Demo 3: Reactive Transport

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Outline

- Introduction to reactive transport with Amanzi-ATS
  - Flow: Demo 1
  - Transport: Governing equations
  - Reactions: Third-party solvers
  - Coupling: Processes & Domains
- Surface reactive transport demo
- Subsurface reactive transport demo
- Integrated hydrology and reactive transport demo

Outline

These slides

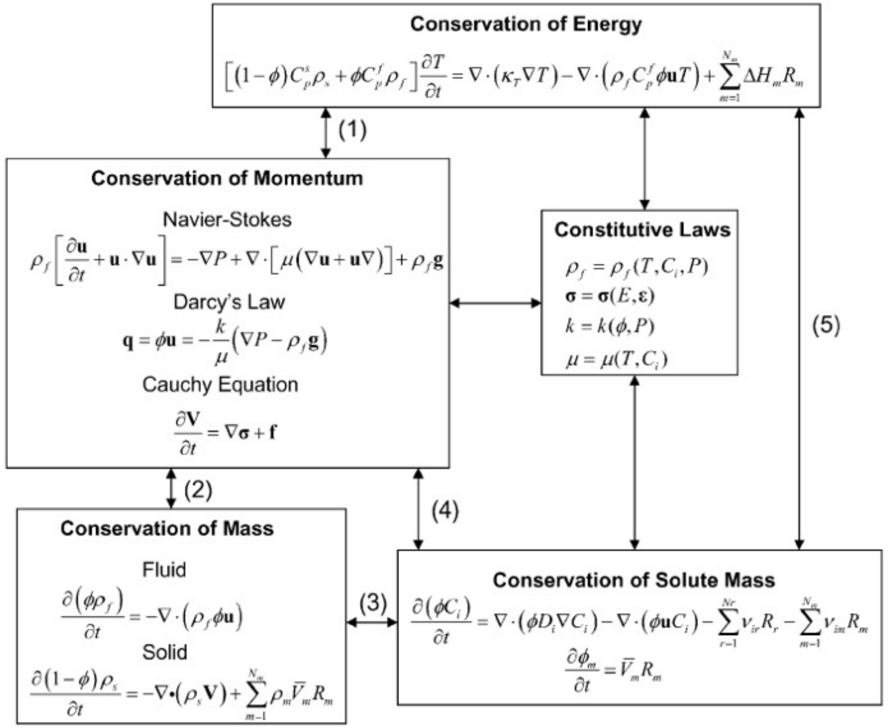
- Introduction to reactive transport with Amanzi-ATS
  - Flow: Demo 1
  - Transport: Governing equations
  - Reactions: Third-party solvers
  - Coupling: Processes & Domains

Jupyter Notebooks

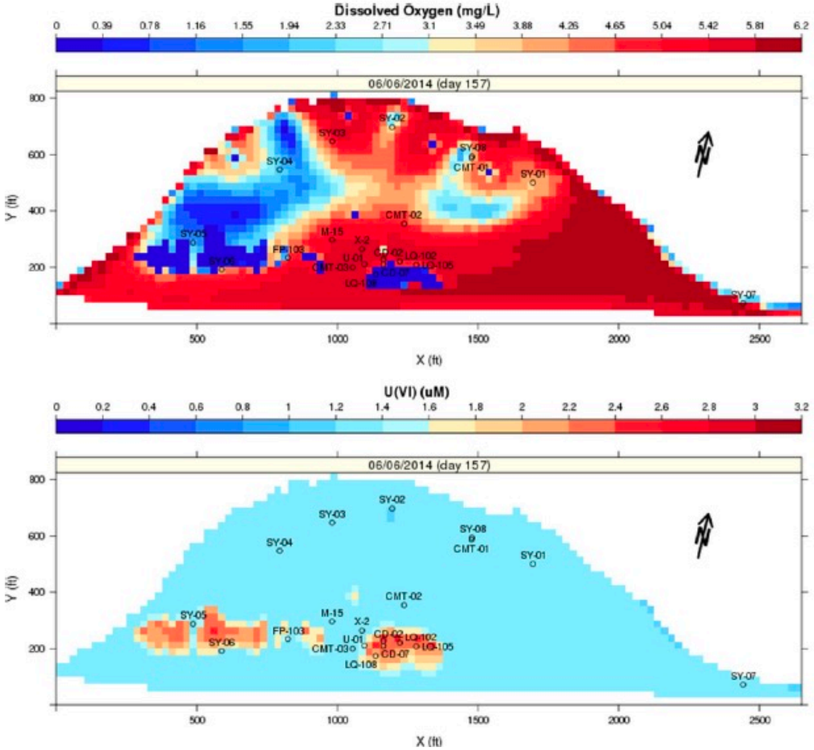
- Surface reactive transport demo
- Subsurface reactive transport demo
- Integrated hydrology and reactive transport demo

Reactive transport

- Reactive transport modeling has become an essential tool for the analysis of coupled physical, chemical, and biological processes



Steefel et al 2005



Yabusaki et al 2017

Reactive transport with Amanzi-ATS

- Meshing and workflow tools (Demo 2, lightning talks)
- Multiphysics framework to manage process complexity, specifically (weak, strong) coupling between processes
  - Surface and subsurface flow (Demo 1)
  - Surface and subsurface transport
  - Transport and reactions
  - Reactions: PFLOTRAN or CrunchFlow (via Alquimia)

Transport PK

```
<Parameter name="PK type" type="string" value="transport ats" />
```

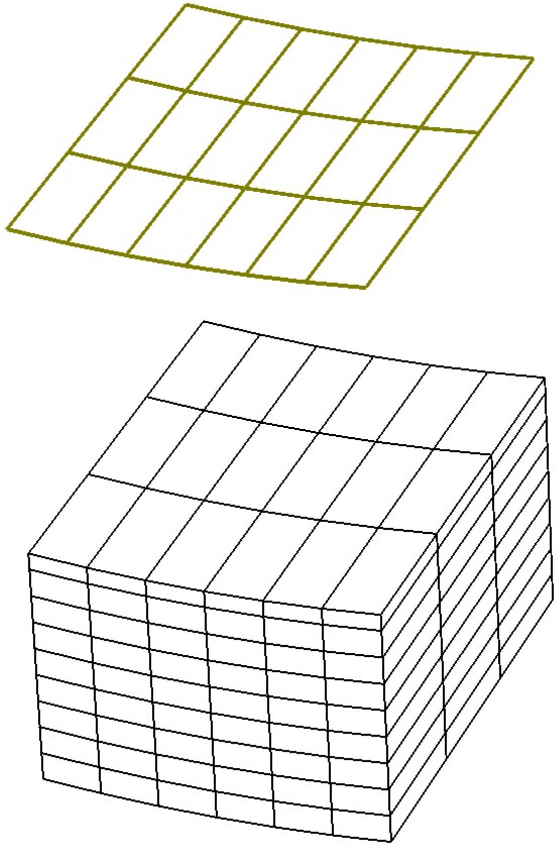
- Surface Transport

$$\frac{\partial \Theta_s \chi_i}{\partial t} - \nabla \cdot (h D \nabla \eta \chi_i) + \nabla \cdot (\mathbf{q}_s \chi_i) = Q_s \chi_s$$

- Subsurface Transport

$$\frac{\partial \Theta_g \chi_i}{\partial t} - \nabla \cdot (\theta S_w D \nabla \eta \chi_i) + \nabla \cdot (\mathbf{q}_g \chi_i) = Q_g \chi_g$$

surface domain



subsurface domain

Reactive Transport PK

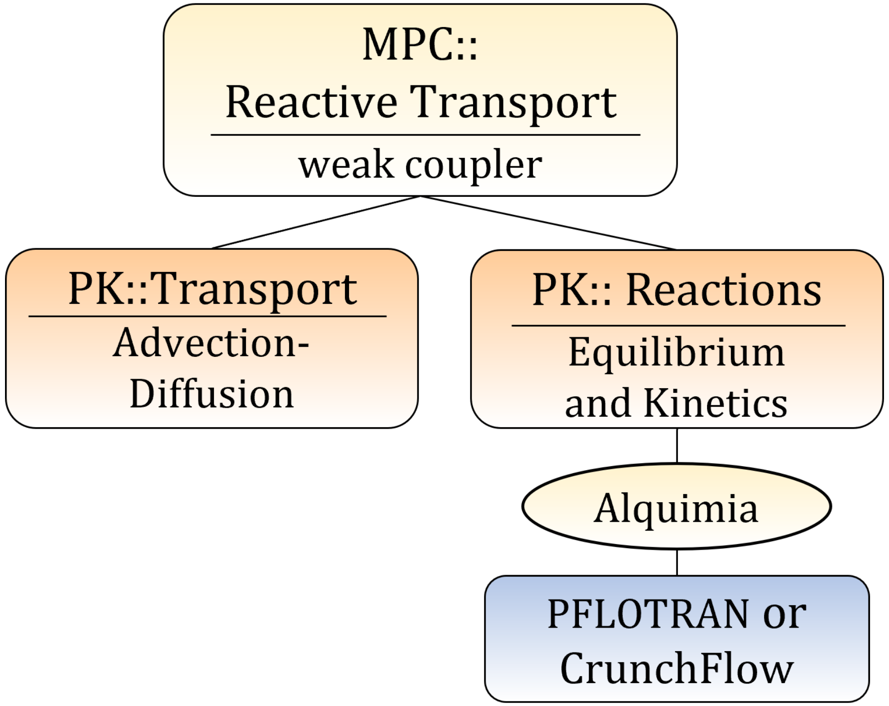
```
<Parameter name="PK type" type="string" value="reactive transport" />
```

- Operator Splitting (weak) coupling between transport and reactions
- Canonical Approach:
  - Transports total component concentrations

$$C_i = c_i + \sum_{j=1}^{N_x} \xi_{ij} c_j$$

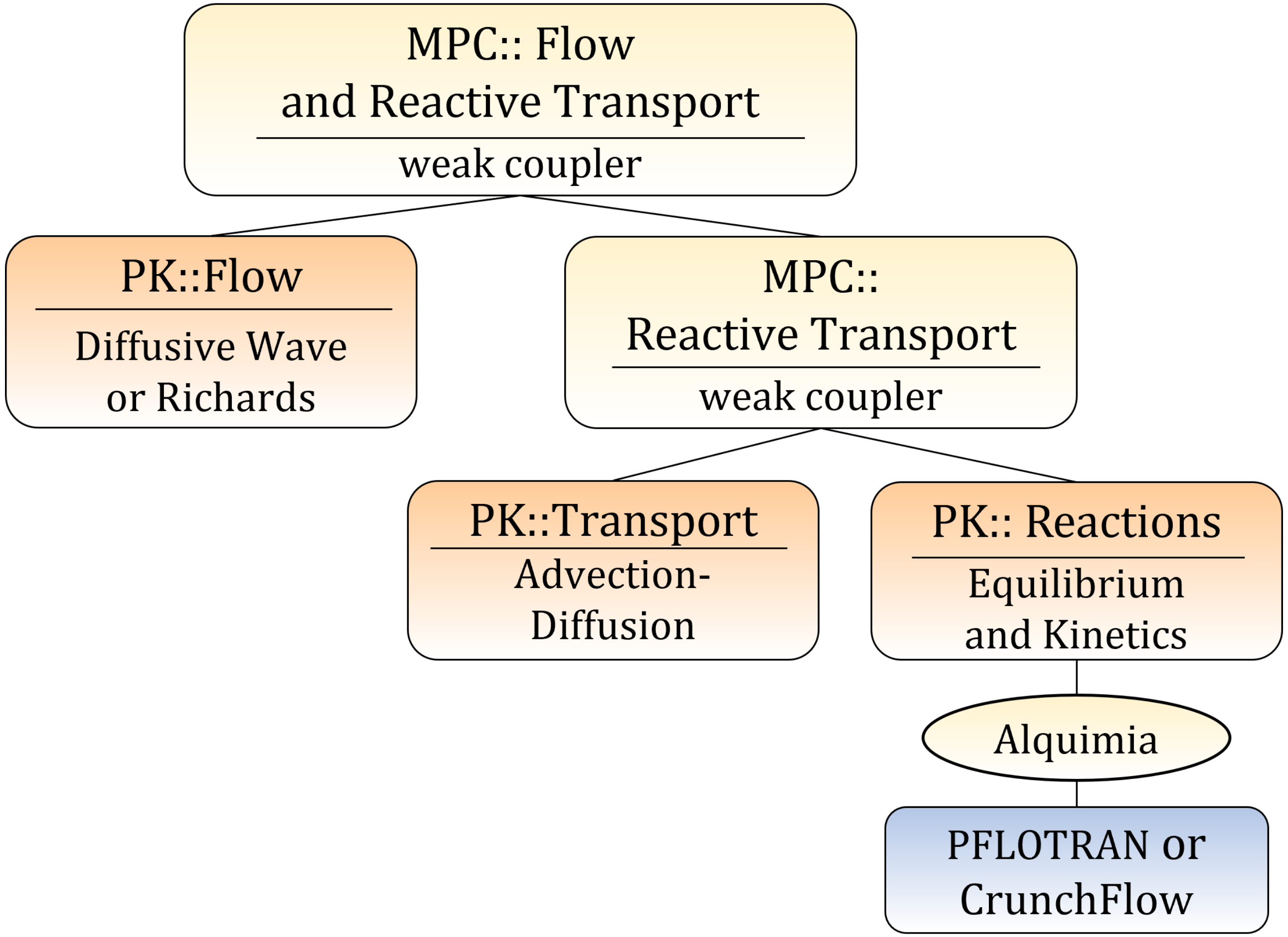
  - Does geochemical calculations cell by cell

$$c_j = (K_j \gamma_j)^{-1} \prod_{i=1}^{N_c} (\gamma_i c_i)^{\xi_{ij}}$$



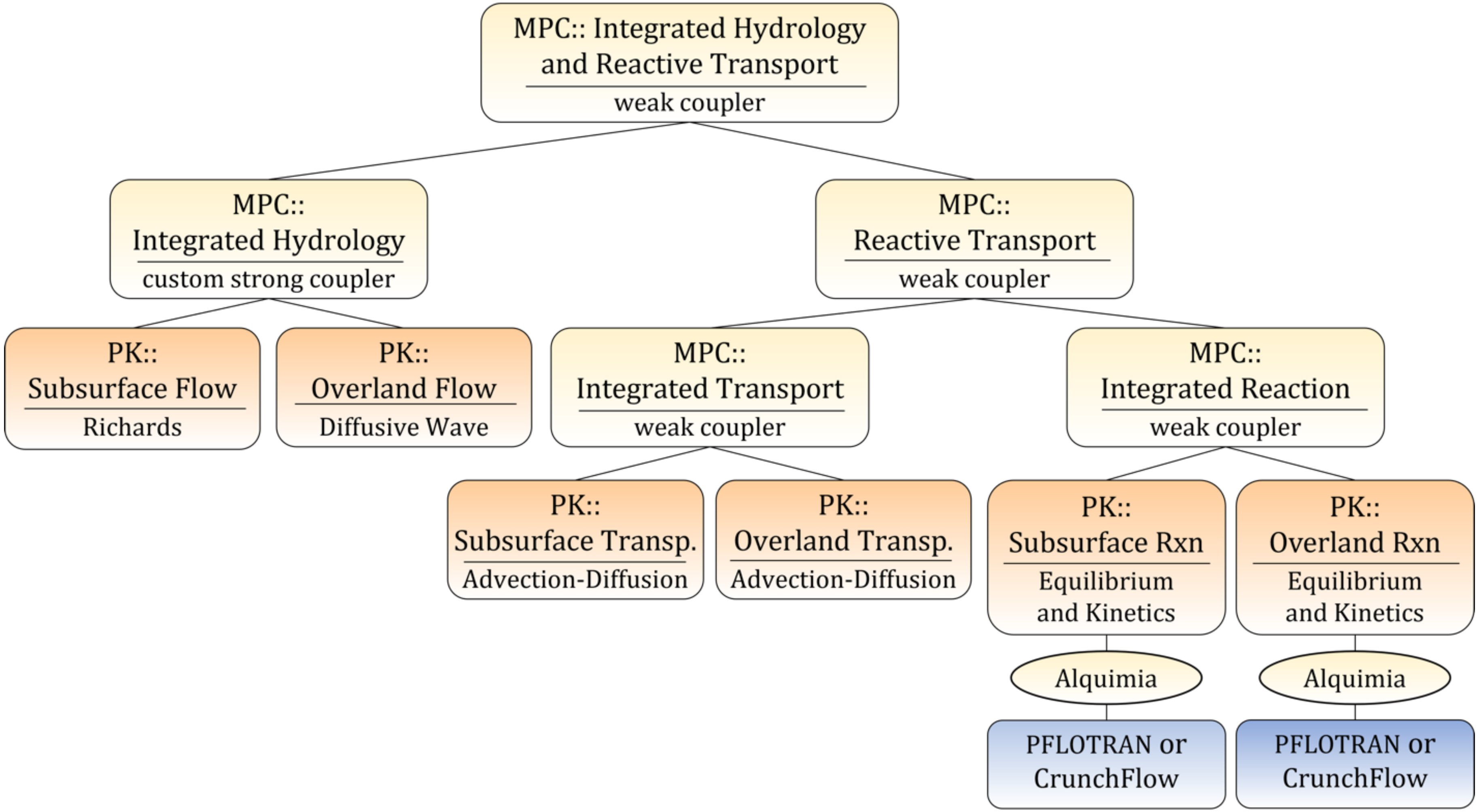
Flow and Reactive Transport PK

```
<Parameter name="PK type" type="string" value="flow reactive transport" />
```

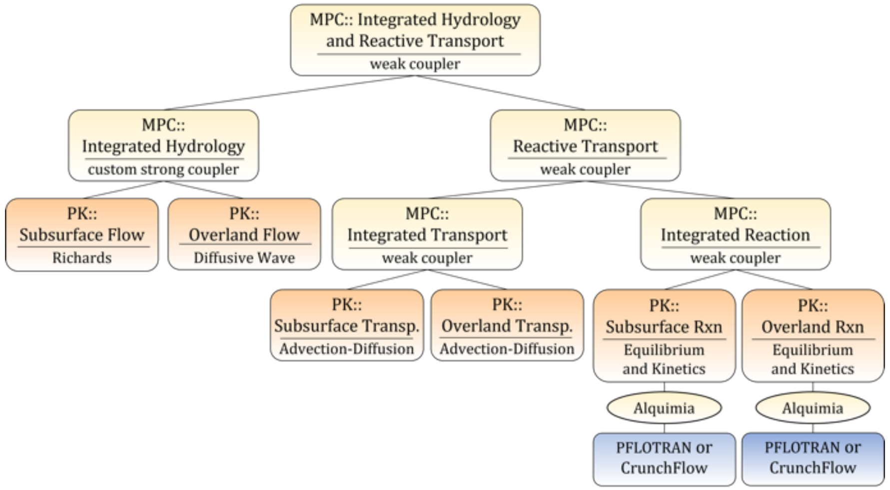


Integrated Flow and Reactive Transport PK

```
<Parameter name="PK type" type="string" value="flow reactive transport" />
```



Integrated Flow and Reactive Transport PK




```xml
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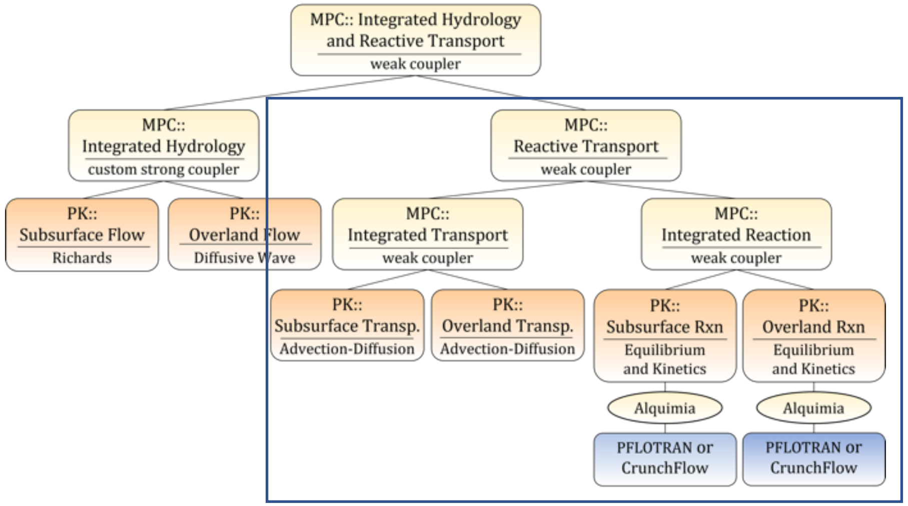
  <Parameter name="start time" type="double" value="0.0" />
  <Parameter name="end time" type="double" value="300.0" />
  <Parameter name="end time units" type="string" value="d" />
  <ParameterList name="PK tree">
    <ParameterList name="flow and transport">
      <Parameter name="PK type" type="string" value="flow reactive transport" />
      <ParameterList name="surface-subsurface flow coupler">
        <Parameter name="PK type" type="string" value="coupled water" />
        <ParameterList name="flow">
          <Parameter name="PK type" type="string" value="richards flow" />
        </ParameterList>
        <ParameterList name="overland flow">
          <Parameter name="PK type" type="string" value="overland flow, pressure basis" />
        </ParameterList>
      </ParameterList>
      <ParameterList name="reactive transport" type="ParameterList">
        <Parameter name="PK type" type="string" value="coupled reactive transport" />
        <ParameterList name="chemistry coupler" type="ParameterList">
          <Parameter name="PK type" type="string" value="weak MPC" />
          <ParameterList name="chemistry surface" type="ParameterList">
            <Parameter name="PK type" type="string" value="chemistry alquimia" />
          </ParameterList>
          <ParameterList name="chemistry subsurface" type="ParameterList">
            <Parameter name="PK type" type="string" value="chemistry alquimia" />
          </ParameterList>
        </ParameterList>
        <ParameterList name="surface-subsurface transport coupler">
          <Parameter name="PK type" type="string" value="surface subsurface transport" />
          <ParameterList name="subsurface transport">
            <Parameter name="PK type" type="string" value="transport ATS" />
          </ParameterList>
          <ParameterList name="surface transport">
            <Parameter name="PK type" type="string" value="transport ATS" />
          </ParameterList>
        </ParameterList>
      </ParameterList>
    </ParameterList>
  </ParameterList>
</ParameterList>
```

Integrated Flow and Reactive Transport PK

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        </ParameterList>
      </ParameterList>
    </ParameterList>
  </ParameterList>
</ParameterList>
```

Integrated Flow and Reactive Transport PK

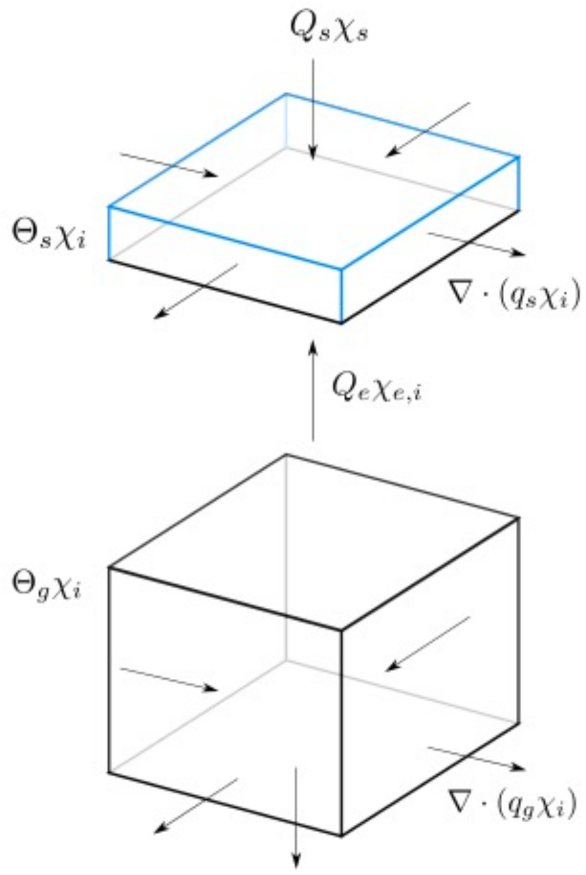
- Surface Reactive Transport

$$\frac{\partial \Theta_s \chi_i}{\partial t} - \nabla \cdot (hD\nabla \eta \chi_i) + \nabla \cdot (\mathbf{q}_s \chi_i) = Q_s \chi_s + Q_e \chi_{e,i} + Q_{r,s}$$

- Subsurface Reactive Transport

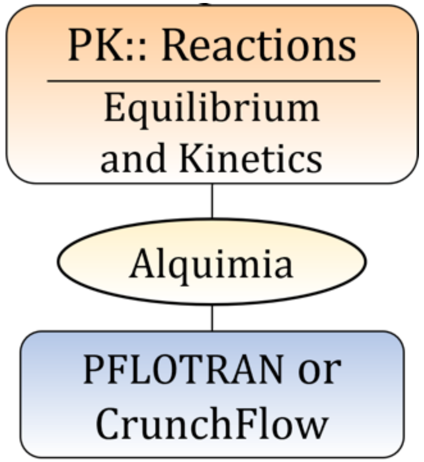
$$\frac{\partial \Theta_g \chi_i}{\partial t} - \nabla \cdot (\theta S_w D\nabla \eta \chi_i) + \nabla \cdot (\mathbf{q}_g \chi_i) = Q_g \chi_g + Q_{r,g}$$

$$-\nabla \cdot (\mathbf{q}_g \chi_i)|_{\partial\Omega} = Q_e \chi_{e,i}$$



Chemistry PK

- The geochemical problem is set up in a separate input file (either PFLOTRAN or CrunchFlow).
- The demos will focus how to connect input from Amanzi-ATS and the geochemical engine.
  - Driver-side (Amanzi-ATS)
  - Engine-side (PFLOTRAN or CrunchFlow)



Amanzi-ATS

Engine

specify engine and its input file name

```
<Parameter name="engine" type="string" value="PFloTran" />
<Parameter name="engine input file" type="string" value="./data/calcite.in" />
```

set up input and database files

```
RUNTIME
time_units       years
timestep_max     1.0
timestep_init    1.E-10
time_tolerance   0.01
correction_max   1.0
debye-huckel     true
database         ./data/calcite.dbs
```

```
DATABASE ./calcite.dat
LOG_FORMULATION
ACTIVITY_COEFFICIENTS TIMESTEP
MAX RESIDUAL TOLERANCE 1.d-15
```

define primary species

```
PRIMARY_SPECIES
H+
HCO3-
Ca++
END
```

```
PRIMARY_SPECIES
  H+
  HCO3
  Ca++
/
```

specify number and name of components to be transported (Transport PK)

```
<Parameter name="component names" type="Array(string)" value="{H+, HCO3-, Ca++}" />
<Parameter name="number of liquid components" type="int" value="3" />
```

define reaction network

(notebooks)

specify ICs, BCs, and sources using named geochemical conditions

```xml
<ParameterList name="initial condition" type="ParameterList">
  <ParameterList name="geochemical conditions" type="ParameterList">
    <ParameterList name="initial" type="ParameterList">
      <Parameter name="regions" type="Array(string)" value="{computational domain}" />
    </ParameterList>
  </ParameterList>
</ParameterList>
<ParameterList name="source terms">
  <ParameterList name="geochemical" type="ParameterList">
    <ParameterList name="Tracer injection" type="ParameterList">
      <Parameter name="regions" type="Array(string)" value="{surface domain}" />
      <Parameter name="solutes" type="Array(string)" value="{H+, HCO3-, Ca++}" />
      <Parameter name="times" type="Array(double)" value="{0.0,8640000.0}" />
      <Parameter name="geochemical conditions" type="Array(string)" value="{rain, rain}" />
      <Parameter name="time functions" type="Array(string)" value="{constant}" />
      <Parameter name="ats units [moles/m^3]" type="bool" value="true" />
    </ParameterList>
  </ParameterList>
</ParameterList>
```

define the geochemical conditions

```
Condition initial
units      mol/kg
temperature        25.0
SolidDensity       2700.0
pH                 charge
HCO3-              Calcite
Ca++               1.0e-3
!Mineral          <volume
Calcite            1.0e-2
END
```

```
Condition rain
units      mol/kg
temperature        25.0
pH                 charge
HCO3-              CO2(g)
Ca++               1.e-10
!Mineral          <volume
Calcite            0.0
END
```

```
CONSTRAINT initial
  CONCENTRATIONS
    H+       1.d-8 Z
    HCO3     1.d-3 M  Calcite
    Ca++     1.d-3 T
  /
  MINERALS
    Calcite 1.d-2 1.0d0
  /
END
```

```
CONSTRAINT rain
  CONCENTRATIONS
    H+       5.       Z
    HCO3     3.15e-4  G  CO2(g)
    Ca++     1.d-10   T
  /
END
```

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pH                   charge
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Calcite              0.0
END
```

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