Table 1: Computational Thinking Practices

Computational Thinking	Description	Example for Groundwater Contamination
Discretization	Analyzing change over a continuous space requires dividing the space into discrete chunks or cells. Values can then be assigned to these cells and analyzed within a computer model. The number and size of the cells has trade-offs in accuracy, precision, and performance, depending on the data available or the size of the system being modeled.	The three-dimensional volume of an aquifer is divided into discrete cells to be represented in the model.
Parameterization	A parameter is a characteristic of a system that gets assigned a value within the model. Parameterization is the process of identifying those characteristics and assigning values.	One key parameter relevant to modeling groundwater is the permeability of the Earth materials composing the aquifer. Each discretized cell is assigned a value for permeability associated with the local strata.
Interpolation	Parameter values for the discretized cells are based on data, but one rarely has data for every cell within a model. Interpolation is the process of estimating values from a set of known data points.	In a groundwater system, the exact permeability can only be measured in locations where there are wells. Interpolation is needed to calculate the permeability parameter values for the locations in between.
Writing Rules	For a computer model to produce representations, rules (also called algorithms) are written to instruct the model how to use the information in each cell. These rules reflect model-based principles of the relevant discipline.	For a simple groundwater system, two rules are needed to instruct the model how to trace water and contamination through the aquifer[1]. 1. Direction rule: Water flows from high potential energy to low potential energy. 2. Velocity rule: Water moves more easily through high permeability materials, such as gravel, than low permeability materials, such as clay.
Iteration	Computer models are especially efficient at performing repeated calculation routines to converge towards approximations of a solution.	Tracing contamination of water through a model of a discretized system requires repeatedly running the model, with each run representing a next step in time.

[1] Darcy's law, the equation for modeling groundwater flow, incorporates permeability and change in pressure (related to gravitational potential energy in an unconfined system and pumping in a well) to produce one value for the volume of water that moves past a given point in a given time. For pedagogical purposes, we disaggregated permeability and potential energy so that students can recognize how changes in substrate (e.g., sand, gravel, clay) and elevation or pumping might influence the rate and direction of groundwater flow.