Rethinking how we train researchers to apply numerical models to earth systems

RCN: Community-based educational infrastructure for numerical simulation in the Earth Sciences: a reactive transport use case

Alexis Navarre-Sitchler - Colorado School of Mines

Kate Maher - Stanford University

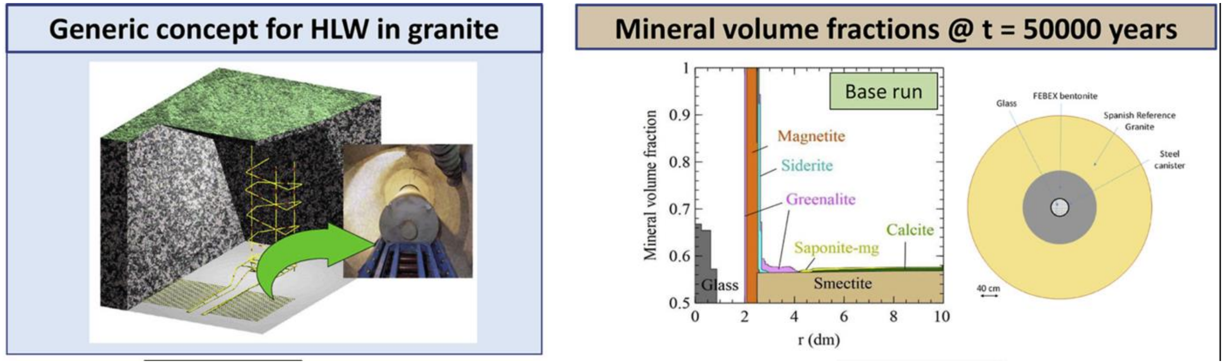
Jenny Druhan - University of Illinois

Award number 1935321

From NSF: The goal of the RCN program is to advance a field or create new directions in research or education by supporting groups of investigators to communicate and coordinate their research, training and educational activities across disciplinary, organizational, geographic and international boundaries.

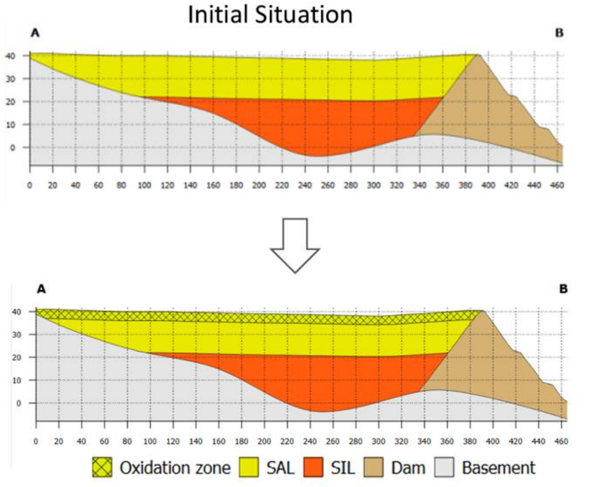
The promise of Reactive Transport Simulation

Waste disposal and isolation



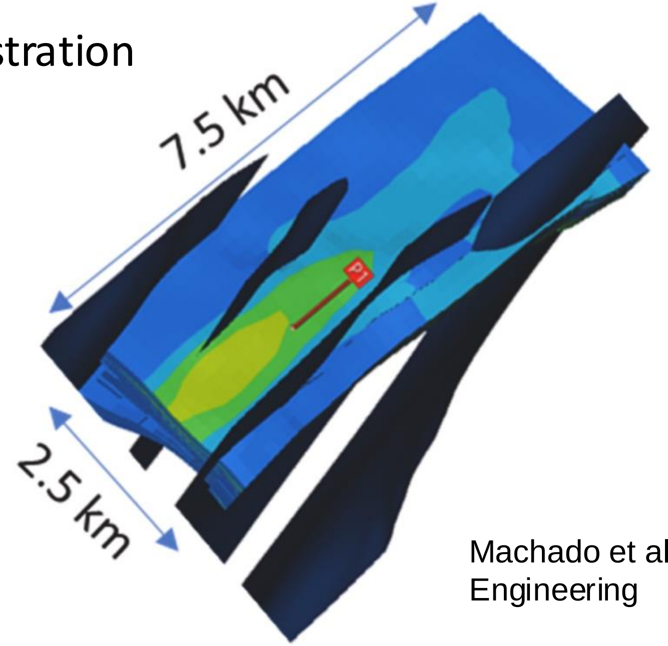
Samper et al., 2024, Applied Geochemistry

Mine tailings impact and management



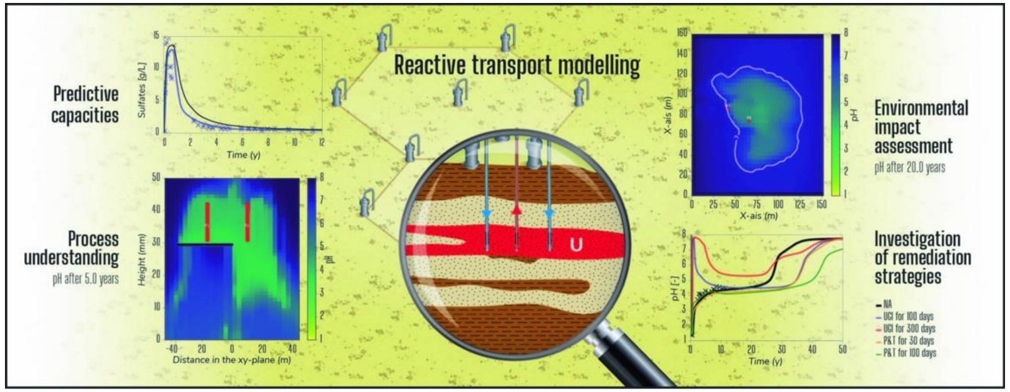
Garcia et al., 2024, Processes in Mine Tailings

Carbon Sequestration



Machado et al., 2024, Geoscience and Engineering

Environmental Remediation



Seigneur et al., 2024, JCH

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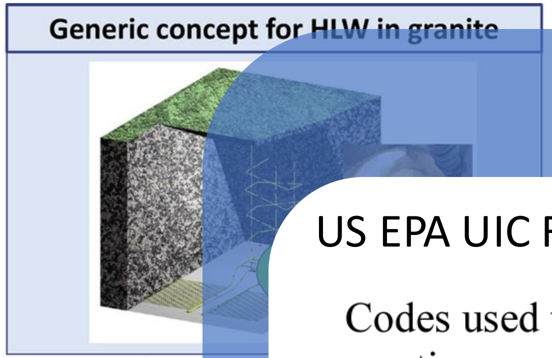

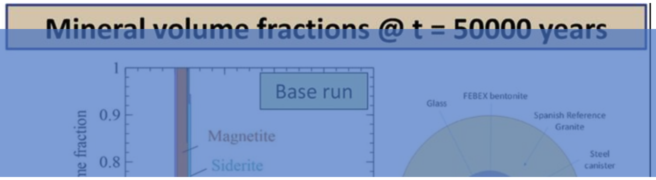

Samper et al., 20

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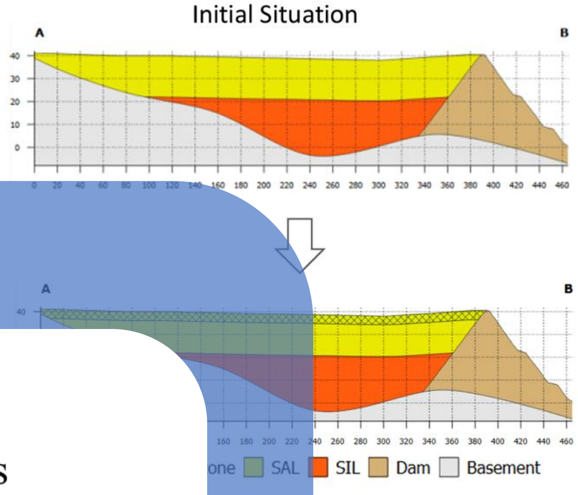
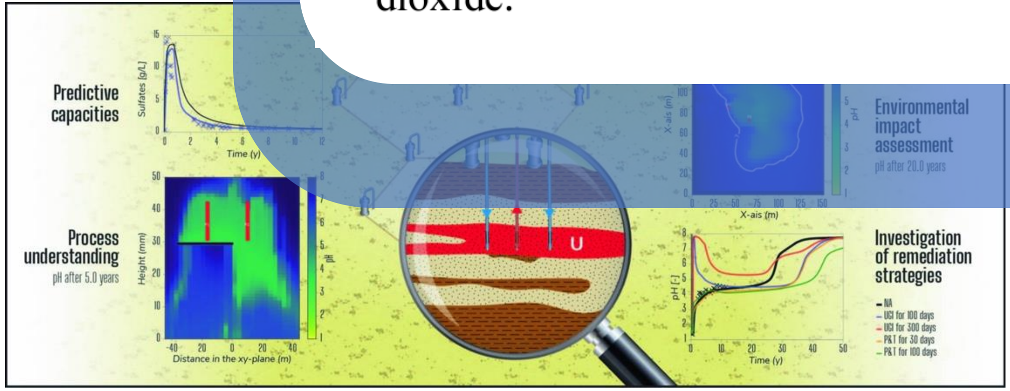


2024, Processes in Mine Tailings

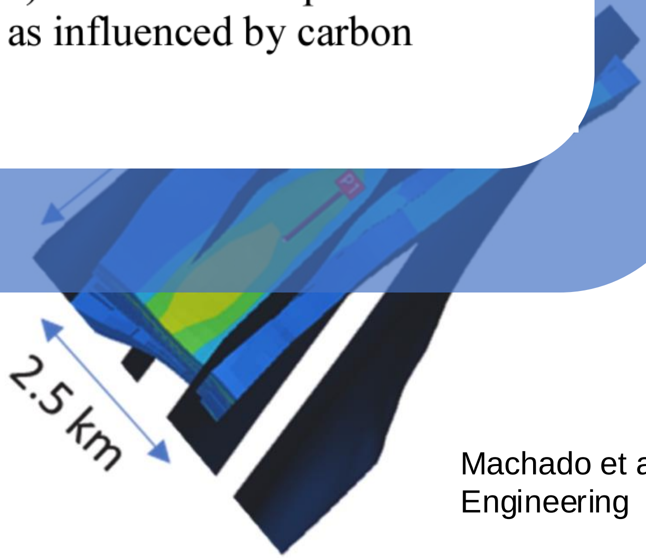
US EPA UIC Regulations and permitting

Codes used to simulate reactive transport generally incorporate rate-limited intra-aqueous reactions, mineral dissolution and precipitation, changes in porosity and permeability due to these reactions, and multi-component gas mixtures. Reactive transport models can be used to determine the impact of carbon dioxide and its co-injectates (e.g., hydrogen sulfide, sulfur dioxide) on aquifer acidification, the concomitant mobilization of metals, and any mineral trapping of carbon dioxide (e.g., precipitation of carbonate minerals). Reactive transport models can also be used to assess corrosion of well construction materials as influenced by carbon dioxide.

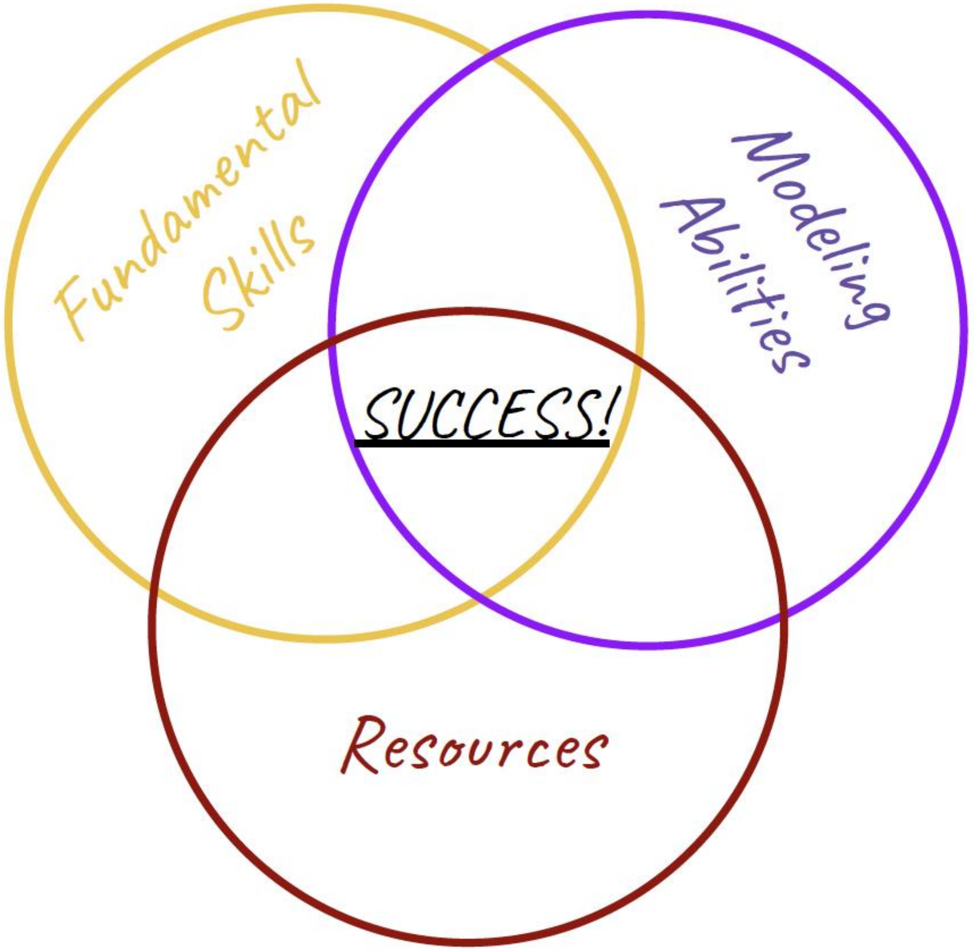
Environm



Seigneur et al., 2024, JCH



Machado et al., 2024, Geoscience and Engineering



Resources

RTM-HUB

- Website based community for announcements and papers.
- Instructional materials with metrics and rubrics available for download.

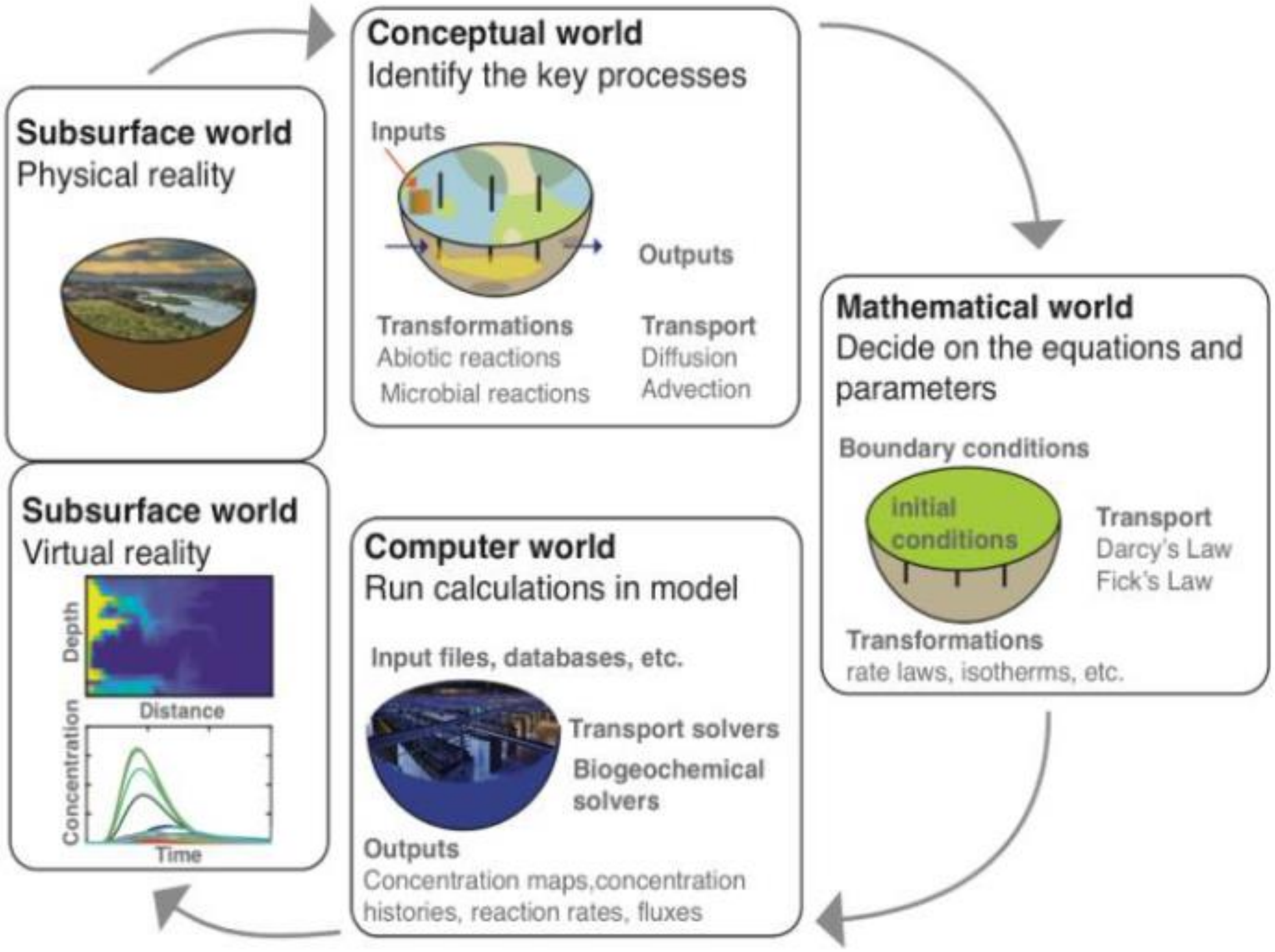
Summer Institute

- Workshops in an open loop learning model.
- Draw on community as instructors.

Based on the 3 components for success in research (Lovitts, 2005; 2008) and *creative work* (Sternberg and Lubart, 1995; Amabile, 1996)

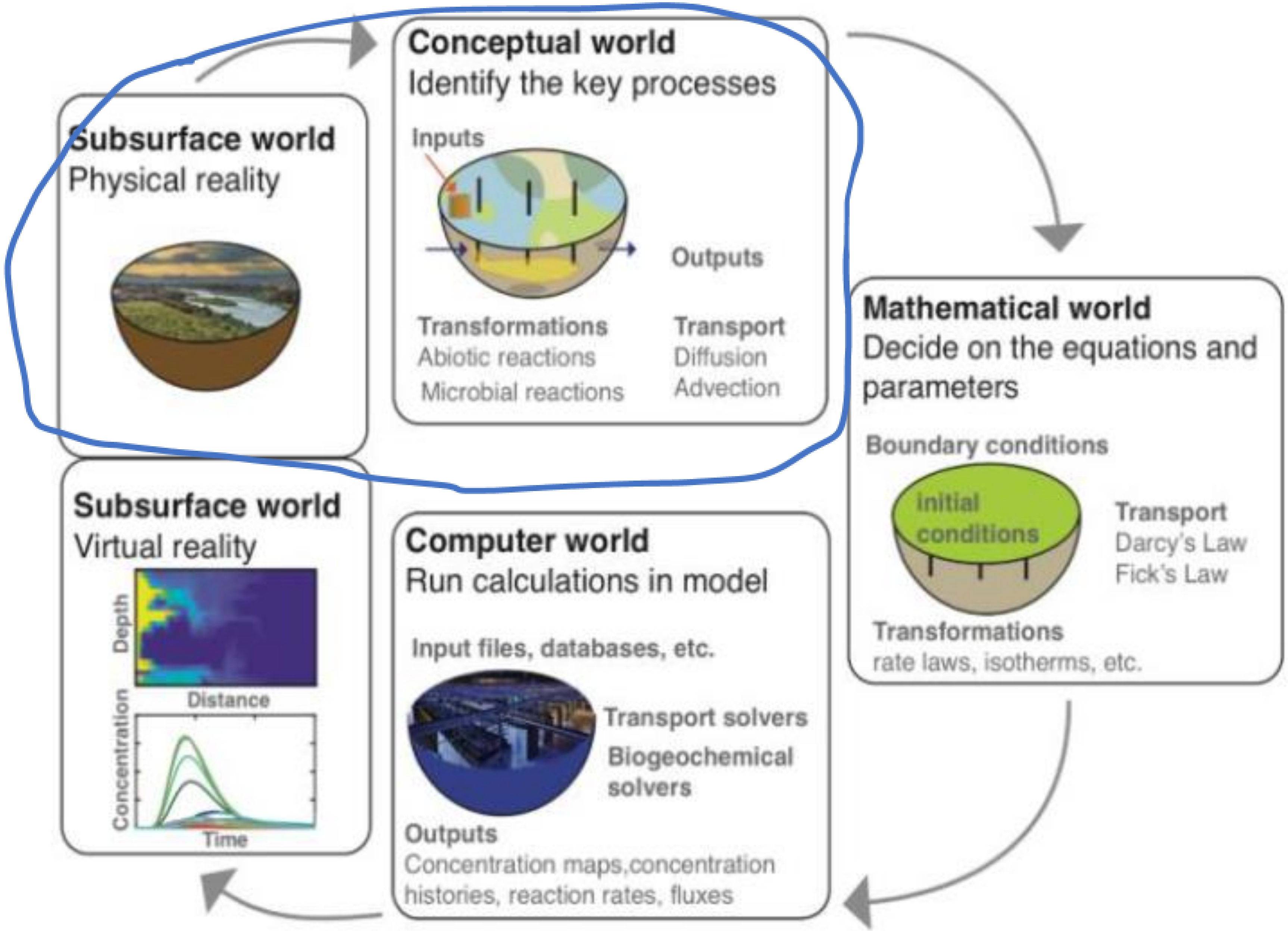
Increasing need for curriculum in reactive transport modeling

The process of modeling

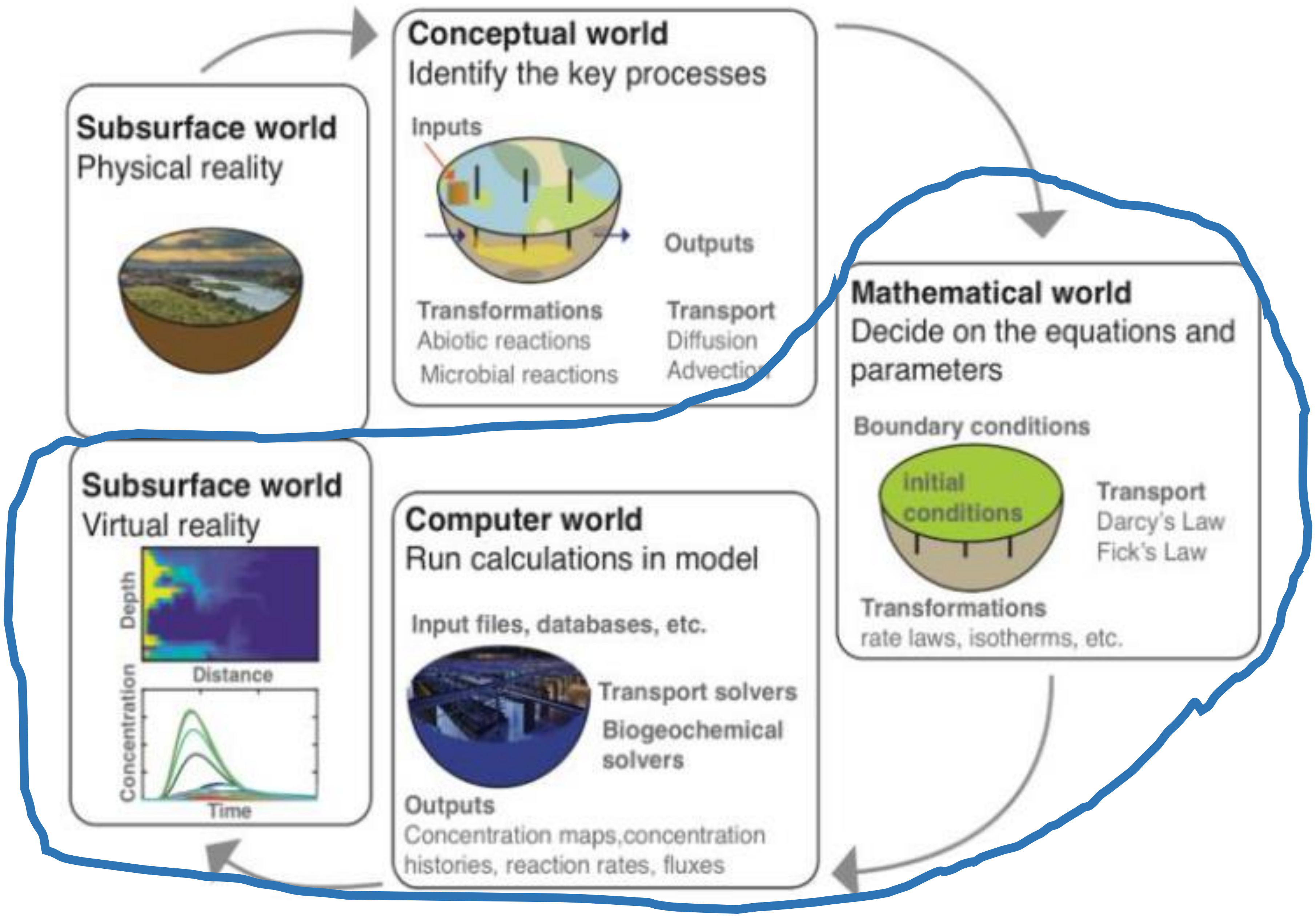


Maher and Meyer 2019

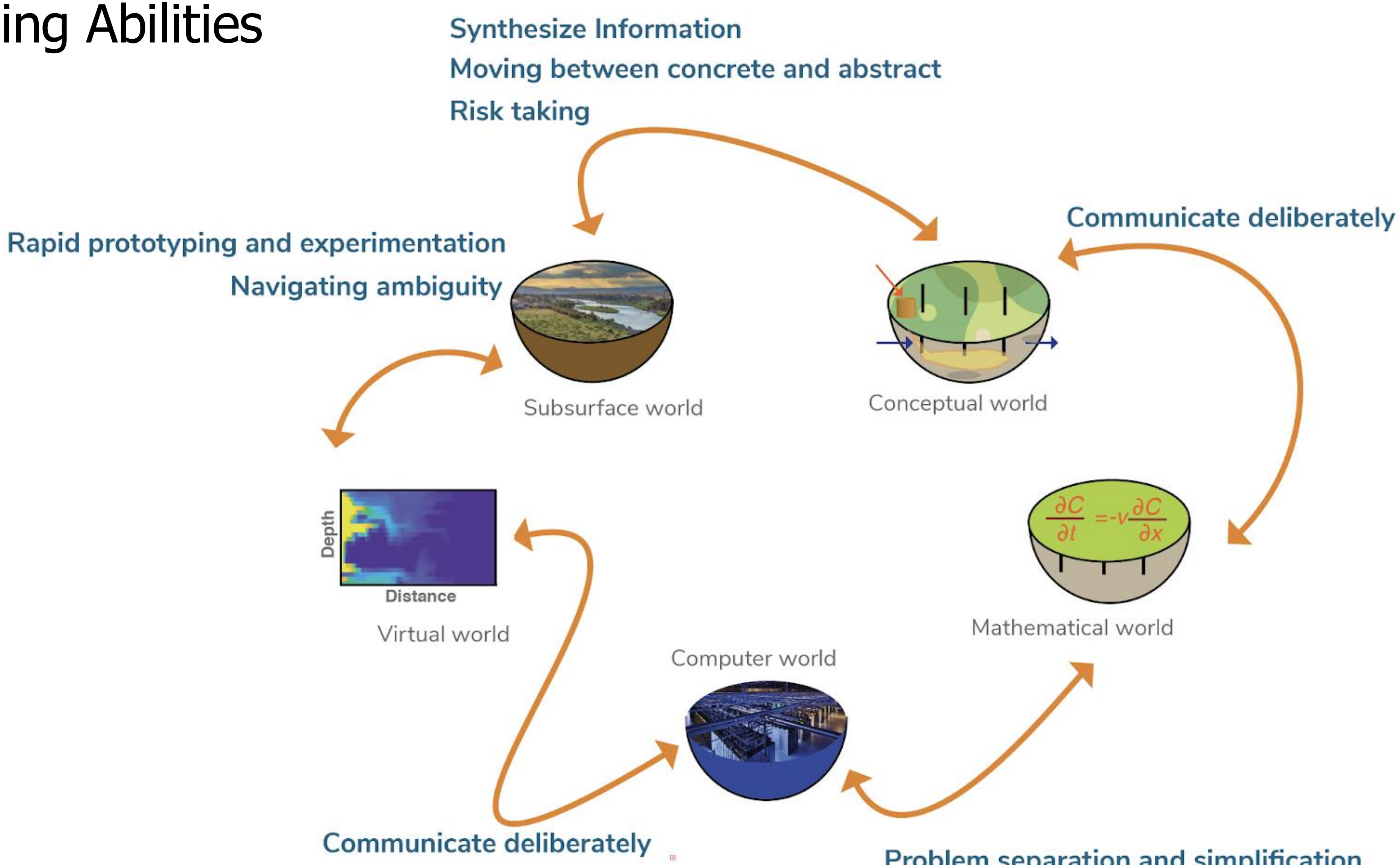
The question and conceptualization part



The computer calculations part:



Modeling Abilities



Conceptualized and developed by J. Druhan, K. Maher, A. Navarre-Sitchler (NSF Award Number 1935321)

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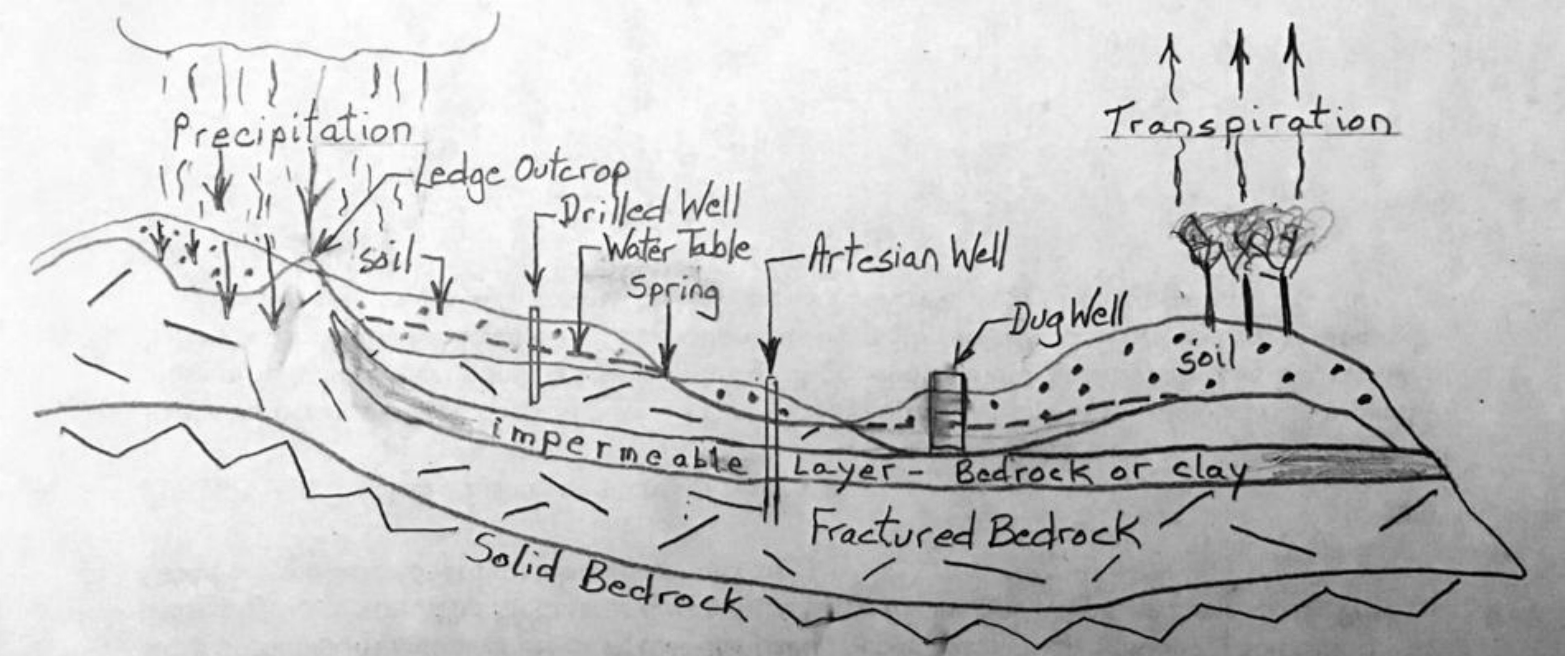
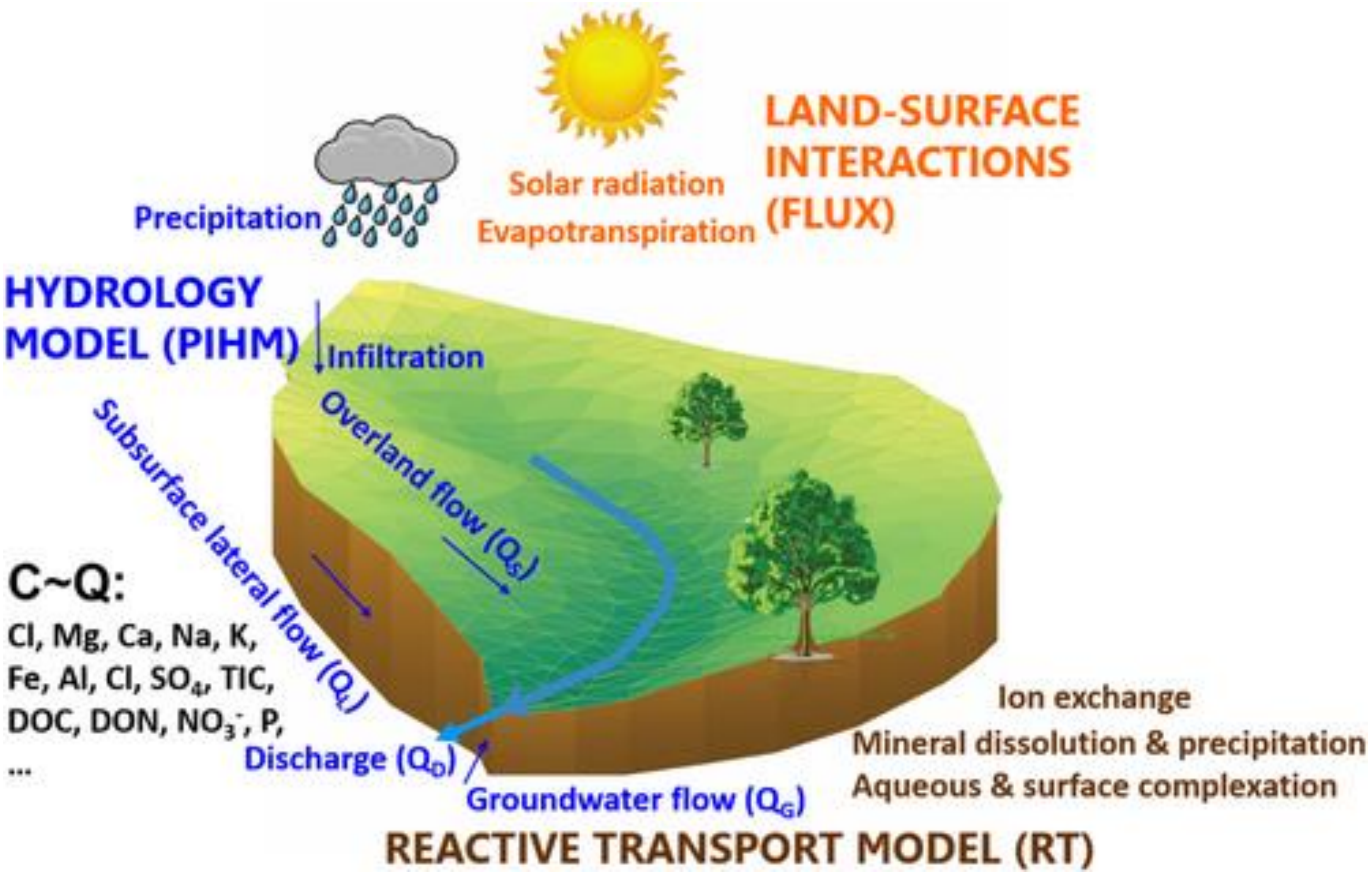


Sketching is an important part of the thinking and design process

Relationships, boundaries, inputs, outputs

https://www.northstarmonthly.com/features/the-water-under-our-feet/article_33335764-3313-11eb-b7b9-cba7627aa838.html

A good numerical model starts with a good conceptual model!



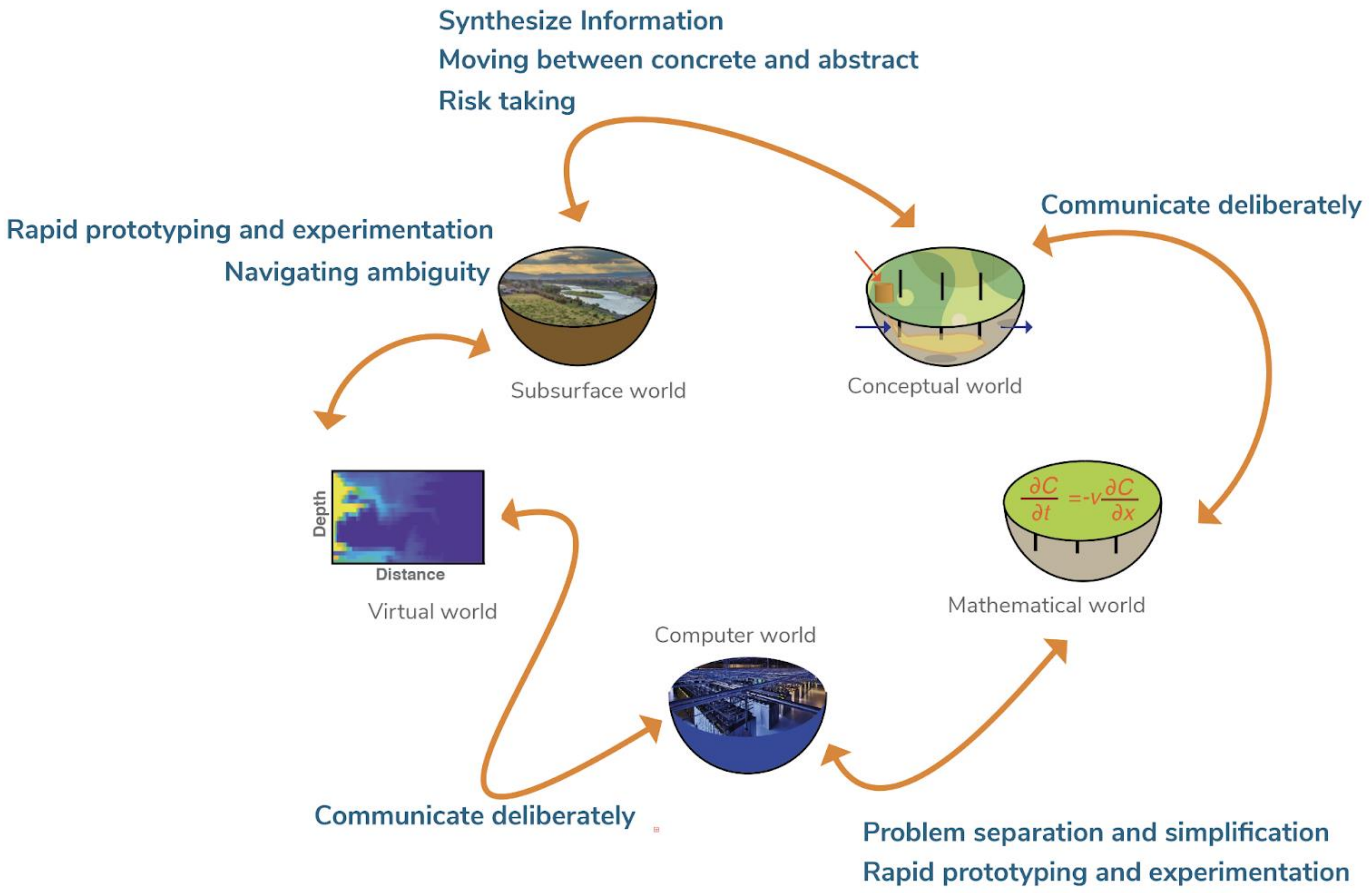
Li et al., 2017

Inputs, outputs, internal processes, boundary conditions, initial conditions

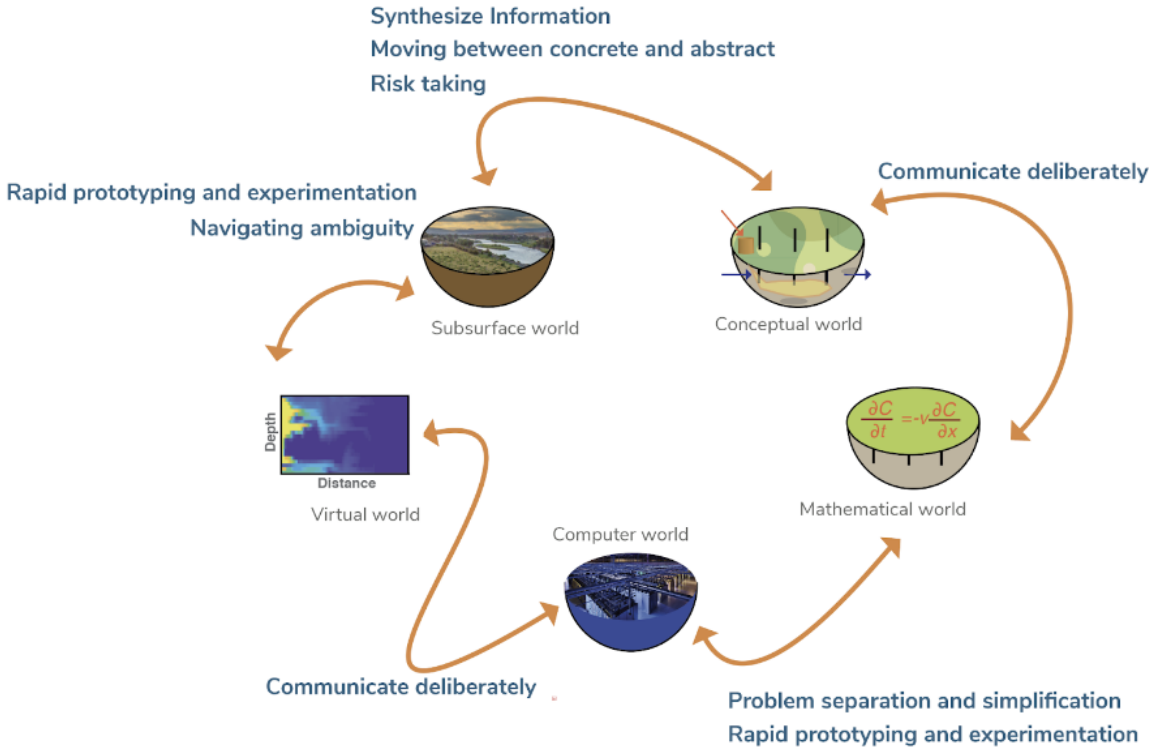
Fundamental Skills (aka domain-relevant skills)

(1) Space for time - specific set of conditions, lead into 5 (**#fs-space4time**)
(2) Temporal evolution (quasi-steady state, relaxation time, reaction-limited) (**#fs-tempevo)**
(3) Adding dimensions - dimensionality, heterogeneity (maybe leave out 3d)(**#fs-dimensions**)
(4) Mass balance (reactor models to plug flow, mass flux vs concentrations) (**#fs-massbalance**)
(5) Site conceptualization (communication, abstraction, scaling - dimensionless numbers) - same conceptual model for different systems (what is common?), same system different models for different questions. (**#fs-siteconceptual**)
(6) Numerical conceptualization (from discretization to troubleshooting, dimensionless numbers) (**#fs-numconceptual**)
(7) Computer literacy (terminal use, etc.) (**#fs-computerliteracy**)

But what about all the other stuff?



Introduction to Modeling Abilities

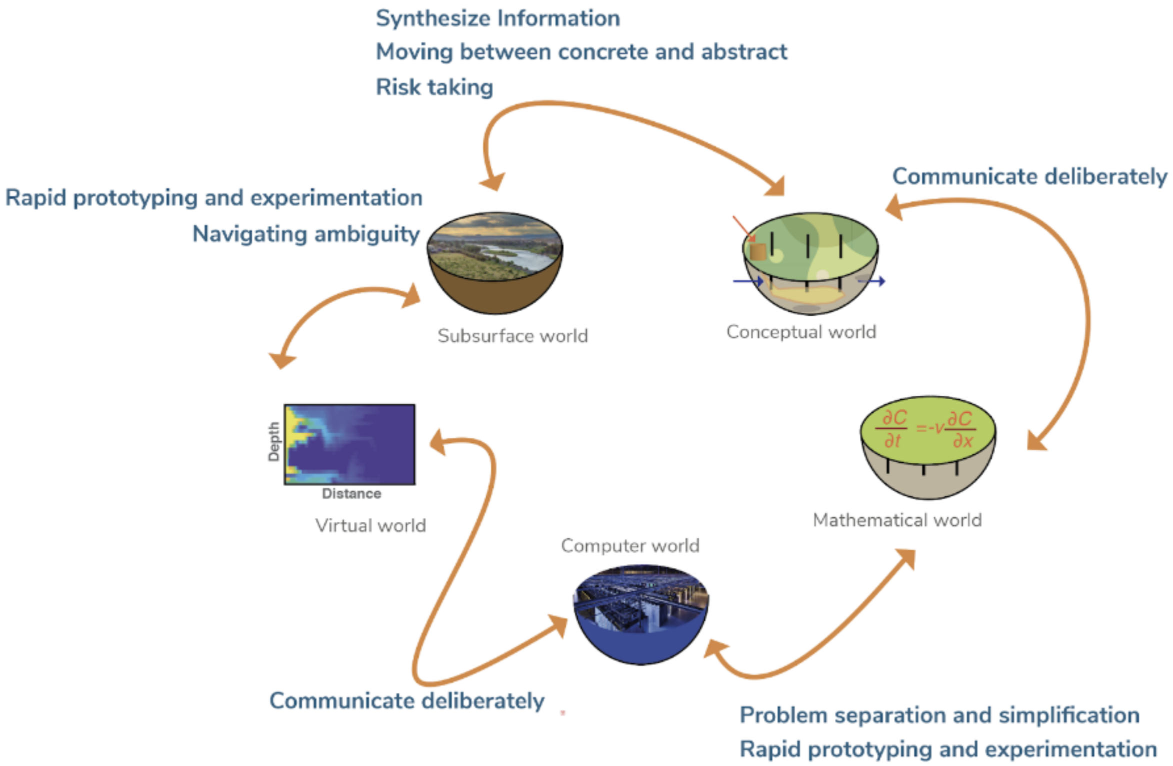


Synthesize Information: Synthesis is the ability to make sense of information and find insight and opportunity within. A modeler must draw from a range of field observations and modeling studies to incorporate existing knowledge into conceptual and numerical models. How do we bring together insights from field and experimental studies to define model inputs and metrics? (#ma-synthesis)

Moving between concrete and abstract: This ability contains skills around extrapolating from general theoretical frameworks to local conditions and conversely abstracting on concrete systems to theoretical and conceptual frameworks. Seeing the connections across scales, contexts and concepts, to abstract out for meaning and principles, as well as zooming in to define details and features of data and models. How do we extrapolate knowledge across scales or models? (#ma-abstract)

Risk taking: This is the ability to follow a divergent path and explore new designs, new models of thinking and new paradigms, even if they are likely to fail. Divergent thinking is critical to advancing understanding but requires an acceptance of risk (#risktaking).

Introduction to Modeling Abilities

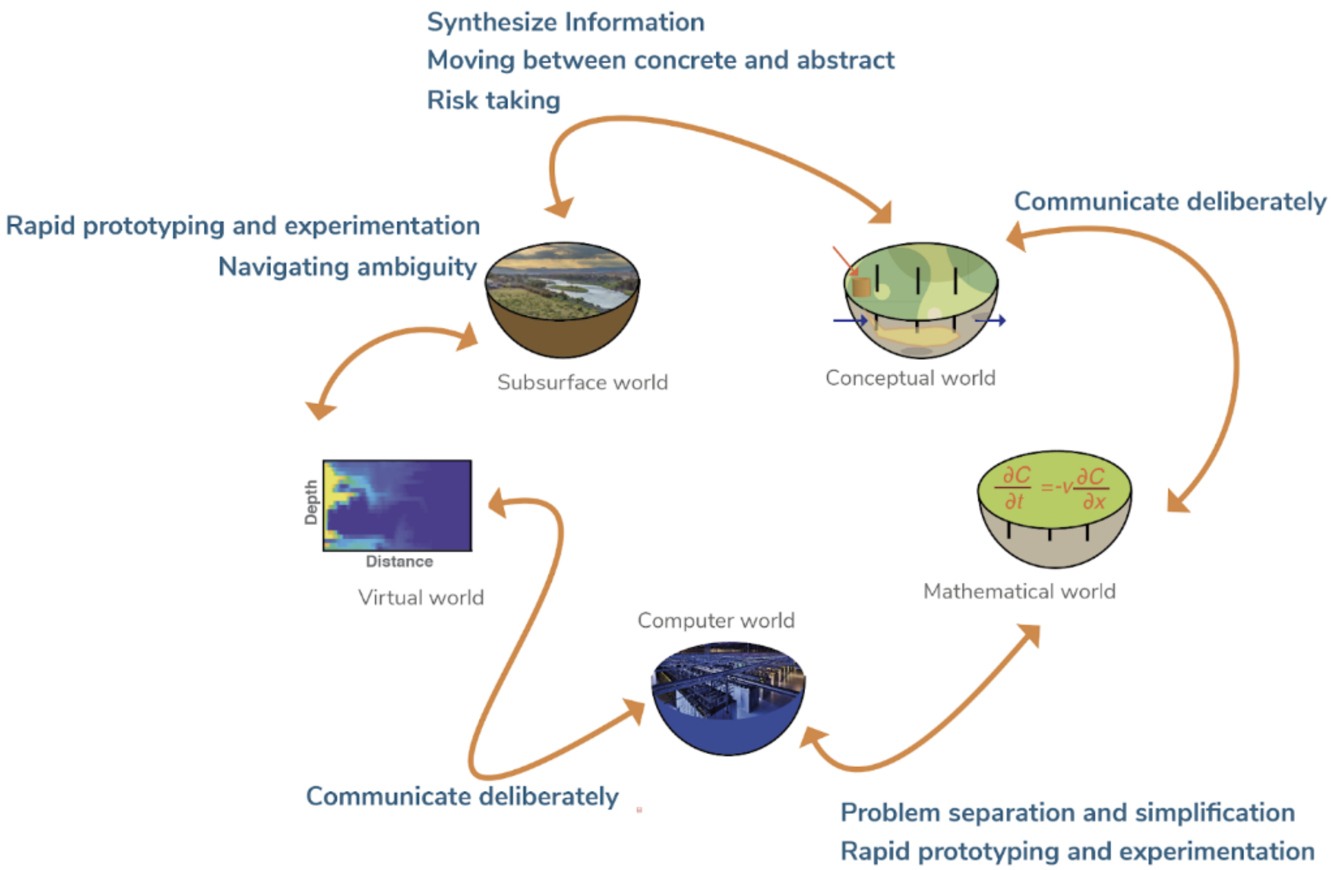


Communicate deliberately: This is the ability to form, capture, and communicate ideas, observations, concepts and learnings between the model and appropriate audience. Knowledge of the theoretical and conceptual foundations of the model and ability to translate a conceptual model into that framework and vice versa. How is knowledge embedded in input files? (#ma-deliberatecom)

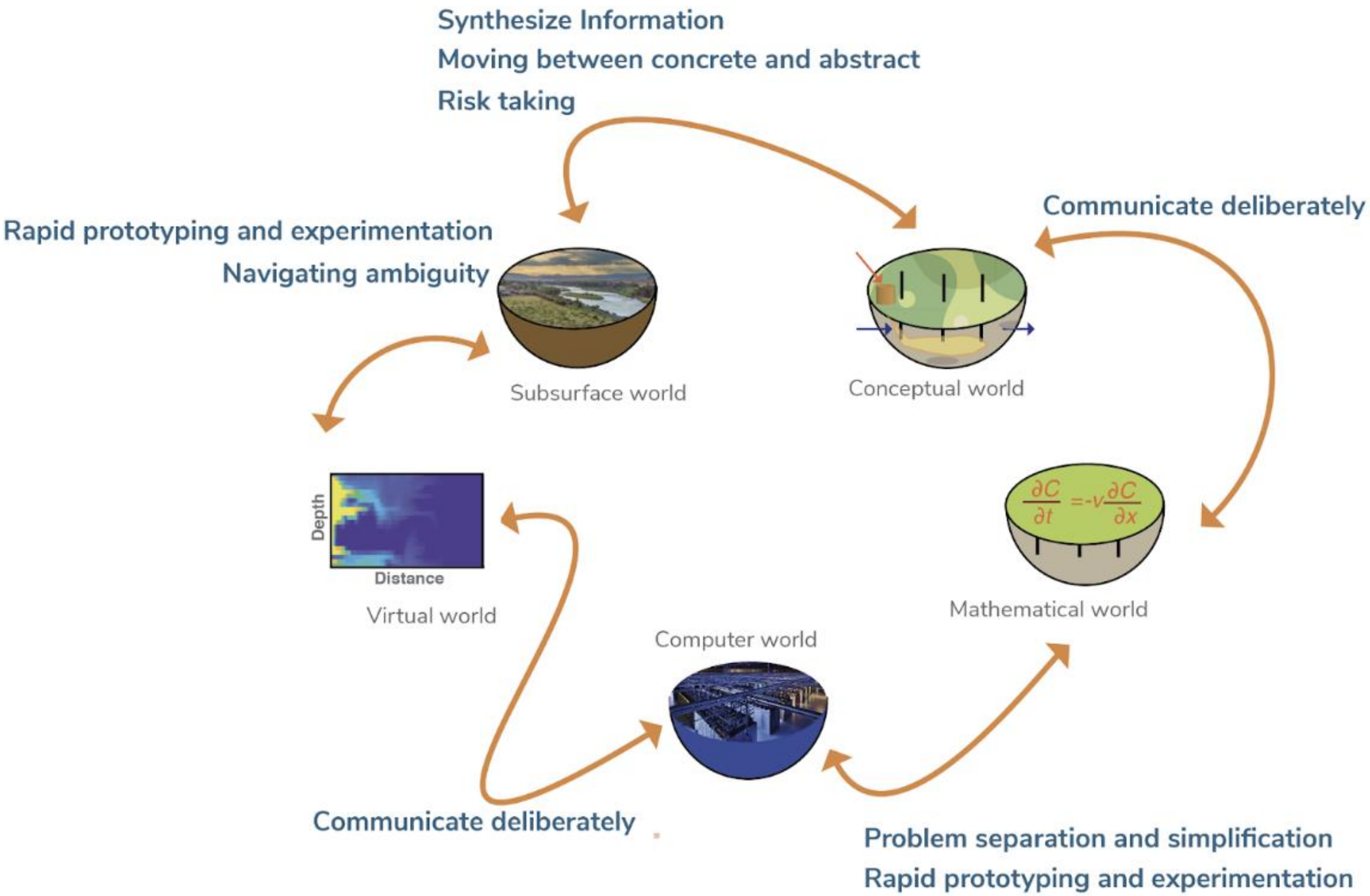
Problem separation and systematic simplification: This is the ability to isolate parts of a complex system and/or systematically identify evaluate simplifying assumptions in order to evaluate their function and operation, either early in the process of building a model or as a form of communicating understanding (#problemsep).

Rapid prototyping and experimentation: This ability is about being able to quickly generate ideas and test them, whether using equations, sketches or numerical models. How do you scaffold model experiments to advance a project rapidly by starting simple and then build complexity. Where do you start? ? (#ma-prototype)

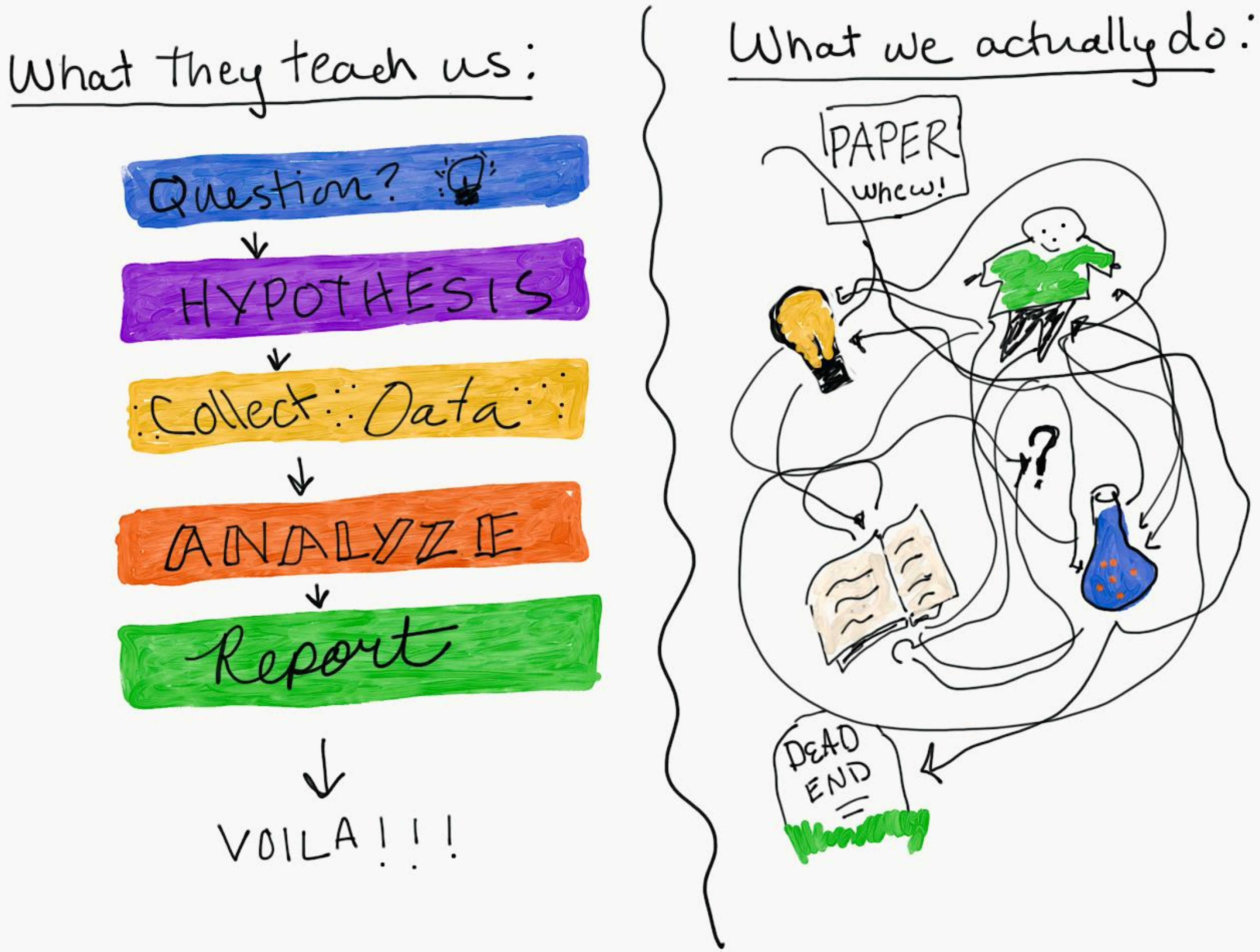
Introduction to Modeling Abilities



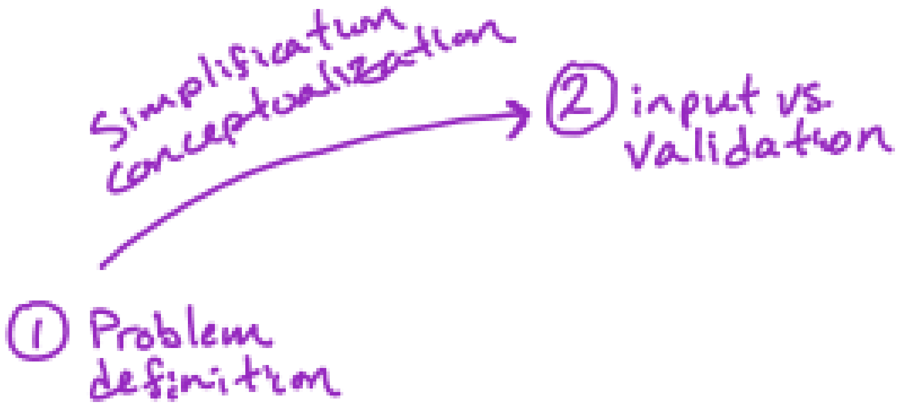
Navigating ambiguity: This is the ability to recognize and manage the discomfort of not knowing, and then to develop strategies to navigate towards an objective. Modeling is rife with uncertainty and the ability to reframe problems, find patterns in data or model output, and persist through ambiguity are important skills for advancing research (#ma-navigateambiguity).



The process does not just move around the circle smoothly and in one direction.


What they teach us:
Question?
HYPOTHESIS
Collect Data
ANALYZE
Report
VOILA!!!
What we actually do:
PAPER
whew!
?
DEAD END

We asked an experienced modeler to sketch the process of modeling……



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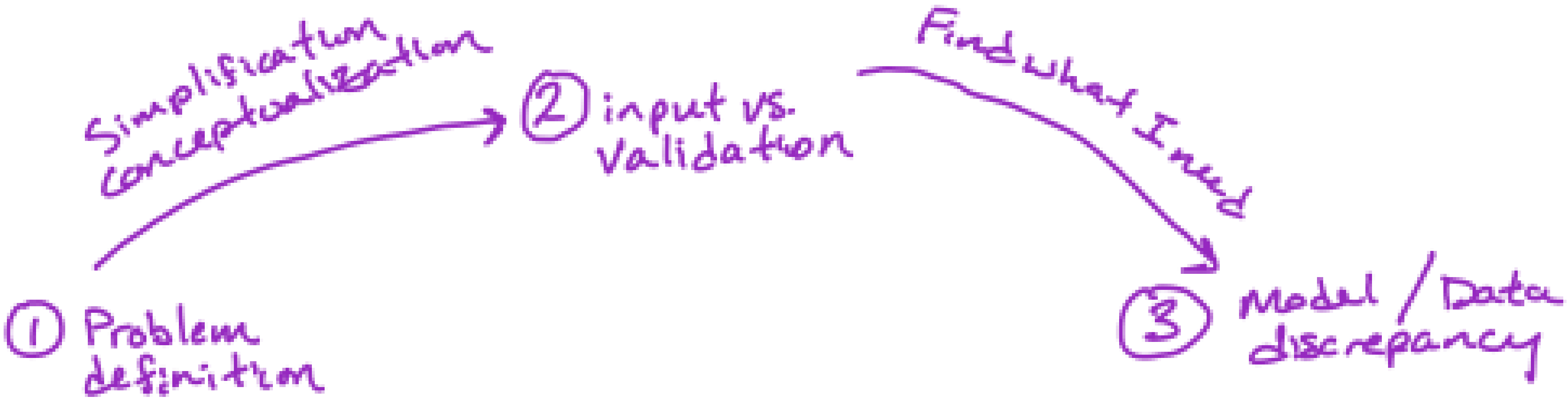

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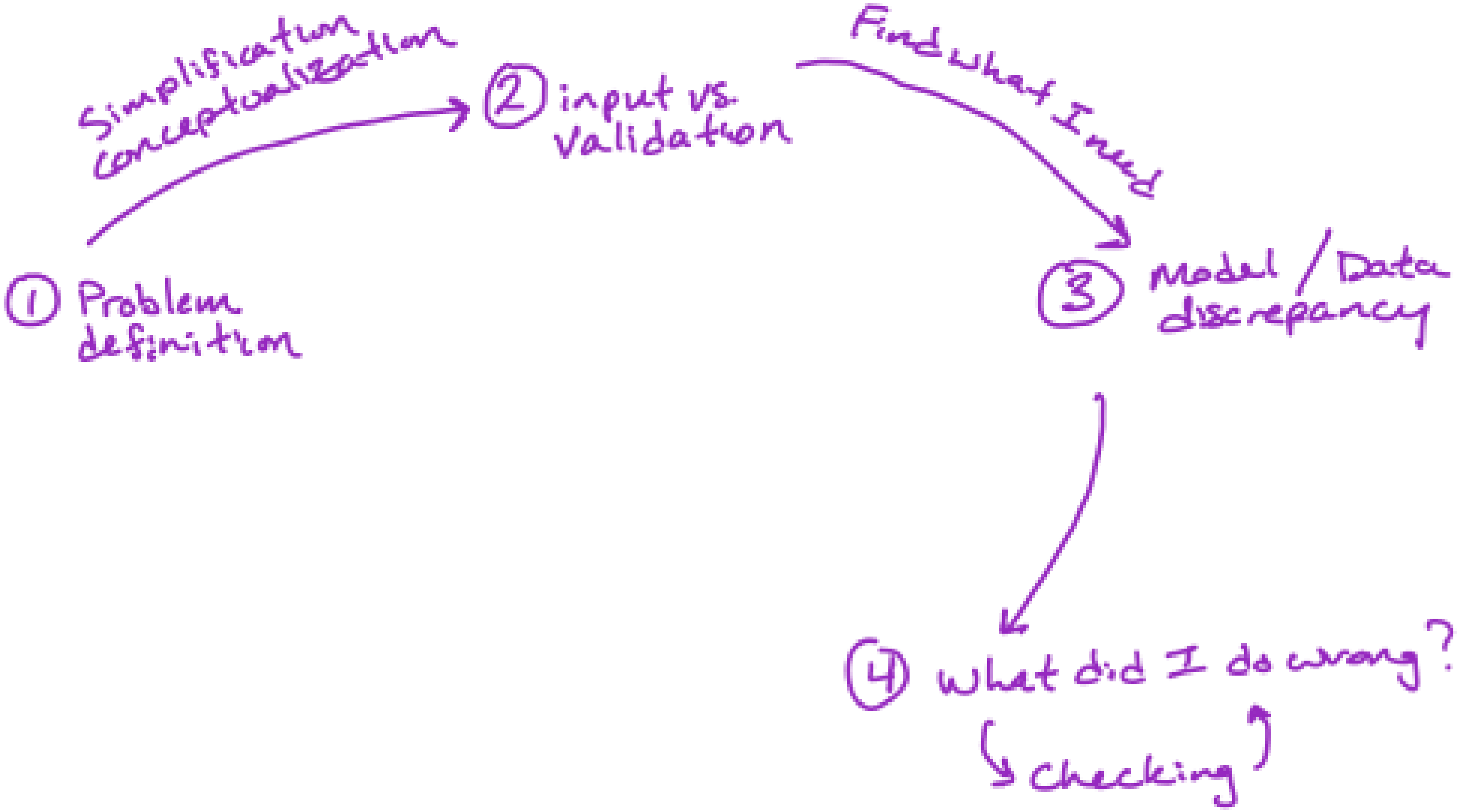

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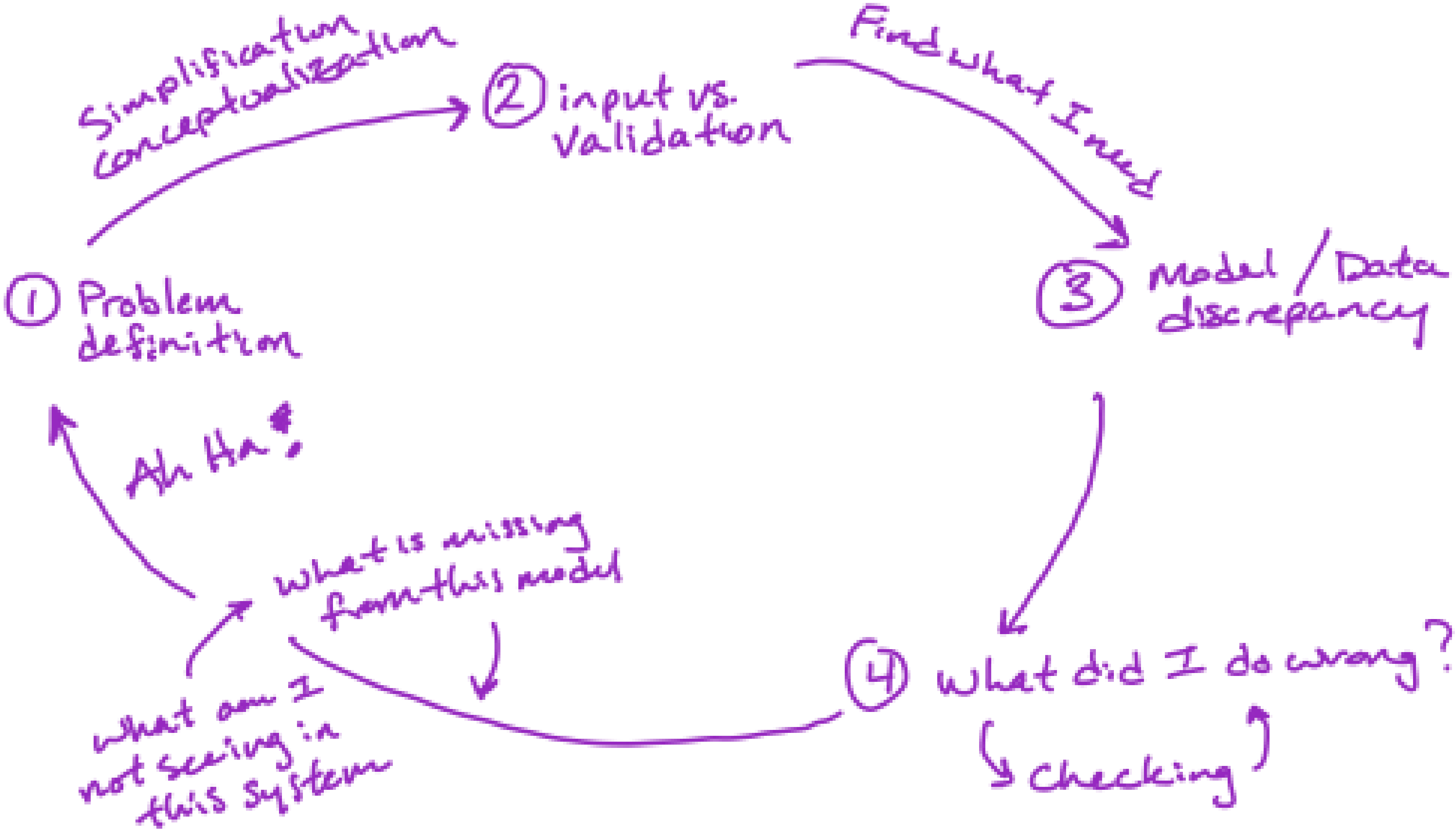

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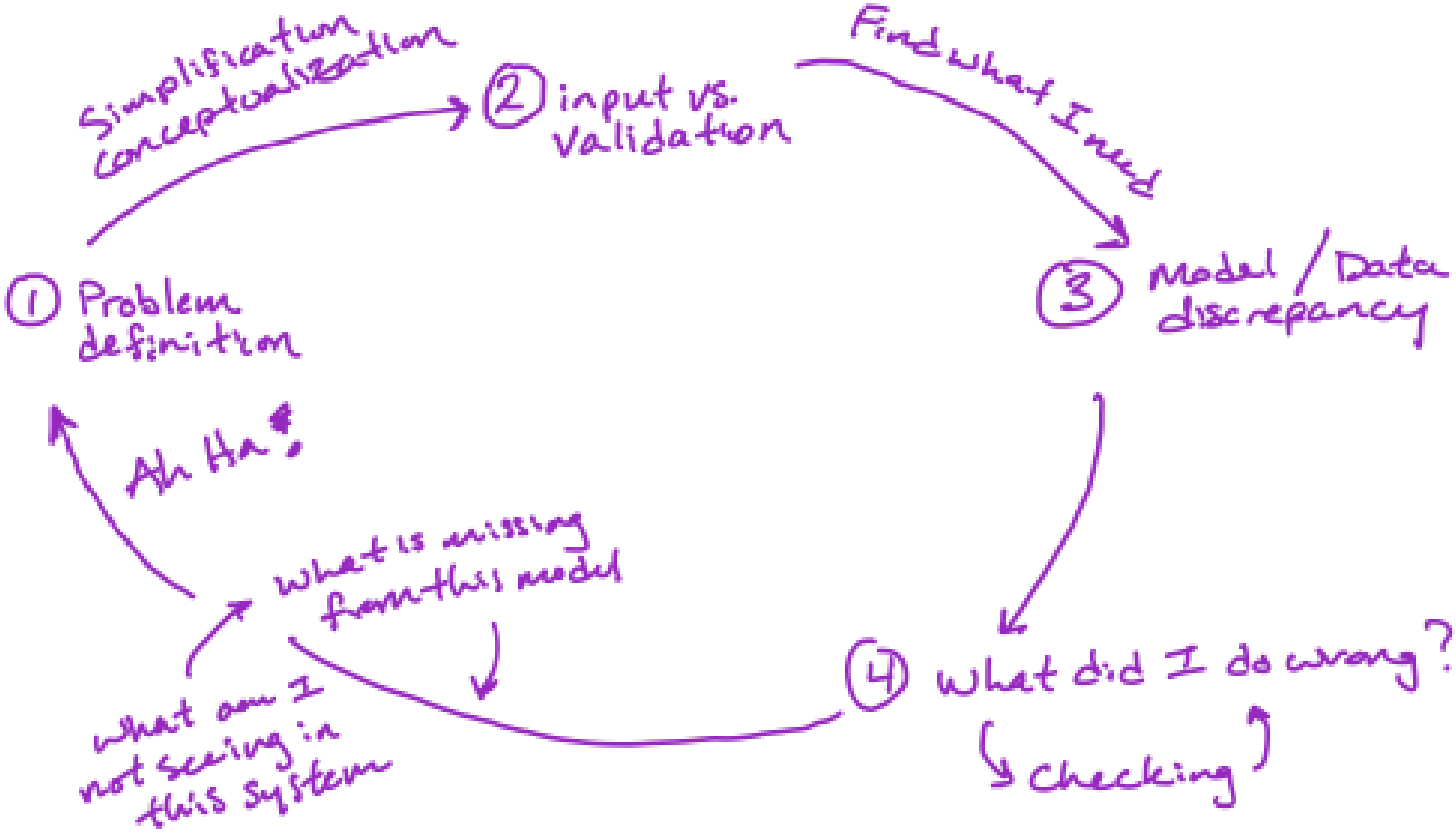

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Two things in the workshop schedule:

2024 RTM Workshop Schedule

TLDR: We will mostly start everyday at 9 am in Room 108, Berthoud Hall

Monday: Introduction to Reactive Transport Modeling I

9:00-9:30	Introductions
9:30-11:30	Fundamentals of Transport
11:30-12:30	Lunch
12:30-2:30	Building Models, Part I: Conceptualizing
2:30-5:00	Fundamentals of Geochemistry

Tuesday: Introduction to Reactive Transport Modeling II

9:00-10:00	Building Models, Part II:
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12:30-2:00	Surface complexation
2:30-4:00	Building Models, Part III

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9:00-11:30	Sediment DIffusion, Kinetics Redox
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12:30-2:00	Heterogeneity and multiple dimensions
2:30-3:30	Chemical Weathering Case Study
3:30-4:30	Building Models, Part IV: Parameter Space to Input File
4:30-5:00	Ta da! Workshop Wrap-up

Thursday: Advanced Modeling Strategies I

9:00-10:30	New Participant on-boarding (new participants)
10:30-11:30	Introduction to advanced modeling (all participants)
11:30-12:30	Lunch
12:30-1:30	Sampling from parameter distributions, Exercise 8-2
1:30-3:30	Analyzing many simulations, Exercise 8-3
3:30-4:00	Introduction to sensitivity analyses
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1. Working through individual models from conceptualization to getting something running.

2. Exercises built to introduce and practice modeling abilities.

Model Conceptualization - 1 Transport

Conceptualize. Sketch a site conceptual model of a system you would like to interrogate with a model. Visualize as much as you know. Think about (1) key boundary conditions, (2) Key initial conditions. Give them labels.

Simplify. Pick a key region from your larger site conceptual model that you can simplify to a 1-dimensional transport problem (or a single flow path line). It may be an interface or a long flow path. Focus on the transport processes only. What would a tracer diagnostic test look like? Is it steady state or transient? Sketch the concentration profile(s) and the concentration history at a key control point.

domain size/discretization (# grid cells and their size):

how will water FLOW occur? Specify relevant parameters/sources.

what TRANSPORT processes are important? Specify relevant processes.

BOUNDARY CONDITIONS on the inlet and exit of the domain:

INITIAL CONDITIONS in the boundary condition and in the domain:

Translate. What would you tell a model? Focus on identifying the domain size, boundary conditions, initial conditions, flow and transport properties. We want to write down the information we will put into an input file. Write some notes about where you think the parameter might come from. Is it fitted? Pulled from literature? Etc.

Model Conceptualization - 2 Chemical Systems

Scaffolding a chemical system. We will start by building the PRIMARY SPECIES (or basis) for your model. Write down the chemical system you envision on the left and then translate that into primary species on the right. Iterate until you have simple and comprehensive primary species.

Key equilibrium aqueous species:

Key kinetic aqueous species (usually redox):

surface reactions (cation exchange, sorption):

Kinetic mineral reactions:

Microbial reactions:

Other:

Primary species:

Secondary species:

Kinetic reactions. For heterogeneous kinetic reactions we have to specify the "mineral", the volume fraction, surface area and a kinetic rate law. Pick a few of the minerals from your list above and decide how you would represent the rate constant, rate law and the initial condition for that mineral. Where would values come from? What type of rate law is needed?

	Rate Law	Initial Condition
Mineral 1:		
Mineral 1:		
Mineral 1:		

Model Conceptualization - 3

Building blocks

These are the core building blocks of a model.

PRIMARY SPECIES

RUNTIME

MINERALS (KINETICS)

DISCRETIZATION

Get specific about what you will build

Look to examples to decide what goes in your model blocks

AQUEOUS (KINETICS)

FLOW & BOUNDARY CONDITIONS

TRANSPORT

Where is there the most uncertainty?

Which parameters will you assume are fixed and which might be "fit" by a calibration procedure? Put a star by the ones you might fit using the model.

Model Conceptualization - 3 Conditions

Conditions are used to populate both the boundary conditions and your domain. As you build your model, keep track of where you need to design a condition. On the map, sketch your domain and show where each condition exists, then identify how you will populate it.

Condition 1:
Where/How?
Primary Species:
Solid Phases:

Condition 2:
Where/How?
Primary Species:
Solid Phases:

Condition 3:
Where/How?
Primary Species:
Solid Phases:

Condition 4:
Where/How?
Primary Species:
Solid Phases:

Model Conceptualization - 4 Planning

First Iteration: What is the first model experiment you will build?

For example, will you focus on transport using only a tracer, or build a batch reactor to let you build up a more complex reaction network before you integrate with transport considerations?

Variables you will assume you know:
These can be model inputs or testing data

Variables you are curious or unsure about:
These can be response variables, parameters you aren't sure how to set, etc.

Second Iteration: What is the next step after your first experiment?

Perhaps you want to layer in chemical reactions? Perhaps you want to test your transport against experimental data? What is the next step that enables you to understand your system?

Variables you will assume you know:

Variables you are curious or unsure about:

Model Target: What is the final objective you hope to achieve with the model you are building?

This might not be the model that yeilds the amazing paper, but rather a model that helps you to advance your understanding of the problem, beyond the simple cases above. Is there a complex feedback or dynamic you want to start to understand? Is there a scaling question?

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Redox reactions across a diffusive front

Overarching Themes:
Fundamental Skills: Numerical conceptualization, dimension, temporal evolution
Modeling Abilities: Abstraction

Project Objective: Evaluate controls on a diffusive reaction front.

Domain expertise challenge:
Fate and transport of nutrients in natural systems are highly connected to redox conditions. One system where a redox gradient develops is the sediment-water interface at the bottom of surface bodies of water (e.g. lakes, estuaries, continental shelf) where waters are oxygenated through contact with the atmosphere and oxygen is consumed in benthic sediments by oxidation of organic carbon. These are inherently complex systems but with some problem simplification and abstraction, numerical simulations provide insight into the processes controlling nutrient cycling across the redox gradient. You will first conceptualize a sediment-water interface in 1D and then develop a simulation of an oxygen diffusion profile in a reactive environment with organic carbon in the sediment. You will test the results of the model against numerical choices of grid discretization and time stepping.

Design questions:

1. How many dimensions will you use for this model?
2. How do you model the oxidation of organic matter by biodegradation simply? Do you have to model organisms themselves?
3. How do you constrain initial aqueous concentrations in the seawater sediments without data?

Domain=Green

Exercise 1

You will start to explore diffusion across a sediment-water interface by first analyzing diffusion of a non-reactive tracer. Set up a conceptual model of this system by defining boundary conditions, equations for transport, initial conditions, and material parameters.

1. Draw a conceptual model of a sediment water interface and label the different aspects of the model. ***(#dk-siteconceptual)***
2. Abstract to a 1D diffusion type model and evaluate diffusion of a non-reactive tracer into the sediment.
3. Draw anticipated diffusion profiles with time (conceptual, not quantitative) and then calculate the diffusion profile analytically using the equation below (you can use the Jupyter Notebook provided if you would like). Use a tracer concentration in the seawater of 1 mmol/kg and in the sediment of 0 mmol/kg.

$$C(x,t) = C_s erfc\left\{\frac{x}{2\sqrt{Dt}}\right\}$$

4. Model a diffusion profile using the same concentrations and compare to your anticipated profile and the analytical solution. Are there differences?

Domain = Green/Blue

Exercise 2

Evaluate the ***#dk-numconceptualization*** of this problem by testing your choice of grid discretization to determine the impacts on the results of a reactive diffusion model. You will modify the input file starting with the input for Exercise 1.

1. First add a solid organic carbon mineral to the seawater sediments, use the mineral DOM(s) that has been added to the database (example on next page). You will also need to add additional primary and secondary species to the input file – try to run the file before adding these so you can see what the error is when you don't add them.
2. Examine the organic matter oxidation reaction in the database and write out the chemical reaction. What are your initial thoughts on this approach to modeling biodegradation of organic matter? (***#ma-abstract***)
3. Run the model and compare the O2 profile to the tracer profile. How does comparing these profiles help inform the behavior of O2 (a reactive species)?
4. Compare the O2 profile to the mineral organic carbon profile. What do you notice about distances where there are changes in slope in both profiles? What is happening here? Think back to the Damkohler number, if you decrease the rate of organic carbon oxidation/dissolution, how would you expect these profiles to change? Test your idea by changing the log rate constant in the input file to -6.

```
MINERALS
DOM(s)                    -label  default -rate -6
END
```

As you just explored, the sharpness of the reaction front is controlled by the reaction rate. In numerical simulations, the sharpness of the reaction front can also be a function of the grid discretization due to numerical dispersion. Refine the grid by using 100 cells as the length but keep the model length to 20 cm.

```
DISCRETIZATION
distance_units      centimeters
xzones             100 0.2
END
```

A place anyone can start:

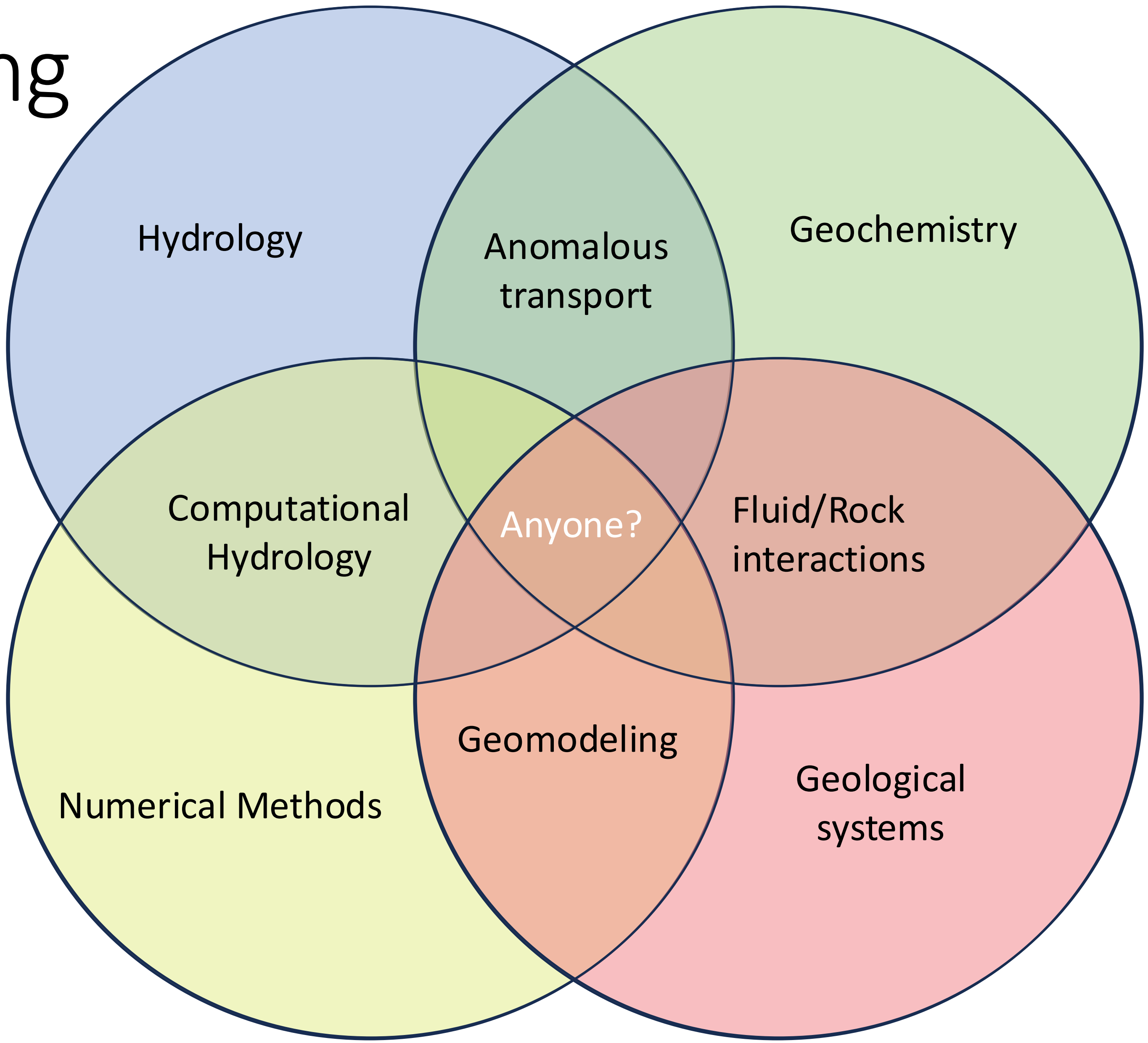
Draw a conceptual model of your system
Include:

Boundaries and boundary conditions – open, closed, isolated
System properties – porosity, permeability, pressure, temperature, chemistry, mineralogy
Inputs – mass flux, concentrations, gases?
Processes inside the system – reactions, diffusion, advection, dispersion
Different parts of the system with different properties and their relationships

Think of a question you want to ask of this model – does this conceptual model have the right information to answer that question?

Adoption and training

What is the fundamental disciplinary curriculum need?



2025 Reactive Transport Summer Institute

June 1-6 at Centre Paul-Langevin, Ile de Oleron, France

Lead instructors: Jenny Druhan, Kate Maher, Alexis Navarre-Sitchler

apply here!

Learn key skills needed to create, apply, and interpret reactive transport models and build a network of colleagues in the modeling community. A background in hydrology and geochemistry is required, and some experience modeling is beneficial.

Introduction to RTM
- Basics of RTM: advection, diffusion, reaction
- Redox driven nutrient cycling
- Mineral dissolution kinetics
- Cation exchange and surface complexation

Advanced topics
- Dimensionality and heterogeneity
- Sensitivity Analyses
- And more!

Participants will be responsible for the cost of travel to Ile de Oleron. During the workshop, lodging and meals for all participants will be provided by NSF award 1935321.

NSF

Reactive Transport Summer Institute
https://www.mines.edu/reactivetransporthub/

Continue this training under a new funding and logistics model.

Online course modules on fundamental disciplinary knowledge.

Reactive Transport "office hours" at conferences.