Upscaling and Automation: Pushing the Boundaries of Multiscale Modeling through Symbolic Computing

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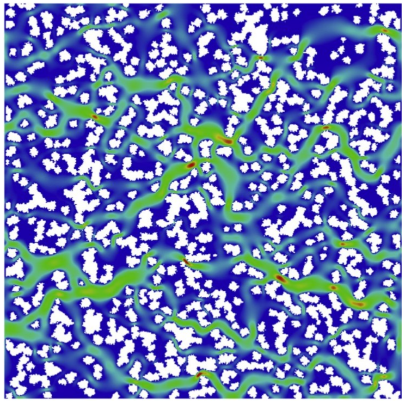
Coarse-grained Models

What are they?

- Models that describe physics on coarser scales
- Use "enhanced" equations to accurately account for small scale effects
- Reduce computational costs

Porous Media



Flow through a porous material
L. Germanou *et al., J. Nat. Gas Sci. Eng.* (2018)

Navier-Stokes Equations

$$\rho\left[\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u}\cdot\nabla\boldsymbol{u}\right] = -\nabla p + \mu\nabla^2\boldsymbol{u}$$

Capture "large-scale" fluid flow (flow rate)

Darcy's Law

$$Q = -\frac{kA}{\mu L}\Delta p$$

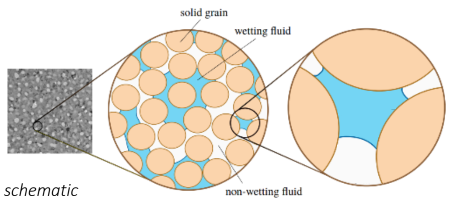
k : Permeability

Applications in Porous Media

- Complex geometries exist at the micro-scale, but interest often lies in the dynamics at larger scales
- Resolving such geometries would be computationally infeasible for large-scale analysis
- Instead, coarse-grained models are relied upon for prediction

Pore Scale

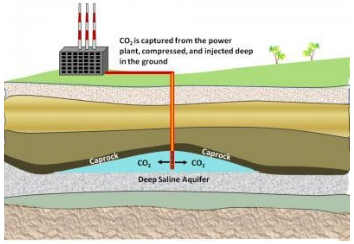
$\mathcal{O}\,(\mu m)$



Pore-scale schematic
www.uib.no

Reservoir Scale

$\mathcal{O}\,(km)$



Reservoir schematic; www.eurekalert.org

Mass Transport

$$\frac{\partial c}{\partial t} + \boldsymbol{u}\cdot\nabla c = D\nabla^2 c + R$$

Mass Transport Model

?

Heat Transfer

$$\rho C_p\frac{\partial T}{\partial t} = k\nabla^2 T$$

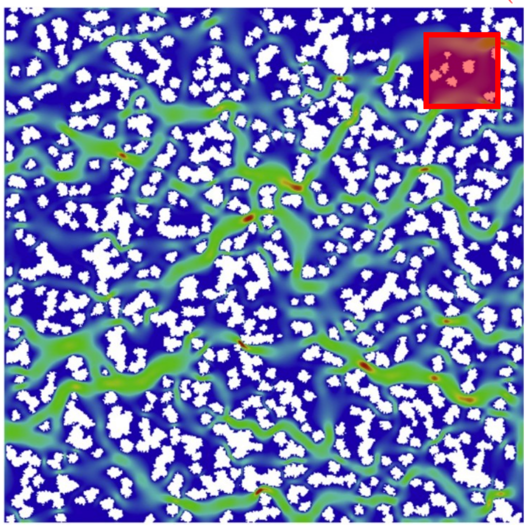
Heat Transfer Model

?

Upscaling Methods

- Generate mathematical models for the evolution of *upscaled* quantities
    - i.e., averaged quantities

REV: $\mathcal{V}(\boldsymbol{x})$



Flow through a porous material
L. Germanou *et al.*, *J. Nat. Gas Sci. Eng.* (2018)

- Define an average:

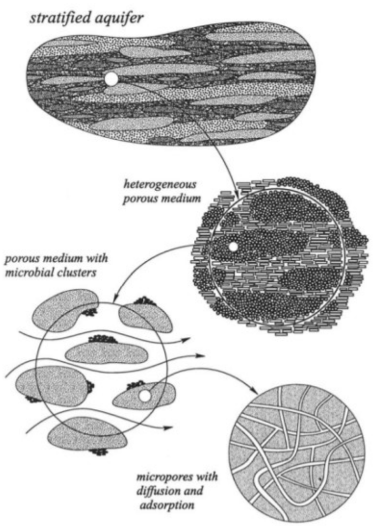
$$\langle \psi \rangle_{\mathcal{V}(\boldsymbol{x})} = \frac{1}{|\mathcal{V}|} \int_{\mathcal{V}(\boldsymbol{x})} \psi_\epsilon(\mathbf{y}) \, d\mathbf{y}$$

- General goal:

$$\langle \mathcal{L}_1[\psi] \rangle_{\mathcal{V}(\boldsymbol{x})} = 0 \quad \rightarrow \quad \mathcal{L}_2\left[\langle \psi \rangle_{\mathcal{V}(\boldsymbol{x})}\right] = 0$$

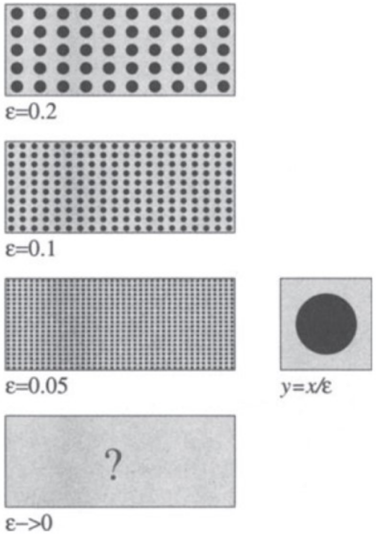
$$\mathcal{L}_1[\cdot] = \partial_t[\cdot] + \boldsymbol{u} \cdot \nabla[\cdot] + \nabla^2[\cdot]$$

Volume Averaging



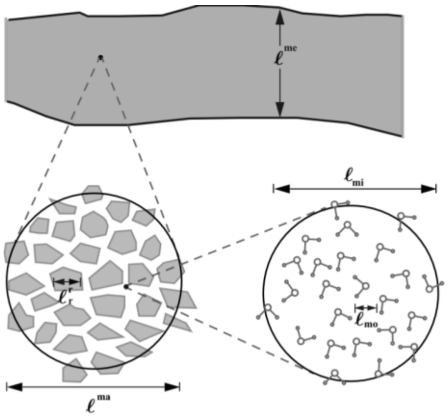
Averaging volumes diagram
S. Whitaker (1999)

Homogenization



Homogenization limit
U. Hornung (1997)

Thermodynamically Constrained Averaging Theory

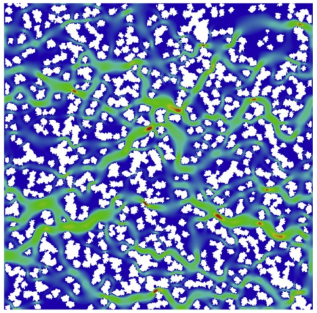


The five length scales of TCAT
W. G. Gray and C. T. Miller (2014)

Homogenization Theory

Real Porous Medium

$\psi(\boldsymbol{x}, t)$

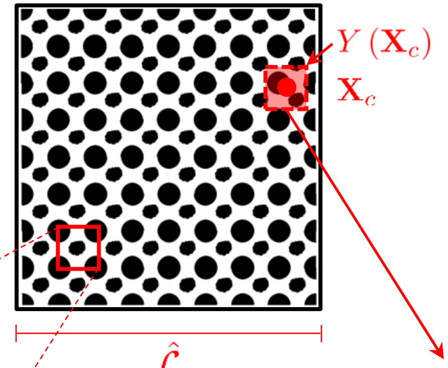


Flow through a porous material
L. Germanou *et al., J. Nat. Gas Sci. Eng.* (2018)

Periodic $\approx$

Pore-scale Domain

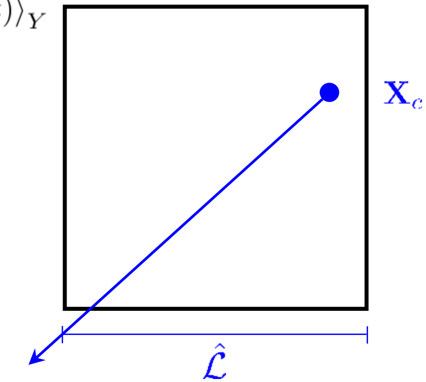
$\psi_\epsilon(\boldsymbol{x}, t)$



Mathematical Derivation $\longrightarrow$

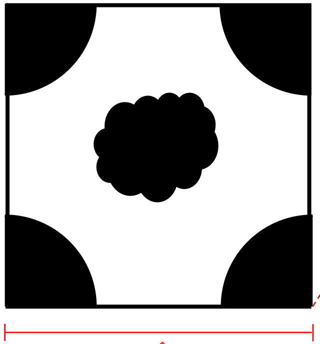
Continuum Domain

$\langle \psi(\boldsymbol{x}, t) \rangle_Y$



$$\frac{1}{|Y|} \int_{Y(\mathbf{X}_c)} \psi_\epsilon(\mathbf{y}, t)\ d\mathbf{y} \sim \langle \psi(\mathbf{X}_c, t) \rangle_Y$$

Periodic Unit-cell Domain, Y



$$\epsilon = \frac{\hat{\ell}}{\hat{\mathcal{L}}} \ll 1$$

Pore-scale Equation

$$\frac{\partial \psi_\epsilon}{\partial t} + \boldsymbol{u}_\epsilon \cdot \nabla \psi_\epsilon - D \nabla^2 \psi_\epsilon = 0$$

$\longrightarrow$

Continuum Equation

$$\frac{\partial \langle \psi \rangle_Y}{\partial t} + \mathbf{V} \cdot \nabla \langle \psi \rangle_Y - \nabla \cdot (\mathbf{D} \cdot \nabla \langle \psi \rangle_Y) = 0$$

Effective Velocity: $\mathbf{V}$, Effective Diffusion: $\mathbf{D}$

e.g., $\mathbf{D} = \langle D(\mathbf{I} + \nabla_{\boldsymbol{\xi}} \boldsymbol{\chi}) \rangle_Y$

Example Closure Problem

$$\nabla_{\boldsymbol{\xi}} \cdot [D(\mathbf{I} + \nabla_{\boldsymbol{\xi}} \boldsymbol{\chi})] = \mathbf{0}$$

$$-\mathbf{n} \cdot [D(\mathbf{I} + \nabla_{\boldsymbol{\xi}} \boldsymbol{\chi})] = \mathbf{0} \quad \text{on } \Gamma$$

Advantages

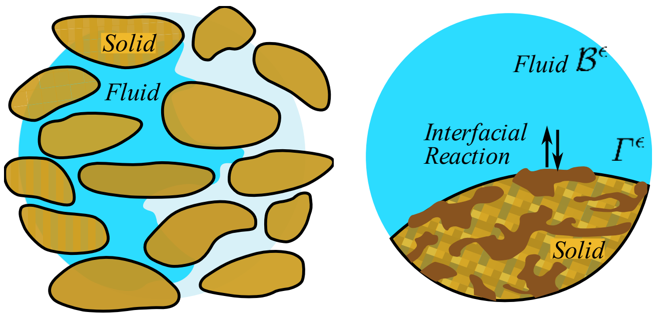
- Significantly reduce computational costs
- Models offer known *applicability conditions*
- Models offer guaranteed error limits

Disadvantages

- Time-consuming derivations that are prone to error
- Requires expertise in mathematical formulation
- Quickly becomes analytically intractable for complex systems

Complex Reactive Porous Media in Application

Pore Scale



Pore-scale Equations in $\mathcal{B}^\epsilon$:

$$\frac{\partial c_\epsilon^{(i)}}{\partial t} + \boldsymbol{u}_\epsilon \cdot \nabla c_\epsilon^{(i)} - D^{(i)} \nabla^2 c_\epsilon^{(i)} = R_\epsilon^{(i)}$$

$$R_\epsilon^{(i)} = \sum_{j=1}^{N} (-1)^{p_L^{(i,j)}} \mathcal{K}_L^{(i,j)} c_\epsilon^{(j)} + \sum_{j=1}^{N} \sum_{k=j}^{N} (-1)^{p_{NL}^{(i,j,k)}} \mathcal{K}_{NL}^{(i,j,k)} c_\epsilon^{(j)} c_\epsilon^{(k)}$$

Boundary Conditions on Γ^ϵ :

$$-\mathbf{n} \cdot D^{(i)} \nabla c_\epsilon^{(i)} = \mathcal{K}_S^{(i)} \left({c_\epsilon^{(i)}}^{n_i} - {C^{(i)}}^{n_i} \right)$$

$$i = 1, 2, \ldots, N$$

Upscaling $\longrightarrow$

~~Time~~

~~Expertise~~

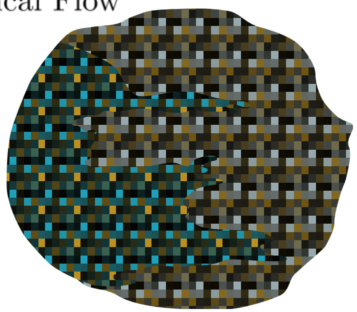
~~Intractability~~ $\longrightarrow$

Allocate work to computational resources

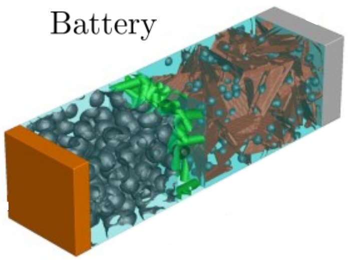
Symbolica

Continuous Scale

Geological Flow



Battery



Battery model
M. Vasilyeva *et al.*, *J. Comput. Appl. Math.* (2018)

Upscaled Equations

$$\frac{\partial \left\langle c^{(1)} \right\rangle_Y}{\partial t} + \ldots = \ldots$$

$$\frac{\partial \left\langle c^{(2)} \right\rangle_Y}{\partial t} + \ldots = \ldots$$

$$\vdots$$

$$\frac{\partial \left\langle c^{(N)} \right\rangle_Y}{\partial t} + \ldots = \ldots$$

Closure Problems

$$\nabla^2 \boldsymbol{\chi}^{(1)} + \ldots = \ldots$$

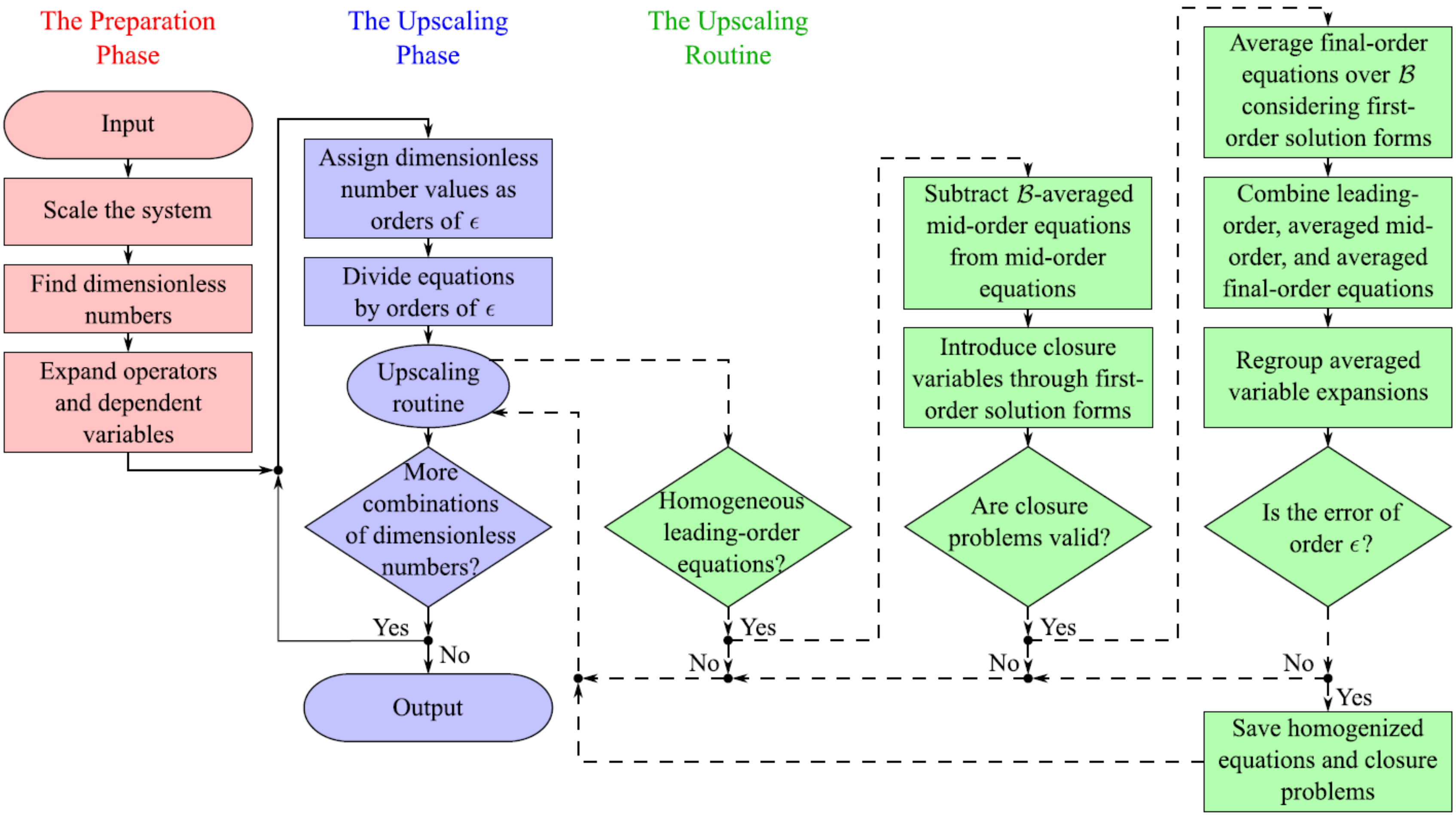
$$\nabla^2 \boldsymbol{\chi}^{(2)} + \ldots = \ldots$$

$$\vdots$$

$$\nabla^2 \boldsymbol{\chi}^{(N)} + \ldots = \ldots$$

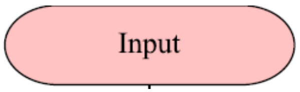
Symbolica's Homogenization Procedure

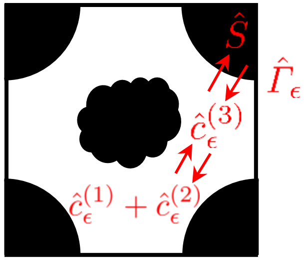
Symbolica in



Three Species, Non-linear Homogeneous Reaction

The Preparation Phase



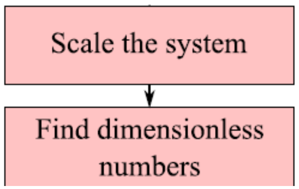


Reactions: $\hat{c}_\epsilon^{(1)} + \hat{c}_\epsilon^{(2)} \rightleftharpoons \hat{c}_\epsilon^{(3)} \rightleftharpoons \hat{S}$

Variables: $\left\{\hat{c}_\epsilon^{(i)}, \hat{D}^{(i)}, \hat{\mathcal{K}}^{(i,j)}, \ldots\right\}$

Scales: $\left\{\hat{\mathcal{C}}^{(i)}, \hat{\mathcal{D}}^{(i)}, \hat{\mathcal{K}}^{(i,j)}, \ldots\right\}$

Symbolica



Scaled equations:

$$\frac{\partial c_\epsilon^{(1)}}{\partial t} + \mathrm{Pe}\,\boldsymbol{u}_\epsilon \cdot \nabla c_\epsilon^{(1)} - D^{(1)}\nabla^2 c_\epsilon^{(1)} = -\mathrm{Da}_1 c_\epsilon^{(1)} c_\epsilon^{(2)} + \mathrm{Da}_2 c_\epsilon^{(3)}$$

$$\frac{\partial c_\epsilon^{(2)}}{\partial t} + \mathrm{Pe}\,\boldsymbol{u}_\epsilon \cdot \nabla c_\epsilon^{(2)} - D^{(2)}\nabla^2 c_\epsilon^{(2)} = -\mathrm{Da}_1 c_\epsilon^{(1)} c_\epsilon^{(2)} + \mathrm{Da}_2 c_\epsilon^{(3)}$$

$$\frac{\partial c_\epsilon^{(3)}}{\partial t} + \mathrm{Pe}\,\boldsymbol{u}_\epsilon \cdot \nabla c_\epsilon^{(3)} - D^{(3)}\nabla^2 c_\epsilon^{(3)} = \mathrm{Da}_1 c_\epsilon^{(1)} c_\epsilon^{(2)} - \mathrm{Da}_2 c_\epsilon^{(3)}$$

Scaled boundary conditions:

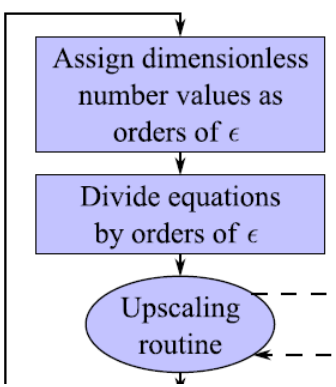
$$-\mathbf{n} \cdot D^{(1)}\nabla c_\epsilon^{(1)} = 0 \quad \text{on } \Gamma_\epsilon$$

$$-\mathbf{n} \cdot D^{(2)}\nabla c_\epsilon^{(2)} = 0 \quad \text{on } \Gamma_\epsilon$$

$$-\mathbf{n} \cdot D^{(3)}\nabla c_\epsilon^{(3)} = \mathrm{Da}_3\left(c_\epsilon^{(3)} - \eta_1\right) \quad \text{on } \Gamma_\epsilon$$

Dimensionless numbers: $\mathrm{Pe} = \frac{\hat{\mathcal{U}}\hat{\mathcal{L}}}{\hat{\mathcal{D}}}$, $\mathrm{Da}_1 = \frac{\hat{\mathcal{K}}_{NL}^{(1,2)}\hat{\mathcal{L}}^2\hat{\mathcal{C}}^*}{\hat{\mathcal{D}}}$, $\mathrm{Da}_2 = \frac{\hat{\mathcal{K}}_L^{(3)}\hat{\mathcal{L}}^2}{\hat{\mathcal{D}}}$, $\mathrm{Da}_3 = \frac{\hat{\mathcal{K}}_S^{(3)}\hat{\mathcal{L}}}{\hat{\mathcal{D}}}$, $\eta_1 = \frac{\hat{\mathcal{C}}^{(3)}}{\hat{\mathcal{C}}^*}$

The Upscaling Phase



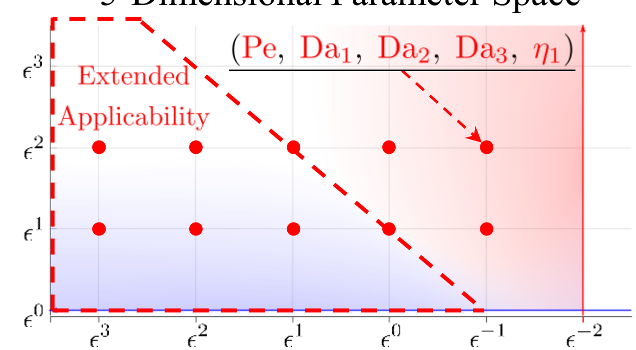
Create and upscale family of differential equations:

Let: $\mathrm{Pe},\ \mathrm{Da}_1,\ \mathrm{Da}_2,\ \mathrm{Da}_3 \in \left\{\epsilon^{-2}, \epsilon^{-1}, \epsilon^0, \epsilon^1, \epsilon^2\right\}$, $\eta_1 \in \left\{\epsilon^0\right\}$

Upscaling Results:

- Execution Time: In 8.5 minutes, 72 upscaled systems were found out of 625 attempted cases
- Found extended region of applicability (reactive regime)

5-Dimensional Parameter Space



Pore-scale and Upscaled Equations Summary

Pore-scale equations:

$$\frac{\partial c_\epsilon^{(1)}}{\partial t} + \mathrm{Pe}\boldsymbol{u}_\epsilon \cdot \nabla c_\epsilon^{(1)} - D^{(1)}\nabla^2 c_\epsilon^{(1)} = -\mathrm{Da}_1 c_\epsilon^{(1)} c_\epsilon^{(2)} + \mathrm{Da}_2 c_\epsilon^{(3)}$$

$$\frac{\partial c_\epsilon^{(2)}}{\partial t} + \mathrm{Pe}\boldsymbol{u}_\epsilon \cdot \nabla c_\epsilon^{(2)} - D^{(2)}\nabla^2 c_\epsilon^{(2)} = -\mathrm{Da}_1 c_\epsilon^{(1)} c_\epsilon^{(2)} + \mathrm{Da}_2 c_\epsilon^{(3)}$$

$$\frac{\partial c_\epsilon^{(3)}}{\partial t} + \mathrm{Pe}\boldsymbol{u}_\epsilon \cdot \nabla c_\epsilon^{(3)} - D^{(3)}\nabla^2 c_\epsilon^{(3)} = \mathrm{Da}_1 c_\epsilon^{(1)} c_\epsilon^{(2)} - \mathrm{Da}_2 c_\epsilon^{(3)}$$

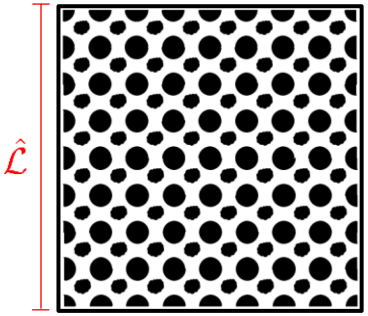
Pore-scale boundary conditions:

$$-\mathbf{n} \cdot D^{(1)}\nabla c_\epsilon^{(1)} = 0 \quad \text{on } \hat{\Gamma}_\epsilon$$

$$-\mathbf{n} \cdot D^{(2)}\nabla c_\epsilon^{(2)} = 0 \quad \text{on } \hat{\Gamma}_\epsilon$$

$$-\mathbf{n} \cdot D^{(3)}\nabla c_\epsilon^{(3)} = \mathrm{Da}_3 \left(c_\epsilon^{(3)} - \eta_1\right) \quad \text{on } \hat{\Gamma}_\epsilon$$

Pore-scale domain



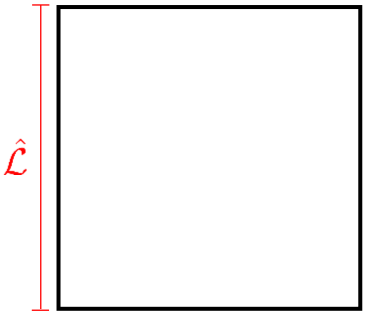
Sample upscaled equations: $\left(\mathrm{Pe} = \epsilon^{-\frac{1}{2}},\ \mathrm{Da}_1 = \epsilon^{-1},\ \mathrm{Da}_2 = \epsilon^{-1},\ \mathrm{Da}_3 = \epsilon^{\frac{1}{4}},\ \eta_1 = \epsilon^{0}\right)$

$$\frac{\partial \langle c^{(1)}\rangle_Y}{\partial t} + \epsilon^{-\frac{1}{2}}\nabla_{\boldsymbol{x}} \cdot \left(\langle \boldsymbol{u}\rangle_Y \langle c^{(1)}\rangle_Y\right) - \nabla_{\boldsymbol{x}} \cdot \left(\mathbf{D}^{(1)} \cdot \nabla_{\boldsymbol{x}} \langle c^{(1)}\rangle_Y\right) = -\epsilon^{-1}\langle c^{(1)}\rangle_Y \langle c^{(2)}\rangle_Y + \epsilon^{-1}\langle c^{(3)}\rangle_Y$$

$$\frac{\partial \langle c^{(2)}\rangle_Y}{\partial t} + \epsilon^{-\frac{1}{2}}\nabla_{\boldsymbol{x}} \cdot \left(\langle \boldsymbol{u}\rangle_Y \langle c^{(2)}\rangle_Y\right) - \nabla_{\boldsymbol{x}} \cdot \left(\mathbf{D}^{(2)} \cdot \nabla_{\boldsymbol{x}} \langle c^{(2)}\rangle_Y\right) = -\epsilon^{-1}\langle c^{(1)}\rangle_Y \langle c^{(2)}\rangle_Y + \epsilon^{-1}\langle c^{(3)}\rangle_Y$$

$$\frac{\partial \langle c^{(3)}\rangle_Y}{\partial t} + \epsilon^{-\frac{1}{2}}\nabla_{\boldsymbol{x}} \cdot \left(\langle \boldsymbol{u}\rangle_Y \langle c^{(3)}\rangle_Y\right) - \nabla_{\boldsymbol{x}} \cdot \left(\mathbf{D}^{(3)} \cdot \nabla_{\boldsymbol{x}} \langle c^{(3)}\rangle_Y\right) = \epsilon^{-1}\langle c^{(1)}\rangle_Y \langle c^{(2)}\rangle_Y - \epsilon^{-1}\langle c^{(3)}\rangle_Y - \epsilon^{-\frac{3}{4}}\frac{|\Gamma|}{|Y|}\left(\langle c^{(3)}\rangle_Y - \eta_1\right)$$

Continuum domain



Dispersion tensor:

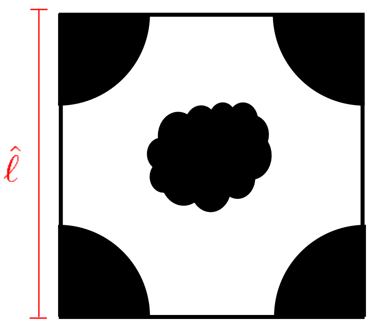
$$\mathbf{D}^{(i)} = \left\langle D^{(i)}\left(\mathbf{I} + \nabla_{\boldsymbol{\xi}}\boldsymbol{\chi}^{(i)}\right)\right\rangle_Y - \epsilon^{\frac{1}{2}}\left\langle \boldsymbol{\chi}^{(i)} \otimes \boldsymbol{u}_0\right\rangle_Y$$

Closure problem:

$$\epsilon^{\frac{1}{2}}\left[\boldsymbol{u}_0 \cdot \left(\mathbf{I} + \nabla_{\boldsymbol{\xi}}\boldsymbol{\chi}^{(i)}\right) - \langle \boldsymbol{u}_0\rangle_{\mathcal{B}}\right] - \nabla_{\boldsymbol{\xi}} \cdot \left[D^{(i)}\left(\mathbf{I} + \nabla_{\boldsymbol{\xi}}\boldsymbol{\chi}^{(i)}\right)\right] = \mathbf{0}$$

$$-\mathbf{n} \cdot \left[D^{(i)}\left(\mathbf{I} + \nabla_{\boldsymbol{\xi}}\boldsymbol{\chi}^{(i)}\right)\right] = \mathbf{0} \quad \text{on } \Gamma$$

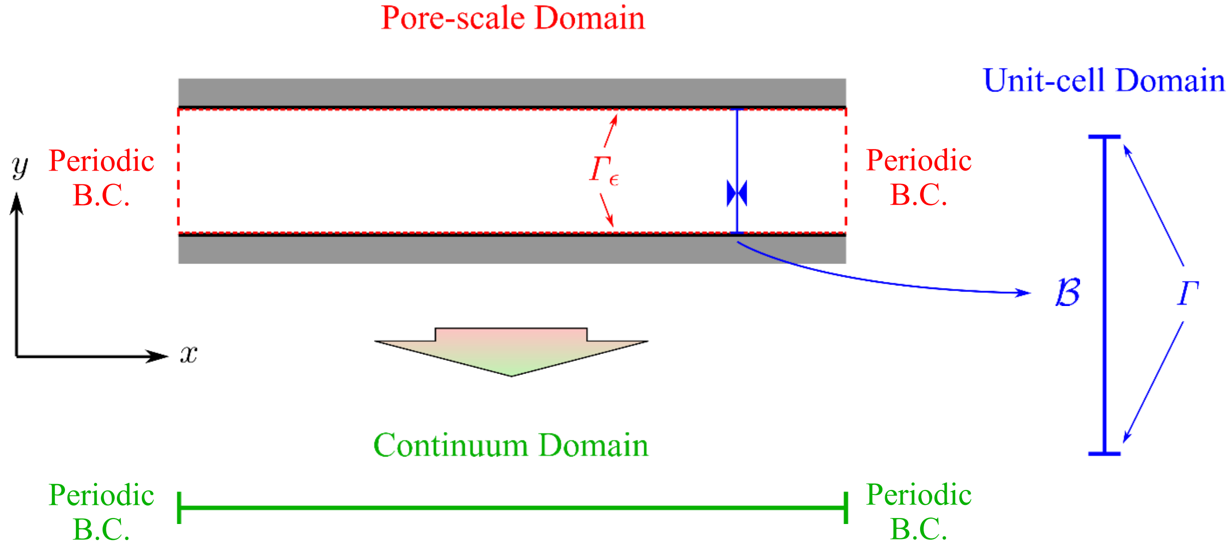
Unit-cell domain



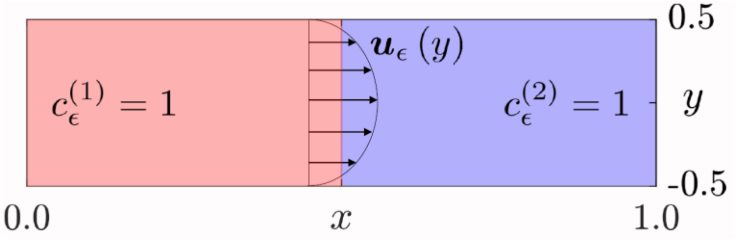
Numerical Validation: System Setup

Three Species, Non-linear Homogeneous Reaction

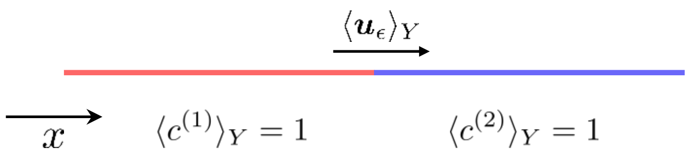
Geometry considered:



Pore-scale domain initial condition:



Continuum domain initial condition:
(averaged over channel width)

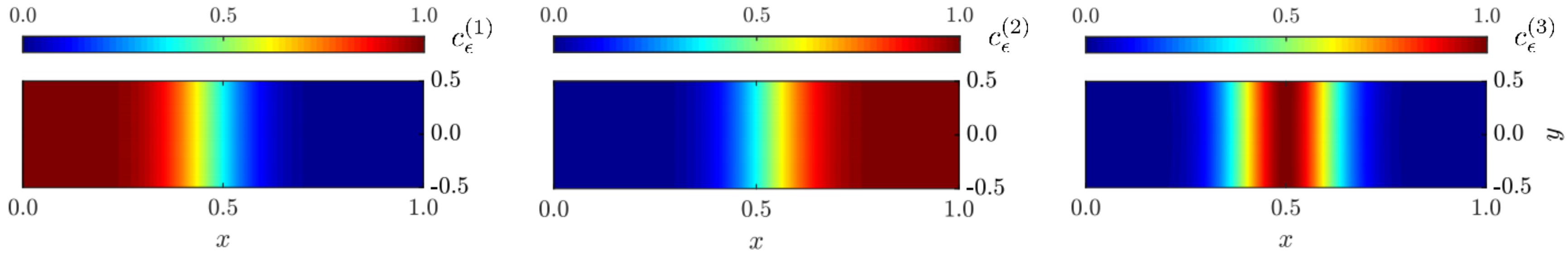


Numerical Validation: Results

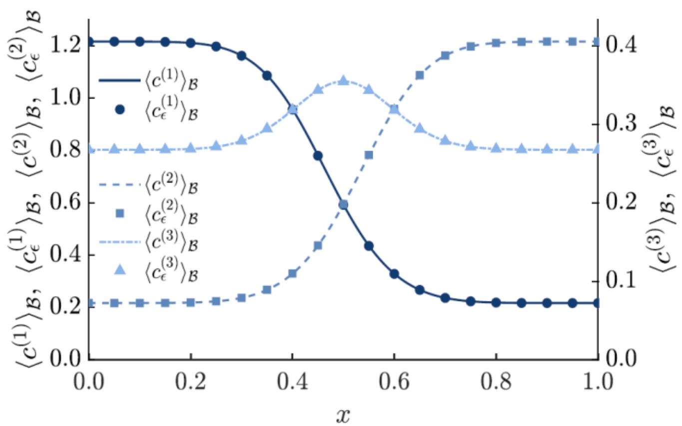
Three Species, Non-linear Homogeneous Reaction

Reactive Regime: $\mathrm{Pe} = \epsilon^2, \quad \mathrm{Da}_1 = \epsilon^{-7/4}, \quad \mathrm{Da}_2 = \epsilon^{-7/4}, \quad \mathrm{Da}_3 = \epsilon^{1/4}, \quad \eta_1 = \epsilon^0$

Pore-scale Simulation:



Averaged Concentrations vs. x at $t = 0.00625$

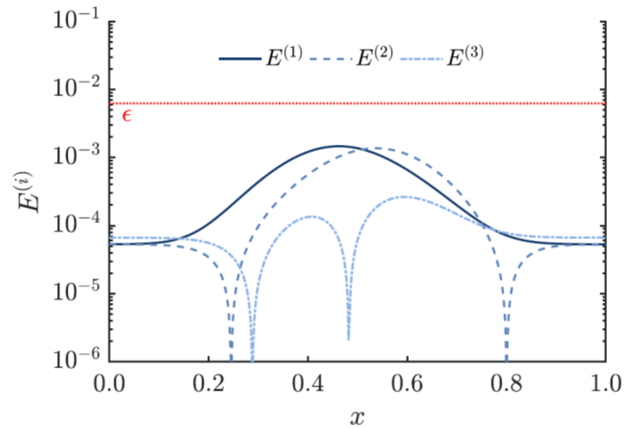


$\langle c_\epsilon^{(i)}\rangle_\mathcal{B}$: Averaged pore-scale (symbols)

(Averaged over width of channel)

$\langle c^{(i)}\rangle_\mathcal{B}$: Upscaled (lines)

Absolute Error vs. x



$$E^{(i)} = \left|\langle c_\epsilon^{(i)}\rangle_\mathcal{B} - \langle c^{(i)}\rangle_\mathcal{B}\right|$$

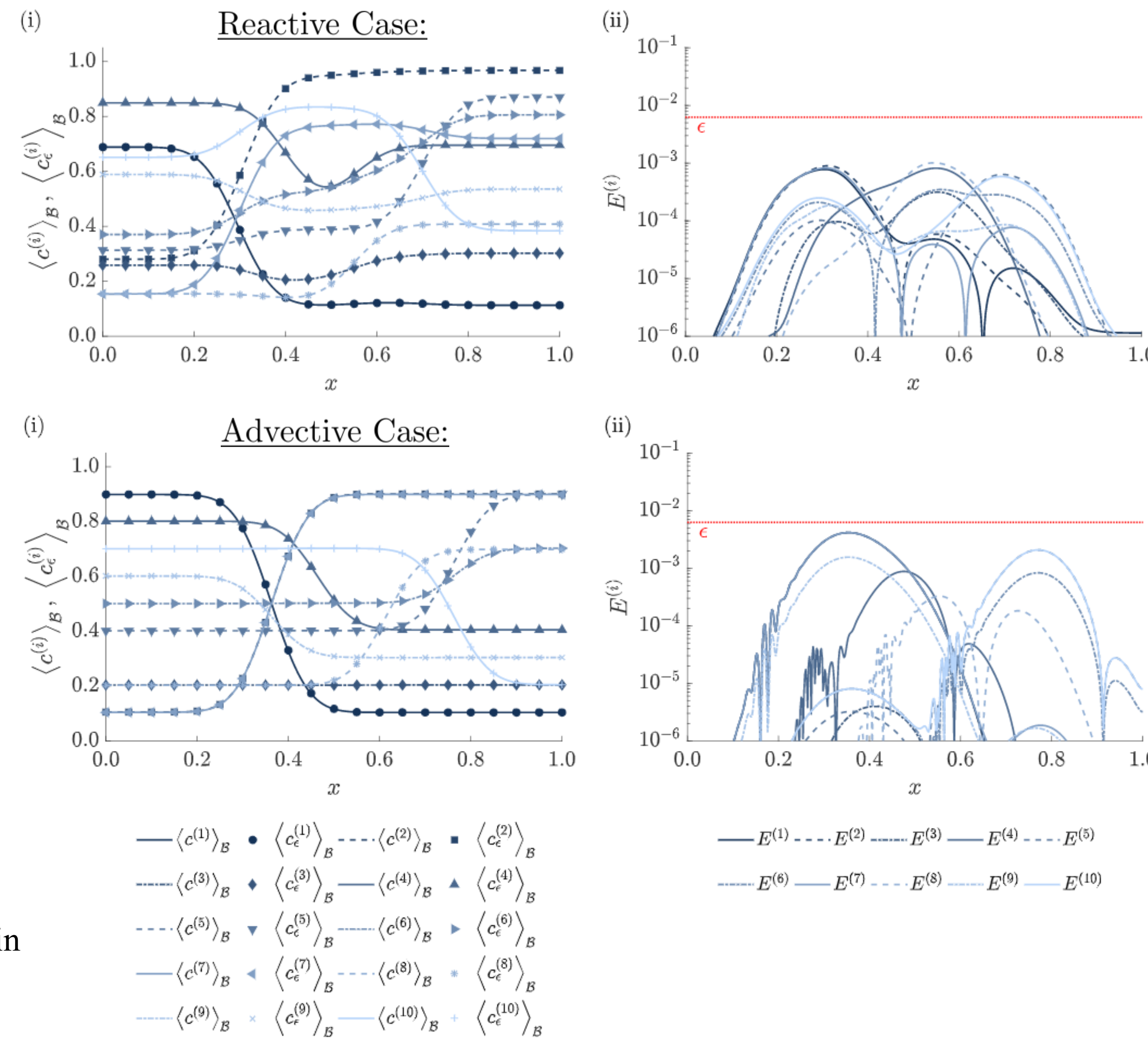
ϵ : Guaranteed error limit

Ten Species, Non-linear Homogeneous Reaction

Symbolica

Input:

$$A + B \rightleftharpoons C,$$
$$C + D \rightleftharpoons S,$$
$$S \to K + D,$$
$$K \to T,$$
$$T + A \to B,$$
$$W + K \rightleftharpoons M,$$
$$G + A \to C,$$

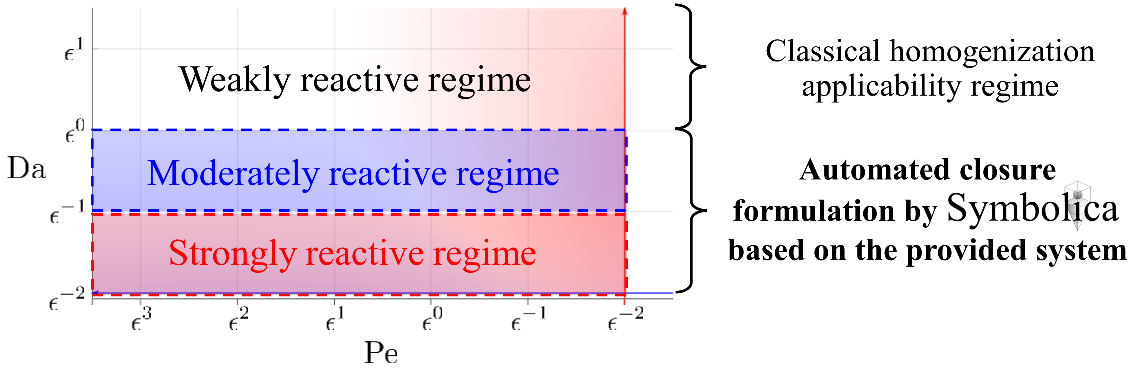


Results:

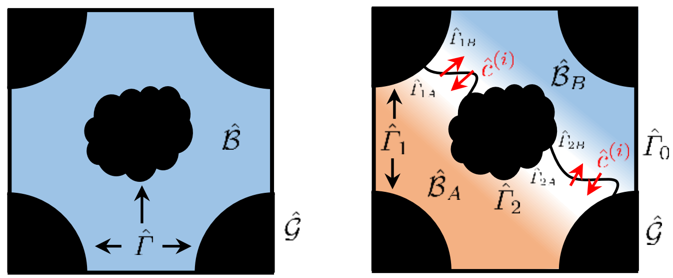
- Execution Time: 65 seconds to upscale the two cases
- Solved for channel geometry with discontinuities in initial conditions
- Successfully upscaled large system in reactive and advective cases

Work in Progress

Extended Applicability through Generalized Closure Formulation

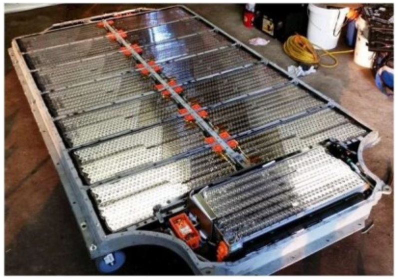


Multi-domain Unit-cell Formulation



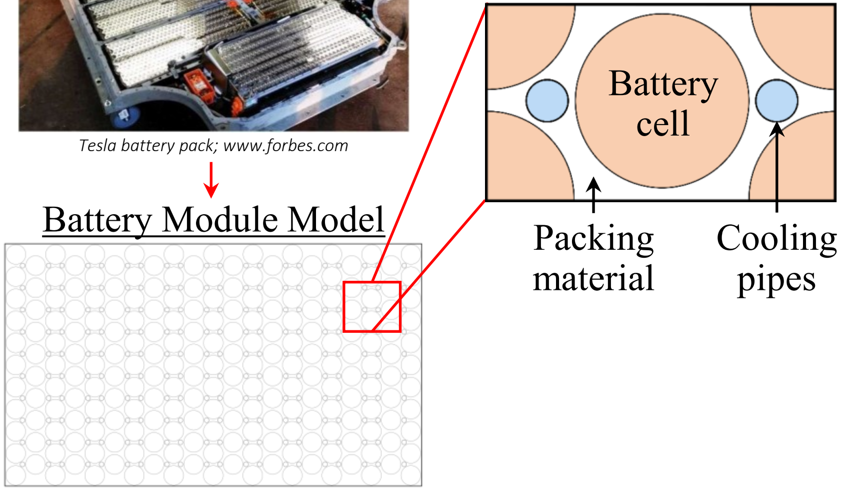
Thermal Runaway Analysis of a Li-ion Battery Pack

Vehicle Battery Pack



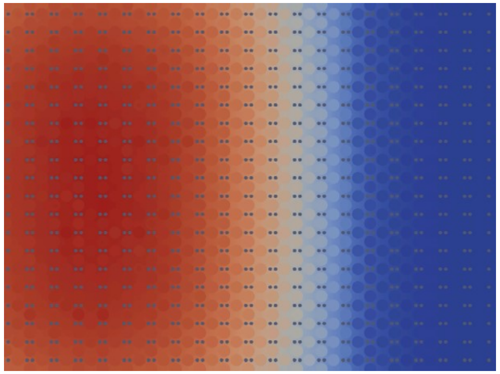
Tesla battery pack; www.forbes.com

Battery Module Model



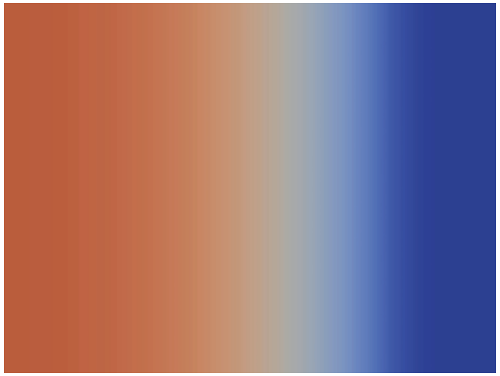
Pore-scale Simulation Temperature

~10 days to run in serial



Upscaled Simulation Temperature

> 1 day to run in serial

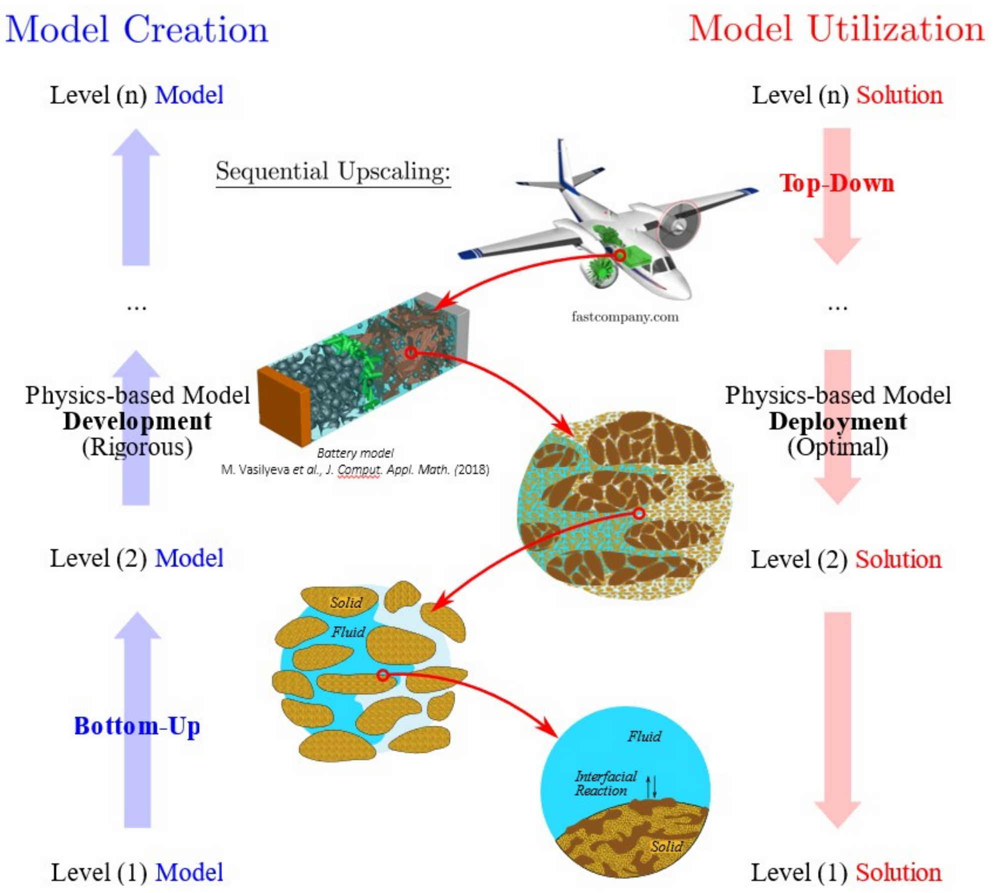


(Symbolica takes 30 seconds to upscale)

Summary

- Introduced Symbolica, a symbolic computational code for automated and accelerated upscaling
  - Automated homogenization theory
  - K. Pietrzyk *et al., Transp. Porous Med.* (2021).
- Enables efficient implementation of homogenization theory in complex, scientific investigations
- Democratizes rigorous, analytical model development methods for practical applications
- "Provide access to model development methods in a similar fashion to how computational physics softwares provide access to numerical methods"

Symbolica



Acknowledgments

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Thank you!

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