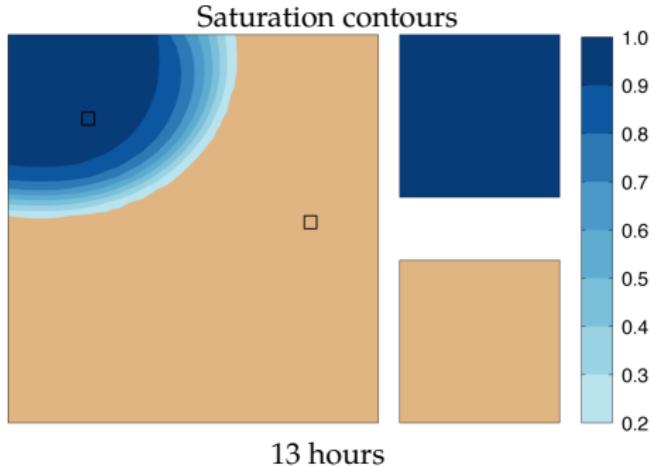
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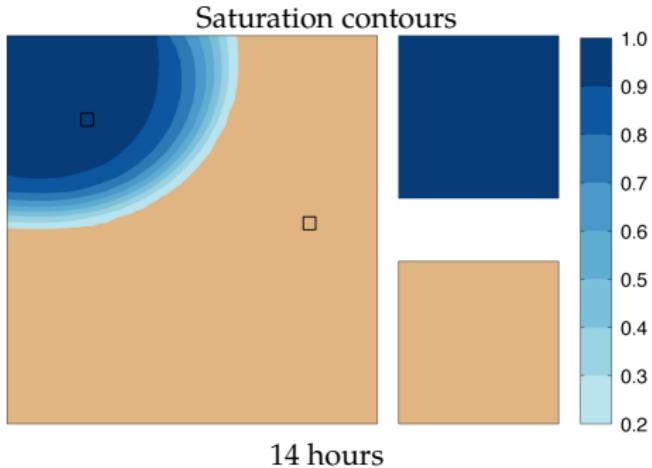
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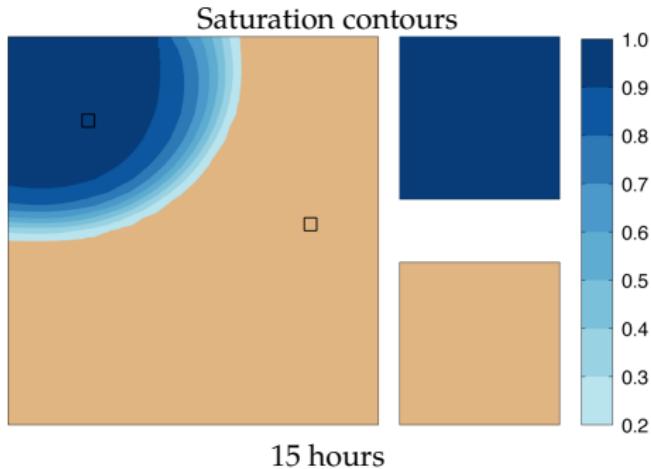
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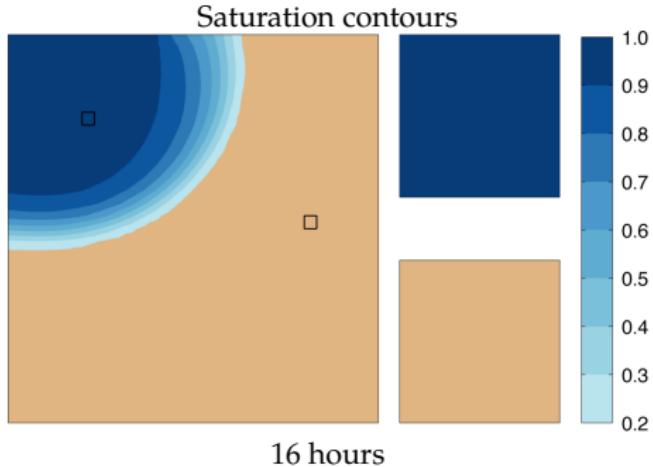
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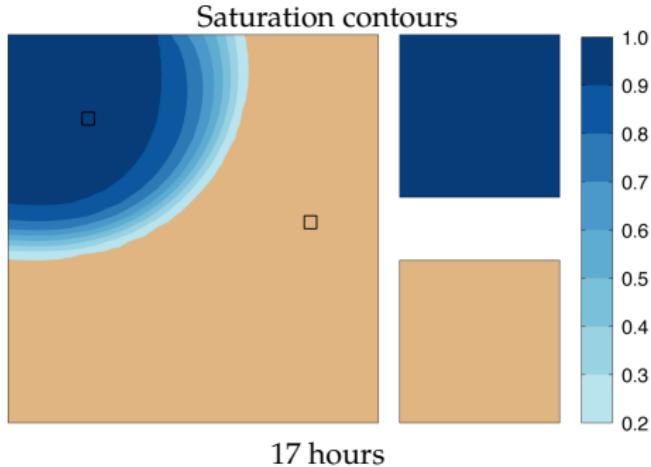
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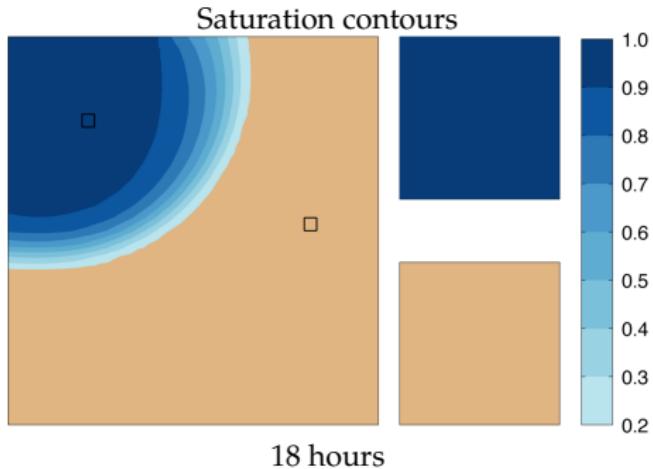
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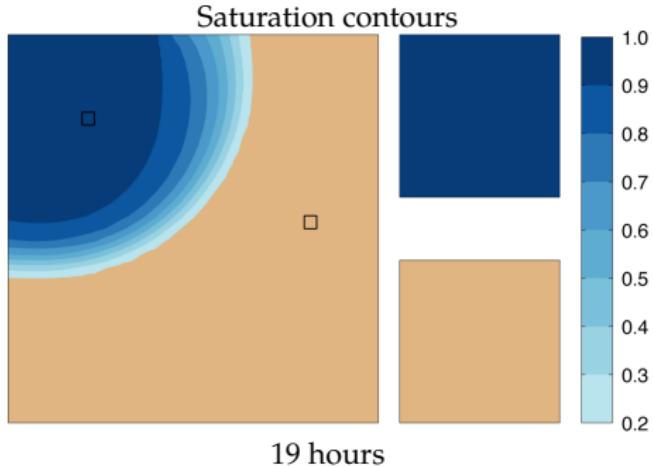
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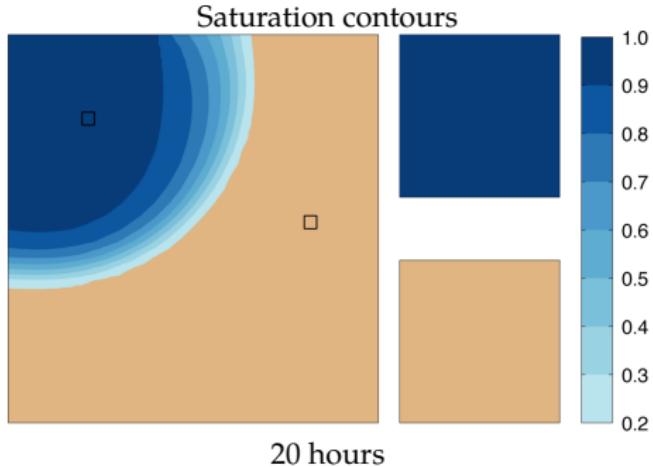
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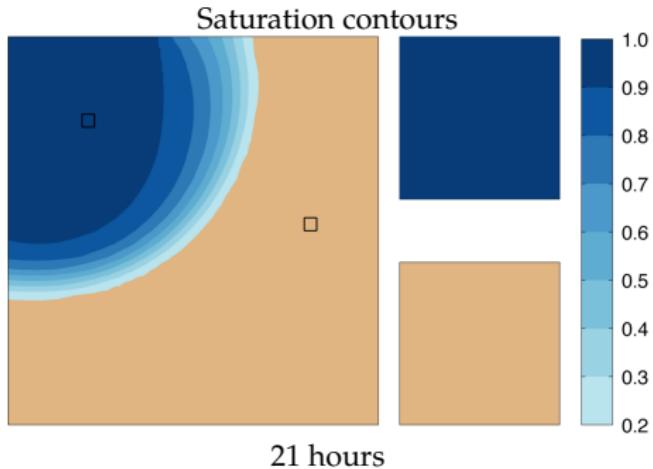
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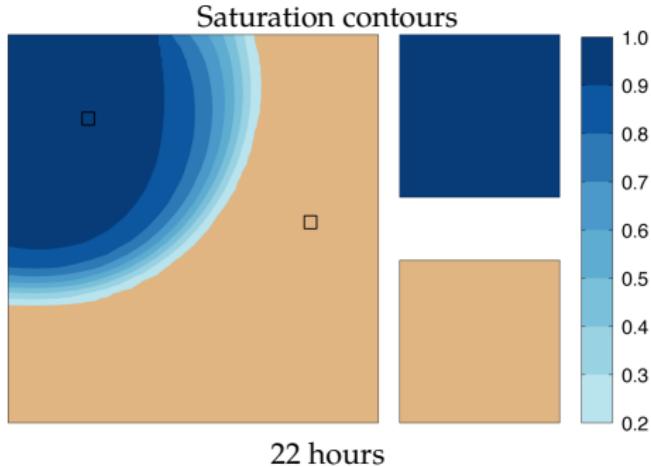
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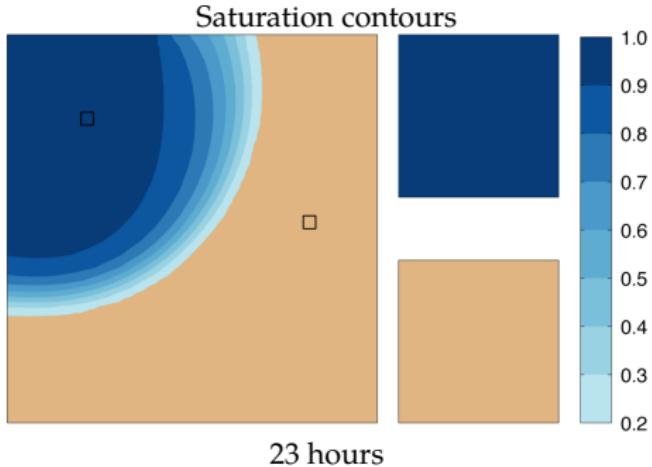
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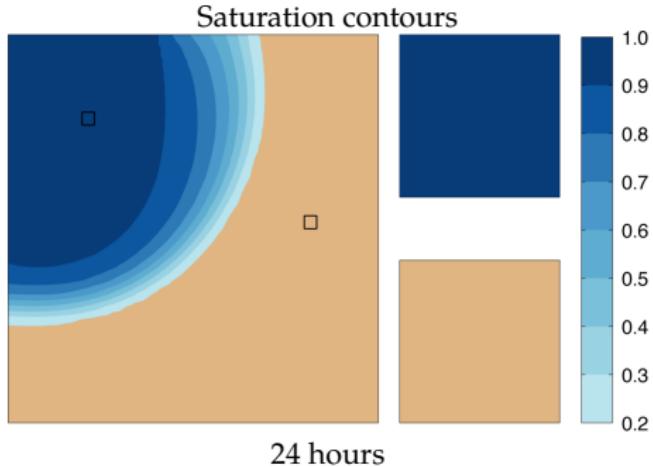
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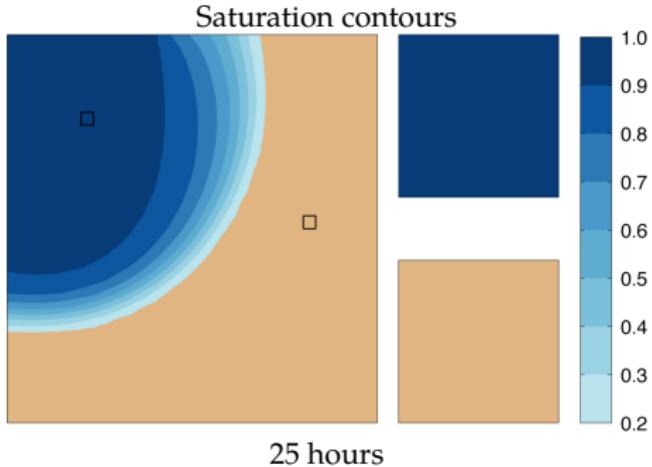
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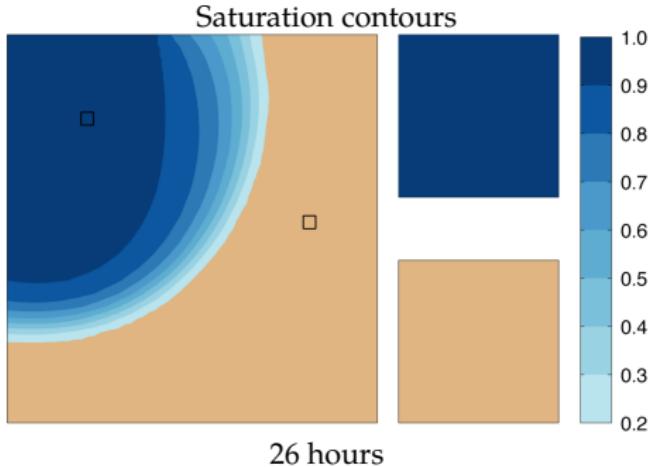
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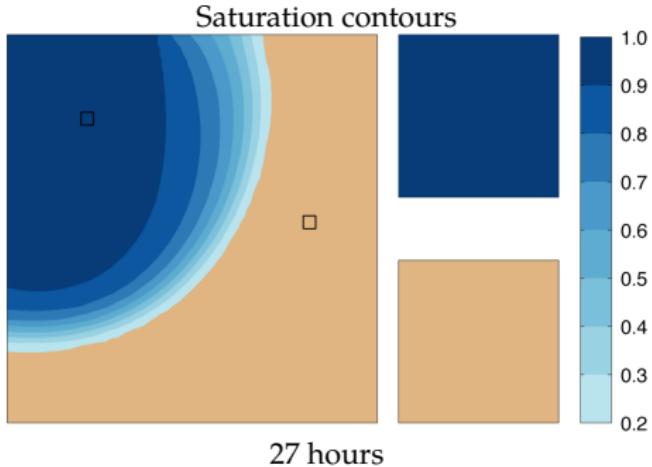
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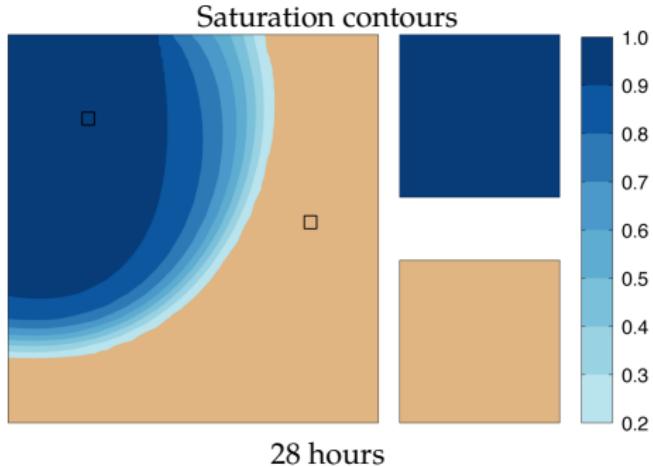
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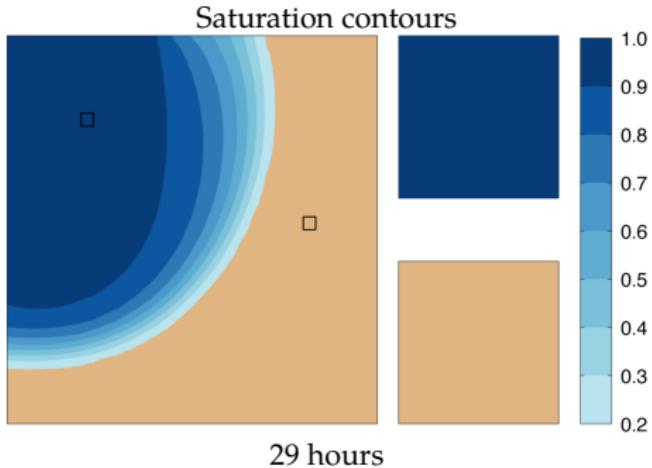
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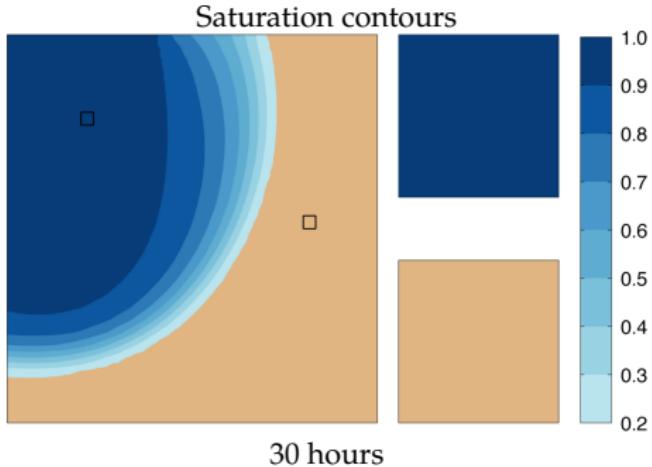
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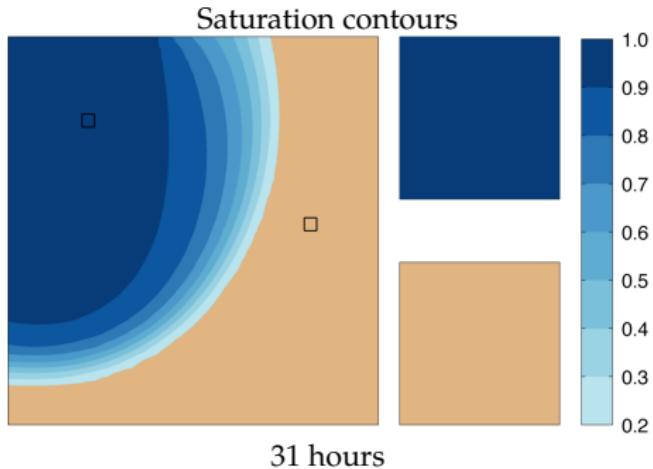
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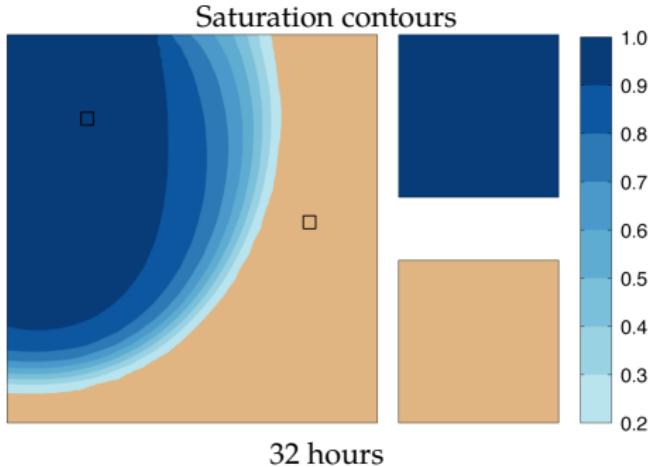
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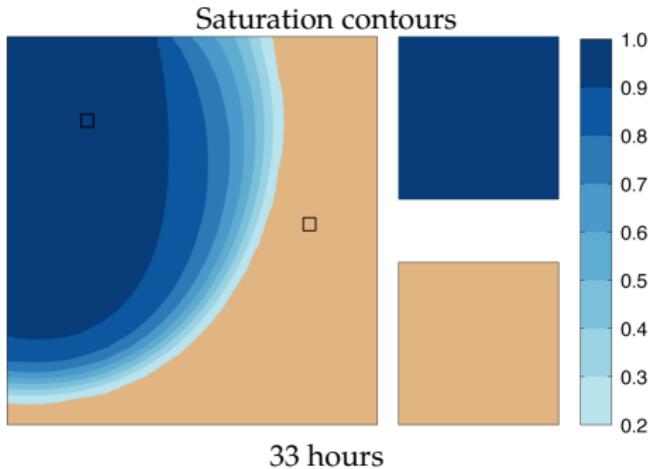
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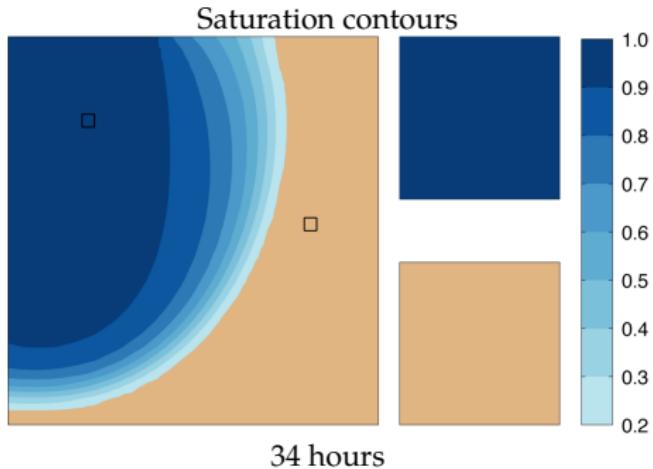
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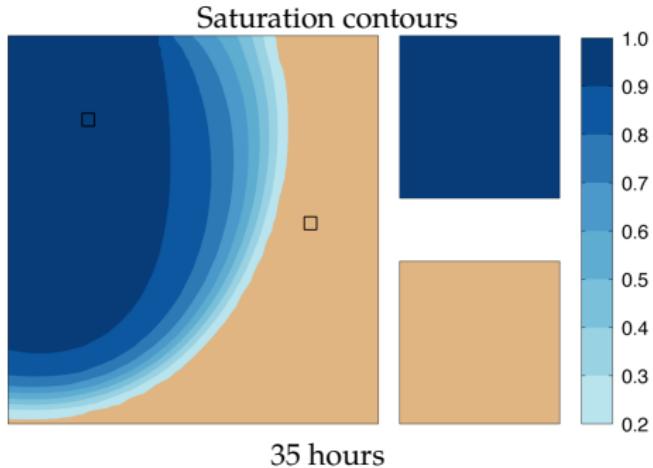
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Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



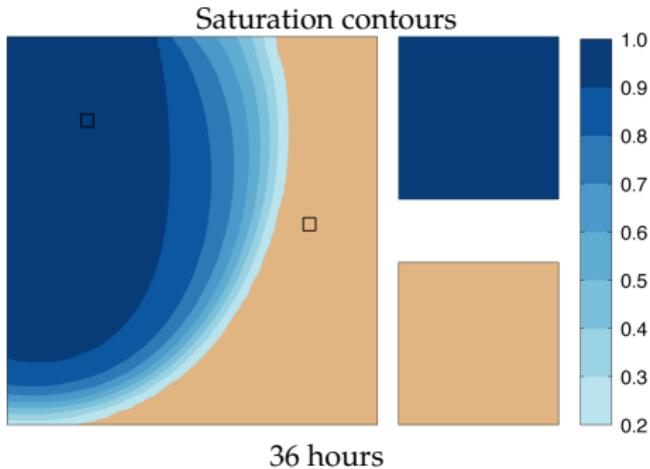
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



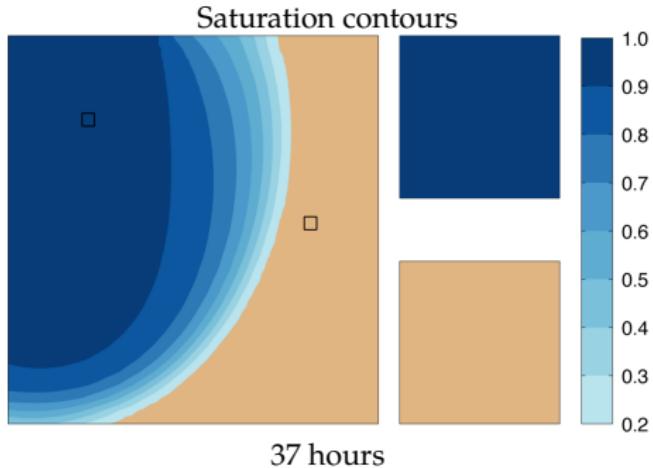
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



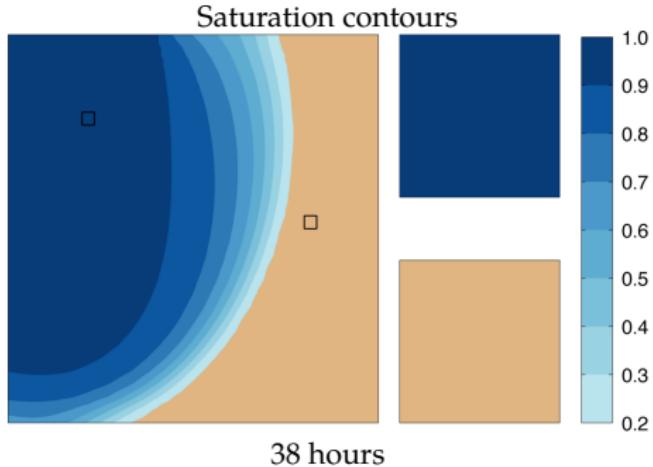
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



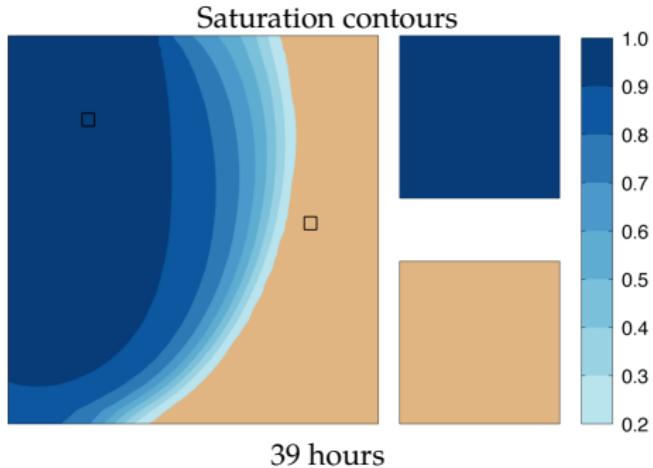
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



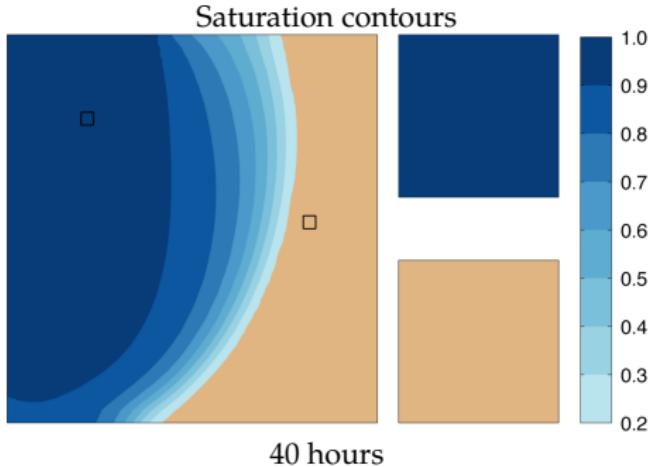
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



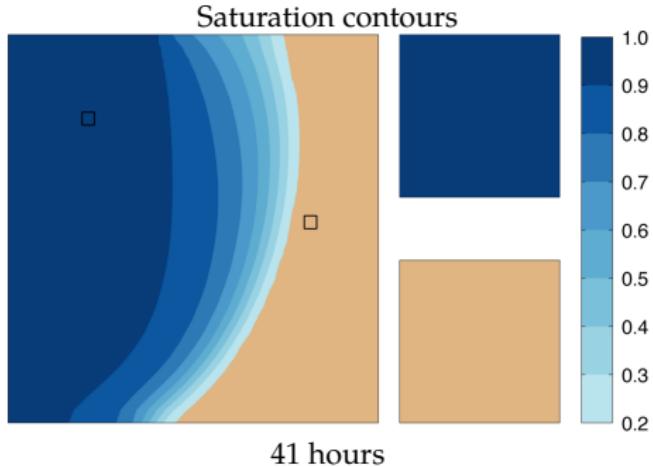
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



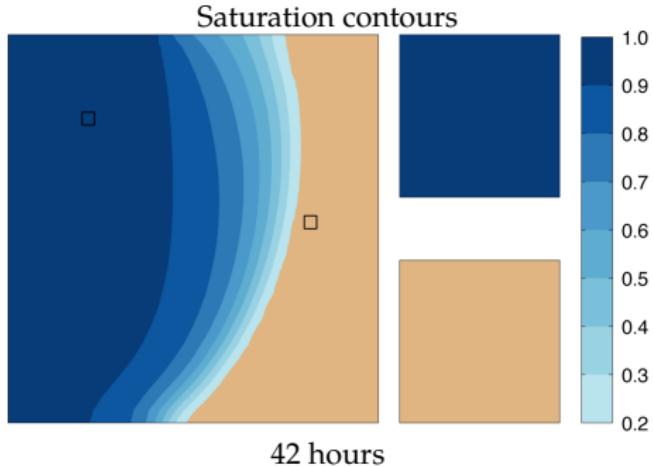
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



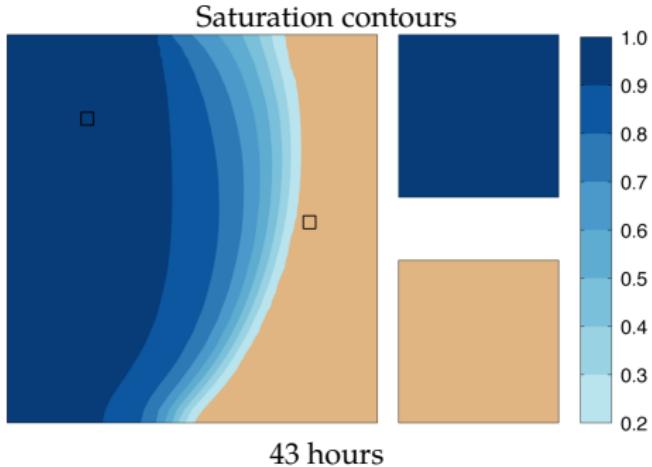
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



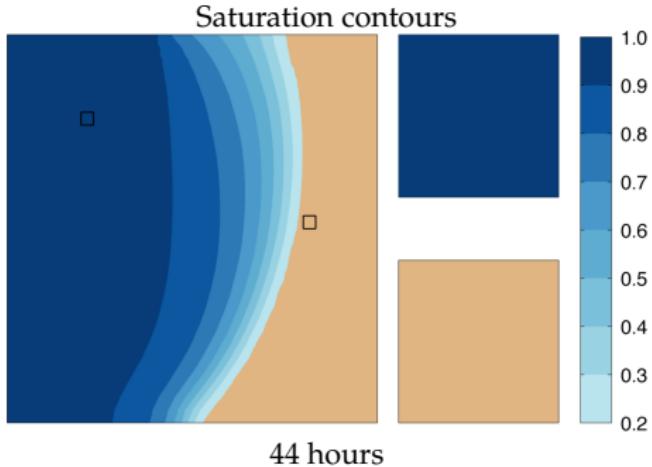
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



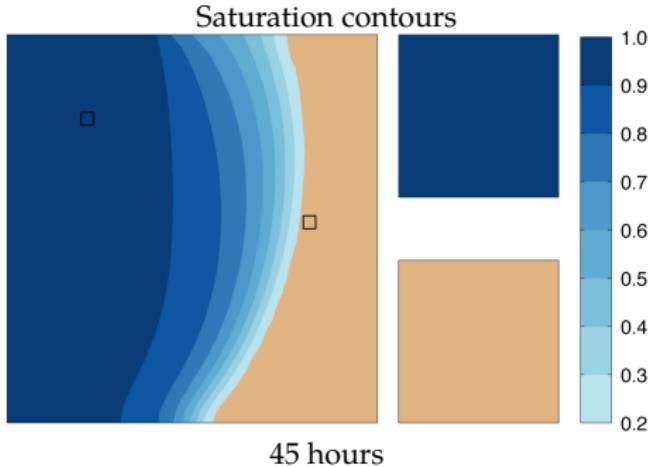
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



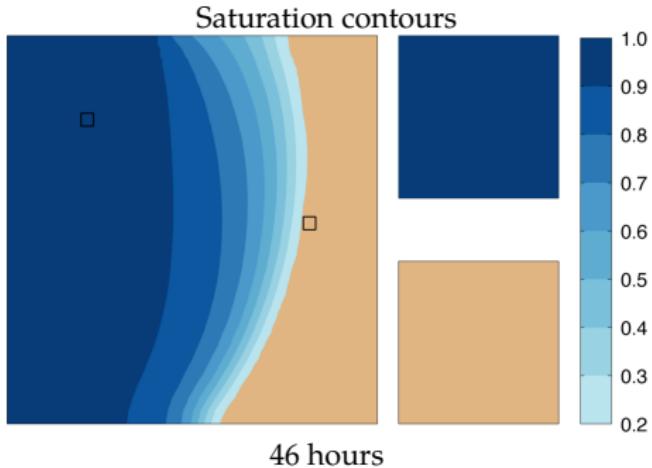
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



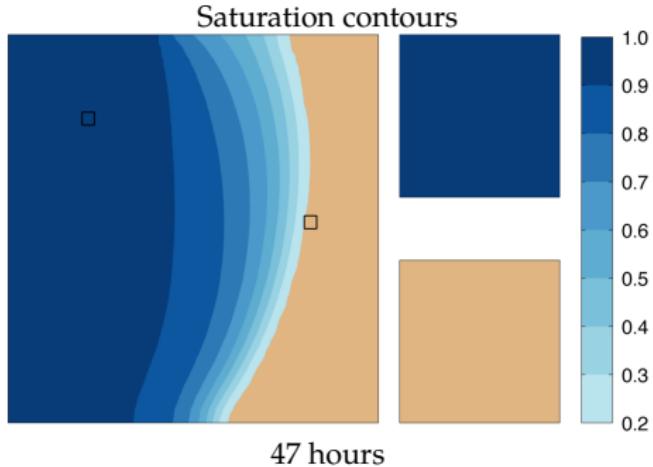
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



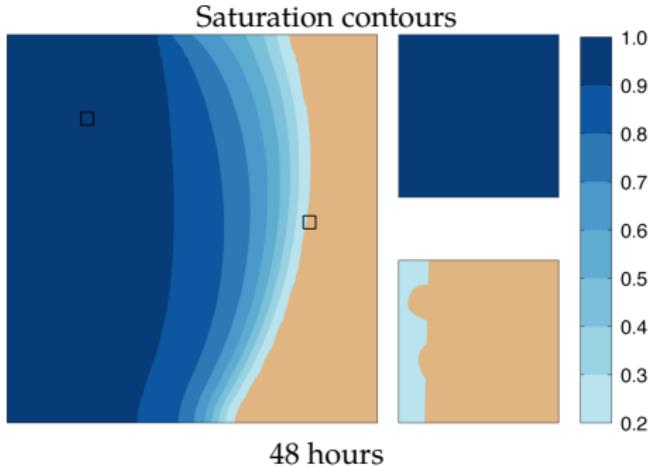
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



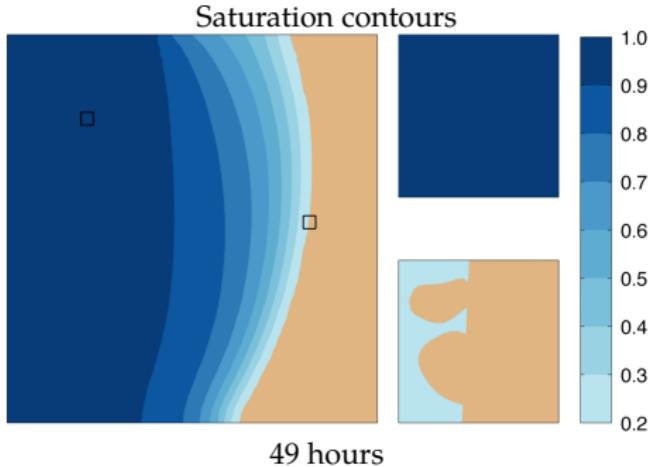
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



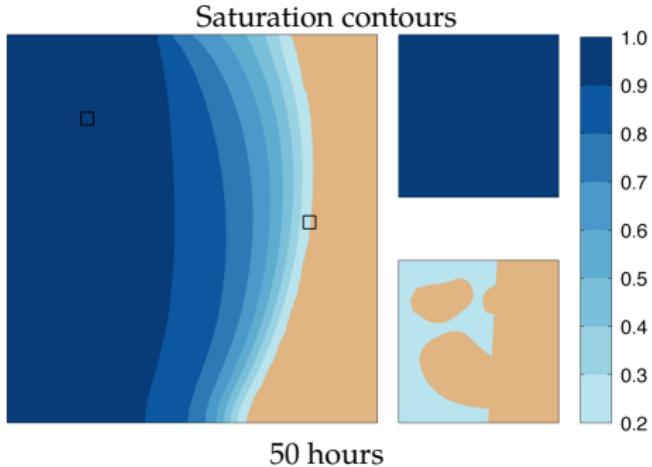
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



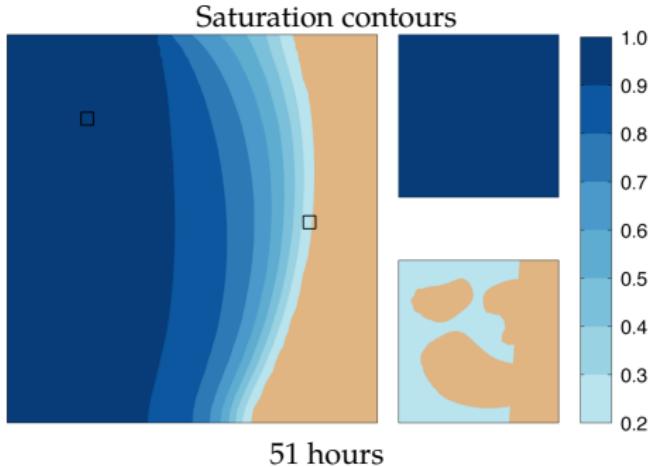
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



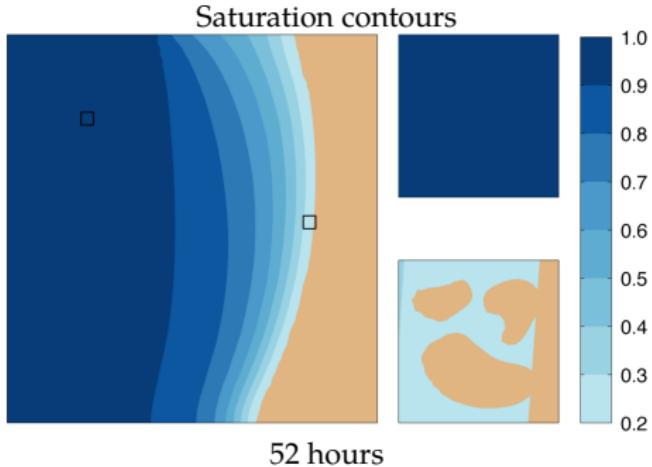
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



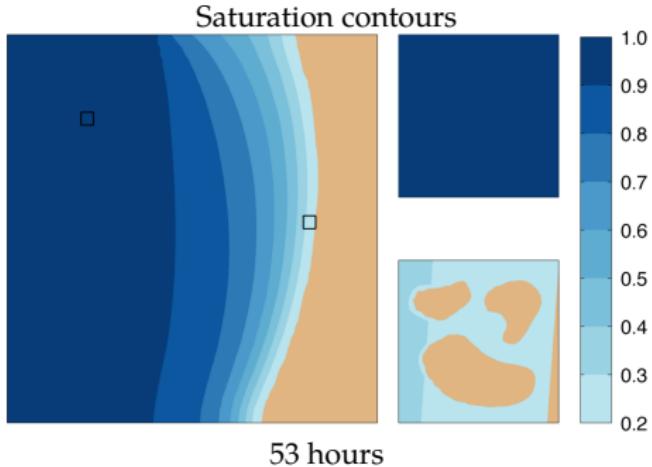
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



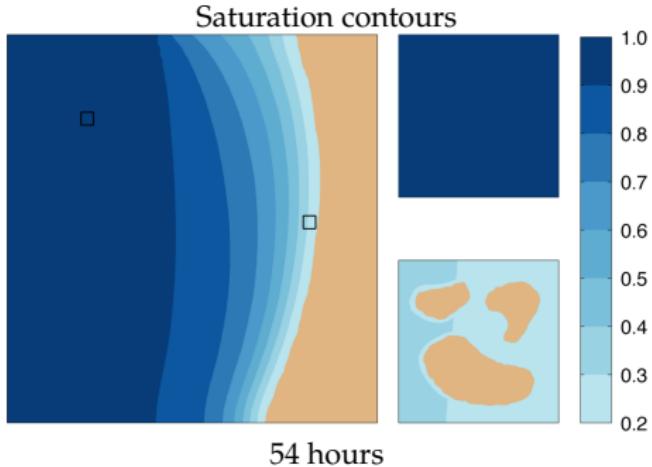
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



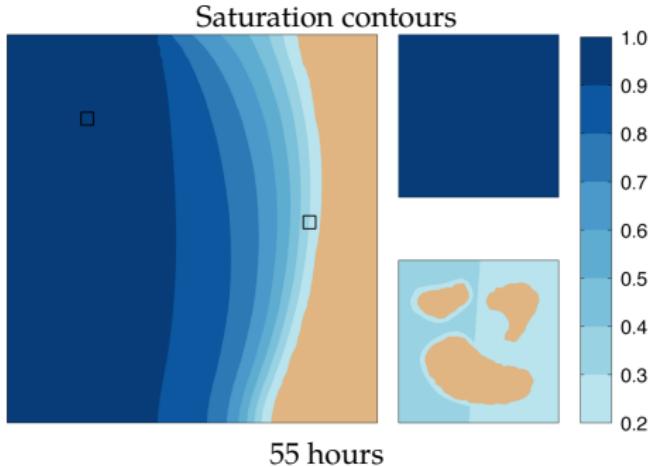
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



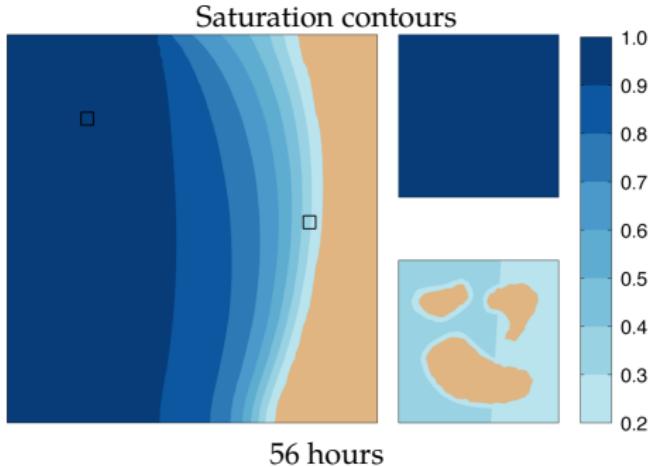
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



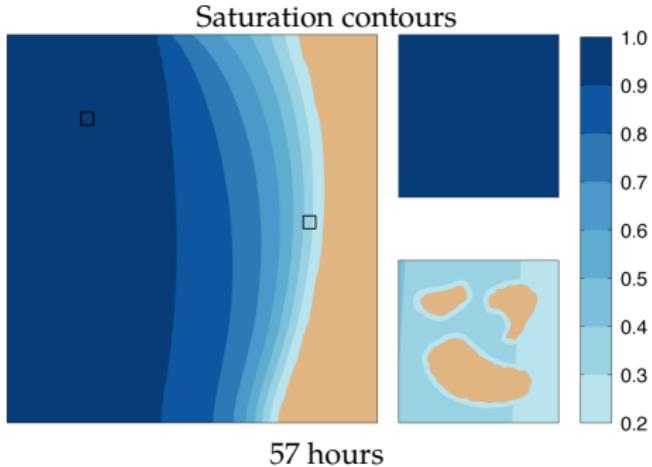
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



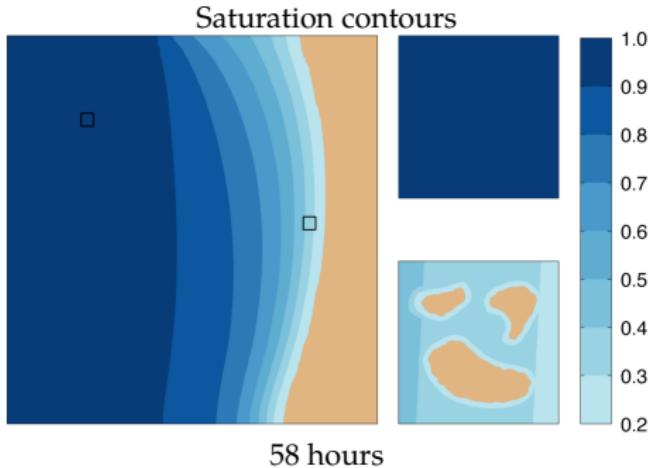
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



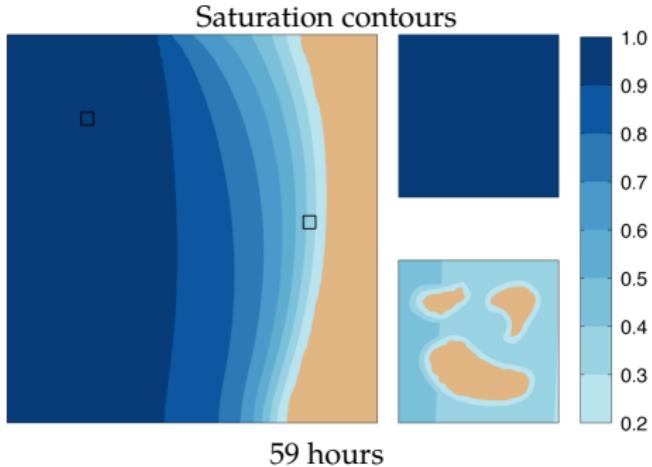
	Serial	1 core	2 cores	4 cores	8 cores
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Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



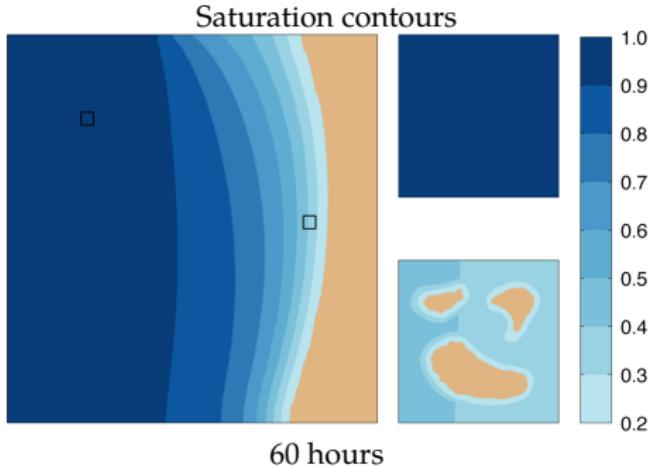
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



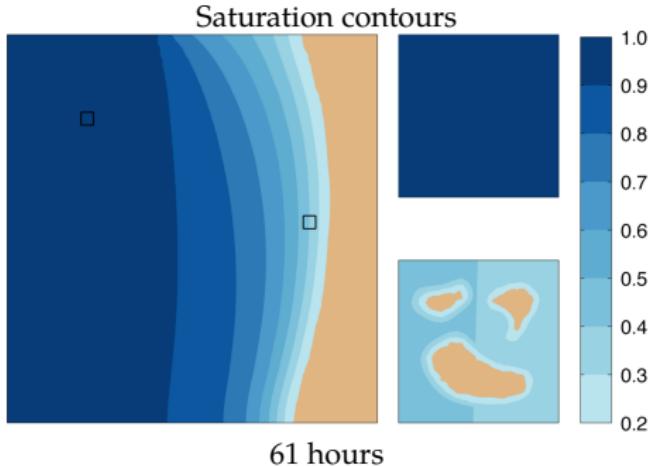
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



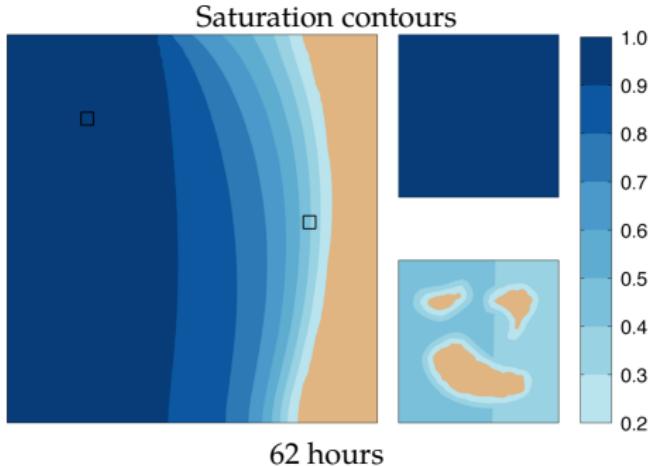
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



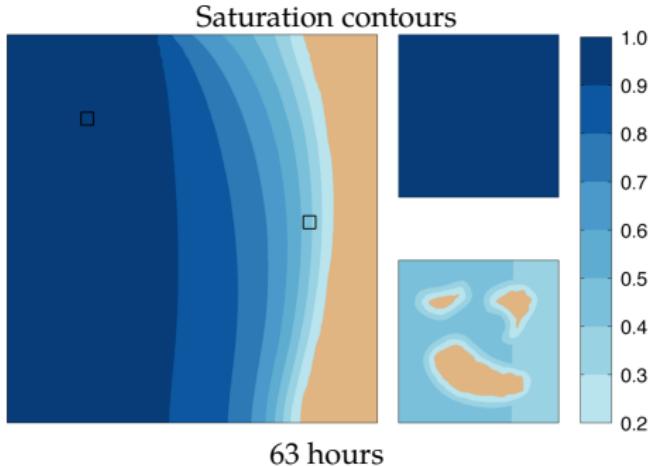
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



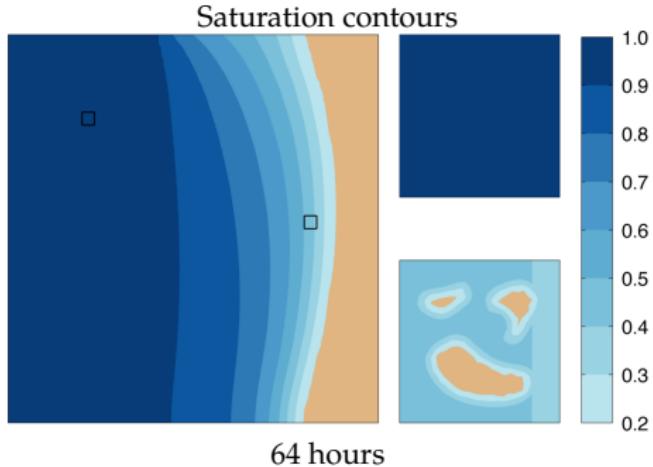
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



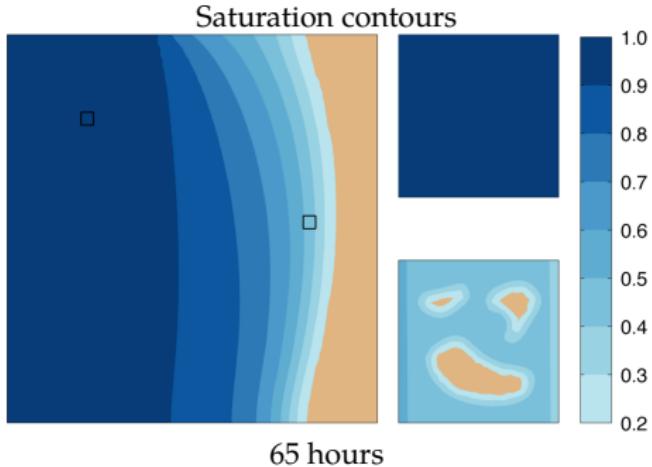
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
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Simulation: unsaturated water flow



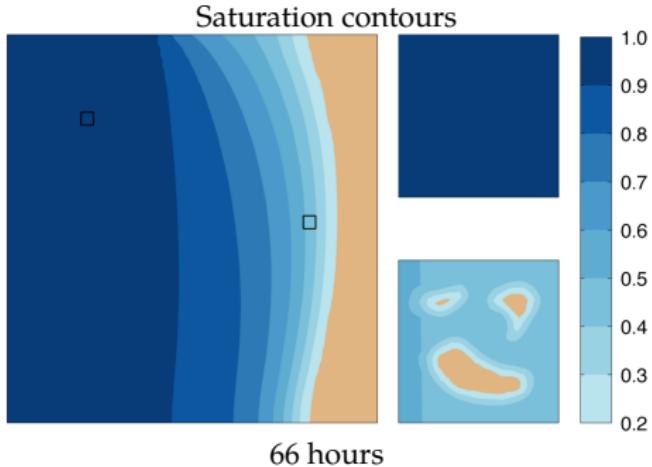
	Serial	1 core	2 cores	4 cores	8 cores
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Simulation: unsaturated water flow



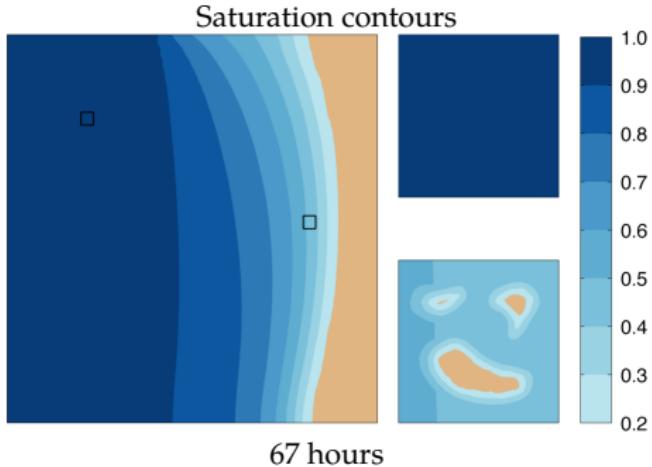
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



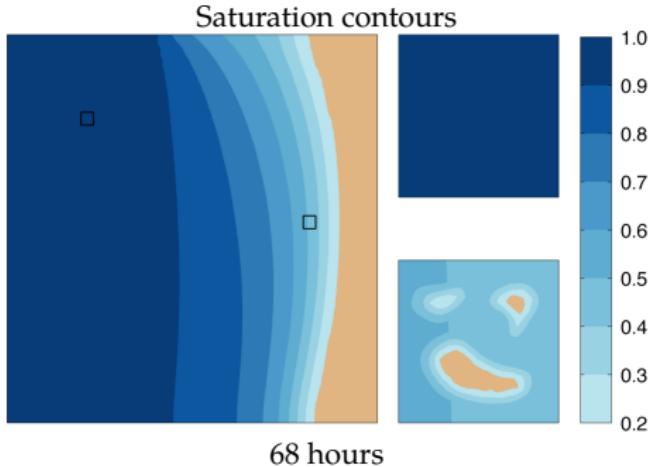
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
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Simulation: unsaturated water flow



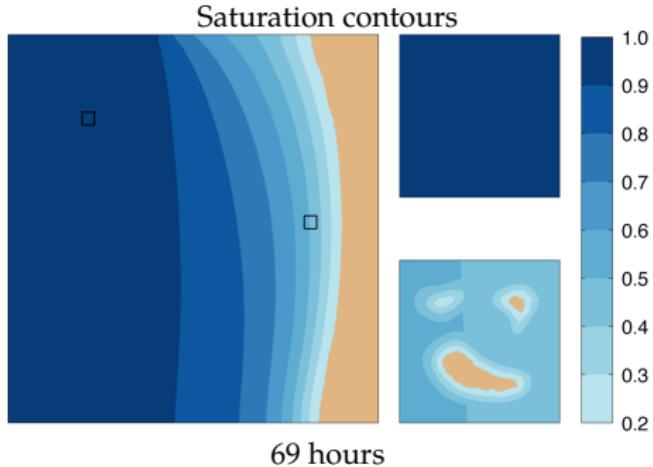
	Serial	1 core	2 cores	4 cores	8 cores
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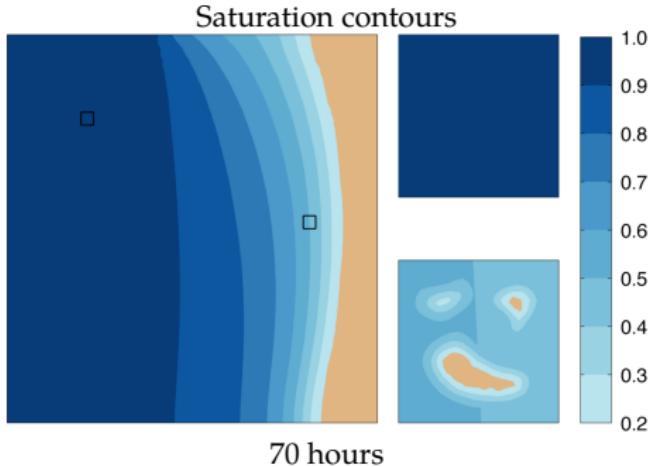
	Serial	1 core	2 cores	4 cores	8 cores
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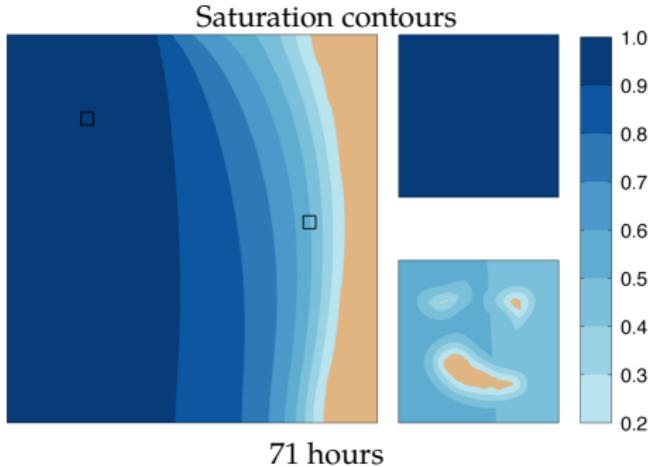
	Serial	1 core	2 cores	4 cores	8 cores
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Simulation: unsaturated water flow



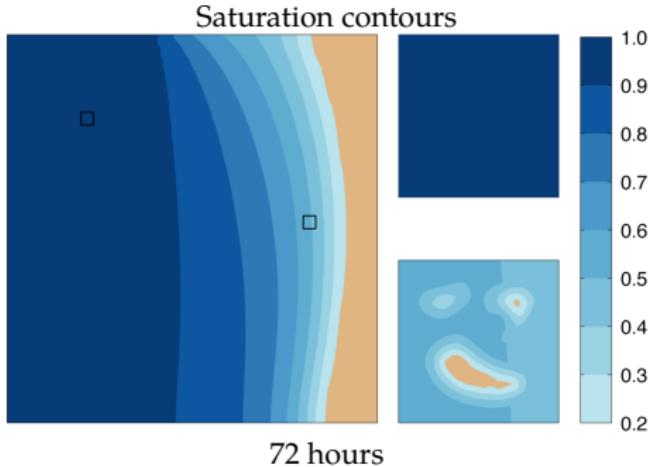
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
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Simulation: unsaturated water flow



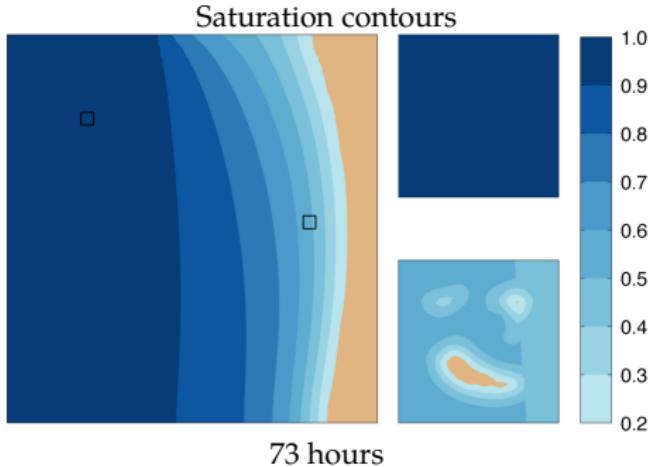
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



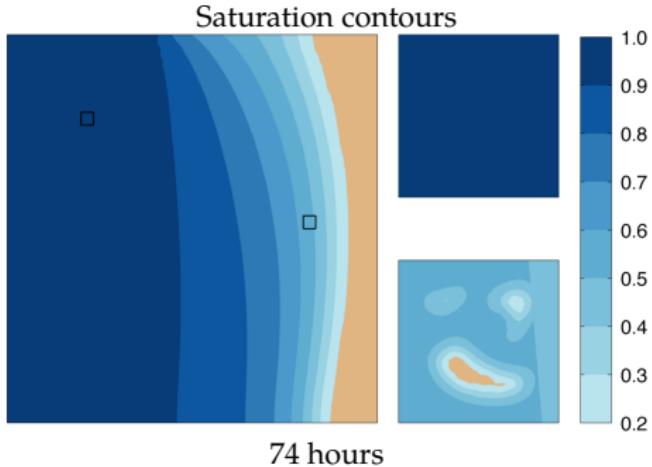
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



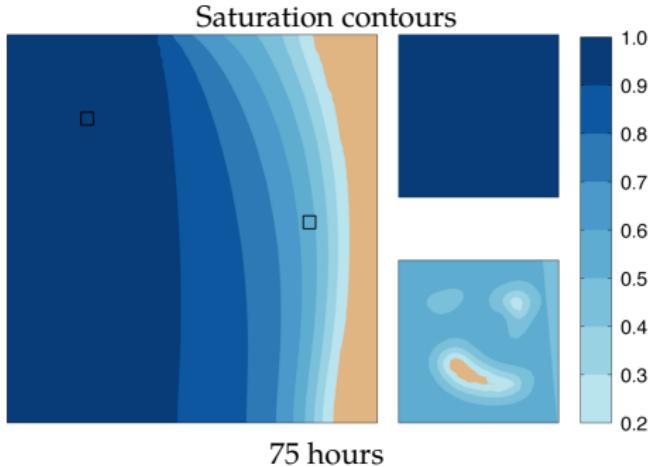
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
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Simulation: unsaturated water flow



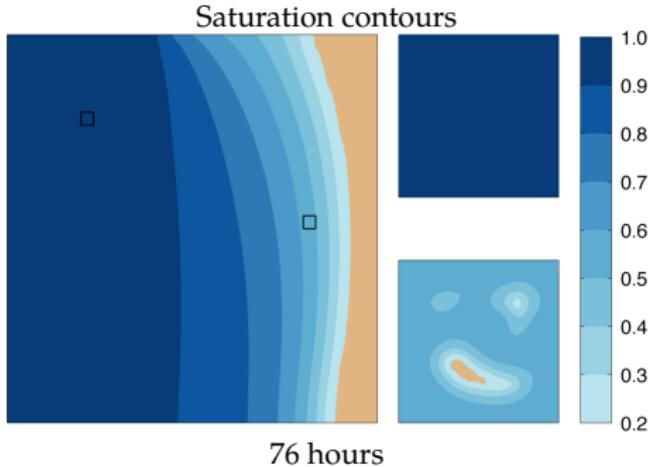
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
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Simulation: unsaturated water flow



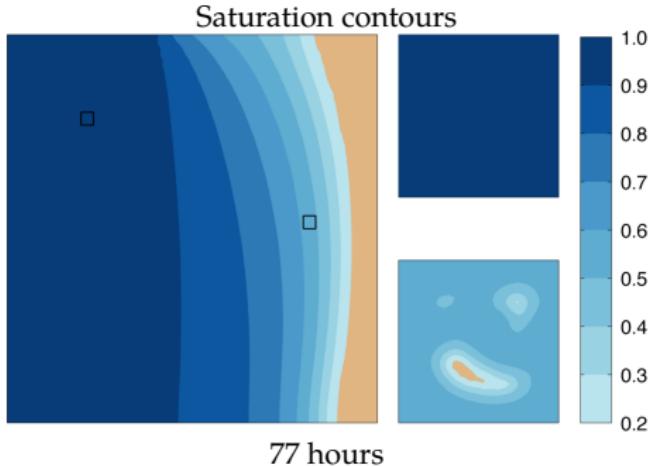
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
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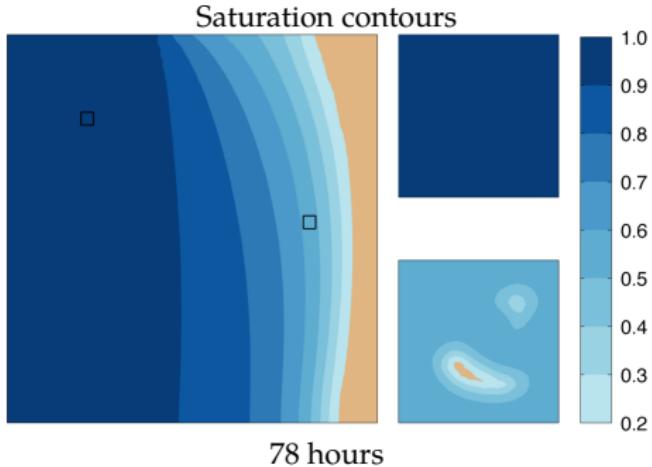
	Serial	1 core	2 cores	4 cores	8 cores
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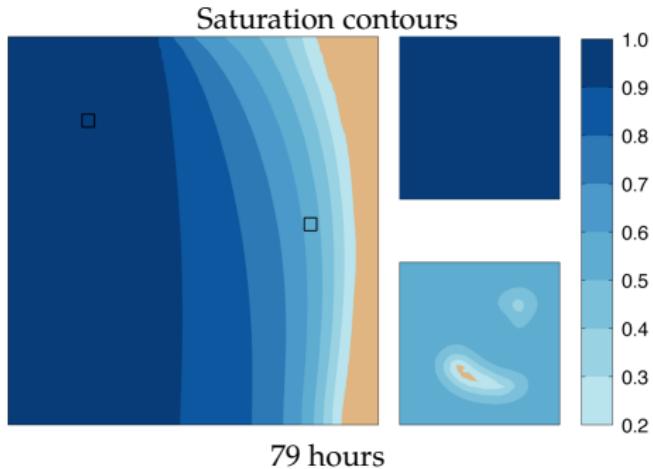
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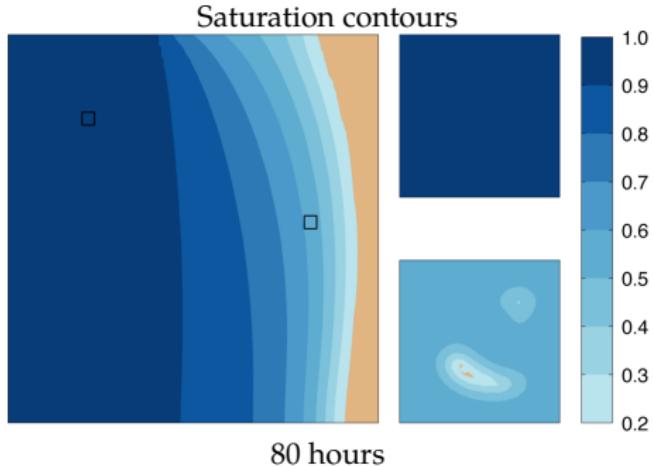
	Serial	1 core	2 cores	4 cores	8 cores
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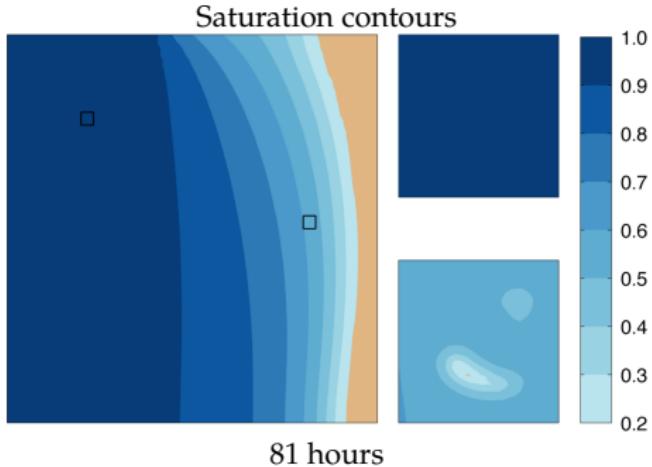
	Serial	1 core	2 cores	4 cores	8 cores
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Simulation: unsaturated water flow



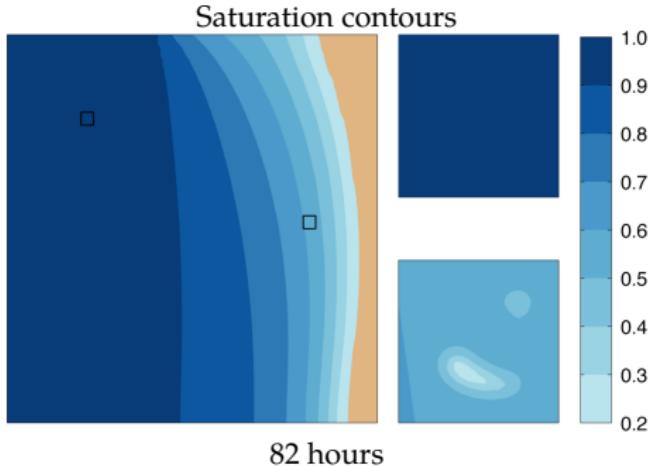
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



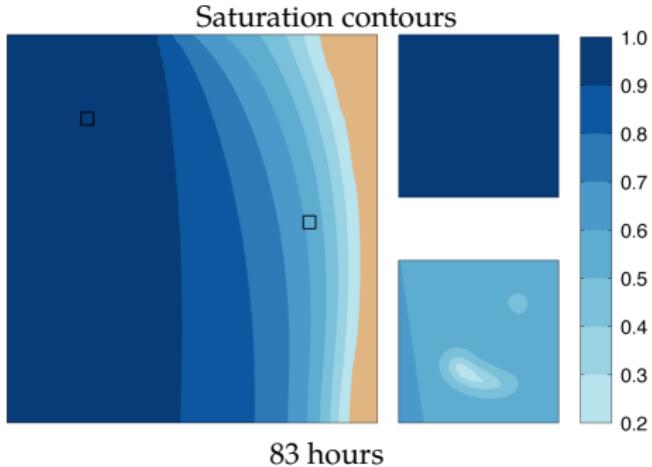
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

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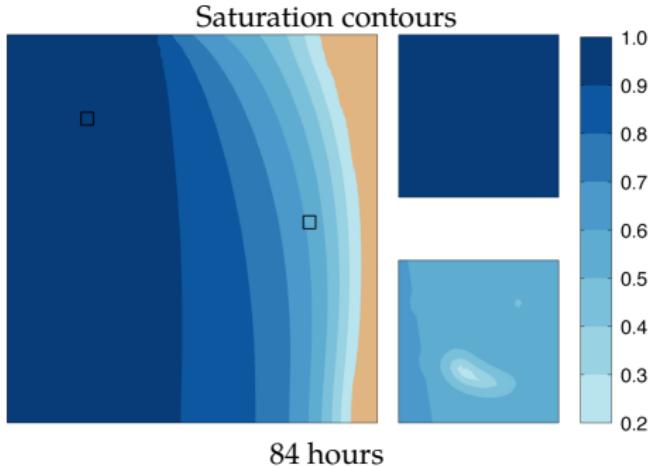
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



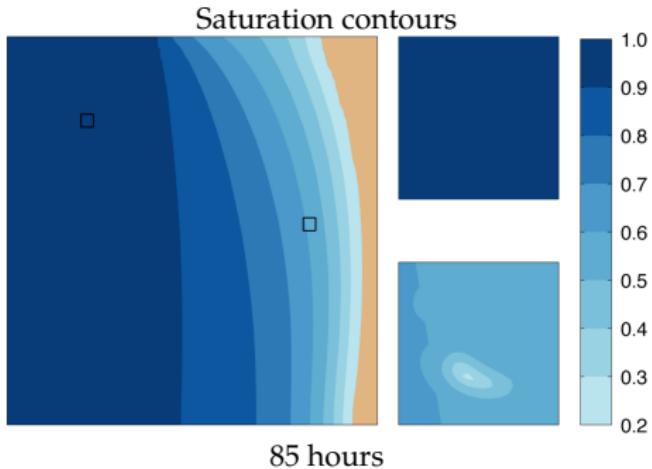
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
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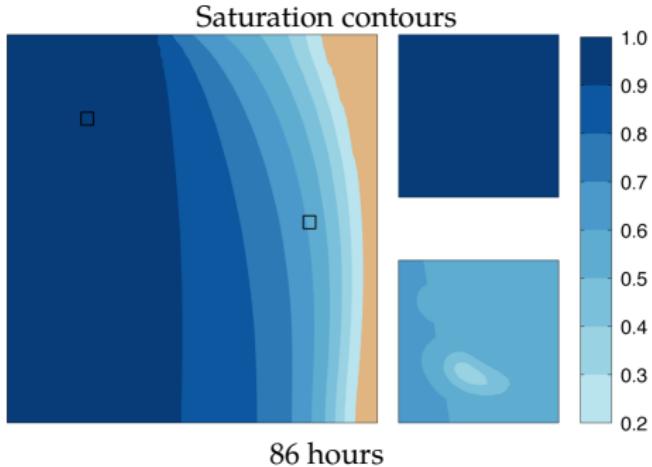
	Serial	1 core	2 cores	4 cores	8 cores
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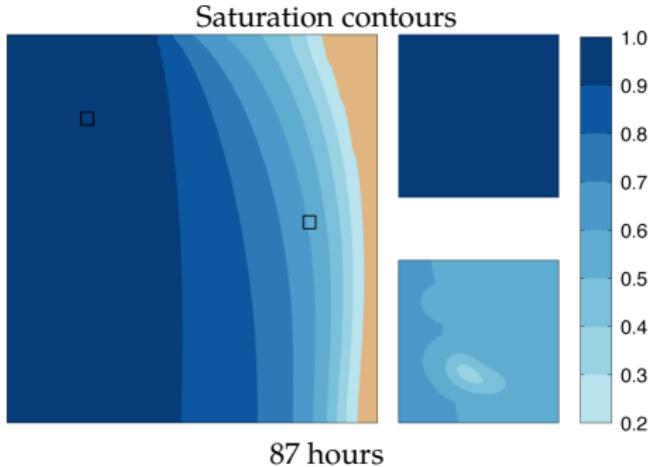
	Serial	1 core	2 cores	4 cores	8 cores
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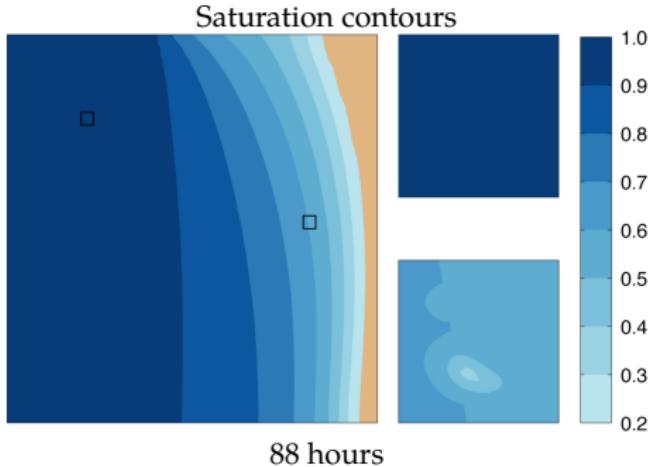
	Serial	1 core	2 cores	4 cores	8 cores
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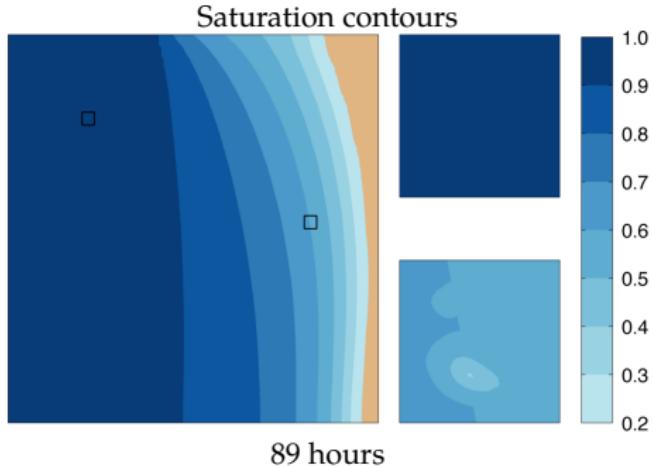
	Serial	1 core	2 cores	4 cores	8 cores
Wall time (min)	179	182	94	51	31
Speedup	1.00	0.98	1.90	3.50	5.84

Simulation: unsaturated water flow



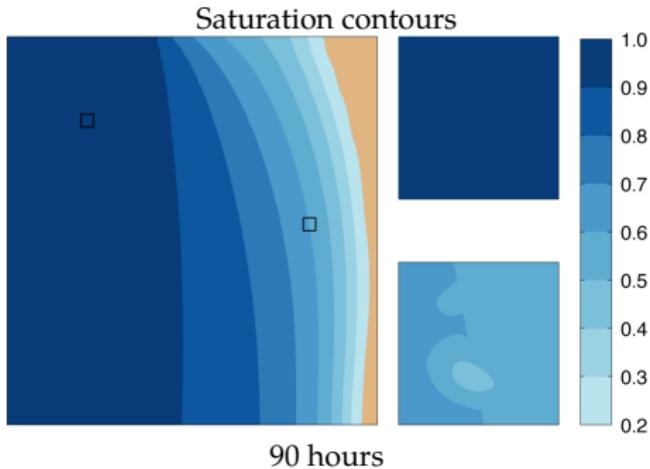
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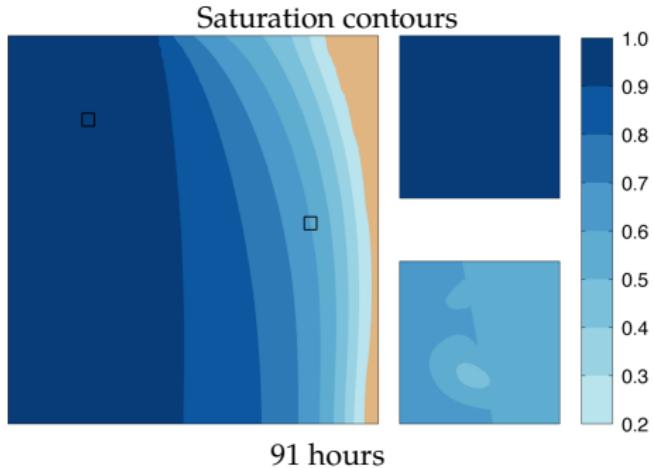
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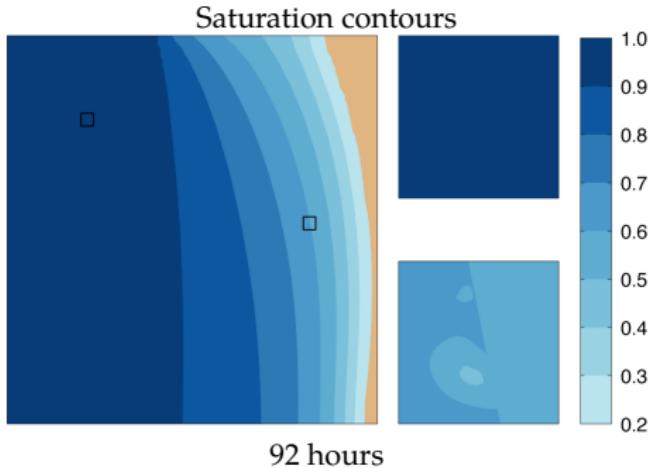
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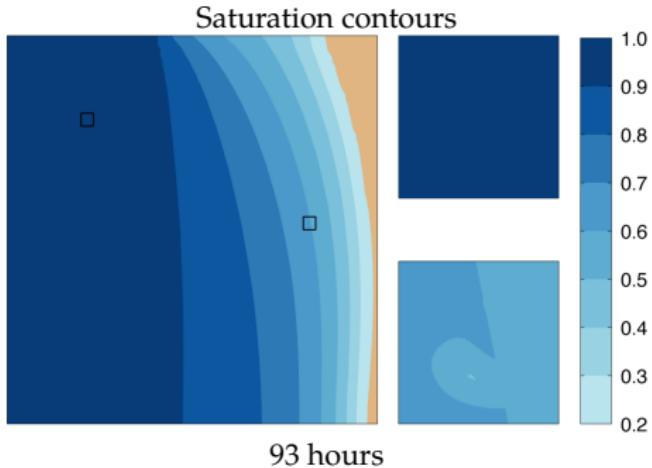
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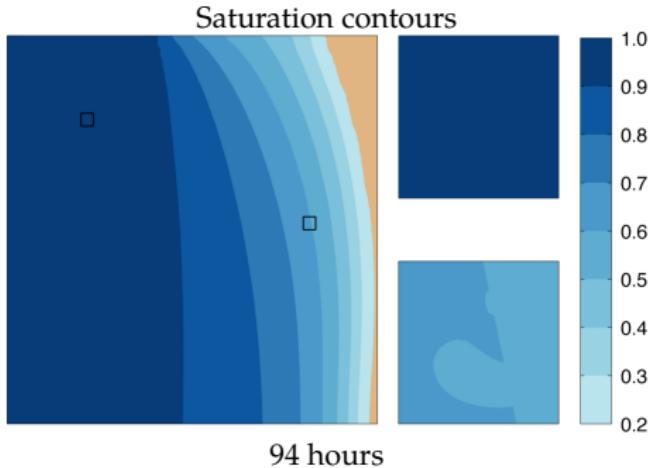
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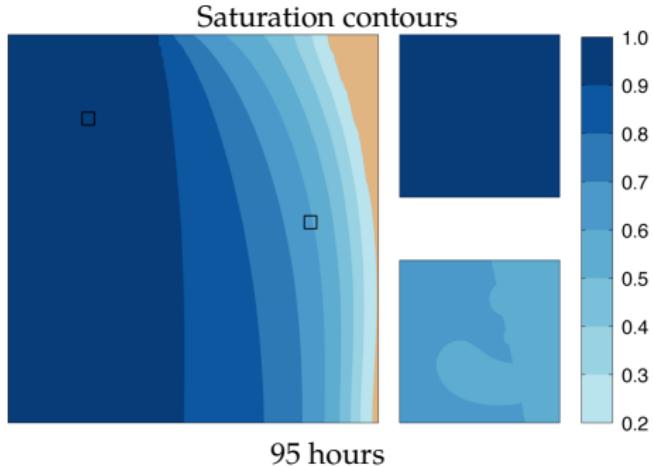
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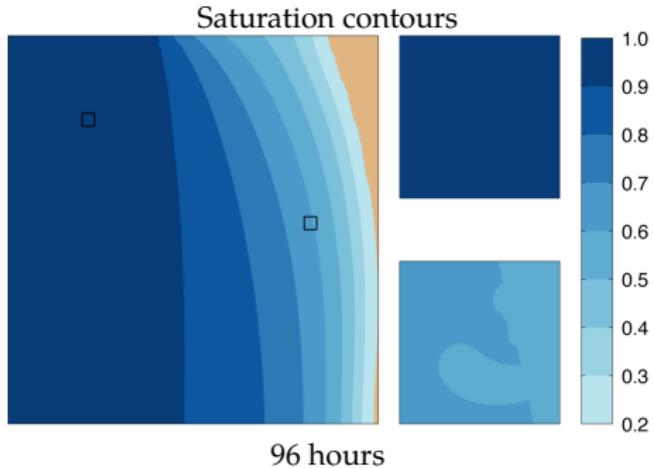
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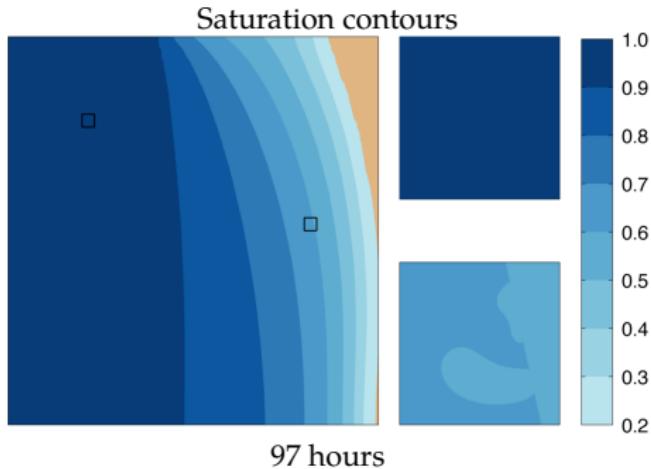
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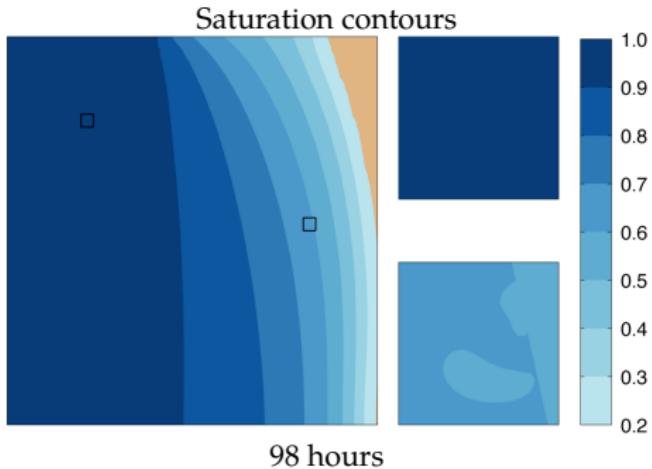
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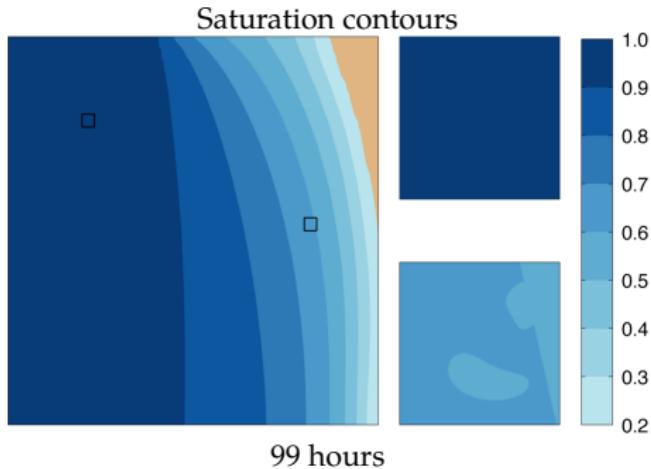
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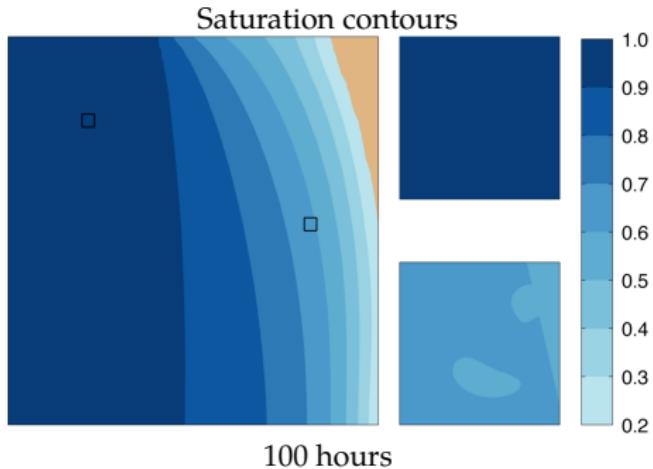
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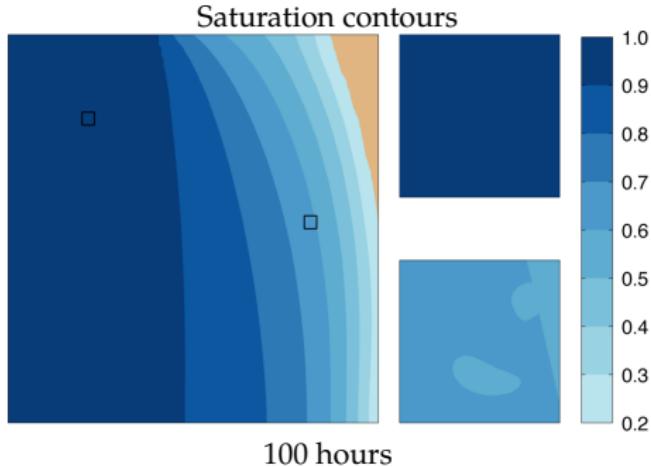
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Summary and conclusions

Pros:

- ✓ Ability to capture fine-scale detail in the full heterogeneous problem
- ✓ Produces good qualitative agreement with fine-scale model
- ✓ Significant reduction in simulation time (compared with fine-scale model)
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Thank you!

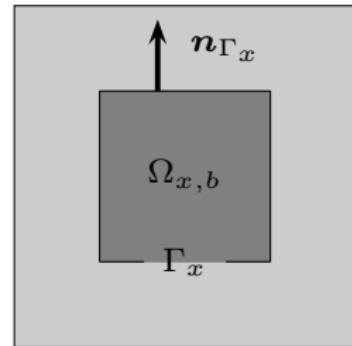
Effective hydraulic conductivity

- $(\mathbf{K}_{\text{eff}})_{*,j}$ is a matrix with j th column equal to

$$(\mathbf{K}_{\text{eff}})_{*,j} = \frac{1}{|\Omega_x|} \int_{\Omega_{x,a}} K_a(h_a) \nabla_y (u + y_2) \, dA$$

where u is a solution of the periodic cell-problem:

$$\begin{cases} \nabla_y \cdot (K_a(h_a) \nabla_y (u + y_2)) = 0 & y \in \Omega_{x,a} \\ K_a(h_a) \nabla_y (u + y_2) \cdot \mathbf{n}_{\Gamma_x} = 0 & y \in \Gamma_x \\ u \text{ is } \Omega_x\text{-periodic} & \end{cases}$$



- Pre-processing step:
 - Compute entries of \mathbf{K}_{eff} using a suitable range of values of h_a
 - Use interpolation to compute \mathbf{K}_{eff} at any given value of h_a

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