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Instituto de Pesquisas Hidráulicas – IPH

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Iporã Brito Possantti

A synthesis on hydrological models and their applications in watershed revitalization planning

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Thesis presented to the Graduate Program in Water Resources and Environmental Sanitation at the Federal University of Rio Grande do Sul, as a partial requirement for obtaining the doctoral degree.

Advisor: Prof. Dr. Guilherme Fernandes Marques

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Acknowledgements

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palavras-chave — Oornare arcu dui; mauris augue; lacus sed turpis.

Abstract

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keywords — Oornare arcu dui; mauris augue; lacus sed turpis.

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Acronyms

`CN` *Curve Number*. 67–69, 76, 109

`ET` evapotranspiration. 45, 47, 48, 63

`GLUE` *Generalized Likelihood Uncertantiy Estimation*. 10, 55

`HAND` Height Above Nearest Drainage. 96, 97

`MDE` Digital Elevation Model. 92, 96

`NBS` Nature-based solutions. 95

`SCS` *Soil Conservation Service*. 64, 67–69, 76

`TWI` Topographic Wetness Index. 91, 92, 95, 97

Symbols

Chapter 1 – Theories and evidences

$\mathcal{L}$	Informal likelihood
μ	Mean
Ω	Space of possibilities
σ	Standard deviation
σ^2	Variance
Θ	Parameter vector
Υ	Input data vector
ε	Error
E	Evidence
H	Hypothesis
M	Model
n	Sample size
O	Observation
P	Probability
S	Statement
s^2	Sample variance

Chapter 2 – Sistems and models

Δt	Time step
μ_M	Mean of simulated points
μ_O	Mean of observed points
Ω_Θ	Parametric space
σ_M	Standard deviation of simulated points
σ_O	Standard deviation of observed points
KGE	Kling-Gupta efficiency
MAE	Mean absolute error
RMSE	Root mean square error
R^2	Coefficient of determination
Θ	Set of parameters
Υ	Exogenous variables, input data
E	Evapotranspiration

I	Input material flow into a compartment
k	Mean residence time
O	Output material flow from a compartment
P	Precipitation, rain
Q	Runoff, discharge
R	Rapid surface runoff
r	Correlation coefficient
S	State or level of a compartment
$s_{\max}$	Storage capacity
s_a	Activation level
s_c	Connectivity level
$y_{M,i}$	Simulated point (value)
$y_{O,i}$	Observed point (value)

Chapter 3 – Hydrology

α	Drainage area per unit contour
β	Slope of the terrain
Δz	Difference in hydrostatic potential (Darcy's Law)
κ	Lateral hydraulic conductivity, transmissivity
$\kappa_{\max}$	Maximum lateral hydraulic conductivity
λ	Topographic wetness index
$\nabla\Phi$	Hydrostatic potential gradient (Darcy's Law)
ν	Hydrogram volume
ω	Scaling factor
$\mathbf{C}$	Vegetation canopy
$\mathbf{D}$	Gravitational deficit
$\mathbf{D}_{\mathrm{v}}$	Capillary deficit
$\mathbf{G}$	Phreatic zone
$\mathbf{O}$	Organic horizon
$\mathbf{S}$	Soil surface
$\mathbf{V}$	Vadose zone
HT	TWI enhanced by HAND
H	HAND - Height Above the Nearest Drainage
$\mathrm{H}_{\max}$	Upper threshold of HAND
T	TWI - Topographic Wetness Index
$\mathrm{T}_{\max}$	Upper threshold of TWI
V_{c}	Capillary water in the vadose zone
V_{g}	Gravitational water in the vadose zone

$\tilde{\mathrm{H}}$	Normalized HAND
$\tilde{\mathrm{T}}$	Normalized TWI
A	Cross-sectional area of the pipe (Darcy's Law)
c_{max}	Interception capacity
e_{c}	Evaporation in the canopy
e_{g}	Transpiration in the phreatic zone
e_{o}	Transpiration in the organic horizon
e_{pot}	Potential evapotranspiration
e_{s}	Evaporation at the surface
e_{v}	Transpiration in the vadose zone
f	Infiltration
f_{max}	Infiltration capacity
g	Mean residence time of the aquifer
H_w	Dominance factor of HAND
H_α	Threshold for drainage initiation
K	Hydraulic conductivity
k	Mean detention time of linear reservoir
l	Length of the pipe (Darcy's Law)
m	Vertical uniformity of the soil
n	Effective number of linear reservoirs
o_{max}	Field capacity of the organic horizon
P	Precipitation, rain
P_{s}	Effective rain
P_{x}	Excess rain
Q	Runoff, flow, discharge
Q_{gt}	Translational runoff
$q_{\mathrm{g},i}$	Lateral base flow per unit contour
$Q_{\mathrm{g,max}}$	Aquifer production capacity
Q_{g}	Base flow
q_{o}	Percolation between horizons
q_{se}	Direct rain, excess saturation runoff
q_{si}	Runoff, surface flow
q_{ss}	Exfiltration, subsurface runoff
q_{v}	Recharge
s_{max}	Surface detention capacity
u	Darcy velocity (Darcy's Law)
v_{max}	Field capacity of the mineral horizon

Chapter 0

Motivação

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On February 16, 2023, at 3:23 PM, two black swans were observed in the park behind the Palácio das Laranjeiras, Rio de Janeiro, Brazil. A single black swan would already be sufficient to prove that *not all swans are white*.

Chapter 1

Theories and evidences

I had long observed that, with regard to customs, it is sometimes necessary to follow opinions that we know to be uncertain as if they were indubitable; but, as I then wished to concern myself solely with the search for truth, I thought it was necessary to do the opposite, and reject as absolutely false everything in which I could imagine the slightest doubt, in order to see if anything would remain in my beliefs that was entirely indubitable.

René Descartes, *Discourse on the method*, p. 15 [1]

It is clearly possible to develop and use environmental models without any underlying philosophy. Many practitioners do so, although most perhaps ultimately want to develop and use models that are *as realistic as possible*, given the constraints of current knowledge, computational capabilities, and observational technologies.

Keith Beven, (2002, p. 2465) [2]

1.1 Electronic circuits

Simulating a hydrological model consists of applying electrical voltages to electronic circuits. This is *literally* what happens during a simulation. The manner and order in which the voltages are applied directly correspond to the instructions provided to the central processing unit (CPU) of a machine, usually a digital computer. In this case, we provide the operating system with code in a high-level language (such as `Fortran` or `Python`), which is interpreted into a lower-level version, processable by the machine. Thus, all information, including data and instructions, is converted into binary digits

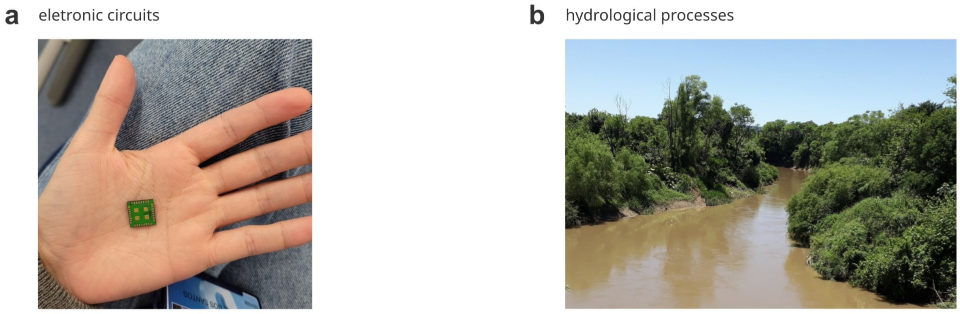

Figure 1.1 — From electronic circuits to hydrological processes. a. — Applying a hydrological model consists of *literally* applying voltages to digital electronic circuits. The simulation results refer literally and objectively to the processing of the binary states of transistors. **b.** — Hydrological model users generally accept that the electronic results are a *realistic representation*, albeit approximate, of various hydrological processes, whether it be rainfall infiltration, surface runoff q_{si}, or river discharge. How is this possible? The photograph in (**a**) was kindly provided by electrical engineer Karina Kerne; the photograph in (**b**) was taken by the author on the bridge over the Pardinho River south of Lago Dourado, Santa Cruz do Sul, Rio Grande do Sul, Brazil.

(*bits*) stored by states of electronic circuits called **transistors**. The processing, in turn, happens through logic gates that perform *boolean* operations of conjunction $\wedge$, disjunction $\vee$, and negation $\neg$ on the bits. All the graphs, maps, and animations we see after a simulation objectively refer to the recorded states of sections of the machine's digital memory—numbers represented in binary form by transistors. That said, how is it possible that binary patterns in digital circuits have *anything to do* with rainfall, river runoff, or soil saturation?

As highlighted by Keith Beven in the epigraph of this chapter, it is rare for applications of hydrological models[1] to ground this issue with an *explicit philosophy* [2]. Even so, model users generally believe that simulation results provide a *realistic representation* of processes and phenomena that indeed exist in the world, not just in electronic circuits, such as soil erosion, river runoff, plant transpiration, etc. Of course, no one thinks that hydrological model simulations provide an *exact* description of reality, but it is generally accepted that they offer an *approximate* description of reality and that this approximation can be improved as new computing and observation technologies become available. This belief is further accentuated when simulation results are directed to assist in important decision-making related to water resource management in State organizations or private companies. If material and human resources are allocated based on these results, they had better agree with reality!

Beven calls this common implicit philosophy among hydrological model users **pragmatic realism**. He classifies this stance as naïve, demonstrating that the much-desired realistic representation, when taken seriously, becomes an extraordinary goal in light of the **empirical uncertainty** that exists in hydrological modeling. If water resource management genuinely wishes to build **evidence-based policies**, scientific advice must adopt a *critical stance* toward the use of models and their results. As highlighted by Ongaro and Andreoletti, uncertainty is a pervasive attribute in the decision-making process [3]. In this context, they argue that the proper role of scientific authorities is to inform about empirical uncertainties so that other interest groups can deliberate on the ethical and political uncertainties at play. However, this critical stance is only possible from an explicit philosophical perspective, referred to here as **instrumentalism**, which brings to the fore several problems that need to be addressed before affirming the correspondence between electromagnetic fields in electronic circuits

[1] Although Beven actually refers to environmental models in general, including atmospheric and geochemical models, I will here limit the discussion to hydrological models.

and hydrological processes in watersheds.

In this spirit, the aim of this chapter is to establish the instrumentalist philosophical foundations that will be explicitly used throughout this thesis. I will articulate the following issues from the Philosophy of Science: the problem of justification, Bayesian epistemology, the falsifiability of theories, the concept of paradigms, and the underdetermination problem. The ontology of models, which is also a relevant topic, will be addressed in the next chapter. For the purposes of this chapter, one must consider that **a model is a symbolic vehicle of a theory**. The intention is not to exhaust the presented topics (as this would require writing many other theses!). On the contrary, this chapter should be understood as a panoramic view, as if we were standing atop a mountain. This analogy is particularly useful, as the summit provides a good understanding of the landscape stretching below our feet. At the same time, it is a hostile territory. The air is thin, and we feel dizzy. Movement is complicated, possible only through labyrinths of trails surrounded by cliffs and caves. Care must be taken not to get lost and never return.

1.2 Justification

Epistemology is the branch of Philosophy that investigates the nature of human knowledge itself. The epistemological question is: *how is it possible to know something*? From this perspective, a **theory** is a *universal statement* that provides a definitive explanation about a particular phenomenon. Thus, creating a theory is relatively easy. Someone might profess, for example, the theory that forest fairies are responsible for making household objects disappear, especially socks. We have a phenomenon (the disappearance of things) and a definitive explanation (the fairies). The difficult part, however, is *justifying the truth* of a theory—the so-called **problem of justification**. Here, the epistemological question becomes a bit more complicated: *how is it possible to know something* ***true***? In the given example, if someone claims that, in fact, the dog is responsible for making the socks disappear, how can one defend the fairy theory? How do we separate the true from the false? The example of forest fairies might seem ridiculous at first glance. But just a few centuries ago, people were tortured and burned alive in public squares over issues like this (especially women accused of being witches). Even today, in fact, it is a very serious issue, with significant social and political implications. According to Daniel Kahneman, research in the field of psychology shows that humans exhibit numerous **cognitive biases** that compromise their ability to distinguish the true from the false [4].

The epistemological problem of justifying theories was assimilated by two different philosophical schools of thought during the birth of the **scientific method** in modernity [5]. One of these schools, **rationalism**, holds that *Logic* must be the justification for the truth of theories. After all, it is clear that an incoherent explanation cannot be true. This position is commonly associated with Descartes (1596-1650), Spinoza (1632-1677), and Leibniz (1646-1716) — the so-called continental rationalists. René Descartes, one of the greatest rationalists of his time, propagated the notion that the senses are deceptive and elected reason as the guide for his opinions, establishing a program he called the *method of doubt*. In his *Discourse on the Method*[2], he went so far as to doubt the existence of everything, claiming that reality could be indistinguishable from a mere dream [1]. With that, he concluded that the simple act of *doubting* existence guarantees at least one absolute certainty: the existence of oneself[3]. The other philo-

[2]Descartes delves deeper into his ideas in *Meditations*.

[3]Descartes' idea that "I think, therefore I am" (*cogito, ergo sum*) guarantees the existence of a *Self*

sophical school, **empiricism**, argues that a theory is justified by *empirical evidence*, that is, through a collection of direct observations of events and phenomena. This line of thought is associated with philosophers Locke (1632-1704), Hume (1711-1776), and Reid (1710-1796), the so-called British empiricists. Locke, for instance, became known for spreading the idea that all people are born equal, like a blank slate, a *tabula rasa*, and acquire knowledge through experience, by interacting with their environment [6].

Although not exactly opposing, what these philosophical schools favor, in essence, are different methods of *inference*. While rationalists prefer **deductive inference**, empiricists prefer **inductive inference**. In the first case, statements are justified when they logically follow from their premises, that is, they are deduced [7]. For example, considering the premises that "*all Gauchos like mate*" and that "*Clara is a Gaucho*", then we deduce that "*Clara likes mate*". Typically, the process of deductive inference follows a structure in which a conditional statement (if S_1 is true, then S_2 is also true) is followed by an *antecedent* sentence, which can be either an affirmation (*modus ponens*: S_1) or a negation (*modus tollens*: $\neg S_1$), leading to the conclusion of the *consequent* sentence. In the affirmative form (*modus ponens*):

$$\begin{aligned} S_1 \implies S_2 \quad & \text{if someone is from the Pampas, then that person likes drinking mate} \\ S_1 \quad & \text{Clara is from the Pampas} \\ \therefore\ S_2 \quad & \text{therefore, Clara likes drinking mate} \end{aligned}$$

deductive inference guarantees the truth of the consequent sentence as long as its antecedent premises are true. In the affirmative mode illustrated, it deduces *singular statements* from *universal statements*. inductive inference, on the other hand, goes in the opposite direction. Empiricists seek to build theories (universal statements) by *generalizing* from evidence (singular statements) obtained through empirical experience. This gives rise to the notion of a **hypothesis**: a draft of a theory to be *confirmed* or *verified* by evidence. For example, if we observe that the Gauchos we know like to drink mate, we can infer, by induction, that *all* Gauchos must like mate. With a bit more caution and empirical rigor, we might eventually state that the *probability* of any given Gaucho liking mate is high, since 99% of respondents in a survey of a thousand Gauchos said that yes, they like to drink mate. For empiricists, the observation of phenomena justifies the construction of generalizations that are plausible or *probable*.

Both lines of reasoning are problematic. The strict use of Logic as a justification for theories produces the **infinite regress problem** [8]: if a statement S_1 is justified by another statement S_2 ($S_2 \implies S_1$), what justifies S_2? Perhaps statement S_3 justifies S_2, and statement S_4 justifies S_3, and so on, *ad infinitum* ($\infty \implies ... \implies S3 \implies S_2 \implies S_1$). An alternative is to establish a circular chain of statements ($S_1 \implies S_2 \implies S_3 \implies S_1$), but this is, logically speaking, even worse than the previous situation, as ultimately the statements end up self-justifying. Infinite regress is easily noticed when children, being naturally curious, learn to ask "*why?*". One can stop the regress (or at least *stop the questions*) by establishing fundamental truths, unquestionable axioms, as happens in Mathematics. But in Science, this only produces *dogmatic* theories based on relatively arbitrary conventions, which are easy targets for empiricist criticism. On the other hand, using empirical experience as a justification for theories brings with it an insoluble problem, described by David Hume (1711-1776) and known today as the **induction problem**. inductive inference is fragile because

that asks questions. Descartes uses this to attempt to prove the existence of God as well. However, Descartes' proof of God is questionable, which can easily lead us to **solipsism**: the thesis that the *Self* is alone, floating in the void, imagining a reality that fundamentally does not exist. After all, how can *you*, the one reading this text, be certain that *I*, the author, exist? How can you be sure that all your memories were not just created right now, at this very instant? And what if your entire life is nothing but an immaterial hallucination?

it is based on the **principle of uniformity**: the assumption that the regularities of nature observed in the past will be the same as those observed in the future. This assumption is the foundation of all Physics, after all, the laws observed today are often used to predict future events and reconstruct past events. Despite being intuitive, it is not possible to rationally justify the principle of uniformity. If we invoke the fact that it has always proven functional or correct, we fall into a circular, logically invalid argument that *evokes the very principle of uniformity to justify the principle of uniformity* [9]. In other words, one cannot defend inductive inference through an inductive argument! Thus, the principle of uniformity is ultimately the fundamental dogma of the empiricists[4].

The progress of modernity gradually reduced the intellectual rivalry between thinkers from the European continent and the British Isles. empiricism, although revised and moderated, triumphed over rationalism — especially after the work of Immanuel Kant (1724-1804). In his *Critique of Pure Reason* (1781), this thinker proposes a synthesis between rationalism and empiricism [todo:cite]. In it, Kant agrees with the empiricists — that empirical experience justifies knowledge — but makes a concession to rationalism, establishing that theoretical concepts about the objects to be known are necessary *a priori*. Without what he called **transcendental categories**, we cannot do much with the perceptions we collect about the external world. The hegemony of empiricism in modernity culminated in the early 20th century with the philosophical movement of **logical positivism**. This movement established the common sense that scientific theories are *verified* or *confirmed* through the collection of observations and statistical analyses. However, this conception was surpassed in the mid-20th century, mainly due to the remarkable transformations in Physics. This reignited the debate about how Science justifies its theories and changes them in the long term, with new perspectives proposed by Karl Popper (1902-1994) and Thomas Kuhn (1922-1996), creating the conditions for the contemporary debate in the Philosophy of Science: scientific realism and the purpose of Science.

1.3 Confirmation

In the previous section, we saw that the empiricist school holds that a hypothesis represents a draft of a theory that must be *confirmed* by empirical experience. In this sense, the ideas of the philosopher and statistician Thomas Bayes (1701-1761) provide a particularly useful method of inductive inference for the confirmation of hypotheses through the mathematics of probabilities [10], [11]. The central idea of the so-called **Bayesian epistemology** professes that knowledge is not an all-or-nothing matter, black or white, but presents subtleties, with various shades of gray between true and false. The reason for this stems from the recognition that empirical observations are inevitably subject to *random noise*, meaning there is **statistical uncertainty** in the sampled data. For this empiricist approach, the subtleties of knowledge consist in the **credence** in the truth of a hypothesis. This credence should be updated as favorable or unfavorable evidence is obtained through empirical experience.

Before proceeding, it will be useful to establish an intuitive example.

[4] Hume's ideas inevitably lead us to **skepticism**. Beyond the induction problem, Hume argued that **causality** between phenomena is an imaginary concept, never *directly* experienced in reality. Imagine a billiard ball colliding with another ball at rest. Then, the ball at rest begins to move as well. Newton would say that this happened *because of* the law of conservation of motion. But this law requires several imagined theoretical concepts, such as mass and energy. What we can actually experience are events happening one after the other, but never the cause-and-effect connection between them. For Hume, *this connection does not exist.*

Consider that you are at the airport of a distant country, in the food court of a busy international terminal. You want to know if the person at the table in front of you will take the same flight as you to Brazil. With no information available, your credence in this hypothesis is relatively low, as there are dozens of flights scheduled from this terminal to various other countries. But if you suspect that the person is Brazilian, your credence increases — after all, your flight is likely full of other Brazilians. At the same time, caution is needed, as being Brazilian does not necessarily imply traveling to Brazil. Even if the person were not Brazilian, there would still be a small chance that they are traveling to Brazil on the same flight as you, for tourism or business. One thing is certain: *favorable evidence that the person is Brazilian will lead you to update your degree of conviction.* Bayesian epistemology articulates how to do this in a mathematically precise way.

A good starting point to formalize the concept of credence in terms of probabilities is to note that a given hypothesis H and its favorable evidence E are distributed in a **space of possibilities** Ω. From a Bayesian perspective, each of these possibilities is assigned a credence, which can be considered probabilistic as long as they are *mutually exclusive* (they cannot both be true at the same time) and *jointly exhaustive* (at least one of them is true). Given these conditions, the **principle of probabilism** is observed based on the following axioms:

- **Non-negativity**. The probability of a given possibility A must be a non-negative real number: $P(A) \geq 0$;
- **Normalization**. The probabilities of all possibilities must sum to one: $P(\Omega) = 1$, and;
- **Additivity**. Because they are incompatible, the probability of two possibilities A and B is the sum of their individual probabilities: $P(A \cup B) = P(A) + P(B)$.

In the airport example, there are four possibilities: the person is Brazilian and on the same flight (E is true and H is true); the person is Brazilian and not on the same flight (E is true and H is false); the person is not Brazilian and on the same flight (E is false and H is true); and the person is not Brazilian and not on the same flight (E is false and H is false). This space of possibilities can be more easily visualized through a table with illustrative numbers, as in Table 1.1. So, consider that in the international terminal, there are 200 scheduled flights (only one of them to Brazil) and that each plane carries 500 passengers. In total, there are 100,000 passengers circulating in the terminal. Additionally, there are 800 Brazilians in the terminal, with 450 on your flight and another 350 with other destinations.

	same flight (H)	**different flight ($\neg H$)**	totals
is Brazilian (E)	450	350	800
is not Brazilian ($\neg E$)	50	99150	99200
totals	500	99500	100000

Table 1.1: Possibility space for the airport example. The numbers represent the distribution of passengers in the different combinations between hypothesis H (on the same flight) and evidence E (nationality is Brazilian)

By inspecting the table, we can easily see that the probability of your hypothesis being true, that any given passenger is on your flight, is $P(H) = 0.005$ (0.5

$$P(H|E) = \frac{P(H) \cdot P(E|H)}{P(E)} \tag{1.1}$$

Where $P(H|E)$ is the probability of hypothesis H being true given that evidence E is true (posterior probability); $P(H)$ is the probability of hypothesis H being true (prior

Hypothesis *i*	$P(H_i)$	$P(E\|H_i)$	$P(H_i) \cdot P(E\|H_i)$	$P(H_i\|E)$
H_1: $X < x_1$	0.143	0.008	0.001	0.008
H_2: $x_1 \leq X < x_2$	0.143	0.026	0.004	0.026
H_3: $x_2 \leq X < x_3$	0.143	0.084	0.012	0.084
H_4: $x_3 \leq X < x_4$	0.143	0.171	0.024	0.171
H_5: $x_4 \leq X < x_5$	0.143	0.208	0.03	0.208
H_6: $x_5 \leq X < x_6$	0.143	0.275	0.039	0.275
H_7: $X \geq x_6$	0.143	0.227	0.032	0.227
totals	1.0	1.0	0.14	1.0

Table 1.2: Illustrative example of the conditioning of the probability distribution of a random variable X. In this case, the prior distribution $P(H)$ was defined as uniform by observing the principle of indifference (objective Bayesianism).

probability); $P(E|H)$ is the probability of evidence E being true given that hypothesis H is true, called the **likelihood**, and $P(E)$ is the probability of the evidence being true under all possibilities. In the case of the airport:

$$P(H|E) = \frac{\frac{500}{100000} \cdot \frac{450}{500}}{\frac{800}{100000}} = \frac{450}{800} = 0.56\,(56\%)$$

What Bayes' Theorem tells us is that the estimate of the probability of the hypothesis being true given favorable evidence must take into account both the space of possibilities reduced *by the favorable evidence* (in this case, the fact that there are few Brazilians in the international terminal) and the chance *that the evidence does not guarantee the hypothesis* (in this case, the fact that not everyone on your flight is Brazilian). Or simply:

$$\text{Posterior} = \text{Prior} \times \text{Likelihood} \div \text{Evidence}$$

The update of the credence is only possible *provided that* the evidence favorable to the hypothesis is true. For this reason, this is called the **principle of conditionalization** of Bayesian epistemology. In the airport example, everything is quite clear because the absolute numbers of passengers were provided in the table. The probabilities calculated this way are objective, based on the *frequency* of each set in the space of possibilities Ω. But in a practical situation, we usually only have access to the degrees of conviction in the space of possibilities Ω, which must change as new evidence is obtained. To remain consistent with the axioms of probabilism, conditioning or **conditioning** [5] with the evidence must *zero out*, *rescale*, and *normalize* the probability values. In the airport example, when we find out that the person in the airport is definitely Brazilian, we must zero out the probabilities that they are not Brazilian, which implies proportionally rescaling the probability of the other possibilities and *normalizing their values* so that their sum equals one, as $P(\Omega) = 1$. On the other hand, if we only infer that the person at the table ahead speaks Portuguese (perhaps by reading a book), this is not enough to zero out the probability that they are not Brazilian (after all, other nationalities also speak Portuguese!).

The principle of conditionalization allows for the application of Bayes' Theorem to a finite number of N hypotheses H_1, ..., H_N, as long as they are mutually exclusive and collectively exhaustive possibilities. In this case, Bayes' Theorem takes the following form:

$$P(H_i|E) = \frac{P(H_i) \cdot P(E|H_i)}{\sum_{j=1}^{N} P(E|H_j) \cdot P(H_j)} \tag{1.2}$$

The denominator in this equation is a constant that plays the role of normalizing the probability values, ensuring that $P(\Omega) = 1$. Here, it is noted that normalization pro-

[5] The terms *conditioning* and *conditionalization* will be used equivalently here.

Hypothesis *i*	$P(H_i)$	$P(E\|H_i)$	$P(H_i) \cdot P(E\|H_i)$	$P(H_i\|E)$
H_1: $X < x_1$	0.227	0.008	0.002	0.022
H_2: $x_1 \leq X < x_2$	0.273	0.026	0.007	0.088
H_3: $x_2 \leq X < x_3$	0.229	0.084	0.019	0.236
H_4: $x_3 \leq X < x_4$	0.146	0.171	0.025	0.306
H_5: $x_4 \leq X < x_5$	0.082	0.208	0.017	0.208
H_6: $x_5 \leq X < x_6$	0.036	0.275	0.01	0.12
H_7: $X \geq x_6$	0.008	0.227	0.002	0.022
totals	1.0	1.0	0.08	1.0

Table 1.3: Another illustrative example of conditioning of the probability distribution of a random variable X. In this case, the prior distribution $P(H)$ was defined subjectively, by expert opinion (subjective Bayesianism).

vides an opportunity to assign *non-probabilistic* degrees of conviction to the likelihood $P(E|H)$ without violating the principle of probabilism, as long as they are non-negative values. In other words, the likelihood $P(E|H)$ can be interpreted as a *weight* given by the evidence. If this is the case, the notation for likelihood should be modified to an **informal likelihood function**, denoted by $\mathcal{L}(E|H)$[6]. Either way, the posterior distribution of a random variable must be conditioned by an empirically estimated probability (or weight) distribution. To do this, it is necessary to discretize the values of the variable into N intervals, which are the hypotheses H_1, ..., H_N in Equation (1.2). For each hypothesis H_i, its prior $P(H_i)$ must first be assigned. Next, empirical evidence must be obtained to derive the likelihood $P(E|H_i)$ for each hypothesis. The posterior of each hypothesis is then conditioned through the application of Equation (1.2). Finally, if we consider the posterior distribution obtained as the prior distribution for the next stage, the confirmation of the probability distribution of the variable occurs incrementally as new evidence accumulates. Table 1.2 shows an example of the conditioning of the probability distribution of a random variable X, which in this case was divided into seven discrete intervals defined by thresholds $x_1, ..., x_6$.

A controversial issue in the conditioning process is the definition of prior probabilities in the very first stage when there is still no evidence. In the case of Table 1.2, what justifies the prior distribution $P(H_i)$ being uniform? This is the so-called **problem of priors** in Bayesian epistemology, which divides the field into two main branches of Bayesianism: the *subjective* and the *objective*. To proceed, one must decide between the two. On the one hand, the **subjective Bayesianism** branch accepts any prior distribution as long as it does not violate the principle of probabilism. The obvious problem here is that the posterior distribution may become more sensitive to the values of the prior distribution than to the evidence itself, as demonstrated in Table 1.3. Figure 1.2 clearly shows the difference between the posterior results $P(H|E)$ between Tables 1.2 and 1.3, even though exactly the same likelihood distribution $P(E|H)$ was used for the conditioning. Defenders of this branch argue that it is legitimate for different subjective opinions to be compared objectively. Moreover, if the evidence is consistent, divergent opinions about the prior distribution become irrelevant in the long run, dissipating during successive conditioning stages. On the other hand, the **objective Bayesianism** branch prefers to eliminate any bias when defining the prior distribution. To this end, the **principle of indifference** is recommended: the credence in two or more hypotheses should be equal in the absence of sufficient reasons to the contrary. In the case of Table 1.2, there may not be enough reasons to differentiate the values of $P(H_i)$, which is why a uniform distribution was adopted. This principle may seem natural, but it is nothing more than an arbitrary convention: in the face of complete ignorance, any

[6]This is the basis of the *Generalized Likelihood Uncertantiy Estimation* (`GLUE`) method for uncertainty analyses, introduced in the next chapter

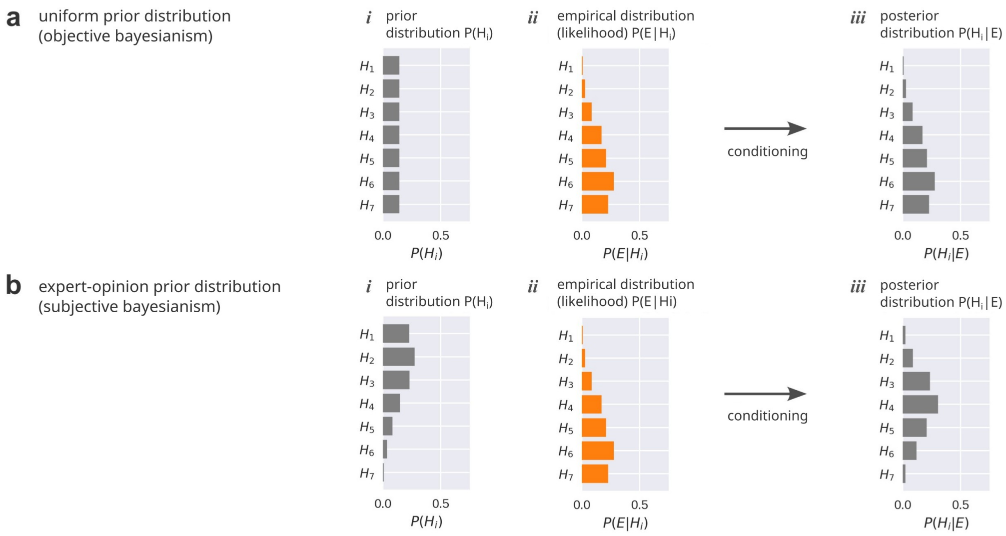

Figure 1.2 — Conditioning the prior distribution of a random variable. This visually presents the illustrative data from Tables 1.2 and 1.3. In both cases, the evidence is the same; what changes are the assumptions used in the prior distribution. **a** — Uniform distribution, considering the *principle of indifference* of objective Bayesianism. **b** — Distribution defined by opinion, a practice considered valid in subjective Bayesianism.

prior distribution is equally probable, with the uniform distribution being, in fact, an extremely specific case.

Another open issue in the conditioning process is how to obtain the likelihood $P(E|H)$ from the evidence. After all, without precise details about the entire space of possibilities Ω, as in the airport example, the evidence usually consists of sampled data that does not automatically translate into probabilities. This issue becomes even more pronounced in the case of a continuous random variable when we seek to estimate a probability distribution from the available data. Similar to the problem of priors, the solution to this question requires a decision-making process, which involves establishing a set of assumptions about *the behavior of random noise*[7]. In this direction, a particularly useful example for our future discussion on hydrological models is the fitting of mathematical curves that relate two phenomena, such as in the case of the **rating curve** that describes discharge as a function of the observed level at a river section (see Highlight 1.3). In this case, the mathematical curve represents the hypothesis, or **model**, for which we are interested in knowing the credence. A general relationship for this problem is as follows [12]:

$$O(x,t) = M(x,t,\Theta) + \varepsilon(x,t) \tag{1.3}$$

In which $O(x,t)$ is the empirical observation obtained at the independent variable x and time t; $M(x,t,\Theta)$ are the predictions of the model M at x,t given the parameter vector Θ, and; $\varepsilon(x,t)$ is the **error**[8] of the empirical observation at x,t. Of course, in this context, the random variables of interest for estimating the likelihood of the model M are the parameters Θ themselves. A typical set of assumptions[9] about the behavior of random noise is that the error ε exhibits:

[7] An ironic fact about the Bayesian approach is that the hypothesis about the behavior of the noise can only be justified through logic, never by the evidence, under penalty of entering an infinite regression of decisions about the noise of the noise. After all, to justify the hypothesis about random noise based on evidence, we would need to repeat the Bayesian method *ad infinitum*, evaluating the noise of the noise, and the noise of the noise of the noise, and so on.

[8] Also referred to as **residual**.

[9] The introduction of bias, temporal autocorrelation, and other distributions can also be made within a mathematically formal, albeit more intricate, framework.

1. zero mean, i.e., $\mu_\varepsilon = 0$;
2. constant (stable) variance σ_ε^2;
3. independence over time, and;
4. normal distribution: $p(\varepsilon) = \frac{1}{\sigma_\varepsilon\sqrt{2\pi}}e^{-(\varepsilon-\mu_\varepsilon)^2/(2\sigma_\varepsilon^2)}$, where μ_ε is the error mean (zero) and σ_ε is the standard deviation of the error.

The rational justification for considering the normal distribution is based on the **central limit theorem**, which states that the sample mean of any population is normally distributed[10]. Thus, the problem of the likelihood of the parameters Θ is resolved by estimating the population variance of the error σ_ε^2 by its sample variance, which is defined as $s_\varepsilon^2 = \frac{1}{df}\sum_{i=1}^{n}(\varepsilon_i - \bar{\varepsilon})^2$, where $\bar{\varepsilon}$ is the sample mean of the error; n is the sample size, and; df is the degrees of freedom[11] [13]. The error ε_i of each n observation is the difference between the observation O_i and the prediction of the model curve M_i defined by the parameters Θ adjusted with optimization techniques, such as the least squares method. Next, the uncertainty associated with the variance of the error must be assimilated in some way by the parameters Θ. For linear models, this can be done analytically, based on the principles of linear combination of random variables. A robust alternative, applicable to models in general, is the **Monte Carlo simulations** method. In this method, numerous *resamplings* of the error ε are performed, i.e., simulations of statistically equivalent realizations[12]. For each simulation, new values for the parameters Θ are adjusted using optimization techniques. Thus, the database generated by these simulations allows the estimation of the empirical probability distribution of the parameters Θ of the model $M(x, t, \Theta)$, which can finally be used in the conditioning process.

Figures 1.3 and 1.4 present an illustrative example for the conditioning process of a model. The goal was to condition a linear model of the type $M(x, \Theta) = c_1x + c_0$ using the available empirical evidence[13]. Note that $\Theta = \{c_0, c_1\}$, meaning the problem consists of obtaining the posterior distribution of the parameters c_0 and c_1. Let's first consider the case of the initial situation (Figure 1.3), when the first sample of empirical data was obtained ($n = 50$). Given the data, the model $M(x, \Theta)$ was fitted using the least squares method. The exact values obtained for the parameters in the initial fit are *irrelevant*, as we are interested in obtaining a probability distribution, not precise values. The initial fit of the model only serves to estimate the dispersion of the error ε. By simple visual inspection, it can be seen that the distribution of the model's errors is well-symmetrical around zero with stable dispersion. Assuming that the error ε follows a normal distribution with zero mean and constant variance, the Monte Carlo method was applied with a thousand resamplings, which were done by approximating the population variance by the sample variance (i.e., $\sigma_\varepsilon^2 \approx s_\varepsilon^2$). In each simulation, new fits for the model were performed, allowing the estimation of the uncertainty bands for the model $M(x, \Theta)$. Finally, the likelihood distribution $P(E|H)$ of the parameters c_0

[10]What this theorem means is that sums of random numbers (note that the mean is a sum) tend to naturally produce the normal curve pattern simply by combining high values with low values. For example, consider rolling a fair six-sided die. The probability of each top face showing one of the values from the set $\{1, 2, 3, 4, 5, 6\}$ is the same, $1/6$. However, the probability of the *mean* of the values sampled in n rolls tends to be much higher among intermediate values as n increases, since high values are offset by low values. This is the fact that produces the bell-shaped pattern modeled by the normal curve.

[11]$df = n - 2$ for models with two parameters.

[12]In the case of small samples, with $n < 30$, the error ε should be simulated using the Student's t distribution with $n - 1$ degrees of freedom.

[13]The data here is synthetic, generated for the purpose of illustrating the Bayesian approach.

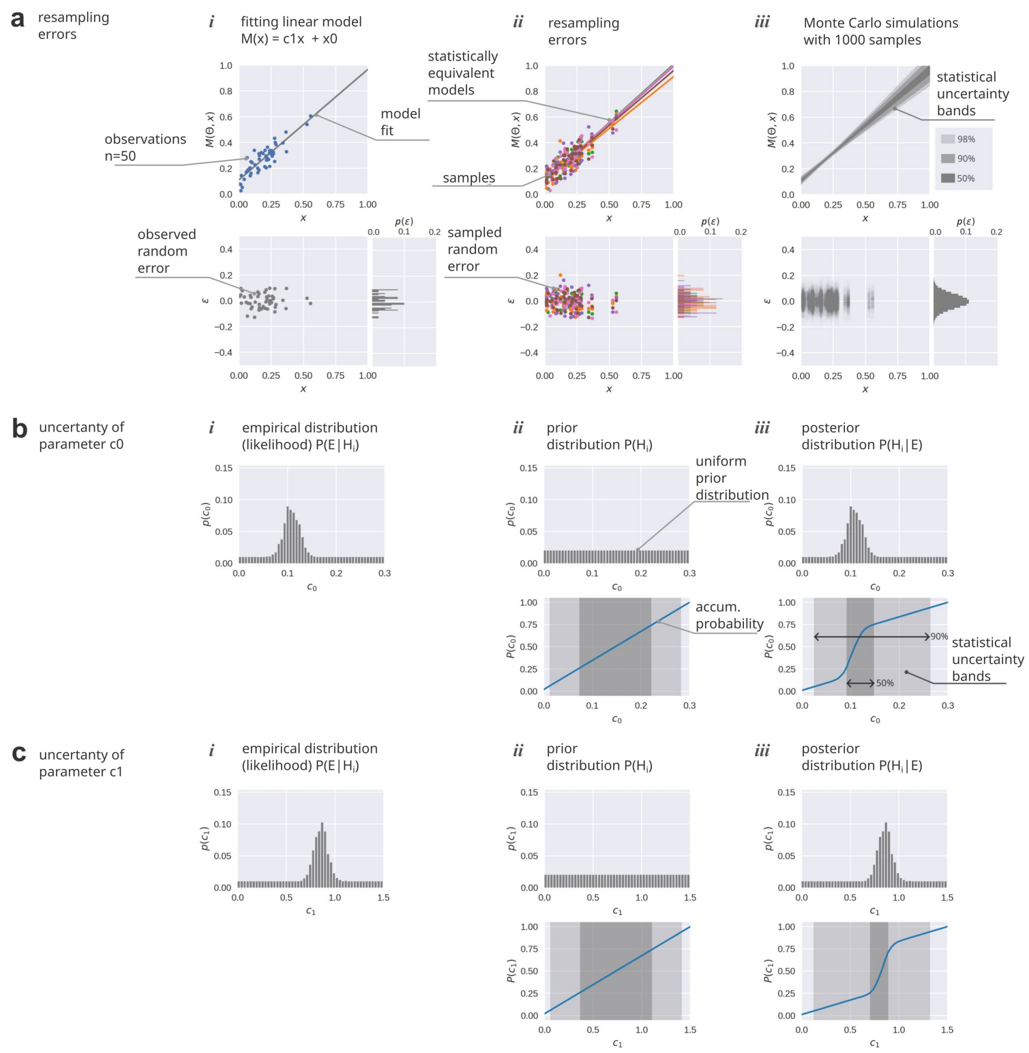

Figure 1.3 — First stage of conditioning of a linear model of the type $M(x,\Theta) = c_1x + c_0$**.** **a** — Fitting a linear model using the least squares method. This first fit allows estimating the behavior of the error ε (detail a.i.). If the assumptions about the error are met, numerous error resamplings are performed (Monte Carlo simulations, details a.ii. and a.iii). For each resampling, new models are fitted. The resampling database allows the estimation of the empirical probability distribution of the parameters c_0 and c_1. **b** — Application of Bayes' Theorem to obtain the posterior distribution of parameter c_0 (detail b.iii.). The empirical distribution (detail b.i.) was obtained from the results of the Monte Carlo simulation. **c** — Application of Bayes' Theorem to obtain the posterior distribution of parameter c_1 (detail c.iii.). The empirical distribution (detail c.i.) was obtained from the results of the Monte Carlo simulation. In both cases, the prior distribution was considered uniform (b.ii.; c.ii.).

and c_1 was estimated from the histogram of the list of a thousand statistically equivalent values generated by the simulations. Since the prior distribution $P(H)$ was uniform, the posterior distribution pattern $P(H|E)$ was completely influenced by the likelihood. Now let's consider the second stage (Figure 1.4), when a new sample of empirical data was introduced ($n = 50$). In this stage, the new data was mixed with the old, and the same procedure was followed: a model was fitted to the data, and new error ε simulations were conducted by approximating its population variance with its sample variance. The exception was that the prior distribution is now the posterior distribution obtained in the initial situation. With this, the arrival of new empirical observations can both *reinforce* or *weaken* the previously obtained credence for the parameters c_0 and c_1. In the illustrated case, it is clear that the new observations slightly weakened the credence for parameter c_1, slightly widening the 50% uncertainty band obtained in the first stage and generating a bimodal posterior distribution.

In Equation (1.3), the embedded assumption is that the error ε is *linearly*

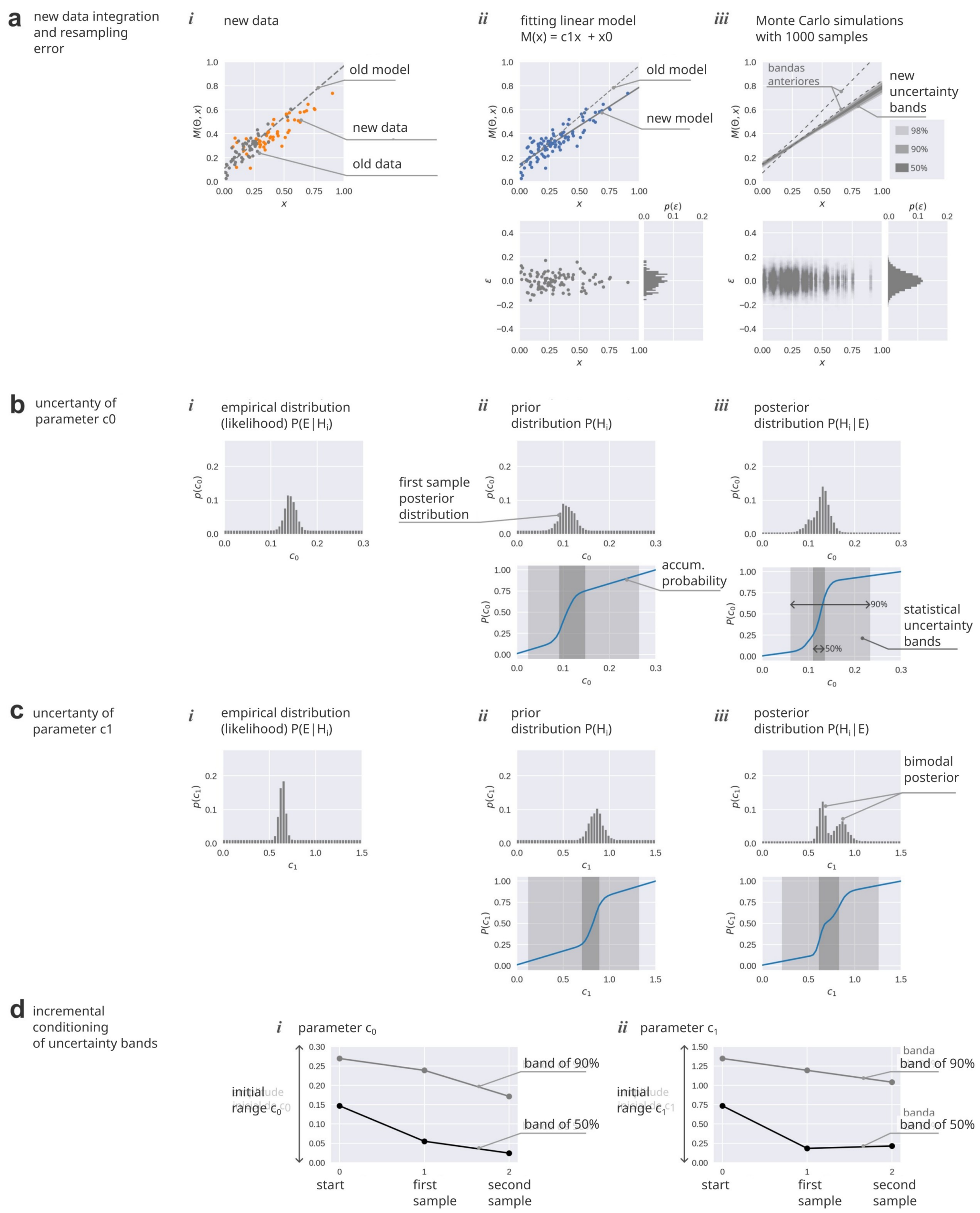

Figure 1.4 — Second stage of conditioning of a linear model of the type $M(x, \Theta) = c_1x + c_0$. **a** — Second stage of conditioning. The same procedures are carried out as in the first stage, with the difference that new data obtained is integrated with previous observations and that the prior distribution used is the posterior distribution from the first stage. **b** — Application of Bayes' Theorem to obtain the posterior distribution of parameter c_0. **c** — Application of Bayes' Theorem to obtain the posterior distribution of parameter c_1. **d** — Analysis of the uncertainty bands of the parameters as new samples are taken. The uncertainty bands of the model's predictions and parameters have been reduced, except for the 50% uncertainty band in the second stage of parameter c_1. This occurred because the evidence in the second sampling is highly inconsistent with those obtained in the first sampling, resulting in a bimodal posterior distribution (detail c.iii.).

additive to the model. However, it could be *multiplicative*, which would make Equation (1.3) take the following form:

$$O(x,t) = M(x,t,\Theta) \cdot \varepsilon(x,t) \tag{1.4}$$

This assumption makes sense when the random noise increases as the independent variable grows. In the case of rating curves, it is reasonable to expect that proportionally larger errors are present in the measurement of high flows from the water level, especially (but not only) due to greater uncertainties in the geometry and roughness of the channel

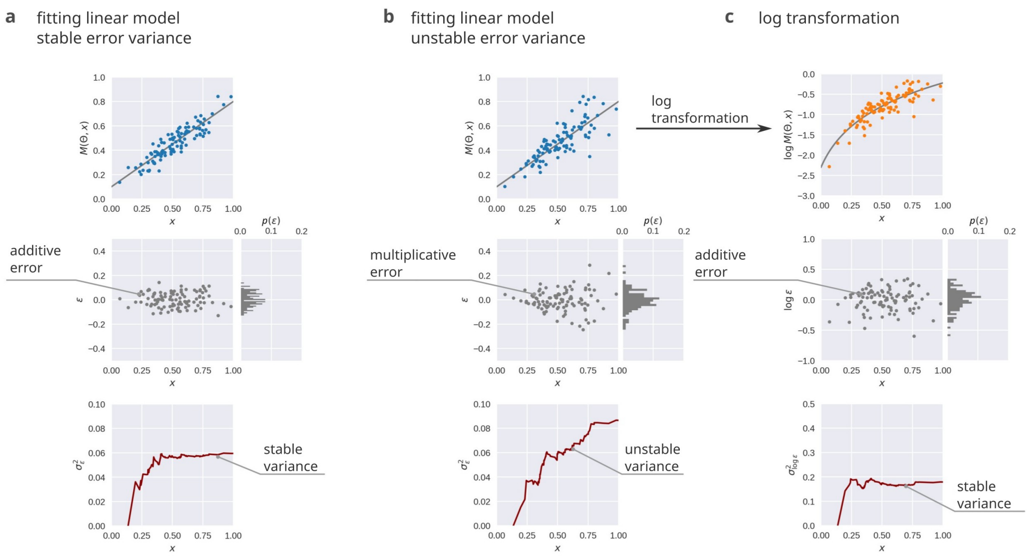

Figure 1.5 — Additive error and multiplicative error in the fitting of a linear model. **a** — Additive error in a linear model, with stable error variance (homoscedastic). **b** — Multiplicative error in a linear model, with unstable error variance (heteroscedastic). **c** — Stabilization of the multiplicative error variance through a logarithmic transformation. The logarithm of the error is additive.

section. When this occurs, the error variance is not constant but gradually increases. In this case, the variance is heteroscedastic (unstable), as opposed to homoscedastic (stable). An alternative to address this case is through **variable transformation**, converting the problem to an additive case by taking the logarithm on both sides of Equation (1.4), since $\log(ab) = \log(a) + \log(b)$. Thus, the assumptions mentioned earlier can be evaluated over $\log(\varepsilon)$, which possibly shows stable variance. To apply the Monte Carlo method, the resampling of the error can be done directly on $\log(\varepsilon)$ and then converted back into Equation (1.4) for fitting the model $M(x, \Theta)$ through optimization techniques. Figure 1.5 illustrates this process.

1.4 Rejection

Despite the success of empiricism as the hegemonic current in the Philosophy of Science during modernity, the remarkable changes in Physics in the 20th century gave another chance to rationalism, that is, the deductive approach to the problem of justification. The impact of Albert Einstein's (1879-1955) work is a good example of this historical moment. In this case, Einstein revolutionized Physics with what he called *thought experiments*. If theories are products of empirical experience, as empiricists claim, Einstein would never have written his first papers, since at the time he worked at a patent office and had no access to laboratories or other resources to collect empirical data. On the contrary, it was other scientists who, through observations and experiments, supported Einstein's theory *a posteriori*, that is, *after* his ideas were already published. Something was definitely wrong with the empiricist theory justification current.

The exponent of this new rationalist movement was the philosopher Karl Popper (1902-1994), especially with his work *The Logic of Scientific Discovery*. He introduced the current now known as **critical rationalism**, also called the **hypothetico-deductive approach** [todo:cite]. On one hand, Popper was aware of the seriousness of the induction problem, which remained (and still remains) unsolved since its formulation by Hume – for him, inductive empiricism clearly could not be sustained. On the other hand, the philosophical currents of his time, called Conventionalists, also did

Destaque 1.3.1– Flow uncertainty bands from rating curves

Flow in rivers is almost never measured directly, as it requires a specialized technical team. It is much easier and cheaper to observe the **water level** in rivers using staff gauges. In fact, the water level of many rivers in Brazil is observed twice a day at streamflow stations of the National Hydrometeorological Network. Thus, the rare feasible flow observations are used to construct a **rating curve**, which is usually a power-type model:

$$Q = a \cdot (h - h_0)^b$$

Where Q is the flow in m^3/s; h is the observed level, and; h_0, a, and b are the parameters of the model. This curve can then be used to estimate flow from routine level observations.

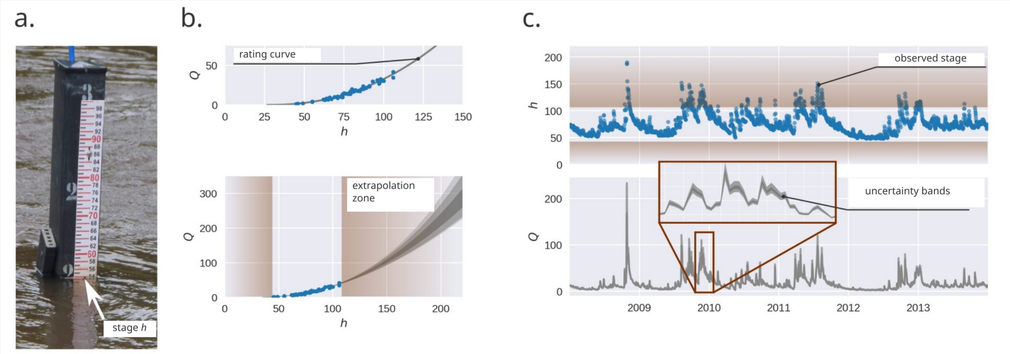

Figure 1.6 — Flow uncertainty bands from rating curves. a — Water level observation h on a staff gauge. **b** — Fitting a power-type model and estimating uncertainty through error resampling methods. **c** — Historical series of water level and flow uncertainty bands.

As illustrated in Figure 1.6, the confirmation of this model based on water level and flow evidence begins by fitting the parameters to the available data using optimization techniques. The behavior of random error can then be evaluated. If the error variance is stable, statistically equivalent resamplings of the data (Monte Carlo simulations) can be performed. Thus, the uncertainty bands of the rating curve reflect the uncertainty in the flow estimates in the historical series. In the presented example, **extrapolation zones** can be observed at the extremes, where the uncertainty expands disproportionately. This is expected, as extreme flow events are rare or difficult to measure. On the other hand, capturing a few extreme events can drastically reduce the uncertainty in these zones.
An interesting approach in this context is presented by Thomas Morlot and colleagues, who highlight that in addition to statistical uncertainties, rating curves exhibit temporal dependency associated with changes in the river section morphology [14]. Other complexities also exist, such as hydraulic hysteresis, which can manifest under different flow regimes.

not appeal to him, even though they represented deductive approaches to theory justification. In this sense, Popper concluded that the great epistemic power of empirical evidence is to justify, by the deductive method, the *falsity* of a theory. In other words, it is through **rejection**[14] of theories by evidence that true knowledge is obtained.

A simple example conveys the strength of this argument.

Consider the universal statement that "*all swans are white*". To definitively establish the truth of this statement by the inductive method, it would be necessary to observe all the swans that exist in the universe, including swans in the past and future, which is obviously impossible in practice. On the other hand, it only takes seeing a *single black swan* (or any other color) in time and space to definitively refute the theory that all swans are white. After all, if the singular statement "*a certain swan is black*" is true (because it was empirically verified), then we deduce that the universal statement

[14] Here, the terms *rejection*, *refutation*, and *falsification* are used interchangeably.

"*all swans are white*" is false:

$$\begin{array}{rl} S_1 \implies S_2 & \text{if all swans are white, then a certain swan is white} \\ \neg S_2 & \text{a certain swan is } \textbf{not} \text{ white} \\ \therefore\ \neg S_1 & \text{therefore, not all swans are white} \end{array}$$

This mode of deductive logic, involving negation, is called *modus tollens*, in contrast to *modus ponens*, which involves positive affirmation. What Popper demonstrates is that there is a fundamental asymmetry between these two modes of logic when we want to deduce universal statements from singular statements (make generalizations from specific observations), with *modus tollens* being the only way to obtain secure knowledge (in this case, the falsity of a universal statement). Hence, observations and empirical experiences are important for refuting theories, not for confirming them. As long as a theory survives rigorous empirical tests, it is said that the theory is *corroborated* by empirical evidence – but never confirmed.

Armed with this argument, Popper turns to what he calls the **demarcation problem**, initially raised by Kant: the difficulty of distinguishing whether a theory is *scientific* or merely *metaphysical*, based solely on abstractions. Unlike empiricists, who claim that experience is the origin of all knowledge, for Popper the origin of where theories arise is irrelevant. As long as they are logically consistent, they can emerge either from some motivating empirical observation (like the example of white swans) or from creative intuition (such as Einstein's thought experiments). What matters is the theory's ability to not survive the tests of empirical experience, that is, its ability to be rejected. This ability, called **falsifiability**, is the *demarcation criterion* that categorizes a theory as scientific. In summary, from the perspective of critical rationalism, a scientific theory must be falsifiable. Here, it is important to emphasize that *being falsifiable* does not mean *being false*. Being falsifiable means that the structure of the theory allows for observations to be used to demonstrate its potential falsity. If *in principle* it is impossible to prove that a theory is false through observations or experiments, then that theory is not scientific. This generally implies that scientific theories must be precise enough to produce observable predictions. In Einstein's case, his theory was precise and made observable predictions that were, in Popper's jargon, *corroborated* by other scientists (but could have been perfectly refuted). A more intuitive example of a non-falsifiable theory is the Multiverse theory, a cosmological theory that postulates the existence of Universes parallel to the one we inhabit. As enticing as it may be to *explain* some cosmological mysteries, this theory is not scientific because it does not allow for any *test* with empirical observations – in principle, there is no way to observe beyond our own Universe. In Popper's words:

> (...) a theory is something the mind attempts to prescribe to nature; something nature often does not allow to be prescribed to her; a hypothesis we attempt to impose on nature, but which can be contradicted by her – Karl Popper [15].

Once falsifiability is designated as the demarcation criterion for scientific theories, Popper moves on to the so-called **problem of simplicity**. This epistemological problem consists of the difficulty in explaining why simpler theories should be preferred over more complex ones (also known as *Occam's Razor*). For example, consider a series of point observations of a given phenomenon plotted in a system of coordinates. If there is a theoretical law that describes this phenomenon, this law will be a curve connecting all the observed points. However, for a finite number of points, it is always possible to fit an infinite number of curves using various mathematical formulas. If a straight line provides a good fit, so can the asymptotic part of a hyperbola. As we saw in the previous section, while Bayesian empiricists have methods to update the credence in the fit of a given curve as new observations are collected, they have nothing to say about the justification for *choosing that curve in the first place*, except for its supposed *simplicity*. This is indeed a confusing problem, as it depends on what we mean by simplicity. For some, it means an aesthetic aspect, something related to mathematical elegance – like the fact that circular orbits for planets seem more beautiful than elliptical orbits. For others, it means a pragmatic aspect, something related to time and resource economy – a simpler method for solving a task should be preferred over a more intricate one. The statistician George Box (1919-2013), for instance, advocates for what he calls the **principle of parsimony** in mathematical models based on purely practical criteria, such as cognitive load, better precision, and objectivity [12].

In view of this, Popper removes any aesthetic or pragmatic aspect, equating the simplicity of a theory with its **degree of falsifiability**: the simpler it is, the more falsifiable. This logically solves the problem of simplicity, because, in his words:

> Simple statements (...) tell us more because they contain greater empirical content and are susceptible to more rigorous testing – Karl Popper [16].

In other words, as long as a simpler, more *restrictive* theory survives empirical tests, it makes no logical sense to adopt a less simple, more *flexible* theory. This becomes clearer in mathematical terms, since the number of parameters in a curve is inversely associated with its degree of falsifiability. Consider a curve with three parameters, such as a second-degree polynomial (a parabola): $f(x) = c_2x^2 + c_1x + c_0$. This curve is much more flexible for fitting data than a curve with two parameters, such as a first-degree polynomial (a straight line): $g(x) = c_1x + c_0$. After all, if we make the quadratic parameter c_2 small enough, we can fit the data equally well with the straight line $g(x)$ without falsifying the theory that the studied phenomenon is described by the parabola $f(x)$, because $\lim_{c_2 \to 0} f(x) = g(x)$. The same logic applies to circular and elliptical orbits: the theory of the circle, being a specific case of an ellipse, should be rejected before the theory of the ellipse not for its aesthetics, but for its ease of being demonstrated false by observed evidence.

The concept of simplicity in Popper makes logical sense, but it doesn't exactly answer how to proceed when faced with observed evidence that presents random noise. In practice, it is impossible to obtain data that perfectly adheres to a mathematical relationship based on some theoretical principle, such as a linear, quadratic, or power function. Before proceeding, it is important to differentiate a theory from a **statistical model**. Theories establish mathematically precise models about specific phenomena. Statistical models, on the other hand, are a very specific type of theory that precisely define *the mathematical pattern of a dataset*, without theoretical links to the underlying phenomena[15]. In the case of theories, the open question in Popper's rationalist approach is when anomalies in the data should be taken seriously enough to reject a simple theory in favor of a more complex one. That is, how much should the data deviate from the proposed model for the theory to be considered falsified by the evidence? This question inevitably introduces a decision, which is the prior definition of a **rejection criterion**. The decision on the rejection criterion needs to be *before* the evaluation of the theory (*a priori*) because if it is *after*, nothing prevents the theory from never being rejected

[15] An intuitive example of this difference is to consider a population of, say, a thousand triangles with random sizes. If we look at the data for perimeter and area, we can easily create a statistical model between these two variables: large perimeters are generally accompanied by large areas. But this is not a theoretical law about triangles, as some very acute triangles have large perimeters and small areas. The mathematical theory is that the area of a triangle is its base times height divided by two – the perimeter is only partially and indirectly related.

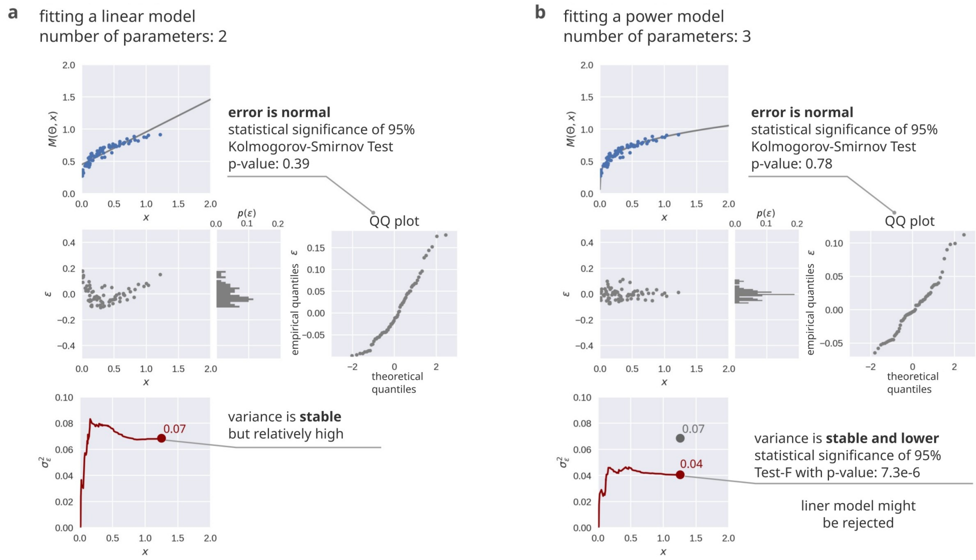

Figure 1.7 — Rejection criteria for model selection. **a** — Fit of a linear model of the type $M(x, \Theta) = c_1 x + c_0$. **b** — Fit of a power model of the type $M(x, \Theta) = c_1 x^k + c_0$. Both models are fitted to the same set of observed data. Both fits satisfy the assumptions of normal error and stable variance (homoscedasticity). Only by the principle of parsimony (simplicity), the linear model should be preferred as it has fewer parameters. But the power model shows significantly lower error variance with 95% statistical significance. This could be a rejection criterion for the linear model.

– one just needs to establish a criterion that is known to be lenient. Popper himself criticizes theories that, in the face of clearly falsifying evidence, resort to subterfuges and *ad hoc* explanations to try to survive. This dilemma becomes evident in the case of the premises mentioned in Section 1.3 regarding the statistical model of random noise: zero mean, constant variance, independence over time, and normal distribution. For example, one can evaluate the premise of normality of the error ε using a Quantile-Quantile plot or hypothesis tests, such as the Kolmogorov–Smirnov test. In the case of the Quantile-Quantile plot, the interpretation is purely visual. If the plot deviates significantly from a straight line, the premise should be rejected. In the case of the hypothesis test, the confidence level for the null hypothesis is defined *a priori*. If the desired confidence level is set at 95%, a p-value less than or equal to 0.05 indicates that the probability of normality given the considered data is less than 5%, and the premise should be rejected. Is there a logical justification for the 95% level? There is none. Another example, illustrated in Figure 1.7, is when all the premises about the residuals are satisfied by both a simple model and a complex model, but the complex model is more *accurate* than the simple model, meaning the error dispersion is *less*. How much should the dispersion be less to reject the simpler model? Again, one could apply a hypothesis test for equal variances, the F-Test, and obtain an answer for a previously defined confidence level. If the variances are statistically significantly different, the simpler model should be rejected. One way or another, there is subjectivity involved in rejection, as criteria or thresholds defined *a priori* are necessary.

1.5 Paradigms

In the Philosophy of Science, there is an important distinction between **context of justification** and **context of discovery**. The first context addresses the epistemological problem of how to justify the truth of a theory. The second context investigates the historical and sociological problem of how progress occurs in Science – if indeed progress exists. The different philosophical currents mentioned in the previous sections fit into the first context, as they provide solutions to the epistemological problem of justification. In one way or another, they assign an important role to empirical evidence. For Bayesian empiricists, evidence would be used inductively to confirm the credence in a theory based on the mathematics of probabilities. For critical rationalists, evidence would be essential to falsify theories through deductive logic, leaving theories in an eternal provisional state – they would be corroborated but never confirmed. *Confirmation* and *rejection*, thus, form a somewhat paradoxical dichotomy, as both make sense in the practice of Science, but contradict each other. This paradox is resolved by the perspective of the context of discovery. In his work *The Structure of Scientific Revolutions*, Thomas Kuhn (1922-1996) provides substantial contributions in this regard.

As a historian, Kuhn warns that Science does not exist in a vacuum: rather, it is composed of a *community* of human beings who interact over History, across successive generations, within a larger society. The existence of the **scientific community** implies that one must consider not only the History of Science but also the Sociology of Science to understand the context of discovery. This community is obviously not a single block, but a social network of smaller communities across different disciplines and fields of knowledge. In this light, Kuhn proposes that the dynamics of a given scientific community produce a cyclical historical pattern, structured into three interconnected phases: the period of **normal science**, the period of **crisis**, and the period of **revolution**. Thus, the confirmation and falsification of theories predominately occur at different stages of this historical pattern, with confirmation being a dominant process in the normal science period and rejection being an essential characteristic of the crisis period. However, the most important process for change in Science, occurring during the revolutionary period, is the **competition** between theories. In his words:

> (...) the competition between segments of the scientific community is the only historical process that actually results in the rejection of an previously acceptable theory or the adoption of another. – Thomas Kuhn [17].

This process is inevitably intergenerational, as new members of the community need to be reeducated to think within a new worldview. To illustrate this point, Kuhn cites a striking excerpt from the autobiography of physicist Max Planck (1858-1947):

> (...) a new scientific truth does not triumph by convincing its opponents and making them see the light, but rather because its opponents eventually die, and a new generation grows up familiar with it. – Max Planck *apud* Thomas Kuhn [17].

A key idea for Kuhn is that a scientific community shares a common **paradigm**. By paradigm, he refers to a set of exemplary solutions for research problems, meaning a system of theories, instruments, and auxiliary practices that effectively solve certain widely accepted problems and are *promising* for addressing mysterious and controversial issues with great competitive appeal. This competitive appeal is crucial, as the attraction of segments of the community around a paradigm creates a positive feedback: the more segments adopt the paradigm, the more new segments become convinced that they need to adopt it as well, under the penalty of falling behind. The scientific community in the normal period thus operates on both theoretical and applied fronts to reaffirm and articulate the hegemonic paradigm. Scientific research during this period is not explicitly aimed at discovering unexpected novelties; instead, the success of normal research is defined precisely by not encountering any surprises. A successful research effort typically confirms what the prevailing paradigm has already promised by providing a more refined detailing or by expanding the range of applications (for example, through the invention of new technologies). Like a jigsaw puzzle, in normal science, it is presumed in advance what the complete picture that the pieces form looks like – the only challenge is to fit the pieces together. Here, the sense arises that Science is a *cumulative* endeavor: each new member introduced into the scientific community would have the humble mission of laying another small brick in the grand "edifice of human knowledge". In Kuhn's view, this impression of accumulation, besides being misleading in the larger context, is reinforced by the widespread use of textbooks in training new researchers. These textbooks serve as vehicles for the perpetuation of the hegemonic paradigm because, when they are not simply written in an anti-historical manner, they distort History to make it appear as a linear and inevitable process leading to current theories.

Kuhn argues, with various examples from the History of Science, that the pieces of the puzzle studied by normal science eventually do not fit together. While knowledge accumulates during the normal period, empirical and theoretical **anomalies** also accumulate. Typically avoided or ignored, at some point these anomalies begin to cause widespread discomfort within the scientific community, leading it into the crisis period. The most detailed example of crisis provided by Kuhn is that of geocentrism, but he also offers examples in chemistry, mechanics, and electromagnetism. From this perspective, history shows that some crises develop slowly, as in chemistry, while others are sudden, like the one caused by Einstein in Physics. A scientific community in crisis exhibits various symptoms, such as discord, discontent, philosophical debates, and, most importantly, the widespread proliferation of candidate theories to explain the anomalies.

The only way out of the crisis is the revolution brought about by the proposal of a paradigm that is irresistible to the scientific community. As previously noted, the new paradigm must be effective in solving already known problems and make enticing promises for solving open issues. The new ideas must, in some way, offer a **retrocompatibility** with the old ideals without being contaminated by the problems embedded in the fundamental principles of the old ideas. Scientific revolutions, therefore, are episodes in which the supposed edifice of knowledge is demolished so that a new structure can be erected on a new foundation, with a new blueprint. During this revolutionary period, which typically lasts a generation, the scientific community migrates en masse to the new paradigm. New textbooks are then written, and a new historical cycle of normal science is established. An important aspect of this process is that, for Kuhn, a new paradigm is so fundamentally different from the old one that they are *incommensurable*: intellectual communication between them is extremely precarious, as they represent different worldviews. Typical examples of **theoretical incommensurability** occur with the concepts of mass, space, and time in Newtonian physics and in Einstein's physics. Despite having the same name and symbol, these concepts have distinct meanings under the different paradigms, with distinct theoretical implications[16]. Thus, Kuhn brings forth a troubling conclusion: that there is *no absolute progress* in Science towards the truth about reality, only *relative* to what we are concerned with explaining. More than that, with his thesis, Kuhn highlights the depth of the social dynamics surrounding Science, which is often portrayed as the most rational of human endeavors[17].

[16]In the Newtonian paradigm, gravity is an attractive force related to mass that acts instantaneously at a distance. In the Einsteinian paradigm, gravity is not a force but a *consequence* of the distortion of space itself, implying the existence of gravitational waves. For Kuhn, Einstein does not merely extrapolate the limits of Newton: he produces a new worldview that is irreconcilable with the previous one.

[17]Kuhn's emphasis on the relativity of knowledge, historical contingency, and the presence of paradigms has invigorated the emergence of the philosophical current of **postmodernism**, bringing with it the notion that human knowledge is a **discourse**. Thus, postmodernists reject grand absolutist narratives and emphasize the linguistic, cultural, and especially political influences that permeate the production of knowledge.

As previously outlined, Thomas Kuhn's thesis on the context of discovery eliminates the paradox between confirmation and rejection, which are contradictory solutions in the context of justification. However, a cautious look reveals that Kuhn's approach is essentially empiricist: he seeks to *confirm* the ideas of paradigms and scientific revolutions based on examples from the History of Science, that is, based on *empirical evidence*. Kuhn employs inductive inference to justify a theory about the context of discovery. From the perspective of critical rationalism, no matter how well corroborated, a single counterexample would be sufficient to falsify Kuhn's theory. The problem is that this fact, paradoxically, *resurrects the dichotomy between confirmation and falsification*. To make matters worse, if Kuhn's theory is scientific (i.e., falsifiable), wouldn't it itself be a *paradigm* for how to explain the context of discovery? Here arises a recursive loop of self-reference. Recursion in an argument is typically an indicator of the infinite regress problem mentioned earlier. This is a typical terrifying situation of being endlessly caught in circles that Philosophy provides. Karl Popper, perhaps because he was a philosopher and not a historian, seems to have foreseen these problems and pre-established that the theory on the scientific method cannot itself be scientific – falsifiable by evidence – but only a theory based on Logic.

1.6 Underdetermination

What we have seen so far fits into the broader philosophical current known as **scientific realism**. This current essentially defends the thesis that the purpose of Science is to provide theories that are true descriptions of reality [18]. For example, we began this chapter by mentioning that Keith Beven classifies the philosophy of most users of hydrological models as *pragmatic realism*, which is the tacit understanding that models provide an approximate description of reality that can be improved with new technologies. The pragmatic realism, for Beven, would be a branch of scientific realism. The origins of scientific realism can be traced back to the ideas of René Descartes [19]. Here, it is important to establish that **realism** itself consists of the conception in Metaphysics that admits the existence of an *objective* reality, meaning that the world does not depend on anyone to observe it. In this sense, when a person enters a room and observes a table, it is assumed that the table was there before they entered. The table did not come into existence at the moment of observation. Objects, like tables, exist independently of subjects. This conception opposes **idealism**, a current that considers reality strictly as a product of subjects, that is, *subjective*. If we agree on the existence of a supposed object, like a table, it is because it manifests similarly in our minds, that is, *intersubjectively*. Descartes flirts with idealism when he questions his own existence in the *Discourse on the Method*, particularly with the branch of solipsism—the idea that the mind of the person reading this text is the only thing that truly exists. Descartes basically points out that, although we have absolute certainty about the ideas in our minds, it is difficult to guarantee that they correspond to external reality. In his terms, *likelihood does not imply truth*. To try to resolve this problem, Descartes describes the method of doubt, which inspired the formation of the modern scientific method, contributing to the debate around the problem of justification that we have addressed so far. Ultimately, the problem of justification is inherently contaminated by the *assumption that objective reality exists*, with the concept of **truth** being precisely the *correspondence* between theories and reality.

The thesis of scientific realism seems obvious, but defending it is not so straightforward. In fact, Bas van Fraassen [18] and Nancy Cartwright [20] provide a profound critique, proposing a radically empiricist viewpoint known as **instrumentalism**[18] [21].

[18]Instrumentalism is a broad and neutral term. For example, van Fraassen self-identifies his thesis

Both argue that the objective of Science is to produce theories that exhibit *empirical adequacy*—and nothing beyond that. Since empirical adequacy does not logically imply a true description of reality, the claim of scientific realism is too ambitious in epistemological terms. This viewpoint does not deny the existence of reality (it is not an idealist current): what it denies is the ambition of obtaining a true description of reality. Theories and their models would merely be *instruments* constructed by scientists to explain empirical evidence. One of the main reasons for this claim is the **underdetermination problem**, which is the difficulty of ensuring that the observed evidence determines the truth of a theory without there being empirically equivalent theories [22], [23]. Popper's orientation to always prefer the simplest theory works well only for theories that are completely falsifiable by empirical evidence. This is not the case for most theories, which almost always postulate the existence of *unobservable entities* to explain phenomena that are directly observable. For example, in Physics, the existence of electrons and electromagnetic fields (unobservable) is invoked to explain the lightning and thunder of a storm (observable). This complicates matters, as no matter how we detect unobservable entities, like electromagnetic fields, indirect evidence will always be contaminated with a *theoretical load* that establishes the existence of these entities in the first place. This type of theoretical approach involves a kind of reasoning that is non-deductive, called **inference to the best explanation**, or abduction. Because it is not deductive, this reasoning does not guarantee the truth of the consequent and is also subject to the induction problem postulated by Hume. Thus, a theory that instantiates unobservable entities pays the price of being underdetermined by observable empirical evidence.

One of the main defenses of scientific realism consists in evoking the success of Science as evidence that scientific theories, even when instantiating unobservable entities, progress toward describing reality in an increasingly true manner [24]. From the critical rationalist perspective, although the ultimate truth about reality remains permanently shielded, the rejection of theories allows for the incremental isolation of a set of potentially true ideas. Indeed, it is undeniable that the theoretical predictions and technological applications that Science has produced in recent centuries are impressive and unprecedented in historical terms. Given all this success, it even sounds somewhat absurd to consider that modern Science does not describe reality. Although inference to the best explanation does not guarantee a logical implication, as instrumentalists correctly point out, defenders of scientific realism argue that it would be *a miracle* extremely unlikely for current theories to achieve good results for the wrong reasons. However, Donald Hoffman introduces the possibility that scientific theories describe the behavior of a *cognitive interface* with remarkable empirical adequacy [25]. He argues that cognitive systems, when subjected to natural selection, are pressured to operate through **heuristic**. That is, those systems that condense the necessary information to make useful decisions gain a competitive advantage. The evolution of these systems results in a perceptual interface optimized for survival and reproduction, but whose probability of being equivalent to reality is *precisely zero*. As an analogy, consider the graphical interface of a computer. In this case, we can easily observe the behavior of buttons and icons to identify patterns without knowing anything about the underlying electronic mechanisms. The information from the graphical interface tells us absolutely nothing about the *hardware*. For Hoffman, the truth about reality may simply have nothing to do with space, time, energy, matter, etc.—in Kantian terms, these would be the transcendental categories we use to condense and integrate perceptual information [19]

as *empiricism constructivist*. Realists, on the other hand, classify instrumentalism as *anti-realism*.

[19]Donald Hoffman subverts the paradigm of material physicalism by proposing that reality is not fundamentally constituted of subatomic particles, but rather of an infinite network of interactions among

The underdetermination problem has direct and relevant implications for users of environmental models, including hydrological models. In this context, Naomi Oreskes and colleagues point out that underdetermination occurs because various processes represented by the models are not observable *in practice*, meaning that information about the modeled system is *incomplete* both in time and space [27]. This milder version of underdetermination is also referred to as the **equifinality problem** [28]. For example, consider the groundwater flow occurring in watersheds. It is evident that this process exists: a field expedition makes this clear by directly observing the springs of streams, the places where groundwater flows to the surface. In fact, piezometers can be installed to monitor the water table level, providing more direct evidence of this process. However, the extent and complete dynamics of these underground flows are practically impossible to monitor, being observable only in specific points. Oreskes *et al.* argue that the partiality of the information renders the modeled natural systems *logically open*. Unlike logically closed systems, such as algorithms and mathematical equations, they point out that it is impossible to verify or validate a logically open system in light of *extenuating circumstances* that often ensure empirically equivalent explanations, or *equifinal*. This is intuitive: when we do not have complete information about some event we observe, it is natural for rival and equally valid explanations to emerge. Indeed, it is precisely for this reason that scientific experiments are designed to reduce the logical openness of the evaluated system, that is, to lessen the influence of extenuating circumstances. Thus, models of natural systems present themselves as a **main hypothesis** that requires the assistance of **auxiliary hypotheses** — such as parameters, input data, the adopted scales, and, especially, the underlying theoretical assumptions. This gives rise to a paradox: it is precisely due to the lack of information that the application of models is sought in the first place. If the information were already completely available, it is unlikely that a model would be relevant for decision-making. But without complete information, a model becomes underdetermined by the available evidence—the inexorable underdetermination problem in model application.

For Keith Beven, recognizing the underdetermination problem in hydrological modeling brings radical consequences for the confirmation of models in light of observed evidence, specifically the need to evaluate the **total error** associated with a given hydrological model [29]. From this perspective, Equation (1.3) would be incomplete, as the error ε there represents only the random noise related to the observed evidence. It is necessary to include not only the **statistical uncertainty**, resulting solely from sampling noise, but also the epistemic uncertainty, which arises from the auxiliary hypotheses necessary to address the underdetermination problem [30]. Thus, the **total error equation** for hydrological models takes the following form:

$$O(x,t) + \varepsilon_O(x,t) + \varepsilon_\Delta(\Delta x, \Delta t, x, t) = M(\Theta, \Upsilon, \varepsilon_\Upsilon, x, t) + \varepsilon_M(\Theta, \Upsilon, \varepsilon_\Upsilon, x, t) + \varepsilon_r \quad (1.5)$$

where $O(x,t)$ is the observation obtained at the independent variable x[20] and at time t; $\varepsilon_O(x,t)$ is the **measurement error** of the observation; $\varepsilon_\Delta(\Delta x, \Delta t, x, t)$ is the **commensurability error** at the modeling scale Δx and Δt; $M(\Theta, \Upsilon, \varepsilon_\Upsilon, x, t)$ is the prediction of the model at x, t based on the vector of parameters Θ, the vector of input data Υ, and the **input data error** ε_Υ; $\varepsilon_M(\Theta, \Upsilon, \varepsilon_\Upsilon, x, t)$ is the **model structural error**, and; ε_r is the **random error** remaining. The commensurability error ε_Δ results from the conversion between scales, representing the epistemic uncertainty of the

conscious agents [26]. The interactions of these agents produce cognitive interfaces that eventually instantiate self-referential ties, that is, realize a *Self*, an "I". This hypothesis simultaneously explains why subjective experiences exist (note that they are not predicted within material physicalism) and why realism definitely does not hold at quantum scales (the supposedly physical properties are realized instantaneously at the moment of observation).

[20] In hydrological models, the independent variable is usually two-dimensional space, meaning x should be replaced by x, y.

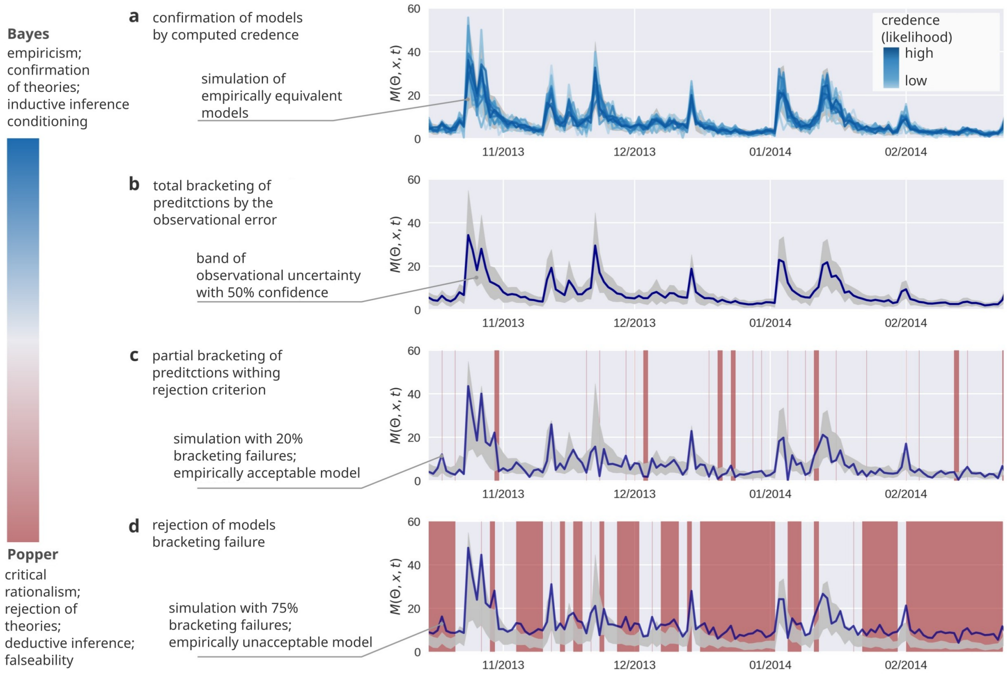

Figure 1.8 — Instrumentalist approach to hydrological modeling. In this approach, both Bayes' confirmation and Popper's rejection are employed under the recognition of the underdetermination problem (equifinality). **a** — Confirmation of models through Bayesian conditioning, where degrees of confirmation (informal likelihood measures) are assigned to empirically equivalent models. In this case, all models are encapsulated by the observational uncertainty band within the pre-established rejection threshold. **b** — Total (no failures) encapsulation of a simulation (time series) by the effective observational error of the empirical evidence. In the illustrated case, the uncertainty band has a confidence level of 50%. A more or less comprehensive band should be defined *a priori*. **c** — Partial encapsulation (with 20% failures) of a simulation by the effective observational error. As the band is at 50% confidence, the failures are within the rejection threshold, and the model can be considered empirically acceptable. **d** — Rejection of models due to insufficient encapsulation (75% failures). In this case, the failures exceed the 50% confidence level, and the model must be considered empirically unacceptable.

difference in meaning between an observation obtained at x, t and the corresponding modeled variable at $\Delta x, \Delta t$. For example, while the observed flow of a river is instantaneous and refers to a specific section of the channel, the modeled flow integrates some time step and refers to a discrete spatial extent. The measurement error ε_O and the commensurability error ε_Δ are kept on the left side of Equation (1.5) to denote that together they constitute the **effective observational error**. The input data error ε_Υ originates from the aggregation of uncertainties in both boundary conditions (such as maps of topography, soil, vegetation, etc.) and the forcing variables of the model (such as rainfall, temperature, wind speed, etc.). In this case, the uncertainty is generally statistical, so representative samples tend to reduce its impact. However, it can also take on an epistemic nature when the input data correspond to **scenarios**, which adds a conceptual burden. Finally, the model structural error ε_M results from the epistemic uncertainty of the theoretical and numerical configuration of the hydrological model. This component is strongly influenced by the theoretical assumptions previously defined about the system and its hydrological processes.

With Equation (1.5), Keith Beven operationalizes an instrumentalist paradigm for hydrological modeling that, beyond confirmation, *allows for the rejection of models*. This approach follows the recommendations discussed by Albert Tarantola, to consider both the empiricist confirmation of Bayes and the rationalist rejection of Popper for a philosophically explicit approach to environmental modeling [31]. In this line, the critique of the hegemonic modeling paradigm, dominated by pragmatic realism, is that model confirmation occurs at the cost of underestimating epistemic uncertainties, masking them as random error minimized through optimization techniques, as seen in Equation (1.3). This leads to the **overfitting problem** of models to the available data used. Through the conventional **calibration process**[21], one reaches the (incorrect) conclusion that the adjusted model identified is the only empirically adequate representation. On the other hand, the new instrumentalist approach, in Beven's words:

> (...) There is, however, another approach. That is to accept that it is very unlikely that our current model structures are truly realistic descriptions of the enviromental systems of interest so that there may indeed be many different models that can be shown to provide predictions that are acceptably consistent with whatever observed data are available. That is to treat the problem of identifiability as one of equifinality of model structures and parameter sets in reproducing the known behaviour of the system. – Keith Beven (2009. p. 15) [32].

It is important to note that this new approach does not abandon the confirmation process through the Bayesian conditioning of the posterior distribution of the parameters Θ. Although the total error equation makes a formal treatment of the likelihood $P(O|M)$ impossible, it remains possible to assign different degrees of conviction, or weights, to the **empirically equivalent models** through informal likelihood measures $\mathcal{L}(O|M)$. The novelty of the approach lies in establishing that an **empirically acceptable model**[22] occurs when its structural error ε_M is less than its effective observational error $\varepsilon_O + \varepsilon_\Delta$. Otherwise, the model must be rejected. This implies that the predictions of any model must be *encapsulated* by a confidence interval defined *a priori* as a rejection criterion. In other words, for a confidence level of $\alpha\%$, the **bracketing inequality**:

$$O_{100-\alpha\%}(x,t) < M(\Theta, \Upsilon, \varepsilon_\Upsilon, x, t) < O_{\alpha\%}(x,t) \quad \forall \quad x,t \tag{1.6}$$

must hold true with a frequency of at least $\alpha\%$; where $O_{100-\alpha\%}$ and $O_{\alpha\%}$ are the lower and upper thresholds of the confidence interval of the effective observational error at each sample point x, t. This approach has exactly the same structure as statistical hypothesis tests: 1) a rejection criterion is pre-defined by a confidence level $\alpha\%$; 2) a test statistic is calculated, in this case the encapsulation rate of the simulation, and; 3) the p-value of the test is evaluated, which in this case is the failure rate of encapsulation. If the p-value is greater than the confidence level, the model should be rejected. On the other hand, all models that pass the minimum encapsulation test are considered empirically equivalent and can be confirmed based on likelihood measures. Figure 1.8 illustrates the approach for encapsulating a time series of any hydrological variable, but it is generally the discharge in a river section. It is noted that the pre-definition of the confidence level implies more or less comprehensive observational uncertainty bands. This fact introduces the following dilemma: when high certainty about predictions is desired, the observational band may be very wide, resulting in various empirically acceptable simulations and little precision in structural error. This creates the need to obtain more evidence, so that the observations themselves present narrow bands for high confidence levels. Another aspect that differs from the hegemonic paradigm, which operates solely through confirmation, is that nothing prevents the eventual *rejection of all tested models* by the bracketing inequality. If this is the case, Beven emphasizes, a valuable opportunity arises to transform modeling into a learning process, forcing users to review both the auxiliary hypotheses and the main hypothesis, that is, the very theoretical assumptions adopted in the conception of the modeled hydrological processes. Ultimately, total rejection imposes the need for new theories and explanations [33]. Without this, the scientific community in this field will be forever trapped in the same paradigms. ■

[21] Also referred to as the *inverse problem*

[22] Keith Beven refers to empirically acceptable models as *behavioral models*.

1.7 Chapter Summary

In this chapter, I aimed to establish the foundations of an instrumentalist philosophy for the application of hydrological models. The distinction between rationalism, with its emphasis on deduction, and empiricism, which values induction, was highlighted. From the empiricist side, I presented Bayesian epistemology, which proposes a gradual confirmation of hypotheses based on probabilities. From the rationalist perspective, I articulated the deductive rejection of theories, a stance defended by Karl Popper. In his thesis on scientific paradigms, Thomas Kuhn explains the alternation between periods of normal science and crises. The problem of underdetermination, raised by critics of scientific realism, is applied to hydrological modeling, culminating in an instrumentalist proposal that addresses epistemic uncertainty in the acceptance of empirically adequate models.

- **The problem of justification**. There is a difficulty in justifying the truth of theories, in establishing definitive explanations for events and phenomena. On one hand, rationalists appeal to the use of deductive inference, which guarantees the truth of statements as long as their premises are true. On the other hand, empiricists prefer to use inductive inference, which employs empirical evidence to generalize observed patterns.
- **Inductive confirmation of hypotheses**. Bayesian epistemology describes the process of empirical conditioning to confirm hypotheses. By recognizing the existence of random noise in empirical observations, the truth of a hypothesis must be described as a credence, or probability. In this process, the probability distribution of hypotheses is incrementally adjusted through the application of Bayes' Theorem.
- **Deductive rejection of theories**. Karl Popper, when analyzing the Logic of scientific research, argues that the only safe way to acquire knowledge is through deductive refutation. In this sense, the role of empirical evidence is to test a hypothesis against counterexamples that prove its falsehood. For this reason, Popper claims that scientific theories must be falsifiable theories that allow for their own rejection.
- **Paradigms and the context of discovery**. Thomas Kuhn, by exploring the History of Science, eliminates the apparent contradiction between confirmation and rejection of theories. He argues that the dynamics of the scientific community plays a profound role in the production of knowledge, especially in the advent of paradigms. For him, confirmation occurs in periods of normal science, while rejection predominates in crisis periods. Crisis periods end only when the competition of new ideas leads to a new paradigm.
- **The problem of underdetermination**. scientific realism is deeply questioned by Bas van Fraassen and Nancy Cartwright. They establish an instrumentalist perspective, where the goal of Science is solely to produce empirically adequate theories. This mainly stems from the instance of unobservable entities, which renders theories underdetermined by the evidence. A version of this occurs in hydrological modeling due to many modeled processes being practically unobservable – the so-called equifinality problem. In this line, Keith Beven proposes an instrumentalist paradigm for the application of models, allowing for the rejection of models based on the encapsulation test of predictions by observational uncertainty. Models that pass the test are deemed empirically acceptable and equivalent.

The whole is not merely the sum of its parts. If it were, chairs could not exist. Similarly, people could not exist. The **form** unifies in **dynamic systems** the parts that, when isolated, bear no resemblance to the whole.

Chapter 2

Sistems and models

> Everything we think we know about the world is a model. Every word and every language is a model. All maps and statistics, books and databases, equations and codes are models. So are the ways I imagine the world in my head – my mental models. None of these is or ever will be the real world.
>
> Donella Meadows (2008, p. 86) [34]

> If validation is impossible and all models are wrong, why do we bother to build them? As a leader, you must recognize that you will be using a model – mental or formal – to make decisions. Your choice is never whether to use a model, but which model to use. Your responsibility is to use the best model available for the purpose at hand, despite its limitations. Delaying actions in the vain search for a perfect model is, in itself, a decision, with its own consequences.
>
> John Sterman (2000, p. 850) [35]

2.1 The Modeling Process

Donella Meadows (1941-2001) may have been the most brilliant environmental systems modeler to ever live, leading the ambitious initiative proposed by the book *Limits to Growth*, published in 1972 and revised in two subsequent editions. This book issued an unprecedented warning about the ecological scenarios that the current industrial society, based on non-renewable resources, may face by the year 2100, including the possibility of a catastrophic collapse [36]. Her argumentation was based on simulations of a comprehensive model of the world, the model `World3`, mapping the availability of numerous stocks and flows of natural resource consumption, from arable land to oil

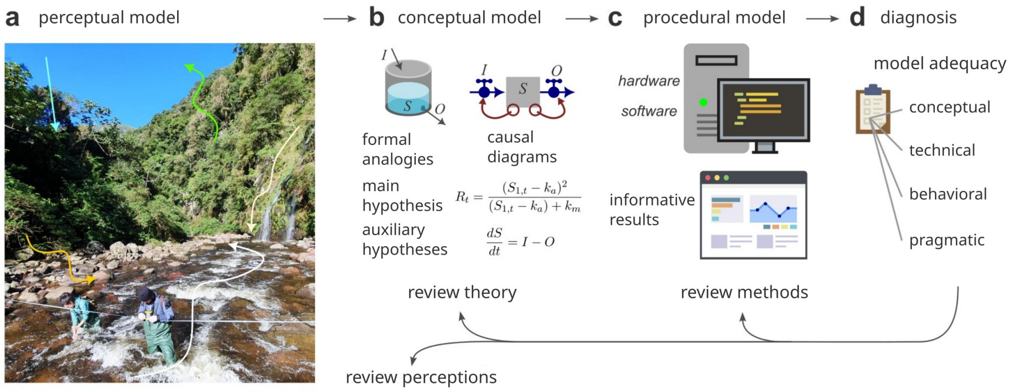

Figure 2.1 — The modeling process. Hydrological modeling can be understood as an iterative learning process. **a** — The first stage consists of the perceptual model (mental models), which is a collection of subjective and personal perceptions acquired through empirical experience (field expeditions) and theoretical experience (textbooks, lectures, classes, etc). **b** — The second stage consists of the conceptual model, which instantiates formal (mathematical) analogies and causal diagrams (structures) to obtain an objective main hypothesis in the form of equations. Various auxiliary hypotheses are generally required, making the conceptual model a logically open system (underdetermined). **c** — The third stage consists of the procedural model, which is the synthesis of the computational methods used (*hardware* and *software*) to simulate the conceptual model and produce results in symbolic forms such as tables, graphs, maps, animations, etc. **d** — Finally, the diagnostic stage applies various procedures to assess the adequacy of the models in conceptual (theoretical problems), technical (computational problems), behavioral (empirical justification), and practical (decision-making impacts) terms. The diagnosis is iterative, reviewing all created models and closing the learning cycle. The photograph in (**a**) was kindly provided by hydrologist Marina Fagundes, who is measuring the flow of a mountain river during a field expedition in Rio Grande do Sul, Brazil.

reserves. Despite the significant social, political, and economic impact of her work, Meadows contributed little toward the more philosophical direction, such as the epistemological problems addressed in Chapter 1. Still, as emphasized in the above epigraph, she left evidence of sharing the Kantian tradition, according to which pure reason has access only to transcendent categories or, in her terms, to **mental models**. These mental models would then be expressed in various forms, including diagrams, texts, equations, and computer programs. Her line of thought eventually suggests an instrumentalist view, in which we will never have the conditions to establish the truth about the world, but only empirically adequate theories:

> Our models usually have a strong congruence with the world. That is why we are such a successful species in the biosphere. Especially complex and sophisticated are the mental models we develop from direct, intimate experience of nature, people, and organizations immediately around us. However, and conversely, our models fall far short of representing the world fully. That is why we make mistakes and why we are regularly surprised. In our heads, we can keep track of only a few variables at one time. We often draw illogical conclusions from accurate assumptions, or logical conclusions from inaccurate assumptions. – Donella Meadows [34].

Regardless of Meadows' position on philosophical currents, her view is clear in that modeling is a *process* that begins in a *subjective and personal* manner with mental models, and then becomes increasingly *objective and impersonal* through texts, equations, and computer programs.

In the field of Hydrology, Keith Beven emphasizes Meadows' perspective, proposing that the modeling process consists of at least three stages represented by models of different natures: the *perceptual* stage, the *conceptual* stage, and the *procedural* stage[1] [37]. Figure 2.1 illustrates this conception, including a final diagnostic

[1]Two additional stages in the modeling process include the calibration and validation of the procedu-

stage. The **perceptual model** begins with the hydrologist's subjective and qualitative understanding of how a watershed responds to precipitation events. This model is profoundly influenced by individual experiences, studies, analyzed data, and the hydrologist's field experience. It is an inherently personal model and varies substantially from person to person. Moving to the **conceptual model**, Beven describes a transition to a more formalized and simplified representation of the processes identified in the perceptual model. This model involves creating hypotheses and adopting assumptions to *abstract* the complex processes of reality into tangible and objective forms, often utilizing mathematical formulations. Finally, the **procedural model** represents the practical implementation of the conceptual model in a computer program. At this stage, the equations and concepts from the conceptual model are translated into code, allowing simulations and predictions of flows and levels based on input data through the application of tensions in electronic circuits. In the case of digital computers, this process involves the application of numerical methods and may introduce additional errors or approximations, making precision and care in execution extremely important. It is these electronic computations that produce the supposedly informative results we see in tables, graphs, maps, etc. For Beven, the interaction and evolution between these three models are crucial in the modeling process in Hydrology. With several caveats, he includes two additional stages, which would be the *calibration* and *validation* of the model against empirical evidence. These are jargons of pragmatic realism. An instrumentalist nomenclature would be *conditioning* and *testing* against empirical evidence. One way or another, a final stage of **diagnosis** should lead to the review and refinement of the previously developed models, giving rise to an *iterative learning cycle* and potential *scientific revolutions* in understanding hydrological processes.

It is with this perspective that the objective of this chapter is to establish the necessary details about the modeling process so that we can soon discuss hydrological models properly. At a certain point in the previous chapter, it became essential to define a model as a **symbolic vehicle of a theory**, a typically instrumentalist conception that resonates with Nancy Cartwright's view [todo:cite] – which is effective in articulating the epistemological problems that underlie modeling practices. In this perspective, models are seen as mere translators of our theories or hypotheses about real phenomena, such as the hydrological cycle. However, this is still a generic and abstract definition that does not provide a concrete understanding of the exact nature of models. As emphasized at the beginning of the first chapter, hydrological models materialize in the states of electronic circuits in digital computers, but they are also other things before this materialization. To articulate the enigma of what exactly models are, this chapter will abandon the domain of Epistemology and the Philosophy of Science, delving into the field of Ontology of models. I will address the problem of representation, the paradigm of systems, Systems Dynamics, and model diagnostics. If in the previous chapter we were on a panoramic view with thin air, like at the top of a mountain, we are now certainly descending from the heights, following the valleys of the streams. The analogy remains interesting, as the path is still difficult and steep, but the landscape is becoming increasingly familiar. Hope grows that soon we will be on gentle and open ground.

2.2 Representation

Models serve the function of representing a **target system**. That is, precisely because they symbolically convey a theory, models aim to re-interpret a given phenomenon or entity that supposedly exists and develops in the real world. The problem of justifying

ral model, but these stages are not models themselves; rather, they are steps of empirical justification.

the correspondence between the model and reality was the subject of the first chapter. Here, however, we have a new problem: *how is it possible to create the representations themselves*? The solution to this **representation problem** consists of establishing a process of **idealization** of the target system combined with the application of **analogical inference**, that is, the construction of a **analogy** between the target system and the model. In this line, Mary Hesse proposes that such analogies manifest both through *material models*, semantic structures realized by physical objects, and through *formal models*, syntactic structures expressed by mathematical equations implemented by computer programs [38].

The process of idealization is the foundation of all modeling and is characterized by *deliberate simplifications*, which make the model more tangible and understandable than the target system itself, emphasizing crucial aspects while ignoring supposedly less relevant details. According to R. Frigg and S. Hartmann [39], there are two forms of idealization that are not mutually exclusive: **Aristotelian idealization** and **Galilean idealization**. In the case of Aristotelian idealization, the key lies in the process of **abstraction**, when all supposed superficialities of the target system are removed, leaving only a supposed *essence*. In other words, abstraction aims to preserve the truth, albeit only the part that is relevant. In a hydrological model, for example, the vegetation canopy is usually treated as a single reservoir that intercepts rainwater. It is clear that each leaf and twig plays a role in interception, but this individual process is considered irrelevant and abstracted as a general process occurring throughout the canopy. Alan Musgrave, however, notes that abstraction can also result in falsehoods, especially when **negligibility premises** are introduced, that is, when a *knowingly true* causal factor is neglected [40]. He initially brings this critique to neoclassical economic theories, but it is also the case, for instance, when hydrological models ignore the importance of solar radiation and terrain shading on evaporative processes. The Galilean idealization, on the other hand, consists of applying a controlled experimental distortion, which can be incrementally reversed from the simple to the complex, from the ideal to the real [41]. In other words, idealization exhibits an *asymptotic behavior* that, in the limit, makes the model identical to the target system. The reference to Galileo Galilei (1564-1642) relates to his famous experiments with inclined planes, which led him to conclude that objects fall at the same time, regardless of their mass. In this case, the inclined plane idealized free fall, allowing for a better understanding of the physical process. In hydrological models, an example of this type of idealization is the spatial discretization into response units, sub-basins, or drainage networks – when taken to the extreme of small parcels, it asymptotically approaches the watershed.

Among the available forms of analogies, a somewhat direct alternative is to construct a *copy* of what is understood as the target system, at a scale suitable for manipulation by humans. These material models are referred to as **scale models** reduced or enlarged, illustrated in Figure 2.2a and Figure 2.2b. To some extent, we are all accustomed to models of this type, as the toys we played with as children are like reduced-scale models. A scale model of a building or a car in a wind tunnel, for example, is a reduced-scale model used for engineering applications. Atoms of chemical elements with fittings to form more complex molecules, on the other hand, are enlarged-scale models for educational purposes. In a highly technological age, scale models may seem crude or simplistic, but they are actually extremely interesting options for investigating, visualizing, and experimentally testing the implications of a given theory or hypothesis. A notable example in the History of Science that involved the contribution of an enlarged-scale model was the discovery of the structure of DNA by Watson and Crick in the early 1950s [42]. Despite their appeal, the **scale similarity** of representation is only feasible in special cases or for certain characteristics. For example, if a model of a city is built to observe the shading effects of buildings, the reduction of scale does not interfere

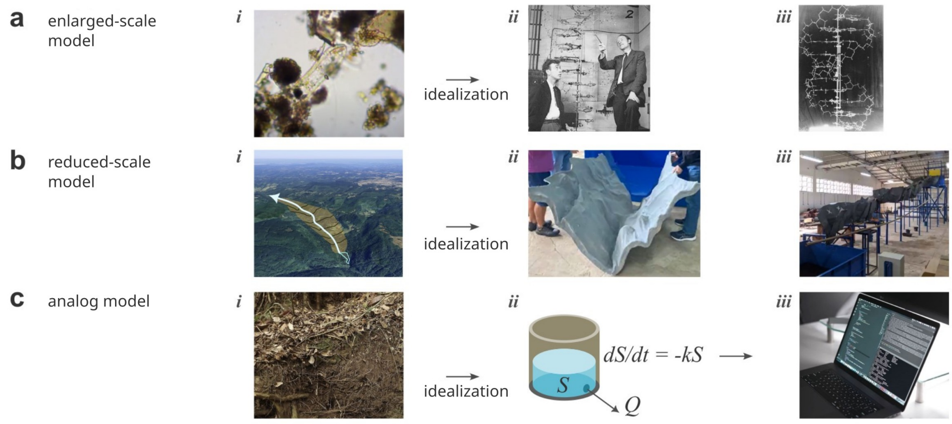

Figure 2.2 — Representation of systems by models. idealization is necessary to represent target systems in sufficiently tractable models. **a** — A famous enlarged-scale model in the History of Science was the double helix model for the DNA molecule, which stores the genetic code of organic cells (detail i); Francis Crick and James Watson handling the model (detail ii); the original DNA model (detail iii). **b** — A reduced-scale model for empirical studies of dam breakage. In this case, the model represents 5.5 km of the valley downstream from the Canastra dam, Canela, Rio Grande do Sul (detail i); the topobathymetric representation of the valley (detail iii) with cross-section modules and steel long beams, filled with fiberglass and resin (detail ii). **c** — A typical analog model of Hydrology for water storage in the soil and groundwater (detail i); the formal analogy (homology) is made with a linear reservoir, as if it were a bucket with a porous outlet at the bottom (detail iii); the model is realized in a digital computer, from the interaction of *hardware* with *software* (detail iii). Credits for the images: (**a**) the author (detail i) and from Chadarevian [42] (details ii and iii); (**b**) the author (detail i) and Flávia Pereira [43] (details ii and iii); (**c**) the author (detail i) and Pinterest (detail iii).

with the shadow patterns produced by light, as the geometry is completely preserved at both scales. However, a reduced-scale water channel or pipe may exhibit viscosity and surface tension effects much greater than those observed at the real scale, making the conversion between scales a non-trivial problem. In fluid mechanics problems like this, the conversion is usually solved through dimensional analysis, which seeks to establish a characterization of the target system that is scale-free, such as the Mach, Reynolds, and Froude numbers.

Depending on the target system in question, representation by reduced or enlarged scale models may not be possible due to some fundamental principle or simply due to a lack of material resources. An epidemiological model at a reduced scale is clearly not possible for ethical reasons, for example. Meanwhile, a reduced-scale model of an environmental system, such as a floodplain or the atmosphere itself, can be very expensive. Given this condition, it is necessary to resort to a form of analogical representation. In other words, it is essential to adopt a modeling approach that establishes a formal analogy, or **homology**, with the target system, that is, an equivalence between the *mathematical structures* of the target system and the model. In Hydrology, this is often achieved by establishing that the soil (or any other compartment of the hydrological cycle) functions *as if* it were a linear reservoir, like a bucket with a porous hole at the bottom, as illustrated in Figure 2.2c. The conjunctive phrase “as if” is crucial, as it establishes the analogy that underpins the idealization of modeling. The implementation of the formal analogy, that is, the realization of its mathematical structure, generally occurs through the programming of digital computers (which is the case for hydrological models), although it is also possible to create material models of the analogous system. In this sense, formal models make the symbolic conveyance of the theory or hypothesis about the target system much clearer than scale models, as they seek to test a mathematical structure based on a supposedly analogous system. Just like deduction, induction, and abduction mentioned in the context of justification of theories in the first chapter, the analogy also constitutes a form of inference, which presents the following logical structure [44]:

1. The objects $O_1, O_2, O_3, ...O_n$ share the properties $P_2, P_3, P_4, ...P_k$.
2. The objects $O_2, O_3, ...O_n$ share the property P_1.
3. Therefore, it is likely that the object O_1 possesses the property P_1.

Thus, analogical inference allows for multiple items to be evaluated, although generally the relationship is made between only two objects – in the case of modeling, the target system and the model. Another characteristic is that, unlike abduction, analogical inference is not a special form of induction, as it does not involve a universal generalization from singular statements. Still, it is also not as secure as deduction, as there is no guarantee of the truth of the consequent statement. For this reason, analogical inference is considered an independent form of inference.

In many cases of research and scientific investigation, obtaining an empirically adequate representation of a given target system is not necessarily the ultimate goal of model construction, but rather the *exploration* of the implications of the theory that the model conveys. In other words, instead of confronting the models with empirical evidence to test or confirm the hypotheses embedded in their structure, they can also serve the epistemic function of *articulating* the theory itself. In this sense, Axel Gelfert introduces the concept of **exploratory experimentation** with models, a process that has the potential to reveal various new hypotheses and elucidations in the theoretical field [45]. The advantage of **exploratory models**, often maintained as **minimalist models** to facilitate understanding, is that the analogy with the target system suggests that unexpected and surprising behaviors of the exploratory model may eventually be empirically observed in the target system, under limit conditions. One example that Axel Gelfert highlights from the History of Science is the experiments with the Lotka-Volterra ecological model, which explored predator-prey dynamics. Although the model did not provide empirically precise predictions, it offered several important qualitative *insights* about the interdependencies among different species in a situation of complete isolation: it was demonstrated that oscillations in populations can emerge even without external interference. In the environmental and hydrological field, for example, exploratory models can contribute to understanding the impacts of *scenarios* never observed in the historical record, such as the ongoing climate changes. In this conception, exploratory models are versatile tools in scientific research, serving various roles, from providing starting points for future investigations, demonstrations of *proof of principle*, formulating potential explanations, to evaluating the adequacy of the model. Furthermore, they are particularly valuable in situations where established theories are in crisis, allowing new paradigms to be proposed based on experimental explorations.

2.3 Systems

When we deal with models, a central concept arises, which is the notion of **system** – after all, models convey a theory by representing a target system. A system is defined as *a set of parts with relationships among themselves*. This definition may seem simple, but it carries with it a holistic worldview that instantiates things that transcend materiality. As has been pointed out, by exploring the essence of "things", we enter the field of **Ontology**, which is the study of what exists. The ontological question is: *what exists*? Consider, for example, a classic ontological question: the existence of chairs [46]. Whether chairs exist or not, the answer varies depending on the interpretation of the nature of fundamental elements. From a reductionist perspective, which considers atoms of matter as the only possible entities, chairs are merely collections of atoms and, therefore, *do not exist*. This bottom-up perspective leads to a disquieting conclusion: nothing exists, *not even people*, except matter being scattered in a great flow from nothing to nothing. However, it is evident that chairs do exist; otherwise, we would all be sitting on the floor. Even more evident is the fact that there are people; otherwise, I could not write this text and no one could read it. The solution to instantiate the existence of objects like chairs or people consists of adopting a holistic approach, that is, a top-down view. This perspective understands objects and subjects as entities that **emerge** from the relationship and interaction among their fundamental components, their elements, their parts. In this sense, a chair exists independently of its material, whether it is metal, wood, or plastic. At the same time, it is useless to obtain a pile of wood and expect a chair to emerge from it: **organization** is necessary. A chair would then be the system that emerges from an organized structure that serves the function of providing a seat.

The roots of systems thinking date back to Antiquity, especially in the ideas of Aristotle (384-322 B.C.). This Greek philosopher developed a concept known as **hylomorphism**, which permeates various aspects of his philosophy, ranging from natural science to politics. With this perspective, Aristotle argued that every existing object is composed of both **matter** and **form**, with the latter being essential for the *unification* of the object into a single entity [todo:cite]. For example, in living organisms, the body represents the matter and the soul, the form. In politics, citizens would be the matter and the constitution, the form. With the advent of the scientific method in modernity, primarily influenced by the ideas of Descartes, there was a decline in the conception of form as an ontological unifier. In his *Discourse on Method*, Descartes introduced an analytical, reductionist, and mechanistic approach to the world. For example, one of the essential steps of his method to dispel doubts involves isolating difficulties into as many parts as necessary for easier resolution, gradually building the complete vision of the whole, from the simplest to the most complex. In this regard, the focus should remain on the individual parts, with the whole being merely an overlay or linear concatenation. Here lies a **principle of additivity**, which allows understanding larger scales from smaller scales. Descartes illustrates this view by describing the human heart in terms of a hydraulic pump that functions to distribute blood, suggesting that the human body is actually a machine, with each organ performing a specific function. This movement gained traction from Newtonian physics, with a landmark of its peak being Laplace's celestial mechanics and later, in the 19th century, classical thermodynamics, which established blind and relentless laws that describe random and disorganized complexity.

The renaissance of systems thinking in the 20th century was substantially marked by the work of the biologist Ludwig von Bertalanffy (1901-1972). Criticizing the hegemonic mechanistic and reductionist paradigm, Bertalanffy initiated the **General Theory of Systems** starting in the 1920s, although it only consolidated in the 1960s. The influence of biology in this contemporary movement of systems thinking was partially related to the refutation of vitalist theories about living organisms. Given that living beings are completely composed of the same matter as their environment, the need arose to explain the enigma of how simple molecules can form cells, tissues, organs, individuals, and societies. But there were also influences from other theories and disciplines of the time, such as cybernetics and the theory of information, which introduced the concepts of **feedback** and signals among the components of a system. The generality of the theory lies in what Bertalanffy calls **structural isomorphism**, which is the formal analogy (homology) between completely different phenomena in material terms, but which present the same relationships among the parts, that is, the same form. In this sense, the proposal becomes somewhat ambitious, as Bertalanffy suggests that there is a unifying potential for a Science that was overly compartmentalized:

> The systemic point of view has penetrated and proved indispensable in a wide variety of scientific and technological fields. This ultimate fact that it represents an original paradigm in scientific thought (to use Thomas Kuhn's expression) has the consequence that the concept of system can be defined and developed in different ways as required by research objectives. – Ludwig von Bertalanffy [47].

Bertalanffy's theory, in essence, advocates for a holistic understanding of living organisms and systems in general, treating them as **open systems** that constantly interact with the environment and are subject to the flow of matter, energy, and information. This view contrasts with the perspective offered by classical thermodynamics, which focuses on closed systems governed by random disorganization. Open systems, on the other hand, allow for the emergence of homeostasis, metabolism, and steady states, phenomena that, according to Bertalanffy, help explain the apparent violations of the laws of thermodynamics in biology. In the mechanistic view of the world, the fate of any system is rigidly determined by blind laws and its initial conditions. But Bertalanffy emphasizes that this does not occur in open systems, exemplifying with the phenomenon of equifinality[2], which occurs when different initial conditions lead to the same final state, a process observed mainly in the embryonic development of living organisms. Darwinian evolution itself, Bertalanffy points out, also apparently violates the dictates of the second law of thermodynamics, as it allows for the accumulation of information and complexity over time. It is clear that the laws of thermodynamics are not violated in any of these cases, but it is the capacity to import free energy from degrading sources that allows open systems to remain stable against the natural flow of disorder, in a process of constant *self-organization*.

Although Bertalanffy admits that the General Systems Theory can be broadly applied from what he called *verbal models*, he illustrates that *formal models* of systems can be derived from a more or less general mathematical formulation. In this case, this formulation involves a system of simultaneous differential equations. Thus, for n elements characterized by a quantitative measure S:

$$\begin{aligned} \frac{dS_1}{dt} &= f(S_1, S_2, ..., S_n) \\ \frac{dS_2}{dt} &= f(S_1, S_2, ..., S_n) \\ &... \\ \frac{dS_n}{dt} &= f(S_1, S_2, ..., S_n) \end{aligned} \tag{2.1}$$

In other words, any variation in S_i is a function of the overall state of the system, which includes all other elements. This formulation also allows for the destruction of the relationship between the parts: it is enough to make the state S of an element solely a function of itself, that is, $dS_i/dt = f(S_i)$. In this case, the system as an ontological entity ceases to exist, and the final state of the whole is completely reduced to the superposition of the states of the individual elements. However, when there are relationships, no matter how trivial they may be, Bertalanffy shows that from the differential equations emerges a rich variety of *end behaviors*, such as exponential growth or decay and processes described by the logistic curve, like saturation and autocatalysis. With just two elements, the system of linear constant coefficients assumes the following

[2] Keith Beven adopted the term "equifinality" to describe the underdetermination problem in hydrological models based on Bertalanffy's General Systems Theory [todo:cite].

general form:

$$dS_1/dt = c_{11}S_1 + c_{12}S_2$$
$$dS_2/dt = c_{21}S_1 + c_{22}S_2$$

In this simple system, the Taylor series expansion allows solutions to be obtained for S_1 and S_2 through mathematical analysis. The different solutions demonstrate the emergence of different **stability conditions** (Figure 2.3 a). This can be visualized graphically through a **phase plane** in which the trajectories of the states of the two elements are drawn, as well as the evolution of the variables in the temporal domain. Thus, the multiple configurations of parameter values (coefficients) and also of initial conditions reveal the **attractors** that act on the system. For example, under certain conditions, the system is stable and migrates from a *source* to a final state (S_1^*, S_2^*), or node, in a *drain*. This can occur smoothly or through **damped oscillations** (Figure 2.3 b, details *i* and *ii*). Under other conditions, the system is unstable, migrating eternally, either in a fixed direction ($-\infty$ or $+\infty$) or through **amplified oscillations** (Figure 2.3 c, details *i* and *ii*). Alternatively, the system may exhibit **stable oscillations**, remaining eternally in a loop when visualized in the phase plane (Figure 2.3 b, detail *iii*). A famous example of stable oscillations is the non-linear system of Lotka-Volterra mentioned in Section 2.2, which simulates the interaction between the prey populations S_1 and the predator population S_2:

$$dS_1/dt = r_1S_1 - c_1S_1S_2$$
$$dS_2/dt = -r_2S_2 + c_2S_1S_2$$

where r_1 and r_2 are growth and decay rates, respectively. The product S_1S_2 aims to represent the rate of encounters between prey and predators, weighted by the coefficients c_1 and c_2, creating a feedback that balances the populations in cycles. Bertalanffy emphasizes that these are simple examples that help illustrate the versatility of systems in representing patterns observed in nature. If the system of interest has various relationships or even greater complexities, such as partial terms, the analytical solution of the model can be extremely difficult or even impossible, necessitating the application of numerical methods to solve the equations in any domain, whether in time or space (or both).

Although Bertalanffy admits that the General Systems Theory can be broadly applied from what he called *verbal models*, he illustrates that *formal models* of systems can be derived from a more or less general mathematical formulation. In this case, this formulation involves a system of simultaneous differential equations. Thus, for n elements characterized by a quantitative measure S:

$$\begin{aligned}
\frac{dS_1}{dt} &= f(S_1, S_2, ..., S_n) \\
\frac{dS_2}{dt} &= f(S_1, S_2, ..., S_n) \\
&... \\
\frac{dS_n}{dt} &= f(S_1, S_2, ..., S_n)
\end{aligned} \tag{2.2}$$

In other words, any variation in S_i is a function of the overall state of the system, which includes all other elements. This formulation also allows for the destruction of the relationship between the parts: it is enough to make the state S of an element solely a function of itself, that is, $dS_i/dt = f(S_i)$. In this case, the system as an

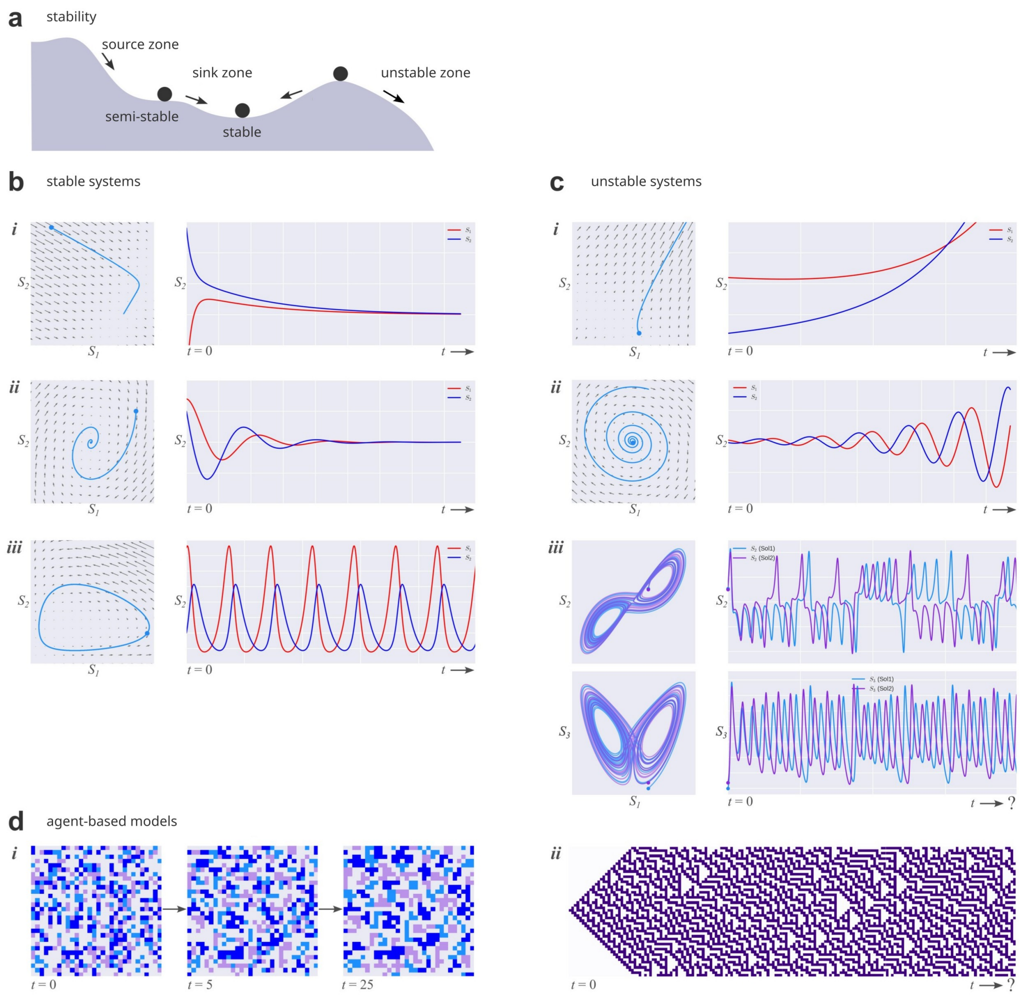

Figure 2.3 — Stability and behavior of systems. A system is defined by a set of parts with relationships among them. Since it is the relationships that unify the whole, similar final behaviors emerge in different scientific fields. **a** — The behavior of a system can be classified as stable or unstable, depending on its initial and boundary conditions. **b** — Stable systems with two elements (S_1 and S_2): exponential decay (detail i) and damped oscillations (detail ii) make an asymptotic movement toward an equilibrium point, being variations of the homogeneous linear system. A stable system can also exhibit eternal oscillations around the equilibrium point, as in the case of the Lotka-Volterra predator-prey model, a non-linear system (detail iii). **c** — Unstable systems with two elements (S_1 and S_2): exponential growth (detail i) and amplified oscillations (detail ii) make a movement toward $+\infty$ or $-\infty$ (or both), also being variations of the homogeneous linear system. Instability can also be chaotic, as in the Lorenz model, a non-linear system with three elements (S_1, S_2, and S_3; detail iii). In the case of the chaotic system, two solutions (in blue and purple) are visualized for very close initial conditions, but diverge in the long run (high sensitivity to initial conditions). **d** — Agent-based models illustrate that complex behaviors can emerge from simple interactions in the immediate neighborhoods of each agent. The Schelling model (detail i) illustrates the emergence of ordered clusters from random initial conditions. Wolfram's Rule 30 (detail i) illustrates computational irreducibility: the only way to understand the final behavior of the system is to simulate the model step-by-step.

ontological entity ceases to exist, with the final state of the whole completely reduced to the overlay of the states of the individual elements. But when there are relationships, however trivial, Bertalanffy demonstrates that from the differential equations emerges a rich variety of *final behaviors*, such as exponential growth or decay and processes described by the logistic curve, such as saturation and autocatalysis. With just two elements, the linear system of constant coefficients takes the following general form:

$$dS_1/dt = c_{11}S_1 + c_{12}S_2$$
$$dS_2/dt = c_{21}S_1 + c_{22}S_2$$

In this simple system, the Taylor series expansion allows solutions to be obtained for S_1 and S_2 through mathematical analysis. The different solutions demonstrate the emergence of different **stability conditions** (Figure 2.3 a). This can be visually represented graphically from a **phase plane** where the trajectories of the states of the two elements are drawn and also by the evolution of the variables in the time domain. Thus, the multiple configurations of values of the parameters (coefficients) and also the initial conditions reveal the **attractors** acting on the system. For example, under certain conditions, the system is stable and migrates from a *source* to a final state (S_1^*, S_2^*), or node, in a *drain*. This can occur smoothly or through **damped oscillations** (Figure 2.3 b, details i and ii). Under other conditions, the system is unstable, eternally migrating, either in a fixed direction ($-\infty$ or $+\infty$) or through **amplified oscillations** (Figure 2.3 c, details i and ii). Alternatively, the system may exhibit **stable oscillations**, remaining forever in a loop when viewed in the phase plane (Figure 2.3 b, detail iii). A famous example of stable oscillations is the non-linear system of Lotka-Volterra mentioned in Section 2.2, which simulates the interaction between the populations of prey S_1 and the population of predators S_2:

$$dS_1/dt = r_1 S_1 - c_1 S_1 S_2$$
$$dS_2/dt = -r_2 S_2 + c_2 S_1 S_2$$

Where r_1 and r_2 are growth and decay rates, respectively. The **strange attractor** of this system is illustrated in two phase planes in Figure 2.3c, in detail iii. The detail also illustrates two trajectories that started very close but take on different behaviors in the long run. On the other hand, the problem of computational irreducibility relates (mainly) to the application of **agent-based models**. The agent-based models represent systems through fundamental elements – the agents – that follow simple rules in their immediate neighborhood. When represented in a regular matrix, such as a board, these models are called **cellular automata**. An exemplary agent model is the **model of segregation by Schelling** [todo:cite]. In this model, the agents have qualitative categories. At each time step, the agents evaluate their immediate neighborhood and decide whether to move or stay, depending on their tolerance rate with agents of different categories. This system with simple rules spontaneously produces organized clusters, as illustrated in Figure 2.3d, detail i. In this line, Stephen Wolfram demonstrates that simple rules in certain systems can generate unpredictable complexity, accessible only through simulations that evaluate the system *step-by-step* [todo:cite]. This computational law arose from experiments with cellular automata that followed simple rules of Boolean conversion (from 0 to 1 and vice versa) based on binary representation. Some rules, such as **Rule 30**, exhibit computational irreducibility (Figure 2.3d, detail ii). Both deterministic chaos and computational irreducibility convey the same message: these are issues that cast doubt on the *predictive capacity* of theories when it comes to dynamic and non-linear systems. At the same time, they are concepts that reinforce the importance of empirical adequacy and estimation of epistemic uncertainties so that policies are based on *evidence*, not just on *theories*, as explored in the previous chapter.

2.4 Dynamics

The advent of the paradigm sistêmico in the 1960s allowed for the emergence of the discipline of **Systems Dynamics**, which is, in fact, a fusion of control engineering with management science and decision-making. Systems Dynamics, as the name indicates, studies the evolution of complex systems over time. Furthermore, John Sterman argues that Systems Dynamics is fundamentally a method for *learning* about the behavior of complex systems [35]. As emphasized in the second epigraph of this chapter, Sterman asserts that models ultimately allow for gaining *insights* into the structure and behavior of systems, exploring **leverage points** to achieve desired outcomes in policy formulation and decision-making. The ability of a model to accurately predict the state of a given system, from this perspective, is not as important as understanding its functioning and developing action strategies. The creation of this discipline is attributed to Jay Forrester (1918 - 2016), who sought to understand the behavior of systems from a technological and managerial perspective, that is, focused on solving problems and achieving pre-established goals, from capturing a market share by an industry to reducing the concentration of greenhouse gases in the atmosphere. This is illustrated by his account that the fundamental ideas of this discipline emerged from a challenging industrial problem at *General Electrics*, related to long-term fluctuations in jobs. After studying the decision-making processes of the industry, he used a simple simulation, with pencil and paper, which revealed a potential for oscillations in the internal organization of the system:

> (...) even with constant incoming orders, one would get employment instability as a consequence of commonly used decision-making policies within the supply chain. That first inventory-control system with pencil and paper simulation was the beginning of the System Dynamics field – Jay Forrester [48].

Despite its beginning with pencil and paper, Systems Dynamics clearly requires the use of digital computers to simulate highly complex models in industrial, urban, social, economic, environmental, and global contexts. A global application example is the world model `World3`, whose simulations were explored by Donella Meadows in *Limits to Growth*, who was part of Forrester's research group at MIT. Currently, the application of concepts and the construction of Systems Dynamics models are typically carried out using software such as `Stella` and `Vensim`, which utilize advanced graphical interfaces to facilitate the development of complex systems.

Systems Dynamics formalizes the basic architecture observed in hydrological and environmental models. This architecture, in philosophical terms, is a singular ontology that consists of **compartment model**, illustrated in Figure 2.4a. In Hydrology, it corresponds to the reservoir or "bucket" model. This approach has consolidated in the environmental field, primarily due to the ease of abstraction and the (relative) low computational demand. Another contributing aspect is that empirical evidence about environmental processes often results from aggregated processes, such as the flow of a river or the concentration of a substance in water or air, a fact that is changing with the advent of high spatial and temporal resolution remote sensing technologies. However, Sterman argues that compartment models are not the only form of representation in Systems Dynamics. It also allows for architectures with disaggregated, heterogeneous, or even individualized parts, such as the previously mentioned agent-based models [49]. In light of this, Sterman establishes a pragmatic attitude, arguing that the decision regarding the architecture of the model should be considered from the perspective of the problem being evaluated, but without losing the ability to manage the model with ease. As an example, he mentions that the SIR epidemiological model[3] is a compartment model that exhibits practically the same aggregated final behavior as any other more detailed version. The justification for introducing heterogeneities, such as age groups, spatialization, or even agents that follow more or less social distancing rules, should reside in the final purposes of the study, within the scope of relevant recommendations for policy formulation and decision-making. Otherwise, one incurs in a practically infinite regression of details: after all, why model only the host agents if it is possible to model their organs, cells, and even the bacteria or viruses themselves? Another relevant issue regarding detailed architecture is its high computational demand. Although

[3] The acronym SIR stands for Susceptible, Infectious, and Recovered.

currently accessible and somewhat seductive, Sterman emphasizes that highly detailed simulations with long simulation times introduce cognitive biases in the modeling process, especially in the iterative component. In this case, there arises resistance both to reviewing deeper conceptual aspects and to diagnosing the model through sensitivity and uncertainty analyses, which require many simulations.

In the compartment architecture, the **causal structure** of the modeled system is defined by the arrangement of compartments connected by flows that can be material (transfer rates) or informational (positive and negative feedback loops). From the Aristotelian perspective, the *matter* of the system consists of the compartments, while the *form* of the system consists of the flows. Thus, two identical sets of compartments, when connected by different material and informational flows, reveal themselves to be completely different systems. In Systems Dynamics jargon, the emphasis on form is often expressed by the fact that *the causal structure of a system defines its behavior*. The model should initially be visualized through a **causal loop diagram**, as shown in Figure 2.4a. Here, it is crucial to properly establish the **system boundary** that the model represents, that is, which flows beyond which the subsequent compartments do not have significant causal effects on the modeled system[4]. A compartment consists of a *level* of a state variable S that accumulates over time, meaning it has *memory*. An easy way to identify a level is to consider what happens if the material flows cease: in this situation, the levels in the compartments continue to exist, inert. The only way to change the level is through the action of the material flows. The level in the compartments is governed by some **conservation principle**, generally the conservation of *mass*[5]. In practice, this implies the application of a **balance equation**, where any variation in the level of a compartment results from the net effect of the input rates (positive) minus the output rates (negative). Mathematically:

$$\frac{dS}{dt} = I - O \tag{2.3}$$

In which the material input flows I and output flows O are rates of change of the level S, and have units of S divided by the adopted time unit. A compartment can have multiple input and output flows, with Equation (2.3) being the simplest possible version. These flows are defined as *functions* of both the **state variable** S (when feedback exists) and of **exogenous variables** Υ (outside the system boundaries[6]) and a set of **parameters** Θ (constants adjusted to reproduce the expected behavior of the system). In general terms:

$$\begin{aligned} I &= f(S, \Upsilon_I, \Theta_I) \\ O &= g(S, \Upsilon_O, \Theta_O) \end{aligned} \tag{2.4}$$

By including feedback, the equations that define the material flows also capture the flows of *information* that connect the compartments. Ultimately, they capture the structure of the system, and thus, its final behavior. The behavior of the system is so sensitive to them that, to some extent, the flow equations become intertwined with much of the hypotheses postulated by the theory that the model is conveying[7]

Equation (2.3) expresses the balance of a compartment as an instantaneous and *continuous* process over time, which generally corresponds to the expectations for the

[4]As it is a decision, the boundary design has the dangerous potential to be a premise of neglect, to use Musgrave's term.

[5]In environmental models, it is generally assumed that water is an incompressible fluid of constant density, which enables a simple volumetric balance of water.

[6]In environmental models, the exogenous variables are generally referred to as **external forcings** of the system. In a typical hydrological model, for example, precipitation is an exogenous variable.

[7]Evidently, the underlying theory is also represented by the instantiated compartments, by the boundary design, and even by the balance equations.

modeled target system. For example, the volume of water in a bathtub that is being filled by a faucet increases continuously, not in discrete jumps. Other systems, such as the population in an ecological model, exhibit discrete transitions over time as new generations replace the previous ones. In one way or another, it is impossible to program a digital computer to solve continuous differential equations directly, necessitating the application of numerical methods. This technological limitation of digital computers, while allowing significant advances in other aspects, such as multifunctionality, leads to the so-called **numerical integration problem**. In essence, this problem consists of the **truncation error** associated with the numerical scheme used in modeling. In the case of the balance, this problem involves the difficulty of accurately determining the level S_{t+1} from the known level S_t and the selection of a time interval Δt. After all, how do you calculate the average of the input and output flows during the time interval? Especially when there is feedback, any minimal variation in S directly influences the rates of input or output flow. In light of this issue, Jay Forrester advocates the need to sacrifice the numerical accuracy of simulated results in favor of gaining useful knowledge about the target system [50]. Forrester's guidance, which can be viewed as a *pragmatic convention*, suggests defining a time interval Δt that is sufficiently small relative to the time scale of the modeled flows and then applying the **Euler method** for numerical integration. Figure 2.4d illustrates the truncation error in the numerical solution of the differential equation $dS/dt = -kS$ (a linear reservoir), whose analytical solution $S = S_0 e^{kt}$ is easily obtained. In this case, the Euler method was applied with different time intervals Δt, demonstrating the improvement in integration with smaller intervals. For more complex systems without an analytical solution, it is expected that adopting a sufficiently short time step will ensure that the flow between one moment and another is approximately constant.

The choice of the Euler method for numerical integration is certainly controversial, as there are other numerical methods that are recognized as more efficient (such as the Runge-Kutta methods), but that require greater computational demand. John Sterman advances this debate by establishing the **temporal insensitivity principle**[8]: a crucial test that a model must pass is to demonstrate that different time intervals do not influence (for practical purposes) the results of the simulations [35]. After all, the results of a model sensitive to the time interval defined in numerical integration are devoid of theoretical meaning. As long as the model shows numerical instabilities depending on the time step, it is necessary to adopt progressively smaller time steps until reaching behavior that is independent of the chosen time interval. In the extreme case that the behavior of a modeled system fails to remain stable across the range of viable time intervals with the available technology, then one must consider using a more efficient numerical integration method. In the case of the Euler method, the numerical arrangement of finite differences from Equation (2.3) exhibits the following form:

$$S_{t+1} = S_t + I_t \Delta t - O_t \Delta t \quad \forall t \tag{2.5}$$

That is, it is assumed that the input flows I and output flows O are constant during the course of the time step Δt, with the value of the rates always computed at time t and then *extrapolated* to $t + 1$. For a compartment with N input flows and M output flows:

$$S_{t+1} = S_t + \sum_{i}^{N} I_{t,i} \Delta t - \sum_{j}^{M} O_{t,j} \Delta t \quad \forall\, t \tag{2.6}$$

Starting from the indexing of t, the algorithm to simulate the system on a

[8]The term principle of insensitivity is my own.

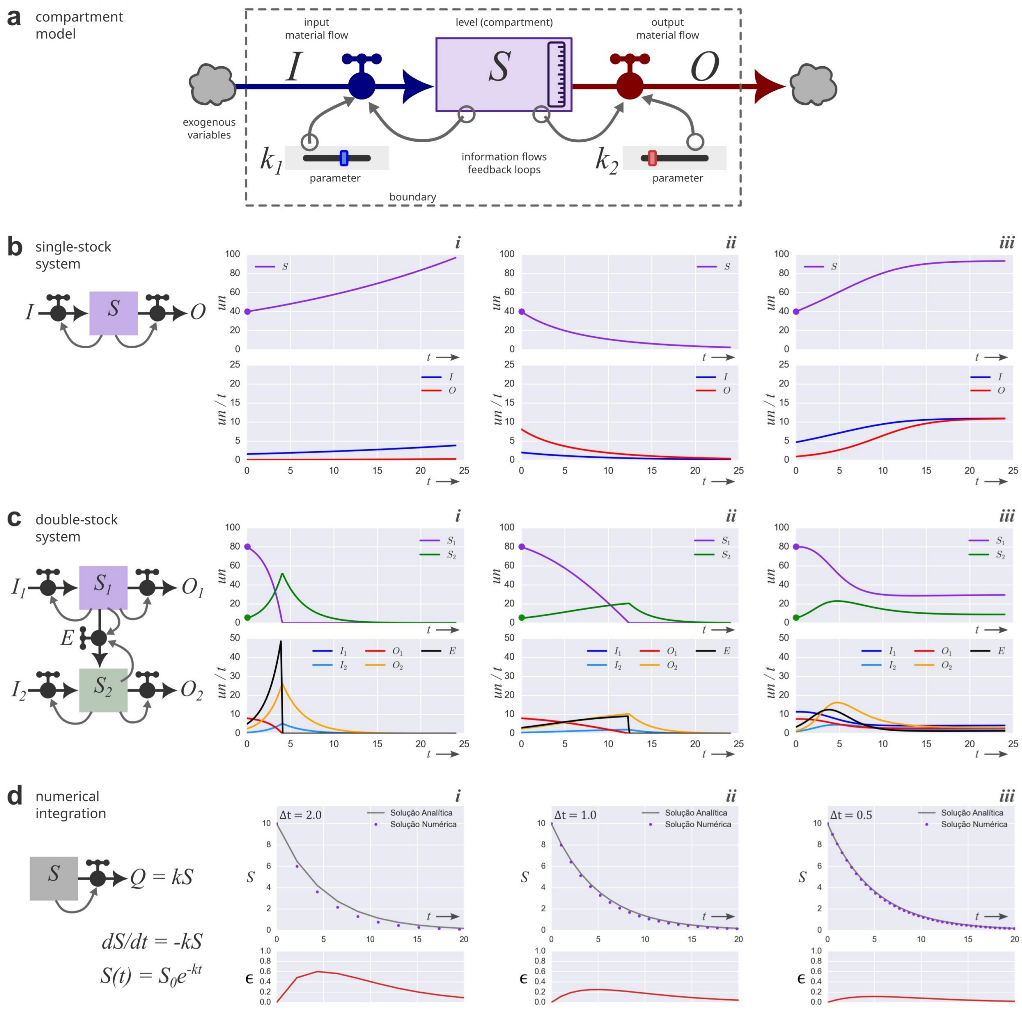

Figure 2.4 — Systems Dynamics and the compartment model. The compartment model consists of the basic architecture for constructing models within Systems Dynamics. The system is solved numerically, revealing complex patterns. **a** — Causal loop diagram: the level of the compartment S changes due to the action of material inflows I and outflows O. Information flows relate the level to the material flows through feedback, which is regulated by parameters of the model (such as k_1 and k_2). The **boundary** of the system should not neglect significant feedbacks with the exogenous variables. **b** — Simulations with the single stock model, with different dominances between material inflows and outflows: exponential growth (detail i); exponential decay (detail ii), and; logistic curve (detail iii); **c** — Simulations with the double stock model, where level S_2 depletes S_1 with an extraction flow E: overload and rapid collapse (detail i); overload and delayed collapse (detail ii), and; sustainable equilibrium (detail iii). **d** — Numerical integration introduces the truncation error ϵ, which can be minimized with sufficiently short time steps Δt (details i to iii). The overall behavior of the system should not be sensitive to the time step Δt.

computer basically consists of inserting Equation (2.5) within a loop[9]. This loop then iterates through all values of t, incrementally calculating the states of the levels and subsequently updating the value of the flows based on the values from the previous step. In addition to the flow balance equations, Forrester suggests that a procedural model of a system (i.e., the computer code itself) should also include **auxiliary equations** and **supplementary equations**. The auxiliary equations are derived directly from the balance and flow equations, implemented to simplify the understanding of the computational steps by humans. The supplementary equations, on the other hand, define variables of interest that are not part of the modeled system, such as statistics accumulated over time or in moving time windows.

As previously mentioned, understanding the *structure* of a modeled system is

[9]Note that, depending on the simplicity of the system, a typical spreadsheet can perform the computation, where each row of the table consists of a time step.

key to predicting its *behavior*. In this regard, the structural isomorphism postulated by Bertalanffy becomes, within the realm of Systems Dynamics, what Donella Meadows refers to as a "zoological garden of systems": a set of systems that exhibit *archetypical behaviors*, which can be generalized across a wide range of real examples [34]. A good starting point in this context is to consider the simplest possible model, which is one that has a single compartment, governed by Equation (2.3) (Figure 2.4b). Although simple, different behaviors manifest depending on the *dominance* of one flow over another. In the case where the inflow I predominates over the outflow O, the level S of the compartment will tend to increase (detail i in Figure 2.4b). If there is positive feedback, the pattern will be that of **exponential growth curve**. Conversely, if the outflow predominates, the tendency will be for the level S to decrease (detail ii in Figure 2.4b). Here, the existence of feedback produces **exponential decay curve**. A concrete example of this archetypical system is a culture of cells (such as bacteria or fungi), growing on a Petri dish without significant nutritional limitations. The more microorganisms reproduce (inflow), the more new generations are added to the total population, which grows exponentially. Simultaneously, the increasing confinement of cells leads to the accumulation of toxic waste from their own metabolism, which also increases mortality (outflow). These two flows act as a **reinforcing loop** and a **balancing loop**, competing for dominance over time, producing patterns more intricate than mere growth or decay, such as the **logistic curve** (detail iii in Figure 2.4b).

A second step in this direction is to consider the behaviors that emerge from the *coupling* of two or more compartments. Meadows explores the basic model with two compartments, particularly when the level S_1 of the first acts as a source of inputs E for the level S_2 of the second (Figure 2.4c). This is the case, for example, when the previously mentioned cell culture has limited nutritional resources. In fact, this arrangement is the archetype of any system producer-consumer, which includes the global economy itself (natural resources and capital). A notable pattern that emerges from this system is the **overshoot and collapse curve**, which occurs when the balancing loop in the consumption of available resources does not exist or is very weak, causing the level of the second compartment to rise rapidly until it exhausts its own source, resulting in a similarly rapid decline (detail i in Figure 2.4c). The introduction of **double feedbacks** and **activation thresholds** to mitigate or even suspend the consumption of resources can either delay the collapse (detail ii in Figure 2.4c) or establish a **sustainable equilibrium** in the long term[10] (detail iii in Figure 2.4c). Moreover, the introduction of **delays** in the flow of information can produce stable oscillations (naturally damped) or unstable oscillations (amplified and chaotic) in the levels. It is easy to see that the complexity and diversity of behaviors grow exponentially as new compartments and feedbacks are introduced into the models. The advantage of Systems Dynamics, with its strictly computational nature, lies in its ability to simulate the system step by step from the basic relationships between the compartments, eliminating the need to explicitly solve systems of non-linear differential equations. Thus, patterns of growth, decay, saturation, collapse, and oscillations simply emerge.

2.5 A prototype

With what has been presented so far, we finally arrive at a suitable position to introduce a prototype of a model hidrológico. In this line, the aim here is to establish the basic implications that Systems Dynamics brings to hydrological modeling through an exploratory and minimalist model. Theoretical and practical deepening, both on

[10] In the case of the global economy, this optimistic scenario is referred to as *prosperous decline* by Odum and Odum [51]

hydrological processes and on more detailed models, will be articulated in the next chapter.

As highlighted in Section 2.1, every modeling process begins from a *model perceptual*. Thus, the minimalist model arises here from some perceptions, especially the one that a watershed has at least two different ways of *responding* to rainfall events: one faster and the other slower. The **hydrological response** fast manifests in the rises of rivers that occur after rains. The hydrological response slow, on the other hand, is evident during dry times, when rivers continue to flow even after many days or even months without rain. In this line, it is assumed that the fast response is more related to surface processes, while the slow response is associated with subsurface processes. The first relationship derives from the perception that highly impermeable watersheds or those with shallow soils produce large runoff (fast response). Conversely, the springs of streams and wet areas in the valley bottoms of more preserved watersheds reinforce the perception of the role of groundwater in sustaining base flow in rivers during dry times. An important perceptual detail that we can introduce here is that not all rain produces a fast response, as it is necessary to surpass a certain *activation level*, such as interception of water in the canopy or filling the depressions in the terrain that are not connected. Once this threshold is surpassed, the incremental *saturation* of the surface produces an increasingly greater fast response, which will only cease when the surface is again dry. This occurs due to the *level of fragmentation* of the surface – that is, more water is needed to connect isolated pockets of water with the available outlets (in channels or macropores). Regardless of the forms of response, water also needs to travel through a network of channels to reach the outlet of the watershed. This reinforces another relevant perception, that the movement of water implies an attenuation of the response pulses due to energy dissipation effects. Finally, one last perception refers to the outflow of evapotranspiration (`ET`). In this case, it is expected that transpiration from plants through the canopy is the initial flow, followed then by evaporation of water from the surface.

Once a perceptual model is established, we can move on to a conceptual model from the perspective of Systems Dynamics. The diagram of this model is displayed in Figure 2.5a. Thus, the first step in this process is to define the system boundary of the modeled system. In the case of typical hydrological models, the aim is to represent a watershed, which is an area of land traversed by the hydrological cycle. The watershed, therefore, is an open system to water flows that enter through atmospheric precipitation P (rain, snow, and dew) and to outflows, which can occur through both runoff Q and evapotranspiration, denoted here as E. Thus, the flows P and E are maintained as exogenous variables, obtained from **input data** and acting outside the boundary of the target system. It is assumed, therefore, that the internal state of the system does not exert causal influence over the value of these variables[11]. It is clear that, as an outflow, evapotranspiration depends on the water available in the system, but its *potential* flow is determined without causal links. Runoff Q, on the other hand, is a flow calculated by the model itself through the application of its flow equations. Models with this characteristic are often called "rain-runoff" models, although this designation obscures the fact that many other flows are calculated to estimate the outflow.

The second step in building a conceptual model involves configuring the reservoirs[12] of the system under study. For this, it is essential to mobilize the concept of hydrological response provided by the perceptual model. To keep the model in a minimalist condition, we define only two response reservoirs: one for the fast response, S_1,

[11] This assumption becomes increasingly fragile as the scale of the watershed evolves from a small area to larger regions or continents [todo:cite] to cite examples and references.

[12] In the context of hydrological models, I will use the term *reservoir* as a synonym for *compartment*.

and another for the slow response, S_2. These reservoirs are vertically coupled, so that the water must pass through the fast response reservoir (upper) before reaching the slow response reservoir (lower). This scheme aims to represent the water balance in the soil, intuitively relating the fast response to surface processes and the slow response to subsurface processes. However, due to the simplification of the model, this interpretation should be considered with caution: the representation in only two reservoirs is essentially a synthesis of several subprocesses that could be more specifically defined in a more detailed model. In addition to the coupled reservoirs, a third reservoir, S_3, collects both the fast and slow flows, acting as a filter over the signal of both. The purpose of this reservoir is to model the effects of attenuation and storage during the propagation of runoff through the channel network before reaching the watershed outlet. Just as in the case of the water balance in the soil, this reservoir encompasses several subprocesses that, in a more complex model, could be explored in detail. Considering that the area of the watershed is constant, it is convenient, though not mandatory, to express the levels of the reservoirs S_i in mm of water column and the flows in $mm/\Delta t$. The reservoirs S_1 and S_3 (surface and channel network, respectively) have unlimited total capacity, while the reservoir S_2 (soil and subsurface) reaches its maximum capacity from a certain level, such that:

$$S_{2,t} \leq s_{2,\max} \quad \forall; i,t \tag{2.7}$$

Where $s_{2,\max}$ is the *maximum storage capacity* of S_2, a parameter expressed in level units (mm).

The third step, finally, is to define the flow equations that govern the water balance in each reservoir. In this sense, all three reservoirs operate as a **linear reservoir**, which implies that they exhibit an outflow Q_t directly proportional to the level S_t, that is:

$$Q_{i,t} = \frac{1}{k_i} \cdot S_{i,t} \quad \forall\; i,t \tag{2.8}$$

Where k_i is a parameter with time units that is equivalent to the mean residence time of the reservoir S_i. This implies that the *greater* the value of k_i, the more *slow* its emptying is, as illustrated in Figure 2.5b (details i and ii). A linear reservoir is analogous to a water tank with vertical walls and a porous outlet, which allows a laminar flow directly proportional to the water column. In the case of the fast response reservoir S_1, the outflow Q_1 is the flow of vertical transfer of water to the reservoir S_2, interpretable as the *infiltration* from the surface into the soil, with the necessary effectiveness caveats. In the case of reservoir S_2, the outflow Q_2 is the very slow response of the watershed, interpretable as the *base flow* that the soil produces directly into the drainage network. Finally, the outflow Q_3 is the final *outflow rate*, resulting from the attenuation of the runoff through the propagation process. The rapid outflow from reservoir S_1, denoted by R, has a specific formulation, corresponding to a hypothesis of how rapid processes, such as surface runoff q_{si}, develop in the watershed. Just like in the outflow of a linear reservoir, R is directly proportional to the stored level, with the difference that the level must exceed a minimum value s_a before it begins to overflow:

$$R_t = \begin{cases} 0 & \text{if} \quad S_{1,t} \leq s_a \\ c \cdot (S_{1,t} - s_a) & \text{if} \quad S_{1,t} > s_a \end{cases} \tag{2.9}$$

Where s_a is the **activation level** of the fast response, a parameter of the model expressed in level units; and c is a *runoff coefficient*, with units of t^{-1}. However, unlike the linear reservoir, the value of c is not constant, but rather a function of the level S_1 itself. For the purposes of this chapter, we will simply establish that the fast response

R results from a *saturation process* of the reservoir S_1, such that:

$$c = \frac{(S_{1,t} - s_a)}{(S_{1,t} - s_a) + s_c} \frac{1}{\Delta t} \quad \forall\, t \tag{2.10}$$

Where s_c is the **fragmentation level**, a parameter with the same units as the level S_1 that regulates the speed of the saturation process. The level s_c represents 50% connectivity, so that the greater the value of s_c, the more slowly the saturation of the reservoir occurs. As the reservoir level increases, the runoff coefficient c asymptotically approaches 1[13], as illustrated in Figure 2.5b (details *iii* and *iv*). The term $1/\Delta t$ was retained in the definition of c to clarify its units, even though it is effectively eliminated in the balance equation (Equation (2.5)). By substituting Equation (2.10) into Equation (2.9), we arrive at the flow equation for R (in the case of $S_{1,t} > s_a$)[14]:

$$R_t = \frac{(S_{1,t} - s_a)^2}{(S_{1,t} - s_a) + s_c} \quad \forall\, t \tag{2.11}$$

In this minimalist model, the external evapotranspiration flow E acts on the soil water balance, affecting reservoirs S_1 and S_2, such that $E = E_1 + E_2$. The drainage of water, in this case, occurs from the bottom up, meaning that the flow E only starts to act on the upper reservoir S_1 when the lower reservoir S_2 is empty. That is, the outflow E_2 in S_2 corresponds to the transpiration of plants, which removes water from the soil, and the outflow E_1 in S_1 corresponds to surface evaporation. Thus, it is noted that the reservoirs S_1 and S_2 are *simultaneously depleted* by more than one outflow. For S_1, the outflows are E_1, R, and Q_1. For S_2, the outflows are E_2 and Q_2. This is a good point to introduce two practical problems in compartment models within Systems Dynamics, which are the **congested output problem** and the **simultaneous depletion problem**. The first problem consists of the difficulty in determining a given outflow $O_{t,j}$ that *is also an input* in a compartment with limited storage capacity. In the case of the minimalist hydrological model, this occurs in the flow Q_1 (infiltration), which goes from S_1 (surface) to S_2 (soil and subsoil). However, since the reservoir S_2 is limited by $s_{2,\max}$ (Equation (2.7)), there is a negative feedback from S_2 on Q_1, which can be interpreted by the notion that the infiltration flow is *congestible* by the moisture present in the soil. After all, if the soil pores are already filled with water, it doesn't matter how much water is available for infiltration stored on the surface. The **actual flow** $Q_{1,t}$, thus, is obtained by confronting the **potential flow** outflow $Q^*_{1,t}$ with the **maximum flow** possible input to the next reservoir, which in the case of S_2 is defined by the **storage deficit** $D_{2,t}$ divided by the time step Δt:

$$Q_{1,t} = \begin{cases} Q^*_{1,t} & \text{if} \quad Q^*_{1,t} \leq D_{2,t}/\Delta t \\ D_{2,t}/\Delta t & \text{if} \quad Q^*_{1,t} > D_{2,t}/\Delta t \end{cases} \tag{2.12}$$

Where $D_{2,t}$ is calculated by:

$$D_{2,t} = s_{2,\max} - S_{2,t} \tag{2.13}$$

This solution can be generalized for other congestible outflows[15]. When a compartment with limited capacity has *multiple* simultaneous inflows, then the solution

[13]Equation (2.10) presents a typical form of saturation processes found in distinct fields, such as the **Michaelis-Menten Equation** in the kinetics of chemical reactions.

[14]A cautious look reveals that Equation (2.11) has exactly the same structure as the empirical formula of the CN method proposed by the Soil Conservation Service to estimate effective runoff from rainfall events and types of land cover. This is an intriguing fact that deserves further study.

[15]In this context, it is worth noting that John Sterman argues against using conditional structures like `IF... THEN... ELSE` in simulation code, suggesting that an alternative for Equation (2.12) of the form $Q_{1,t} = \mathtt{MIN}(Q^*_{1,t}, D_{2,t}/\Delta t)$ is more robust and readable [35].

Componente	Nome	Dimensão	Unidade	Categoria
S_1	quick response reservoir (surface)	L	mm	level
S_2	slow response reservoir (subsurface)	L	mm	level
S_3	drainage network reservoir	L	mm	level
P	precipitation	L/T	mm/h	flow (exogenous)
E	potential evapotranspiration	L/T	mm/h	flow (exogenous)
R	quick runoff ($S_1 \rightarrow S_3$)	L/T	mm/h	flow
Q_1	infiltration ($S_1 \rightarrow S_2$)	L/T	mm/h	flow
Q_2	slow runoff ($S_2 \rightarrow S_3$)	L/T	mm/h	flow
Q_3	outflow from S_3	L/T	mm/h	flow
E_1	evaporation	L/T	mm/h	flow
E_2	transpiration	L/T	mm/h	flow
k_1	residence time of S_1 (surface)	T	h	parameter
k_2	residence time of S_2 (subsurface)	T	h	parameter
k_3	residence time of S_3 (drainage network)	T	h	parameter
s_a	activation level of quick response	L	mm	parameter
s_c	fragmentation level of S_1	L	mm	parameter
$s_{2,\text{max}}$	maximum capacity of S_2	L	mm	parameter

Table 2.1: Summary of the hydrological model prototype developed, listing the components of levels, flows, and parameters. Due to the high degree of aggregation of the model, the names and meanings of the components should be interpreted with caution, as they are in fact effective processes that could be better detailed and disaggregated in more complex versions.

needs to adopt an analogous (but inverse) approach to the other problem mentioned, which is the simultaneous depletion problem. This problem, in turn, consists of the difficulty in *preventing negative values* in a level subjected to multiple outflows that is numerically integrated using the Euler method. In a mathematically continuous system, the various outflow rates smoothly act on a given level S_t, so it tends asymptotically toward zero. However, the Euler method, by considering that the rates are constant during a discrete time interval Δt, introduces the risk that S_{t+1} may take on negative values. The solution to this problem is to compute the outflows in three steps. In the first step, the total *potential* outflow O_t^* is calculated by summing the individual potential outflows. More generically, for M potential outflows $O_{t,j}^*$:

$$O_t^* = \sum_{j}^{M} O_{t,j}^* \quad \forall\, t \tag{2.14}$$

Next, the *actual* total outflow O_t is determined by confronting the potential flow with the *maximum* possible outflow, which is the value of the level S_t of the reservoir divided by the time step Δt:

$$O_t = \begin{cases} O_t^* & \text{if} \quad O_t^* \leq S_t/\Delta t \\ S_t/\Delta t & \text{if} \quad O_t^* > S_t/\Delta t \end{cases} \tag{2.15}$$

Finally, the third step consists of calculating the values of the *individual* actual outflows. Since the Euler method assumes constant flow rates, the actual outflows are directly proportional to the *allocation* of the potential outflows:

$$O_{t,j} = \frac{O_{t,j}^*}{O_t^*} \cdot O_t \quad \forall\, t \tag{2.16}$$

Such problems, inherent to the computational nature of Systems Dynamics, indicate the next step in the modeling process: the development of a *model procedural*, that is, a computer program. In the form proposed above, the conceptual model is simple enough to be implemented in a *spreadsheet*, where the columns represent different storage and flow variables and the rows represent the time steps of the simulation. To follow the Euler method, the formulas in the reservoir balance cells should refer to the previous row, in the flow columns. Some auxiliary columns should be created to implement the intermediate steps of the potential flows and maximum flows. Additionally, certain static cells should be kept isolated, such as the values of the parameters $\Theta = \{k_1, k_2, k_3, s_a, s_c, s_{2,\max}\}$, the initial conditions values $\mathbf{S}_{t=0} = \{S_{1,t=0}, S_{2,t=0}, S_{3,t=0}\}$, and the exogenous variables values $\Upsilon = \{P_t, E_t\}$. A more robust alternative, however, is to implement the procedural model from code, such as `C`, `Fortran`, `Python`, etc. A simple code structure should be based on the functional programming paradigm, with three interconnecting steps:

1. importing input data;
2. processing the model, and;
3. exporting the output data.

Each step has its typical characteristics and technical limitations, from defining the format of the data files to using efficient structures offered by the chosen programming language. In this regard, a code presents two fundamental advantages: one cognitive and the other operational. The cognitive advantage is that a code completely makes explicit the equations and the computational algorithm itself[16]. Spreadsheets and other graphical interfaces, in contrast, tend to obscure the formulas and the algorithm structure, making the procedural model somewhat inaccessible in cognitive terms. The operational advantage, on the other hand, is that a code allows the *nesting* of the simulation process in a larger hierarchy of processes, such as running batches (multiple simulations in series or parallel) and coupling with other models (where the output of one is used as input data in another). As we will see later, this operational advantage is essential for the diagnosis and research of models.

Before conducting any computational simulation with the developed hydrological model prototype, it is important to highlight some valuable aspects that the formalization of the perceptual model into a conceptual model brings. As mentioned earlier, Systems Dynamics has an exploratory spirit that seeks not only to make reliable predictions about a target system but also to use models to *learn* about the behavior of this system, thereby identifying useful leverage points in decision-making. That said, let us consider for a moment that the theory conveyed by the proposed model is *justified*, which frees us from the issues raised in Chapter 1. If that is the case, what can we deduce *a priori* about the behavior of the watershed? What are its critical leverage points when considering, for example, the problem of water security[17]?

In light of these issues, the first aspect to note is that **the system is stable**, dominated by feedbacks that cause the levels of the reservoirs to *tend towards zero*, as illustrated by the simulation in Figure 2.5c. In other words: the reservoirs S_1, S_2, and S_3 empty on their own[18], even without any external action (when $P = 0$ and $E = 0$). Unlike ecological, social, and economic systems, no form of exponential growth or oscillations is expected from the proposed system. A second aspect is to classify the final behavior of the system in terms of sensitivity to the input flow P. At one extreme, we have low sensitivity behavior, characterized by the dominance of the slow response mechanism in S_2 and high residence time in S_3. The simulations in both Figure 2.5d and Figure 2.5f illustrate possibilities of this behavior. At the other extreme, we have high sensitivity behavior, characterized by the dominance of the rapid response mechanism in S_1 and low residence time in S_3, as shown in the simulation in Figure 2.5e. Maintaining

[16] Highly efficient codes often imply a sacrifice in readability, which reinforces the importance of supplementary materials such as documentation and comments.

[17] This problem will be explored in Chapter 4

[18] In physical terms: through the action of gravity.

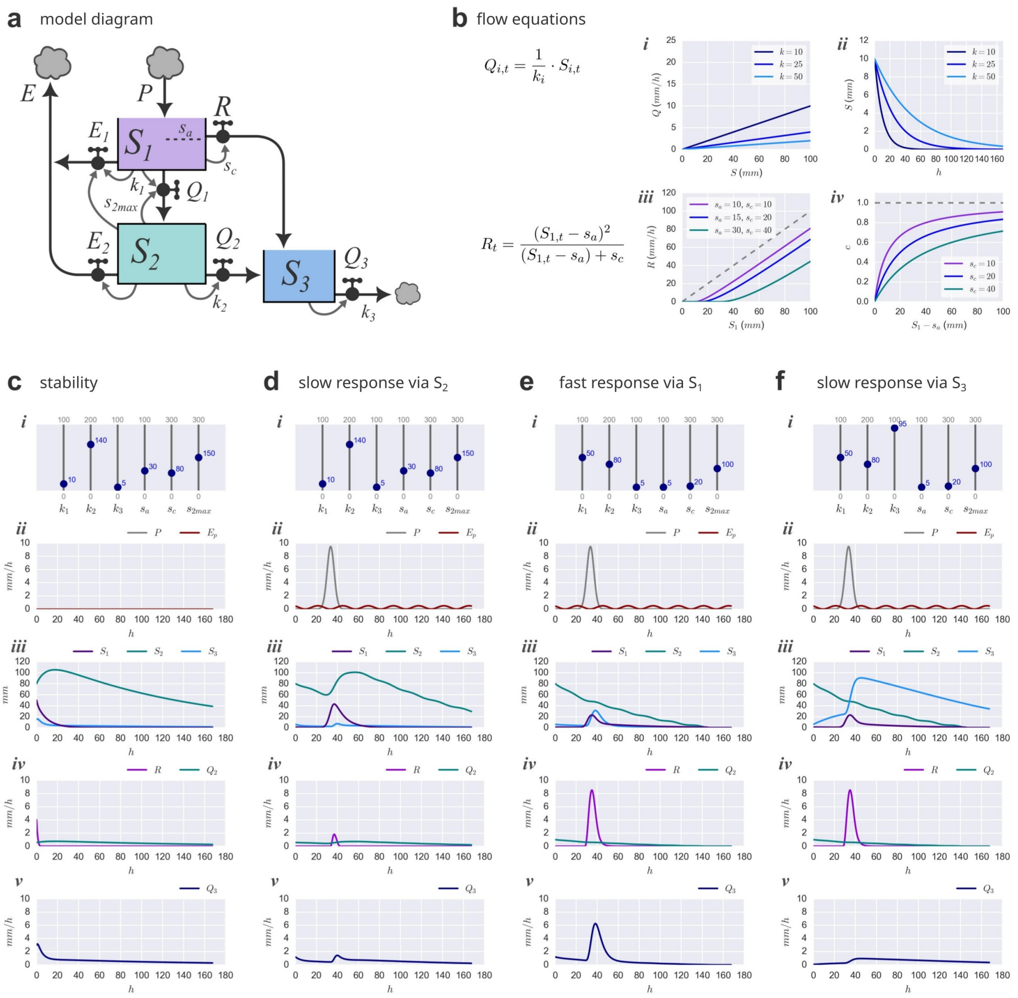

Figure 2.5 — A prototype of a hydrological model and its behavior. The model is kept minimalistic for exploratory purposes. **a** — The structure of the model is designed with three reservoirs (S_1, S_1, and S_3) to represent mechanisms of slow or fast hydrological response. S_1 represents the surface, S_2 represents the subsurface, and S_3 represents the drainage network. With six parameters regulating internal flows, the system is subjected to the exogenous flows of evapotranspiration E and precipitation P. The reservoir S_2 is the only one with limited capacity ($s_{2\text{max}}$). **b** — Two equations regulate the flows (Equation (2.8) and Equation (2.11)). The exponential decay equation for the reservoirs ($Q_i = S_i/k_i$, detail i), where k_i is the residence time. The larger the value of k, the more slowly the reservoir empties (detail ii). The quick response equation ($R = c \cdot (S_1 - s_a)$, detail i) is similar, but c results from a saturation process of the surface ($c = (S_1 - s_a)/(S_1 - s_a + s_c)$, detail ii). This process is regulated by the activation threshold s_a and the fragmentation level s_c. **c** — The system shows stable behavior – it empties by itself, even when P and E are null (detail ii). In this case, S_2 showed a peak as water from S_1 infiltrated (detail iii). But soon after, all reservoirs emptied. **d** — A configuration of parameters (detail i) that defines a slow response through the action of S_2 (subsurface). Here, a rainfall pulse P with a maximum of 9.5 mm/h and a daily oscillation of E (detail ii) result in an attenuated flow Q_3 (detail iv); R has a maximum of only 2 mm/h, while the base flow Q_2 sustains the flow during most of the simulated period (detail iii). **e** — A configuration of parameters (detail i) that defines a fast response through the action of S_2 (surface). The same pulse of P and E results in a typical hydrograph of Q_3, with a maximum of 6 mm/h (detail iv); R shows a maximum of 8 mm/h and the base flow Q_2 is extinguished in about 140 hours (detail iii). **f** — A configuration of parameters (detail i) similar to (**e**), but defining a slow response through the action of S_3 (drainage network). The same pulse of P and E results in an attenuated flow Q_3 (detail iv) – the flow is sustained by damping in the drainage network.

the proposed structure and the same exogenous flows P and E, it is clear that behavior will strictly depend on the set of parameters $\Theta = \{k_1, k_2, k_3, s_a, s_c, s_{2,\text{max}}\}$, although different values may eventually result in similar behaviors (high or low sensitivity). For example, it is possible to reduce the sensitivity of the system by increasing both the activation threshold of the rapid response ($\uparrow s_a$) and the residence time in the drainage network ($\uparrow k_3$), or both simultaneously[19]. This leads us to the third and final

[19] This ambiguity is directly associated with the equifinality problem. As presented in Chapter 1,

aspect, which is the leverage points of the system in relation to practical problems, such as water security. For the purposes of this chapter, the problem of water security is defined as the difficulty in *ensuring the availability of water in adequate quantity and quality* for human activities. Therefore, it is concluded that any leverage strategy in the system should aim to reduce its sensitivity to the input flow, seeking a **regularization effect**. In the soil water balance, this translates to reducing the dominance of the rapid response mechanism: increasing the activation threshold, reducing surface connectivity, and reducing surface residence time. In the case of the drainage network, the only available alternative is to increase residence time through detention basins, ponds, or even dams.

The aspects raised above illustrate that the simple deductive logic applied to the developed conceptual model allows for the identification of important *insights* about the behavior and the leverage points in the system. Furthermore, if the model captures the essence of the target system, it is expected that more detailed versions do not eliminate the essence of the conclusions drawn, but rather introduce the necessary nuances in the decision-making process based on hydrological models, depending on the problem at hand. Heterogeneities in lithology, pedology, land cover, and topography should certainly expand the range of theoretical understandings and practical recommendations. Despite the leap observed between the perceptual model (mental models) and the conceptual model, it is clear that this reasoning can hide surprises from blind spots and non-intuitive interactions among the parts of the system. Moreover, the assumption that the conveyed theory is justified was a provisional move: it is necessary to test the model against empirical evidence. Thus, the only way to make stronger assertions is to simulate the model using diagnostic techniques, which are presented next.

2.6 Diagnosis

The **model diagnostics** consists of a vast set of techniques applied to evaluate the *adequacy* of a model. Before empirical justification, which is a crucial test, a model needs to be adequate from the conceptual, technical, practical, and behavioral angles. After all, an extremely well-fitting statistical model in empirical terms can be directly obtained with optimization techniques, such as machine learning. But what can one *learn* about the target system with a statistical model? An overfitted statistical model to the available data, for example, may be useful for *interpolations*, but not for *extrapolations*. Such a model does not contribute much to understanding how the system would *behave* in response to a given leverage policy or a future scenario that has never been observed. The search for learning, in the context of Systems Dynamics, implies that modeling is a process of *deductive* inference, which requires a robust and reliable definition of the antecedent statements (main and auxiliary hypothesis) before producing their consequent statements (simulated results). In this regard, John Sterman suggests a list of twelve general strategies for diagnosing[20] these adequacies, displayed in Table 2.2, enhancing Jay Forrester's initial proposals [35]. However, given the highly practical nature of Systems Dynamics, perhaps the diagnosis *of zero order* of a model is to evaluate the **adequacy of the problem** it is being addressed. This primary diagnosis assesses whether the model was *tailored* to answer the truly relevant questions of the practical problems at hand. Although obvious, this diagnosis can pose significant challenges, even forcing modeling teams to *abandon* comfortable modeling strategies as the

the largest number of possible empirical evidences should be employed to *condition* the behavior of the model.

[20] Originally, he uses the term "model testing", but here the term "test" will be reserved for when a *rejection criterion* is explicitly defined.

Diagnosis*	Purpose	Procedures
0. Problem Adequacy	Diagnose if the model is suitable for the practical problem being addressed.	Explicitly state the questions implied by the problem that need to be answered by the model.
1. Boundary Adequacy	Diagnose if the exogenous variables of the model do not imply serious causal neglects.	Explicitly define the system and its endogenous and exogenous variables in causal loop diagrams.
2. Structural Adequacy	Diagnose if the structure (including flow equations) aligns with the perceptual model and does not violate basic theoretical principles. The degree of aggregation also needs to be useful in practical terms.	Inspect equations and causal diagrams; clarify decision-making questions related to expected outcomes.
3. Dimensional Consistency	Diagnose if the equations and parameters are consistent and make sense concerning real phenomena.	Inspect equations; dimensional analysis; rationalize the underlying theory.
4. Parameter Distribution	Diagnose how distributions of values align with conceptual and empirical expectations.	Obtain prior distributions from expert opinion.
5. Comparative Studies (System Families)	Diagnose if the distribution of parameters is consistent across target systems of the same family. E.g., different watersheds;	Obtain distributions of parameters consistent with the largest possible number of system members (generalist model).
6. Integration Error	Diagnose if the results are not sensitive to the time step and numerical integration method.	Reduce the time step; change the numerical integration method.
7. Extreme Conditions	Diagnose how robust the procedural model is to very high or very low values.	Simulate the model under synthetic conditions with extreme shocks to values.
8. Sensitivity Analysis	Diagnose how variations in the parameters of the model affect the results, identifying critical parameters for the behavior of the system.	Apply exploratory techniques, such as the Monte Carlo Method, for random sampling in the parameters space. Use search techniques to identify critical scenarios and reveal unusual leverage policies.
9. Anomalous Behavior	Diagnose unexpected behaviors of the model that may indicate formulation errors or important *insights* about the modeled system.	Subject the model to encapsulation testing; discard.
10. Empirical Adequacy	Diagnose if the model can reproduce observed behaviors in the target system, adjusting parameters to improve adherence to empirical data.	Compare the outputs of the model with observed data, using metrics like MAE, RMSE, and coefficients such as determination and KGE.
11. Surprising Behavior	Diagnose if the modeling results surprise the target audience in some way, revising their mental models.	Effectively communicate results; reveal nuances and details; demonstrate non-intuitive mechanisms.
12. Positive Practical Impacts	Diagnose if modeling has brought positive practical impacts on the decision-making process.	Prepare impact indicators from the model; technical documentation; reproducibility.

Table 2.2: Model Diagnostics in the context of Systems Dynamics. — Summary of the twelve "Model Tests" proposed by John Sterman, following the tests suggested by Jay Forrester. Adapted from Sterman [35].

nature of the problem is understood more deeply. From the decision-making side, that is, the clients of model sellers, this type of diagnosis is essential to avoid uneconomical situations when the model sold is disproportionate.

Among the conceptual diagnostics, it is essential to evaluate the **boundary adequacy**. As illustrated in the prototype of the hydrological model, an important assumption is that the storage and flows of water in the watershed (the endogenous variables) do not influence precipitation and potential evapotranspiration (the exogenous variables). This assumption may be questionable for large watersheds, where evapotranspiration in one region converts into precipitation, either locally (cloud condensation nuclei [todo:cite]) or in other areas (flying river effect [todo:cite]). Thus, as one shifts from a local scale to a continental scale, neglecting the causal interactions of the meteorological and climatic system with terrestrial hydrological processes tends to become increasingly inadequate. Another basic conceptual evaluation is the **structural adequacy** of the model, both in theoretical terms (physical principles) and practical terms (decision-making). The structure of the model must ensure that physical principles, such as mass conservation, non-negativity of levels, and certain irreversible processes, are not violated. For example, Sterman describes an economic model that produced remarkable results in simulating the leather market, but this occurred because the model reverted produced leather *back* into cows whenever necessary [35]. Similarly, it is important to evaluate whether the level of aggregation of the model meets the pre-established needs of the decision-making process. In hydrological modeling, the aforementioned prototype would hardly be useful for identifying priority action areas within a watershed, due to its highly aggregated nature.

Two other related conceptual diagnostics involve **dimensional consistency** and **parameter distribution**. This evaluation relates to the *meaning* of the parameters in the flow equations and the distribution of their values. When starting from a deductive logic, the flow equations need to make theoretical sense (after all, *they convey a theory*), and their parameters should have consistent names and units that are equivalent (at least in effective terms) to real processes. According to Sterman, parameters and variables with names and units that do not make sense in the real world are *symptoms that the theory about the target system is poorly formulated*. Moreover, the values of the parameters themselves also need to meet conceptual expectations. Since different combinations of parameters can result in similar final behaviors (the equifinality problem), certain combinations of parameters may be empirically adequate but theoretically questionable. For example, in a mountainous watershed without artificial reservoirs, one would expect low attenuation of the flow pulse in the drainage network, or at least lower than in flatter watersheds with floodplains. Thus, **comparative studies** between different systems but of the same *family*, and the definition of prior distributions through **expert opinion**, help to discard inconsistent parameters values[21].

On the technical side, a crucial diagnostic is the **test of numerical integration**, which was described in Section 2.4. It is important to emphasize that *no simulation is informative if its result stems from numerical instabilities*. Thus, this test consists of evaluating whether the behavior of the system adheres to the temporal insensitivity principle. Another diagnostic in this vein is to subject the model to **extreme and boundary conditions**, such as very high values of input and output flows. This is an assessment of technical robustness, as it is under these unusual (but possible) conditions that problems in the procedural model may arise, such as errors in the numerical representation of data structures (*overflow* and *underflow*) and violations of non-negativity in the simulated levels. For example, a discrete level variable (like a population) can be instantiated by a data structure with positive, integer numbers of 16 bits—which offers interesting memory gains, unlike 64-bit floating-point numbers. However, this data structure has an upper numerical limit of 65535—values above this will wrap around to low numbers, causing an *overflow* error that can render simulation results meaningless. In this case, it is necessary to ensure that a more efficient code does not compromise the robustness of simulations under extreme but feasible conditions.

Diagnostics that evaluate the behavior of the model include **sensitivity analysis**, **anomaly detection**, and **empirical adequacy**. These evaluations form a spectrum in terms of justification. On one side, sensitivity analysis seeks to understand how the system responds to changes in its elements, such as input flows and parameters values. In this case, the approach is exploratory, without major commitments to justification. On the other side, empirical adequacy seeks to find the sets of parameters that condition the modeled system to reproduce the observed behavior. Clearly, this is the only test capable of pointing out the need for significant revisions in the modeling process, as it is here that the theory is directly confronted with the available evidence. Still, the rejection of the proposed model is only possible through the modeling paradigm discussed in Section 1.6 (Chapter 1), which applies an encapsulation test of a set of empirically adequate models. A purely confirmatory approach, in contrast, seeks to "calibrate" the parameters of the model in order to identify a single set of parameters deemed adequate.

One way or another, behavior diagnostics generally require a broad assessment of the **parametric space** Ω_Θ, the mathematical space with N dimensions created by the N instantiated parameters in the conceptual model. Here, a technical barrier

[21] It is expected that expert opinion will *inform* about the prior distribution of parameters with qualitative empirical evidence from their perceptual models that have not been transformed into quantitative data. Still, care must be taken not to turn this process into a **confirmation bias**, keeping an openness for empirical anomalies to act as a means to refute the theories posited by the models. One way to achieve this is to maintain posterior probabilities within a minimum threshold.

arises, which is the **dimensionality problem**: the difficulty of thoroughly evaluating the parametric space Ω_Θ in a reasonable simulation time. For example, consider a **exhaustive sampling**[22] approach with M regular intervals across the estimated range for each parameter Θ_i, with $i \in \{1, ..., N\}$. It follows that the number of simulations n_s in a exhaustive sampling approach is $n_s = M^N$. This number can grow exorbitantly quickly: with $M = 100$, one would need to simulate the proposed hydrological model ($N = 6$) one trillion times, $100^6 = 1,000,000,000,000$. With a simulation time of one second, this evaluation would take around *31 thousand years* to complete. A simulation time of one millisecond would require 31 years. To be practical, exploration in the parametric space Ω_Θ should last a maximum of a few days, preferably a few hours or minutes.

More powerful computers greatly help in overcoming the dimensionality problem, but in practice, the sampling strategy also employs more efficient methods than exhaustive sampling, which can be divided into **exploratory techniques** and **search techniques**, although they are largely related. Exploratory techniques are variations of the Monte Carlo Method, mentioned in Section 1.3, that perform random sampling over the expected value ranges for the parameters Θ. The goal here is merely to reveal regions of the parametric space. If a prior distribution for the parameters is available (from expert opinion, for example), this sampling can be *weighted by the density* of the distribution, which directs the exploration more towards certain regions than others. An efficient variation of the Monte Carlo Method consists of random sampling *without replacement*, known as **Latin Hypercube Sampling**, which ensures a more spaced distribution of the sampled parameter sets, avoiding the risk of redundant samples. Search techniques, in turn, consist of optimization techniques aimed at identifying regions of the parametric space that meet predefined specifications regarding the behavior of the system. In the jargon of Operations Research, these techniques maximize or minimize a given **objective function**. A wide variety of optimization algorithms can be implemented for this purpose, such as linear programming, dynamic programming, gradient ascent, evolutionary algorithms, Markov chains, etc. The criterion for selection, however, depends on various technical issues, especially in nonlinear models that exhibit objective functions with multiple local optima.

In sensitivity analysis, exploratory techniques are applied to quantify the numerical sensitivity of each parameter. This analysis can be either *local*, performed by varying one parameter while keeping the others constant, or *global*, conducted through a more comprehensive exploration of the parametric space Ω_Θ [52]. Andrea Saltelli and colleagues emphasize the importance of the latter, demonstrating that only global analysis has the potential to capture interactions and synergies that emerge when a given set of parameters changes simultaneously [53]. However, sensitivity analysis also employs search techniques in explorations designed to **discover critical scenarios** and reveal unusual leverage policies. To illustrate this approach, John Miller applied two optimization techniques (genetic algorithms and gradient ascent) to the model `World3` used by Donella Meadows and colleagues in *Limits to Growth*, in order to discover alternative scenarios for world population up to 2100 [54]. The results obtained from these searches indicated that it is possible to maximize the world population by up to six times the amount projected by Meadows' base scenario (4 billion, peaking at 9 billion in 2050), but it is also possible to minimize the population to half of the forecasted amount. These different modes of behavior of the same system help to better understand the critical parameters and flows necessary for policy development. For instance, a global population of 2 billion by 2100 might be desirable, not due to wars, pollution, and famine, but because of economic, technological, and cultural changes that improve

[22] Also known as enumeration method or brute-force method.

people's quality of life.

On the side of empirical adequacy and anomaly detection, exploratory techniques are related to the uncertainty analysis of the parameters. A method of particular relevance proposed in hydrological modeling is the *Generalized Likelihood Uncertantiy Estimation* (GLUE) method, introduced by Keith Beven and Andrew Binley, which applies Bayes' Theorem (Equation (1.4)) with an informal likelihood function $\mathcal{L}(E|H)$ [55]. Thus, the posterior distribution of the parameters is obtained by conditioning the prior distribution with the normalized histogram of the likelihood $\mathcal{L}(E|H)$. This histogram, in turn, is calculated from a robust exploration of the parametric space Ω_Θ. Search techniques, on the other hand, act to "calibrate" the model by maximizing the likelihood $\mathcal{L}(E|H)$, resulting in a single set of parameters deemed empirically adequate[23]. In any case, when it comes to models in Systems Dynamics, the informal likelihood $\mathcal{L}(E|H)$ is usually equated to some point-to-point statistic or fit metric that seeks to measure the adherence of the simulated variables to the observed data. Therefore, the closer a simulated point $y_{M,i}$ is to its corresponding observed point $y_{O,i}$, the greater its empirical adequacy. A typical fit metric is the mean absolute error MAE:

$$\text{MAE} = \frac{1}{n}\sum_{i}^{N} |y_{M,i} - y_{O,i}| \tag{2.17}$$

An alternative that disproportionately penalizes larger errors more and smaller errors less is the root mean square error RMSE:

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i}^{N}(y_{M,i} - y_{O,i})^2} \tag{2.18}$$

Both the MAE and RMSE metrics are positive and have the same units as the evaluated variable y, which makes them difficult to compare with other models or even other variables. A more universal metric is the coefficient of determination R^2 [56]:

$$R^2 = 1 - \frac{\sum_i^N (y_{M,i} - y_{O,i})^2}{\sum_i^N (y_{M,i} - \bar{y}_O)^2} \tag{2.19}$$

where $\bar{y}_O$ is the mean of the observed data. In this sense, the coefficient of determination R^2 can be interpreted as a measure of how much the model M is better at determining the observed values compared to the simple mean of the observed data O. In the context of hydrological simulation, the coefficient of determination is also referred to as the Nash-Sutcliffe Efficiency NSE [57]:

$$\text{NSE} = R^2 \tag{2.20}$$

A commonly used alternative in Hydrology is the Kling-Gupta Efficiency KGE, which establishes a decomposition among the correlation coefficient r, the mean μ, and the standard deviation σ of the modeled and simulated data [58]:

$$\text{KGE} = 1 - \sqrt{(r_{M,O} - 1)^2 + \left(\frac{\mu_M}{\mu_O} - 1\right)^2 + \left(\frac{\sigma_M}{\sigma_O} - 1\right)^2} \tag{2.21}$$

Finally, an important practical diagnosis involves assessing how the modeled system produces a **surprising behavior** against the mental models (perceptual) of the

[23] In multi-objective approaches, the set of parameters considered empirically adequate corresponds to a Pareto frontier.

interest groups involved in the modeling process, changing opinions. If the use of Systems Dynamics models has a *null* effect on the ingrained preconceptions of the target audience (including scientists), then their use has no cognitive learning value. In the worst-case scenario, modeling becomes a **fallacious appeal to authority** that ultimately blinds its users from making evidence-based decisions (confirmation bias). Thus, the obtained results must be communicated effectively to surprise the target audience, revealing at least new *nuances and details* in the results and, at most, *non-intuitive* mechanisms of system behavior[24]. For example, considering the use of a hydrological model in the context of watershed revitalization, it may be that the target audience overestimates the capacity of the system to mitigate rapid response mechanisms through nature-based solutions. However, this same audience may underestimate the potential of these solutions to improve water quality. Along this line, another relevant diagnosis is to identify whether the model results actually produced **practical changes in decision-making**, in formulating strategies and action plans. Changing the personal opinions of involved actors is one thing; effectively altering the decision-making process is another. This category of diagnosis should include the evaluation of whether the developed model is *usable by third parties*, known as the **reproducibility problem**. A model accessible only by its developers, no matter how good, will likely leave a small legacy, producing low practical impact outside the scope of the project for which it was conceived. In this sense, Sterman emphasizes strategies to maximize reproducibility, such as low computational demand, ease of installation and operation, and maintaining accessible documentation, including *websites* with training, tutorials, etc. In the pragmatic spirit of Systems Dynamics, evaluating the positive impact of a model is the essence of the modeling endeavor and should be carefully planned with impact indicators from the outset of any project. The relevance of preparing the diagnosis *a priori* is to avoid **anecdotal evidence** and minimize the **retrospective bias** in assessing the success of the model. It is clear that important decisions always involve ethical and political issues at play, but the use of models in scientific advisory roles, including their uncertainties, should have at least some positive impact. ■

[24] From the perspective of Thomas Kuhn's paradigms, this diagnosis assesses whether the modeling results are embedded in the *normal cycle* of science, articulating and enhancing the prevailing theory.

2.7 Chapter Summary

In this chapter, I presented modeling as a learning process, where perceptions are refined into computational models. The discussion on representation highlighted idealizations and analogies as tools to make target systems understandable. Hydrological modeling was treated as an example, emphasizing the importance of identifying leverage points to influence hydrological responses. Finally, the chapter underscored the significance of diagnostics, ensuring that models are both technically sound and practically applicable.

- **Modeling is a learning process.** In Hydrology, this involves an iterative learning cycle that begins with the perceptual model (subjective impressions), moves through a conceptual model (objective expressions), and culminates in a procedural model (computation). A diagnostic step reviewing adequacies closes the cycle, revisiting methods, theories, and perceptions.

- **The problem of representation.** Idealizations are deliberate simplifications used to make the target system tangible. Scaled-down or scaled-up models are idealizations in the form of copies of target systems. Conversely, analog models are formal analogies. In any case, analogical inference is employed.

- **Systems are an ontological paradigm.** Systems are a set of parts with relationships among them. Stable or unstable behaviors emerge from these relationships. This Aristotelian paradigm sees *form* as the unifying element of the object. Ludwig von Bertalanffy proposed the General Systems Theory as a unification of Science. deterministic chaos and computational irreducibility pose challenges to the predictive capability of systemic theories.

- **Structure defines behavior.** Systems Dynamics is an applied discipline where the goal of modeling is to understand modes of behavior and identify leverage points in systems for better decision-making. The compartment architecture allows modeling of levels connected by material flows and feedback loops. Parameters act in the flow equations, regulating the levels. The system is solved numerically using the Euler method, allowing complex and nonlinear behaviors to emerge from simulations.

- **Rapid and slow hydrological responses.** A hydrological model is created for exploratory purposes. The concepts of slow and rapid hydrological response are introduced. Three reservoirs interact based on two basic flow equations regulated by six parameters. The model demonstrates equifinality, with slow responses produced by more than one mechanism. It is possible to evaluate where to act in the system to maximize water availability by reducing the dominance of rapid responses.

- **Adequacy diagnostics.** John Sterman asserts that model adequacy should be tested across conceptual, technical, behavioral, and practical aspects. The test of empirical adequacy, while crucial, should integrate other assessments: adequacy of the boundary; adequacy of the structure; dimensional consistency; parameter distribution; comparative studies; integration error; extreme conditions; sensitivity; anomalies; surprises; and practical impacts. An empirically inadequate model with practical impacts is harmful; but an empirically adequate model without practical impact is devoid of meaning.

The soil mantle acts as a natural reservoir for rainwater, storing it in its internal cavities. The fauna and flora, by excavating macropores, not only create pathways for water infiltration but also accelerate its release, especially in the upper horizons.

Chapter 3

Hydrology

> The assertion or assumption that all rises are caused by surface runoff has persisted in articles and even in some hydrology textbooks, despite much evidence to the contrary in forestry and agricultural research.
>
> Hewlett & Hibbert (1967, p. 275) [59]

> A box, objectively defined by distinct dynamics of groundwater, soil solution chemistry, or isotopic composition, with defined area, depth, and porosity, is a much better modeling building block than a myriad of elements in landscapes that are notoriously heterogeneous both vertically and laterally!
>
> Jeffrey McDonnell (2003, p. 1872) [60]

3.1 Zero-order Basins

Hydrology is the science that studies continental waters, seeking to understand how water is distributed on continents after precipitating from the atmosphere and before returning to the oceans [61]. In other words, Hydrology investigates how the **hydrological cycle** manifests in its terrestrial phase, in contrast to Meteorology (which focuses on the atmosphere) or Oceanography (which studies the oceans). When contemplating this, it is easy to imagine large rivers, such as the Amazon and Paraná, as well as other notable rivers like the Danube, Nile, Yellow, Indus, Ganges, and Mississippi. In the case of Brazil, images of lush nature arise, including the vast Amazonian and Pantanal floodplains, as well as the spectacular Iguaçu Falls. Visions related to large-scale human intervention also emerge, such as the hydroelectric complex, with its dams spread throughout the country, and the major transposition and irrigation projects, exemplified by the reservoirs in the Cantareira Mountains, the transposition of the São Francisco River, and the central pivots in the São Marcos River basin. The recent floods that devastated the cities located in the river valleys of Rio Grande do Sul also illustrate

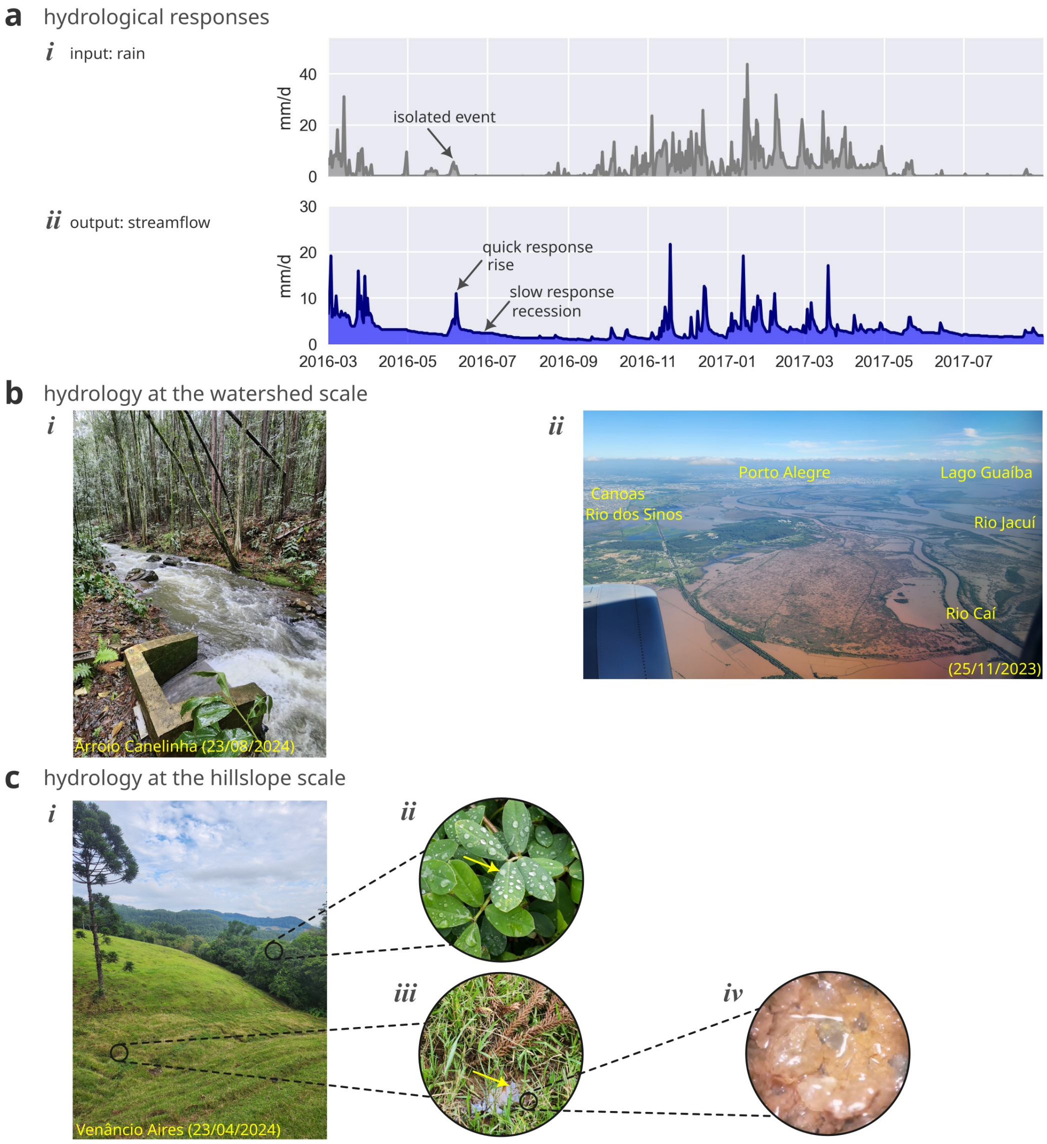

Figure 3.1 — Hillslopes: where it all begins. The most intuitive scale when thinking about hydrological processes is the flow of water in rivers, which are channels that drain water to the ocean. However, the hydrological responses to rainfall events originate in the slopes, in zero-order basins, where rain interacts with the landscape. **a** — The alternation between fast responses (rises, detail i) and slow responses (recessions, detail ii), observed in a medium-sized drainage area in the Paraíba do Sul basin (342 km², Rio de Janeiro). Daily rainfall obtained from `INMET 83738` Station (Resende) and daily flow obtained from `ANA 58287000` Station (Rialto). **b** — The evident hydrological processes at the basin scale include the propagation of flow through the drainage network, downhill (detail i) and the flooding of plains, when river flow exceeds the larger section of the channels, invading adjacent dry lands (detail ii). **c** — The water that supplies river flow comes from the interaction of rain with the slopes (detail i), resulting in surface processes (such as interception, in detail ii) and subsurface processes (such as soil saturation, details iii and iv).

that rivers are crucial not only for energy and food production but also for ensuring the basic health and physical safety of the inhabitants of vast urban metropolises. In this regard, it is not uncommon for textbooks on Hydrology to mention how the first city-states, which emerged in Mesopotamia and Egypt, developed an almost symbiotic relationship with large rivers and their floodplains. Water and society are closely linked.

This intuitive interpretation of Hydrology, however, results from two particular perceptions. The first is the **engineering bias** that permeates Hydrology, which has always been marked by a **science-management duality**. This duality implies that Hydrology exists in a fluid interface between theoretical investigation of nature (problems that are *important* for human knowledge) and practical solutions to social, environmental, and economic impasses (problems that are *urgent* for people). James

Dooge (1988) [62] argues that the field was born relatively distinct from other scientific disciplines, such as Physics or Biology, being essentially pragmatic in its formation. Throughout history, hydrological problems generally presented themselves directly from their application, leading to new data being obtained and ultimately some knowledge being produced. For example, Dooge illustrates that, according to Pliny the Elder (24-79 AD), the level of the Nile River was measured in antiquity not in terms of flow but on a scale of the socio-economic impact involved: famine (low level), safety (medium level), and disaster (above flood stage). In this regard, Murugesu Sivapalan and Günter Blösch suggest that the field evolved from a phase based on reductionist and pragmatic engineering methods (Empirical Era) to becoming, during the twentieth century, an Earth Science (Geoscience Era), holistic and integrative, merging with important branches of Physical Geography, Geology, Pedology, Ecology, and recently, Sociology (Co-evolution Era) [63], [64]. The second perception is the **fluvialist bias** that dominates the field, especially in areas traversed by large rivers, such as Brazil, the United States, China, and Central Europe. This view directs hydrological studies toward essentially hydraulic problems at a continental scale, such as the propagation of flow in the channels of the drainage network, the flooding of adjacent plains, and, with the advent of remote sensing, continental water balance. The efficiency of economic activities such as electricity production, navigation, basic sanitation, irrigation, etc., fundamentally depends on this type of knowledge. This bias makes sense in much of the continents but carries less weight in regions dominated by small and medium rivers, such as the archipelagos of Japan, New Zealand, and the British Isles. The fluvial perspective is illustrated by the account reported by a Brazilian hydrologist during a visit to the United Kingdom:

> When I was in England, I went to visit a certain reference gauging station on a famous river in the region. They talked about that river all the time, but when I arrived at the site, I was somewhat perplexed and disappointed. That was not a river: it was a stream. With a little push, it was even possible to jump to the other bank. – Walter Collischonn (2023, in personal communication).

With the influence of these two biases, it is somewhat easy to forget that water only flows in rivers as a consequence of processes occurring on the hillslopes and, ultimately, in the vertical profile that starts at the vegetation canopy, passes through the surface and horizons of the soil, and ends in the underground rock foundation. The propagation of flow through the channels and the flooding of plains are nothing more than processes of transport and dissipation of rises produced by the interaction of rain with the higher and mountainous terrain of the landscape. This importance of the *slope scale* was initially highlighted in Japan by Tsukamoto (1973) [65] in the early 1970s, who expanded the systematic hierarchization of channels proposed by Strahler (1957) [66] by introducing the concept of **zero-order basin** (in Japanese: 0 次 谷). Although Tsukamoto's emphasis on the slopes and valleys of the terrain advances specific issues of erosion and sediment production, its primordial importance in the hydrological cycle is evident. As illustrated in Figure 3.1, *it is in zero-order basins where it all begins.* The alternation between rises and recessions, a primordial observation in Hydrology (Figure 3.1**a**), does not originate from the propagation of water downstream or from the flooding of plains (Figure 3.1**b**), but from the interaction of rain with the landscape, at the slope scale (Figure 3.1**c**). In this same regard, Mediondo & Tucci (1997) [67] use the term **drainage basin**, which they also argue is the starting point for understanding the diversity of hydrological processes, reflecting both at the micro and macro scale. I will use the term zero-order basin here, considering that, according to Godoy et al. (2021) [68], this term has become popular in the international literature.

Table 3.1 organizes the nomenclature regarding the hydrological processes that occur on hillslopes and valleys of the terrain, to be explored in more detail in this chapter. Although relevant in theory, is this entire diversity relevant *in practice*? When considering the application of hydrological models to assist in decision-making and strategy formulation, how much can the complexity present in zero-order basins be simplified or even neglected? After all, as we saw in Chapter 2, modeling systems needs to utilize idealizations, which are deliberate simplifications to make the target system more tangible. Moreover, in the face of rivers that travel continental distances, the minute details about hydrological processes in zero-order basins lose any practical sense. The mere confluence of two medium-sized rivers or a floodplain inundation can completely erase the hydrological signature left by some typical feature produced by processes on the hillslopes. The mass of water and sediments, energy, and momentum are necessarily preserved by the laws of conservation, but detailed information is progressively attenuated and mixed in the large flow moving toward the ocean. In this sense, as long as a model presents empirically adequate quantitative results, the details about the processes in zero-order basins would be irrelevant.

This *appeal for simplification* becomes a seductive objection, as it greatly facilitates the modeling process. But it is merely a reflection of the fluvialist bias: a perspective that frames questions to be understood and problems to be solved from upstream to downstream, riverward. In this regard, the most popular hydrological models, at least in Brazil, such as `SWAT`, `HEC-HMS`, `MGB`, `SWMM`, treat zero-order basins as hermetic units or black boxes, making it impossible to recover details about hydrological processes on the hillslopes and valleys of the terrain, except in average and aggregated terms. At the end of the computational simulations, the most informative visualization possible is a mosaic of sub-basins[1]. It is clear that this simplification is justified when the objective of a given study is to understand phenomena and solve downstream hydrological problems, i.e., fluvial ones. However, to address much of the issues related to water security, such as the revitalization of watersheds, it is necessary to take a look from downstream to upstream, hillslope above, representing the zero-order basins with sufficient detail, because it is at this scale that the relevant processes occur and actions need to be specified. Therefore, a useful model must take seriously what hydrological theories say about runoff generation in zero-order basins. Otherwise, there is a risk of instantiating a model that fails both the boundary adequacy test and the structural adequacy test (see Section 2.6).

That said, this chapter marks the point at which I will articulate how theories about hydrological responses in zero-order basins can be conveyed by hydrological models. This is a critical point because here we will encounter all the philosophical, scientific, and technical challenges and problems exposed in the previous two chapters, but now from a hydrological perspective. The topics will all be revisited directly or indirectly, such as the rise and fall of paradigms, the refutation and confirmation of hypotheses, the problems of structure, dimensionality, and underdetermination, etc. Essentially, it will be seen that the complexity of hydrological processes in the soil and on the hillslopes brought by empirical evidence, combined with the difficulty of obtaining direct observations in any given basin, makes any attempt at modeling based on continuous and spatially distributed mathematical formalizations a disproportionate effort. As we will see, a unifying solution to this problem, recently proposed by Jeffrey McDonnell (2021) [69], consists of adopting conceptual models that *effectively* represent the processes of **connectivity** at the scale we need to address to answer our research questions. Returning to the analogy of the landscape that I introduced at the beginning of this thesis, we are clearly moving out of the narrow valleys of abstract and philosophical subjects

[1]It is also possible to recover information in the hydrological response units within each sub-basin. However, as we will see later, this representation is irretrievably static, while the processes at the scale of zero-order basins are dynamic in time and space.

Component	Name	Dimension	Unit	Category
C	vegetation canopy	L	mm	reservoir
S	soil surface	L	mm	reservoir
O	organic horizon	L	mm	reservoir
V	vadose zone, mineral horizon	L	mm	reservoir
$\mathbf{V}_\mathrm{c}$	capillary water in the vadose zone	L	mm	reservoir
$\mathbf{V}_\mathrm{g}$	gravitational water in the vadose zone	L	mm	reservoir
$\mathbf{D}_\mathrm{v}$	capillary deficit	L	mm	reservoir
G	groundwater zone	L	mm	reservoir
D	saturation deficit	L	mm	reservoir
p	precipitation, rain	L/T	mm/h	flow (exogenous)
p_s	effective rain	L/T	mm/h	flow
p_x	excess rain	L/T	mm/h	flow
Q	river flow, fluvial runoff	L^3/T	l/h	flow
q	specific river flow, fluvial runoff	L/T	mm/h	flow
f	infiltration	L/T	mm/h	flow
q_si	runoff, runoff by excess of infiltration	L/T	mm/h	flow
q_se	direct rain, surface runoff due to saturation excess	L/T	mm/h	flow
q_ss	exfiltration, subsurface runoff, lateral runoff	L/T	mm/h	flow
q_o	percolation between horizons	L/T	mm/h	flow
q_v	recharge, final percolation	L/T	mm/h	flow
Q_g	base flow, slow groundwater discharge	L^3/T	l/h	flow
Q_gt	translational flow, rapid groundwater discharge	L^3/T	l/h	flow
e_pot	potential evapotranspiration	L/T	mm/h	flow (exogenous)
e_c	evaporation in the canopy	L/T	mm/h	flow
e_s	evaporation at the surface	L/T	mm/h	flow
e_o	transpiration in the organic horizon	L/T	mm/h	flow
e_v	transpiration in the vadose zone	L/T	mm/h	flow
e_g	transpiration in the groundwater zone	L/T	mm/h	flow
f_max	infiltration capacity	L/T	mm/h	parameter
K	hydraulic conductivity	L/T	mm/h	parameter
g	aquifer detention time	T	h	parameter
c_max	interception capacity	L	mm	parameter
s_max	surface detention capacity	L	mm	parameter
o_max	field capacity of the organic horizon	L	mm	parameter
v_max	field capacity of the mineral horizon	L	mm	parameter
m	vertical uniformity constant of the soil	L	mm	parameter

Table 3.1: Hydrological processes in zero-order basins — Relation of reservoirs, flows, and parameters related to hydrological processes in zero-order basins.

to enter a broader field of more tangible and applied questions. Here, the mountain streams converge, forming mighty rivers that flow through bars and banks.

3.2 Infiltration

In Section 2.5 of the previous chapter, I organized a prototype of a hydrological model aimed at illustrating and articulating how Systems Dynamics can be employed in the modeling process. The obtained conceptual model, maintained in a minimalist condition, was constructed primarily based on the perception that a watershed exhibits **fast and slow responses** to rainfall events, thus producing the phenomenon of alternation between **rises** and **recessions** in rivers [59]. This is a fundamental perception in Hydrology: when it rains, rivers become agitated, the water gets muddier, and levels rise (fast response); between rains, rivers calm down, the water becomes clearer, and levels fall (slow response); if too much time passes before it rains again, smaller streams begin to dry up (the system tends to empty). With some empirical rigor, this phenomenon in any given watershed can be measured and reproduced in graphs with the aid of a rain gauge and a level stick. With a bit more empirical rigor, the perception of this phenomenon becomes sharper through field expeditions, observing the spatial and tem-

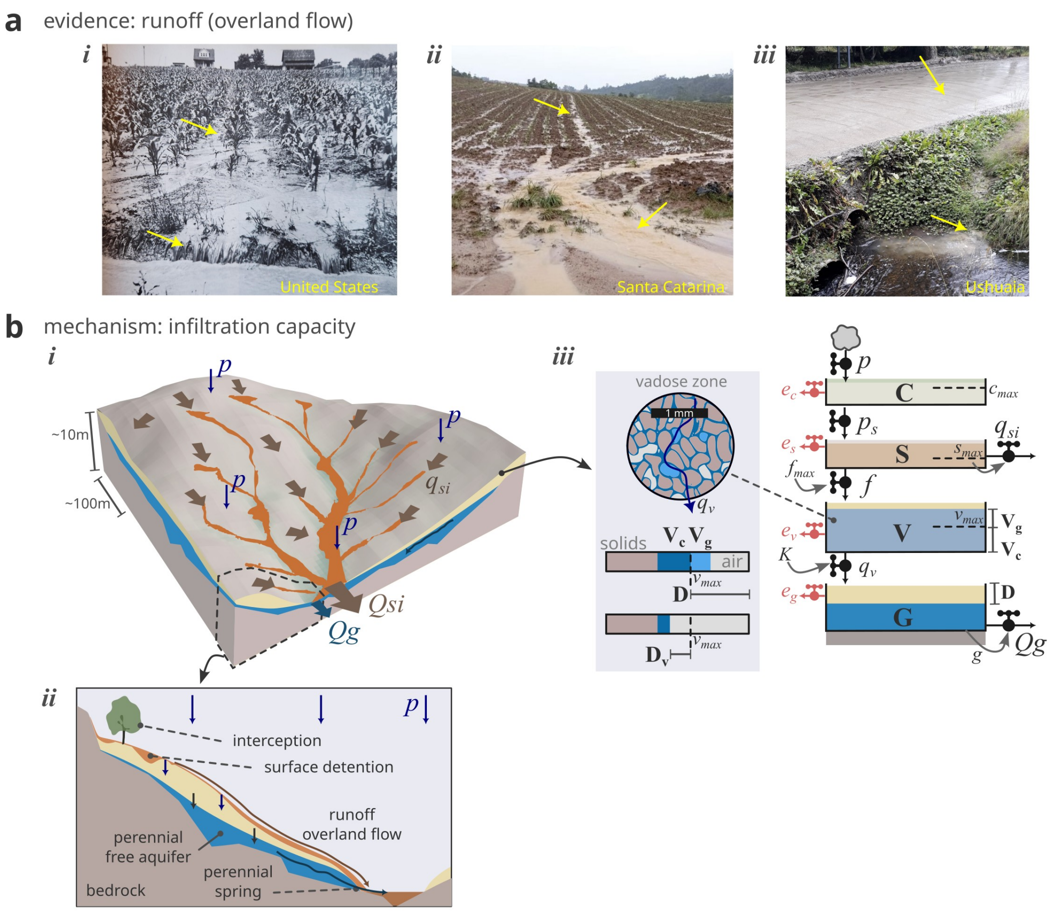

Figure 3.2 — The Hortonian paradigm. The Hortonian paradigm explains the alternation between rises and recessions based on the concept of the soil's infiltration capacity f_{max}. **a** — The motivating empirical evidence includes the surface runoff observed after rains when water fails to infiltrate: runoff in the United States reported by the SCS [70] (detail i); runoff in Santa Catarina reported by EPAGRI [71] (detail ii), and; rural road runoff in Ushuaia, authored by me (detail iii). **b** — The surface runoff q_{si} occurs generally in the basin (detail i) from the moment when the rainfall flow exceeds the interception capacity c_{max} and the surface detention capacity s_{max} (details ii and iii).

poral dynamics of springs and puddles (where groundwater slowly surfaces) and the rapid runoff (caused by more intense rains).

In the context of zero-order basins, the dominant scientific theory today postulates that hydrological responses to rainfall events are the consequence of **multiple mechanisms of runoff generation**, both surface and subsurface, encompassing fast and slow responses, whether simultaneous or not, which will be described in the next section. These mechanisms were revealed and corroborated by successive experimental investigations in small basins, hillslopes with trenches, and soil plots during a scientific revolution in Hydrology that took place throughout the second half of the twentieth century. Before this revolution, however, the hegemonic scientific explanation for the fast and slow responses of hillslopes was primarily based on the hydrological theory of Robert Horton (1875-1945) [72], [73]. Once published, the perceptual model described by Horton solidified as a true paradigm in the following years and decades, marking the so-called **Infiltration Age** – a long period of normal science in which the scientific community developed research in both pure and applied fronts to articulate its implications [74], [75]. Although ultimately surpassed by a more complex explanation, Horton's theory, being scientific (i.e., falsifiable), greatly contributed to elevating Hydrology from its Empirical Era, focused on engineering applications, to being understood as a Geoscience, aimed at explaining natural phenomena.

The central idea of Horton's perceptual model is established in the paper *The role of infiltration in the hydrological cycle* (1933) [72], in which the soil is conceived as a *separating surface* for rain: a portion of the rainwater infiltrates into the hillslopes, lodging in the soil matrix, while another portion runs off superficially as **runoff**, causing dramatic increases in river flow downstream (Figure 3.2**a**). Thus, **infiltration** f would be the key process for understanding the hydrological cycle in its terrestrial phase:

> Infiltration divides rainfall into two parts, which thereafter pursue different courses through the hydrologic cycle. One part goes via overland flow and stream-channels to the sea as surface-runoff; the other goes initially into the soil and thence through ground-water flow again to the stream or else is returned to the air by evaporative processes. The soil therefore acts as a separating surface, and the author believes that various hydrologic problems are simplified by starting at this surface and pursuing the subsequent course of each part of the rainfall as so divided, separately. – Robert Horton (1933, p. 446–447) [72].

To articulate this perceptual model, Horton instantiates various flows, reservoirs, and important parameters of the system representing the zero-order basin. Figure 3.2**b** illustrates the modeled system (the evapotranspiration flows in each reservoir are denoted by E). The primordial flow consists of **effective rainfall** $\boldsymbol{p_s}$, that is, the flow of rain that actually reaches the soil after the rain p exceeds the interception capacity $c_{\max}$ in the vegetation canopy **C**. The soil, in turn, consists of a porous matrix of solid minerals that stores water in films maintained by the surface tension of its particles, thus forming the **vadose zone V**. The accumulation of water in the films in this zone occurs up to a certain limit, which is the characteristic **field capacity** $\boldsymbol{v_{\max}}$ of the soil. This water in the vadose zone **V**, which is trapped in the pores, is referred to as **capillary water** $\mathbf{V_c}$. In addition to the field capacity $v_{\max}$, the films of water on the particles, when mixed, create a relatively mobile mass of water, termed **gravitational water** $\mathbf{V_g}$. This water then percolates vertically through the pores due to gravity, forming a **phreatic zone G** above the impermeable layer, which is the solid rock foundation (i.e., this zone forms an unconfined aquifer). Horton refers to **recharge** $\boldsymbol{q_v}$ as the vertical flow of water suspended in the vadose zone **V** to the aquifer of the phreatic zone **G**, a process that can eventually raise the groundwater level (thus increasing the hydraulic load in this porous system). In this context, **gravitational deficit D** represents the amount of gravitational water $\mathbf{V}_{\mathrm{g}}$ in the vadose zone **V** necessary to achieve complete soil saturation and, consequently, the emergence of the groundwater table at the surface. Here, the maximum flux of recharge q_{v} is limited by the **hydraulic conductivity** K of the soil: the closer the vadose zone **V** is to saturation, the vertical percolation tends to be dominated by the hydraulic load, overcoming surface tension.

At this point, Horton introduces a crucial parameter in his perceptual model: the **infiltration capacity** $\boldsymbol{f_{\max}}$, that is, the maximum maximum flow of infiltration that the soil surface can offer at any given moment. It is important to highlight that this capacity is an attribute of the thin top layer of soil and, according to Horton, tends to be lower than the hydraulic conductivity K of the soil matrix, functioning as a critical limiting factor in the system. Thus, water from a effective rainfall p_{s} with an intensity less than or equal to infiltration capacity $f_{\max}$ is completely absorbed by the soil matrix. On the other hand, when a effective rainfall p_{s} has an intensity greater than infiltration capacity $f_{\max}$, the water from the **excess rainfall** p_x begins to fill the small surface depressions. If the excess rainfall p_x persists long enough, the **surface detention capacity** $\boldsymbol{s_{\max}}$ is exceeded, and the process of surface runoff q_{si} or **runoff by excess of infiltration** begins, where the rainwater flows through furrows and ravines downhill until it reaches the channels of the streams.

The infiltration capacity $f_{\max}$ depends on soil type, texture, and management practices, which implies variability in the response of different basins, even when subjected to identical rainfall events. In addition to spatial variability, Horton argues that the infiltration capacity $f_{\max}$ of the soil varies over time, dynamically oscillating between extremes of minimum and maximum capacity, in a **decay and restoration cycle** (Figure 3.3**a**). In this cycle, the decay phase occurs during rainfall events due to the expansion of colloidal particles, clogging by fine particles, and compression caused by the impact of raindrops. On the other hand, the restoration phase occurs during dry periods as new cracks and pores open up due to the retraction of colloidal particles, thermal expansions, and the activity of soil fauna, such as insects and earthworms. With this conception, it is expected that a long rain, even of relatively low intensity, will eventually produce surface runoff q_{si} if the ongoing decay leads the soil's infiltration capacity $f_{\max}$ to a value *below* the intensity of the effective rainfall p_{s}. Furthermore, this concept introduces the effect of **antecedent moisture conditions**, such as the difference in responses between the beginning and the end of a rainy season or during the onset of a cold front with persistent rains. In this case, if the restoration speed of the soil's infiltration capacity $f_{\max}$ is relatively slow, subsequent rains, even if *less* intense, tend to produce *more* surface runoff q_{si} than the initial rains. In other words, the behavior of the system becomes highly non-linear.

With the theory regarding the role of infiltration in the hydrological cycle, Horton then advances to definitively explain the phenomenon of rises observed in rivers, proposing a method for separating the hydrograph (Figure 3.3**b**). To this end, he argues that total runoff consists of two separable flow components: (1) the groundwater flow, which is a slow response from the unconfined aquifer, and; (2) the surface runoff, which is a rapid response of runoff produced on the hillslopes. Both responses are controlled, in whole or in part, by the soil's infiltration capacity $f_{\max}$:

> In accordance with this theory, total runoff consists of two parts: (1) Suface-runoff, which is dependent on rainfall-amount, rain-intensity, and infiltration-capacity and is practically independent of evaporation-rate. (2) Ground-water runoff. This is dependent on (a) total infiltration and hence indirecty on the same factors which control surface-runoff and is also dependent on (b) vegetational activity and evaporation, which in part determine the water losses, and on (c) the complex interrelations between infiltration-capacity, field moisture-capacity, vegetational activity, and accretion to the water-table. – Robert Horton (1933, p. 454) [72].

Assuming that the phreatic zone **G**, the unconfined aquifer, functions as a linear reservoir, the **recession curve** of the ground flow, or flow of discharge, consists of a typical exponential decay curve of the type $Q_g = Q_{g,o}e^{-t/g}$. This curve is a physical characteristic, and the aquifer detention time g can be extracted from hydrographs during dry periods when water losses due to evapotranspiration are minimal (for example, in the colder months in temperate and subtropical climates). Once obtained, the recession curve can be horizontally shifted on the hydrograph, allowing for the separation of the surface component of river flow from the purely subsurface contribution. Thus, Horton proposes that there are four possible typologies of hydrological response to rainfall events. The **Type 0** response occurs when the intensity of effective rainfall p_{s} is less than infiltration capacity $f_{\max}$ and the total infiltrated water is below the capillary deficit $\mathbf{D}_{\mathrm{v}}$ (there is *no* surface runoff q_{si} and *no* recharge). In this situation, even though it has rained, there is no detectable change in the river's recession curve. The **Type 1** response occurs when the intensity of effective rainfall p_{s} is less than infiltration capacity $f_{\max}$, but the total infiltrated water is greater than capillary deficit $\mathbf{D}_{\mathrm{v}}$

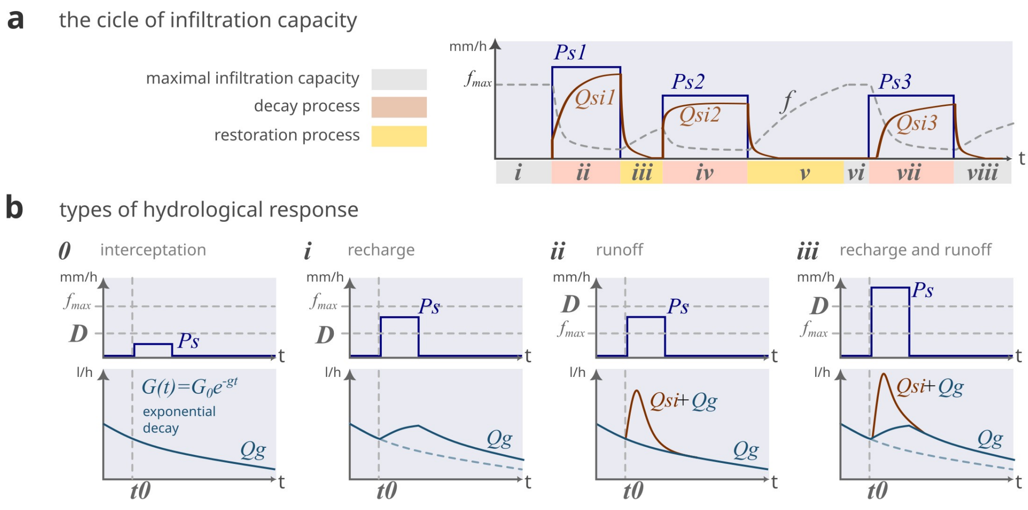

Figure 3.3 — Implications of the Hortonian model. **a** — The capacity for infiltration f goes through cycles of decay and restoration, generating non-linearities, such as the fact that identical rains ($P_{g,2}$ and $P_{g,3}$) produce different fast responses ($Q_{s,2}$ and $Q_{s,3}$) (details *iv* and *vii*). **b** — It is also possible to deduce different typologies of hydrological response: Type 0, when rain produces neither recharge nor runoff (no response, detail *0*); Type 1, when rain produces only recharge (slow response, detail *i*); Type 2, when rain produces only runoff (fast response, detail *ii*), and; Type 3, when rain produces both a slow and a fast response (detail *iii*).

(there is *no* surface runoff q_{si} but *there is* recharge q_{v} from the aquifer). In this case, the recession curve is shifted, depending on how much the recharge q_{v} exceeds (or falls short of) the discharge flow, potentially producing a (relatively slow) pulse in the river flow purely from the increase in hydraulic load in the aquifer system. The **Type 2** response occurs when the intensity of effective rainfall p_{s} exceeds infiltration capacity f_{max} and the total infiltrated is very low, below capillary deficit $\mathbf{D}_{\text{v}}$ (there is *sf-runoff* but *no* recharge q_{v} from the aquifer). This type of response consists of a rapid pulse of surface runoff water superimposed on the recession curve that was developing before the event. Finally, the **Type 3** response happens when both the fast and slow responses occur simultaneously: both surface runoff q_{si} and recharge q_{v} from the aquifer manifest as overlapping pulses. These four typologies illustrate the complexity that emerges from Horton's perceptual model, providing significant leeway for explanations of rises that vary according to the characteristics of the surface, soil, subsurface, rainfall, and antecedent moisture conditions.

In light of this perceptual model, various conceptual models have been developed through physical approaches (when physical principles are applied *a priori*) and empirical approaches (when equations are fitted to data *a posteriori*) [76]. In the realm of the physical approach, notable advancements include those by Philip (1957) [77], who laid the foundations for a mathematically formal theory of infiltration as a special case of the Darcy-Richards equation, that is, the movement of water in an unsaturated porous medium. On the empirical side, Robert Horton himself maintained an applied research line, proposing a conceptual model of exponential decay for the soil's infiltration capacity f_{max} [78]. Consequently, the production of experimentally standardized infiltration curves enabled a more sophisticated technique for estimating total surface runoff q_{si}, in contrast to the rational method, which is based on a simple runoff coefficient [74]. Another empirically influential method produced in this context was the **Curve Number Method (*Curve Number* (`CN`))**, developed by the *Soil Conservation Service* (`SCS`) in 1954 and presented as a technical guideline in the following decades. According to Rallison & Miller (1981) [79], the `CN` method from the `SCS` emerged from the results of experimental research in small basins, but was primarily motivated by the passage of environmental protection legislation in the United States.

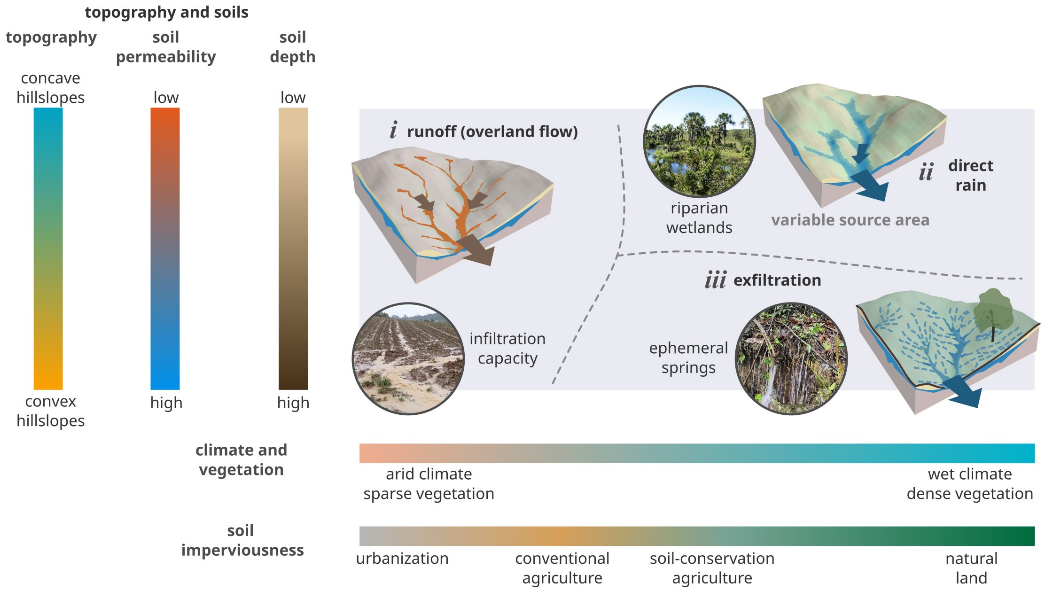

Figure 3.4 — Differentiation of rapid response mechanisms. Schematic view proposed by Thomas Dunne (1983) [81] on the new paradigm of rapid response mechanisms in zero-order basins. Runoff, considered the only mechanism in the Hortonian paradigm, has been reserved for special conditions in arid climates or anthropized environments, such as farms or cities, where the soil's infiltration capacity is very low (detail i). At least two new mechanisms are differentiated: rapid responses due to saturation excess, or direct rain on riparian wetlands (detail ii), and; rapid responses due to exfiltration in ephemeral springs, dominant in deeper, structured soils with macropores (detail iii).

It is noted that Horton was a consultant for the `SCS`, but his infiltration curve method did not gain much traction, yielding to the aggregated approach of Mockus (1949) [80], which evaluates the relationship between total rainfall and runoff for individual events. Justified by this evidence, the equation of the `CN` method seeks to express the supposed *transition* from a *non-linear* response (when infiltration and surface detention dominate the surface water balance) to a *linear* response (when the intensity of effective rainfall p_{s} exceeds infiltration capacity $f_{\max}$ and surface detention). The CN parameter, in this sense, calibrates the effect of non-linearity for different types of soil, land covers, management practices, and antecedent moisture conditions. Rallison & Miller point out that the choice of this approach by the `SCS` had a strong convenience bias, as the data used were readily available on a national scale (in the United States). Nevertheless, the essence of the `CN` method reproduces Horton's perceptual model, as surface runoff q_{si} is regarded as the only rapid response of the watershed and is determined by the estimate of excess rainfall p_x.

3.3 Differentiation

In Section 1.5, I highlighted that, according to Thomas Kuhn, the success of a scientific theory is primarily associated with its *competitiveness* in relation to other ideas circulating within the scientific community. Thus, a theory tends to establish itself as the hegemonic paradigm when it efficiently explains known phenomena and opens promising avenues for investigation for new generations of researchers. In the absence of structured competing theories in this sense, Horton's perceptual model for explaining rapid and slow hydrological responses provided these two attributes to a scientific community strongly marked by engineering bias and fluvialist bias. These two characteristics have a shielding effect on perceptions that are technically irrelevant for solving typical downstream problems, as they do not require details about what happens in zero-order basins. Ironically, this was precisely the objective of the `SCS` – to protect the soil on the hillslopes. The Hortonian model, whether partially or completely incorrect, did not prevent good estimates of design flows for bridges, dams, and water balance in large basins, among others. After all, the equifinality of systems allows similar behaviors to manifest from distinct mechanics (until the day everyone is surprised). In strictly technical terms, to some extent, the development of the `CN` method by the `SCS` *perpetuated* the ideas of the Infiltration Age, being generally the basic method required or accepted by technical guidelines in engineering projects and the main module for generating runoff in various distributed hydrological models in software such as `SWAT` and `SWMM`.

Although the paradigm of infiltration may have consolidated simply due to a lack of competitors, its crisis has been present since its formation in the 1930s and 1940s. For example, the rainfall intensity and soil infiltration capacity $f_{\max}$ data measured by Horton's own laboratory suggest that it is highly *unlikely* he observed widespread surface runoff q_{si} in his experimental basin at La Grange Brook (14.4 ha, New York) [82]. The laboratory data, evaluated by Keith Beven, indicate that the soil in the main covers of the basin (fields and orchards) exhibited a relatively high infiltration capacity $f_{\max}$ compared to the recorded rains. In fact, the reconciliation between Horton's infiltration capacity $f_{\max}$ measurements of the soil *in situ*, the **field value**, and estimates at the basin scale, the **effective value**, possibly never made much sense with each other, requiring numerous auxiliary hypotheses and negligibility premises (the **scale problem**, which we will address later). This was made clear in Betson's (1964) article [83], which achieved excellent fittings of a conceptual model to observed data only after *relaxing* the Hortonian model, implying a **partial contribution area** concept of surface runoff. From a rationalist perspective, Betson attempted to "save" Horton's theory by admitting *ad hoc* modifications to avoid its refutation. Even though statistically well-fitted, the results hinted that a small and relatively constant fraction of the basins in the Tennessee River valley produced surface runoff q_{si} (basins ranging from 500 ha to 8.4 km^2, North Carolina).

However, it was throughout the 1960s that the Infiltration Age faced its ultimate crisis in the scientific realm. Not coincidentally, this period witnessed the **International Hydrological Decade** (1965-1974), a United Nations (`UNESCO`) program developed to promote research in Hydrology. The revolution in perceptions within the scientific community occurred after a profusion of empirical evidence accumulated in the literature, reporting the observation of new mechanisms of hydrological response from hillslopes, which will be described in the following sections. At least three new rapid response mechanisms (or potentially rapid) can be summarized beyond those posited by Horton: (1) **exfiltration** $q_{\mathbf{ss}}$, (2) **direct rainfall** $q_{\mathbf{se}}$, and (3) **translational flow** $Q_{\mathbf{gt}}$. The first two refer to new rainwater contributing to rises. The last consists of old water stored underground, which also contributes to the rapid response (with surprisingly high prevalence rates). The nomenclature surrounding these mechanisms is somewhat confusing in the literature even today, perhaps due to the fact that water lacks a visible label, complicating differentiation out of context (for example, water emergence in springs can represent either a slow or fast response). In contrast to the Hortonian model, these rapid responses include surface and subsurface pathways controlled by other parts of the system beyond the topsoil, such as **macroporosity** (preferential lateral and vertical pathways in the soil) and topography (dynamic patterns of soil saturation). Essentially, empirical evidence in the second half of the twentieth century irreversibly exposed the complexity of processes in zero-order basins.

A landmark for the beginning of the end of the Infiltration Age was Mike Kirkby's (1969) article [84], which reviewed results from various experimental studies and presented a new way to understand and name hydrological processes in zero-order basins. At this point, Kirkby (1969) definitively marks the importance of rapid responses of water moving through the soil via a network of macropores (subsurface runoff). After more than a decade of accumulating new empirical evidence, a landmark for the rise of the new paradigm was Thomas Dunne's (1983) article [81], which definitively organized a new schematic view of rapid hydrological responses, illustrated in Figure 3.4, proposing a promising new research program in both pure and applied fronts. Dunne (1983) makes clear the idea that different climates, scales, and landscapes favor the *dominance* of one mechanism over another, even though they may occur simultaneously or alternate seasonally. For example, in semi-arid climates, factors such as long dry periods and the formation of soil crusts favor Horton's mechanism—the infiltration capacity $f_{\max}$ tends to be insufficient, and there are often no saturated areas in valley bottoms at the end of the dry season. In contrast, in humid tropical climates, the formation of deep soils or excess water during the rainy season may favor either mechanism. Ultimately, this revolution produced new understandings of the complex relationships between these mechanisms, as demonstrated by Jeffrey McDonnell (1990) [85] in the case of the MaiMai Experimental Basin (New Zealand). However, McDonnell (2013) [86] also critiques the entrenched paradigm: the hegemonic research program primarily focuses on *differentiating* the multiple hydrological responses, reaffirming the idea of complexity and uniqueness of each environment. While this attitude may continue *ad infinitum*, he argues that the true objective of hydrological science might be to produce *generalizations*, theories that are *unifying*. In this spirit, the prevailing hydrological paradigm might deserve the title of **Differentiation Age**.

3.3.1 Macropores

In the late 1930s and early 1940s, the scientific literature already recognized the weaknesses of Horton's model, asserting that the rapid response of small basins should include one or more *subsurface* mechanisms. Snyder (1939) [89], for example, suggests using the term direct runoff to denote the rainwater that contributes to the river flood *without ever having moved through the soil*. In this context, Barnes (1939) [90] divides the components of river flow into *three* (rather than *two*): (1) surface runoff; (2) storm seepage; and (3) base flow. By "storm seepage", Barnes referred to a rapid subsurface flow of rainwater that moves *laterally* through the vadose zone $\mathbf{V}$, feeding the stream channels at a much faster rate than expected from the aquifer detention time g:

> This consists of water which has penetrated only the upper soil-layers during a rainstorm or a thaw and has filtered more or less horizontally through the soil to discharge into the stream-system by seepage. It was observed by the writer in 1936 while analyzing discharge records of Zumbro River in Minnesota and called by him "secondary base-flow". – Bertram Barnes (1939, p. 721) [90].

Thus, a distinction is made between **perennial springs**, fed by the flow of true groundwater (unconfined aquifer), and **ephemeral springs**, fed by the subsurface flow of rainwater (suspended aquifer). This response mechanism was greatly reinforced by studies conducted by Charles Hursh at the Coweeta Experimental Forest (North Carolina, United States), with results reported for various forested basins ranging in size from 16 to 760 hectares [87], [91], generating the model illustrated in the details of Figure 3.5**c**. For example, Hursh & Brater (1941) [92] claim that surface runoff q_{si} was never observed on the hillslopes of one of the monitored basins, despite the rapid responses observed in river flow:

> Surface storm-runoff as overland-flow has not been observed on this

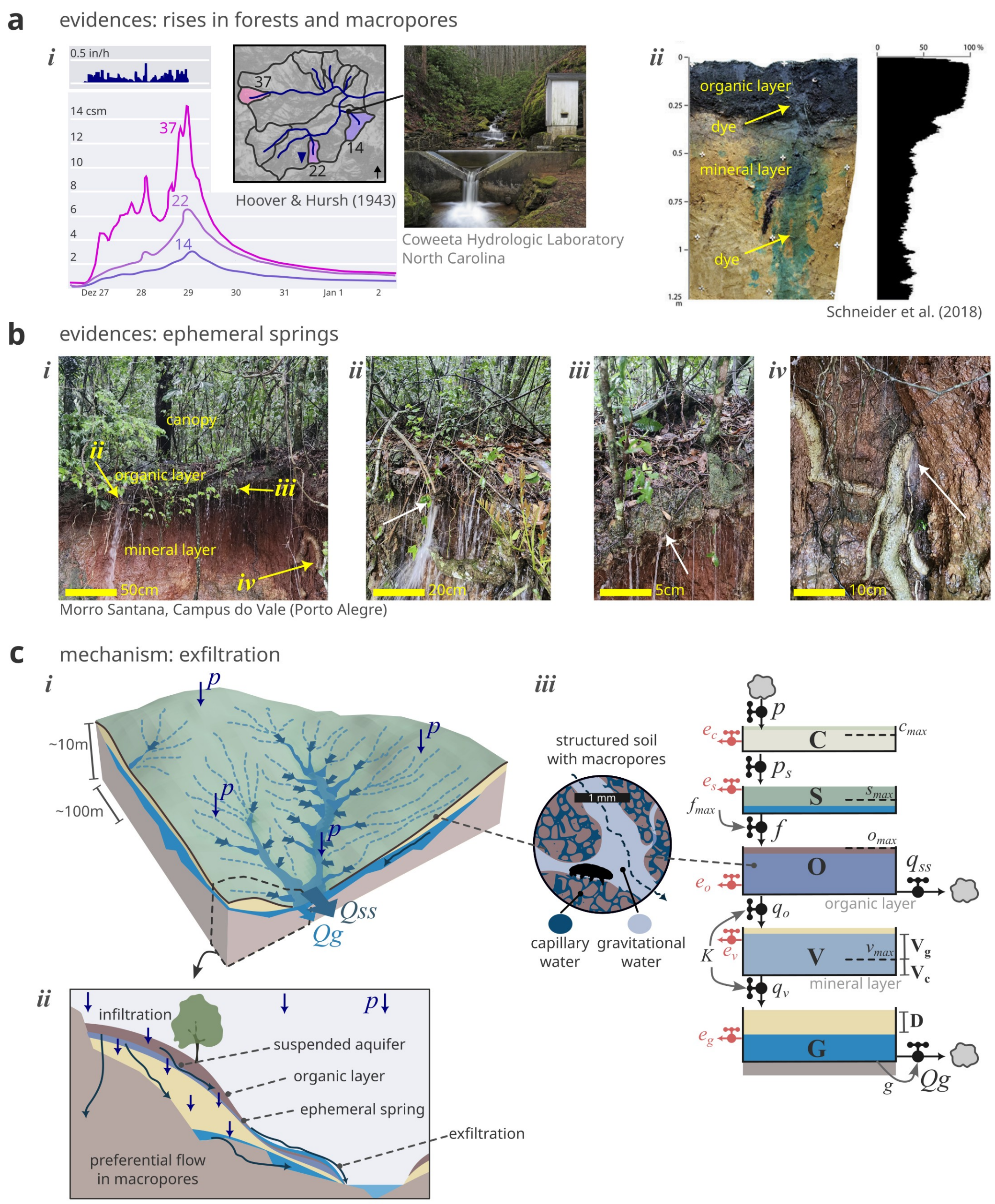

Figure 3.5 — Rapid exfiltration through macropores. Macropores and preferential subsurface pathways produce rapid exfiltration q_{ss} responses, especially in forests. **a** — Evidence: rises without runoff in basins at the Coweeta Experimental Forest (North Carolina, United States) reported by Hoover & Hursh (1943) [87] (detail i), and; the distribution of macropores in the soil profile highlighted by dyes, reported by Schneider et al. (2018) [88] (detail i). **b** — Evidence: ephemeral springs observed on June 16, 2023, at a road cut on the Vale Campus of the Federal University of Rio Grande do Sul (Morro Santana, Porto Alegre). Despite the extraordinary rain on that day (141.7 mm in 24 hours), no runoff was observed in the forest soil. i – profile of the bank; ii – preferential flow; iii – flow at the interface between horizons; iv – turbulent flow in a fracture in granite, created by a root. **c** — Systematization of the ephemeral springs mechanisms: rainwater infiltrates rapidly, creating a suspended aquifer at the transition between the organic and mineral horizons. This suspended aquifer emerges at various points in the basin, facilitated by macropores and preferential subsurface pathways, creating ephemeral springs during and shortly after rainfall. Source of the photograph in **a**: https://www.be-roberts.com/se/cwta/cwta1.htm .

> drainage-area; nevertheless, characteristic flood-hydrographs are produced by heavy rains. – Hursh & Brater (1941, p. 863) [92].

This claim, followed by data in subsequent studies (see Figure 3.5**a**, in detail i), inevitably introduces a *counterexample* to the theory of infiltration capacity f_{max}. After all, if there is no surface runoff q_{si}, the only available response in Horton's perceptual model is the *slow* response caused by the recharge q_{v} from the aquifer, which is responsible for the recession curve. Among other mechanisms at work in the basin, detailed later, the authors point to the existence of *rapid subsurface responses* that include both water flow in highly permeable soil layers (unsaturated flow) and the formation of temporary suspended aquifers (saturated flow), which develop in different parts of the landscape during rainfall. In this regard, Hursh & Fletcher (1942) [93] emphasize the importance of soil macroporosity. Especially in forests, this property would help explain the dominance of preferential subsurface flows, significantly increasing the soil's gravitational water $\mathbf{V}_\mathrm{g}$, in contrast to capillary water $\mathbf{V}_\mathrm{c}$:

> The exact nature of this macro-pore space occurring in different horizons of the soil profile has yet to be described. It includes all large underground channels formed from decayed roots, fractured rock, insect and animal burrows, and larger spaces that may exist. It also includes macro-pore spaces formed through the complex structural patterns created by the aggregation of soil particles in the presence of organic materials. In the upper horizons of natural soils these biological openings and structural patterns built up from lattice-like aggregates are far more important in determining noncapillary porosity than the single grain soil particle size. Root channels and animal burrows are of particular significance in the detention storage and draining of gravitational water. A single earthworm burrow may be far more important in draining through a block of heavy soil than the entire cross sectional area of the pore space. In like manner, it is conceivable that a few continuous void spaces may give rise to rapid discharge of groundwater through a soil profile which, when viewed as a uniformly pervious medium, would be expected to transmit water slowly. – Hursh & Fletcher (1942, p. 485) [93].

Unlike recent studies with dyes, which clearly demonstrate the existence of macropores (as shown in detail *ii* of Figure 3.5**a**, with recent results from Schneider et al. (2018) [88]), the authors from Coweeta presented no evidence beyond observations of aggregated processes, such as rain, flow, and well levels. This research gap was permanently addressed in the 1960s when a new wave of studies provided more detailed quantitative results obtained through a more experimental approach than observational. Still in the context of the Coweeta Experimental Forest, Hewlett and Hibbert (1963) [94] used a lysimeter to demonstrate the critical role of water flow in the vadose zone $\mathbf{V}$ in sustaining base flow in streams. Whipkey (1965) [95] detailed lateral flows in the soil profile of a hillslope in Ohio (USA). The hillslope was monitored by a trench at its base, demonstrating the dynamics of exfiltration q_ss, especially in the upper organic layers, where high hydraulic conductivity K was measured due to the presence of macropores. Here, the function of **permeability transitions** between the soil horizons appears, especially between the organic horizon **O** (upper) and the mineral horizon (lower). This discontinuity generates a loss of hydraulic head that results in *lateral* flow in the vadose zone **V**. I personally observed this process during a severe storm on June 16, 2023, at the Vale Campus of the Federal University of Rio Grande do Sul, at the base of Morro Santana, Porto Alegre (see details in Figure 3.5**b**). According to the `INMET` Station `83967`, June 16, 2023, recorded 141.7 mm of rain, which is above the monthly average for that month (around 130 mm). Despite such extreme rain and streams practically overflowing, I did not observe surface runoff in the forested areas of the campus, except where the terrain's channel forced the emergence of the suspended aquifer (i.e., through the expansion of riparian wet areas).

Other trench studies reaching similar conclusions to Whipkey's (1965) in the United States include: Ragan (1968) in Vermont [96]; Beasley (1976) in Mississippi [97], and; Harr (1977) in Oregon [98]. In the latter case, it was reported that exfiltration q_ss was 6 to 9 times greater in the upper soil layers than in the lower layers, corroborating the function of macroporosity. In the same study, the authors report that exfiltration q_{ss} was responsible for about 97% of the rapid response during rises. This was consistent with earlier results from Patric and Swanston (1968) [99], who cut down all the trees on a slope in Alaska and applied sprinkler irrigation. They observed no surface runoff q_{si} – the applied water traveled through preferential subsurface pathways, emerging rapidly at the base of the slope. In the British Isles, Weyman (1970) [100] reported that unsaturated subsurface runoff constitutes the main rapid response in an experimental basin, while Jones (1971) [101] noted that the widespread occurrence of the phenomenon known as *piping* – the formation of natural tunnels in the soil profile – contributes to high velocities in subsurface response. Consolidating this new generation of field research, results from the MaiMai experimental basin (New Zealand) established a new experimental research program, combining water balance, trenches, and the novelty of chemical tracers, dyes, and isotopes. In the case of MaiMai, Mosley (1979) [102] reaffirms (almost forty years after Hursh) the crucial role of macroporosity and natural tunnels in exfiltration q_{ss} while addressing some theoretical objections:

> Freeze [1972, p. 1282] considerou que um valor limiar de condutividade hidráulica saturada da ordem de 0,002 cm/s é necessário para que a exfiltration q_{ss} seja significativa, mas em um solo que contém canais de raízes, túneis e zonas de afloramento, a condutividade hidráulica saturada não é um fator limitante. O fluxo de corante traçador através de macroporos no solo foi observado a taxas até 3 ordens de magnitude maiores, e a resposta sensível e rápida da exfiltration q_{ss} às variações na precipitação sugere que o fluxo por macroporos, e não pela matriz do solo, contribui para as enchentes nos canais.[2] – Paul Mosley (1979, p. 806) [102].

3.3.2 Topography

The Hortonian paradigm has not only been refuted by the recognition of exfiltration q_{ss}, as empirical evidence has also accumulated to support the existence of two additional, less intuitive rapid response mechanisms occurring in **riparian wetlands**. These mechanisms, illustrated in Figure 3.6, result from the interaction of rain with a shallow and dynamic groundwater table, one being direct rainfall q_{se}, and the other translational flow Q_{gt} (details in the next section). Both are interrelated, are strongly controlled by the terrain's topography, and also have consequences for the manifestation of exfiltration q_{ss} in macropores, as we will see later. The first of these emerges in the literature when direct precipitation in the area surrounding channels and springs is cited by Hursh & Brater (1941) [92] as one of the sources of river runoff in the basins of the Coweeta Experimental Forest:

> Contributions from areas of normally shallow water-tables located in close proximity to the stream, and occurring in soil-profiles which are quickly saturated. Where such conditions occur along a stream, it is expected that there will be an actual increase in the width of the channel and subsequent increase in the amount of channel-precipitation. Areas of high water tables adjacent to spring-heads would be expected to contribute similarly. – Hursh & Brater (1941, p. 870) [92].

[2] Tradução livre de: *Freeze [1972, p. 1282] considered that a threshold value for saturated hydraulic conductivity of the order of 0,002 cm/s is necessary for subsurface stormflow to be significant, but in a soil that contains root channels, pipes, and seepage zones, saturated hydraulic conductivity is not a limiting factor. Flow of dye tracer through macropores in the soil was observed at rates up to 3 orders of magnitude greater, and the sensitive as rapid response of subsurface flow to variations in precipitation suggests that flow through macropores rather than through soil matrix contributes to channel stormflow.*

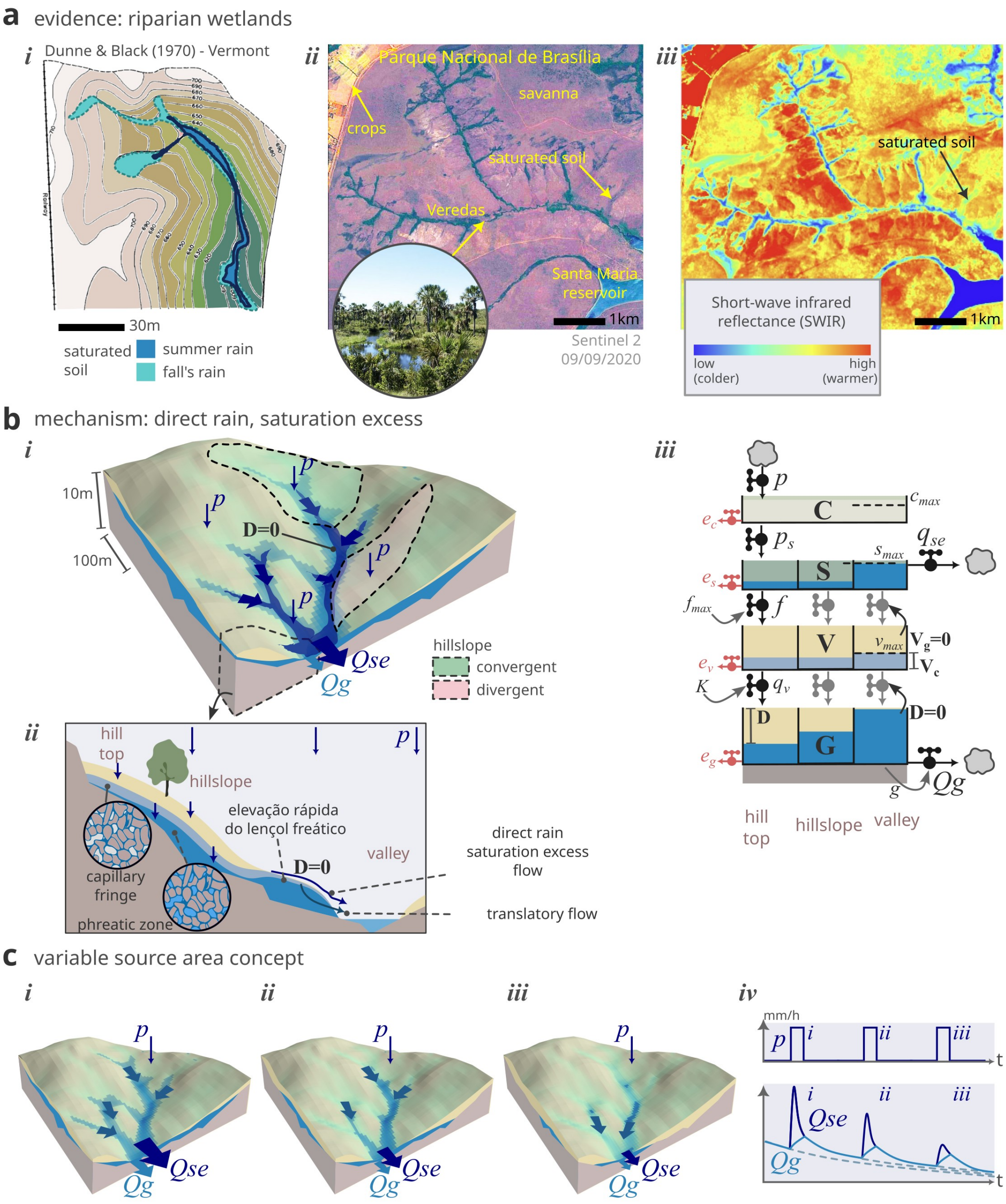

Figure 3.6 — **Topography and the variable source area.** Topography plays a crucial role in the formation of riparian wetlands that vary in extent during rainfall and throughout the seasons. These saturated soil areas thus produce direct rainfall q_{se}, as well as rapid subsurface responses from translational flow Q_{gt}. **a** — Evidence: map by Dunne & Black (1970) in Vermont (United States), demonstrating the extent of riparian wetlands at different times of the year (detail i), and; wet veredas in the dry season at the Brasília National Park, observed through short-wave infrared reflectance from a Sentinel-II scene on September 9, 2020 (details ii and iii). **b** — Systematization of the mechanism of runoff due to saturation excess. The soil in different parts of the basin (valley bottom, hillslope, and hilltop) saturates at different rates, generating rapid responses primarily in the valley bottoms. Convergent slopes tend to produce more direct rainfall q_{se} than divergent slopes, where recharge q_{v} and baseflow Q_{g} prevail. **c** — Schematic representation of the retraction of riparian wetlands during a dry spell (seasonal dynamics). This process also exhibits ephemeral dynamics during and shortly after rainfall events. Source of the photograph in **b**: https://commons.wikimedia.org/wiki/File:Veredas.jpg .

This is certainly one of the pioneering descriptions of the concept of **variable source area**: the generation of surface runoff q_{si} as a function of the *expansion and contraction of wet areas* in valley bottoms, adjacent to streams. This mechanism, illustrated in Figure 3.6**c**, allows any effective rainfall p_{s} to transform into excess rainfall p_x when it falls on saturated soil areas, which helps explain the prevalence of rises even in basins with high infiltration capacity $f_{\max}$ soils (as in the case of La Grange Brook, near where Robert Horton lived [82]). This concept was well organized by Cappus (1960) [103] in a study in the Alrance Experimental Basin (315 ha, France). The author claimed to have evidence for a “new theory of surface runoff”, in which the basin area can be divided into a *surface runoff zone* and an *infiltration zone*. The former includes a *fixed* part of impermeable areas and a *variable* part of permeable areas that are nearly completely saturated with water:

> The experimental basin can be divided into two zones S_r and S_i of variable extents: — The runoff zone S_r of area A_r includes, on one hand, fixed extent impermeable zones (roads, paved paths, compacted dirt paths from repeated traffic of people or livestock, rocky surfaces, etc.) and, on the other hand, variable extent zones consisting of permeable land, but almost completely saturated with water. The rain that falls in the zone S_r entirely transforms into surface runoff q_{si} or subsurface runoff. — The infiltration zone S_i of area A_i consists of unsaturated permeable land. The sandy-textured soil, which forms the surface layers of the experimental basin, is characterized by a very high infiltration capacity $f_{\max}$ f that exceeds the intensity of all rains that may fall on this basin—except for those of extremely rare occurrence. Thus, except in very exceptional cases, the rain that falls in the zone S_i is completely absorbed by infiltration and consequently generates no runoff. [3] – Cappus (1960, p. 503) [103].

Tsukamoto (1963) [104] also structured a similar theory, based on results obtained in a basin at the University of Tokyo Forest (106.7 ha, Japan). In his paper, he points out that riparian areas exhibit rapid saturation responses due to the influence of the **capillary fringe** of groundwater, generating surface runoff q_{si} in this part of the slope, as opposed to the higher and well-drained parts of the terrain. The experimental results from Ragan (1968) [96], mentioned above, also demonstrated rapid rises in the water table near the stream during monitored rainfall events. Even Betson (1964) [83], while attempting to uphold the Hortonian perceptual model, noted that half of the runoff was possibly generated by a swamp area in one of the basins analyzed in his study.

To corroborate the theory of variable source area, Dunne & Black (1970) [105], [106] published detailed results for a small experimental basin in Vermont (United States). In this study, the authors present maps of saturated soil areas that follow the terrain’s channel (detail *i* in Figure 3.6**a**), which showed variations both throughout the year (seasonal dynamics) and during rainfall events (ephemeral dynamics). The seasonal dynamics of these wet areas is explained by the increase in recharge q_{v} of groundwater during the wetter season, which expands the extent of spring emergence zones in the valley bottoms. Detail *ii* in Figure 3.6**a** demonstrates evidence of seasonal dynamics from short-wave infrared (`SWIR`) reflectance with a Sentinel-II scene on September 9, 2020, in the Brasília National Park. This period is marked by dry conditions, but the riparian areas remain moist, forming the Veredas. On the other hand, the ephemeral dynamics are explained by a rapid rise of the phreatic zone **G** when the capillary fringe is very close to the surface (more details ahead).

[3] Freely translated from: *Le Bassin expérimental peut être partagé en deux zones S_r et S_i d’étendues variables: — La zone de ruissellement S_r de superficie A_r comporte, d’une part, des zones imperméables d’étendue fixe (routes, chemins empierrés, chemins de terre tassée par le passage répété des hommes ou du bétail, surfaces rocheuses, etc.) et, d’autre part, des zones d’étendue variable constituées de terrains perméables, mais à peu près complètement saturés d’eau. La pluie tombant sur la zone Sr se transforme entièrement en ruissellement superficiel ou hypodermique. — La zone d’infiltration S_i de superficie A_i est constituée par les terrains perméables non saturés. Le sol de texture sableuse, qui forme les couches superficielles du Bassin expérimental est caractérisé par une capacité d’infiltration f très forte qui dépasse l’intensité de toutes les pluies pouvant tomber sur ce bassin — à l’exception seulement de pluies d’une rareté extrême — ainsi, sauf en des cas très exceptionnels, la pluie tombant sur la zone S_i est entièrement absorbée par infiltration et ne donne lieu par conséquent à aucun ruissellement.*

The unequivocal observation of the dynamics of saturated areas by Dunne & Black (1970) solidified the perception that *topography* exerts an important control in the Hydrology of zero-order basins, and not just the *surface* of the soil, as postulated by the infiltration paradigm. In this sense, Anderson & Burt (1978) [107] demonstrated that, in a basin in the Quantock Hills (England), the rapid rise of the water table along the channels of the **convergent slopes** is much greater than in the **divergent slopes**. The former tend to generate relatively more direct rainfall q_{se} and also more exfiltration q_{ss}, as the sudden rise of groundwater activates the macropore network in the soil. In the divergent slopes, on the other hand, slower processes of recharge q_{v} and baseflow Q_{g} predominate.

In this context, the mechanism of surface runoff q_{si} defended in Horton's theory (infiltration excess) was not exactly refuted but reserved as a response mechanism limited to extraordinary precipitation events or areas with altered soil, whether in natural environments (such as rocky outcrops and arid regions) or anthropized environments (such as agriculture and urban areas). This implies that the use of the `CN` method from the `SCS` is justified when its application is directed towards extreme rainfall events or in urban and rural basins where the Hortonian mechanism is clearly dominant. However, this restriction is not explicitly stated in the official manuals of the method, which also include `CN` values for forests and other natural land covers. Additionally, simulation models such as `SWAT` and `SWMM` utilize continuous simulation (various rainfall events) and represent any land cover. It is worth noting that Horton (1936) [108] came close to analytically deducing this mechanism in one of his papers, as he highlights that sloping soil hillsides induce the water table to intercept the surface above the valley bottom level, causing the emergence of a saturated surface in this convergent part of the topography [109].

3.3.3 Paradoxes

Translational subsurface runoff, in turn, is conceptually speculated by Hewlett & Hibbert (1967) [59], in a clearly revolutionary article in the field of Hydrology [114]. While criticizing the hegemonic paradigm of the time (the infiltration capacity theory), the authors organize new relevant concepts, such as the terms "rapid and slow responses" and "variable contributing area", paving the way for the advent of the new paradigm. In this direction, the authors suggest a mechanism of *instantaneous* subsurface response that occurs when the field capacity v_{max} of the soil is exceeded by the infiltration of rainwater in the riparian zones, where there is greater influence from capillarity fringes. In summary, they postulate that this response, although rapid, would not exactly be rainwater but water that had settled in the soil matrix *before* the event occurred. In this process, the thickness of water films on soil particles in the vadose zone $\mathbf{V}$ suddenly reaches a limit where the pore network becomes pressurized by gravity. Therefore, the **new water** from the rain (event water) triggers a pulse, a pressure wave, that expels the water stored in the soil at the base of the slope, referred to as **old water** (pre-event water):

> However, of the part contributed to direct runoff, a fraction will be some of the actual drops that fell during the storm – that is, some new rain – and the other fraction will be what we might call translatory flow, or flow produced by a process of displacement. This is a contribution to direct flow of water already stored in the soil mantle before rainfall began. It will be released in large quantities only when the soil is within field capacity range or wetter. Above the zone of saturation, we may regard such movement as due to thickening of the water films surrounding soil particles and a resulting pulse of water flux as the saturated zone is

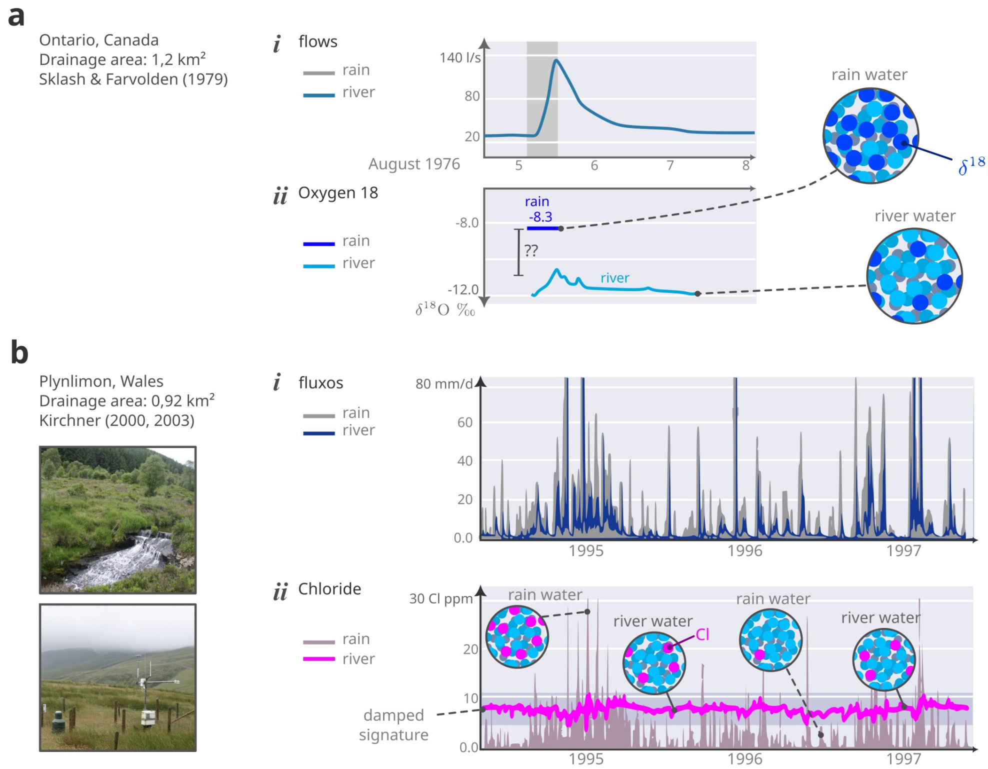

Figure 3.7 — The old water paradox. Analyses of isotopic signature and geochemistry of rainwater and river water during rises make it clear that they are waters of different ages, thus creating a paradox. **a** — Evidence provided by Sklash & Farvolden (1979) [110] in a rural basin in Ontario, Canada (1.2 km² drainage area). The flows clearly denote a rapid response from the basin (flood) to the rainfall event (detail i). However, the isotopic signature with Oxygen-18 shows that the water in the flood is not the same as the rainwater (detail ii). **b** — The same paradox observed with Chloride (marine aerosol) by Kirchner et *al.* (2000, 2003) [111], [112] in an experimental basin in Plynlimon, Wales (0.92 km² drainage area). The flows are typical rapid responses (detail i), but the river signature shows a pronounced damping over the years, suggesting a long-duration mix (detail ii). Source of the photographs: Ecological Continuity Trust [113].

approached. – Hewlett & Hibbert (1967, p. 279) [59].

Although the theory makes sense and cites laboratory studies, the text by Hewlett & Hibbert (1967) does not provide empirical evidence obtained in the field to justify the reality of this mechanism. However, this gap was filled by Pinder and Jones (1969) [115], who evaluated the separation of flood hydrographs in three monitored basins in Nova Scotia (ranging from 647.5 ha to 13.5 km², Canada). Unlike conventional graphical methods, they inferred the separation between surface runoff q_{si} and subsurface flow using chemical tracers and a simple mass balance model[4]. In the presented case, sodium, calcium, bicarbonate, magnesium, and sulfate concentrations were monitored before and during flood events. The results indicated a substantial prevalence of groundwater flow during rises, accounting for 32% to 42% of the maximum hydrograph flow. However, this did not eliminate the alternative explanation of a subsurface response from rainwater (new water) that dissolved the monitored solutes while rapidly moving through the soil. Evidence in favor of groundwater (old water) became much more robust with the advent of hydrogen and oxygen isotope monitoring, such as Deuterium (^{2}H), Tritium (^{3}H), and Oxygen-18 (^{18}O), which are ideal markers that are part of the water molecule itself[5]. In locations with significant variability in the **isotopic signature** of the precipitated water, it is possible to estimate how much

[4] The developed model consists of two mixing compartments: $C_{tr}Q_{tr} = C_{dr}Q_{dr} + C_{gw}Q_{gw}$, where: C is the concentration of some conservative solute; Q is the flow; tr denotes total flow; dr denotes direct runoff, and; gw denotes groundwater flow.

[5] Unlike common solutes, the concentration of ^{18}O is measured by the difference in parts per thousand

of this new water is present during rises[6]. This strategy was suggested by Dinçer et al. (1970) [116] in a study in the mountains of Czechoslovakia that demonstrated the effect of **thermal fractionation**[7] on the concentrations of ^{3}H and ^{18}O in snow layers that precipitated and melted over the seasons. Subsequently, the results published by Martinec et al. (1974) [118] noted that river water in the Swiss mountains exhibited a relatively low variability in ^{18}O concentration, approaching the long-term average of seasonal oscillations observed in precipitation. The strategy then took on well-defined contours with the article by Sklash et al. (1976) [117], which, in addition to organizing the logic of the method, showed that in two monitored basins in Ontario (Canada), the contribution of groundwater to the maximum flood flow ranged from 55% (in upstream basins) to 70% (in downstream basins draining an area of 700 km^2). These results carry revolutionary implications:

> The most important finding is that the pre-storm component of storm runoff for the 16 May storm was large. For example, at peak total discharge, the pre-storm component of Big Otter Creek at Vienna was 70 ± 9% of storm runoff. These results substantiate the findings of Pinder & Jones (1969) and Fritz et al. (1974), even though the basins in the present study are one to two orders of magnitude larger in areal extent.These results are not consistent with the simulated results of Freeze (1972b), the field results of Dunne & Black (1970a,b), and Hewlett & Hibbert (1967), or the theoretical implications of Horton (1933). The results are particularly encouraging, though, in light of the large subsurface (prestorm) component of snowmelt noted by Dinçer et al. (1970). – Sklash et al. (1976, p. 276) [117].

Michael Sklash continued studies of this type, corroborating the existence of this process in basins in Canada, New Zealand, and the British Isles [110], [119], [120]. For example, the article by Sklash & Farvolden (1979) [110] in Canada presents similar results for a basin with intensive agriculture (1.2 km^2, in the Hillman Creek Experimental Basin, Ontario, Figure 3.7**a**) and two highly forested basins (1.0 km^2 and 3.9 km^2, in the Ruisseau des Eaux Volées Experimental Basin, Québec). In addition to reporting the surprising prevalence of old water in rises (between 80% to 94% of total runoff), the authors contribute to the theory of rapid rises in groundwater in valley bottoms to explain the phenomenon. In the MaiMai Experimental Basin (New Zealand), Sklash et al. (1986) [119] present results that drastically revise the interpretations of Mosley (1979) [102]. As mentioned above, Mosley (1979) argues for the dominance of exfiltration q_{ss} (new water) in this basin. The unequivocal prevalence of old water in rises, obtained with isotopic markers, created a certain impasse in the scientific community, which since then has proposed plausible mechanisms [121]. In this context, McDonnell (1990) [85] synthesizes the response mechanisms in the MaiMai basin, introducing the concept of **activation of subsurface flow** from the entry of rainwater into the macropore network of the hillslopes, i.e., through exfiltration q_{ss}. In this scheme (illustrated in Figure 3.8**a**), he emphasizes the role of *vertical* shortcuts in the soil profile, created by macropores, which allow the new rainwater to rapidly lodge in the capillary fringes of

(δ^{18}O ‰) of the ratio of ^{18}O/^{16}O of a standard and the sample: $\delta^{18}\mathrm{O} = (\frac{^{18}\mathrm{O}/^{16}\mathrm{O\,sample}}{^{18}\mathrm{O}/^{16}\mathrm{O\,standard}} - 1) \times 1000$. The standard is usually the mean ocean water (`SMOW`). Waters depleted of ^{18}O relative to the standard exhibit negative δ^{18}O, and vice versa.

[6] Obviously, if the rainwater is isotopically indistinguishable from the river water just before the event, then it is impossible to extract any relevant information.

[7] The main cause of the fractionation of these isotopes in the atmosphere arises from the difference in vapor pressure between isotopically heavy and light water molecules: $H_2{}^{18}O$ has a lower vapor pressure than $H_2{}^{16}O$ and, therefore, $H_2{}^{16}O$ remains preferentially in the liquid phase during both evaporation and condensation processes. Thus, the observed concentrations of δ^{18}O in precipitation tend to be incrementally negative as moist air masses move over continents [117].

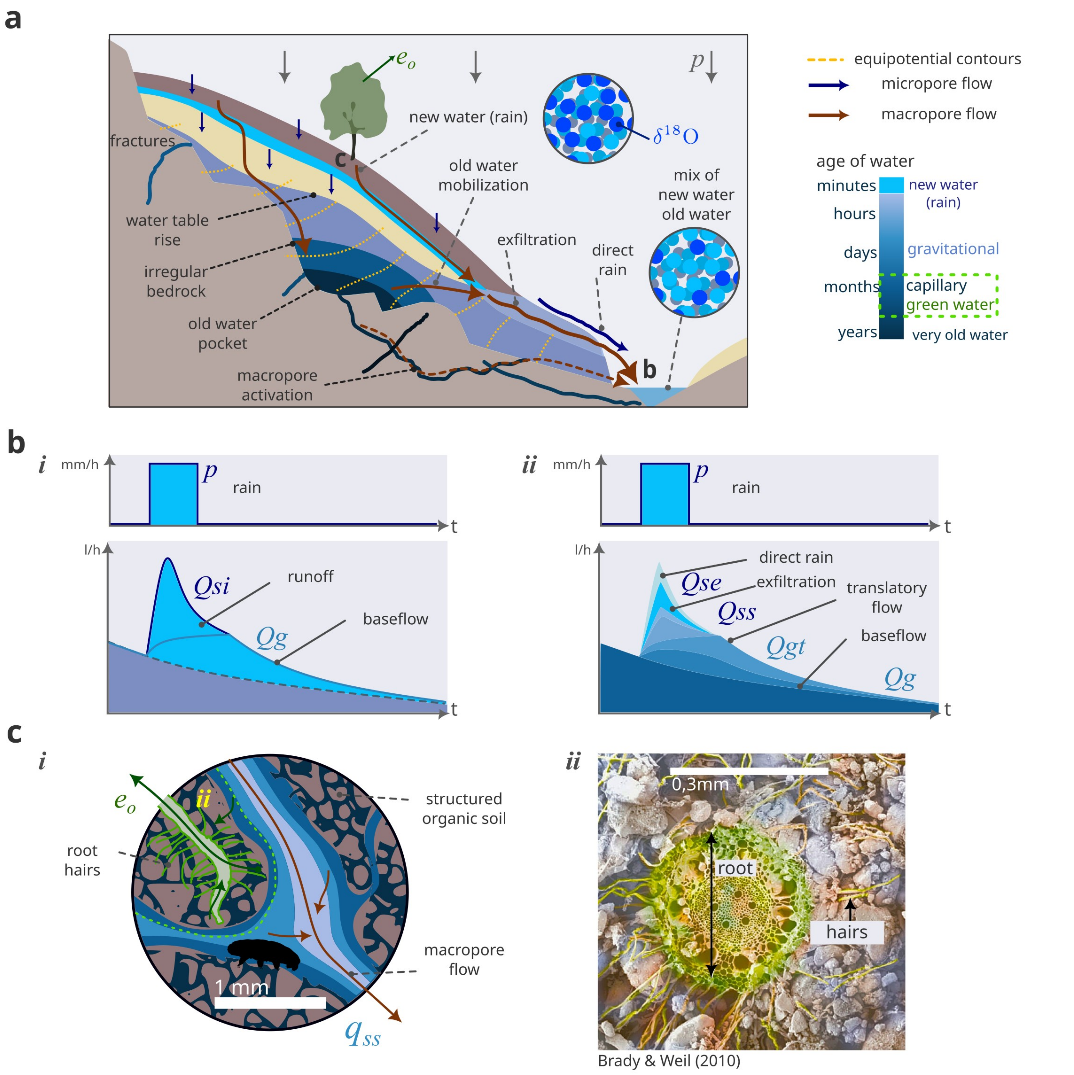

Figure 3.8 — Mobilization of old water. a — The rise of the water table combined with flow through macropores (fractures and preferential pathways) helps explain the dominance of old water in the rapid responses of rivers. Vertical shortcuts allow new water (rain) to mix with older water in stagnation zones (pockets) at the aquifer's threshold, activating hydraulic head in fractures and preferential pathways, resulting in the rapid expulsion of old water. **b** — Differences between the Hortonian model of rapid response (Type 3 flood) and the model obtained from isotopic analyses. **c** — Water in the soil also shows an age differentiation, which is perceived in the evapotranspiration flows of plants (detail i). The capillary water **V**$_c$ is absorbed by fine roots, while gravitational water **V**$_g$ drains to the base of the slope (detail ii). Photograph from electron microscopy adapted from Brady & Weil (2010) [124].

the phreatic zone **G**, thereby activating the hydraulic head necessary to quickly expel the old groundwater at the base of the slope. A new review by McGlynn et al. (2002) [122] also highlights the relevant effect of the **bedrock topography** of the slope (the underlying relatively impermeable bedrock). It is suggested that the irregularities of this layer can create **stagnation zones** or **pockets** that store water underground for much longer than expected. The eventual hydraulic activation of these relatively inaccessible parts expels old water at the base of the slope, facilitated by the presence of macropores. Indeed, the influence of underlying geological structures (fractures) on the emergence of groundwater had already been mentioned by Huff et al. (1982) [123], but without analyzing the age of the water using isotopes.

The evidence, impasses, and plausible mechanisms proposed to explain the dominance of old water in rapid responses further increase in complexity given the results of **geochemical signature**, which tend to exhibit high variability. In this sense, Burns et al. (2001) [125] suggest that the surface responses in the Panola Mountain

Experimental Basin (Georgia, United States) end up mixing with groundwater in the riparian zone before entering the channels. Seibert et al. (2003) [126] also emphasize the difference in geochemical signature between the water in the riparian zone (anoxic conditions) and the water in well-drained hillslope soils (greater aeration). This complexity has led to some perplexity, expressed by Kirchner (2003) [112] in the so-called *double paradox of catchment hydrology and geochemistry*, or simply **old water paradox**. For him, this paradox has two components that, although related, are somewhat contradictory: (1) Hydrology: the rapid mobilization of old water—the quick replacement of old water by new, as postulated by translational flow Q_{gt}, and; (2) Geochemistry: the chemical variability of old water—the fact that old water assumes different chemical signatures depending on the flow velocity. In this sense, based on chloride concentrations[8] monitored in a basin in Wales, Kirchner et al. (2000) [111] propose a **hydrogeochemical compartmentalization** of the soil, where pores and fractures exhibit a fractal structure of residence times (see Figure 3.7**b**). This implies why the slopes of the basins transmit *hydrological signals* much faster than *geochemical signals*. This concept becomes clearer through Iorgulescu et al. (2007) [127], who reinforce the difference between the *wave* speed (**celerity**) of water and the *molecular* speed of water—beyond material, flood flow is an energy flow. In the same spirit, McDonnell (2014) [128] also draws a new perspective on evapotranspiration flows, particularly regarding the age of the water that plants consume, proposing the possibility of a **hydro-ecological compartmentalization** of the soil, which he refers to as **two-world hypothesis**. In this situation, the water consumed by the roots and **fine roots** of plants (known as *green* water) would be capillary water $\mathbf{V}_{\text{c}}$, relatively older than gravitational water $\mathbf{V}_{\text{g}}$ (see Figure 3.8**b**). Evaristo et al. (2015) [129] provide evidence supporting this hypothesis, showing that ecological separation is common in various biomes—plants use soil water with an isotopic signature distinct from the water contributing to the recharge q_{v} of groundwater and to river runoff.

3.4 Models and Limitations

Accompanying the scientific revolution brought about by empirical evidence regarding runoff mechanisms on hillslopes, the 1960s was also marked by the advent of the first hydrological models simulated on digital computers. This occurred largely due to a confluence of factors, such as the intellectual context of von Bertalanffy's General Systems Theory and the practices of Jay Forrester's Systems Dynamics, following the emergence of digital mainframe computers. Keith Beven reports that by 1971, he had counted over a hundred hydrological models in the literature, which were basically versions of the Stanford University model, the *Stanford Watershed Model IV* (`SWM`) [130]. The model was developed starting in 1959 as Norman Crawford's doctoral thesis, supervised by Ray Linsley, and later gave rise to a program called the *Hydrologic Simulation Program, Fortran* (`HSPF`), developed for and with the support of the U.S. Environmental Protection Agency (`USEPA`) [131]. This pioneering model clearly exemplifies the influence of the ontology offered by Systems Dynamics: a network of reservoirs connected by flows that is solved numerically. In this case, the SWM is only slightly more intricate than the minimalist model presented in the previous chapter, with four reservoirs (canopy, vadose zone $\mathbf{V}$, phreatic zone $\mathbf{G}$, and drainage channels) and three response mechanisms (including a subsurface response in addition to surface runoff q_{si} and groundwater flow). However, the model does not represent water storage on the surface, nor does it differentiate topographic aspects in a way that surface runoff

[8] An analogous strategy to that used with isotopes is possible in basins with marine aerosol deposition, with chloride being an inert marker that can be analyzed in rainwater.

can be separated into surface runoff q_{si} or direct rainfall q_{se}. But this is not exactly a problem in Systems Dynamics; it is sufficient to add a new compartment and connect the flows. The flexibility provided by Systems Dynamics, in this sense, introduced it as a conceptual and procedural paradigm in hydrological modeling, resulting in both a proliferation of models from this period and an increased theoretical understanding of the importance of **scale** throughout the modeling process.

3.4.1 Data and Processes

Before the advent of hydrological simulations, however, the approach to obtaining flood hydrographs from rainfall data primarily relied on the concept of **Unit Hydrograph** of the basin, introduced by Sherman (1932) [132]. This concept is based on the theory that the hydrological response of a basin can be summarized as a linear process of kinematic propagation through the channel network from a rainfall pulse, which can be reduced to a unit pulse. According to the **principle of superposition**, more complex rainfall pulses can be integrated over time (convolution method). In this case, the fundamental parameter of a basin is its **time of concentration**, which is relatively larger in elongated basins than in rounded basins, even if they have exactly the same area. The systemic view allowed this process to be represented as a series of connected reservoirs, a "cascade," resulting in the parameterization of a Gamma distribution, or **Kalinin-Miyukov-Nash model**:

$$Q(t) = \frac{\nu}{k\,\Gamma(n)} e^{-t/k} (t/k)^{n-1} \tag{3.1}$$

Where ν [L^3] is the volume of the hydrograph; n [-] can be interpreted as the effective number of reservoirs; and k [T] can be interpreted as the average residence time of the reservoirs. Reportedly, this parameterization was first obtained independently by Kalinin & Miyukov (1957) [133] in the Soviet Union, and later by Nash (1958) in England [134]. From this, the notion emerged that the response of the basin is analogous to a *function* or *filter* that acts on the rainfall signal (or other input signals). This approach to obtaining hydrographs, which represents a modeling paradigm with its own ontology, evolved into what Todini [135] refers to as **data-driven models**, in contrast to **process-driven models**. The data-driven models today encompass a set of techniques that include, for example, artificial neural networks. This approach is visibly contaminated by the fluvialist bias; after all, it is impossible to *explain* exactly where and how runoff was generated based on a truly hydrological theory—the basin is treated as a black box. In this regard, Todini argues that this family of models sought to maximize **predictive capability** at the expense of **explanatory capability**, that is, to produce results that have "physical meaning." An attempt to re-establish the explanatory capability of data-driven models is the modeling approach termed *Data Based Mechanistic* (`DBM`), schematized by Young (2002) [136]. This technique results not only in predictions of flow but also identifies internal structures and parameters that possess explanatory capability. In this context, Todini argues:

> Although the DBM modelling approach recognises the importance of the physical coherence of the identified model structure, it derives it from the observations, thus disregarding de facto the results of at least 50 years of research efforts aimed at specifying the physical hydrological mechanisms that generate rises. This contrasts with the Bayes principle which would combine the observations with all possible a priori knowledge on the hydrological processes and possibly on the parameter values to obtain less uncertain a posteriori forecasts. – Todini (2007, p. 471) [135].

As highlighted in Chapter 1, *models are symbolic vehicles for theories*. In this sense, data-driven models are, in their essence, **statistical models**: they establish a theory about the data *themselves*, about their internal relationships. As mentioned in Chapter 2, such models tend to be *overfitted to the data*, allowing for good interpolations but making extrapolations problematic, not contributing to the learning process that Systems Dynamics offers. Process-based models, on the other hand, instantiate a representation of a *target system* that exists in an objective reality *beyond* the data—the watershed. Therefore, a truly hydrological model, based on processes, is capable of simulating the behavior of a basin *even without any empirical observation available* (a synthetic scenario, for example), as modeling is a process of **deductive inference**. The role of empirical evidence, in this sense, is to reject or corroborate the theory conveyed by the model.

3.4.2 Incommensurability

Despite the appeal in terms of explanatory capability, process-driven models, enabled by Systems Dynamics, have also begun to demonstrate their limitations, especially in light of the evidence supposedly associated with the parameters. Even when representing known hydrological response mechanisms, the highly *aggregated* nature of the instantiated compartments has made it increasingly clear that defining the parameters of a hydrological model to achieve good results is not a trivial practice, requiring a long process of trial and error, marked by many nuances[9]. To make matters worse, the parameters values that produced results adhering to empirical observations rarely coincided with field-measured values. For instance, Amorocho & Hart (1964) [138] draw attention to unrealistic results obtained internally within this type of model, due to **compensating effects** in the mass balance imposed on the compartments. For these reasons, Todini suggests that calibrating hydrological models with optimization methods without greater concern for the physical coherence of the parameters ultimately transforms a process-based model into a data-based model, as the focus tends to be on adjusting input data (rain) and output (flow), rather than explaining phenomena in an objective reality [135]. This limitation arises from two inexorable and inseparable problems in hydrological modeling: (1) the **equifinality problem** and, (2) the **scale problem**.

The equifinality problem was explored in Chapter 1 (Section 1.6), being a milder version of the underdetermination problem of theories that postulate unobservable entities. The term "equifinality" was introduced by von Bertalanffy in General Systems Theory (Chapter 2, Section 2.3), conveying the notion that open systems systems can converge to similar structures. In modeling, it is associated with the fact that systems with different structures or even parameters can exhibit similar *behaviors*, as in the case of slow responses illustrated in the prototype model from Section 2.5. Thus, the calibration process of a model with partial information about its processes (only observed flow, for example) **does not** guarantee that other internal processes are adequately represented in empirical terms—hence the discrepancy between observed and adjusted parameters. But even if *complete* information exists, the scale problem, discussed below, implies that the differences between the scale represented by the model and the scale of observations are *incommensurable*, or incompatible, introducing the commensurability error ε_Δ in the results of the model (see Equation (1.5), the total error equation). It is noteworthy that the issue of scale similarity was a problem promptly

[9] According to Keith Beven, in the early days of rainfall-runoff modeling, there was a story that the only person who could truly calibrate the Stanford Model, with all its parameters, was Norman Crawford, who wrote the original version of the model as part of his doctoral thesis (Beven 2012, p. 233 [137]).

recognized in the field of reduced scale models, but was only appreciated from the 1980s onward in hydrological modeling.

3.4.3 Vector Fields

In light of the difficulties in reconciling field observations with adjustments of modeled systems and the increasing computational capacity available through *mainframes*, Freeze & Harlan (1969) inaugurated a new perspective on hydrological modeling, originating what they termed **physically based models**. This form of modeling, like that in Systems Dynamics, is based on the description of processes. The difference, however, is that the processes described by these models are derived *directly* from laws postulated by Physics: the conservation of mass, momentum, and energy. The article by Freeze & Harlan established a "design" of a physically based model that fundamentally differs from Systems Dynamics in its ontological aspects. Unlike the systemic paradigm, which is based on aggregated compartments connected by flows and feedbacks, the physical paradigm consists solely of **velocity vector fields** that act continuously, distributed in three-dimensional space $\mathbb{R}^3$ and modulated by initial and boundary conditions. With this, the authors aimed to provide a superior alternative to systemic models:

> With hydrologic systems models, it is possible to simulate streamflow hydrographs with a high degree of accuracy for a variety of hydrologic and geographic conditions. The Stanford Watershed Model IV (Crawford and Linsley), is the best-known and most successful model of this type. If the model we espouse is to offer promise for the future, it must be able to compete with the systems approach in terms of practical results and utility. A case could then be made for its superiority on the basis that a better understanding of the internal processes and their effects on the overall hydrologic system is desirable and could be beneficial to the solution of practical problems. – Freeze & Harlan (1969, p. 242) [139].

In other words, the authors believed that the solution to avoid the apparent problems in the calibration process of Systems Dynamics models was to apply the laws of Physics (Fluid Mechanics) directly to describe the hydrological cycle in the basins—after all, there was no need to reinvent the wheel. The only hindrance might have been the available computational capacity, although on the other hand, it would not be necessary to calibrate the models through any intensive search method, as the *truly* physical parameters could be defined *a priori*, such as channel roughness or hydraulic conductivity. Another promised advantage was the ability for continuous integration among the parts of the system, such as surface runoff q_{si} and subsurface flow. They pointed out that, although certain processes of the hydrological cycle at the time still lacked physically based studies (such as evaporation processes), unidimensional flow in channels and three-dimensional flow in porous media were already well established by the St. Venant and Darcy-Richards equations, respectively. Variations for different boundary conditions or negligibility premises could be developed, and solutions obtained in new theoretical studies.

A good example of the physically-based approach (and its problematic aspects) is the modeling of flow in porous media, specifically water in soil. In this case, the logic emerges from **Darcy's Law**. This law was experimentally derived by Henry Darcy (1803-1858) using a pipe filled with sand, where he observed that the flow of water in the pipe Q [$\mathrm{L^3T^{-1}}$] is directly proportional to the cross-sectional area of the pipe A [$\mathrm{L^2}$] and to the difference in hydrostatic potential between the inlet and outlet Δz [L] [140]. At the same time, the flow is inversely proportional to the length of the pipe l [L]. To transform these relationships into a dimensionally consistent equation, the **hydraulic conductivity** K $[\mathrm{L\,T^{-1}}]$ is introduced [10]:

$$Q = K\frac{A}{l}\Delta z \tag{3.2}$$

This is an analysis at the **global scale**, that is, evaluating the *aggregated* behavior of the system of the pipe. But then a crucial analytical move is made to migrate to the **local scale**. This is done by *assuming* that it is possible to represent *infinitesimal elements* of the soil, which leads to the definition of the gradient of hydrostatic potential $\nabla\Phi$ $[\mathrm{LL^{-1}}]$:

$$\nabla\Phi = \frac{\Delta z}{l} \tag{3.3}$$

Therefore, from Equation (3.2) it follows that:

$$Q/A = K\nabla\Phi \quad \Rightarrow \quad u = K\nabla\Phi \tag{3.4}$$

Where u $[\mathrm{M\,T^{-2}}]$ is the **Darcy velocity**[11] of the fluid. For a three-dimensional spatial domain $\mathbb{R}^3 = \{x, y, z\}$:

$$u_x = -K\frac{\partial\Phi}{\partial x} \quad u_y = -K\frac{\partial\Phi}{\partial y} \quad u_z = -K\frac{\partial\Phi}{\partial z} \tag{3.5}$$

Which makes the Darcy's Law assume the following differential and vector notation[12]:

$$\mathbf{u} = -K\nabla\Phi \tag{3.6}$$

The maneuver to *collapse* the global scale into a local scale of infinitesimal elements is a typical **idealization** of the Galilean type, where a mathematical representation in a *limit condition* is deduced from the representation of an *observed condition* (see Section 2.2). Galileo used the inclined plane to then idealize the limit condition of the vertical angle for freely falling objects. In the case of flow in porous media, the Darcy's Law for a pipe filled with sand assumes the form of Equation (3.6) in the limit of infinitesimal soil elements. The complete formulation to describe the movement of water in soil, including flows in the vadose zone $\mathbf{V}$, is described by the Richards Equation (or Darcy-Richards). Richards (1931) [141] coupled the Darcy Equation with the mass balance in the local scale (in the assumed infinitesimal elements), producing a system of partial differential equations that need to be solved over time and in three-dimensional space[13].

The innovative modeling proposal made by Freeze & Harlan (1969) was explicitly termed a "project", as it was not readily operational. However, it already pointed to directions for new research in both theoretical and applied fronts so that a fully integrated model could eventually be realized beyond the equations. This process was, in part, led by Freeze himself, in a series of articles where he presents the results of various experimental simulations in the realm of groundwater flow [142]. In a typical

[10] For any fluid and any porous medium, K is defined as: $K = \frac{c}{\mu}$, where c $[\mathrm{M\,T^{-2}}]$ is the permeability of the porous medium, and; μ $[\mathrm{M\,L^{-1}\,T^{-1}}]$ is the viscosity of the fluid.

[11] The **real velocity** of the fluid is higher since the fluid must flow through a relatively smaller section, where there are connected pores.

[12] The negative sign denotes that the direction of velocity is opposite to the gradient of hydrostatic potential.

[13] The Richards Equation can take different notations, but generally it establishes the expansion of hydrostatic potential to include, in addition to gravitational potential Δz, also the capillary potential of water, so that: $\Phi = \Delta z + \psi$. Thus, the hydraulic conductivity of the fluid becomes variable in saturated conditions, even exhibiting hysteresis effects.

demonstration of exploratory modeling, Freeze begins this movement by organizing the theoretical mathematical details (the differential equations) and numerical details (the solution methods) to simulate transient flow in unsaturated porous media within the three-dimensional domain of an idealized slope [143]. The result obtained by Freeze consists of a solution using the **finite difference method**, with a regular **computational grid** that can be applied to any surface geometry of slope and geological subsurface pattern (for example, impermeable beds and different soil horizons). Alternatively, Beven (1977) [144] demonstrated that it is also possible to implement numerical solutions using the **finite element method**, employing an **irregular computational grid**. With a focus on the plan and profile of the simulated variables, virtual experiments with models of this type show in detail the behavior of groundwater in response to spatial patterns of rainfall and water extraction by wells or channels. In subsequent advances, Freeze seeks to engage with the empirical evidence regarding the new flow mechanisms being reported by the scientific community at the end of the 1960s, emphasizing that the physically based model developed naturally produced such phenomena, depending only on the boundary conditions, that is, the geometry of the slope [145], [146]. In this context, the physical theory would indicate that exfiltration q_{ss} would be dominant in convex convergent slopes (incised valleys) while saturation excess would dominate in concave convergent slopes (amphitheater-shaped valleys).

3.4.4 El Dorado

The project envisioned by Freeze & Harlan (1969) was thus realized in various models, some more and some less integrated with the hydrological cycle, including models like `HEC-RAS` (focused on surface runoff) and `MODFLOW` (focused on groundwater) [147]. Among the pioneering and fully integrated models, the model Système Hydrologique Européen (SHE) stands out, developed starting in 1976 through a collaboration between the Danish Hydraulic Institute, the British Hydrology Institute, and the French consulting company SOGREAH. After ten years of development, operational results began to be released, and the structure of the model was published in a series of articles in 1986 [148], [149]. According to its authors, the model was explicitly inspired by the project of Freeze & Harlan (1969), although they implemented a simplified version of the flow in the vadose zone $\mathbf{V}$, with a unidimensional formulation of the Darcy-Richards equation. Despite all the effort allocated and the computational complexity compared to models based on Systems Dynamics, the authors of the model `SHE` readily acknowledge its limitations, especially the scale problem:

> In principle, because the parameter values are based on physical measurements, models such as the SHE should not require calibration. In practice, though, problems such as inadequate representation of the hydrological processes and the possible difference in scale between the measurement and the model grid square mean that some calibration is likely to continue to be required. In a SHE context this is regarded as a selective improvement of initial parameter estimates, by a comparison between observed and simulated hydrological variables, e.g. stream discharges or phreatic surface levels. At present this is carried out on a trial and error basis. – Abbott et al. (1986, p. 53) [148].

This fact clearly breaks the promise made by Freeze & Harlan (1969) that a physically-based model would be free from such nuances, with the definition of parameters made *a priori*, without the need for manual or automated adjustments *a posteriori*.

The practical limitations of the model `SHE` opened a gap for a crisis in hydrological modeling, providing inputs for a theoretical and philosophical discussion on scale and uncertainty issues in the 1990s and 2000s. This crisis was laid bare in the critical essay by Beven (1989) [150], who systematically organizes the problems of physically based models. At this point, Beven points out that, in practice, physically-based modeling applies a **scalability premise**, which is as idealizing as the other simplifications seen in Systems Dynamics, with the advantage that the latter is more intuitive. For example, Beven cites the application of the model `SHE` in a catchment in England that instantiated computational grid elements with a length of 250 meters, as if the physics of velocity fields were applicable at this scale. The variables simulated in a mesh element hundreds of meters long are clearly not commensurable with point empirical evidence. Furthermore, even with relatively small mesh elements (on the scale of centimeters), the models underrepresent the processes that are known to occur *below* this scale. Unlike free flow in channels or in extensive, homogeneous aquifers, which are well represented by velocity fields, empirical evidence about macroporosity in slopes with structured soils brings fundamental incompatibilities with the ontology of physically based models [130], [151]. As emphasized by Hursh & Fletcher (1942), cited above, "A single earthworm tunnel can be much more important in draining a mass of soil than the entire cross-sectional area of the porous space". By instantiating continuous velocity fields, the Darcy-Richards equation simply does not capture the local complexity of the soil's macropore structure (or, equivalently, fractures in a fractured aquifer). From a scientific standpoint, Kirchner (2006) [152] reminds us that elegant differential equations do not guarantee good results for good reasons—this is a role reserved for empirical evidence and hypothesis testing.

With the advent of strong criticisms and discussions, the defense of physically based models took on a pragmatic tone, with a much milder discourse compared to that articulated by Freeze & Harlan (1969). In this vein, Woolhiser (1996) [153] suggests that the development of models that realistically represent hydrological processes directly from physical theory may have been a great illusion of the scientific community, analogous to the search for "El Dorado". On the other hand, Simmons et al. (2020) [147] argue that the central spirit of Freeze & Harlan's project was to promote the *coupling* between the various compartments of the hydrological cycle, such as the atmosphere, soil, subsurface, and rivers—and not to obtain a supposedly true description of reality. Since most of the criticisms revolved around the representation of continuous fields (the ontology) and their philosophical consequences, the essence of the project remains alive and produces important *insights* by integrating various sciences, such as Hydrology, Climatology, and Ecology, into a modeling platform. For this reason, they emphasize that the term "physically-based" leads to a false interpretation of the ultimate purposes, with "integrated models" being a more appropriate designation. An undeniable pragmatic fact that contributes to this direction, brought by Fatichi et al. (2016) [154], is that complex problems often require complex solutions. That is, various practical applications need **distributed models**, which represent hydrological processes in sufficient detail in two- or three-dimensional space to aid in decision-making regarding water resource management, such as flood mapping and land use changes. Moreover, Clark et al. (2017) [155] argue that the philosophical problems of scale and uncertainty, while inevitable, are increasingly assimilated by integrated models, especially with **scaling techniques**, featuring nested parameterizations that can range from the finest mesh element of the local scale, through intermediate scales, to the global scale of the modeling domain.

3.5 Scale

3.5.1 Scaling

The relevance of scale in hydrological modeling took clear shape in the 1990s, particularly following the review by Blöschl & Sivapalan (1995) [156]. These authors present a comprehensive conceptual paper that transforms the scale problem, although inevitable, into something manageable through a structured approach. The starting point of their analysis is the science-management duality, that is, the distinction between **predictive models**, used to solve specific practical issues, and **exploratory models**, aimed at formalizing and articulating theories about the system hydrological. The practical problems of water resource management, the main targets of the application of hydrological models, vary substantially in terms of temporal scale, from hours, for flood alerts, to decades, for the impacts of land use changes. In this context, challenges related to scale in modeling arise when models are configured to operate predictively, with their parameters conditioned by empirical observations under specific time and space conditions, and then applied to produce predictions in different situations. A classic example already mentioned is the difficulty Horton faced when using point measurements of infiltration capacity to make predictions at the watershed scale in La Grange Brooke [82]. This difference in conditions necessitates an information transfer between scales, or **scaling**, which is often non-trivial, as highlighted in the discussion about physically based models. Thus, the concept of scale is defined by the attributes of time and space, which can be summarized as a **characteristic velocity**. The scale problem, therefore, presents itself as a problem of scaling, that is, in the difficulty of transferring information between different velocities.

Blöschl & Sivapalan (1995) also advance to establish the crucial notion that there are three scales to be understood and reconciled in a modeling exercise: the **natural scale**, the **observational scale**, and the **conceptual scale** (Figure 3.9). The natural scale refers to the actual characteristic velocity exhibited by hydrological processes. It can be classified in different ways: as the lifespan of intermittent **events**, such as rises; by the **period** of annual events, such as snowmelt or the arrival of wet seasons; or by the duration of **trends** in long-duration stochastic processes, which exhibit some degree of autocorrelation, such as the depletion or filling of aquifers (Figure 3.9**a**). The authors also expand this idea to spatial scales, defined by extent and trends in space, depending on the nature of the process. Some processes, like precipitation, do not have a preferred scale, as they distribute across multiple scales due to the nesting of subprocesses of both small and large scales, often with **spectral gaps** between them, that is, intervals where certain scales are less frequent. River runoff also follows this nested process structure, with flood peaks resulting from overlapping rapid response mechanisms and slower response mechanisms, such as groundwater or the occupation of large floodplains. Even rapid responses occur at different nested scales, such as flash rises from small soil plots and the formation of riparian wetlands or ephemeral springs, manifesting at the slope scale. The observational scale, in turn, consists of the scale occupied by empirical evidence, arising from the need to manage a finite number of samples. It has three main aspects: the **extent** or coverage of the dataset, the **resolution** or spacing between samples, and the interval of **integration** of the sample (Figure 3.9**b**). If sampling were infinite (or infinitesimal), the observational scale would coincide with the natural scale, capturing even the sample noise. In contrast, a very sparse sampling captures only the trend of the process, at best. A typical example of this is a rain gauge that, when read daily, reports the accumulated rainfall over a one-day interval, which may be much larger than the natural duration of a rain that occurred for only a few minutes. Nevertheless, this reading captures the trend of rainfall

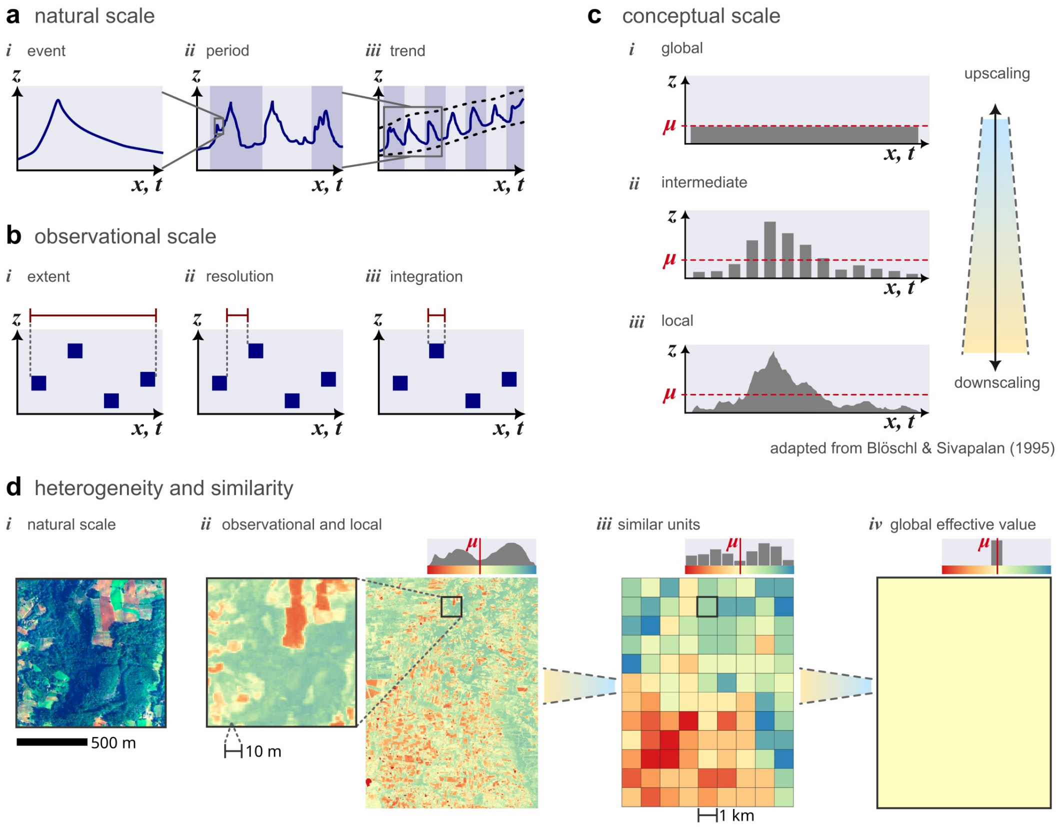

Figure 3.9 — Schematic representation of different scales. Organized system by Blöschl & Sivapalan (1995) [156] on the scales to be reconciled in time and space. **a** — The natural scale of processes varies in: (i) event scale; (ii) period scale, and; (iii) trend scale. **b** — The observational scale presents three aspects: (i) extent; (ii) resolution, and; (iii) integration. **c** — The conceptual scale mediates between the natural scale and observational through scaling methods. The model operates at nested scales: (i) global scale; (ii) intermediate scales, and; (iii) local scale. **d** — Effective values across scales: natural scale, where processes occur (i); the observational scale establishes the lower limit of the local conceptual scale (ii); intermediate scale of similar units (iii), and; effective process value at the global scale (iv).

on a weekly or monthly scale. On the other hand, detailed soil samples can provide information about extremely localized hydraulic conductivity, which does not reflect the actual effect of macropores and preferential pathways at the slope scale. In this case, the process scale is broader, making point samples incomparable. Ideally, observations should be compatible with the scale of the processes of interest, positioning the sampling at an optimal point between the noise range and the trend range.

The natural scale and the observational scale relate in hydrological modeling by being mediated by the conceptual scale, which is the scale of representation of the model itself (Figure 3.9**c**). Here lies the challenge of scaling, as the conceptual scale is often much larger or much smaller than the observational scale, introducing the inevitable commensurability error ε_{Δ}. As previously discussed, both the soil reservoir instantiated by Systems Dynamics and an element of computational grid in a physically-based model represent massive blocks that are incomparable with any point observation obtained in the field. Still, this error can be minimized by representing the target system simultaneously at scales close to the available observations. In practice, this means dividing the model into at least two nested levels: a more aggregated **global scale** and a more detailed **local scale**. Intermediate scales can also be incrementally instantiated, depending on the simulated hydrological processes and the available observations. At the global scale, for example, the highly aggregated processes of the watershed are represented, such as river flow at a river section and the final flow of evapotranspiration, accumulated results of various subprocesses at smaller scales. At the local scale, the details of these subprocesses are represented in small plots or mesh elements, such as rainfall input and runoff generation in different parts of the landscape. In this sense, the storage and flow variables, the parameters, and the input data need to be compatible at all levels, necessitating the transfer of information from one level to another, that is, they need to be scaled.

The solution to this situation, therefore, consists of defining a **scaling function** that is valid between the simulated levels. These functions perform both **upscaling**[14] of information (bottom-up transfer) and **downscaling**[15] of information (top-down transfer). For material levels and flows, which are conserved, the upscaling function can simply be the average or the sum over a given spatial or temporal extent. The global evapotranspiration flow of a watershed, therefore, would be the average of local flows (the integral). The downscaling, on the other hand, generally consists of a non-trivial process that strongly depends on the process in question. In the case of soil and rock properties, such as hydraulic conductivity, the only way to unpack this information is through maps that reveal its pattern or **spatial heterogeneity**. The same mapping strategy applies to parameters related to vegetation or land cover, such as interception capacity $c_{\max}$ and surface detention capacity $s_{\max}$. In the absence of direct information, the use of **co-variables** or indicators can be employed with a downscaling function, or **distribution function**, which adds new auxiliary hypotheses to the theoretical framework of the model. For example, Collischonn et *al.* (2007) [157] assume the hypothesis that the local interception capacity $c_{\max}$ is directly proportional to the Leaf Area Index (LAI), that is: $c_{\max,i} = c \cdot \mathtt{LAI}_i$, where c is a proportionality constant. On the other hand, co-variables can be applied to *group* spatial regions that theoretically exhibit **hydrological similarity**, that is, regions that are sufficiently homogeneous with respect to a given process at the assessed scale. In this context, the co-variable is referred to as the **hydrological similarity index**. The homogeneous regions resulting from this grouping, referred to as **hydrological response units**, significantly reduce computational cost as they execute block processing, as opposed to the mesh processing required at the local scale. Thus, models that apply this approach in downscaling are regarded as **semi-distributed models**, as they do not represent the local scale completely explicitly; the information is still compacted at the intermediate scale of the hydrological response units. Finally, another challenge at the local scale consists of the **regionalization** of values located at points or patches to their lateral neighborhoods, at the same scale, as in the case of point rainfall observations that are interpolated to represent a continuous field in space. Just like in the case of distribution function of parameters, this interpolation process introduces new auxiliary hypotheses (and their uncertainties) into the modeling process.

3.5.2 `TOPMODEL`

An example of scaling that is worth presenting at this moment is the model `TOPMODEL`, initially articulated by Beven & Kirkby (1979) in a study of the Crimple Beck basin (England, 8 km^2) [158]. This model, instantiated in the paradigm of Systems Dynamics, despite exhibiting a relatively simple compartment structure, effectively represents the mechanism of variable source area, producing rapid hydrological responses both through flash rises and through saturation excess in wet areas. During the simulation, the model explicitly represents the expansion and contraction of riparian wetlands along the terrain's thalweg as the watershed receives more or less rain. The flow of effective rainfall p_s that directly impacts the saturated areas eventually becomes part of the rapid

[14] Translation of *upscaling* in English.
[15] Translation of *downscaling* in English.

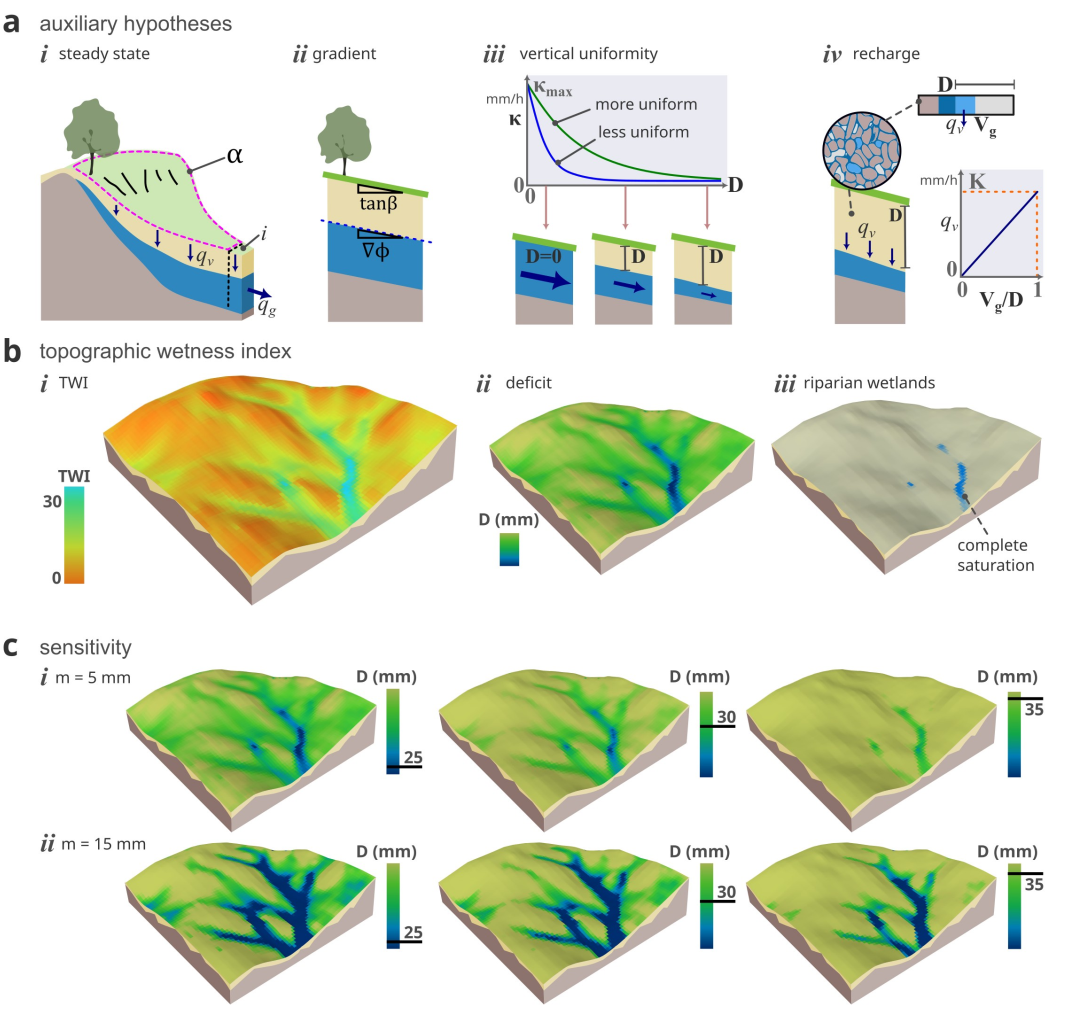

Figure 3.10 — Hypotheses and implications of `TOPMODEL`. The `TOPMODEL` is a model that performs downscaling of soil saturation from a topographic wetness index, the Topographic Wetness Index (`TWI`). **a** — The classic version of the `TWI` in the model is obtained by applying Darcy's Law with three auxiliary hypotheses: the hypothesis of steady-state (detail i); the hypothesis of shallow soils (detail ii), and; the hypothesis of vertical decay of transmissivity (detail iii). A fourth auxiliary hypothesis is the flow of recharge q_v as a linear function of the pressure in the vadose zone **V** (detail iv). **b** — The application of the scaling function of the model uses the distribution of the `TWI` (detail i) to determine the gravitational deficit **D** and the riparian wetlands at the local scale (detail ii and iii). **c** — The details i and ii compare the sensitivity of local deficit distribution for more or less uniform soils (parameter m). A basin with more uniform soil (m high) exhibits a more dispersed deficit distribution than a basin with less uniform soil (m low).

response of flood events, while the remaining portion of effective rainfall p_s falls on dry soil and can then infiltrate.

Unlike the high computational cost of physically based models, which need to numerically solve the Darcy-Richards Equation on a computational grid, the `TOPMODEL` approach identifies the spatial pattern of soil saturation at the local scale through a low-cost computational downscaling function (distribution). In the presence of empirical evidence solely from rainfall and discharge, both approaches are empirically equivalent, with the advantage that `TOPMODEL` is simpler (i.e., it has a greater degree of falsifiability). In this sense, the use of a physically-based model becomes justified only when more detailed evidence becomes available, such as piezometric levels, bedrock topography, and water quality parameters[16].

Soil saturation in `TOPMODEL` is expressed by the gravitational deficit $\mathbf{D}$ at the

[16] For detailed mappings of contamination plume evolution in the subsurface, for example, a physically-based model is the only alternative that offers the ontology compatible with the problem at hand.

local scale in the watershed, denoted by D_i [L], where i is any element of a mesh that divides the basin into N elements. That is, when $D_i = 0$, the soil is completely saturated in element i, and the water from the effective rainfall p_s that falls on this element cannot infiltrate, remaining accumulated on the surface until it reaches the surface detention capacity s_{max}. The compaction function of this variable transfers information across scales through the simple calculation of the average:

$$D = \frac{1}{N}\sum_{i}^{N} D_i \quad \forall\, i \in \{1, 2, ..., N\} \tag{3.7}$$

Where D [L] is the global deficit and; D_i [L] is the local deficit. Thus, the gravitational deficit $\mathbf{D}$ at the global scale consists of the average of the deficits at the local scale D_i. The distribution of gravitational deficit from global scale to local scale, on the other hand, is based on the use of a **saturation index**. This index is thus considered a *co-variable* of the gravitational deficit, such that the *deviations from the mean* between the local scale and global are linearly proportional:

$$D - D_i \propto \lambda_i - \lambda \quad \forall\, i \tag{3.8}$$

Where λ_i [$-$] is the saturation index at the local scale, and; λ [$-$] is the saturation index at the global scale, that is, the average obtained by:

$$\lambda = \frac{1}{N}\sum_{i}^{N} \lambda_i \quad \forall\, i \tag{3.9}$$

The Equation (3.8) becomes an equality when a proportionality constant is introduced:

$$D - D_i = \omega(\lambda_i - \lambda) \quad \forall\, i \tag{3.10}$$

Where ω [L] is the scaling factor. By rearranging the terms, the local gravitational deficit D_i is obtained through the following distribution function:

$$D_i = D + \omega(\lambda - \lambda_i) \quad \forall\, i \tag{3.11}$$

Where D_i must be truncated at zero, so as not to take negative values. In a hydrological model, Equation (3.11) aims to locally distribute the global deficit D at each time step, allowing other variables at the local scale to be specified, such as recharge q_v and surface runoff. In this case, the elements i where $D_i = 0$ correspond precisely to saturated soil areas, the variable source area that will invariably produce rapid runoff responses in the face of rainfall events.

Here, it is worth noting that Equation (3.11) is a generically applicable formulation for any saturation index λ_i. However, Beven & Kirkby (1979) originally deduced it theoretically from Darcy's Law and some auxiliary hypotheses (see Figure 3.10**a**), resulting in the saturation index λ_i then referred to as **Topographic Wetness Index (**`TWI`**)**, which is calculated by:

$$\mathrm{T}_i = \ln\left(\alpha_i / \tan\beta_i\right) \quad \forall\, i \tag{3.12}$$

Where α_i [$L^2 L^{-1}$] is the local drainage area per unit of contour, and; β_i[$-$] is the local slope of the terrain. That is, the local potential for soil saturation (1) is greater the larger the drainage area, and (2) is greater the smaller the slope of the terrain. Maps of `TWI` can thus be obtained directly from a **digital elevation model (**`DEM`**)** using geoprocessing techniques. The local slope β_i, for example, can be estimated using Horn's method (1981) [159] by computing the altitude differences in the west-east and north-south directions in the **mantissa**[17] of the mesh element. On the other hand, determining the local drainage area per unit of contour α_i requires a more computationally intensive analysis, as it is necessary to trace all upstream mesh elements for each given element. This cannot occur before removing spurious depressions in the `MDE`, which cause the method to truncate. Barnes et *al.* (2014) [160] introduce an efficient algorithm for this process, as well as review various other strategies available in the literature. Once a depression-free `MDE` is obtained, the drainage area is computed using flow accumulation methods, such as the unidirectional flow method by O'Callaghan & Mark (1984) [161] or the multidirectional flow method by Freeman (1991) [162]. Quinn et *al.* (1991) [163] demonstrate that there is substantial sensitivity in `TOPMODEL` regarding the choice of flow accumulation method, suggesting that the multidirectional method presents better empirical adequacy. Additionally, the authors also evaluate the possibility of *overlapping* methods to adjust the `TWI` between ephemeral (multidirectional) and perennial (unidirectional) drainage regions.

There are three auxiliary hypotheses that theoretically underpin Equation (3.12). The first is the hypothesis of steady-state (detail i in Figure 3.10**a**), which establishes that a local steady-state condition is achieved at each time step, such that the lateral base flow equals the recharge flow:

$$q_{\mathrm{g},i} = q_{\mathrm{v}} \cdot \alpha_i \quad \forall i \tag{3.13}$$

Where $q_{\mathrm{g},i}$ $[L^2T^{-1}]$ is the lateral base flow per unit of contour; q_{v} $[LT^{-1}]$ is the recharge flow, and; α_i $[L^2L^{-1}]$ is the local drainage area per unit of contour. The second auxiliary hypothesis (detail ii in Figure 3.10**a**) assumes that the soil is shallow enough for the local hydraulic gradient in the water table $\nabla\Phi_i$ $[LL^{-1}]$ to be approximated by the local slope of the terrain $\tan\beta_i$ $[LL^{-1}]$:

$$\nabla\Phi_i = \tan\beta_i \quad \forall i \tag{3.14}$$

The third auxiliary hypothesis (detail iii in Figure 3.10**a**) is that local hydraulic conductivity K_i $[LT^{-1}]$ decays exponentially with gravitational deficit, meaning that the drier the soil, the lower the hydraulic conductivity. This is a hypothesis consistent with empirical observations that the upper soil horizons, with organic layers and macropores, exhibit higher conductivity than the lower, more mineral parts. The hydraulic conductivity per unit of contour is expressed as **hydraulic transmissivity**, leading to the hypothesis taking the following form:

$$\kappa_i = \kappa_{\max} \cdot e^{-D_i/m} \quad \forall i \tag{3.15}$$

Where κ_i $[L^2T^{-1}]$ is the local transmissivity; $\kappa_{\max}$ $[L^2T^{-1}]$ is the maximum transmissivity under saturated conditions; D_i $[L]$ is the local deficit, and; m $[L]$ is the constant of **vertical uniformity of the soil**. The larger the value of m, the more gradual the change in transmissivity as a function of saturation, such that: $\lim_{m\to\infty} T = T_{\max}$. Considering the flows per unit of contour of the terrain, Darcy's Equation (3.6) takes the following structure:

$$u = K\nabla\Phi \Rightarrow q_{\mathrm{g,i}} = \kappa_{\max}\nabla\Phi_i \quad \forall i \tag{3.16}$$

Where the Darcy velocity u $[LT^{-1}]$ corresponds to the lateral base flow per unit of contour $q_{\mathrm{g},i}$ $[L^2T^{-1}]$. Connecting Equations (3.13), (3.14), and (3.15) in Darcy's Equation (3.16):

$$q_{\mathrm{v}}\alpha_i = \kappa_{\max} e^{-D_i/m} \tan\beta \quad \forall i \tag{3.17}$$

[17] In a rectangular mesh of elements, the mantissa consists of the eight neighboring elements surrounding any given element.

The local deficit D_i can be isolated, yielding:

$$D_i = -m \ln \left(q_{\mathrm{v}} \alpha_i / \kappa_{\max} \tan \beta_i \right) \quad \forall i \tag{3.18}$$

By logarithmic properties, the following relationship is also obtained, isolating the terms of static hydrological variables from dynamic hydrological variables and purely topographic terms:

$$\ln(q_{\mathrm{v}}/\kappa_{\max}) = -D_i/m - \ln(\alpha_i / \tan \beta_i) \quad \forall i \tag{3.19}$$

Now, considering that the global deficit D is the average of the local deficits D_i, Equation (3.18) can be applied in Equation (3.7):

$$D = \frac{1}{N} \sum_i^N -m \ln \left(q_{\mathrm{v}} \alpha_i / \kappa_{\max} \tan \beta_i \right) \quad \forall\, i \tag{3.20}$$

Using summation properties and assuming m and $\kappa_{\max}$ are spatially homogeneous, local terms can be isolated from global terms:

$$D = \left[-m \frac{1}{N} \sum_i^N \ln \left(\alpha_i / \tan \beta_i \right) \right] - \left[m \ln \left(q_{\mathrm{v}} / \kappa_{\max} \right) \right] \quad \forall\, i \tag{3.21}$$

Substituting (3.19) into (3.21), we arrive at:

$$D = \left[-m \frac{1}{N} \sum_i^N \ln \left(\alpha_i / \tan \beta_i \right) \right] + D_i + m \ln \left(\alpha_i / \tan \beta_i \right) \quad \forall\, i \tag{3.22}$$

Which is homologous to Equation (3.10), with $\lambda_i = \mathrm{T}_i$ and $\omega = m$:

$$D_i = D + m \left[\left(\frac{1}{N} \sum_i^N \mathrm{T}_i \right) - \mathrm{T}_i \right] \quad \forall\, i \tag{3.23}$$

In total, the version of `TOPMODEL` articulated by Beven & Kirkby (1979) includes seven parameters regulating reservoirs and flows of the water balance in the soil, as well as a flow velocity parameter used in simulating the propagation of flow in the drainage network of channels. In particular, the parameters m and $Q_{\mathrm{g,max}}$ can be estimated *a priori* from the recession curve of the river during observed recessions in cold weather (with low water loss due to evapotranspiration), as the integration of Equation (3.15) over all lateral stretches of channels determines the base flow:

$$Q_{\mathrm{g},t} = Q_{\mathrm{g,max}} \cdot e^{-D_t/m} \quad \forall\, t \tag{3.24}$$

Where Q_{g} $[L^3T^{-1}]$ is the base flow; $Q_{\mathrm{g,max}}$ $[L^3T^{-1}]$ is the production capacity of the aquifer; D_t [L] is the global deficit at time t, and; m $[L]$ is the vertical uniformity of the soil. The details in Figure 3.10**b** demonstrate how sensitive the model is to changes in the vertical uniformity of the soil. The distribution of local deficit, in this regard, becomes increasingly more dispersed as the value of m increases. This occurs evidently because it acts as a multiplier in the scaling function (Equation (3.11)). The practical implication is that a basin with relatively more uniform soil will produce relatively more riparian wetlands. The physical interpretation of this implication is that, keeping the same production capacity of the aquifer $Q_{\mathrm{g,max}}$, a more uniform soil transmits more water, draining the higher slopes more quickly as the global deficit of the basin increases.

The hydraulic conductivity K of the soil is employed in `TOPMODEL` in a revision of the model presented by Beven & Wood (1983) [164], under a fourth auxiliary hypotheses concerning the flow of recharge q_{v} (detail *iv* in Figure 3.10**a**). In this case, the authors assume that the vertical flow of recharge q_{v} at the local scale tends linearly toward the value of hydraulic conductivity K as the vadose zone $\mathbf{V}$ becomes pressurized by hydraulic load[18]:

$$q_{\mathrm{v},i} = K \cdot \frac{V_{\mathrm{g},i}}{D_i} \quad \forall\, i \tag{3.25}$$

Where $q_{\mathrm{v},i}$ $[LT^{-1}]$ is the local recharge; K $[LT^{-1}]$ is the hydraulic conductivity of the soil; $V_{\mathrm{g},i}$ $[L]$ is the local gravitational water in the vadose zone $\mathbf{V}$, and; D_i [L] is the local deficit. That is, the pressurization in the vadose zone $\mathbf{V}$ is represented by the ratio of gravitational water to the saturation deficit, which can also be interpreted as the *capacity* for storing gravitational water in the vadose zone $\mathbf{V}$. Thus, as the gravitational water in the vadose zone $\mathbf{V}$ is constrained by the deficit, the ratio $V_{\mathrm{g},i}/D_i$ tends to 1 when the deficit approaches zero, or $\lim_{D_i \to 0} q_v = K$.

The classic version of `TOPMODEL` is essentially summarized by the concepts and equations organized above, with its main hypothesis being the downscaling function represented by Equation (3.11). Its fundamental hallmark, therefore, is to represent rises produced both by overland runoff and by saturation excess, which is accomplished with simulated maps of riparian wetlands obtained from a topographic indicator (in this case, the `TWI`). On the other hand, the other flow equations, such as the evapotranspiration flow in each reservoir of the system and hydraulic propagation downstream, are couplings to the basic model that can be modified or not. Authors like Ambroise et *al.* (1996) [165] and Iorgulescu & Musy (1997) [166] have indeed implemented generalizations in the auxiliary hypotheses, deriving generic formulations to calculate the topographic wetness index. In the same vein, Beven & Freer (2001) [167] produced a more complex version of the model, called Dynamic `TOPMODEL`, where the local drainage area α_i is replaced by the local recharge area $\alpha_{v,i}$, which needs to be updated at each time step of the simulation (a procedure that makes this version computationally more intensive).

Besides the capacity for modifications, Beven [137] suggests that the classic version can be instantiated as a semi-distributed model, aggregating the mean of the saturation index into discrete ranges of its histogram in hydrological response units. That is, in small incremental ranges of the index, it is assumed that the mesh elements exhibit hydrological similarity. This way, relatively broad regions of elements in space are scaled to a relatively small number of homogeneous blocks, drastically reducing the computational cost of simulating the model. More detailed maps at the local scale can thus be recovered after processing—one just needs to use the source map of the saturation index to position the simulated processes in their respective mesh elements. Although it is a practically oriented strategy related to the procedural model, using a semi-distributed model has implications for the simulated results. For instance, mesh processing in a fully distributed approach allows for the representation of spatial and temporal spatial heterogeneity of other flows and parameters (such as rainfall distribution, for example), which is not possible in a semi-distributed approach. Since the intensive use of simulations in diagnostic techniques requires that the simulation time of the models not be a critical bottleneck (see Section 2.6), these issues must be weighed to arrive at an appropriate strategy for addressing the dimensionality problem.

[18] In fact, the authors introduced a peculiar term of *delay per unit deficit* t_d $[TL^{-1}]$, causing the recharge equation to take the following form: $q_v = V_g/t_d D$. Although identical, this notation does not make much hydrological sense, especially considering that hydraulic conductivity is a well-established concept. In observance of John Sterman's modeling principles (Chapter 2), I maintained a clearer notation.

3.5.3 PLANS

The model PLANS is a version of TOPMODEL that exhibits strategies for both the generalization of the saturation index and semi-distributed modeling. Illustrated in Figure 3.11, the model was developed by myself and colleagues with the explicit purpose of establishing a tool to assist in the formulation of evidence-based policies in the context of expanding Nature-based solutions (NBS)[19] in watersheds in Brazil [168], [169]. The term "Nature-based solutions" serves as a conceptual umbrella for a collection of techniques and approaches at different scales that draw inspiration from or utilize natural processes. We will see later, in the next chapter, that this public policy movement can benefit from the use of modeling within a framework of basic principles. The first version of the model PLANS was a somewhat more complex model than the prototype presented in the previous chapter. This initial version was used in an exploratory modeling study that applied search techniques to optimally allocate the expansion of NBS over time under future scenarios [168]. On one hand, the application of the model successfully highlighted nuances and stimulated revisions of mental models. In this case, the model found that the expansion of the listed NBS yields scaling benefits in relatively more degraded watersheds—the incremental performance in more preserved areas likely does not justify the investment. On the other hand, the highly aggregated nature of this initial version did not allow for an exact assessment of *where* the expansion of NBS should occur, causing the model to fail in addressing the spatial allocation problem. This shortcoming forced me to abandon the initial structure and instead instantiate a version of TOPMODEL tailored to address the issue of expanding NBS both in time and space [169].

In the model PLANS, as in TOPMODEL, the local distribution of water deficit in the soil is done through the downscaling function defined in Equation 3.11, using a topographic wetness index λ_i as a co-variable. However, unlike TOPMODEL, the only hypothesis fundamentally defended by the model in this aspect is the linear relationship that the scaling function implies, which allows testing other topographic indices beyond the TWI (Figure 3.11**b**). This relaxation of the hypotheses of the classic model was primarily motivated by the practical need to address the problem of expanding NBS in Brazil, a country with a wide heterogeneity of soils and landscapes, including tropical soils that are much deeper than those observed in temperate or subtropical climates. Another motivation, of a conceptual nature, is grounded in the empirical observations presented by Crave & Gascuel-Odoux (1997) [170] regarding the distribution of saturated areas in a small watershed in France (1.3 km^2), with soils varying from 40 cm to 2 meters in depth. In the study, the authors report a weak correlation between local soil saturation and the TWI, as well as the relative immobility of the saturation patch at the valley bottom, largely refuting the underlying theory of TOPMODEL. On the other hand, they show that the soil saturation at sampled points i has an inverse relationship with the *altitude difference* $\Delta Z_{i,o}$, or height $\mathrm{H}_{i,o}$, relative to the nearest water outcrop o. This inverse relationship holds up to a certain height threshold $\mathrm{H}_{\max}$, beyond which saturation exhibits a relatively uniform range of values. Given these observations, the authors suggest that in basins with relatively deep and well-drained soils, the landscape divides into two parts: the drier headwater region and the wetter riparian region (Figure 3.11**b**, detail i). Keeping other variables constant, the separation between these two regions is reasonably delineated by the height threshold $\mathrm{H}_{\max}$ above the valley bottom.

This same topographic wetness index, referred to as **Height Above Nearest**

[19]The acronym PLANS stands for *Planning Nature-based Solutions*, meaning "Planning Nature-Based Solutions". The overarching goal of the initiative is to establish a toolkit of concepts and tools to address the challenges of expanding NBS. The model presented here might be designated as the hydrological module of the PLANS project.

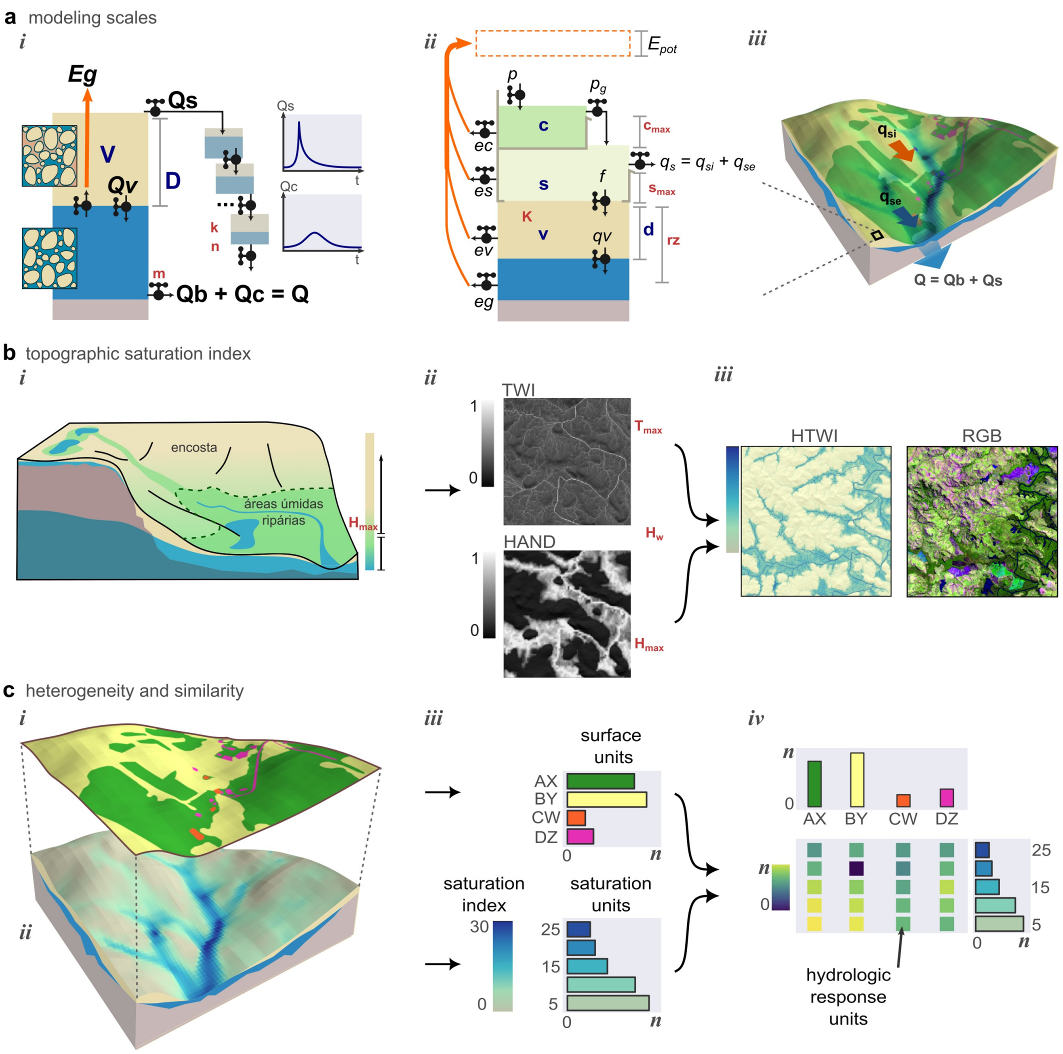

Figure 3.11 — **The model** `PLANS`. The model is a tailored version of `TOPMODEL` designed to address the problem of expanding Nature-Based Solutions. **a** — Modeling scales of the model: global scale (detail *i*); hydrological response units scale (detail *ii*), and; local scale, at the mesh element (detail *iii*). **b** — Topographic wetness index HTWI. The saturation index is based on the hypothesis of dual separation between slope areas and riparian areas (detail *i*). The TWI and HAND indices are normalized by fuzzy logic (detail *ii*). A weighting between the indices generates the HTWI (detail *iii*). **c** — Heterogeneity and spatial similarity: the surface layer of static variables is separated from the subsurface layer of dynamic variables (details *i* and *ii*); the variables at the local scale are grouped into surface units and saturation units (detail *iii*); a two-dimensional histogram, or frequency matrix, is computed to store the hydrological response units (detail *iv*).

Drainage (`HAND`)[20], was articulated ten years later by Rennó et *al.* (2008) [171], who demonstrated its effectiveness in mapping wet areas in the Amazon. However, the differentiating factor of the study by Rennó et *al.* (2008) is that the authors organized the computational method to obtain the `HAND` by applying geoprocessing techniques to `MDE`. In general terms, the technique involves initially establishing a map of the drainage network, which can be done using a drainage initiation threshold H_α [L^2], representing the minimum area for water to outcrop in the soil. Thus, for each mesh element o in the drainage network, their respective altitudes $Z_{o,i}$ and drainage areas (basins) are obtained. Finally, the local `HAND` H_i in each basin area is calculated by the difference between the local altitude Z_i and the altitude of the nearest drainage $Z_{o,i}$. The result is, therefore, a normalized Digital Elevation Model such that the zero altitude is always the level of the nearest river, stream, or valley bottom. The derivation of `HAND` through geoprocessing has led to new applications, such as mapping flood risk of major rivers,

[20]The acronym HAND stands for "Height Above the Nearest Drainage".

since the higher one is above a river channel, the greater the safety [172]. It becomes evident, however, that the value of `HAND` is highly sensitive to the initially established drainage map or area threshold H_α, making applications for mapping floods of major rivers (macro-drainage) very different from mapping soil saturation (micro-drainage).

Thus, the approach adopted in the model `PLANS` encourages that the topographic wetness index λ_i be obtained through fuzzy logic combinations between the `TWI` and the `HAND`, resulting in the index termed *HAND-enhanced TWI*, or the `TWI` enhanced by the `HAND` (`HTWI`), illustrated in detail *iii* of Figure 3.11**b**. This approach was actually suggested tangentially by Quinn et *al.* (1991) [163] to differentiate between ephemeral and perennial drainage regions, but concerning different flow accumulation methods. The proposed index, in this line, retains the characteristic of the `TWI` in increasing the saturation of the landscape from upstream to downstream, but makes this effect relatively more pronounced near the riparian wetlands than on drier slopes. The map is initially calculated by the fuzzy normalization of both variables, requiring the establishment of upper thresholds for each (Figure 3.11**b**, detail *ii*). For the `TWI`, the normalization is ascending:

$$\tilde{\mathrm{T}}_i = \mathtt{MIN}(\mathrm{T}_i/\mathrm{T}_{\max},\ 1) \quad \forall\, i \tag{3.26}$$

Where T_i $[-]$ is the local `TWI`; $\mathrm{T}_{\max}$ $[-]$ is the upper threshold of the `TWI`, and; $\tilde{\mathrm{T}}_i \in \{0,1\}$ $[-]$ is the normalized local `TWI`. In the case of the `HAND`, the normalization is descending:

$$\tilde{\mathrm{H}}_i = \mathtt{MAX}(1 - \mathrm{H}_i/\mathrm{H}_{\max},\ 0) \quad \forall\, i \tag{3.27}$$

Where H_i $[-]$ is the local `HAND`; $\mathrm{H}_{\max}$ $[-]$ is the upper threshold of the `HAND`, and; $\tilde{\mathrm{H}}_i \in \{0,1\}$ $[-]$ is the normalized local `HAND`. Thus, the `HTWI` is determined by the weighted average between these normalized variables and scaled back to the original range of the `TWI`:

$$\mathrm{HT}_i = \mathrm{T}_{\max}\frac{\tilde{\mathrm{T}}_i + H_w\tilde{\mathrm{H}}_i}{1 + H_w} \quad \forall\, i \tag{3.28}$$

Where $\mathrm{HT}_i \in \{0, \mathrm{T}_{\max}\}$ $[-]$ is the `HTWI`, and; H_w $[-]$ is a positive dimensionless factor or weight reflecting the dominance of the `HAND` over the `TWI`. The theory embedded in the derivation of `HTWI` is that there exists a spectrum of hydrological landscapes that extends from the total prevalence of shallow soils and dynamic saturated areas (total dominance of `TWI` over `HAND`) to the total prevalence of deep soils and static saturated areas (total dominance of `HAND` over `TWI`), with intermediate alternatives between these extreme situations. The dominance of one over the other is regulated by the weight H_w, while the mobility of saturated areas is regulated by the thresholds $\mathrm{T}_{\max}$ and $\mathrm{H}_{\max}$. In the special case where $H_w = 0$, the `HTWI` is identical to the `TWI` truncated at $\mathrm{T}_{\max}$. This generalized topographic wetness index, adjustable for any landscape, introduces three additional parameters into the model[21], an epistemological cost that the authors deemed acceptable given the practical need to model hydrological processes in the diverse environments of Brazil. One way to reduce uncertainties in the subsequent distribution of parameters might be to pre-condition the *prior* distribution with other spatial variables obtained from remote sensing, such as moisture indices, surface temperature, or simply shortwave infrared reflectance, as illustrated in Figure 3.6**a**.

Another difference of the model `PLANS` compared to `TOPMODEL` is the representation of surface heterogeneity (Figure 3.11**c**). The classic version of `TOPMODEL` was developed assuming that the surface is homogeneous, which makes sense in the Crimple Beck watershed in England, a rural area dominated by pastures for livestock. However,

[21] In fact, when considering the drainage area threshold H_α for defining the `HAND`, there are four additional parameters.

a model designed to address the problem of expanding Nature-Based Solutions must not only represent the soil and its cover in heterogeneous situations but also enable the simulation of alternative cover scenarios to assess the positive or negative impact of a given expansion policy. For instance, the model should be able to inform whether there is a difference in the behavior of the hydrological system between reforestation in different parts of the landscape. This requirement is recognized by Gao et *al.* (2015) [173], which motivated them to implement a distributed version of `TOPMODEL` to evaluate hydrological impacts of land use and cover change. The model `PLANS`, on the other hand, utilizes a semi-distributed approach, collapsing the local scale into an intermediate hydrological response units scale (Figure 3.11**a**, detail *ii*). This process is accomplished through the cross-tabulation of surface units (similar patches of soil and vegetation) with saturation units (regular intervals of the topographic wetness index)[22] (Figure 3.11**c**, details *i*, *ii*, and *iii*). This tabulation ultimately results in a two-dimensional histogram, or **frequency matrix**, which specifies the area prevalence of each hydrological response unit in the spatial region of interest[23]. As illustrated in detail *iv* of Figure 3.11**c**, the columns represent the histogram of the saturation index in each surface unit. The rows of the matrix, on the other hand, are similar in terms of saturation, which readily facilitates the determination of local deficit through the downscaling function of the model.

3.6 Connectivity

In this chapter, I organized the current twists in Hydrology since the International Hydrological Decade, that is, from the 1960s onward. On one hand, in the experimental front, the Infiltration Age faced its ultimate crisis with the rise of a new paradigm that reaffirms the differentiation and uniqueness of hydrological response mechanisms as functions of climate, topography, soils, vegetation, etc. On the other hand, in the realm of modeling, the advent of digital computers paved the way for ontologically diverse methods, such as Systems Dynamics, vector fields, and statistical models, with the first two based on the theoretical description of processes and the last solely based on empirically obtained data.

As new scientific paradigms do not establish themselves by being perfect, but by being better than the competition, both approaches that have settled in the field are not free from problems. In the case of experimental research, the paradigm of differentiation encountered empirical paradoxes involving the rapid mobilization of old water and the diversity of geochemical signatures, which are difficult to explain by the mechanisms articulated by Dunne's systematization (1983) [81]. Furthermore, the experimental research program is essentially a catalog of the hydrological response mechanisms of each unique watershed. Even though the catalog can be detailed and endlessly expanded, this operational mode does not contribute to a unifying scientific theory [60]. In the case of modeling, crises have affected the various approaches, giving rise to two main inescapable epistemological problems in hydrological modeling: the equifinality problem and the scale problem [175]. Although different, these problems are interconnected, resulting in inexorable epistemic uncertainties that hang over model results. The im-

[22] Although the soil and vegetation maps are maintained as input data for the model, it is important to note that these maps are also the result of a scaling process of other local variables. For example, the vegetation and land use classes provided in the annual maps published by Souza et *al.* (2020) [174], used in the model `PLANS`, were derived from groupings of spectral reflectance and band indices from orbital scene data using machine learning.

[23] The propagation of flow to a given river section, therefore, must be conducted by specifying the prevalence of each response unit in the area of interest basin, which may or may not approximate the prevalence of the total region. This approach, thus, allows for evaluating the final flow in multiple basins of interest.

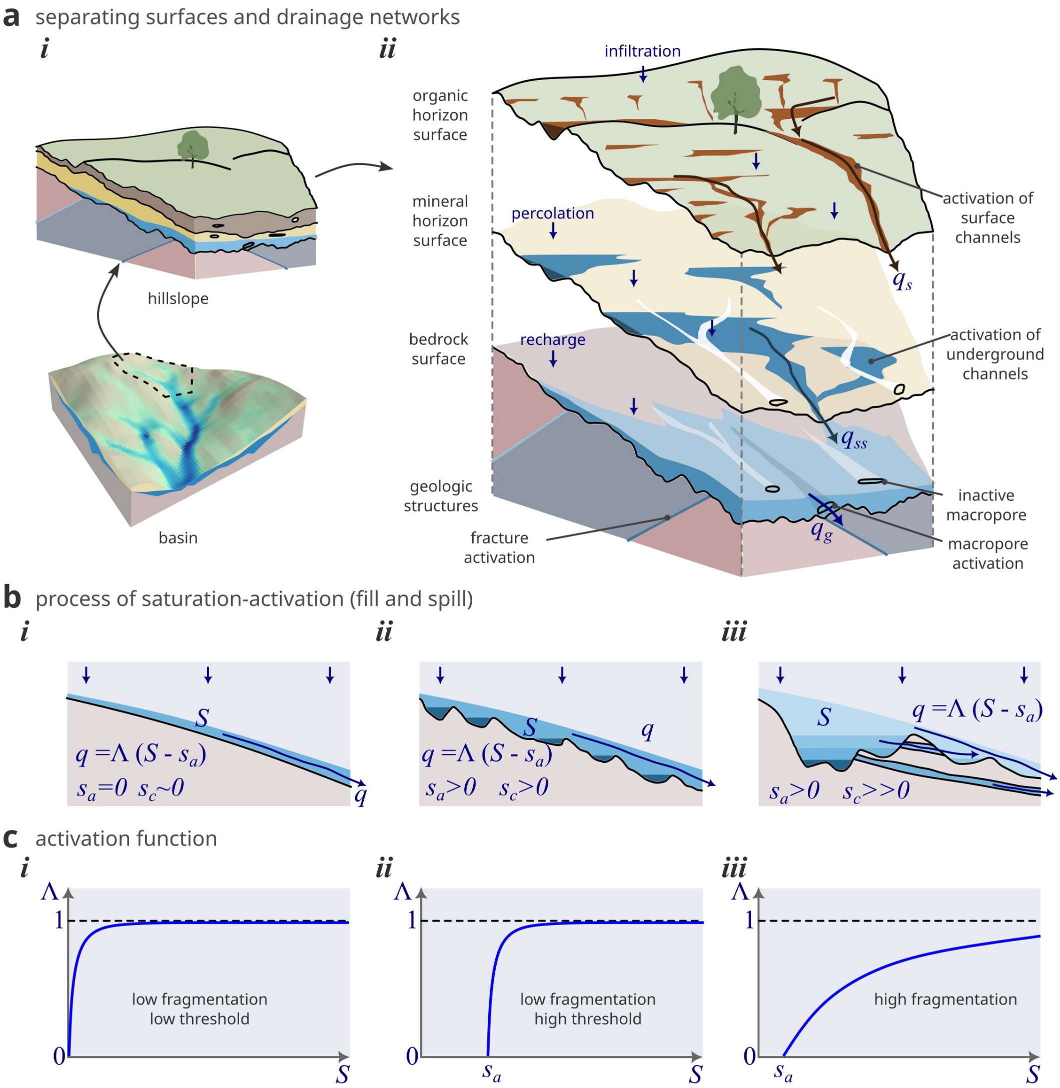

Figure 3.12 — The connectivity paradigm. The Connectivity Theory proposed by Jeffrey McDonnell and colleagues presents a unifying and revolutionary potential in Hydrology. **a** — The perceptual model is based on the principle that all hydrological responses are consequences of the same phenomenon. The vertical permeability transitions create separating surface. Thus, the network of channels on these surfaces can eventually become saturated and activated. Interactions also occur from bottom to top when a layer becomes saturated enough to interfere with the percolation process of the layer immediately above. **b** — The saturation-activation process occurs due to the topology of the channel network that drains the separating surface at various nested scales. The surface can be fully connected (detail i) or require an initial activation level s_a (detail ii). A surface with high fragmentation s_c offers multiple incrementally activated drainage networks, attenuating the response signal (detail iii). **c** — The activation function Λ can be modeled in terms of a saturation process that approaches the potential maximum flux $S - s_a$ as the surface saturates, that is, $\Lambda \rightarrow 1$.

perative of these epistemic problems, while overshadowing the vector field approach (forcing its proponents to appeal to pragmatic advantages), has shed new light on the ontology of Systems Dynamics, making it useful for estimating uncertainties through the application of low-cost computational semi-distributed models.

That said, I will conclude the chapter by articulating the recent revolutionary ideas of Jeffrey McDonnell and colleagues, who have sought over the past two decades to pave the way for a new unifying paradigm in Hydrology. These ideas have a direct impact on the application of hydrological models in the context of zero-order basins, making their assimilation and articulation in future versions of the model `PLANS` of utmost importance. Although widely published, McDonnell's synthesis can be traced through three articles separated by intervals of approximately ten years: McDonnell (2003) [60]; McDonnell (2013) [86], and; McDonnell et *al.* (2021) [69].

Initially, McDonnell (2003) demonstrates the increasing disconnect between hydrological models and evidence, highlighting that the mechanisms from the International Hydrological Decade are based on assumptions that fail to explain the old water paradox. Essentially, he argues that evidence points to both a greater separation between well-drained slopes and riparian wetlands, as well as a greater influence of bedrock topography on the outcropping of groundwater. Together, these two factors produce rapid translational flow of pre-event (old) water with diverse geochemical signatures. In the field of modeling, McDonnell (2003) asserts that the appropriate ontology for the new challenges is Systems Dynamics, not merely for convenience, but because it allows for the representation of the different compartments of the zero-order basin, primarily slopes and riparian zones, and guarantees exploratory experiments at a low computational cost. As highlighted in the chapter's epigraph, Systems Dynamics reaffirms itself as an ontological paradigm that is both intuitive and objective for understanding and learning about environmental systems.

The second step by McDonnell (2013) is to propose the **Connectivity Theory** as the definitive explanation for both the hydrological processes systematized by Dunne (1983) and the (not so) recent findings regarding the old water paradox. Initially reported in Meerveld & McDonnell (2006) [176] to explain processes in a specific experimental basin, McDonnell generalizes his concepts, treating it as a revolutionary and unifying theory that seeks to resolve the crisis established in the field. McDonnell proposes this theory from a question that sounds like heresy: could the rapid and slow responses of basins all be *the same phenomenon*?

> (...) the simple premise that all runoff processes are the same opens up new avenues to explore: Is there common emergent behaviour across all runoff types? – Jeffrey McDonnell (2013, p. 4110) [86].

This provocative question leads him to demonstrate that any system formed by networks of small channels can be modeled by the **Percolation Theory**, a mathematical branch of Network Theory[24] [177]. According to this theory, flow occurs through a network as long as there are connections between the nodes. In the case of a zero-order basin, in the physical world, the different parts of the system each function as a network of small reservoirs connected by small channels (open or closed, macroscopic or microscopic). Here, the relevance of two key concepts from the theory arises: (1) the **separating surface** between compartments, created by the transition of vertical permeability between soil horizons, and; (2) the **activation threshold** of the compartment, which primarily arises from the heterogeneity of the separating surface.

A clear example of this is the generation of flash floods when the soil's infiltration capacity is insufficient. Typically, the level of surface depressions needs to reach an activation threshold, at which point some surface depressions connect for the first time and start to spill water downhill. With more rain, the puddles continue to fill until a point is reached where all the incoming rainwater can flow downhill. The speed at which the connection occurs depends on the heterogeneity of the soil surface: a smooth surface is much more connected than a rough surface.

Although it may seem obvious, McDonnell suggests that the **saturation-activation process**[25] that generates flash floods occurs in all subsurface layers where vertical water flow encounters a transition in permeability, including the relatively impermeable bedrock layer (Figure 3.12**a**). The only difference in the subsurface environment is that the network of channels is composed of the micro and macropores of the

[24] Unlike scientific theories, which require empirical evidence to be corroborated, mathematical theories are based on axioms and deductive inference.

[25] A loose translation of the English term *fill and spill*.

immediately overlying horizon. In this context, the theory even allows for relatively small amounts of event water (new water) to activate the connection between pockets of stored water from before the event (old water). The pressurization in the saturated zone, along with the formation of natural siphons in the subsurface, eventually expels *more* water than what entered, generating a negative mass balance on the slope and a hysteretic behavior of flow pulses. Finally, when a separating surface becomes sufficiently saturated, it propagates this effect from bottom to top, causing saturation of the upper layer, thereby creating conditions analogous to the riparian wetlands we observe on the surface.

Finally, in their third move, McDonnell et *al.* (2021) articulate how to approach the Connectivity Theory in the context of modeling, considering the scale problem. Again, Systems Dynamics is presented as the appropriate ontology for representing the target system, emphasizing the explicit definition of the scale of interest, identifying the saturation-activation processes that manifest at the chosen conceptual scale. The authors' hypothesis is that saturation-activation processes occur at all scales; however, the signals emitted by smaller scales are progressively masked by saturation-activation at larger scales (Figure 3.12**b**). For example, while at the scale of zero-order basins the saturation-activation process is primarily dictated by topography, soil, and vegetation, this signal fades at the scale of higher-order basins, with the saturation-activation effects of the river drainage system and flooding of the plains becoming more dominant. Thus, experimental and modeling research must explicitly question what scale is being addressed and which critical saturation-activation processes are necessary to understand the target system. Relatively simple (yet objective) Systems Dynamics models can capture this knowledge, formalizing the main hypothesis of the **activation function**, which takes the following general form:

$$Q_a = \begin{cases} 0 & \text{if} \quad S \leq s_a \\ \Lambda \cdot (S - s_a) & \text{if} \quad S > s_a \end{cases} \tag{3.29}$$

Where Q_a [LT^{-1}] is the activation flow of the reservoir with level S [L]; s_a [L] is the **activation level** of the reservoir, and; Λ [T^{-1}] is the **activation function** of the reservoir, to be defined based on the auxiliary hypotheses of the model. In the previous chapter, during the development of the hydrological model prototype, I applied these exact principles for the quick response flow R of the surface reservoir S_1 (see Section 2.5). Equation (2.9) has exactly the same structure as Equation (3.29), with $\Lambda = c$, a runoff coefficient defined between 0 and 1 obtained from a activation function with the following structure (Figure 3.12**c**):

$$\Lambda = \frac{(S - s_a)}{(S - s_a) + s_c} \frac{1}{\Delta t} \tag{3.30}$$

Where s_a [L] is the activation level of the reservoir, and; s_c [L] is the **fragmentation level** of the reservoir. This function, when coupled into (3.29), implies that the outflow Q_a caused by activation asymptotically approaches the potential maximum flux $(S - s_a)$ as the reservoir level S increases, because higher levels increasingly activate the drainage network. In other words, $\lim_{S \to \infty} \Lambda = 1$ in (3.30) and $\lim_{S \to \infty} Q_a = (S - s_a)/\Delta t$ in (3.29). The fragmentation level s_c is a parameter that plays the role of regulating the speed of this process, serving as a measure of inverse connectivity (the higher, the less connected the reservoir is). The physical interpretation of the fragmentation level is the level S necessary to reach half of the potential maximum flux. The **Michaelis-Menten equation** [178], which describes an enzyme saturation process, coincidentally has an identical structure, making it a notable homology. Another identical structure is the equation from the **CN method**, empirically proposed based on the results of

Mockus (1949) [80]. The difference in this case is that the creators of the CN method express the level S in terms of accumulated rainfall P, which is only valid for a surface reservoir with unlimited capacity. The fragmentation level, in this regard, is expressed in terms of a dimensionless connectivity coefficient, such that $s_c = (1000/\mathrm{CN}) - 10$. Such homologies and theoretical explanations of old empirical adjustments outline the contours of a legitimately revolutionary scientific theory. ■

3.7 Chapter Summary

In this chapter, I provided a historical and theoretical overview of the evolution of hydrological models, highlighting the main changes in approaches and scientific paradigms. Beginning with slopes, where hydrological processes start, I explored the transition from Horton's infiltration model to more complex concepts that incorporate climatic, geomorphological, and biological variability. I also analyzed the limitations faced by modern computational models, such as scale and equifinality problems, culminating in the Connectivity Theory, which proposes an innovative integration of surface and subsurface flow processes.

- **Slopes are where it all begins.** Rapid hydrological responses (floods) and slow responses (recessions) begin with rain on the slopes or zero-order basins. Simplifying this complexity can lead to inadequate models, especially in the context of watershed revitalization. Therefore, it is crucial to recognize the theories regarding runoff generation at this scale.

- **The Age of Infiltration.** During the mid-20th century, the hegemony of Horton's hydrological model was established, explaining hydrological responses through the soil's infiltration capacity, separating rainfall into runoff and recharge. Although surpassed, this paradigm elevated Hydrology from its empirical phase to a geoscience.

- **The Age of Differentiation.** With the International Hydrological Decade in the 1960s, new evidence and theories emerged that refuted Horton. This new paradigm explores how different hydrological responses arise due to climate, topography, soils, and vegetation. In addition to floods, the roles of macropores and riparian wetlands were highlighted. However, a crisis emerged with the old water paradox.

- **Inevitable Limitations.** Digital computers enabled hydrological models, divided into two families: data-driven (predictions) and process-based (explanations). Systems Dynamics exposed the limitations imposed by equifinality and scale problems, which persisted even with attempts to resolve them using vector field-based models.

- **Information Scaling.** The scale problem refers to the difficulty of reconciling the natural scales of hydrological processes with observational and conceptual scales. The solution is the scaling of information. The `TOPMODEL` achieves this by scaling soil saturation with the `TWI` index. The `PLANS` combines `HAND` and `TWI` to scale saturation across different landscapes and instantiate hydrological response units.

- **The Connectivity Theory.** Jeffrey McDonnell proposes a unifying and revolutionary theory suggesting that surface and subsurface flows are manifestations of a single phenomenon: the saturation-activation of channel networks. In light of the inescapable limitations, Systems Dynamics is deemed the best alternative to model this theory.

Mars has a rocky and sandy terrain. Its atmosphere is composed of approximately 95% carbon dioxide, with an average atmospheric pressure of about 600 Pa. Temperatures vary drastically, with average values around -60℃. The planet has no bodies of liquid water, and its surface is constantly exposed to cosmic and solar radiation due to the lack of a magnetic field.

Chapter 4

Epilogue

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Glossary

abstraction An idealization process that seeks to remove supposedly irrelevant factors and aspects of the target system, leaving only its essence. 32, 40

activation function A formal hypothesis about how the activation of a reservoir develops as saturation occurs. 99, 101

activation level Equivalent to the activation threshold. 99, 101

activation threshold The minimum level required for the connectivity of a reservoir's drainage network (channels or pores) to begin transmitting water. 100

actual flow The flow that actually influences the level of a compartment in the simulation of a dynamic system. 47

agent-based models Agent-based models are computational simulation systems that use autonomous entities, with individual behaviors and interactions,. 39, 40

analog models Representations based on an analogy with the target system, preferably involving systems with supposedly the same mathematical structure (formal analogy). 57

analogical inference Non-deductive and non-inductive reasoning that concludes that a given object O_1 has the property P_1 of object O_2 because they share other properties. 32, 34, 57

analogy A comparison between two or more objects, emphasizing their supposedly similar aspects. Analogy is used in modeling to idealize systems in terms of other, more tangible systems that supposedly have the same mathematical structure. 5, 23, 31–35, 62

antecedent moisture conditions The set of initial conditions of the system on the eve of a rainfall event. 66

aquifer detention time g A characteristic parameter of the aquifer, assuming the phreatic zone behaves as a linear reservoir. 66, 70

Aristotelian idealization (See abstraction). A method of idealization that uses abstraction, a process aimed at removing supposedly irrelevant factors and aspects of the target system, leaving only its essence. 32

attractors A set of final, stable, or unstable behaviors observed in the solution of a given system of differential equations, depending on parameter values and initial conditions. 37, 39

auxiliary equations Equations used in the programming of dynamic systems (procedural model) to break down into steps that are easier for humans to understand. 43

auxiliary hypotheses A set of hypotheses necessary in addition to the main hypothesis of a model. 24, 26, 30, 69, 89–94, 101

balance equation A differential equation that establishes that the variation in a level results from the net effect of the inflow and outflow rates. 41, 47

balancing loop Feedback that acts on both inflows and outflows, reducing the value of this flow, leading to a situation that tends towards a state of equilibrium with or without oscillations. 44

baseflow $Q_\mathbf{g}$ The outflow or drainage of the phreatic zone, usually considered a slow response of the watershed. 74, 76

bedrock topography Irregularities in the bedrock that establish the relatively impermeable bottom of the unconfined aquifer in the phreatic zone. These irregularities can create pockets or stagnant zones in the aquifer. 79, 90, 100

bracketing inequality Inequality used to test whether a model is empirically acceptable. The model's simulated results must be bracketed by the observational uncertainty bands (total observational error) with a predefined level of confidence (rejection criterion). 26

calibration process A procedure to adjust model parameters to increase its degree of confirmation against empirical evidence. 26, 82, 83

capillary deficit $\mathbf{D_v}$ The potential storage capacity of capillary water in the vadose zone. 66, 67

capillary fringe A region in the vadose zone with zero capillary deficit due to its proximity to the phreatic zone, from which water is suctioned. 75

capillary water $\mathbf{V_c}$ Water stored in the vadose zone, held by the cohesive forces (surface tension) of soil particles. This water is more accessible for plant transpiration than for recharge to the phreatic zone. 65, 72, 79, 80

causal loop diagram In systems dynamics, a causal loop diagram is a visual tool that represents cause-and-effect relationships between the variables of a system, highlighting how changes in one variable influence others through reinforcing and balancing loops. 41

causal structure In systems dynamics, the causal structure refers to the set of cause-and-effect relationships that determine a system's behavior over time, including feedback loops and flows between the system's compartments. 41

central limit theorem A theorem that establishes the mathematical fact that the sample mean of any population exhibits a normal distribution. Regardless of the population's distribution (uniform, normal, etc.), the mean obtained from samples will be normally distributed. This happens because the mean is a sum, and in sums of random numbers, low sampled values tend to offset high sampled values, resulting in a bell-shaped pattern similar to a normal distribution. 12

commensurability error Epistemic uncertainty resulting from the difference in scales of time and space between observed processes and modeled processes. 24, 25, 82, 88

compartment model In systems dynamics, a compartment model is a modeling technique that divides a system into different sectors, where each compartment represents an accumulated quantity (level) of a specific variable, and the rates of flow between these compartments describe the changes over time. x, 40, 43

compensating effects Internal discrepancies in hydrological models caused by mass balance constraints in model compartments. These effects can lead to unrealistic results, as mass balances can mask underlying physical processes, compromising the accuracy of simulations. 82

computational grid A spatial discretization structure used in numerical methods to simulate hydrological processes. It consists of dividing the spatial domain into elements or cells, which can be regular or irregular, facilitating the application of techniques such as the finite difference method or finite element method to solve the equations that describe physical processes. 85, 86, 88, 90

conceptual model A formalized and simplified representation of the processes identified in the perceptual model. This model involves creating hypotheses and adopting assumptions to abstract the complex processes of reality in a tangible and objective way, often using mathematical formulations. 30, 31, 45, 48, 49, 51, 53, 57, 63, 67, 69

conceptual scale A level of analysis that serves as a bridge between the natural scale of hydrological processes and the observational scale of empirical evidence, representing the processes and interactions in the model in a structured way. 87, 88, 101

conditioning [synonym of conditionalization] Application of Bayes' Theorem to a hypothesis to update its degree of conviction. It can be done in successive steps as new evidence is obtained. x, xi, 9–14, 25–27

congested output problem The difficulty of applying balance equations using the Euler method when outflows feed into other compartments that may eventually become saturated. One solution is to compute both the maximum and potential flows before defining the actual flow. 47

Connectivity Theory A unifying theory of Hydrology proposed by Jeffrey McDonnell and colleagues to overcome the problems of the differentiation paradigm and address the old water paradox. 99–101, 103

conservation principle A principle used in systems dynamics to apply balance equations to compartments, often referring to the conservation of mass or energy (in physical systems). 41

context of discovery A perspective in the philosophy of science that deals with the problem of understanding the historical change of theories. 19, 20, 22

context of justification A perspective in the philosophy of science that deals with the problem of justifying the truth of theories. 19, 22, 33

convergent slopes Slopes where surface and subsurface drainage converge toward a single region, generally producing riparian wetland areas. 76, 85

credence Measure of belief. Central concept in Bayesian epistemology derived from the idea that knowledge is not a matter of all-or-nothing, but exhibits subtleties between true and false. This concept can be considered a probability under certain circumstances. 7–11, 13, 18, 20, 27

critical rationalism A rationalist philosophical approach proposed by Karl Popper, which establishes falsifiability as the criterion for demarcating scientific theories. In this view, the power of empirical evidence lies in justifying, through deductive logic, the falsity of theories (never their truth). For instance, it takes just one black swan to disprove the theory that all swans are white. While unrefuted, theories are merely corroborated by evidence. 15, 17

Curve Number Method (*Curve Number* (CN)) An empirical method for estimating the water balance in watersheds developed by the Soil Conservation Service in the 1950s. 67

Darcy's Law A principle that describes water flow through porous media. It establishes that the flow is directly proportional to the cross-sectional area of the conduit and the difference in hydrostatic potential, and inversely proportional to the length of the conduit. Mathematically, it is expressed as $\mathbf{u} = -K\nabla\Phi$, where $\mathbf{u}$ is the Darcy velocity, K is the hydraulic conductivity, and $\nabla\Phi$ is the hydrostatic potential gradient. 83, 84, 90, 91

data-driven models Hydrological models that focus on observational data analysis and forecasting, using techniques such as artificial neural networks. They aim to maximize predictive capability (predictive capability), but may compromise the explanatory capability (explanatory capability) of hydrological processes, often treating the watershed as a black box. 81, 82

deductive inference Logical reasoning that establishes the truth of a given statement from antecedent premises. The truth of the consequent statement is guaranteed only if the antecedent premises are also true. 6, 27, 82, 100, 118

demarcation problem The difficulty of establishing the difference between a scientific theory and a merely metaphysical theory, which relies solely on pure abstractions. 17

deterministic chaos Extreme sensitivity produced by nonlinearities in dynamic systems, generally associated with initial conditions. A chaotic system evolves in a highly unstable manner, oscillating between various final states. Rounding errors can amplify this effect even more, though the origin of the process lies in the mathematical formulation itself. 39, 57

Differentiation Age The period from 1970 to the present in which the scientific community in Hydrology seeks to establish how different environments exhibit distinct response mechanisms, depending on climatic, topographic, and land use conditions. 70

digital elevation model (DEM) A digital representation of the Earth's surface that captures the topography of a specific area, used in geoprocessing and hydrological modeling to derive characteristics such as slope, drainage area, and topographic wetness indices. 91

dimensionality problem The difficulty of exploring high-dimensional parametric spaces, requiring exorbitant computational resources to execute simulations in a reasonable time frame. 54, 94

direct rainfall $q_{\mathbf{se}}$ The surface flow produced due to rainfall on saturated soil. It can be generalized but occurs more frequently in riparian wetland areas. Common on convergent slopes, forcing the water table to surface. Considered a fast response. 69, 73, 74, 76, 81

distributed models Hydrological models that represent hydrological processes on a detailed spatial grid, allowing for the simulation of local variations in parameters and flows. These models can capture spatial heterogeneity and provide more accurate results at local scales, though they generally require greater computational power. 86

distribution function A method or function used in hydrological modeling to distribute or adjust parameters or variables from a larger scale to a smaller scale, or vice versa. This function helps transfer information between different levels of spatial detail, ensuring that local characteristics are adequately represented in the model. 89, 91

divergent slopes Slopes where surface and subsurface drainage spread out in different directions, preventing the formation of riparian wetland areas. 74, 76

downscaling The process of transferring information from larger scales to smaller scales in hydrological modeling, which generally involves non-trivial methods and auxiliary hypotheses that consider the heterogeneity of hydrological processes across scales, including the use of co-variables (indicators). 89, 90, 94, 95, 98

effective observational error The overlap of measurement error and commensurability error, representing the uncertainty that a model must be subjected to in order to assess its empirical adequacy. 25, 26

effective rainfall $p_\mathbf{s}$ The flow of rainfall that reaches the soil surface after the vegetation canopy is saturated. 65–68, 74, 89–91

empirical uncertainty The scientific component of uncertainties in the decision-making process based on evidence. It consists of both epistemic and statistical uncertainties about the state of the world. Other non-empirical components include ethical and political uncertainty. 4

empirically acceptable model A model that yields simulated results that satisfy empirical observations with a pre-established level of confidence. 26

empirically equivalent models Different models that yield simulated results with no significant deviations given the total observational error. In this case, there is no empirical reason to favor one model over another, at least concerning the main hypothesis of the models. 25, 26

empiricism Philosophical doctrine that argues that all knowledge originates from empirical experience, that is, observations of the external world. This doctrine opposes rationalism. 6, 7, 15, 23

engineering bias A formative trend in Hydrology that seeks knowledge aimed at solving practical societal problems. 60, 68

ephemeral springs Points and patches in the landscape where small perched aquifers emerge, formed in more superficial organic soil horizons, contributing to exfiltration in the fast response of rivers (rises). 68, 70, 71, 87

epistemic uncertainty A general concept referring to the various non-statistical uncertainties present in the modeling process. Unlike statistical uncertainty, which refers to the available information, epistemic uncertainty is associated with unavailable information. 24, 25

equifinality problem A term coined by Keith Beven for the mild version of the underdetermination problem in the case of environmental numerical models. The underdetermination of models occurs because the information about the modeled processes is incomplete, ensuring the existence of model structures that are empirically equivalent, or equifinal. 24, 27, 50, 82

Euler method A simple numerical integration technique used to solve ordinary differential equations, where the solution is approximated by advancing in small steps, using the known derivative to estimate the value of the function at the next point from the current value. 42, 48, 57

evidence-based policies A concept in public policies that seeks total or partial support from objective evidence to guide decision-making and resource allocation. 4, 95

excess rainfall p_x The excess rainfall that exceeds the soil's infiltration capacity. 65, 68, 74

exfiltration $q_{\mathbf{ss}}$ Flow from ephemeral springs located at the base of slopes, resulting from the rapid passage of water through organic horizons with large amounts of macropores. Common in forests. Considered a fast response. 69, 71–73, 76, 78, 85

exhaustive sampling Also known as brute force, it is a strategy for sampling the parametric space by enumerating all possibilities after uniform discretization. 54

exogenous variables In systems dynamics, exogenous variables are factors external to the modeled system that influence its behavior but are not affected by the system's internal dynamics. They are imposed from outside (external forces) and remain constant or follow a predetermined pattern during the simulation. 41, 43, 45, 49, 52

explanatory capability The ability of hydrological models to provide an understanding of the physical processes that generate runoff. This includes the ability to describe how and why observed hydrological phenomena occur, beyond merely predicting outcomes. 81, 82, 109

exploratory models Models used in scientific research as tools to investigate and develop new hypotheses, especially useful in areas where established theories are insufficient or non-existent, allowing the exploration of theoretical possibilities and potential explanations. 34, 87

exponential decay curve A graph that represents a rapid drop in a compartment's level over time, usually resulting from the dominance of outflows over inflows, associated with the presence of reinforcing loops (positive feedback) on these flows. 44, 66

exponential growth curve A graph that represents the accelerated increase in a compartment's level over time, usually resulting from the dominance of inflows over outflows, associated with the presence of reinforcing loops (positive feedback) on these flows. 44

falsifiability The ability of a theory to be shown as false through empirical experience (observations and experiments). A falsifiable theory is not necessarily false but *can* be proven false by empirical evidence. In critical rationalism, this ability is the criterion for determining whether a theory is scientific. 5, 17, 18

feedback A recursive information loop that acts on a system. It can be positive, reinforcing a given process, or negative, stabilizing a given process. 20, 35, 37, 41–44, 47, 57

field capacity $v_{\mathbf{max}}$ The maximum storage level of capillary water in the vadose zone. 65, 76

finite difference method A numerical technique used to solve partial differential equations, employed in the simulation of transient flows in porous media. This method discretizes the spatial domain into a regular grid, allowing the approximation of the derivatives involved in the physical equations. 85

finite element method A numerical technique used to solve partial differential equations in complex domains, employing an irregular computational grid. It allows for more flexible representation of the domain's geometry and is particularly useful in simulating transient flows in porous media with varied geometries. 85

fluvialist bias A hegemonic trend in Hydrology that focuses on essentially hydraulic problems at the watershed scale, such as flow propagation in river channels and flooding of adjacent plains. 61, 62, 68, 81

fragmentation level A parameter that regulates the speed of activation in the saturation equation. The higher the fragmentation, the more dampened the reservoir's activation becomes. The value of the fragmentation level corresponds to the reservoir value at half the maximum activation speed. 101, 102

Galilean idealization A method of idealization that applies controlled distortions that could be incrementally removed to asymptotically reach the final behavior of the target system. 32

geochemical signature The concentration of solutes that allows identifying or tracing the origin of water from its diffusion process in the soil and rocks. 79, 80

global scale A level of analysis that assesses the aggregated and integrated behavior of the hydrological system as a whole, considering all its parts and interactions from a macroscopic perspective. 84, 86, 88, 91, 96

gravitational deficit D The potential storage capacity of gravitational water in the vadose zone or the effective depth of the water table. 65, 90, 91

gravitational water $\mathbf{V_g}$ Water stored in the vadose zone that is free to percolate vertically to the phreatic zone under the influence of gravity (recharge). 65, 72, 79, 80

Height Above Nearest Drainage (`HAND`) A topographic index representing the height of a point relative to the nearest drainage channel. It is calculated as the difference between the local altitude and the altitude of the nearest drainage point. `HAND` is used to map wetlands and identify flood risks, making it a valuable tool for hydrological modeling and geoprocessing by representing the topography in relation to drainage networks. 95

heuristic A set of problem-solving techniques that do not guarantee an optimal or rational solution but are sufficient to achieve practical decision-making purposes. The main example is solving problems through trial and error. 23

homology A formal analogy made in modeling, which is an equivalence between the mathematical structures of the target system and the model. 33, 101

hydraulic conductivity K The maximum potential percolation flow of water in the phreatic zone of an aquifer. 65, 72, 93, 94

hydraulic transmissivity A soil property that represents the capacity of the porous medium to transmit water per unit of width and depth. Equivalent to hydraulic conductivity per unit of lateral contour. 92

hydro-ecological compartmentalization The concept of separating water in the vadose zone between water widely absorbed by plant rootlets, occupying soil micropores, and water that is rapidly drained (exfiltration and recharge) through soil macropores. 80

hydro-geochemical compartmentalization The concept of separation at multiple scales of water residence times in the pores of the phreatic zone, creating a diversity of geochemical water signatures. 80

hydrological cycle The circular flow of water on Planet Earth, energized by solar radiation. Evaporation transfers surface water to the atmosphere, and this water returns to the surface in the form of precipitation as rain, dew, and snow. 31, 45, 59, 61, 65, 66, 83, 85, 86

hydrological response The way a watershed's outflows (runoff) manifest in response to inflows (rainfall). Typically, there is a clear separation between rapid responses (rises) and slow responses (recessions). 45, 50, 57, 62, 66, 67, 69, 81, 82, 98

hydrological response units Spatial segments or blocks in a watershed that represent hydrologically homogeneous regions in terms of hydrological response, facilitating semi-distributed modeling by grouping areas with similar hydrological behavior. 89, 94, 96, 98, 103

hydrological similarity A condition in which different regions or hydrological units exhibit similar hydrological behavior, allowing them to be grouped or treated uniformly in hydrological models. Hydrological similarity is used to simplify distributed modeling by grouping areas with homogeneous hydrological responses. 89, 94

Hydrology The natural science that studies the hydrological cycle in its terrestrial phase on continents. 30, 31, 33, 40, 55, 57, 59–61, 63, 64, 69, 76, 80, 86, 98, 99, 103

hylomorphism A holistic ontological theory proposed by Aristotle, which states that all things are composed of both matter and form. 35

hypothesis A universal statement in a trial phase, aiming to be elevated to the status of theory after confirmation or corroboration. 6–11, 17, 24, 26, 27, 30, 32, 33, 46, 51, 80, 89, 90, 92, 94–96, 101

idealism A metaphysical conception that opposes realism. In this perspective, which can have ontological or epistemological interpretations, reality is understood as a subjective product of the mind. 22

idealization A fundamental procedure used to construct models, making the representations more tangible and understandable than the target system itself. 32, 33, 84

induction problem Also known as **Hume's induction problem**. A circular invalid argument that arises from the justification of inductive knowledge through the principle of uniformity, as it invokes inductive knowledge to support itself. 6, 7, 15, 23

inductive inference Empirical reasoning based on generalization or extrapolation, establishing a universal statement from observations of singular statements. The truth of the universal statement is not guaranteed but presents degrees of probability. 6, 7, 22, 27

inference to the best explanation [synonym of abduction] Non-deductive reasoning that seeks to define the hypothesis that best explains empirical evidence. 23

infiltration f The flow of surface water into the soil matrix. 65, 67

Infiltration Age The period between 1930 and 1970 when the scientific community in Hydrology operated under the normality of the Hortonian paradigm, which established infiltration as the key process to explain the alternation between rises and recessions in rivers. 64, 69, 98

infiltration capacity $f_{\mathbf{max}}$ The maximum potential infiltration flow determined by the characteristics of the soil surface. 64–71, 74, 75

infinite regress problem The challenge of establishing the ultimate origin of logical or rational knowledge, given that all premises must be deduced from more fundamental premises, leading to an infinite (or circular) chain of premises. 6, 22

input data Input data are the information or values provided to a model for processing or analysis, serving as the basis for generating results or simulating the behavior of the system under study. 24, 31, 45, 49, 82, 89, 98

input data error Statistical and epistemic uncertainty associated with the data used to configure the model. For instance, rainfall data present statistical measurement uncertainty and the epistemic uncertainty of spatial interpolation. 24, 25

instrumentalism An empiricist radical philosophy of science that opposes scientific realism. This doctrine holds that the goal of science is to produce empirically adequate theories and nothing more. It argues that empirical adequacy does not imply a true description of reality. 4, 22, 23

interception The initial flow that fills the vegetation canopy with rainwater. 32, 45, 60, 63

interception capacity $c_{\mathbf{max}}$ The maximum storage level of water in the vegetation canopy before effective rainfall is produced. 64, 65, 89

isotopic signature The concentration of isotopes that allows identifying or tracing the origin of water from its thermal fractionation process in the atmosphere. 77, 80

Kalinin-Miyukov-Nash model A hydrological model representing the response of a watershed as a network of reservoirs arranged in series, known as a cascade. It uses a Gamma distribution to parameterize the hydrograph, incorporating parameters such as the hydrograph volume (ν), the effective number of reservoirs (n), and the mean residence time of the reservoirs (k). Developed independently by Kalinin & Miyukov (1957) and Nash (1958). 81

Latin Hypercube Sampling A statistical sampling strategy used to generate sets of sample points in a high-dimensional space efficiently, ensuring that each dimension is equally represented in all parts of its interval, improving the coverage and representativeness of samples compared to simple random sampling methods. 54

leverage points In systems dynamics, leverage points are strategic locations within a complex system where a small change in one aspect can lead to significant changes in the system's behavior, making them crucial for effective interventions and systemic changes. 39, 49, 51, 57

likelihood The probability that the evidence E is true after considering the probability that the hypothesis H is true. Denoted as $P(E|H)$. 9–13, 22, 25, 26

linear reservoir A compartment that exhibits an outflow directly proportional to its level: $Q_t = S_t/k$, where Q is the reservoir's outflow at time t; S is the reservoir's level at time t, and k is the reservoir's mean residence time. 33, 46, 66

local scale A level of analysis that focuses on infinitesimal elements of the soil, allowing for a detailed and accurate representation of hydrological processes in small areas or units, facilitating the description of hydrological phenomena from a microscopic perspective. 52, 84, 86, 88–91, 94, 96, 98

logical positivism An empiricist philosophical movement from the early 20th century, also known as logical empiricism. 7

logistic curve A graph that represents the alternation between the dominance of reinforcing loops and balancing loops, showing initially rapid growth (or decay) that later stabilizes at a plateau due to balancing effects. 36, 38, 43, 44

macroporosity A network of pores that stores and conducts water in much greater proportion than if considering the apparent porosity of the soil matrix. Higher in structured organic soils with the presence of fauna and flora (bioturbation). Common in weathered rocks, with the presence of fractures and other geological structures. 69, 72, 73, 86

maximum flow The highest possible flow defined by the physical constraint of a given compartment. 47, 65

measurement error Statistical uncertainty resulting from the measurement of empirical evidence. 24, 25

mental models A term from systems dynamics for subjective and personal models that are still in the early stages of the modeling process. 29, 30, 51, 52, 55, 95

minimalist models Models that are simplified to the extreme, used to understand complex phenomena by reducing them to the essentials, focusing on fundamental aspects without the complication of excessive details. 34

model A model is a simplified representation of a real-world phenomenon, often used to explain, predict, or simulate various processes. x, xi, 3–5, 11–16, 18, 19, 24–26, 29, 31–34, 37–57, 62, 63, 67, 69, 70, 77, 79, 80, 82–86, 88–91, 93–99, 101

model diagnostics A broad set of techniques applied to assess the adequacy of a model in various aspects. In systems dynamics, John Sterman lists the following diagnostics: boundary adequacy; structural adequacy; dimensional consistency; parameter distribution; comparative studies; integration error; extreme conditions; sensitivity analysis; anomalous behaviors; empirical adequacy; surprises; and positive impacts. 31, 51

model structural error Epistemic uncertainty associated with the theoretical concepts and computational procedures employed in a given model. 24, 25

Monte Carlo simulations A numerical method in which numerous statistically equivalent resamplings are performed to estimate the final behavior of a model involving random variables (i.e., when $n \to \infty$). The name Monte Carlo refers to a casino in Monaco, alluding to the idea of making numerous "rolls" to perform a robust statistical analysis. 12, 13

natural scale A level of analysis referring to the actual characteristic speeds exhibited by hydrological processes in nature, including the lifespan of intermittent events, annual event periods, and trends in long-term stochastic processes. 87, 88

negligibility premises A concept introduced by Musgrave (1980), referring to the process of ignoring known important causal factors during abstraction, i.e., when abstraction ends up presenting a model with known falsehoods. 32, 69, 83

normal science A concept articulated by Thomas Kuhn referring to the historical period in which a given scientific community shares the same paradigm. Normal science tends to end in a crisis, followed by a revolution imposed by the advent of a new paradigm. 20, 21, 27, 64

numerical integration problem The difficulty of obtaining exact values when solving balance equations in the simulation of dynamic systems on digital computers. See truncation error. 42

objective Bayesianism An approach in Bayesian epistemology that argues that the prior distribution must be defined in such a way as to observe the principle of indifference. 10, 11

objective function A mathematical expression that defines the variable (or set of variables) to be maximized or minimized in an optimization problem. 54

observational scale A level of analysis related to the scale of empirical observations in hydrological modeling, including aspects such as data extent, sampling resolution, and sampling integration intervals. 87, 88

old water paradox The difficulty in explaining the rapid mobilization and high prevalence of old water in rivers after precipitation of new water, as well as the diversity of geochemical signatures of old water. 77, 80, 100, 103

open systems Systems capable of processing an inflow and outflow of matter, energy, and information, in contrast to the closed systems described by classical thermodynamics. 36, 82

organic horizon O A general term for the upper layer of soil with greater macroporosity due to the action of soil fauna and flora. 72

overfitting problem A problem that emerges in model calibration when a model is excessively fitted to the available empirical information, resulting in poorer performance when new empirical observations are evaluated. 26

overshoot and collapse curve A typical graph of systems with two main compartments, where one compartment is drained by the other, producing a pattern of accelerated growth followed by an abrupt drop in levels when resources are exhausted. 44

paradigm A concept articulated by Thomas Kuhn referring to the set of exemplary solutions to research problems, i.e., a system of theories, instruments, and auxiliary practices that solve certain widely accepted problems and are promising for resolving open controversial problems with great competitive appeal. x, 20, 21, 23, 25–27, 31, 35, 36, 39, 49, 57, 64, 68–70, 73, 76, 81, 83, 89, 98–100, 103

parameters Fixed values of coefficients that define the characteristics and behaviors of elements and processes within a model. They are used to adjust the relationships and functions of the system, determining the system's response and dynamics under different conditions. 11, 12, 16, 18, 19, 24, 26, 39, 41, 43, 48–50, 52–55, 57, 63, 65, 81–83, 85, 87, 89, 90, 93, 94, 97

parametric space The set of all possible combinations of a model's parameters, used to explore and analyze how different parameter values affect the system's behavior and results. In general, the parametric space has N dimensions, where N is the number of parameters. 53–55

perceptual model Also called a mental model, it consists of the subjective and highly personal representation of an individual about the target system (object). 30, 31, 45, 49, 51, 52, 57, 64, 65, 67, 68, 71, 75, 99

perennial springs Points and patches in the landscape where the main unconfined aquifer of a watershed surfaces, contributing to the baseflow in the slow response of rivers (recessions). 70

permeability transitions Changes in effective hydraulic conductivity observed between different soil horizons. Generally, hydraulic conductivity increases in more superficial horizons due to macroporosity. 72, 99

phreatic zone G A porous matrix of soil and rock that stores water in an unconfined aquifer under atmospheric pressure. Also known as the saturated zone. 65, 66, 75, 79, 80

physically based models Hydrological models based on fundamental physical laws, such as the conservation of mass, momentum, and energy. They differ from systemic models by using continuous representations of vector fields to simulate hydrological processes, providing a more detailed and theoretically consistent description of watershed behavior. 83, 86, 87, 90

posterior The probability that the hypothesis H is true after considering the probability that the favorable evidence E is true. Denoted as $P(H|E)$. 10, 12

potential flow A calculated inflow or outflow that potentially alters the level of a compartment in the simulation of a dynamic system. The flow needs to be confronted with the imposed physical constraints (usually conservation and non-negativity). 47, 48

pragmatic realism Term proposed by Keith Beven to describe the implicit realism commonly held by environmental model users. In this philosophy, it is accepted that models provide approximate representations of reality and can improve as new technologies become available. 4, 22, 25, 31

predictive capability The ability of hydrological models to predict runoff behavior based on input data, such as precipitation. It refers to the accuracy and reliability of the model's forecasts. 57, 81, 109

predictive models Hydrological models used to solve specific practical problems, focusing on predicting hydrological events under given conditions. These models apply parameters conditioned by empirical observations in specific temporal and spatial contexts to generate forecasts in different situations. 87

principle of conditionalization Principle used in Bayesian epistemology to update degrees of conviction in hypotheses based on evidence. To maintain consistency with the principle of probabilism, conditionalization involves zeroing, scaling, and normalizing the values of updated probabilities. 9

principle of indifference A principle adopted by the objective Bayesianism approach, stating that the degree of conviction in two or more hypotheses should be equal unless there are reasons to the contrary. In the case of complete ignorance, the prior distribution must be uniform. 9, 10

principle of probabilism Principle used in Bayesian epistemology to treat degrees of conviction as probabilities. It has three axioms: non-negativity; normalization; and additivity. 8, 10

principle of uniformity Assumption that the same natural regularities observed empirically in the past will be the same in the future, i.e., that nature is predictable based on its past and that no arbitrary changes will occur in its laws (for example, the Earth suddenly stopping its rotation). 7

prior The probability that the hypothesis H is true before considering the probability that the favorable evidence E is true. Denoted as $P(H)$. 10, 11

problem of justification The challenge of establishing the truth of a particular piece of knowledge or theory. 5, 15, 22

problem of priors The difficulty of justifying the initial definition of degrees of conviction in a hypothesis before any evidence is obtained. In Bayesian epistemology, solutions to this problem are proposed mainly through two approaches: objective and subjective. 10, 11

procedural model A practical representation of a conceptual model in a computer program, where the equations and concepts of the conceptual model are translated into code, allowing simulations and predictions of flows and levels based on input data. 30, 31, 43, 49, 52, 53, 57, 94

process-driven models Hydrological models that represent the physical processes occurring in a watershed. They allow the simulation of watershed behavior even without empirical observations, offering a theoretical basis for runoff generation and enabling deductive inference of hydrological processes. 81, 82

rating curve Functional relationship between the level and flow of a river or channel at a specific section. Typically, the following power function is used: $Q = a(h-h_0)^b$, where Q is the flow; h is the level; and a, b, and h_0 are parameters adjusted by observed data. 11, 16

rationalism Philosophical doctrine that supports the superiority of deductive, intuitive, and innate logic to human knowledge, justifying the truth of theories. This doctrine opposes empiricism. 5, 7, 15

realism A metaphysical conception that admits the existence of objective reality, i.e., reality does not depend on anyone to observe it. 22, 24

recession curve The drainage curve of the phreatic zone displayed on a river's hydrograph during a drought (baseflow). 66, 67, 72, 93

recharge $q_\mathbf{v}$ The vertical water flow (percolation) that transfers water from the vadose zone to the phreatic zone. Also known as ultimate percolation. 65, 67, 71, 74–76, 80, 90, 91, 94

regionalization The process of adapting and applying hydrological models developed for a specific region to other regions with different characteristics, involving the generalization of model parameters and processes to fit new geographical and hydrological conditions. 89

regularization effect The stabilization of water flow over time, minimizing extreme variations and ensuring availability for longer periods. 51

reinforcing loop Feedback that acts on both inflows and outflows, increasing the value of this flow, which can result in exponential behaviors (growth or decay). 44

representation problem The difficulty of constructing a model that performs the semantic or syntactic function of representing a target system. 32

reproducibility problem A typical problem of dynamic systems models pointed out by John Sterman, where models are difficult to use by anyone other than their developers. 56

riparian wetlands Zones in valley bottoms, near watercourses, where the water table frequently surfaces. 68, 73, 74, 87, 89, 90, 93, 94, 97, 100, 101, 103

runoff by excess of infiltration The generalized surface flow produced due to the soil's relatively lower infiltration capacity compared to the effective rainfall. A synonym for **surface runoff**. 63, 65

saturation index A topographic indicator used in hydrological modeling to represent soil saturation in a given area. The saturation index relates topographic characteristics such as slope and drainage area to determine the propensity of an area to become saturated during rainfall events, and it is fundamental for the local distribution of soil water deficit in hydrological models. 91, 94–96, 98

saturation-activation process A hydrological process that manifests at all scales in Connectivity Theory. 99–101

scale models Representations that are literally copies of the target system at a scale suitable for human manipulation, whether scaled-down or enlarged. 32, 33, 83

scale problem The difficulties that arise when the scale represented by the hydrological model differs from the scale of empirical observations. This discrepancy can introduce errors into the model's results, making them incommensurable or incompatible with observed evidence. 82, 85, 87, 98, 101, 103

scale similarity The ability to convert between the real scale of a target system and the scale of a reduced or enlarged model. Similarity is usually not complete, being valid only in certain aspects (e.g., geometrically similar, but not in terms of density or strength). 32, 82

scaling The process of transferring information between different spatial and temporal scales in hydrological modeling, involving the adaptation of data and parameters from one scale to another to ensure model consistency and accuracy. 87–89, 91, 98, 103

scaling function A mathematical function that defines how information is transferred between different scales in hydrological modeling, determining the form of aggregation or distribution of parameters and variables to maintain model consistency and accuracy. 89, 90, 93, 95

science-management duality A characteristic of Hydrology, existing at the interface between theoretical investigation of nature and practical solutions for social, environmental, and economic issues. 60, 87

scientific community The people who practice science at a given period in history. It can refer to the entirety of scientists or a specific subset within a field. Thomas Kuhn argues that, during certain historical periods, the scientific community is characterized by sharing a paradigm. 20, 21, 26, 27, 64, 68, 69, 78, 85, 86

scientific realism A current in the philosophy of science that defends the thesis that the purpose of science is to provide theories that are true descriptions of reality. 7, 22, 23, 27

semi-distributed models Hydrological models that use an intermediate approach between fully distributed models and aggregated models. These models divide the watershed into hydrological response units, allowing for a more detailed representation than aggregated models but with less computational complexity than distributed models. 89, 99

sensitivity analysis A model diagnostic technique that seeks to understand how the modeled system responds to changes in its elements, such as inflows and parameter values. 53, 54

separating surface A surface created by the vertical permeability transition between soil horizons, separating vertical flow into a lateral component. The concept is generalized by the theory of connectivity. 99, 100

simultaneous depletion problem The difficulty of applying balance equations using the Euler method when multiple outflows drain the level of a compartment. A solution is to proportionally allocate between the individual flows if the total outflow exceeds the level in the simulated time step. 47, 48

space of possibilities The set of possibilities generated between hypotheses and evidence in Bayesian epistemology. For probability mathematics to apply to this set, the possibilities must be *mutually exclusive* (cannot be true at the same time) and *collectively exhaustive* (at least one is true). 8, 9, 11

spatial heterogeneity Variability or diversity in the spatial distribution of hydrological characteristics, such as soils, vegetation cover, topography, and hydrodynamic properties. Spatial heterogeneity significantly influences the hydrological response of a watershed, requiring models to accurately represent this diversity to simulate runoff and infiltration processes. 89, 94

statistical model A statistical model is a specific theory about the mathematical behavior of data, without theoretical links to underlying phenomena. 18, 19, 51

statistical uncertainty Uncertainty arising from random noise in the observed data. This type of uncertainty has stationary statistical characteristics that may or may not be structured with bias, heteroscedasticity, and autocorrelation. One way or another, this uncertainty can be modeled by probability distributions. 7, 24

storage deficit The available storage of a compartment that has a maximum capacity. 47

strange attractor A set of states in a dynamic system that, despite being chaotic, possesses a defined geometric structure and attracts the system's trajectories, characterizing an ordered behavior within chaos. 39

structural isomorphism A concept articulated by Ludwig von Bertalanffy to support General Systems Theory, being a formal analogy (homology) observed in different phenomena. 35, 44

subjective Bayesianism An approach in Bayesian epistemology that argues that any prior distribution is valid as long as it does not violate the principle of probabilism. 10, 11

supplementary equations Equations used in the programming of dynamic systems (procedural model) to capture important information that is not part of the modeled system itself, such as statistics of variables. 43

surface detention capacity $s_{\mathbf{max}}$ The maximum storage level in surface depressions. 64, 65, 89, 91

surface runoff q_{si} The generalized surface flow produced due to the soil's relatively lower infiltration capacity compared to the effective rainfall. 4, 46, 64–71, 73–77, 80, 81, 83

system An emergent ontological entity defined by a set of fundamental parts that exhibit relationships with each other. 3, 17, 20, 24, 25, 30, 33–45, 48–57, 63, 65–67, 69, 83, 84, 87, 94, 98, 100, 101

system boundary In systems dynamics, the system boundary defines the limits of what is included or excluded in a system analysis, specifying which compartments exert relevant causal effects on the system without being considered external factors. 41, 45

Systems Dynamics Systems dynamics is a modeling and analysis approach that uses feedback loops, levels, flows, and delays to understand the behavior of complex systems over time, helping to identify and predict behavior patterns and their underlying causes. x, 31, 39–41, 43–45, 47–49, 51, 52, 55–57, 63, 80–83, 85, 86, 88, 89, 98–101, 103

target system A real system that a model supposedly seeks to represent, conveying a theory or hypothesis about this system. 31–34, 42, 45, 49, 51–53, 57, 62, 88, 101

temporal insensitivity principle A guideline by John Sterman, within systems dynamics, that the results of model simulations should not be sensitive to the time step used in numerical integration, regardless of the method adopted. 42, 53

theoretical incommensurability A concept articulated by Thomas Kuhn, referring to the problem of intellectual communication between theories under different paradigms. Two paradigms are fundamentally different, making comparison between their concepts precarious (even if they use the same name and mathematical symbol). 21

theory A universal statement (or system of statements) that definitively establishes the truth of a phenomenon. 5–7, 15–20, 22, 23, 31–36, 41, 49, 51–53, 56, 62, 64, 66–69, 71, 75–78, 81, 82, 85, 86, 95, 97, 98, 100–103

thermal fractionation A change in the concentration of isotopes caused by phase changes of water (evaporation and condensation). The water from a given rain event has a different isotopic signature from ocean water (and other rain events) due to its trajectory of thermal fractionation. 78

time of concentration An effective response time parameter used to determine the unit hydrograph. 81

Topographic Wetness Index (`TWI`) A topographic index used to estimate soil moisture based on terrain slope and drainage area. It is calculated by the formula $\mathrm{T}_i = \ln(\alpha_i / \tan\beta_i)$, where α_i is the local drainage area per unit contour length, and β_i is the local terrain slope. `TWI` helps identify areas prone to saturation and runoff, and is widely used in hydrological models such as `TOPMODEL`. 90, 91

total error equation An equation that includes all sources of errors in a model, both statistical and epistemic. 24, 26, 82

translational flow $Q_{\mathbf{gt}}$ The water flow from the phreatic zone produced by the sudden pressurization of capillary fringes in riparian areas, where the water table is near the surface. Considered a fast response. 69, 73, 74, 80

truncation error The difference between the exact value of a function or analytical mathematical calculation and its approximation resulting from the numerical method employed to calculate the value in a computational environment. 42, 43

two-world hypothesis A testable hypothesis about hydro-ecological compartmentalization proposed by Jeffrey McDonnell. One world of water would be the water for plants (green water), and the other world would be the water for rivers (blue water). 80

underdetermination problem The difficulty of ensuring that the observed evidence determines the truth of a theory without there being other empirically equivalent theories. 5, 23–25, 36, 82

Unit Hydrograph The minimal linear response of a watershed. Complex responses can be constructed from the unit hydrograph through convolution. 81

upscaling The process of transferring information from smaller scales to larger scales in hydrological modeling, often performed through averaging or summation over a specific spatial or temporal extent. 89

vadose zone V A porous matrix of solid soil minerals that stores water in films held by surface tension. Also known as the unsaturated zone. 65, 70, 72, 76, 80, 84, 85, 90, 94

variable source area The phenomenon of expansion and contraction of riparian wetland areas that produces a variable contribution of runoff from direct rainfall. The variation of the source area can occur during a rainfall event or over the course of seasons. 74, 75, 89, 91

vegetation canopy C The leaves and branches of plants that act as a compartment or reservoir that stores water through surface tension before the rain reaches the soil surface. 65

zero-order basin Regions on slopes and higher grounds of the landscape where precipitation interacts with vegetation, soil, and rocks, producing the hydrological responses observed downstream in rivers. Also known as **slope basin**. 61, 65, 100

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