

# A Graph-Theoretic Framework for the Systematic Representation and Generation of Conceptual Hydrological Model Structures

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## Short Summary

- From selecting models to sampling model structures
- Conceptual hydrological models can be represented as directed graphs and transformed into runnable models
- Model structures can systematically generated and sampled
- Structural uncertainty becomes a testable hypothesis space

## Motivation

- Hydrological predictions depend strongly on model structure
- Model selection mostly driven by „legacy, rather than adequacy“
- Structural uncertainty is rarely treated explicitly and equifinality is omnipresent → systematic analysis requires formalization of model structures

### Research Objective:

Enable systematic sampling and evaluation of hydrological model structures through a formalized and unified representation

## Outlook

### Next steps

- Benchmarking with more efficient recursive model generator (incidence based)
- Testing larger and more complex model structure spaces

### Vision

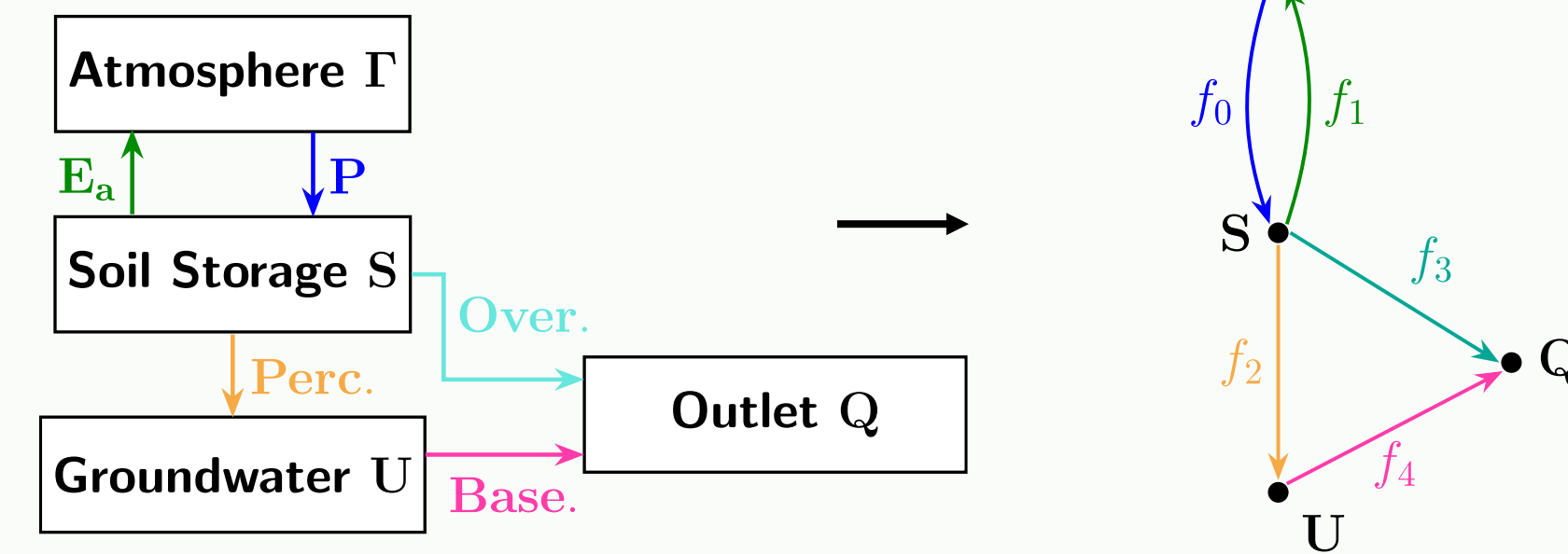
- From ad hoc model choice to systematic structure exploration (hypothesis testing)
- From implicit assumptions to explicit structural uncertainty
- Data-driven identification of the most suitable model structures

## Core Idea

### 1 Representation

Conceptual hydrological models can be represented as directed graphs

- Nodes: compartments (incl. boundaries)
- Edges: fluxes between compartments



### 2 Formalization

Graph structures can be encoded algebraically

#### Adjacency matrix $A$

- Encodes connectivity of compartments and direction of fluxes
- Defines model topology (structure)

	to			
from	$\Gamma$	$S$	$U$	$Q$
$\Gamma$	0	1	0	0
$S$	1	0	1	1
$U$	0	0	0	1
$Q$	0	0	0	0

#### Incidence matrix $B$

- Encodes node-edge relationships
- Shows origin (-) and target (+) of flux  $f$
- Enables direct derivation of model ODE system

	$f_0$	$f_1$	$f_2$	$f_3$	$f_4$
$\Gamma$	-1	1	0	0	0
$S$	1	-1	-1	-1	0
$U$	0	0	1	0	-1
$Q$	0	0	0	1	1

### 3 Consequence

Graph-based encoding enables:

- Systematic generation of model structures
- Formal search and hypothesis testing
- Direct translation into runnable models (e.g. with RAVEN)

## Model Generator

From graphs to automatic sampling of structure spaces

### I Define Structure Space

- Maximum Graph
- All possible connections

	$\Gamma$	$S$	$U$	$Q$
$\Gamma$	0	1	0	0
$S$	2	0	2	1
$U$	0	0	0	3
$Q$	0	0	0	0

Adjacency matrix with process indices

- 2 percolation methods → [linear, power-law]
- 2 evaporation methods → [HBV, VIC]
- 3 baseflow methods → [constant, linear, power-law]

### II Generate Structures

- Constrained matrix permutation enumerates candidate structures

### III Filter Structures

- Overproduce and select

#### Topology Rules (physical plausibility)

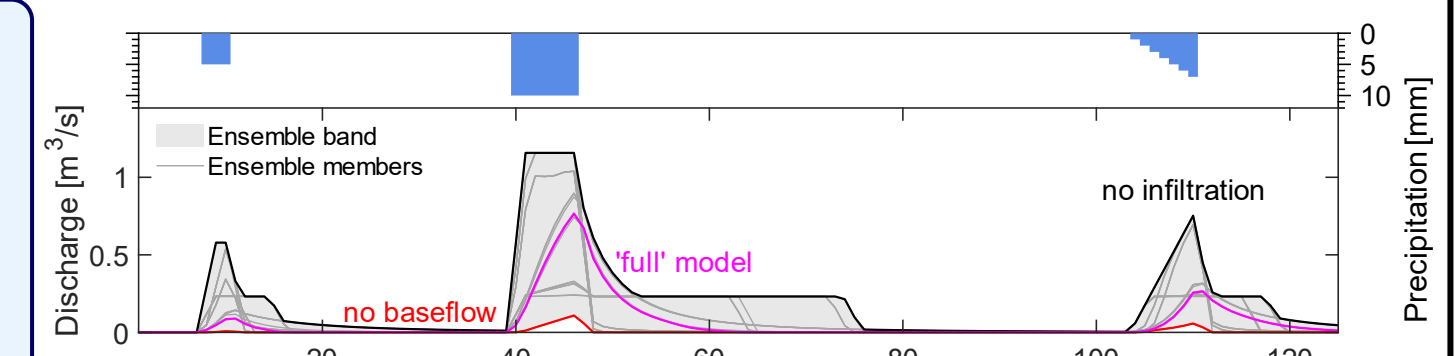
Rule	Matrix	Rule	Matrix	Rule	Matrix
No magic wells	$\begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$	No dead ends	$\begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$	No sub-models	$\begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$

Semantic Rules (user-defined constraints - e.g. „my models require a flux from soil to surface water (direct runoff)“

	$\Gamma$	$S$	$U$	$Q$
$\Gamma$	0	1	0	0
$S$	1	0	1	1
$U$	0	0	0	1
$Q$	0	0	0	0

### IV Execute & Analyse

- Automatic translation into runnable RAVEN models
- Post hoc analysis



### V Answer Key Questions

How many structures are feasible? Which ones explain the data best? What characterizes them? Are they unique?

