Dimension Reduction For Large Systems of ODEs

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Motivation and Objectives

Most dynamic physical processes:

- allow accurate ODE description at the micro-scale (e.g. particle systems, discretization of PDEs);
- have many length scales $\Rightarrow$ system of ODEs is very large;
- allow effective description;
- closed-form effective equations are often unknown.

Our objectives:

- Model effective behavior without solving microscale ODEs
- Develop fast and accurate numerical closures.

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Problem formulation

ODEs of Newtonian particle dynamics (MD, DPD,SPH)

$$\dot{\boldsymbol{q}}_i = \boldsymbol{v}_i, \quad m_i \dot{\boldsymbol{v}}_i = \sum_j \boldsymbol{f}_{ij} + \boldsymbol{f}_i^{(ext)}, \quad i = 1, ...N.$$

N is very large - direct solution is not feasible.
Molecular Dynamics (MD):

$$\boldsymbol{f}_{ij} = \nabla_i \phi_\varepsilon(\boldsymbol{q}_i - \boldsymbol{q}_j),\ \phi_\varepsilon \text{ - potential with support on the order of } \varepsilon$$

Smoothed Particle Hydrodynamics (SPH):

$$\boldsymbol{f}_{ij} = -\left(\frac{P_j}{n_j^2} + \frac{P_i}{n_i^2} + \frac{1}{2}\mu \frac{\boldsymbol{v}_i - \boldsymbol{v}_j}{n_i n_j |\boldsymbol{q}_i - \boldsymbol{q}_j|^2}(\boldsymbol{q}_i - \boldsymbol{q}_j)\cdot\right) \nabla_i w_\varepsilon(\boldsymbol{q}_i - \boldsymbol{q}_j)$$

w_ε is a smooth function with support on the order of ε.
ε is the microscopic length scale.

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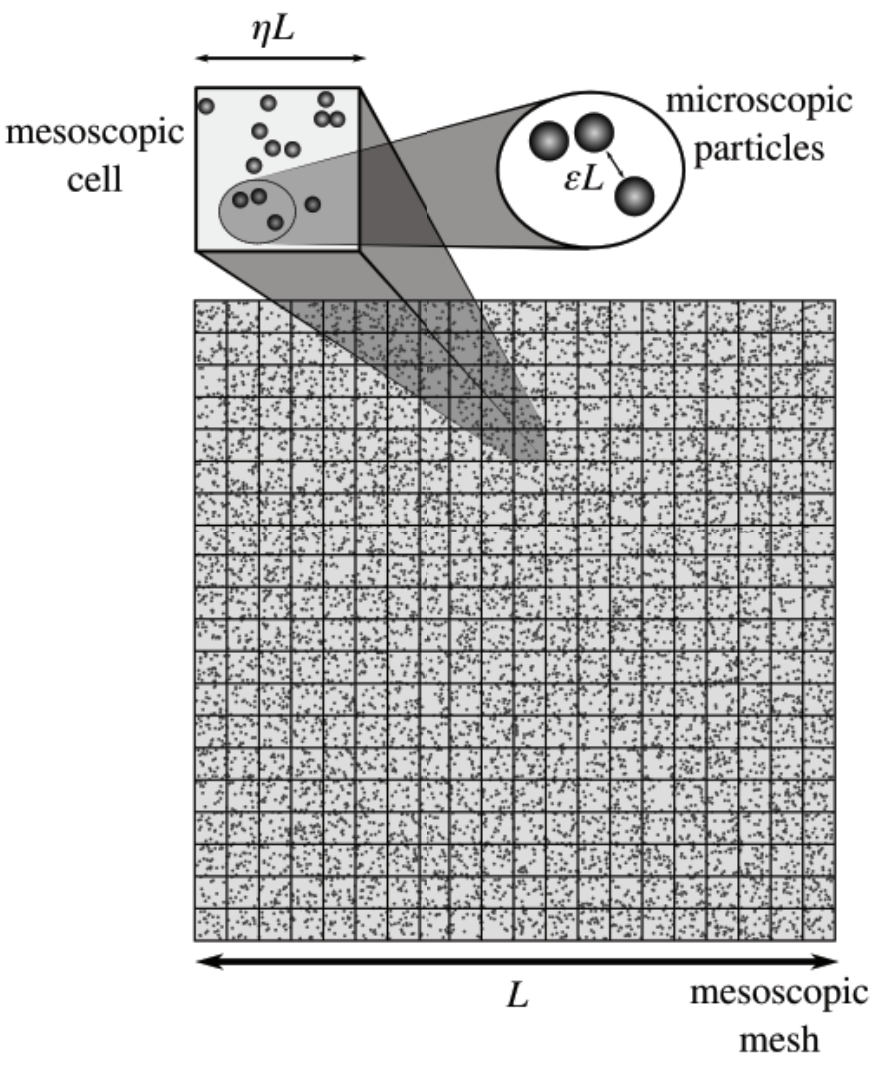
Length scales

ε - microscopic length scale

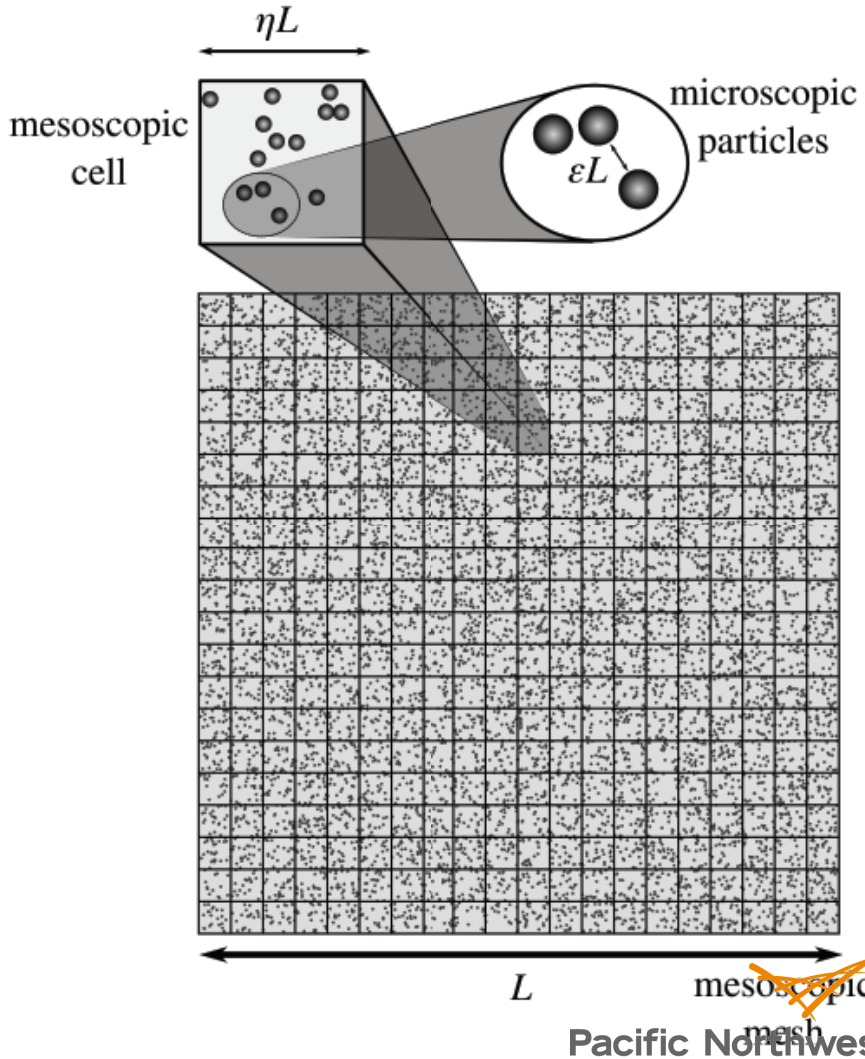
L - macroscopic length scale

Condition for scale separation:
$\varepsilon \ll L$



Dimension Reduction with Numerical Closure (DRNC) Method

1. Choose a spatial resolution scale (meso-scale) η:
$$\varepsilon \ll \eta \ll L.$$
2. Choose primary mesoscale variables (e.g. density and mesoscale velocity).
3. Derive mesoscale balance equations. The mesoscale equations contain fluxes (e.g. stress).



Fluxes are functions of microscale variables.

Approach (continue)

4. **Use a computational closure to calculate the fluxes approximately.**
5. Use deconvolution to approximately reconstruct microscale variables (e.g. particle positions and velocities) from the corresponding mesoscale variables (mesoscale density and velocity).
6. Calculate non-local fluxes.
7. Discretize the mesoscale equations on the mesoscale mesh and integrate with coarse time step.

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Defining mesoscale variables

Mesoscale density,

$$\overline{\rho}^{\eta}(t,\boldsymbol{x}) = \sum_{j=1}^{N} m_j \psi_\eta(\boldsymbol{x} - \boldsymbol{q}_j(t)),$$

Mesoscale momentum,

$$\overline{\rho}^{\eta}\overline{\boldsymbol{v}}^{\eta}(t,\boldsymbol{x}) = \sum_{j=1}^{N} m_j \boldsymbol{v}_j(t) \psi_\eta(\boldsymbol{x} - \boldsymbol{q}_j(t)).$$

Smooth (weighting) function $\psi_\eta(\boldsymbol{x})$ decays fast as $\frac{|\boldsymbol{x}|}{\eta} \to \infty$ and:

$$\int \psi_\eta(\boldsymbol{x}) d\boldsymbol{x} = 1.$$

A possible choice for ψ_η is truncated Gaussian function.

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Integral approximations of the mesoscale variables

Density:

$$\overline{\rho}^{\eta} \approx \int_{\Omega} \rho^{\varepsilon}(\boldsymbol{x}')\psi_{\eta}(\boldsymbol{x}-\boldsymbol{x}')d\boldsymbol{x}',$$

Momentum:

$$\overline{\rho}^{\eta}\overline{\boldsymbol{v}}^{\eta}(\boldsymbol{x}) \approx \int_{\Omega} \rho^{\varepsilon}(\boldsymbol{x}')\boldsymbol{v}(\boldsymbol{x}')\psi_{\eta}(\boldsymbol{x}-\boldsymbol{x}')d\boldsymbol{x}',$$

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Evolution equations for mesocale averages

Conservation of mass: $\partial_t \overline{\rho}^\eta + \mathrm{div}(\overline{\rho}^\eta \overline{\boldsymbol{v}}^\eta) = 0$.
Conservation of the linear momentum:

$$\partial_t(\overline{\rho}^\eta \overline{\boldsymbol{v}}^\eta) + \mathrm{div}(\overline{\rho}^\eta \overline{\boldsymbol{v}}^\eta \otimes \overline{\boldsymbol{v}}^\eta) = \mathrm{div}\boldsymbol{T}^\eta + \sum_{i=1}^N \boldsymbol{f}_i^{(ext)} \psi_\eta(\boldsymbol{x} - \boldsymbol{q}_i)$$

The mesoscale stress $\boldsymbol{T}^\eta = \boldsymbol{T}^\eta_{(c)} + \boldsymbol{T}^\eta_{(int)}$,

- convection component:
  $\boldsymbol{T}^\eta_{(c)}(t, \boldsymbol{x}) = -\sum_{j=1}^N m_j(\overline{\boldsymbol{v}}^\eta(\boldsymbol{x}) - \boldsymbol{v}_j) \otimes (\overline{\boldsymbol{v}}^\eta(\boldsymbol{x}) - \boldsymbol{v}_j)\psi_\eta(\boldsymbol{x} - \boldsymbol{q}_j)$
- interaction component:

$$\boldsymbol{T}^\eta_{(int)}(t, \boldsymbol{x}) =$$
$$\sum_{(j,k)} \boldsymbol{f}_{jk} \otimes (\boldsymbol{q}_k - \boldsymbol{q}_j) \int_0^1 \psi_\eta\left(s(\boldsymbol{x} - \boldsymbol{q}_k) + (1-s)(\boldsymbol{x} - \boldsymbol{q}_j)\right) ds.$$

Murdoch and Bedeaux (1994)

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Reconstruction of a microscale variable f

Mesoscale variable $\overline{f}$ is defined by the convolution operator, R_η:

$$\overline{f}(\boldsymbol{x}) = R_\eta[f](\boldsymbol{x}) = \int \psi_\eta(\boldsymbol{x} - \boldsymbol{y}) f(\boldsymbol{y}) d\boldsymbol{y},$$

R_η is compact $\Rightarrow R_\eta^{-1}$ is unbounded.

Deconvolution (recovering f from $\overline{f}$) is an unstable ill-posed problem.

Deconvolution is the most studied ill-posed problem. Many regularization methods are available in the literature: Tikhonov regularization, iterative methods, reproducing kernel methods, maximum entropy method, dynamical system approach etc.

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Regularized iterative deconvolution[1]

$$f(\boldsymbol{x}) \approx f^{(n)}(\boldsymbol{x}) = \sum_{k=0}^{n} (I - R_\eta)^k [\overline{f}], \quad f_0 = \overline{f},$$

where,

$$R_\eta[\overline{f}](\boldsymbol{x}) = \int \psi_\eta(\boldsymbol{x} - \boldsymbol{y}) \overline{f}(\boldsymbol{y}) d\boldsymbol{y}.$$

and

$$I[\overline{f}](\boldsymbol{x}) = \overline{f}(\boldsymbol{x})$$

$f^{(n)}$ is used to calculate $\boldsymbol{T}^\eta$ in the meso-scale momentum conservation equation.

[1] M. M. Lavrentev, V. Romanov, and S. Shishatskij, Ill-posed problems of mathematical physics and analysis, American Mathematical Society, Providence, RI, 1980.

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Example 1: Poiseuille flow

Smoothed Particle Hydrodynamics (SPH) ODEs:

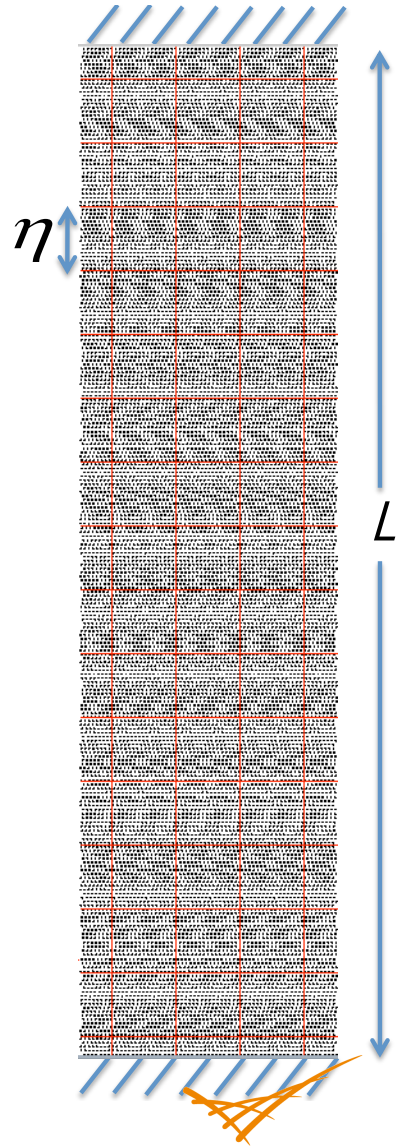
$$\dot{\boldsymbol{q}}_i = \boldsymbol{v}_i, \qquad m_i \dot{\boldsymbol{v}}_i = \sum_j \boldsymbol{f}_{ij} + \boldsymbol{f}_i^{(ext)}.$$

$$i = 1, ..., 32768.$$

$$\boldsymbol{f}_{ij} = -\left(\frac{P_j}{n_j^2} + \frac{P_i}{n_i^2} + \frac{4\mu_i\mu_j}{\mu_i+\mu_j} \frac{\boldsymbol{v}_i - \boldsymbol{v}_j}{n_i n_j |\boldsymbol{q}_i - \boldsymbol{q}_j|^2} (\boldsymbol{q}_i - \boldsymbol{q}_j) \right)$$

$$\cdot \nabla_i w_\varepsilon(\boldsymbol{q}_i - \boldsymbol{q}_j)$$

$\overline{\rho}^\eta = const$, $\overline{\boldsymbol{v}}^\eta = ?$



If $\mu_i = \mu$, then SPH particles behave effectively as a Newtonian fluid with viscosity μ.

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Effect of the mesoscale length on the accuracy of DRNC method

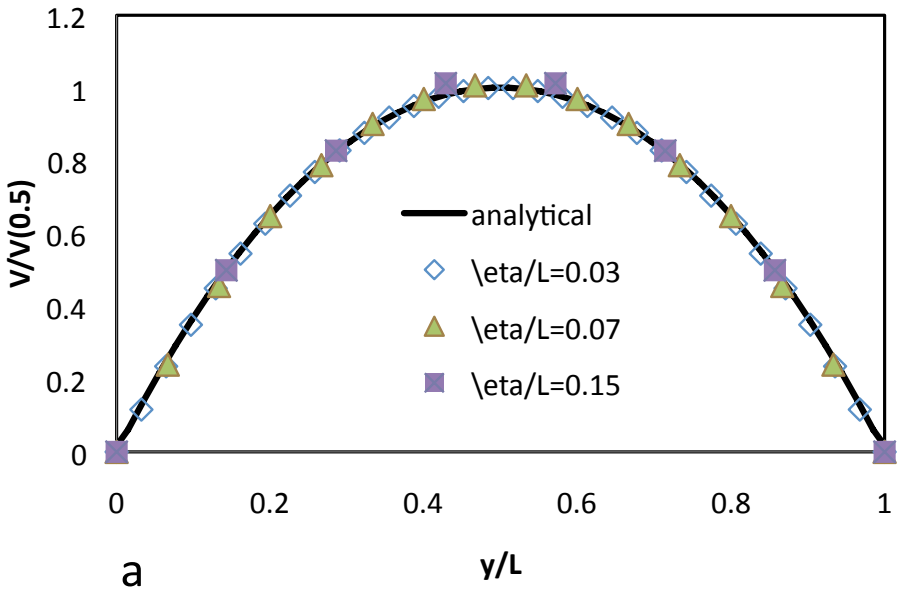

Figure: $\overline{\boldsymbol{v}}^{\eta}$ vs y for different η.

Closure is based on the zero-order deconvolution.

$\overline{\boldsymbol{v}}^{\eta}$ is accurate as long as $\eta/L < 0.1$

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Example 2: Two-phase layered flow

- Fluid is non-newtonian on the scale η
- No effective closed-form description exist

SPH ODEs:

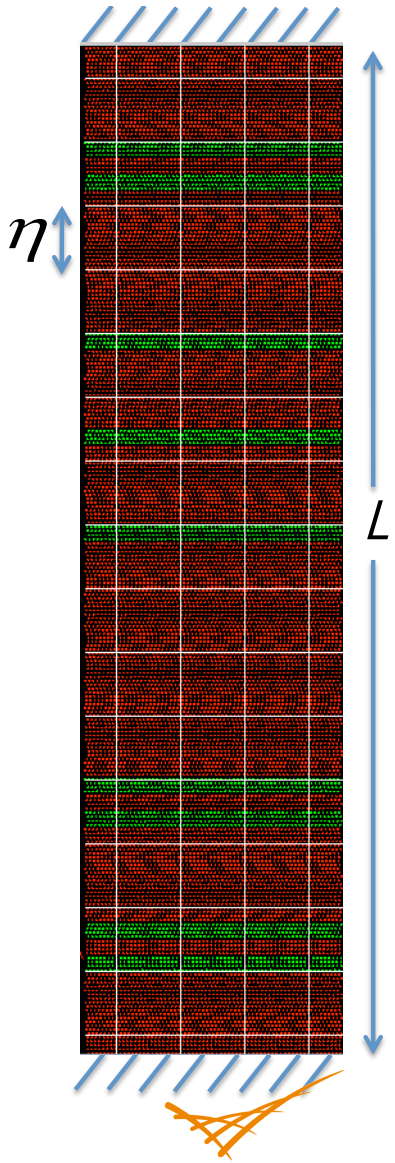
$$\dot{\boldsymbol{q}}_i = \boldsymbol{v}_i, \qquad m_i \dot{\boldsymbol{v}}_i = \sum_j \boldsymbol{f}_{ij} + \boldsymbol{f}_i^{(ext)}, \; N = 32768$$

$$\boldsymbol{f}_{ij} = -\left(\frac{P_j}{n_j^2} + \frac{P_i}{n_i^2} + \frac{4\mu_i\mu_j}{\mu_i+\mu_j} \frac{\boldsymbol{v}_i - \boldsymbol{v}_j}{n_i n_j |\boldsymbol{q}_i - \boldsymbol{q}_j|^2} (\boldsymbol{q}_i - \boldsymbol{q}_j) \right)$$

$$\cdot \nabla_i w_\varepsilon (\boldsymbol{q}_i - \boldsymbol{q}_j).$$

$$P_i = \frac{k_B T n_i}{1 - a n_i} - b n_i^2 \qquad \text{van der Waals EOS}$$

$\overline{\rho}^\eta =?$ and $\overline{\boldsymbol{v}}^\eta =?$



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Example 2: Two-phase layered flow

Comparison of coarse and direct solutions of the SPH equations at different dimensionless times

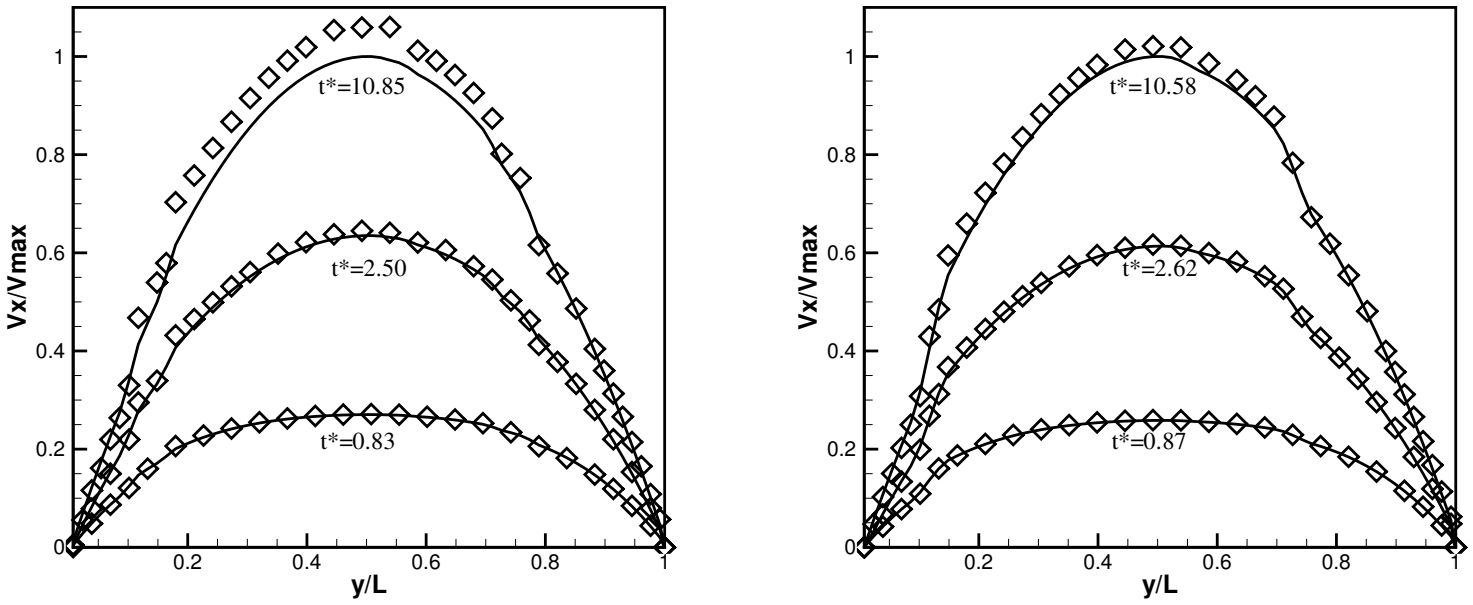

Figure: The width of the layers d is: a) $d = 0.75\eta$; and b) $d = 2\eta$

The second-order deconvolution is used

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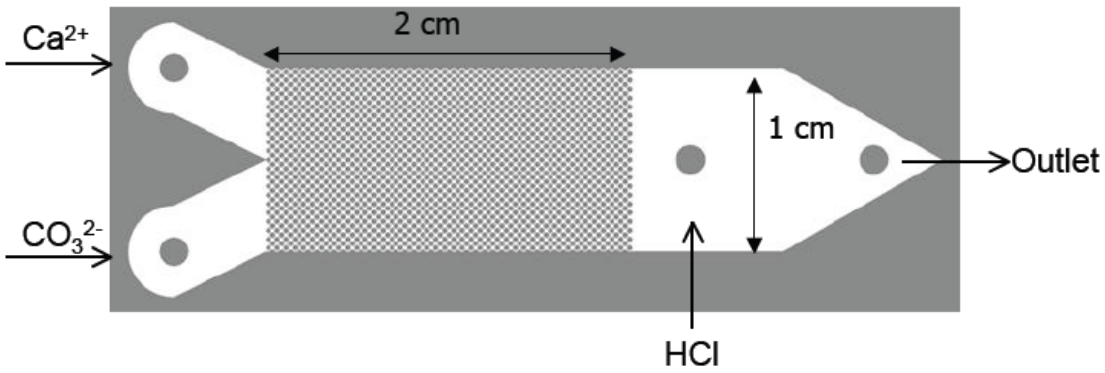
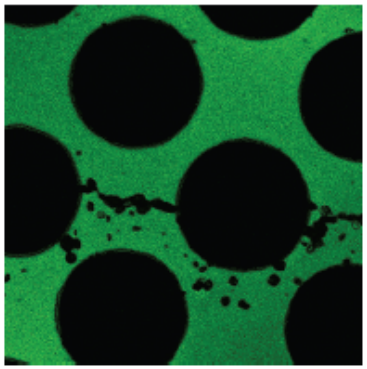
Example 3: Reactive transport and mineral precipitation in porous media

Laboratory experiment. Parallel injection of two solutions containing Ca^{2+} and CO_3^{2-}. Mineral layer of $CaCO_3$ is formed as result of reaction $Ca^{2+} + CO_3^{2-} \rightleftharpoons CaCO_3(s)$. Zhang et al., ES&T, 2011

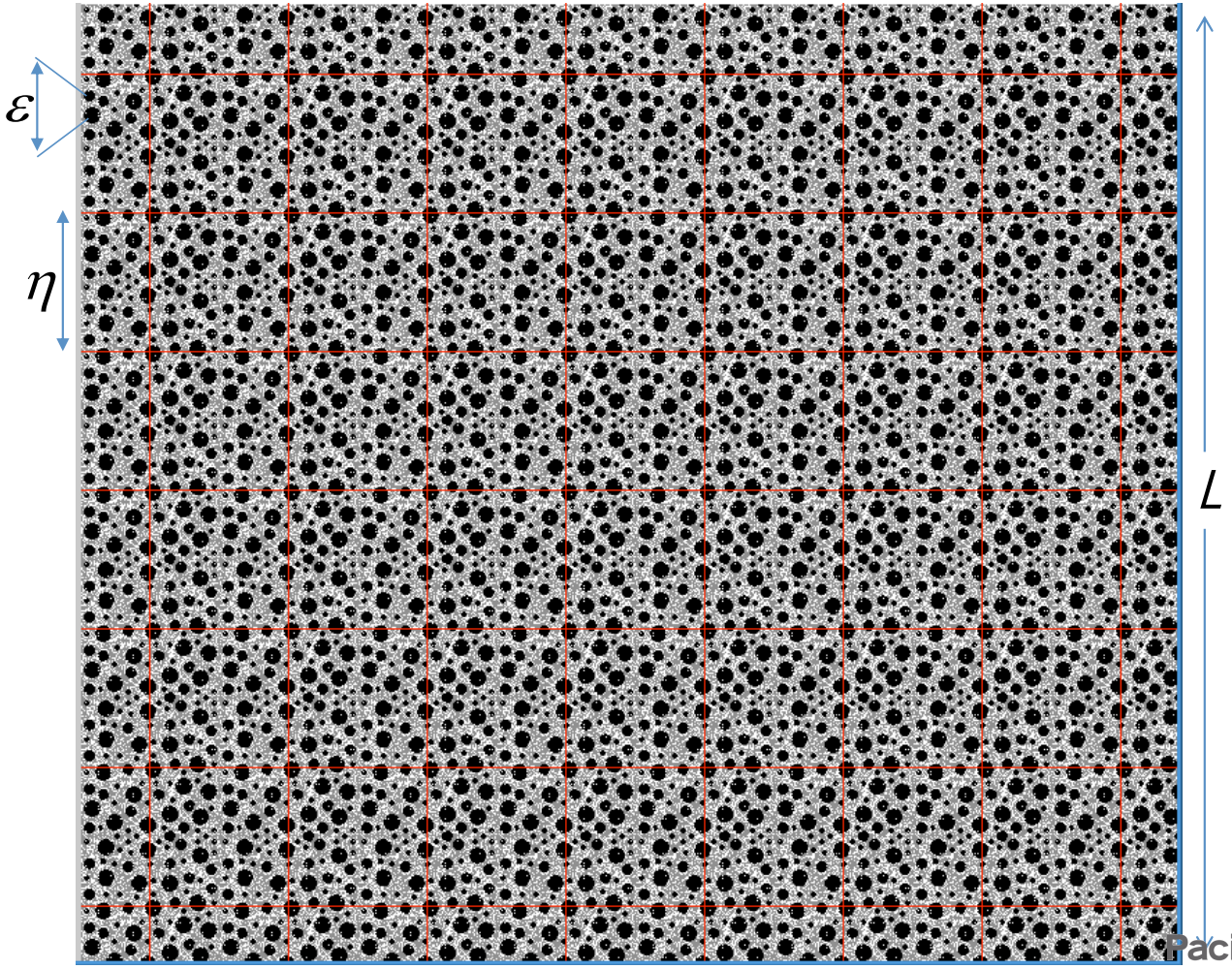




- Existing closed-form effective models are not satisfactory (*WRR*2008, *JCH*2010)
- Microscale (pore-scale) description is very expensive (number of discretization points $\approx$ 24,000,000)

Length scales

Micro-scale $\varepsilon = 1 \times 10^{-5}$ m; meso-scale $\eta = 5 \times 10^{-3}$ m; and macro-scale $L = 4 \times 10^{-2}$m.



Microscale SPH ODEs equations

Momentum conservation equations:

$$\dot{\boldsymbol{q}}_i = \boldsymbol{v}_i, \qquad m_i \dot{\boldsymbol{v}}_i = \sum_j \boldsymbol{f}_{ij} + \boldsymbol{f}_i^{(ext)}, \qquad i \in fluid.$$

Advection-Diffusion-Reaction equation:

$$\frac{dI}{dt} = \sum_{j \in \text{fluid}} p_{ij} - R_i \qquad I = [Ca^{2+}], [CO_2^{3-}]$$

Surface evolution/mineral precipitation:

$$\frac{d(m_{CaCO_3})_i}{dt} = m_0 R_i$$

Reaction term $R_i = k \left(\frac{[Ca^{2+}]_i [CO^{3-}]_i}{K_{sp}} - 1 \right) \sum_j \delta_{ij}$

$$p_{ij} = \frac{1}{m_i} \frac{D^I (m_i n_i + m_j n_j)(I_i - I_j)}{n_i n_j (\mathbf{r}_i - \mathbf{r}_j)^2} (\mathbf{r}_i - \mathbf{r}_j) \cdot \nabla_i W (\mathbf{r}_i - \mathbf{r}_j, h)$$

[18] Tartakovsky et al., JCP 2006

Evolution equations for meso-scale variables

Equations for $\overline{\rho}^\eta$ and $\overline{\boldsymbol{v}}^\eta$ are defined as before.

Meso-scale concentration I, I=Ca^{2+}, CO_3^{2-} and $CaCO_{3(s)}$:

$$\overline{I}^\eta(t,\boldsymbol{x}) = \sum_{j=1}^N \frac{1}{n_j} I_i \psi_\eta(\boldsymbol{x} - \boldsymbol{q}_j(t)),$$

Meso-scale evolution (Advection-Dispersion) equation:

$$\partial_t(\overline{I}^\eta) + \mathrm{div}(\overline{\boldsymbol{v}}^\eta \overline{I}^\eta) = \mathrm{div}\boldsymbol{J}^\eta - \sum_{i=1}^N R_i \psi_\eta(\boldsymbol{x} - \boldsymbol{q}_i),\ \mathrm{I}{=}Ca^{2+},\ CO_3^{2-}$$

The meso-scale flux $\boldsymbol{J}^\eta = \boldsymbol{J}^\eta_{(ad)} + \boldsymbol{J}^\eta_{(dif)}$,

- advection component:
  $\boldsymbol{J}^\eta_{(ad)}(t,\boldsymbol{x}) = -\sum_{j=1}^N m_j(\overline{\boldsymbol{v}}^\eta(\boldsymbol{x}) - \boldsymbol{v}_j)(\overline{I}^\eta(\boldsymbol{x}) - I_j)\psi_\eta(\boldsymbol{x} - \boldsymbol{q}_j)$
- diffusion component:

$$\boldsymbol{J}^\eta_{(dif)}(t,\boldsymbol{x}) = \sum_{(j,k)} p_{jk}(\boldsymbol{q}_k - \boldsymbol{q}_j) \int_0^1 \psi_\eta\left(s(\boldsymbol{x} - \boldsymbol{q}_k) + (1-s)(\boldsymbol{x} - \boldsymbol{q}_j)\right) ds.$$

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Evolution equations for meso-scale variables

Evolution equation for meso-scale calcite concentration:

$$\partial_t(\overline{I}^\eta) = \sum_{i=1}^{N} R_i \psi_\eta(\boldsymbol{x} - \boldsymbol{q}_i), \text{ I=CaCO}_{3(s)}$$

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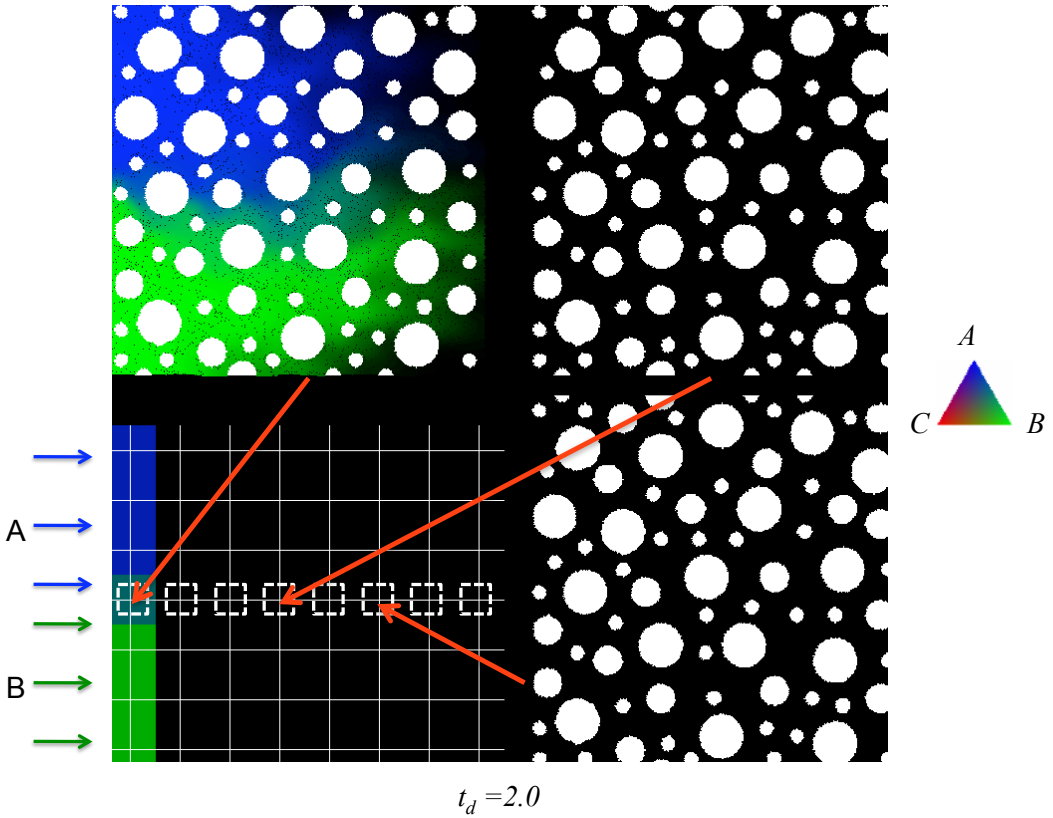
Results: Coarse solution with numerical closure



Parallel injection of two solutions containing A=Ca^{2+} and B=CO_3^{2-}. Mineral layer of C=$CaCO_3$ is formed as result of reaction $Ca^{2+} + CO_3^{2-} \rightleftharpoons CaCO_3(s)$.

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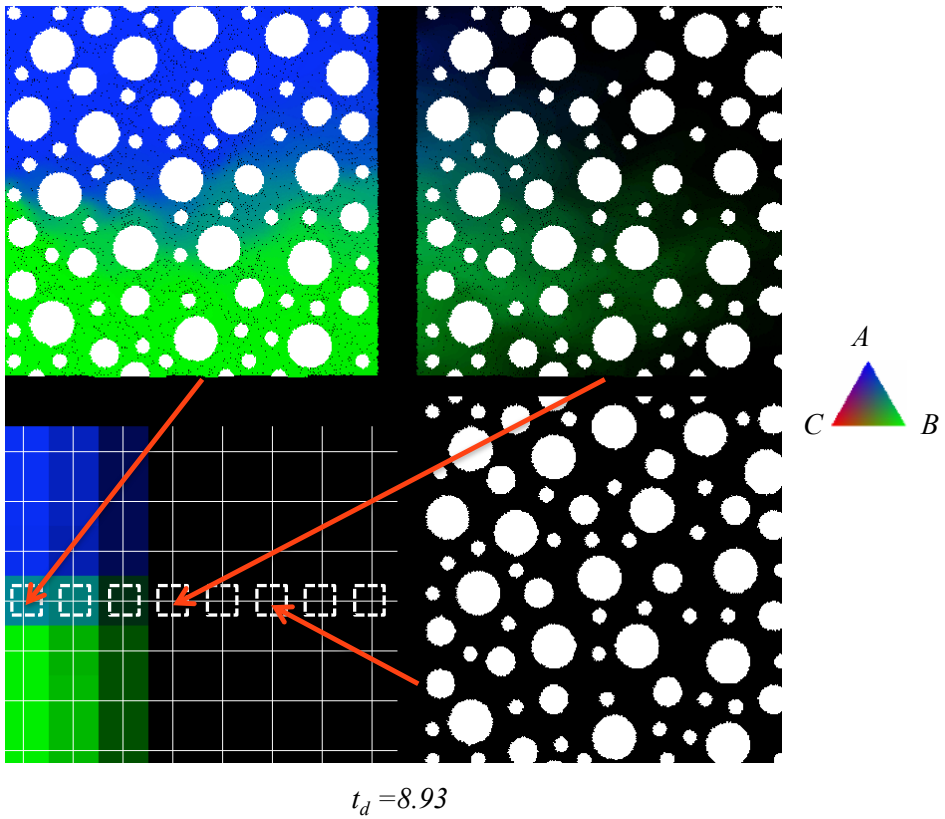

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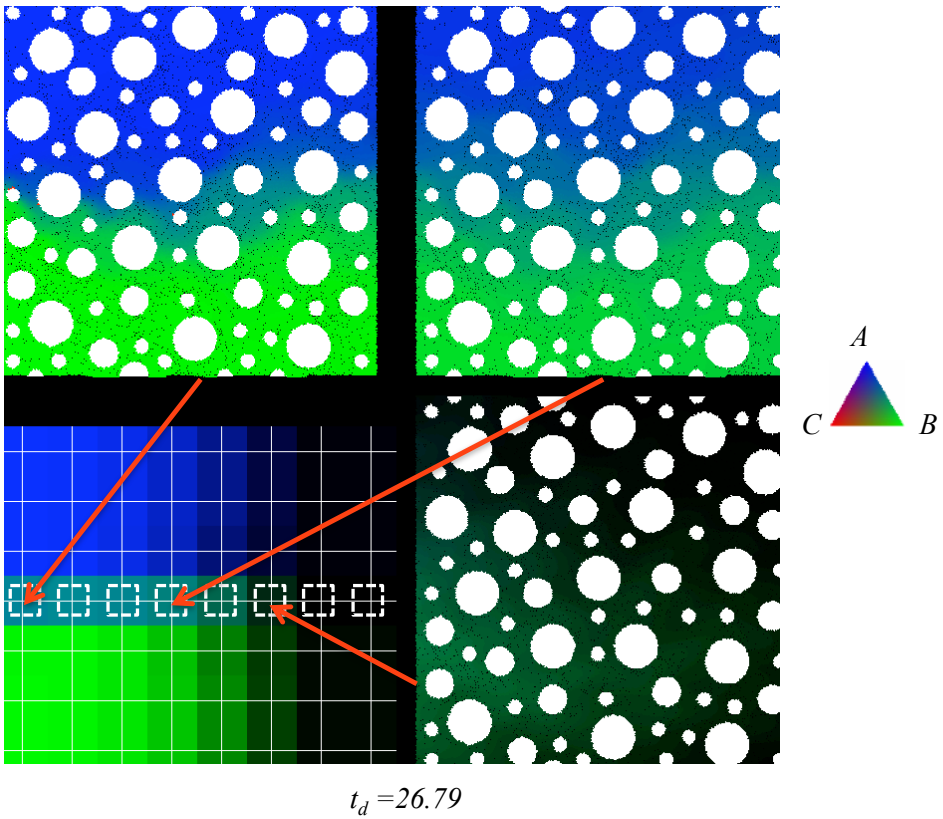

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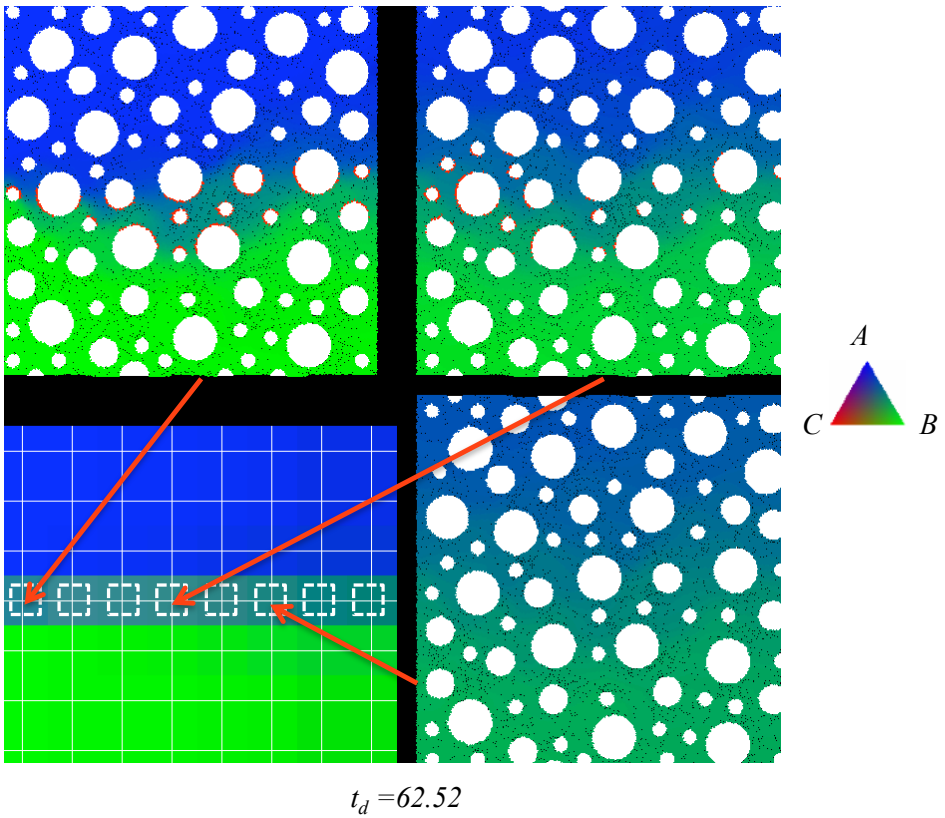

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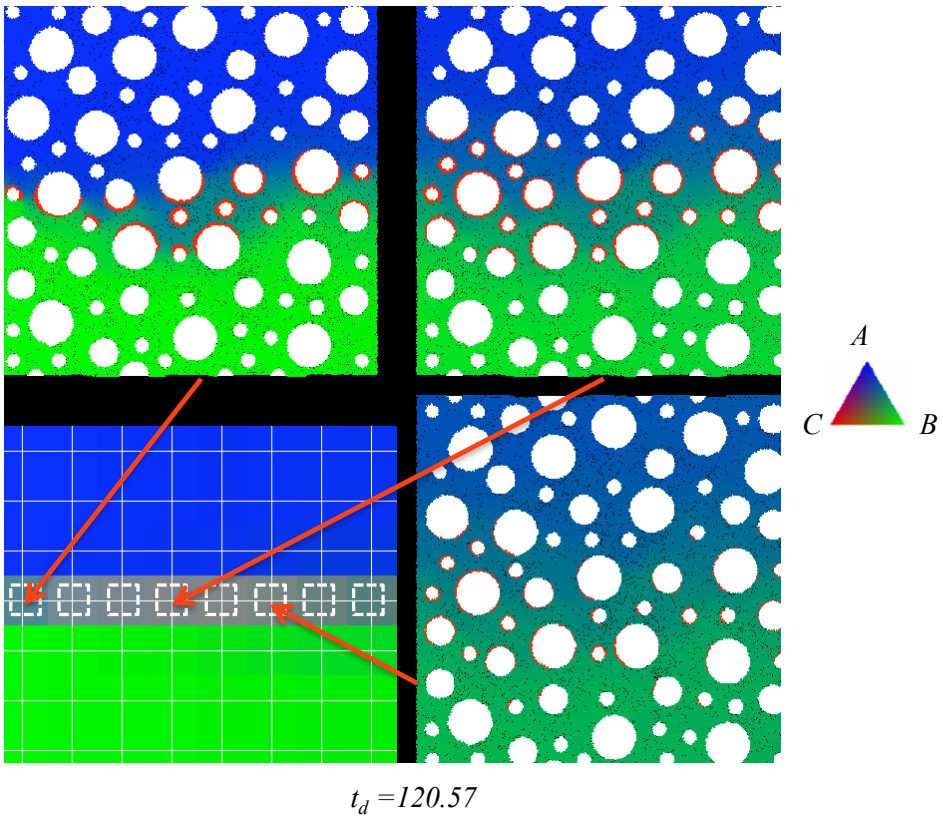

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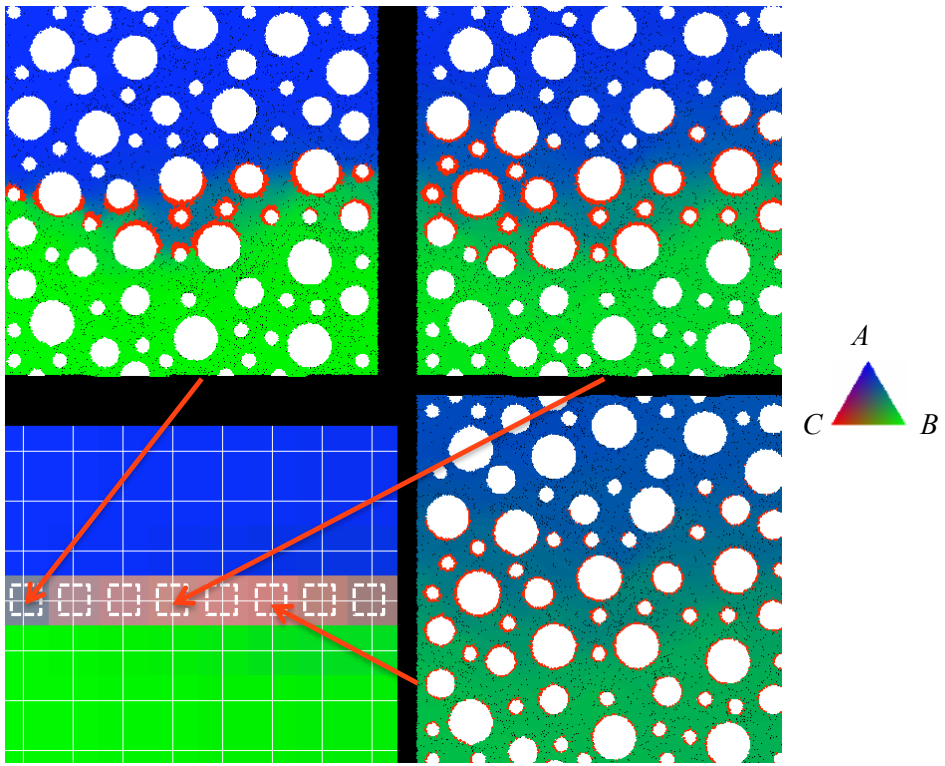

t_d =200.96

Parallel injection of two solutions containing A=Ca^{2+} and B=CO_3^{2-}. Mineral layer of C=$CaCO_3$ is formed as result of reaction $Ca^{2+} + CO_3^{2-} \rightleftharpoons CaCO_3(s)$.

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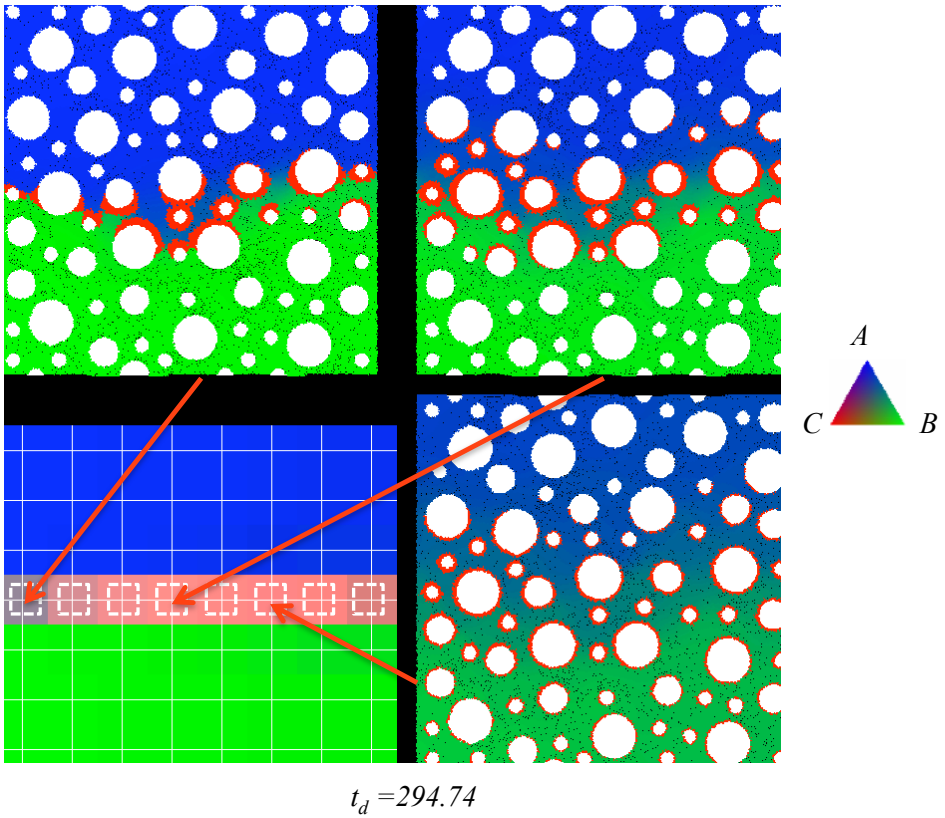

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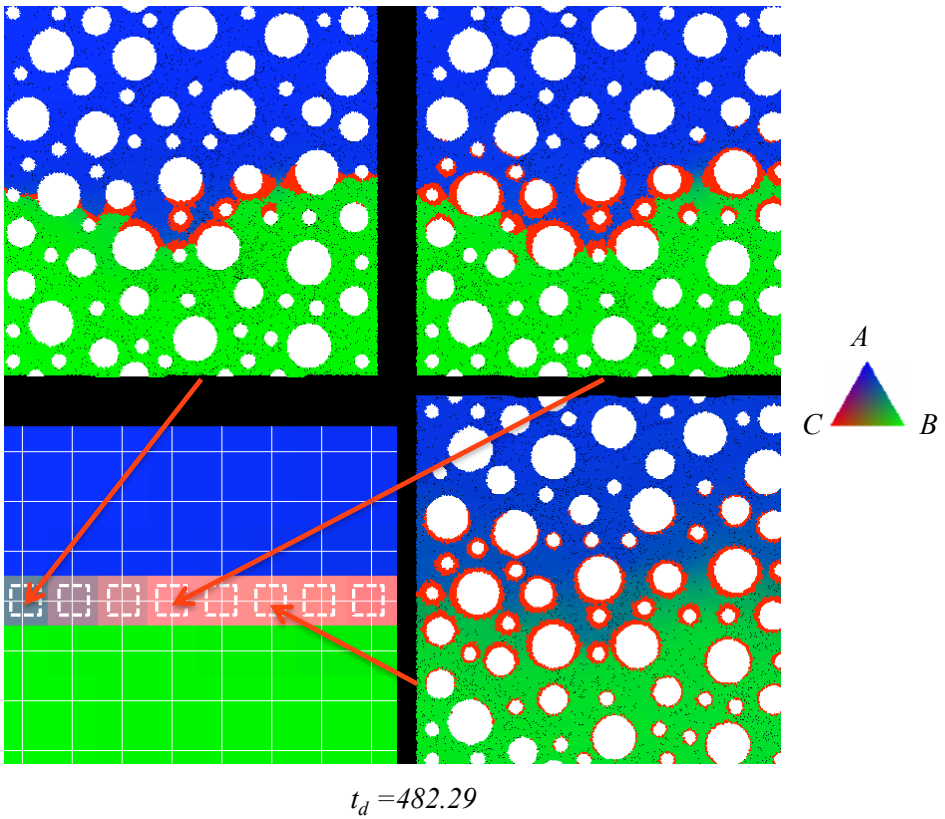

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Comparison of reconstructed microscale variables with the exact solution.

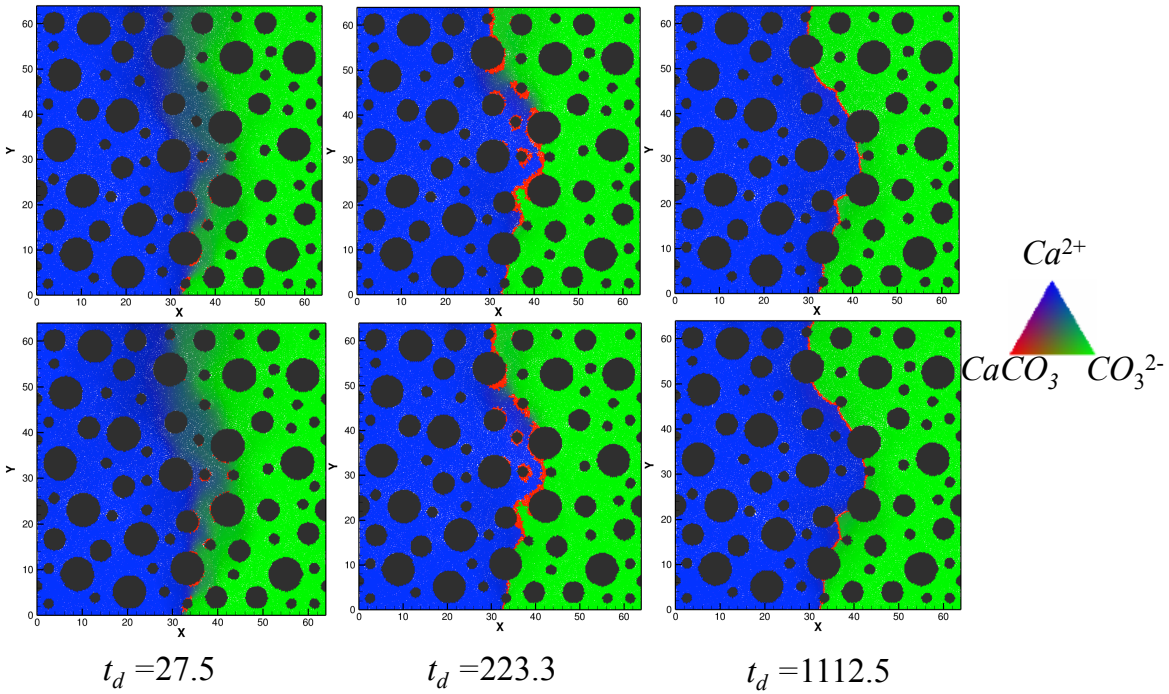

Figure: The first row - direct solution. The second row - reconstructed variables.

Conclusions

- We proposed a new dimension reduction method:
- Other methods based on numerical closures:
  - Equation Free Method of Yannis Kevrekidis (Princeton)
  - Heterogeneous Multiscale Method of Weinan E (Princeton)
- Advantages of DRNC method:
  - Meso-scale equations help to chose an optimal deconvolution
  - Doesn't require a micro-scale solver
- For highly heterogeneous systems we currently use reconstruction based on short bursts of the corresponding micro-scale solver, similar to EFM.

References: Tartakovsky et al., JCP 2011; Tartakovsky and Scheibe, AWR 2011.

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