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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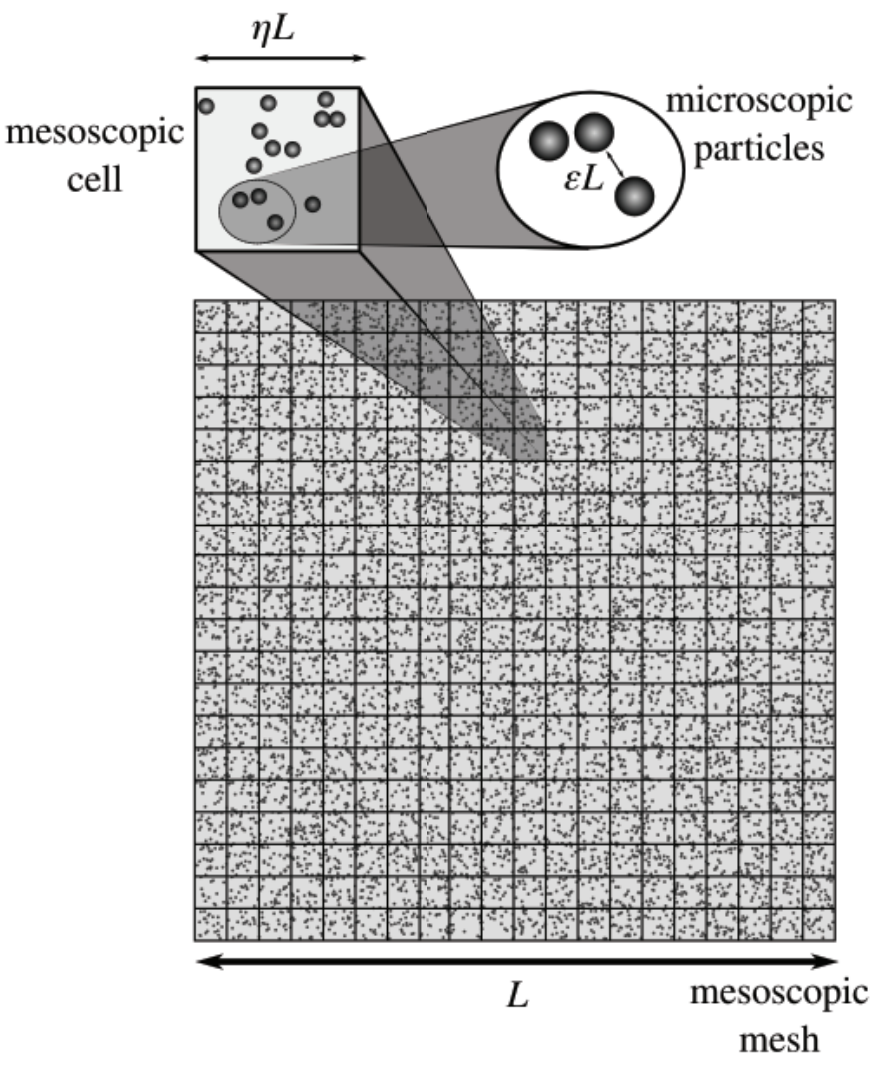
Length scales

ε - microscopic length scale

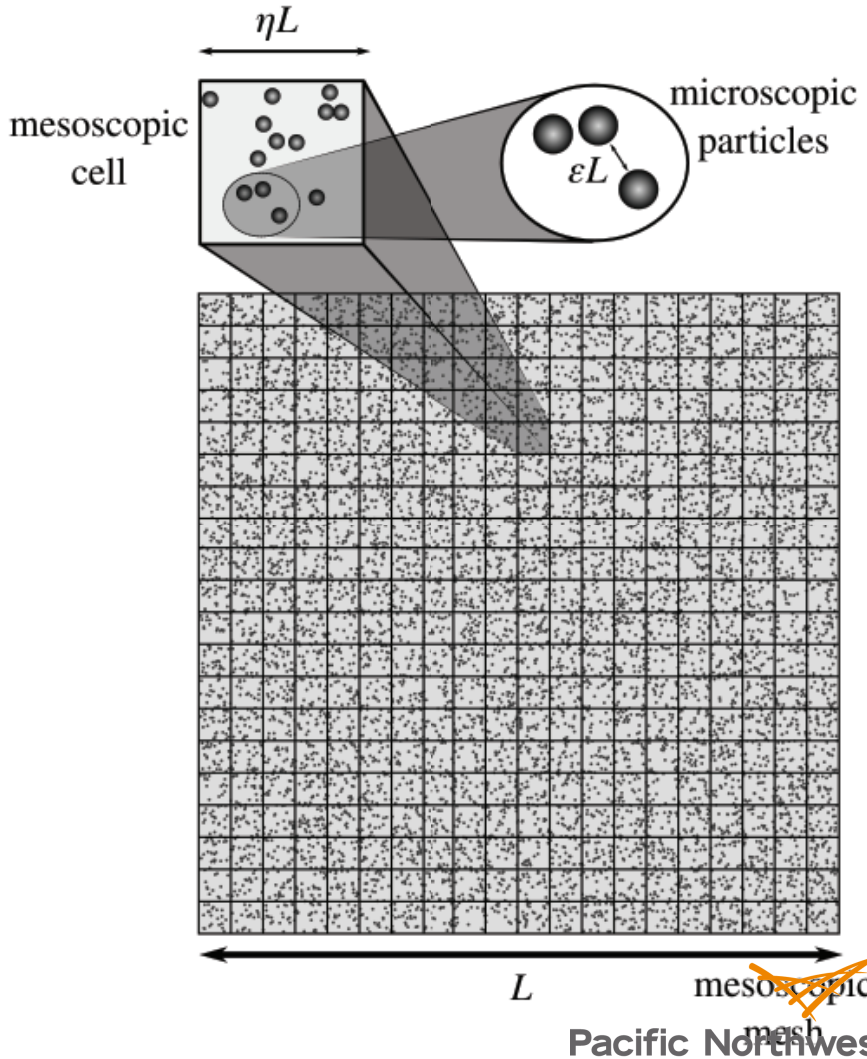
L - macroscopic length scale

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:

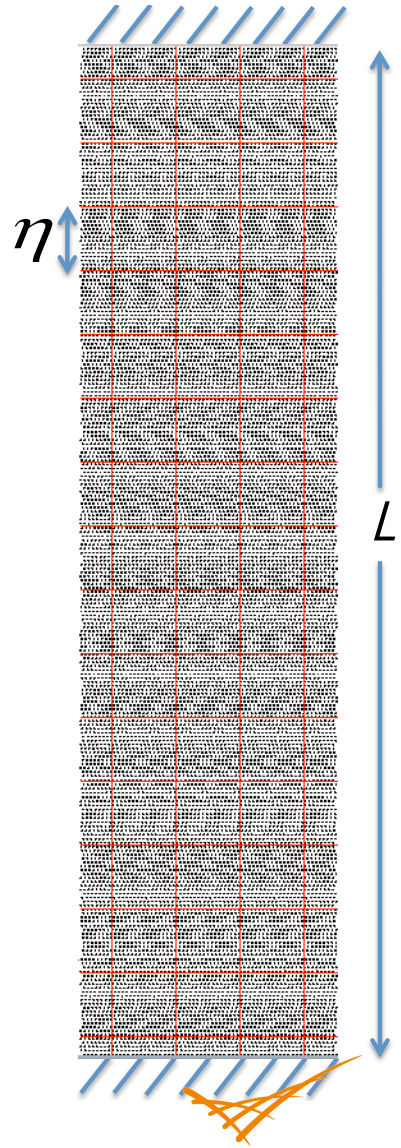
$$\dot{\boldsymbol{q}}_i = \boldsymbol{v}_i, \qquad m_i \dot{\boldsymbol{v}}_i = \sum_j \boldsymbol{f}_{ij} + \boldsymbol{f}_i^{(ext)}.$$

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

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

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

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



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

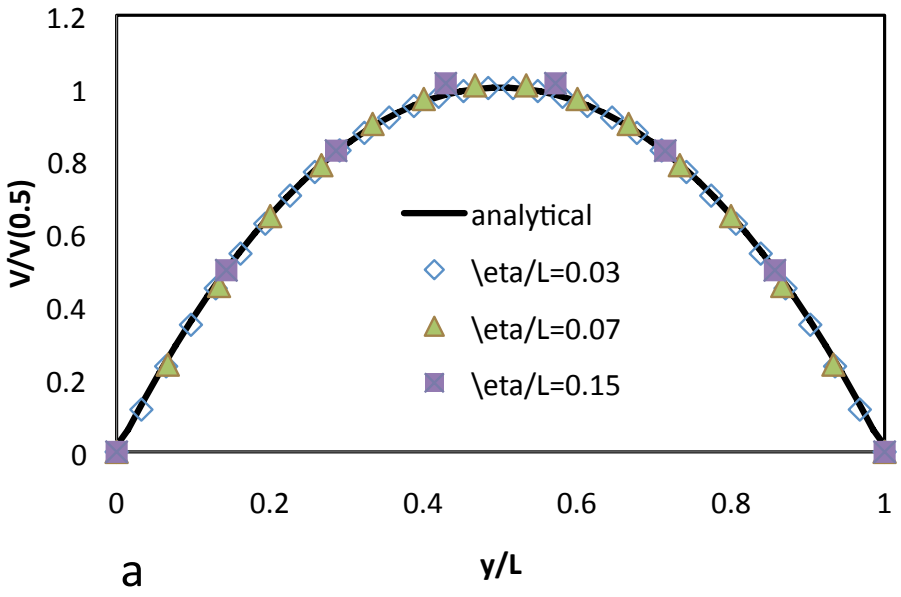

Figure: $\overline{\boldsymbol{v}}^{\eta}$ vs y for different η.

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:

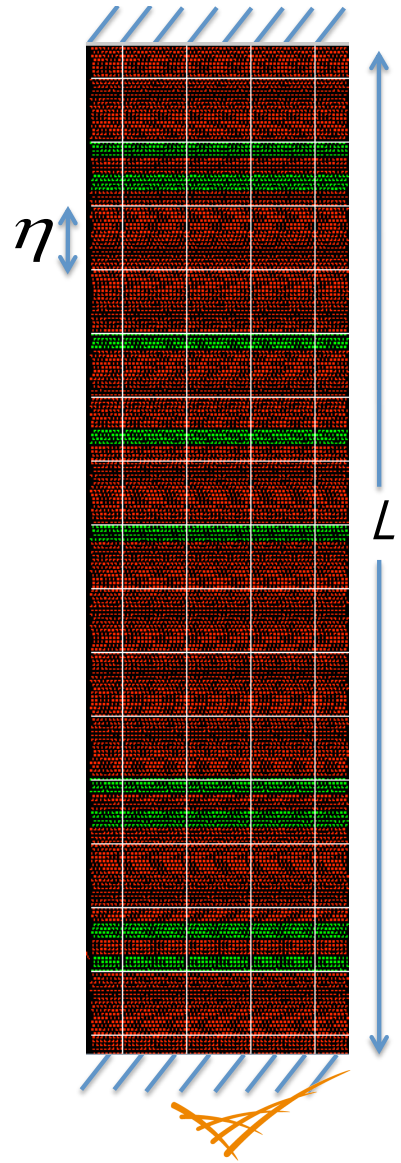
$$\dot{\boldsymbol{q}}_i = \boldsymbol{v}_i, \qquad m_i \dot{\boldsymbol{v}}_i = \sum_j \boldsymbol{f}_{ij} + \boldsymbol{f}_i^{(ext)}, \; N = 32768$$

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

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

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

$\overline{\rho}^\eta =?$ 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

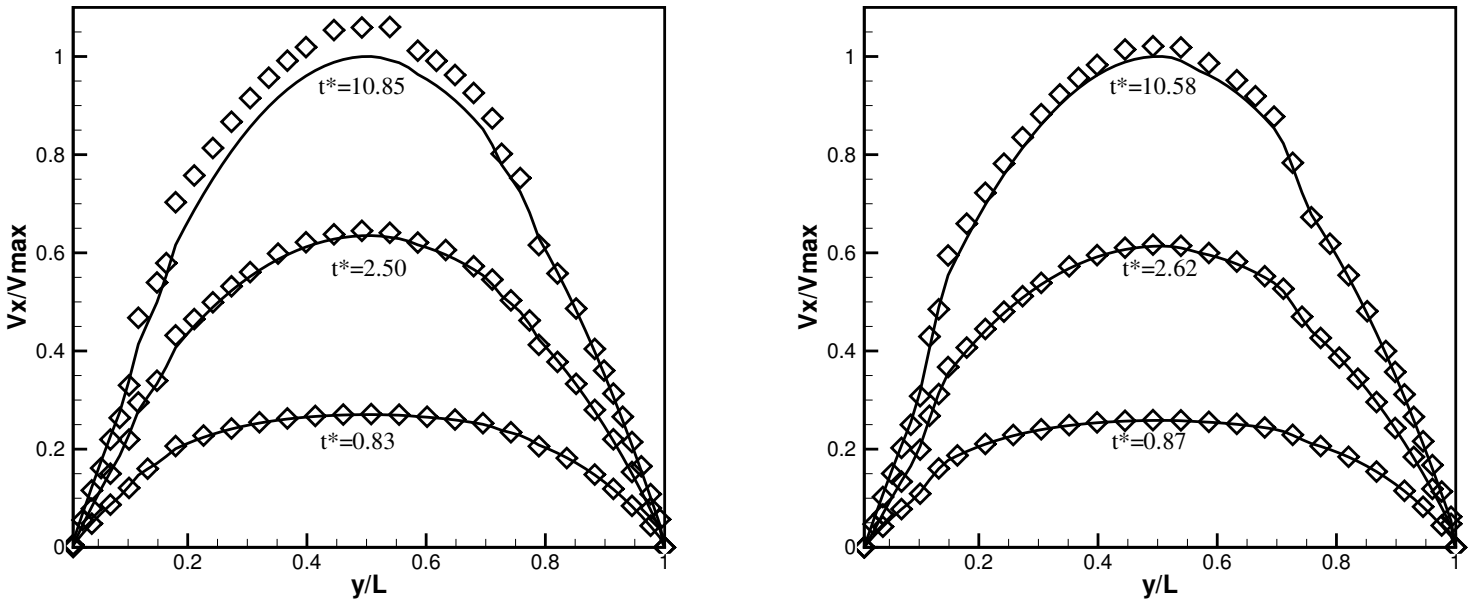

Figure: The width of the layers d is: a) $d = 0.75\eta$; and b) $d = 2\eta$

The second-order deconvolution is used

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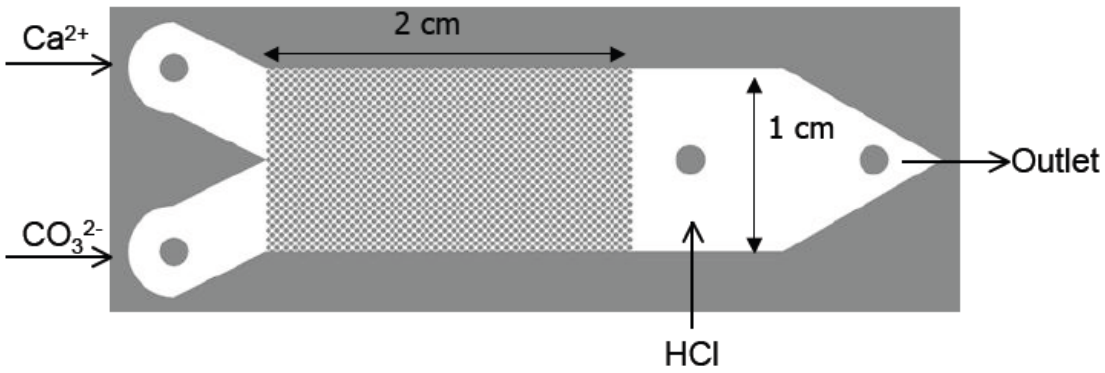
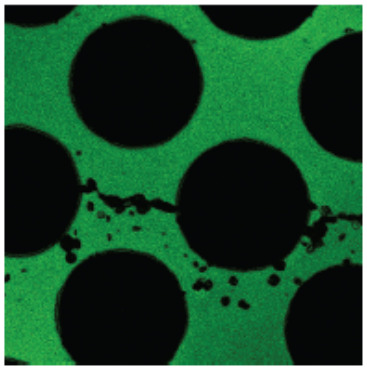
Example 3: Reactive transport and mineral precipitation in porous media

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 $Ca^{2+} + CO_3^{2-} \rightleftharpoons CaCO_3(s)$.

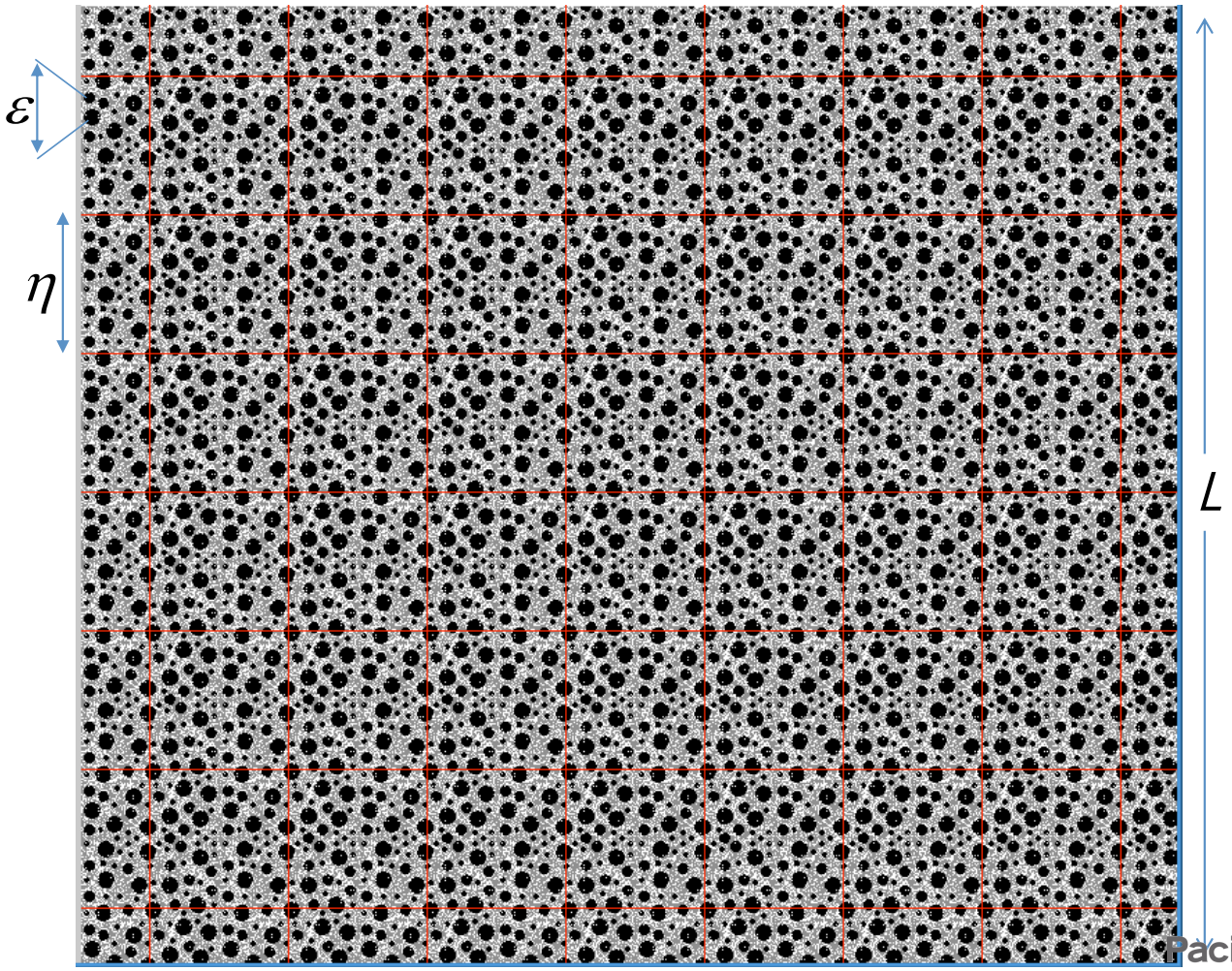




- Existing closed-form effective models are not satisfactory (*WRR*2008, *JCH*2010)
- Microscale (pore-scale) description is very expensive (number of discretization points $\approx$ 24,000,000)

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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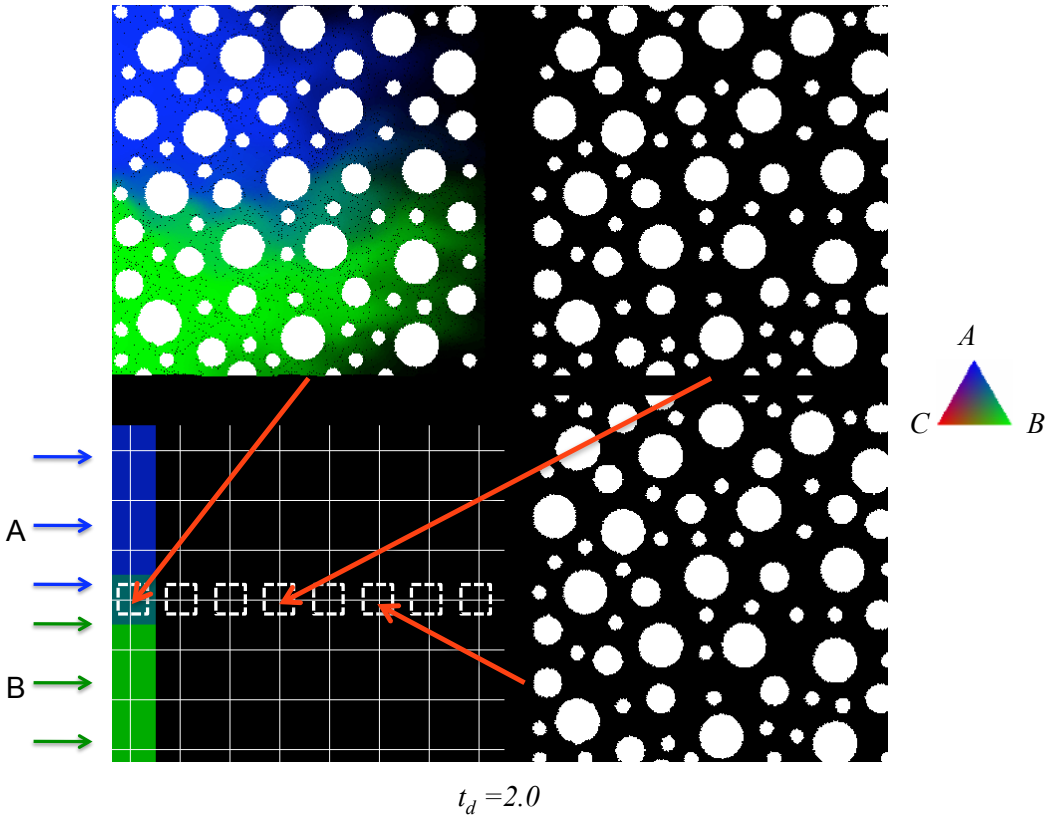
Results: Coarse solution with numerical closure



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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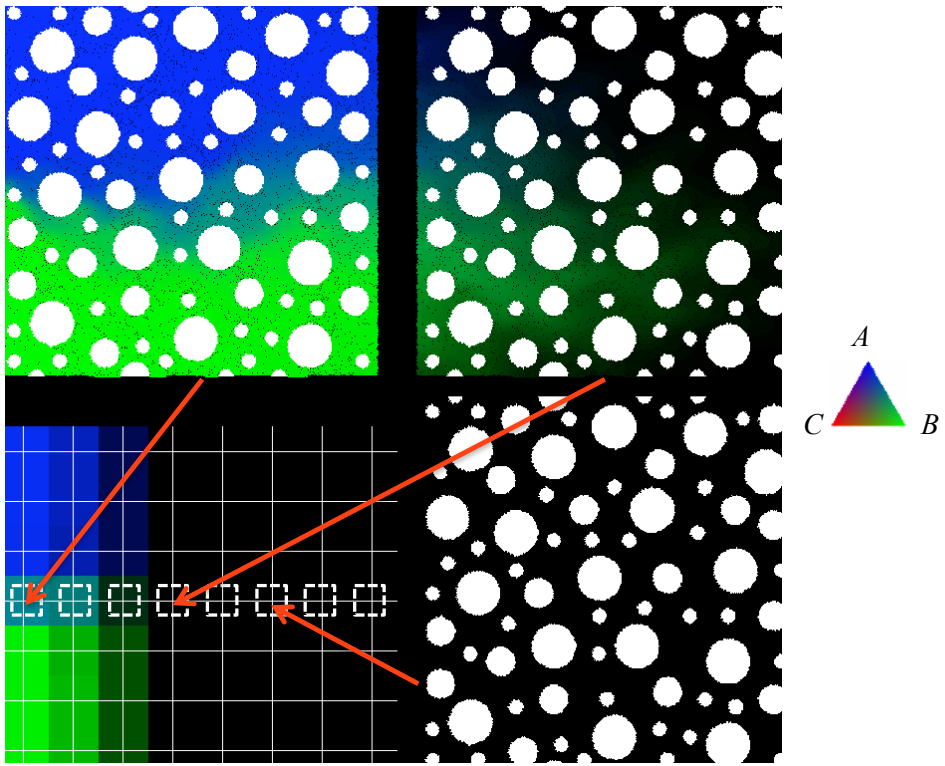

$t_d = 8.93$

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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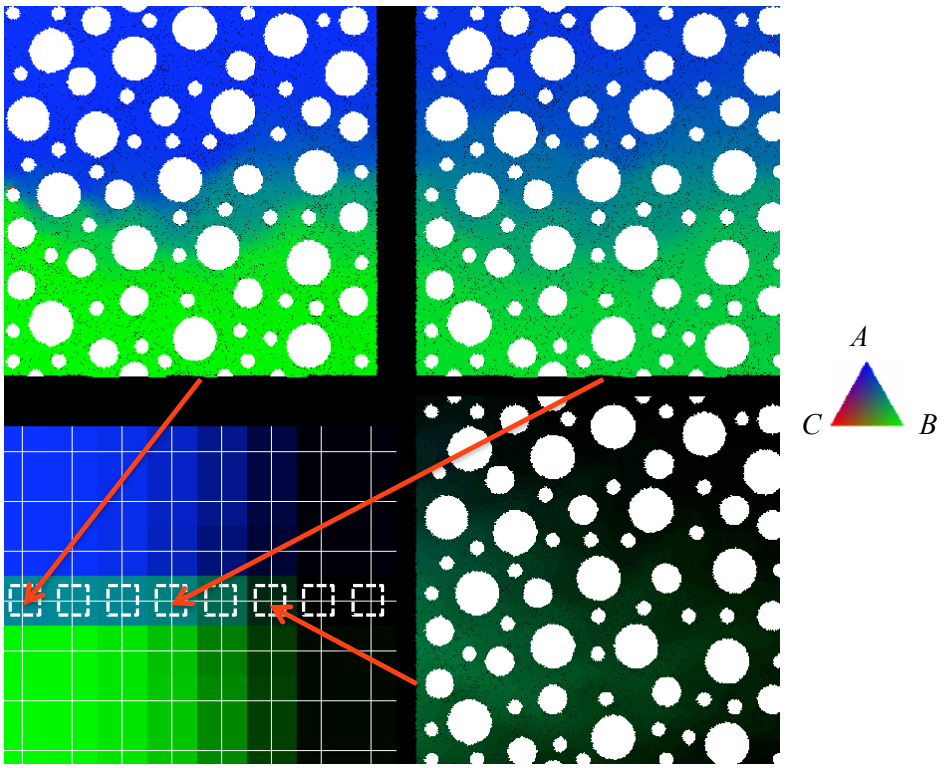
Results: Coarse solution with numerical closure



$t_d = 26.79$

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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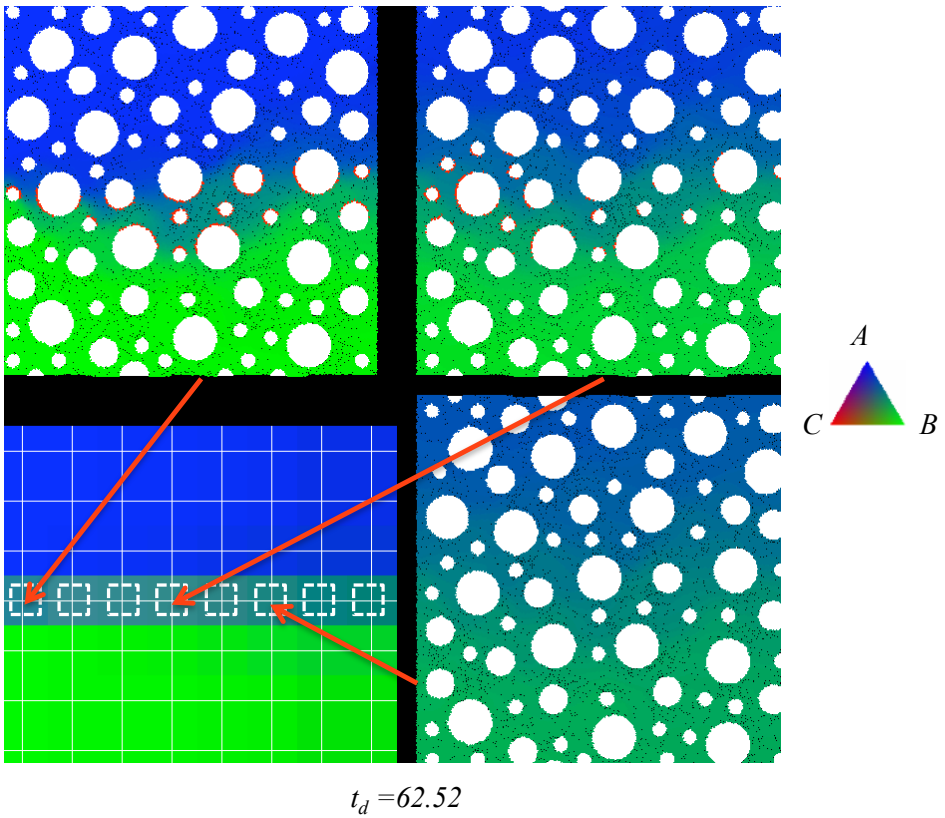
Results: Coarse solution with numerical closure



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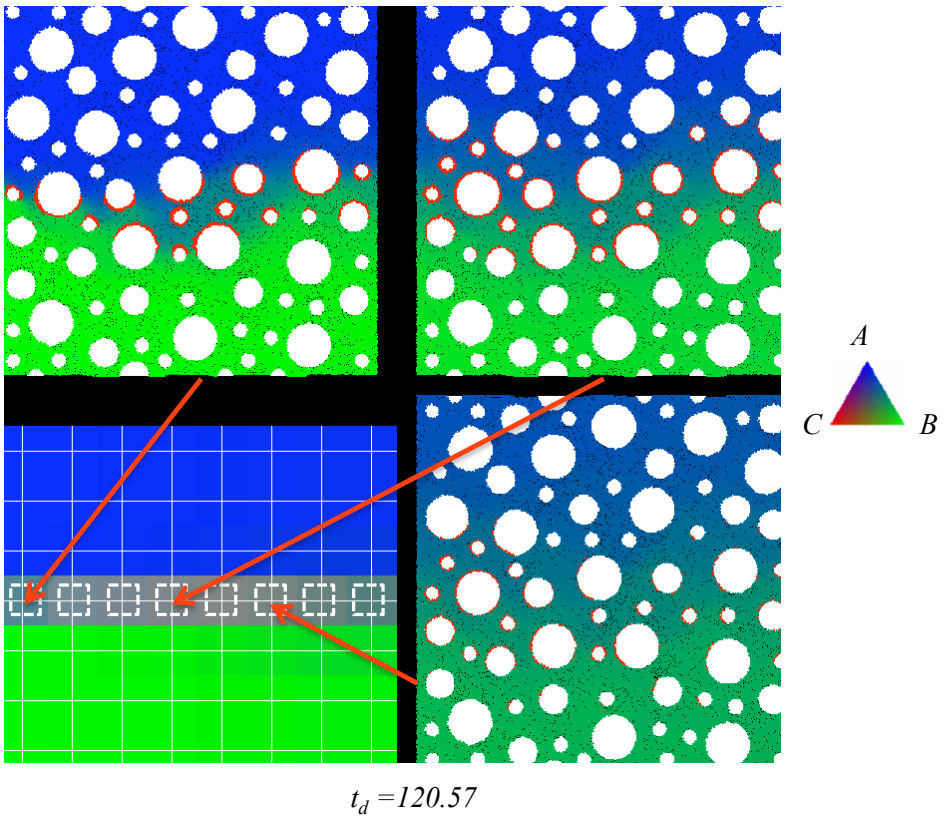

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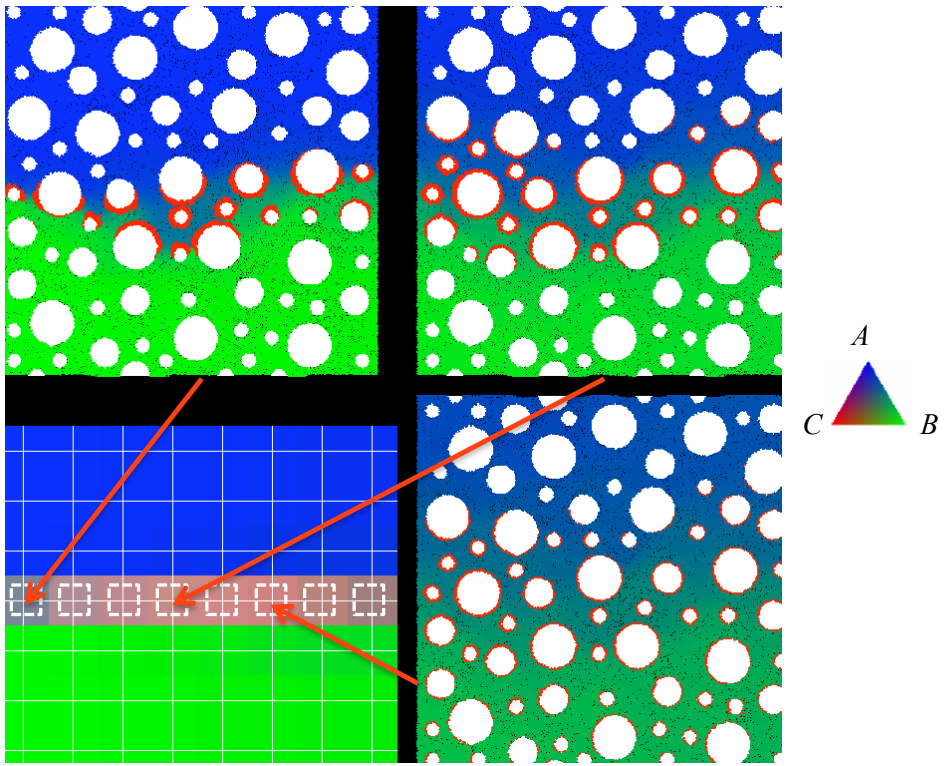

t_d =200.96

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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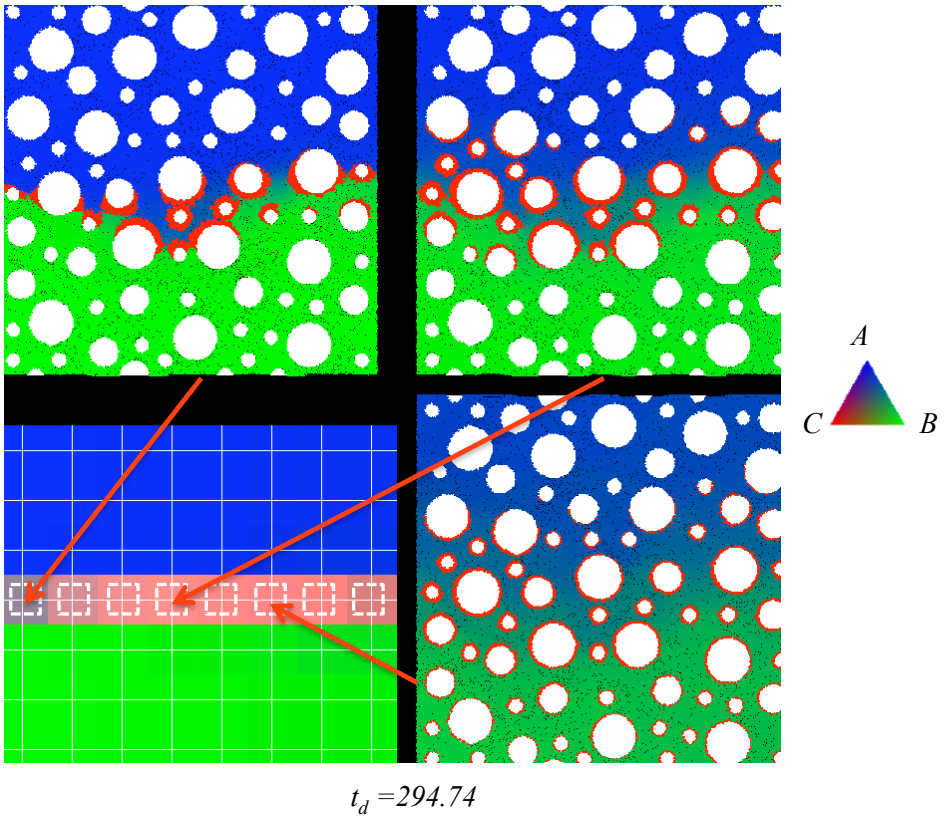
Results: Coarse solution with numerical closure



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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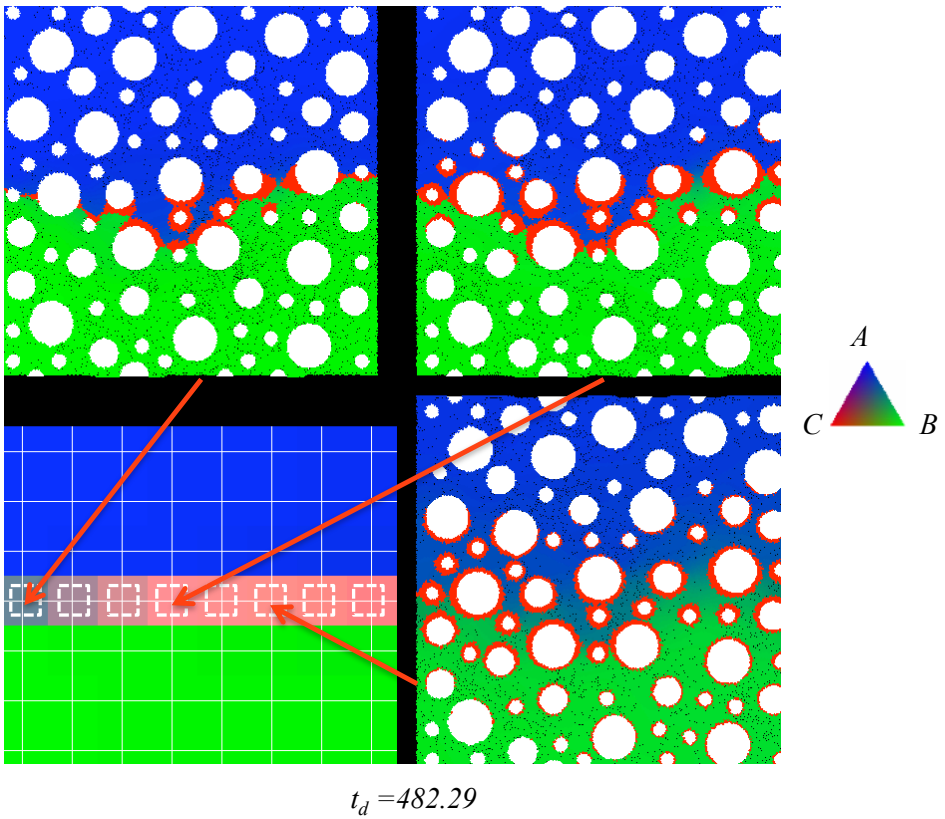
Results: Coarse solution with numerical closure



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Comparison of reconstructed microscale variables with the exact solution.

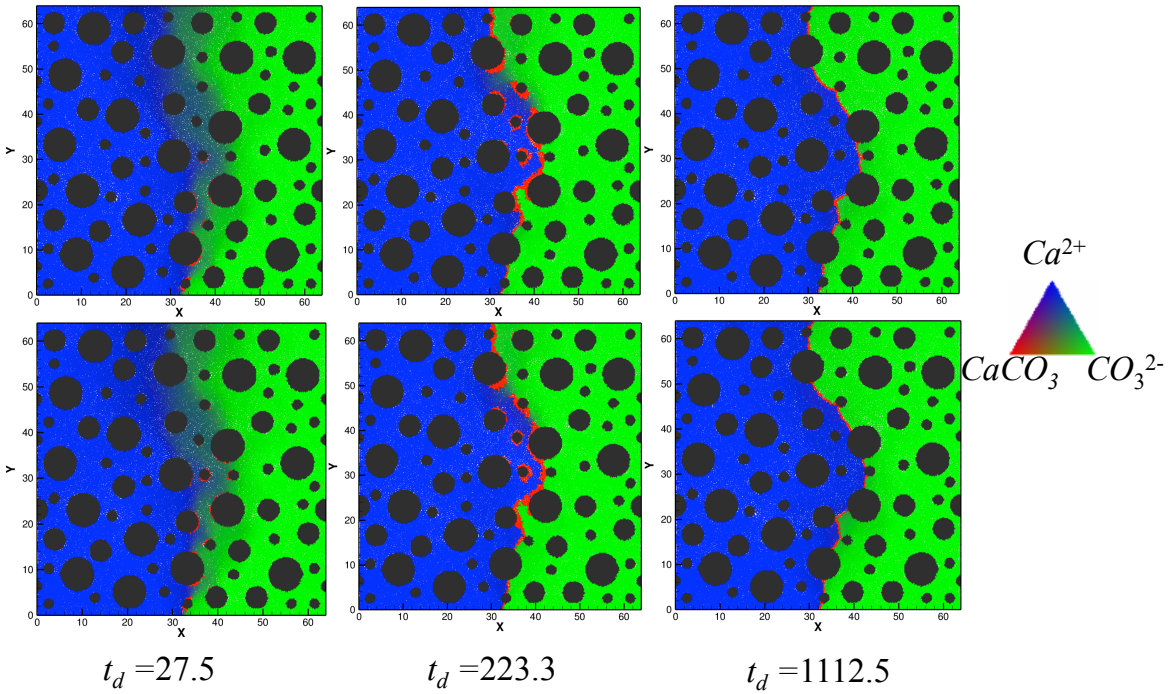

Figure: The first row - direct solution. The second row - reconstructed variables.

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 a micro-scale solver, similar to EFM.

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

Support is provided by the DOE ASCR and BER offices

ODEs for averages

Average velocity: $\frac{\partial \langle \mathbf{v} \rangle}{\partial t} = \langle \mathbf{F} \rangle$

Average concentrations: $\frac{\partial \langle I \rangle}{\partial t} = Q^I_{in} - Q^I_{out} - \langle R \rangle$

Average mass of calcite: $\frac{d\langle m \rangle}{dt} = m_0 \langle R \rangle$

$$\langle \mathbf{F} \rangle = \frac{1}{N_f} \sum_{i \in f} \mathbf{F}_i$$

$$\langle R \rangle = \frac{R}{N_f} \sum_{i \in \text{fluid}} \sum_{k \in \text{solid}} \left(\frac{[Ca^{2+}]_i [CO^{3-}]_i}{K_{sp}} - 1 \right) \delta_{ik}$$

$$Q^I_{in}(t) = \frac{1}{\Omega_P} \int_0^L I(0, y, t) v_x(0, y, t) dy$$

$$Q^I_{out}(t) = \frac{1}{\Omega_P} \int_0^L I(L, y, t) v_x(L, y, t) dy$$

Equations for averages are coupled with the SPH ODEs.

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Computational closure

"Roughly" reconstruct SPH variables from the averages.

1. Run SPH model for N_r time steps (with time step Δt)
2. Use SPH variables to close the equations for averages
3. Integrate the equations for averages with time step ΔT ($\Delta T \gg \Delta t$)
4. Reconstruct SPH variables from the corresponding averages using a fast procedure. *For example*

$$\mathbf{v}^*{}_i(\Delta t N_r + \Delta T) = \frac{\langle \mathbf{v} \rangle (\Delta t N_r + \Delta T)}{\sum\limits_{i \in fluid} \mathbf{v}_i(\Delta t N_r)} \mathbf{v}_i(\Delta t N_r)$$

5. Run SPH model for N_r steps using $\mathbf{v}^*{}_i$ as an initial condition. If $N_r \Delta t >$ relaxation time, then $\mathbf{v}_i(t + \Delta t N_r) \approx \mathbf{v}^*{}_i(t + \Delta t N_r)$.
6. Use reconstructed variables to close the equations for averages

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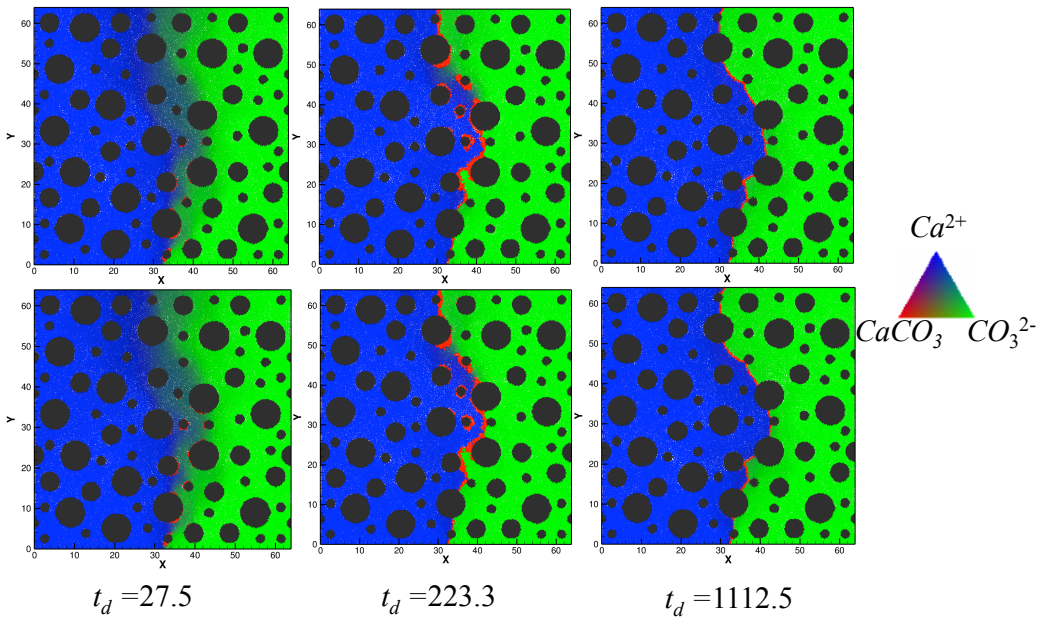
Comparison of DRM and direct solutions of ODEs. Effect of N_r.



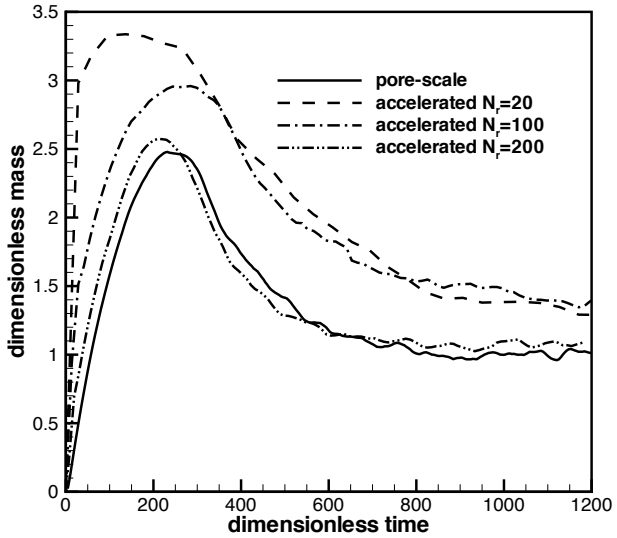


Figure: (a) The first row - direct solution. The second row - DRM solution with $N_r = 200$. (b) Total mass of calcite vs time as function of N_r.

Relaxation time $= 200\Delta t$.

Comparison with the Equation Free Method

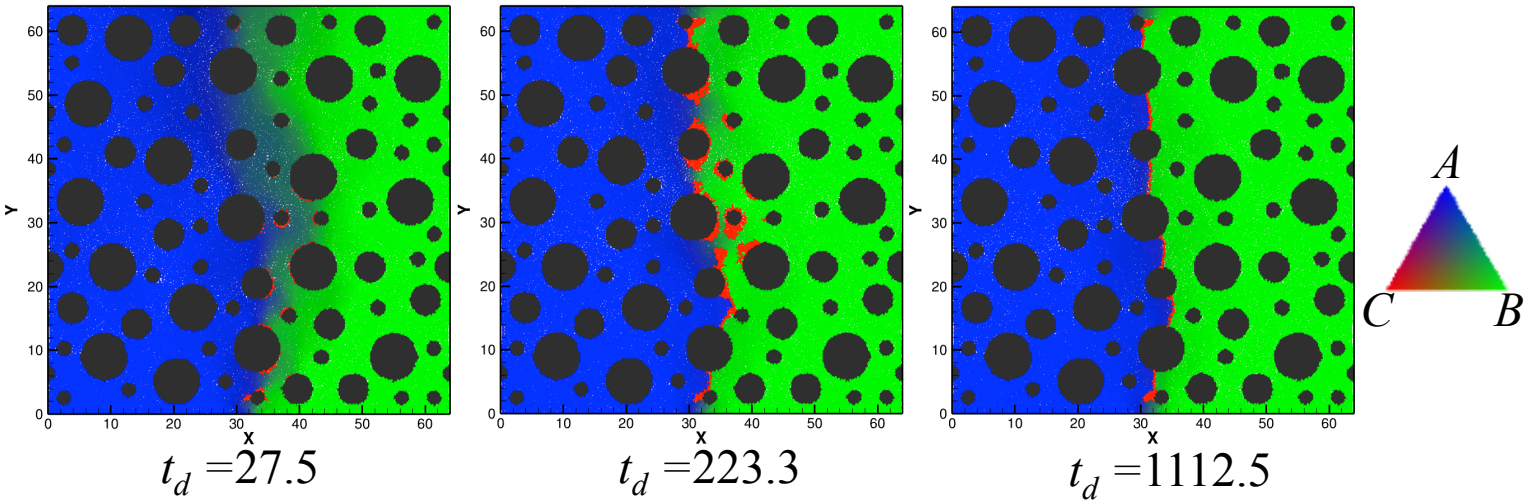


Figure: Precipitation of C (red color) due to mixing of solutes A (blue particles) and B (green particles) at three dimensionless times, t_d, obtained with EFM. The input concentrations are $A^b_{in} = B^t_{in} = 1$ and $A^t_{in} = B^b_{in} = 0$. $N_r = 200$ in the dimension reduction method.

Conclusions

The method significantly accelerates microscale simulations, while providing accurate approximation of the solution and accurate prediction of the average behavior of the system.

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Effect of the deconvolution order on on the accuracy of DRM

Poiseuille flow driven by periodic body force $\rho g \left[1 + A \sin\left(\frac{2\pi y}{L}\right)\right]$

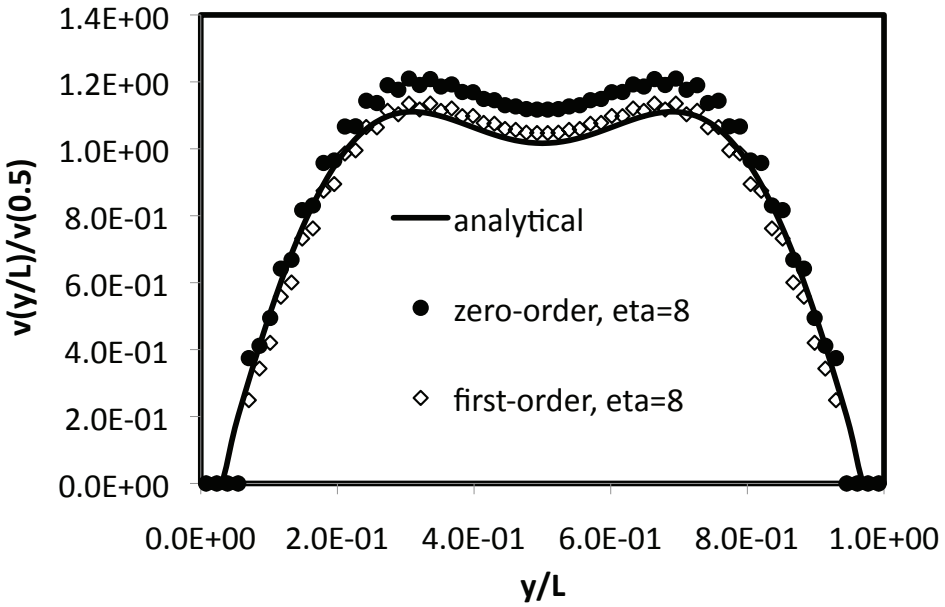

Figure: Mesoscopic velocities obtained with the zero- and first-order deconvolution of particles velocities and $\eta/L = 0.07$. The coarse approximation of T^{η}_{int} with $N/Nc = 32$ is used in the simulations.

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Effect of the mesoscale length and the coarse approximation of T_{int} on the accuracy of DRM

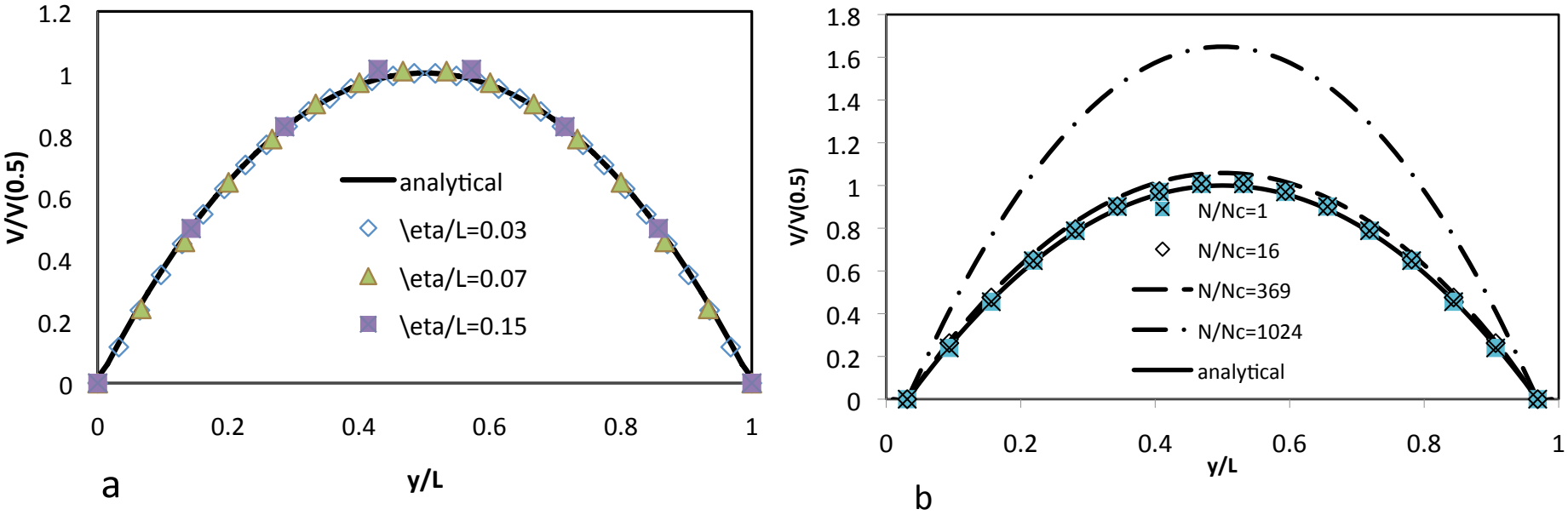

Figure: a) The effect of $\eta' = \eta L$. b) The effect of the coarsened approximation of the interaction stress. The ratio N/Nc is the reduction in the number of operations due to the coarse approximation of the interaction stress.

Closure based on the zero-order deconvolution

Assumptions and Objectives

- The microscale (pore-scale) ODE model is correct
- We are mainly interested in the evolution of averages
  - average concentrations
  - average velocity
  - permeability / distribution of precipitates
- *Accurate* closed-form equations for the averages do not exist
- We want to calculate the averages without solving the microscale ODEs directly

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Motivation

- Many mathematical models of natural and/or engineered systems have a common feature: their discrete approximations are systems of ordinary differential equations (ODEs) which can contain an enormous number of unknowns.
- Direct simulation of these models can be extremely expensive.
- This necessitates development of methods for dimension reduction - methods for approximating mathematical models with a large number of unknowns with mathematical models containing a much smaller number of unknowns.

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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:

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

Stress:

$$\boldsymbol{T}^{\eta}_{(int)}(\boldsymbol{x}) \approx \frac{1}{2}\int_{\Omega}\int_{\Omega} \overline{\boldsymbol{f}}(\boldsymbol{v},\boldsymbol{x}',\boldsymbol{x}'') \otimes (\boldsymbol{x}'' - \boldsymbol{x}') \int_0^1 \psi_{\eta}\left(s(\boldsymbol{x}-\boldsymbol{x}'') + (1-s)(\boldsymbol{x}-\boldsymbol{x}')\right) ds d\boldsymbol{x}' d\boldsymbol{x}'',$$

$\overline{\boldsymbol{f}}(\boldsymbol{v},\boldsymbol{x}',\boldsymbol{x}'') = n(\boldsymbol{x}')n(\boldsymbol{x}'')\boldsymbol{f}(\boldsymbol{v},\boldsymbol{x}',\boldsymbol{x}'')$
$\rho^{\varepsilon}(\boldsymbol{x}) = mn(\boldsymbol{x})$ - microscale density
m - mass of particles
$n(\boldsymbol{x}) = \left[\sum_{j=1}^{N} w_{\varepsilon}(\boldsymbol{x}-\boldsymbol{q}_j(t))\right]$ particle density

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Integral approximations of the mesoscale variables

The integral approximations are an essential part of the computational closure method:

- basis for reconstruction of microscale variables;
- allow to reduce an operation count.

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Reduction of the computational cost: coarse approximation of $\boldsymbol{T}^{\eta}_{(int)}$

Integral approximation of the stress:

$$\boldsymbol{T}^{\eta}_{(int)}(\boldsymbol{x}) = \frac{1}{2}\int_{\Omega}\int_{\Omega}\overline{\boldsymbol{f}}(\boldsymbol{v},\boldsymbol{x}',\boldsymbol{x}'')\otimes(\boldsymbol{x}''-\boldsymbol{x}')\int_0^1\psi_{\eta}\left(s(\boldsymbol{x}-\boldsymbol{x}'')+(1-s)(\boldsymbol{x}-\boldsymbol{x}')\right)dsd\boldsymbol{x}'d\boldsymbol{x}'',$$

Change of variables: $\boldsymbol{R} = \frac{1}{2}(\boldsymbol{x}'+\boldsymbol{x}'')$ and $\boldsymbol{\rho} = \boldsymbol{x}'-\boldsymbol{x}''$.

$$\boldsymbol{T}^{\eta}_{(int)}(\boldsymbol{x}) = \frac{1}{2}\int_{\Omega}\int_{D_{\varepsilon}}\overline{\boldsymbol{f}}(\boldsymbol{v},\boldsymbol{R},\boldsymbol{\rho})\otimes\boldsymbol{\rho}\int_0^1\psi_{\eta}\left(s(\boldsymbol{x}-\boldsymbol{R}+\tfrac{1}{2}\boldsymbol{\rho})+(1-s)(\boldsymbol{x}-\boldsymbol{R}-\tfrac{1}{2}\boldsymbol{\rho})\right)ds\ d\boldsymbol{\rho}\ d\boldsymbol{R},$$

Computational domain Ω can be discretized on the coarse grid with N_C grid points, $N_C \ll N$.

"Microscale" domain D_{ε} should be discretized on the micro-scale grid.

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Reduction of the computational cost: coarse approximation of the interaction stress

The operation count:

- microscale ODEs - $N \times P$
- reduced model (T_{int}) - $N_C \times N_F$

N - number of particles, P - number of neighbors, N_C - number of meso-scale grid points and N_F - number of fine scale mesh points.

N_C and N_F are independent of the number of particles. N_C can be made arbitrary small depending on desired resolution and accuracy.

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Reduction of the computational cost: coarse time stepping

Time step for ODEs and meso-scale equations should satisfy:

- CFL condition: $\Delta t = \kappa_1 \frac{\Delta}{\boldsymbol{v}^*}$
- Constrain due to the viscous term: $\Delta t = \kappa_2 \frac{\rho \Delta^2}{\mu}$ (for SPH and DPD ODEs)

$\Delta = \varepsilon$ for ODEs and $\Delta = \eta$ for the meso-scale equations.

Since η is much larger than ε, **time step in the dimension reduction model can be much larger than time step in the ODE model**.

$\boldsymbol{v}^*$ is the maximum velocity, κ_1 and κ_2 are coefficients that are less than one.

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Microscale SPH ODEs equations

Momentum conservation:

$$\frac{d\mathbf{v}_i}{dt} = \mathbf{F}_i \qquad \frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i$$

$$\mathbf{F}_i = -\frac{1}{m_i}\sum_j \left(\frac{P_j}{n_j^2} + \frac{P_i}{n_i^2}\right) \nabla_i W_\varepsilon\left(\mathbf{r}_i - \mathbf{r}_j\right)$$
$$+\frac{1}{m_i}\sum_j \frac{(\mu_i+\mu_j)(\mathbf{v}_i-\mathbf{v}_j)}{n_i n_j (\mathbf{r}_i-\mathbf{r}_j)^2}\left(\mathbf{r}_i - \mathbf{r}_j\right)\cdot \nabla_i W_\varepsilon\left(\mathbf{r}_i - \mathbf{r}_j\right) + \boldsymbol{g}$$

Density evolution: $n_i = \sum_j W(\mathbf{r}_j - \mathbf{r}_i, h)$

Equation of State: $P_i = P(n_i)$

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