Demo 1: Flow

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Outline

Flow Modeling and Simulation with ATS

- Flow is a critical driver in ecosystem dynamics
- Variably saturated flow
  - Richards' Equation
  - Infiltration in 1D column
- Overland flow
  - Diffusive Wave Equation
  - Simple geometry, rainfall inducing flow, highlight different outflow boundary conditions
  - Realistic catchment with single stream
- Integrated Hydrology
  - Coupling of Surface/Subsurface flow
  - Simple 2D – open-book (V – catchment)
  - 3D open-book to edit/extend.

Motivation/Background

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Flow plays a critical role in driving and coupling processes

- Climate impacts and feedbacks (carbon and nitrogen cycling).
- Contaminant transport and reactions.
- Complex interaction of land surface and subsurface processes.

Subsurface Flow

Richards' Equation

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Variably Saturated Flow: Richards' Equation

Richards (1931) model for variably saturated flow

$$\frac{\partial}{\partial t}(\phi n_l s) + \nabla \cdot \vec{q} = 0$$

$$\vec{q} = -n_l \frac{k_r \kappa}{\mu} (\nabla p + \rho \vec{\mathbf{g}})$$

$$p|_{\partial \Omega_D} = f$$

$$\vec{q} \cdot n|_{\partial \Omega_N} = g$$

- ➢ Φ - soil porosity [-]
- ➢ n_l - molar water density [mol m^{-3}]
- ➢ k_r - relative permeability [-]
- ➢ k - absolute permeability [m^2]
- ➢ μ - dynamic viscosity [Pa s]
- ➢ ρ - mass water density [kg m^{-3}]
- ➢ **g** - gravity [m s^{-2}]

where the unknowns are the water pressure *p* [Pa] and the Darcy flux ***q*** [mol m^{-2} s^{-1}]

Water Retention Models

Nonlinear models for $k_r(p) = k(s(p))$ and for $s(p)$ are defined by van Genuchten and Mualem equations:

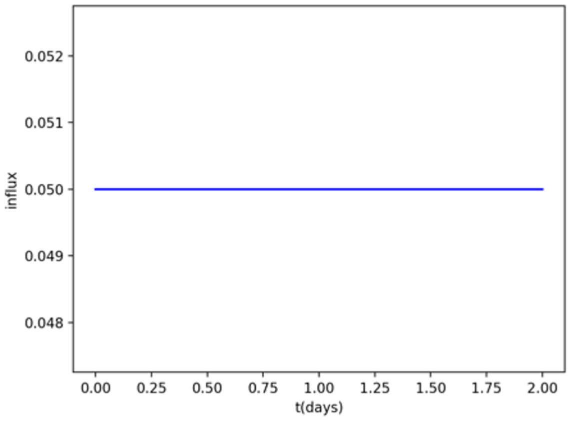
$$k_r = \sqrt{s}\left[1 - \left(1 - s^{1/m}\right)^m\right]^2, \qquad s = \left[1 + (\alpha p_c)^n\right]^{-m}$$

where m, n=1/(1-m) and α are parameters of the water retention model.

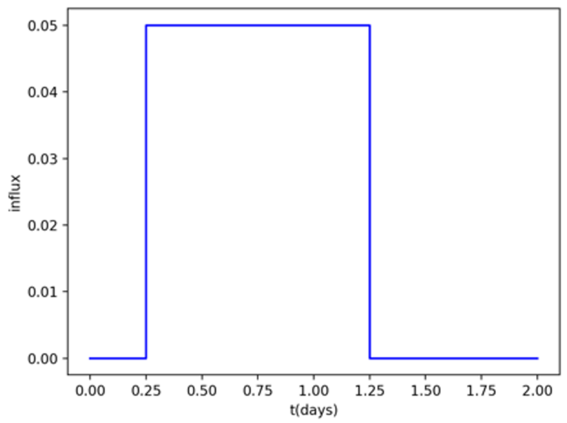
Infiltration into a 1D soil column (Transient)

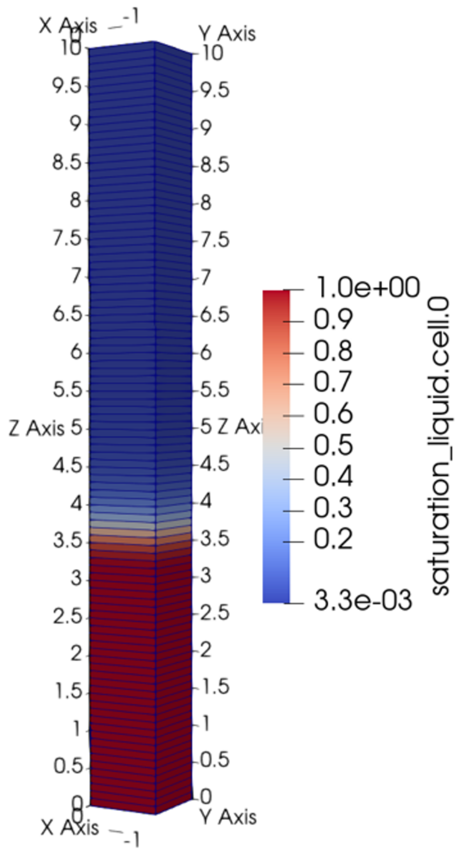
- ➢ Initial condition
  - Hydrostatic pressure with water table at 3m
- ➢ Boundary conditions
  - Infiltration from the top at the rate 0.05 [mol m^{-2} s^{-1}]

A



B





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Overland Flow

Diffusion Wave Model

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Diffusive wave model (DSW)

- This model has been used to simulate overland flow in wetlands and open channels.
- Describe shallow water movement across land surface:
  - rainfall has exceeded the infiltration rate
  - entire soil column becomes completely saturated and water exfiltrates at the surface

Diffusive Wave Model of Overland Flow

Wasantha Lal (1998)

- Q - sources [mol m $^{-2}$ s^{-1}]
- n_{mann}- Manning coefficient [s m$^{-1/3}$]
- Z_s - surface elevation [m^{-1}]
- ε - regularization [m]

$$\frac{\partial}{\partial t}(n_l h) + \nabla_S \cdot \vec{q}_s = Q$$

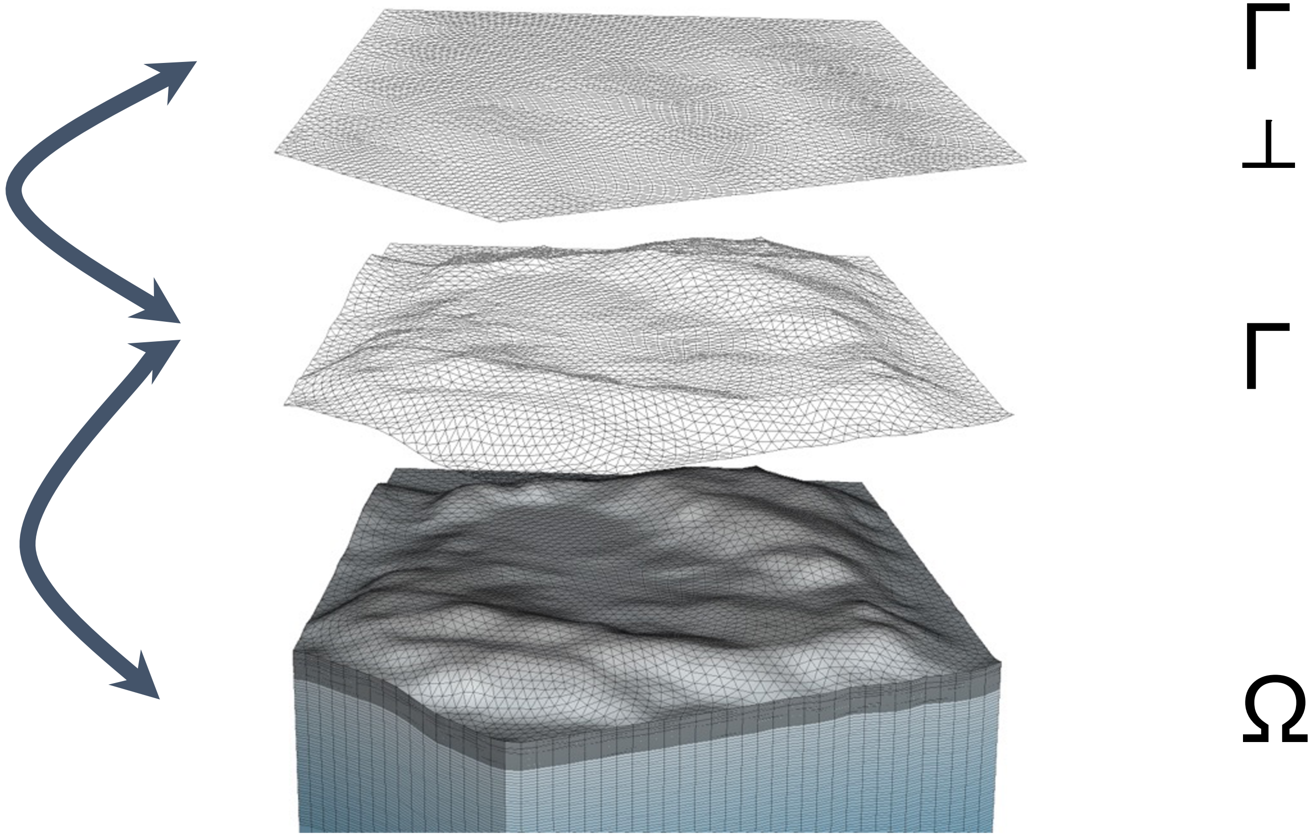
$$\vec{q}_s = -n_l h \frac{h^{\frac{2}{3}}}{n_{mann}\sqrt{|\nabla_S z_s| + \epsilon}} \nabla_S (h + z_s)$$

$$h|_{\partial\Gamma_D^\perp} = f^s$$

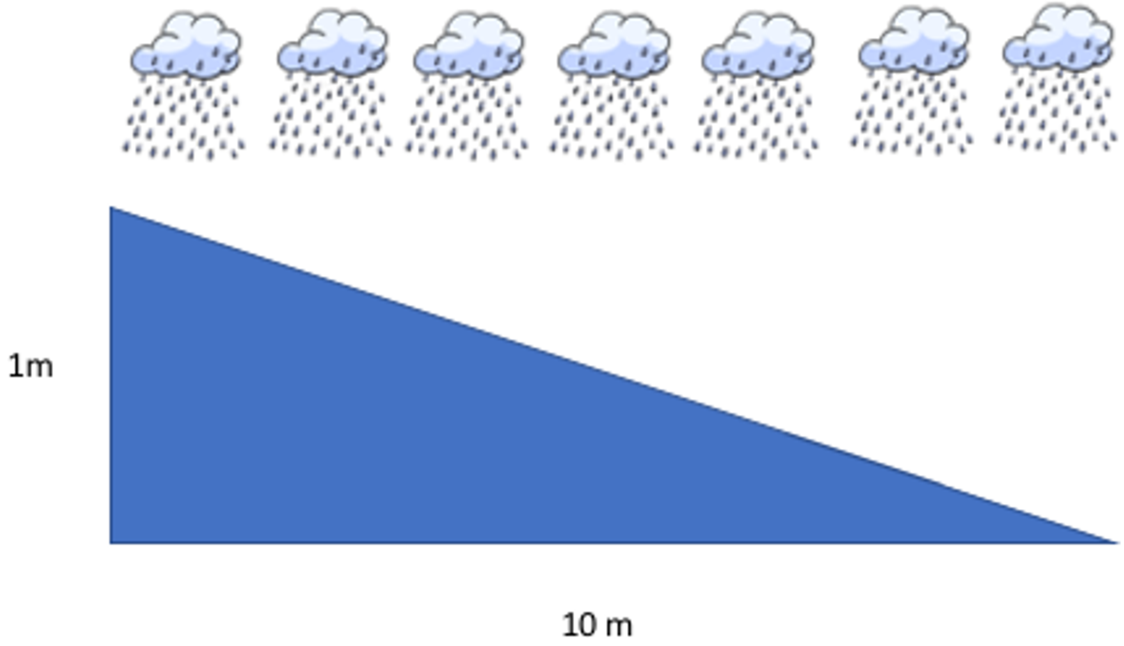
$$\vec{q}_s \cdot n|_{\partial\Gamma_N^\perp} = g^s$$

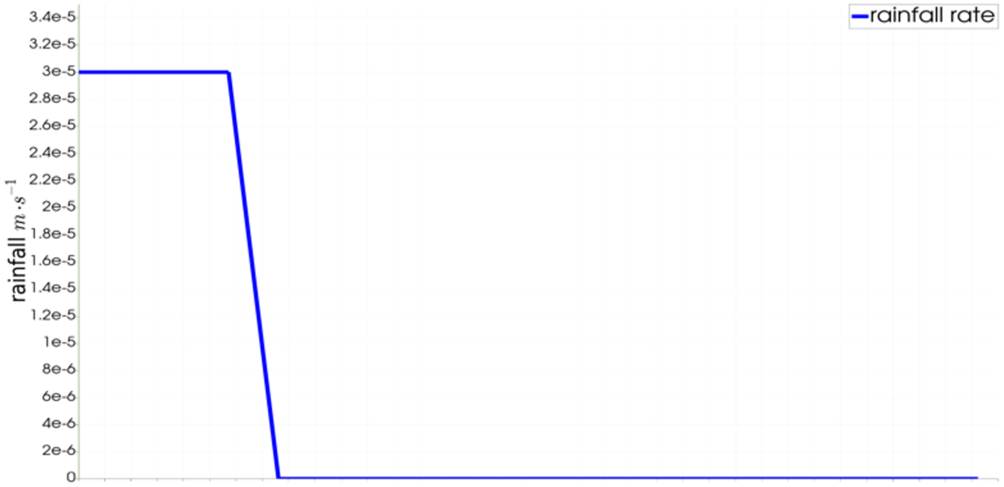
where the unknowns are the ponded depth of water h_w [m], and the flux of surface water $\mathbf{q_s}$ [mol m^{-1} s^{-1}]

Meshes for model design



Overland Flow on a planar hillslope





- Case1: no flow BC
- Case2: critical depth BC
- Case3: zero gradient BC
- Case4: max depth BC

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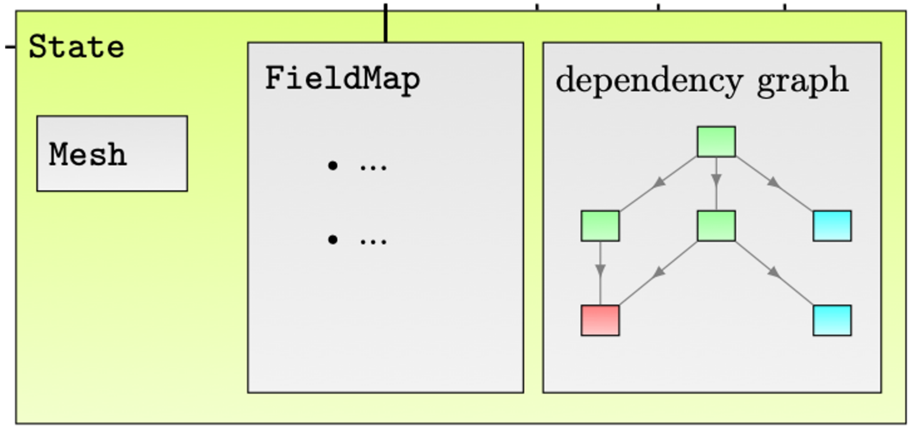
Integrated Hydrology

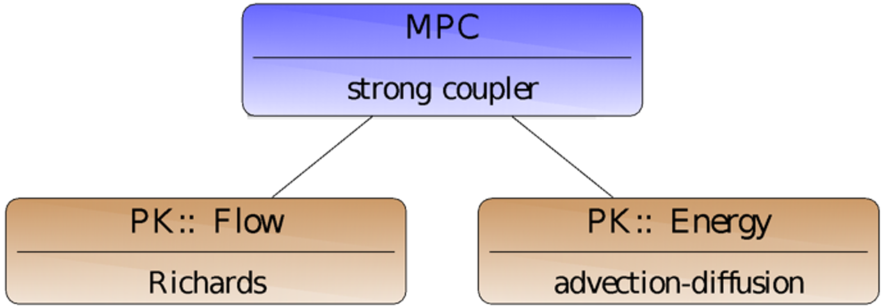
Coupled surface and subsurface flow

Arcos Multiphysics Framework

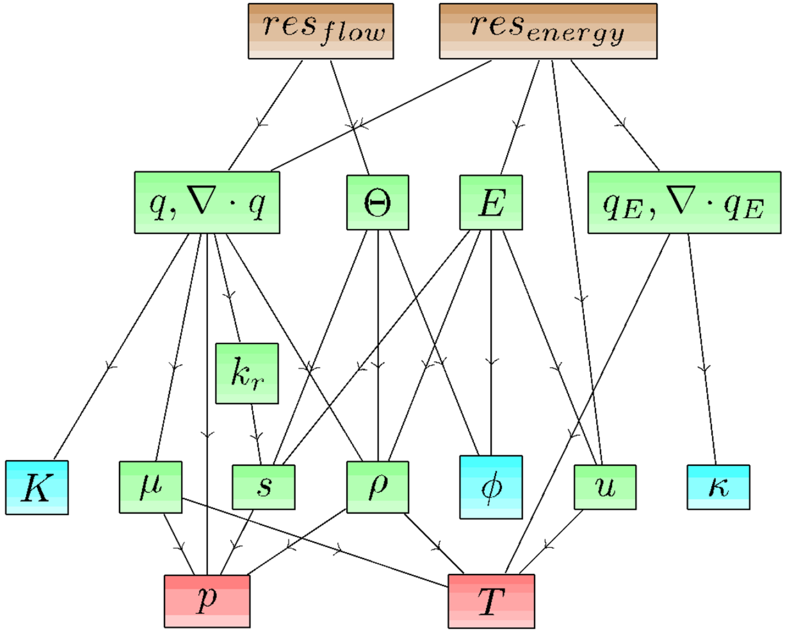
The Arcos multiphysics framework, is a fully functional framework serving Amanzi and ATS, but may also be viewed as a reference implementation to explore interface designs, coupling strategies and outreach to the community.



Dynamic Data Manager



Process Kernel Tree



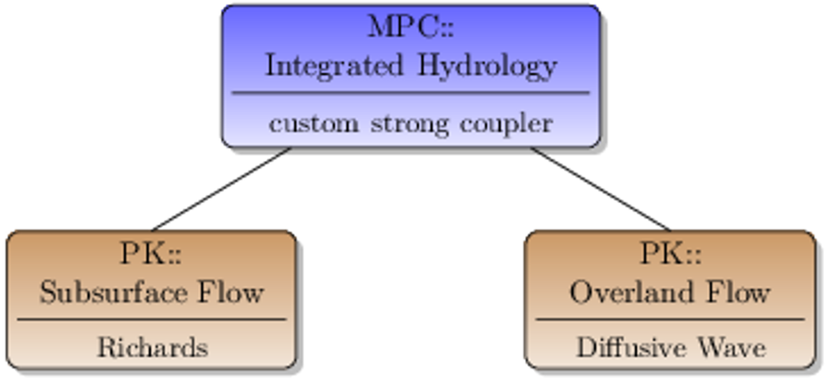
Dependency Graph

Coon et al. Env. Model. & Soft. 2016

Model Coupling: Approach

The Arcos framework supports a flexible and phased approach to development and testing:

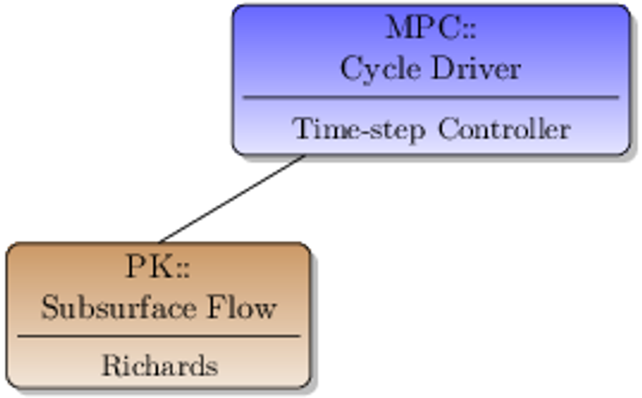
- Develop and test Process Kernels (PKs), such as, flow, transport, and energy in isolation.
- Develop Multi-Process Couplers (MPCs) to create and test an integrated model.
- MPCs fall in two categories:
  - **Strong:** forms and solves a single system of equations (e.g., fully implicit)
  - **Weak:** sequentially steps cycles through the process kernels (typical in flow and transport)
- **Users** are able to express the coupled model at high-level in the input file using PK-trees.



PK-tree describing integrated hydrology.

Model Coupling (PK-Trees)

First, we introduced subsurface flow using Richards Equation:



Schematic of the PK-tree for subsurface flow.

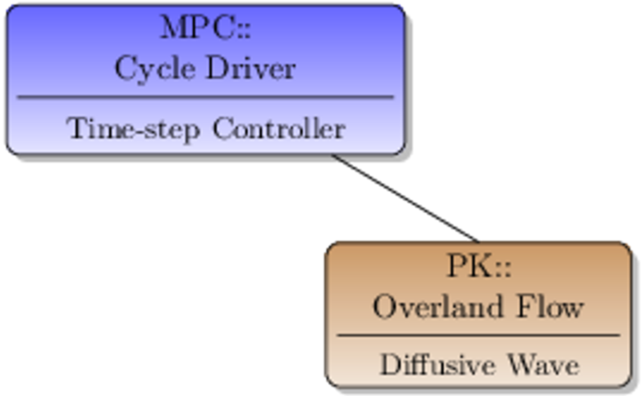
```xml
<ParameterList name="cycle driver" type="ParameterList">
  <Parameter name="start time" type="double" value="0.0" />
  <Parameter name="start time units" type="string" value="s" />
  <Parameter name="end time" type="double" value="10.0" />
  <Parameter name="end time units" type="string" value="d" />
  <ParameterList name="PK tree" type="ParameterList">
    <ParameterList name="Richards" type="ParameterList">
      <Parameter name="PK type" type="string" value="richards flow" />
    </ParameterList>
  </ParameterList>
</ParameterList>
```

Input file showing the “cycle driver” element with the PK-tree sublist for subsurface flow.

A single PK is the simplest PK-Tree you can have and doesn’t need a coupler, just the top-level cycle driver.

Model Coupling (PK-Trees)

Second, we introduced overland flow using a Diffusion Wave Equation:



Schematic of the PK-tree for overland flow.

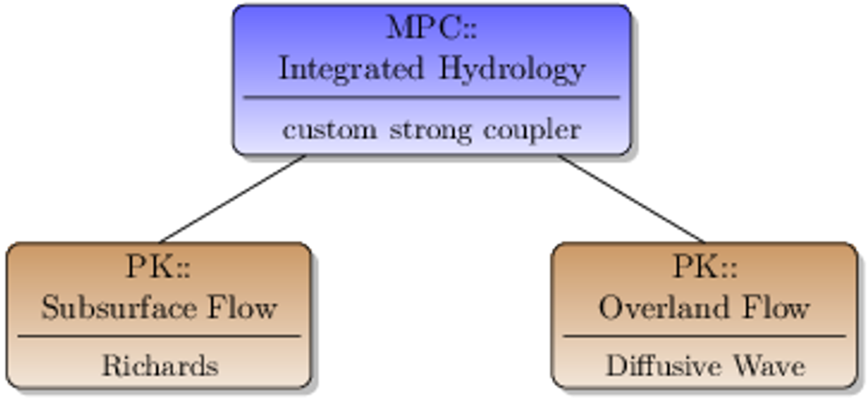
```xml
<ParameterList name="cycle driver" type="ParameterList">
  <Parameter name="start time" type="double" value="0.0" />
  <Parameter name="start time units" type="string" value="s" />
  <Parameter name="end time" type="double" value="10800.0" />
  <Parameter name="end time units" type="string" value="s" />
  <ParameterList name="PK tree" type="ParameterList">
    <ParameterList name="overland flow" type="ParameterList">
      <Parameter name="PK type" type="string" value="overland flow, pressure basis" />
    </ParameterList>
  </ParameterList>
</ParameterList>
```

Input file showing the “cycle driver” element with the PK-tree sublist for overland flow.

A single PK is the simplest PK-Tree you can have and doesn’t need a coupler, just the top-level cycle driver.

Model Coupling (PK-Trees)

Finally, we couple surface and subsurface flow models



Schematic of the PK-tree for Integrated Hydrology (coupled overland and subsurface flow).

```
<ParameterList name="cycle driver" type="ParameterList">
  <Parameter name="start time" type="double" value="0.0" />
  <Parameter name="start time units" type="string" value="s" />
  <Parameter name="end time" type="double" value="10.0" />
  <Parameter name="end time units" type="string" value="d" />
  <ParameterList name="PK tree" type="ParameterList">
    <ParameterList name="surface-subsurface coupler" type="ParameterList">
      <Parameter name="PK type" type="string" value="coupled water" />
      <ParameterList name="flow" type="ParameterList">
        <Parameter name="PK type" type="string" value="richards flow" />
      </ParameterList>
      <ParameterList name="overland flow" type="ParameterList">
        <Parameter name="PK type" type="string" value="overland flow, pressure basis" />
      </ParameterList>
    </ParameterList>
  </ParameterList>
</ParameterList>
```

Input file showing the “cycle driver” element with the PK-tree sublist for coupled overland and subsurface flow (integrated hydrology).

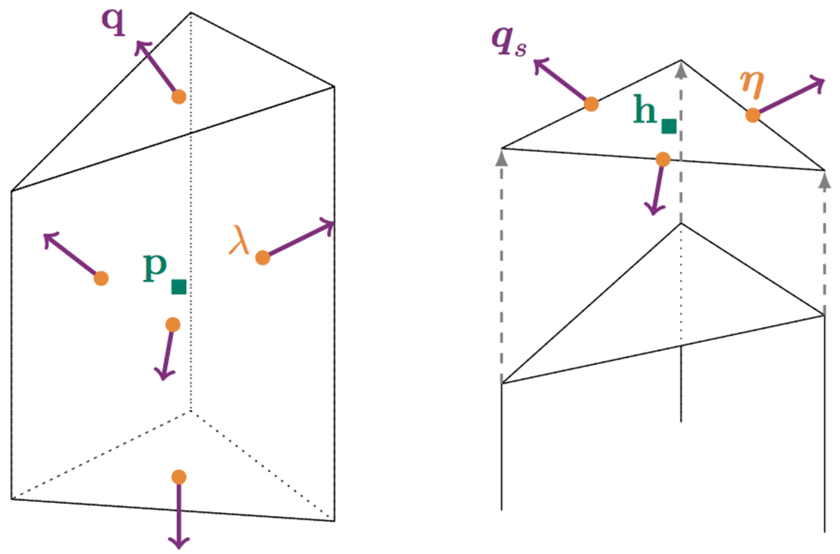
to create the Integrated Hydrology model.

Integrated Hydrology: Coupling Details

Arcos and the low-level infrastructure (e.g., mesh, discretization, and solvers) are helpful but strong couplers a

- Combine matrices (and or Jacobians) of the two models together in a single system.
- Use continuity of normal flux and pressure to create this fully coupled system.
  - rewrite ponded depth as pressure
- Appropriately match entities from one domain to the other, e.g., normal flux from a subsurface face is a source in that cell for surface flow.
- Ensure conservation of mass

Coon E. T., et al., 2020, https://doi.org/10.1016/j.advwatres.2020.103701



Schematic showing the locations on the mesh of the discrete unknowns in the subsurface flow (pressure: p - cells, $\boldsymbol{\lambda}$- faces), q normal flux; and surface flow (ponded depth: h-cells, qs normal flux).

Jump to the notebook

Two examples of integrated hydrology:

- 2D transect of a V (open-book) watershed
  - explore model setup and run existing input file
- 3D open-book watershed
  - given an almost complete input file, fill in the gaps and explore different scenarios