- **Project Topic (by SeonHong Na, Columbia University, New York)**

"Chemo-mechanical coupling problems in saturated porous media"

- **What need to be done using deal.ii**
  - ✓ What is the problem
    : Solving mechanical problem (porous media) coupled with chemical transport & reactions
  - ✓ What results I have
    : Mechanical problem in porous media is already implemented (using deal.ii, trillinos, p4test, etc : so called "poromechanics" code)
    - solving non-linear problem using Newton's method
  - ✓ What I want to do
    - Add additional coupling equation: chemical transport & reaction
    - Chemical transport(diffusion & advection) will be included in global matrix
    - Reaction equation is need to be solved separately(operator splitting method)
    - Include mechanical fracture problem (ex. Phasefield)

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"Chemo-mechanical coupling problems in saturated porous media"

- Governing equation
  - Momentum balance
    (mechanical problem in porous media)

$$\nabla \cdot (\boldsymbol{\sigma}' - Bp\mathbf{1}) = \boldsymbol{f}$$

where $\dot{\boldsymbol{\sigma}}' = \mathbb{C} : \dot{\boldsymbol{\epsilon}}$; $\quad \boldsymbol{\epsilon} = \nabla^s \boldsymbol{u} = \frac{1}{2}[\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^{\mathrm{T}})]$

  - Mass balance equation
    (fluid flow in porous media, seepage velocity)

$$B\nabla \cdot \dot{\boldsymbol{u}} + \nabla \cdot \boldsymbol{q} = 0$$

where, $\boldsymbol{q} = -\frac{k}{\mu_f} \cdot (\nabla p - \rho_f \boldsymbol{g})$

  - Chemical transport equation(3) & reaction equation(1)

$$\frac{\partial(\phi \Psi_j)}{\partial t} + (\boldsymbol{q} \cdot \nabla)\Psi_j - \nabla \cdot \left(\phi \boldsymbol{D}_i \nabla \Psi_j\right) = -I_{cc}$$

$$I_{cc} = -a_{cc} k_{cc} \left(1 - \frac{Q_{cc}}{K_{eq}}\right) \qquad (j = \mathrm{H}^+, \mathrm{Ca}^{2+}, \mathrm{CO_3}^{2-})$$

- Using Newton's method
  - Residuals

$$R = \begin{pmatrix} R_u \\ R_p \\ R_a \\ R_b \\ R_c \end{pmatrix}$$

  - Tangent matrix

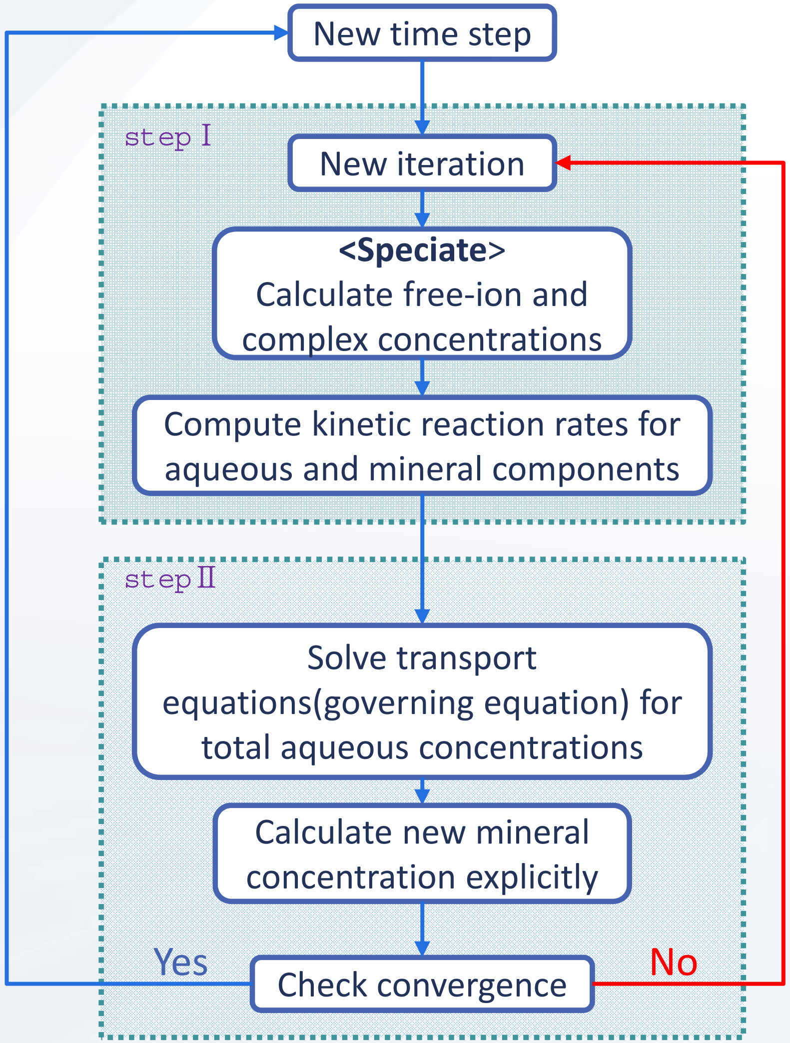
$$R'(X) = \begin{bmatrix} A & B_1 & 0 & 0 & 0 \\ B_2 & C & 0 & 0 & 0 \\ 0 & D_a & E_a & 0 & 0 \\ 0 & D_b & 0 & E_b & 0 \\ 0 & D_c & 0 & 0 & E_c \end{bmatrix}$$

  - Solutions

$$X = \begin{pmatrix} d \\ p \\ \theta_a \\ \theta_b \\ \theta_c \end{pmatrix}$$

2015 DEAL.II WORKSHOP

➢ Approach (Algorithm)



- The first step
  - Compute the free-ion and complex concentrations from the previous iteration's or time step's (in the case of the first iteration) total component concentrations according to prescribed equilibrium equations and uses these concentrations to calculate reaction rates for the transport equations.
- The second stope
  - Involves solving the governing reactive transport equations (including mechanical equations) based on prescribed reaction rate laws and the previous iteration's concentrations
- During the first step
  - Utilize the Newton-Raphson method to carry out "speciation", where individual free-ion and complex concentrations are computed. Then, estimates kinetic source/sink reaction rates as a function of these aqueous concentrations
- In the second step
  - Implements the finite element method along with a specialized matrix solver to compute a solution to the reactive transport equations