Multiscale Modeling of Alkali Silica Reaction Deterioration of Concrete Structures

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Acknowledgments

Collaborators

- Mohammed Alnaggar, RPI, Troy (NY), USA.
- Jianmin Qu, Tufts University, Boston (MA), USA.
- Roozbeh Rezakhani, Northwestern University, Evanston (IL), USA.
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- Nuclear Regulatory Commission

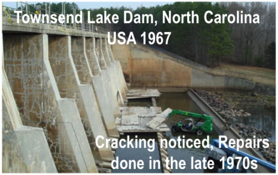
Presentation Outline

Example of Deterioration : Alkali Silica Reaction (ASR)

Dams

Bridges

Nuclear Power Plants



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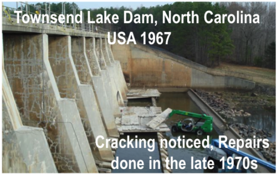

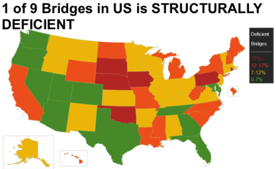

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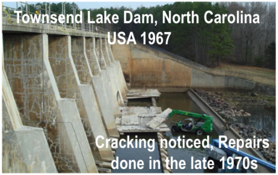
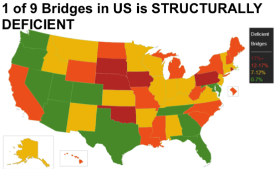
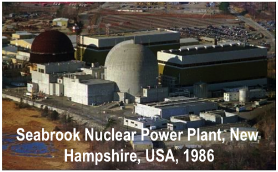
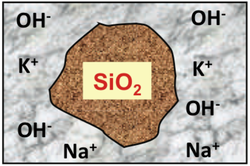


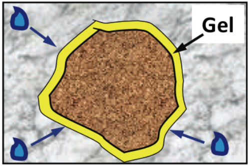


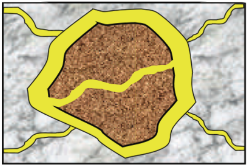


Alkali Silica Reaction (ASR) in a Nutshell

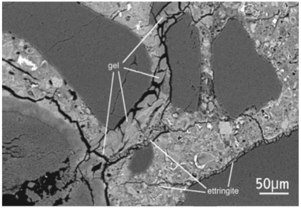
- Chemical Reaction (Very simplistic description)

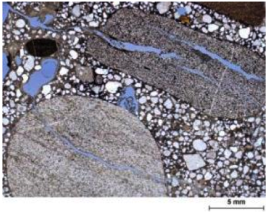


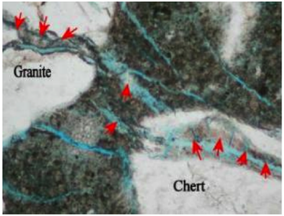




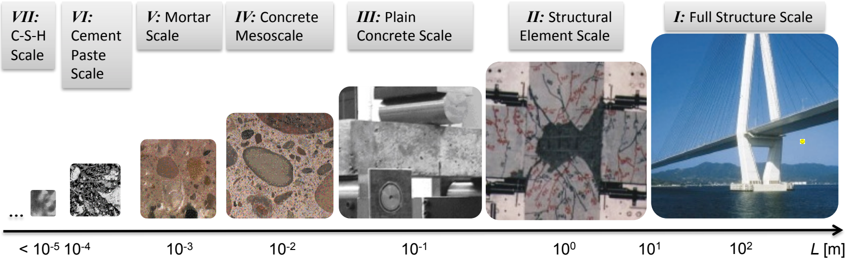
- Mechanical Deterioration







Concrete is a Multiscale Material

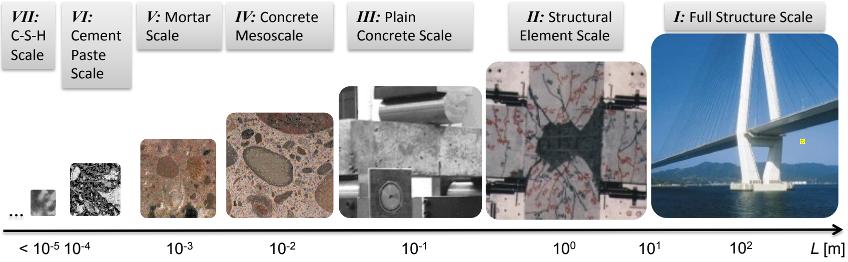


Material Science

Mechanics

Structural Engineering

Concrete is a Multiscale Material



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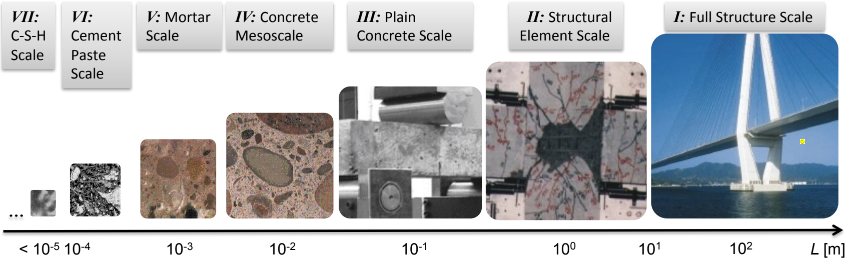

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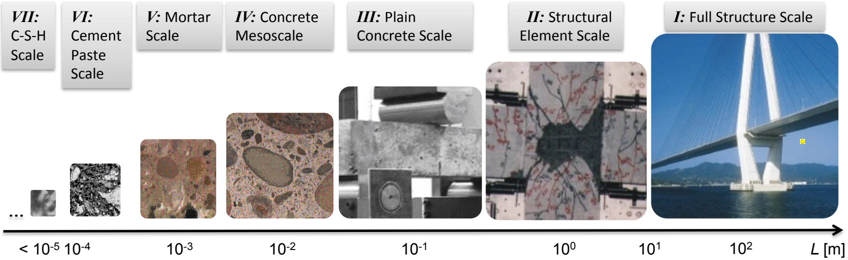

Material Science

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Definition of Multiscale Modeling

Given

1. A specific engineering problem and
2. A fine-scale model of reference

A multiscale model is

an **approximation** of the fine-scale solution characterized by the **max accuracy** for a given **acceptable cost** or the **min cost** for a given **required accuracy**

- *Accuracy* must evaluated against a *Calibrated* and *Validated* fine scale model of reference to avoid "Garbage-down, Garbage-up"
- *Cost* is application and resource dependent.

Available Multiscale Methods

- **Information Passing** - Discretized subscale material element is embedded into a point of the macro-scale continuum (an integration point of a finite element (e.g. Computational homogenization, mathematical homogenization, microplane model, etc.)

- **Concurrent** - A finite region of the macro-continuum coarse mesh is overlapped or replaced by a fine mesh or discrete sub-structure (meso-structure) model representing the subscale (e.g. Variational multiscale method, bridging scale method, multigrid methods).

- **Coarse-graining** Coarse and fine scale models are both discrete and one particle of the coarse scale simulate the behavior of a certain number of fine-scale particles.

Multiscale Computational Framework

Miniscale

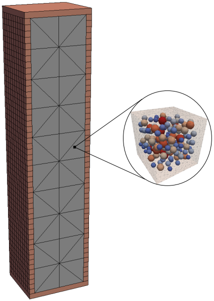
- ASR gel formation
- Water imbibition
- ASR Gel expansion
- Length scale from μm to mm

Mesoscale

- Cracking
- Creep and Shrinkage
- Length scale of mm to cm

Macroscale

- Strength and Stiffness Degradation
- Length scale of cm to m



Presentation Outline

Simplifying a very complex phenomenon

- The aggregate particles are assumed to have spherical shape.
- Silica is assumed to be smeared uniformly over the aggregate volume.
- The dissolution of silica is assumed to progress in a uniform manner in the radial direction inward from the surface towards the particle center.
- The expansion of ASR gel is mostly due to water imbibition.
- Continuous supply of water is needed for the swelling to continue over time.

ASR Model :: Gel Formation

Reaction front :

$$\dot{z} = -a_s(h,T)w_e(h,\alpha_c)/[r_w c_s z\left(1 - \frac{2z}{D}\right)]$$

ASR Gel permeability :

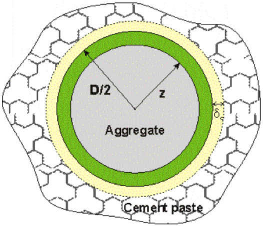
$$a_s = \mathrm{e}^{\left(\frac{E_{ag}}{RT_0} - \frac{E_{ag}}{RT}\right)} a_s^1 \left[1 + \left(\frac{a_s^1}{a_s^0} - 1\right)(1-h)^{nz}\right]^{-1}$$

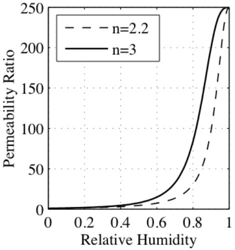
ASR Gel Mass :

$$M_g = \kappa_a \frac{\pi}{6}\left(D^3 - 8z^3\right) c_s \frac{m_g}{m_s}$$

Effect of Alkali Content :

$$\kappa_a = \min(\langle c_a - c_a^0\rangle / (c_a^1 - c_a^0), 1)$$





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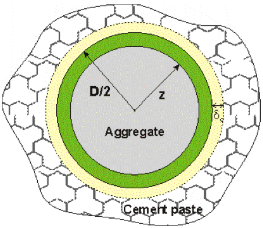

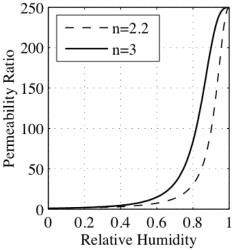

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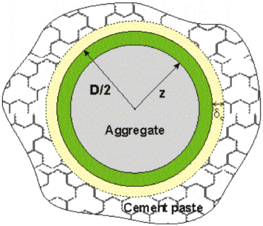

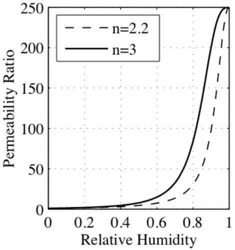

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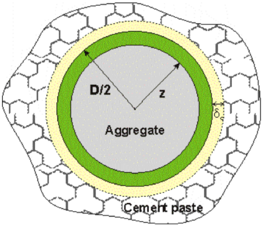

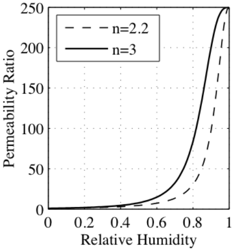

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ASR Model :: Water Imbibition

Driving force (Thermodynamic Affinity) :

$$A_i = \kappa_i^0 \exp\left(\frac{E_{ai}}{RT_0} - \frac{E_{ai}}{RT}\right) M_g - M_i$$

Imbibition Characteristic time :

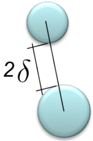
$$\tau_i = \delta^2 / C_i$$

Water Imbibition Coefficient :

$$C_i = C_i^1 \exp(-\eta M_i)(1 + (C_i^1/C_i^0 - 1)(1-h)^{n_M})^{-1}$$

Water Imbibition Rate :

$$\dot{M}_i = A_i / \tau_i$$



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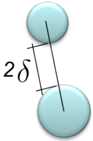

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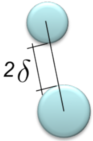

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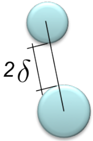

Presentation Outline

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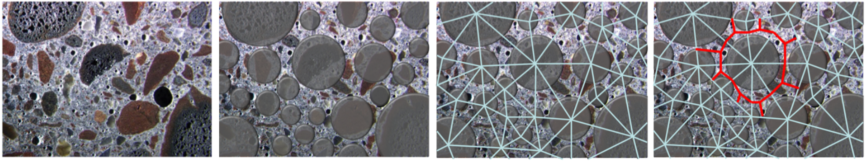
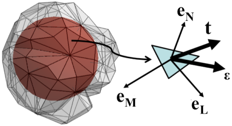
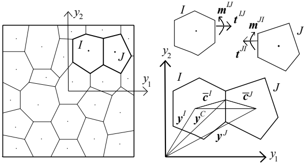
- Geometry



- 3D cell



- Discrete compatibility



Facet Strains

$$\epsilon_\alpha = \frac{1}{r}[\![\mathbf{u}_C]\!] \cdot \mathbf{e}_\alpha; \;\; [\![\mathbf{u}_C]\!] = \frac{1}{r}\left(\mathbf{U}^J + \mathbf{\Theta}^J \times \mathbf{c}^J - \mathbf{U}^I - \mathbf{\Theta}^I \times \mathbf{c}^I\right)$$

LDPM :: Constitutive Equations and Equilibrium

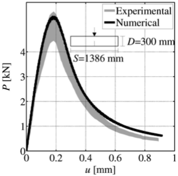
Constitutive Laws

- Fracture and cohesion due to tension and tension-shear
  - $\varepsilon = \sqrt{\varepsilon_N^2 + \alpha(\varepsilon_M^2 + \varepsilon_L^2)}$, $t = \sqrt{t_N^2 + (t_M + t_L)^2/\alpha}$
  - $t_N = (t/\varepsilon)\varepsilon_N$; $t_M = \alpha(t/\varepsilon)\varepsilon_M$; $t_L = \alpha(t/\varepsilon)\varepsilon_L$.
  - $\sigma_{bt} = \sigma_0(\omega)\exp\left[-H_0(\omega)\langle\varepsilon - \varepsilon_0(\omega)\rangle/\sigma_0(\omega)\right]$;
- Compaction and pore collapse from compression
  - $-\sigma_{bc}(\varepsilon_D, \varepsilon_V) \leq t_N \leq 0$; $\sigma_{bc} = \sigma_{c0} + \langle -\varepsilon_V - \varepsilon_{c0}\rangle H_c(r_{DV})$;
- Frictional Behavior
  - $\dot{t}_M = E_T(\dot{\varepsilon}_M - \dot{\varepsilon}_M^p)$ $\dot{t}_L = E_T(\dot{\varepsilon}_L - \dot{\varepsilon}_L^p)$;
    $\varphi = \sqrt{t_M^2 + t_L^2} - \sigma_{bs}(t_N)$
  - $\sigma_{bs} = \sigma_s + (\mu_0 - \mu_\infty)\sigma_{N0}[1 - \exp(t_N/\sigma_{N0})] - \mu_\infty t_N$

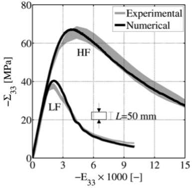
Translational and rotational equilibrium equations of each particle

$$M_u^I \ddot{\mathbf{U}}^I - V^I \mathbf{b}^0 = \sum_{\mathcal{F}_I} A\mathbf{t}^{IJ} \; ; \quad M_\theta^I \ddot{\boldsymbol{\Theta}}^I = \sum_{\mathcal{F}_I} A(\mathbf{c}^I \times \mathbf{t}^{IJ} + \mathbf{m}^{IJ})$$

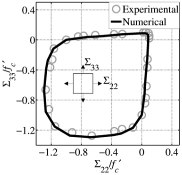
Tensile Fracture



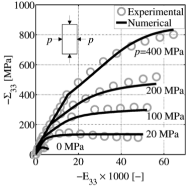
Unconfined Compression

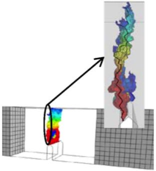


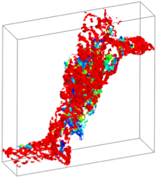
Biaxial Loading

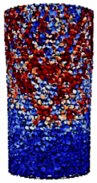


Triaxial Compression









Unconfined Compression, Cont.

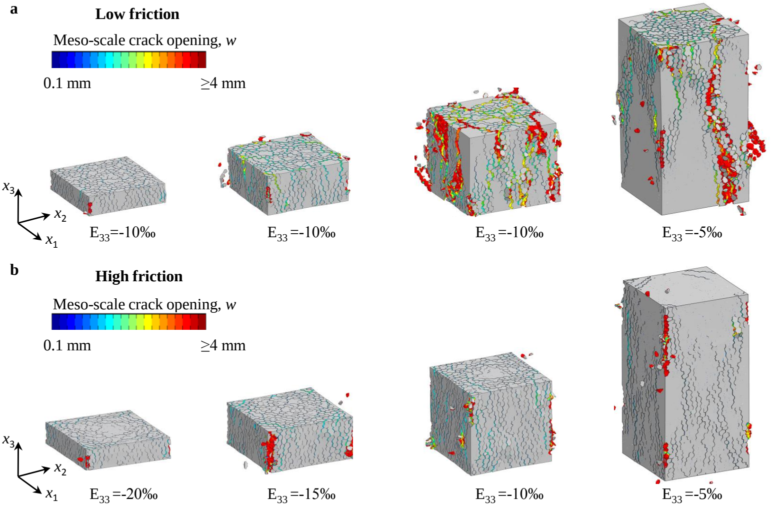


Figure: Unconfined compressive behavior. a) Contours of meso-scale crack opening at failure for low friction boundary conditions; b) Contours of meso-scale crack opening at failure for high friction boundary conditions

Unconfined Compression, Cont.

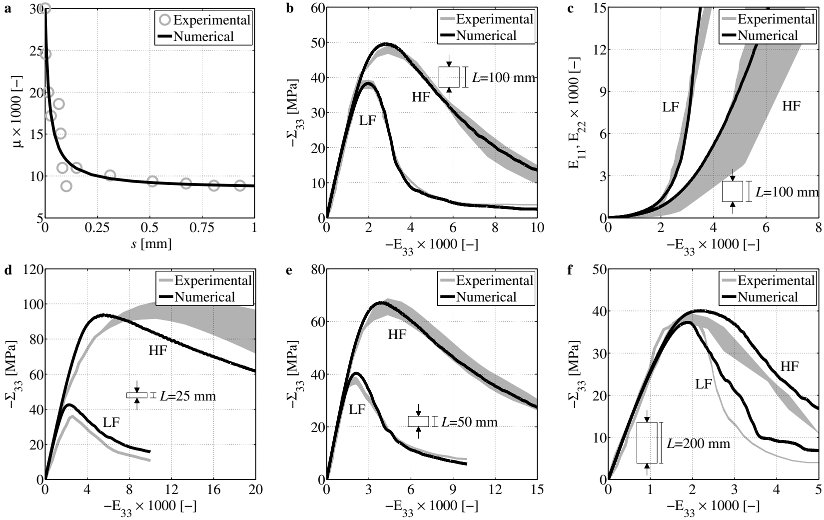
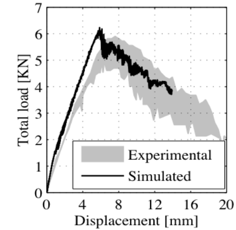
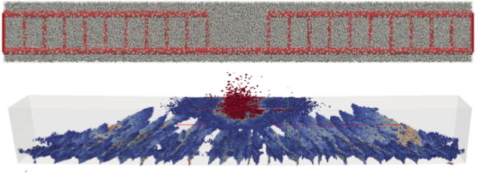


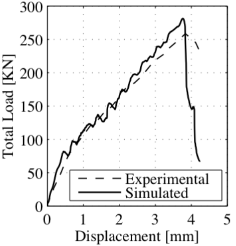
Figure: a) Low friction coefficient $\mu(s) = \mu_d + (\mu_s - \mu_d)s_0/(s_0 + s)$, $\mu_s = 0.03$, $\mu_d = 0.0084$, and $s_0 = 0.0195$ mm; b) Stress-strain curves for cubes; c) Lateral expansion for cubes; d) Stress-strain curves for very short prisms; e) Stress-strain curves for short prisms; f) Stress-strain curves for long prisms.



Over Reinforced Beam



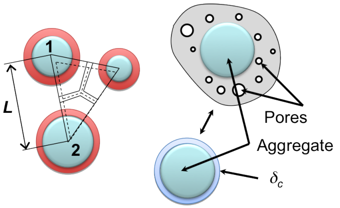
Deep Beam in Shear



Amalgamation of ASR Model with LDPM

- Radius increase of each aggregate particle $r_i = \left(\frac{3M_i}{4\pi\rho_w} + r^3\right)^{1/3} - r$
- **Normal meso-scale eigenstrain** $e^a_N = \langle(r_{i1} + r_{i2})/2 - \delta_c\rangle/\ell$ and $\dot{e}^a_N = 0$ for $\zeta = 0$
- $e^a_M = e^a_L = 0 \rightarrow \boldsymbol{\epsilon}^a = [e^a_N \;\; 0 \;\; 0]^T$
- **Incremental LDPM strain**

$$\Delta\boldsymbol{\epsilon}^* = \Delta\boldsymbol{\epsilon} - \Delta\boldsymbol{\epsilon}^a$$



Limitations. The formulation does not account explicitly for ...

- ... the actual chemistry of gel formation.
- ... multi ion transport.
- ... gel expansion into pores and cracks.
- ... non-uniform silica distribution within the aggregate.
- ... local water diffusion through (a) pores, (b) cracks; and (c) gel.

Amalgamation of ASR Model with LDPM

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- **Normal meso-scale eigenstrain** $e_N^a = \langle (r_{i1} + r_{i2})/2 - \delta_c \rangle / \ell$ and $\dot{e}_N^a = 0$ for $\zeta = 0$
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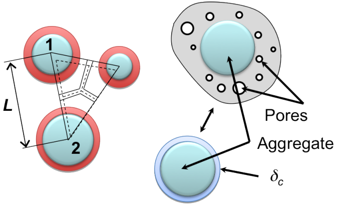

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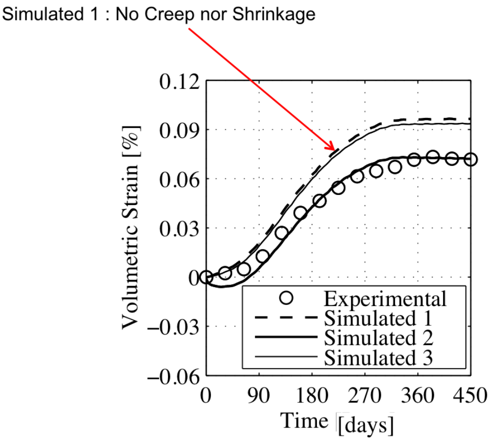
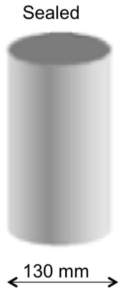
Presentation Outline

Data by S. Multon and F. Toutlemonde, 2006. Cement and Concrete Research, 36:912-920.





Model Calibration

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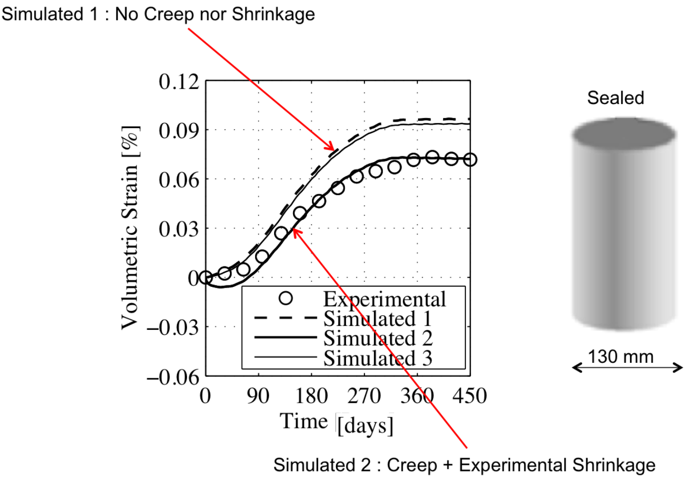

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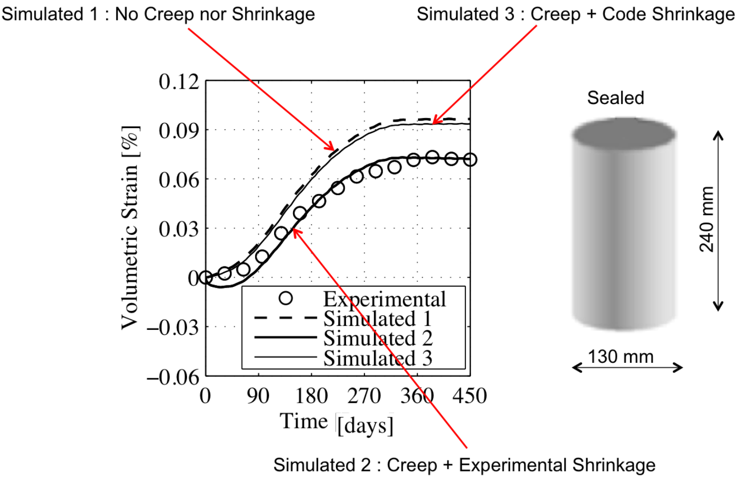
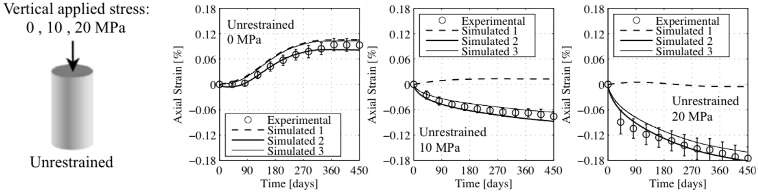


Validation :: Stress Effect - Axial Stresses



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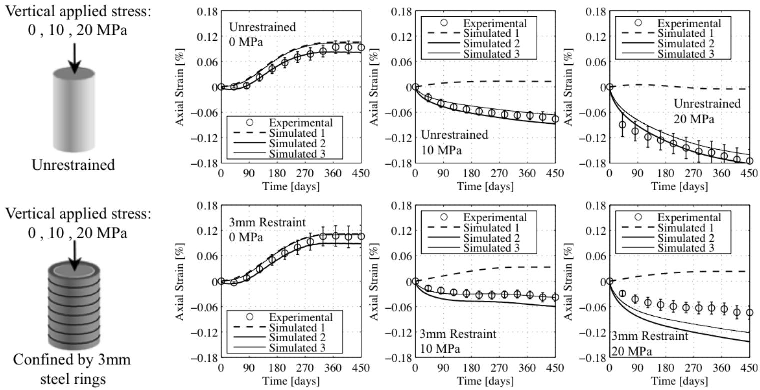
Validation :: Stress Effect - Axial Stresses



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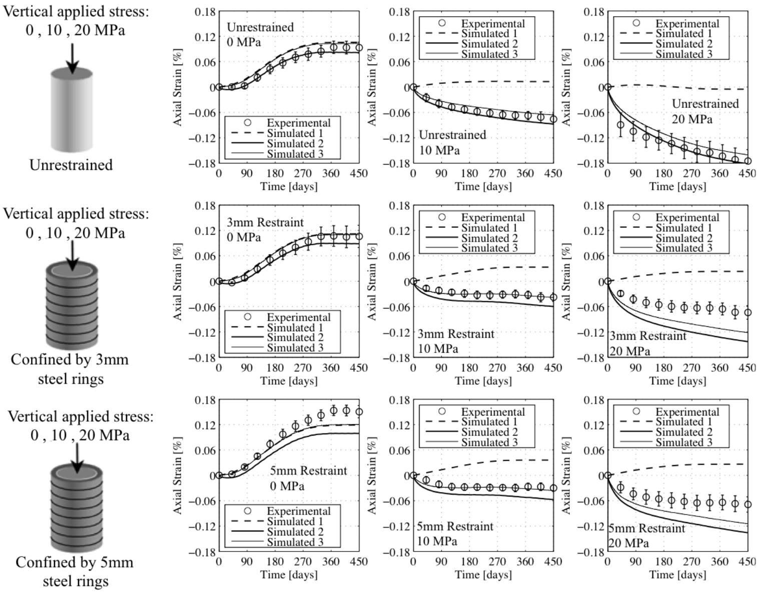

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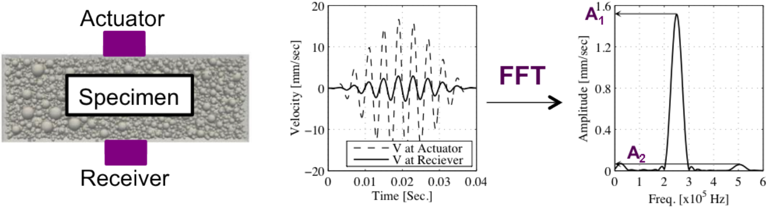
Animation of Damage Evolution

- Free Expansion
- 20 MPa / Unrest.
- 00 MPa / Rest.

Presentation Outline

Nonlinear Acoustic Nonlinearity Techniques



1D nonlinear wave propagation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial X^2}\left(1 + \beta \frac{\partial u}{\partial X}\right)$$

Single harmonic plane wave

$$A_1 \cos(kX - \omega t)$$

Solution with perturbation analysis

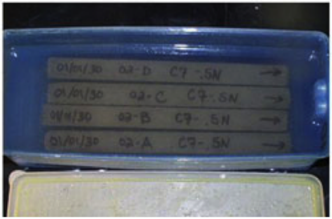
$$u = -\tfrac{1}{8}\beta k^2 A_1^2 X + A_1 \cos(kX - \omega t) + \tfrac{1}{8}\beta k^2 A_1^2 X \cos\left[2(kX - \omega t)\right] + \ldots$$
$$= A_0 + A_1 \cos(kX - \omega t) + A_2 \cos\left[2(kX - \omega t)\right] + \ldots$$

Acoustic Nonlinearity Parameter (ANLP)

$$\beta = \frac{8A_2}{k^2 L A_1^2} \propto A_2 / A_1^2$$

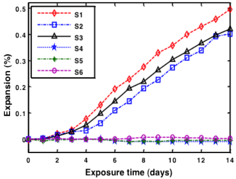
How does it relate to damage?

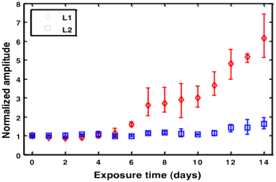
Accelerated Mortar Bar Test with ANLP testing

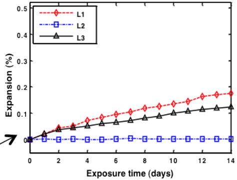


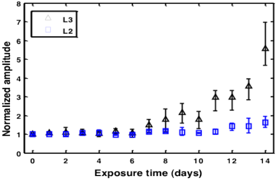
1”x1”x10”

4”x4”x10”









Alkali Ion Macro Diffusion

Nonlinear Alkali ion diffusion model

$$\frac{dc_i}{dt} = \nabla \cdot (D_i(c_i)\nabla c_i) \text{ With } D_i(c_i) = D_i^1 \left[1 + \left(\frac{D_i^1}{D_i^0} - 1\right)\left\langle 1 - \frac{c_i}{c_i^{max}} \right\rangle^{n_i}\right]^{-1}$$

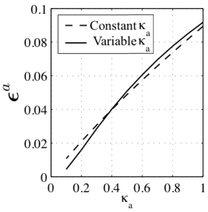
- Modification of ASR-LDPM for Variable Alkali Content

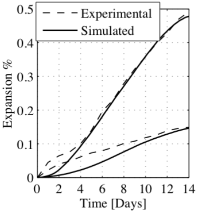
Reaction Front :

$$\dot{z}_\kappa = -\frac{a_s(T) w_s \sqrt[3]{\kappa_a}}{r_w c_s z_\kappa \left(1 - \frac{2z_\kappa}{D}\right)}, \quad z_\kappa = z\sqrt[3]{\kappa_a}$$

Total Mass of Gel per Aggregate :

$$M_g = \frac{\pi D^3}{6}\left(\kappa_a - \left(\frac{2z_\kappa}{D}\right)^3\right) c_s \frac{m_g}{m_s}$$





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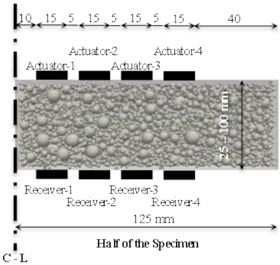

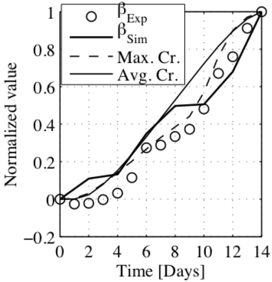

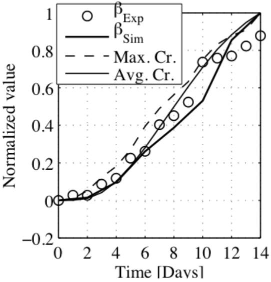

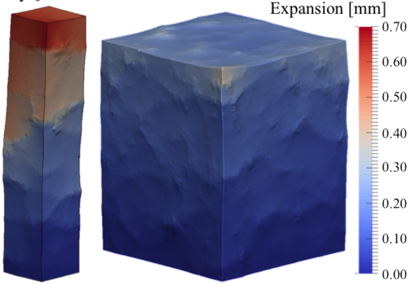

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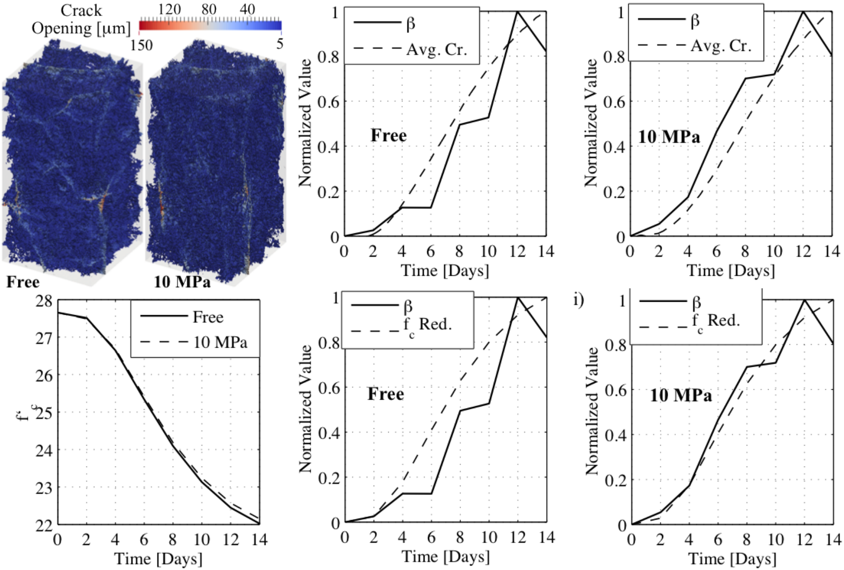

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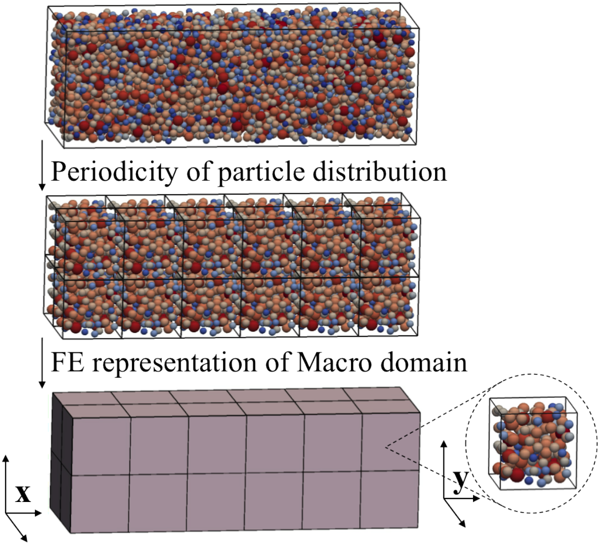
Presentation Outline

Separation of Scales

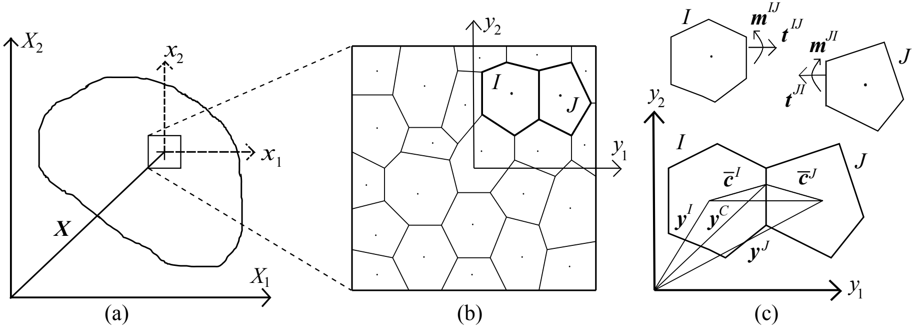


- Separation of scales

$$\mathbf{x} = \eta \mathbf{y}$$
$$0 < \eta << 1$$

- $\mathbf{x}$ is the coarse scale coordinate system
- $\mathbf{y}$ is the fine scale coordinate system

RVE problem at each macroscopic Gauss point



- Asymptotic expansion of particle displacement

$$\mathbf{u}(\mathbf{x},\mathbf{y}) \approx \mathbf{u}^0(\mathbf{x},\mathbf{y}) + \eta\mathbf{u}^1(\mathbf{x},\mathbf{y})$$

- Asymptotic expansion of particle rotation

$$\boldsymbol{\theta}(\mathbf{x},\mathbf{y}) \approx \eta^{-1}\boldsymbol{\omega}^0(\mathbf{x},\mathbf{y}) + \boldsymbol{\varphi}^0(\mathbf{x},\mathbf{y}) + \boldsymbol{\omega}^1(\mathbf{x},\mathbf{y}) + \eta\boldsymbol{\varphi}^1(\mathbf{x},\mathbf{y})$$

Length type variable change $\mathbf{x} = \eta \mathbf{y}$

Taylor expansion of $\boldsymbol{U}^J$ and $\boldsymbol{\Theta}^J$ around $\boldsymbol{x}^I$

Asymptotic expansion of displacement and rotation fields

Facet strain ϵ_α^{IJ} and curvature χ_α^{IJ} definition

Reordering terms of different orders

Multiple scale definition of facet strain and curvature

$$\epsilon_\alpha = \eta^{-1}\epsilon_\alpha^{-1} + \epsilon_\alpha^0 + \eta\epsilon_\alpha^1$$

$$\eta\chi_\alpha = \eta^{-1}\psi_\alpha^{-1} + \psi_\alpha^0 + \eta\psi_\alpha^1$$

$$\underbrace{\eta^{-2}\sum_{\mathcal{F}_I}\bar{A}\,t_\alpha^{-1}\mathbf{e}_\alpha^{IJ}}_{\boxed{\mathcal{O}(\eta^{-2})}}+\underbrace{\eta^{-1}\sum_{\mathcal{F}_I}\bar{A}\,t_\alpha^{0}\mathbf{e}_\alpha^{IJ}}_{\boxed{\text{RVE governing Eqs.}}}+\underbrace{\sum_{\mathcal{F}_I}\bar{A}\,t_\alpha^{1}\mathbf{e}_\alpha^{IJ}-\bar{M}_u^I\ddot{\mathbf{u}}^{0I}+\bar{V}^I\mathbf{b}^0}_{\boxed{\text{Macroscopic governing Eqs.}}}+\mathcal{O}(\eta)=\mathbf{0}$$

$$\overbrace{\eta^{-2}\sum_{\mathcal{F}_I}\bar{A}\,(p_\alpha^{-1}\mathbf{e}_\alpha^{IJ}+q_\alpha^{-1}\mathbf{e}_\alpha^{IJ})}^{\boxed{\mathcal{O}(\eta^{-2})}}+\overbrace{\eta^{-1}\sum_{\mathcal{F}_I}\bar{A}\,(p_\alpha^{0}\mathbf{e}_\alpha^{IJ}+q_\alpha^{0}\mathbf{e}_\alpha^{IJ})}^{\boxed{\text{RVE governing Eqs.}}}$$

$$\underbrace{-\bar{M}_\theta^I\ddot{\boldsymbol{\omega}}^{0I}+\sum_{\mathcal{F}_I}\bar{A}\,(p_\alpha^{1}\mathbf{e}_\alpha^{IJ}+q_\alpha^{1}\mathbf{e}_\alpha^{IJ})}_{\boxed{\text{Macroscopic governing Eqs.}}}+\mathcal{O}(\eta)=\mathbf{0}$$

- Considering facet level elastic constitutive law along with $\boxed{\mathcal{O}(\eta^{-2})}$
  - $\mathbf{u^0}$ and $\boldsymbol{\omega}^{\mathbf{0}}$ are rigid body motion and rotation of the RVE
  - $u_i^0(\mathbf{x},\mathbf{y}) = v_i^0(\mathbf{x}) + \varepsilon_{ijk} y_k \omega_j^0(\mathbf{x})$
  - revise facet strain and curvature definition $\epsilon_\alpha = \epsilon_\alpha^0 + \eta\epsilon_\alpha^1$; $\eta\chi_\alpha = \psi_\alpha^0 + \eta\psi_\alpha^1$

$$\epsilon_\alpha^0 = \bar{r}^{-1}\left(\overbrace{u_i^{1J} - u_i^{1I} + \varepsilon_{ijk}\omega_j^{1J}\bar{c}_k^J - \varepsilon_{ijk}\omega_j^{1I}\bar{c}_k^I}^{\text{Fine-scale displacement jump}}\right) e_{\alpha i}^{IJ} + P_{ij}^\alpha\left(\gamma_{ij} + \varepsilon_{jmn}\kappa_{im}y_n^c\right)$$

$$\boxed{\gamma_{ij} = v_{j,i}^0 - \varepsilon_{ijk}\omega_k^0}$$

$$\psi_\alpha^0 = \bar{r}^{-1}\left(\underbrace{\omega_i^{1J} - \omega_i^{1I}}_{\text{Fine-scale rotation jump}}\right) e_{\alpha i}^{IJ} + P_{ij}^\alpha \kappa_{ij}$$

$$\boxed{\kappa_{ij} = \omega_{j,i}^0}$$

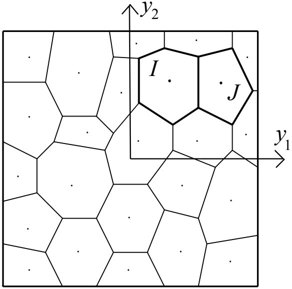
$P_{ij}^\alpha = n_i^{IJ} e_{\alpha j}^{IJ}$ is the projection operator

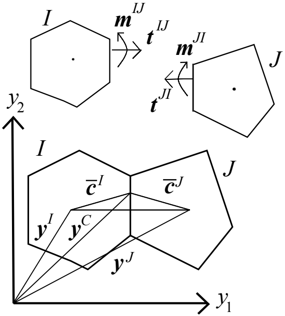
RVE Problem

- Terms of $\boxed{\mathcal{O}(\eta^{-1})}$ state RVE equilibrium equations
  - Force equilibrium equation
  - Moment equilibrium equation

$$\sum_{\mathcal{F}_I} A\, t^0_\alpha \mathbf{e}^{IJ}_\alpha = 0$$

$$\sum_{\mathcal{F}_I} A\,(\mathbf{c}^I \times t^0_\alpha \mathbf{e}^{IJ}_\alpha + m^0_\alpha \mathbf{e}^{IJ}_\alpha) = 0$$





Macroscopic Governing Equations

- Terms of $\boxed{\mathcal{O}(\eta^0)}$ state macroscopic equilibrium equations

  – Macroscopic translational equation of motion

$$\boxed{M_u^I \ddot{u}_i^{0I} = \eta \sum_{\mathcal{F}_I} A \frac{\partial t_i^{IJ}}{\partial \epsilon_\alpha^0} \epsilon_\alpha^1 + V^I b_i^0}$$

$$\Big\downarrow$$

Sum over all particles and divide by the RVE volume and some mathematical work

$$\boxed{\rho_u \ddot{v}_i^0 = \sigma_{ji,j}^0 + b_i \quad ; \quad \sigma_{ij}^0 = \frac{1}{2V_0} \sum_I \sum_{\mathcal{F}_I} A r t_\alpha^0 P_{ij}^\alpha}$$

$\rho_u = \sum_I M_u^I / V_0$ mass density of the macroscopic continuum

Macroscopic Governing Equations

- Terms of $\boxed{\mathcal{O}(\eta^0)}$ state macroscopic equilibrium equations
  - Macroscopic rotational equation of motion

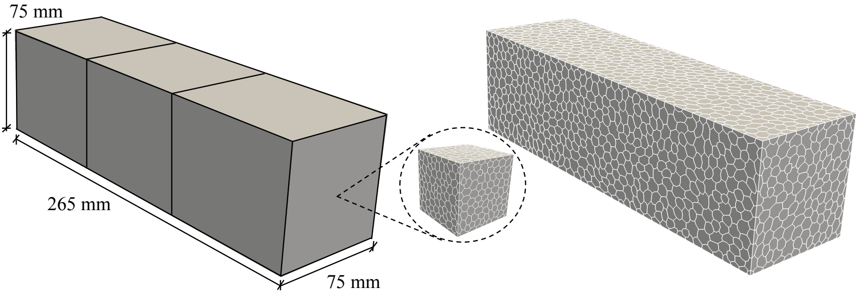
$$\boxed{\begin{aligned} M_u^I \varepsilon_{ijk} X_j^I \left(\ddot{v}_k^0 + \varepsilon_{kmn} \eta^{-1} \ddot{\omega}_m^0 x_n^I \right) + \eta^{-1} M_\theta^I \ddot{\omega}_i^0 = \\ \eta \textstyle\sum_{\mathcal{F}_I} A \left(\frac{\partial w_i^{IJ}}{\partial \epsilon_\alpha^0} \epsilon_\alpha^1 + \frac{\partial m_i^{IJ}}{\partial \psi_\alpha^0} \psi_\alpha^1 \right) + V^I \varepsilon_{ijk} X_j^I b_k^0 \end{aligned}}$$

$$\xrightarrow{\text{Sum over all particles and divide by the RVE volume and some mathematical work}}$$

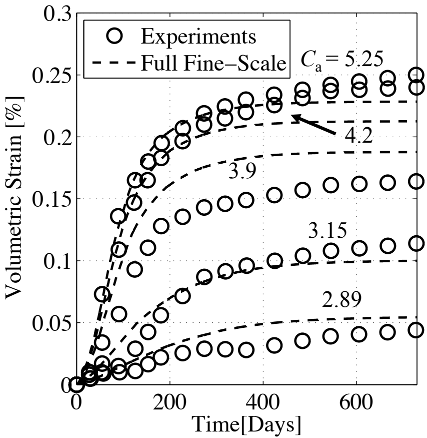
$$\boxed{\rho_{\theta ij} (\eta^{-1} \ddot{\omega}_j^0) = \varepsilon_{ijk} \sigma_{ij}^0 + \frac{\partial \mu_{ji}^0}{\partial x_j} \quad ; \quad \mu_{ij}^0 = \frac{1}{2V_0} \textstyle\sum_I \sum_{\mathcal{F}_I} Ar(m_\alpha^0 P_{ij}^\alpha + t_\alpha^0 Q_{ij}^\alpha)}$$

$\rho_{im}^\theta = \sum_I \left[M_\theta^I \delta_{im} + M_u^I \varepsilon_{ijk} \varepsilon_{kmn} x_j^I x_n^I \right] / V_0$: the inertia tensor of the unit cell

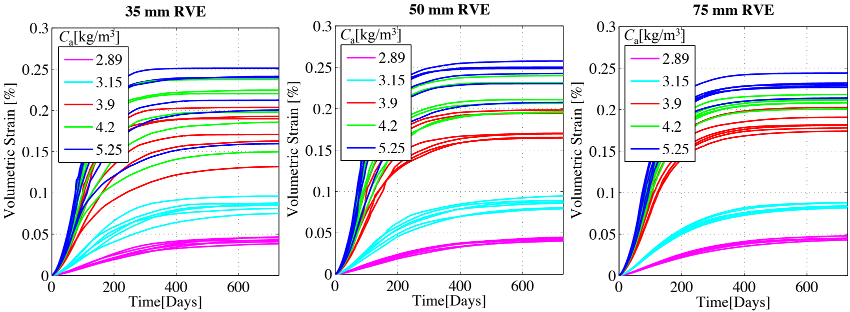
$Q_{ij}^\alpha = n_i^{IJ} \varepsilon_{jkl} x_k^C e_{\alpha l}^{IJ}$: projection tensor



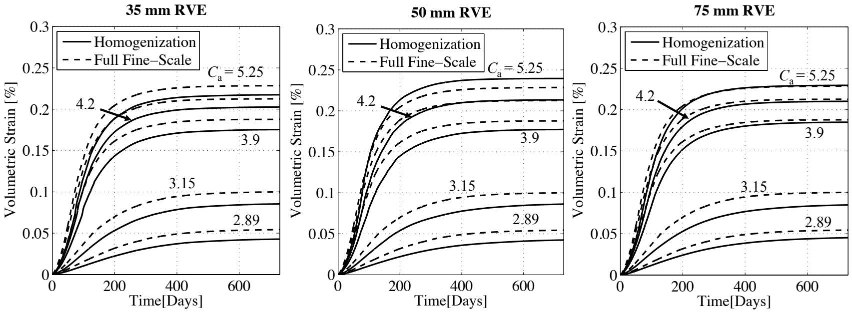
(Left) Two-scale homogenization problem. (Right) Full mesoscale prism model.



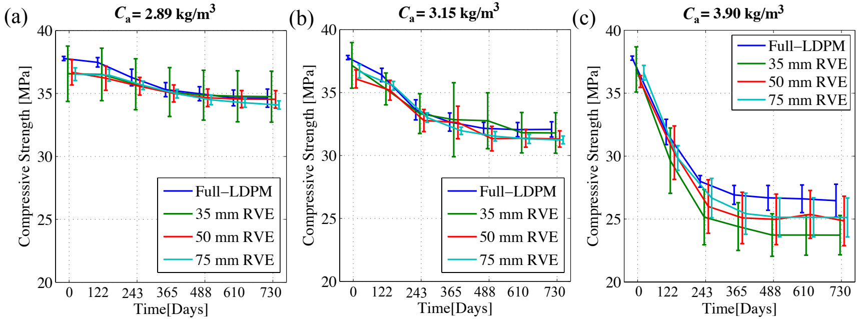
Volumetric expansion of concrete prism for different alkali contents by experiment and full fine-scale analysis.



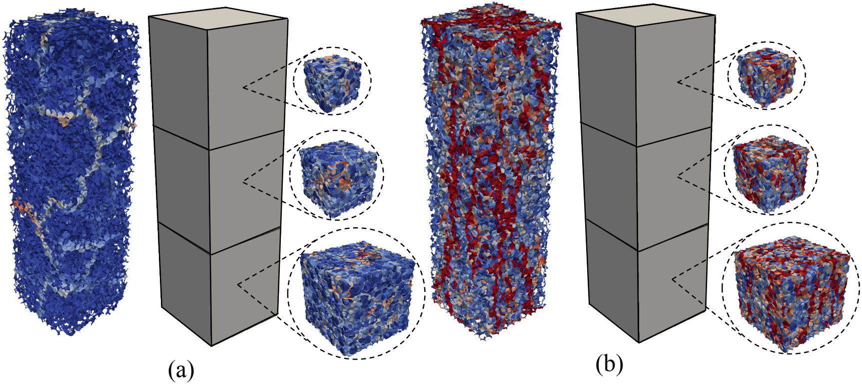
Volumetric expansion using RVE size of (left) 35 mm (center) 50 mm, and (righ) 75 mm.



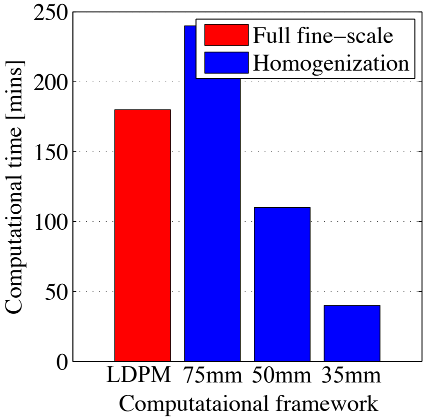
Comparison of the homogenization results using different RVE sizes with the full fine-scale ones.



Comparison of the compressive strength obtained by the full fine-scale simulation and the homogenization framework.



Crack opening contour of the concrete prism and RVEs of different sizes under (a) free expansion due to ASR effect with $C_a = 3.9$ kg/m^3 and (b) uniaxial compression after ASR expansion.



Computational cost in full fine-scale analysis and homogenization framework with different RVE sizes.

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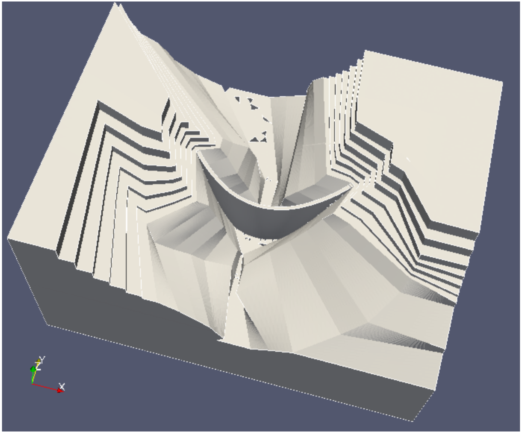
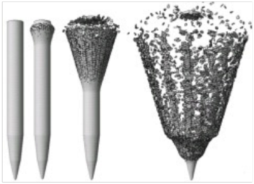


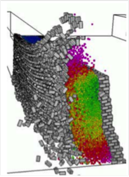
Full scale dam analysis ...

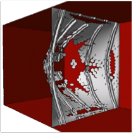
MARS (Modeling and Analysis of the Response of Structures) is a multipurpose object-oriented computational software for simulating the mechanical response of structural systems subjected to short duration events.

It is based on dynamic explicit algorithms and it implements all the capabilities and versatility of a general finite element code.

http://mars.es3inc.com/







Presentation Outline

Conclusions

- Alkali Silica Reaction is a complex multiscale-multiphysics phenomenon affecting the deterioration of concrete structures worldwide.
- Predictive computational models are needed to evaluate existing deteriorated structures.
- A multi scale framework was proposed to simulate ASR deterioration within the LDPM framework.
- LDPM can be extended effectively to account for various aging and deterioration phenomena.
- Classical mathematical homogenezation can be used to upscale LDPM response for durability related structural analysis.
- All LDPM-based algorithms are currently implemented in the commercially available MARS software – **www.mars.es3inc.com**

Thank You ! g-cusatis@northwestern.edu

Free time with my students

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