Groundwater

Issue Paper/

Next Generation Computers Warrant Next Generation Groundwater Models

by Nicholas B. Engdahl

Abstract

Modern hydrologic models have extraordinary capabilities for representing complex process in surface-subsurface systems. These capabilities have revolutionized the way we conceptualize flow systems, but how to represent uncertainty in simulated flow systems is not as well developed. Currently, characterizing model uncertainty can be computationally expensive, in part, because the techniques are appended to the numerical methods rather than seamlessly integrated. The next generation of computers, however, presents opportunities to reformulate the modeling problem so that the uncertainty components are handled more directly within the flow system simulation. Misconceptions about quantum computing abound and they will not be a "silver bullet" for solving all complex problems, but they might be leveraged for certain kinds of highly uncertain problems, such as groundwater (GW). The point of this issue paper is that the GW community could try to revise the foundations of our models so that the governing equations being solved are tailored specifically for quantum computers. The goal moving forward should not just be to accelerate the models we have, but also to address their deficiencies. Embedding uncertainty into the models by evolving distribution functions will make predictive GW modeling more complicated, but doing so places the problem into a complexity class that is highly efficient on quantum computing hardware. Next generation GW models could put uncertainty into the problem at the very beginning of a simulation and leave it there throughout, providing a completely new way of simulating subsurface flows.

Introduction

Models of groundwater (GW) flow processes have continuously evolved in their efficiency and complexity over the last several decades, and the greater GW community now has at our disposal a set of tools that can represent, in some way, nearly every kind of physical interaction important for water resources applications. Advances in parallelization (multithreading and multiprocessing) have also drastically increased the speed of the solvers so these complex, physics-based models (e.g., Kollet et al. 2010; Rasmussen et al. 2011; Clark et al. 2015) are no longer mere speculation. The tradeoff is that more cells and variables means more parameters and this is where GW has some issues to deal with. A classic example is that the hydraulic conductivity, K $[L/T]$, field cannot be known with much confidence away from direct measurements in boreholes, and the same is valid for any other physical properties or parameters. Another example is recharge, which can vary heavily over short distances. Recharge into an aquifer reflects a balance between precipitation, infiltration, runoff, evaporation, and transpiration; all depend heavily on soil and vegetation types and all can be quite difficult to measure accurately. GW modeling is plagued by uncertainty yet it is not common to see articles or model reports that formally present the uncertainty associated with a simulation and/or prediction (Tartakovsky 2013); there may be good reason for this in some cases, but it

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is an issue. Some publications present the K field (or any other parameter field) as if it is a deterministic quantity, uniquely resulting from inverse modeling, adding only brief notes, if any, to suggest that it might be a non-unique field. Calibration and sensitivity analyses can be conflated with uncertainty quantification (UQ) when reporting results to stakeholders. For example, perturbing inputs by plus or minus some amount shows sensitivity not uncertainty, but the layperson is unlikely to recognize the distinction. Hydrologic simulations are becoming increasingly important for large-scale water resources planning and it is important to ensure that their limitations are accurately reported. As many authors have stated before, the balance between realism, runtime, parsimony, and uncertainty in models remains an important topic for debate, but after several decades devoted primarily to making more realistic (i.e., complex) and faster models, it is worth assessing how we can do better regarding uncertainty modeling and reporting in the future (e.g., Hunt et al. 2007; Hunt 2017; White 2017). Next generation GW models are going to play important roles in future water resources management, and the task of building new kinds of models that can do a better job of including uncertainties should at least be equal to building ones that run faster. Interestingly, these two outcomes might not be mutually exclusive.

The objective of this article is to ponder briefly when assessing uncertainty is important in increasingly complex GW simulations, and then explore how we might do a little better with new kinds of models that could potentially do more than just run faster. The structure of this issue paper loosely follows that of a talk given at the 2022 Modflow and More conference titled "*An uncertain future for hydrogeological modeling*" but comments, feedback, and lesson learned since have added new dimensions to the message of that presentation. Most of the discussion will be general and citations of example models (be they superlative or nefarious) are kept to a minimum to avoid any perception of this being a critical review or of it being an attack on any subset of the literature; this article is nothing more than the author's perspective on how GW modelers might best embrace a potential revolution in computational technology. There is no one answer to the question of what future GW models will look like, but the argument made herein is that if the fundamentals of the computers are going to be changing (i.e., quantum computing) then the mathematical approaches to the GW simulation problem should change too.

Confidence in Groundwater Simulations

Uncertainty is a tricky issue to address. Many areas of the physical sciences require reporting of confidence bounds on all results, but GW is unique in that what we might consider "abundant data" is still extremely sparse in all other disciplines. Given the vastness of the subsurface and its inaccessibility, is it really that important to quantify uncertainty in all GW models in the first place? If one inspects the literature, it becomes clear that there are far fewer examples of GW models where uncertainty is reported than those that do not, so it would seem that the answer is no, but it is worth at least a little pondering as to why. UQ is an entire discipline (see Tartakovsky 2013) and uncertainty modeling has been given a great deal of attention in many of the industry standard textbooks on GW modeling (e.g., Domenico and Schwartz 1998; Anderson et al. 2015; Fetter 2018). The approaches range from stochastic perturbation methods (e.g., Rubin 2003; Fiori et al. 2015), Monte-Carlo simulations (e.g., Ballio and Guadagnini 2004; Engdahl et al. 2010), to more recent techniques like the method of distributions (Boso and Tartakovsky 2016) and integrated ensemble smoothing (White 2018; White et al. 2020). The reason UQ is not more widespread in GW modeling is most likely that all of these methods require significantly more effort and resources than just running or calibrating a GW model. This effort might not be possible given time and budget constraints of a client, or certain application/design scenarios might have sufficient margins built in that the likely range of uncertainty would not be expected to change a decision (see Hunt 2017; Barnett et al. 2020). Other cases where UQ is commonly omitted are numerical hypothesis testing studies. These kinds of studies use models to explore system responses, often focusing on relative change due to a perturbation (Engdahl and Maxwell 2015; Wilusz et al. 2017; Visser et al. 2019), or the investigation of feedbacks (Condon and Maxwell 2014; Kollet et al. 2017; Maina and Siirila-Woodburn 2020). It is not that these examples do not have uncertainty, or that given enough time and resources it should not be quantified, rather that the circumstances/conclusions are not expected to change if that uncertainty were to be explored. The catch is that, obviously, this expectation cannot be confirmed for sure without the uncertainty analysis. It would be worthwhile for some new studies to explore this in more detail to provide stronger guidance, but a lack of UQ in applied problems it is generally not considered to be a serious concern.

There is at least one broad class of studies where better UQ could be hugely beneficial in water resources modeling: predictive models. Every calibrated model will contain uncertainty and this will be propagated into predictions, compounding with whatever uncertainty there is regarding model conditions during the prediction phase. Some applications within this arena where uncertainty can make an enormous difference include transport models in systems with preferential flow paths, predictions in the face of unknown climate conditions, unknown timing and severity of abrupt changes like wildfires, and countless others involving a wide range of things we simply cannot know for sure or place reasonable margins on "acceptable" responses. The models currently used to make predictions in many of these cases are either overly simplified or excessively parameterized, depending quite subjectively on who is criticizing the work. Annoyingly, both positions are often valid assessments. For example, travel times

in systems with highly preferential flow can never be reasonably approximated by a homogenized, effective model, and UQ cannot be performed on models will billions of degrees of freedom that take weeks to run one realization on a supercomputer. Both of these examples are systems that involve high degrees of uncertainty where that uncertainty significantly impact predictions, plans, lives, etc. and it is within these areas where improving the connections between uncertainty and forecasts could have the biggest impact given the inevitable time and resource constraints. Progress has been made in this area (e.g., White et al. 2020), but it continues to be difficult to see how we might breakthrough and achieve drastic improvements in predictive UQ given the limitations of current modeling techniques and computers.

What Are the Next Generation Computers?

Next generation means completely different and right now that means quantum. Quantum computers (QCPs) are difficult to define precisely but the unifying feature is that they manipulate "digital" states in ways that follow the rules of quantum mechanical systems, as first proposed by Benioff (1980). This is contrasted to classical binary digital computers (BDCs) that strictly follow rules that can be considered to be based on logic (Deutsch 1985). Conceptually, a BDC is a yes/no engine whereas a QCP can say maybe, similar to the way a person might not always choose to do what appears to be the most logical thing (obviously this is *not* an exact analogy). Information in a BDC is stored as binary digits, or bits, that may only exist in a state of 1 or 0, meaning that a single bit represents one state. Any information can be built up and stored in this way, from numeric values to pictures, within a certain level of precision dictated by the number of bits used to represent that information. The quantum version of this is a quantum bit, termed a qubit, and it is helpful to consider the two, classical, binary outcomes as each representing one of two orthogonal basis vectors (in bra-ket notation): $|\,0\rangle = [1\ 0]^T$ and $|\,1\rangle = [0\ 1]^T$, where ^{T} denotes a transpose to create column vectors. A qubit is made from a linear combination of these basis vectors. Denoting the state of the qubit as ψ, the vector representation of this is:

$$|\,\psi\rangle = a\,|\,0\rangle + b\,|\,1\rangle \tag{1}$$

where a and b are complex numbers, so $|\,\psi\rangle$ is best considered as a sort of mixed state. According to the Born rule (Born 1926), the complex coefficients represent the *probability* of obtaining each state so $|a|^2 + |b|^2 = 1$ and, for example, $|a|^2$ is the probability of being found in the state $|\,0\rangle$. But strangely, unless $|a|^2 = 1$ *or* $|b|^2 = 1$, when we observe the state of $|\,\psi\rangle$ it can only be either $|\,0\rangle$ *or* $|\,1\rangle$. Thus, there is an *indeterminate* nature to the system's information. If the system is re-prepared in the same state and measured a large number of times the probabilities become apparent, but any individual measurement only results in *one* of the possible states. This is called quantum superposition which is a stark contrast to classical superposition where the outcome of the measurement would be *intermediate* between $|\,0\rangle$ and $|\,1\rangle$ forming a weighted average of the vectors instead.

A QCP encodes information using a collection of qubits, called a register, that represents 2^n possible states, where n is the number of qubits. Mathematically, the QCP manipulates this information using the same kinds of linear operators used in quantum mechanics (analogous to matrices of square dimension 2^n in order to operate on n qubits), so the QCP can be considered a "reduced basis, physical analog" to a quantum mechanical system. QCP-based manipulations have some curious requirements such as the fact measuring a state causes it to assume a determinate state, destroying the quantum part of the state, and that all operators must be reversible. For example, x^2 is not a reversible operation since its inverse, $\sqrt{x}$, has a two possibilities. Because of these and other properties, QCPs are suited to an entirely different class of computational complexity problems than most of the algorithms used today in GW flow and transport problems. A key difference is that the QCP is inherently random because of the indeterminate nature of the qubits. This has implications for how deterministic problems can be solved and that the efficiency of something implemented on QCP hardware depends on the computational complexity of the task. For example, many algorithms exist for solving a linear system of equations using BDCs and the same algorithm (e.g., Gaussian elimination, etc . . .) translated onto QCP is seldom (if ever) efficient. However, sometimes a randomized algorithm can be developed and in these cases a QCP can offer significant speedup for some problems. Additional notes on QCPs that are intended for a broad scientific audience can be found in Giani and Goff-Eldredge (2022).

Avoiding a lengthy, jargon riddled discussion, the important summary points are that very little about how a QCP works is the same as how our current BDCs work, and that only specific *complexity classes* of problems are suited to QCP implementation (e.g., non-deterministic polynomial, etc . . .). The architectural, conceptual, and operational differences from contemporary tools are unfamiliar to most of us, but this is always the case with new technologies. Next generation GW models should not just mimic our current models but should instead address frustrations or deficiencies while building new capabilities, like better UQ for predictions. The fact that a QCP is inherently uncertain could be immensely powerful for embedding uncertainty into GW simulations, but, to date, no recipes for doing so have been proposed.

Toward Next Generation GW Models

The main issues under consideration here are (1) what are next generation GW models going to look like (supposing that the next generation computers are indeed quantum), and (2) can we develop GW models that do a better job of dealing with predictive uncertainty. There are already several possible avenues by which QCPs and

QM concepts might find their way into GW workflows. Each of these involves some conceptual and/or technical challenges, but these seem surmountable given a bit of focused research. This section outlines three options for bringing GW models to QCP hardware each with a slightly different goal: option 1 is solving the same linear (or linearized) systems as done today, option 2 is solving a different kind of classical mechanical system that could represent GW flow but in a way conducive to QCPs, and option 3 is creating an "effective quantum model" that uses properties of QM to create new ways of representing complex process in aquifers. These sections by no means comprise an exhaustive list of the possibilities and are only meant as brief overviews of what currently seem like some promising options for GW modeling on QCPs to stimulate further conversation, discussion, and research.

Solving Linear Systems

Suppose for a moment that the goal is just to start running some relatively simple GW models, like those in use today (e.g., confined, Darcy flow), on quantum hardware. Conceptually and mathematically this problem is well defined and it is the solution of a (potentially) large and sparse linear system. An algorithm has already been developed by Harrow et al. (2009) for solving linear systems on QCP systems that requires time proportionate to $\log(N)s^2\kappa^2/\varepsilon$, where N is the size of the linear system, s is the sparsity, κ is the condition number, and ε is the numerical tolerance. Interestingly, the number of qubits required, m, is generally $m = \log_2 N$ (Hidary 2019), so a 1024×1024 system can, theoretically, be solved with 20 qubits, and a 3d domain with $1024 \times 1024 \times 1024$ cells should require only 30 qubits. Using conjugate gradients to solve the same problem requires time proportionate to $Ns\kappa \log(\varepsilon^{-1})$ so the HHL algorithm (HHL is an abbreviation of the authors names) can exhibit speedup relative to current methods under many circumstances, but the speedup is not guaranteed and can rapidly breakdown (Aaronson 2015). The HHL algorithm has been improved and generalized several times (e.g., Childs et al. 2017; Wossnig et al. 2018) but even 20 fault tolerant (error correcting) qubits are out of reach for current gate-based QCP hardware. However, as the technology improves, these techniques will almost certainly become available. Another potential path forward related to the HHL algorithm can be found in Berry (2014) where a method for solving general linear differential equations is presented, but the current limitation is again hardware. A crucial distinction is that all of these techniques would allow solution of the same equations currently in use, using an inherently random QCP to solve deterministic problems (to be fair, "randomized" solutions can be more efficient sometimes, but there is ultimately one solution). It is possible that the potential speedup might accelerate solutions of GW flow systems sufficiently that ensemble-based UQ could be less cost prohibitive, but it would not directly incorporate uncertainty into the governing equations. The HHL algorithm could be a useful stepping stone but it is not clear that this path would provide the kind of speedup that would be necessary to allow robust, ensemble-based UQ to become standard.

Koopman–von Neumann Dynamics

The most efficient QCP implementation for GW models on QCP hardware is likely a model that behaves more like a QM system, yet is not quite quantum. The argument being that, since a QCP obeys QM rules, the more "quantum-like" the quantities being simulated are the less overhead they will incur on a QCP. The result of this should be outstanding speedup if they are in the right class of computational complexity. One way this might be achieved with relatively little discomfort is the connection between the Schrödinger equation and the less familiar Koopman-Von Neumann equation. The latter was developed by Koopman (1931) and von Neumann (1932a, 1932b) in an effort to use the same mathematical framework to describe quantum *and* classical systems. Compare their equations

$$i\hbar\frac{\partial\psi}{\partial t} = \widehat{H}\psi \tag{2a}$$

$$i\hbar\frac{\partial\psi}{\partial t} = \widehat{L}\psi \tag{2b}$$

where ψ is a complex ($\psi \in \mathbb{C}$) state function, $i = \sqrt{-1}$, the operator $\widehat{H}$ is the Hamiltonian operator (Schrödinger equation, abbreviated "SE") and $\widehat{L}$ is the Liouville operator (Koopman-von Neumann equation, abbreviated "KvN") from statistical mechanics (see McQuarrie 2000; Mann 2018) or $\widehat{L}$ may be replaced with a generalized KvN operator (Chirikov et al. 1988). The constant $\hbar$ is typically the reduced Planck's constant, but more generally it represents a fundamental scale of quantization. Choosing (2a) or (2b) and solving for the abstract state function allows one to compute expected values of observables or dynamic quantities in quantum or classical systems (Bohm 1951; Cvitanovic et al. 2005). The main difference between (2a) and (2b) is that $\widehat{H}$ is usually second order and $\widehat{L}$ is first order, but closer inspection shows more. Define a trial solution for ψ such that $\psi = A\exp iS$, where A and S are arbitrary real-valued functions of space and time. Substitution into (2) for typical definitions of $\widehat{H}$ and $\widehat{L}$ reveals that A and S (termed the amplitude and phase, respectively) are decoupled in KvN but coupled in SE, meaning phase interference and other uniquely quantum effects are not possible using KvN (Mann 2018), which is good because they are not observed in classical mechanical systems. The KvN is also posed in a "phase space" representation where the independent variables are position and conjugate momenta, whereas SE is not, but this also means that classical probabilistic systems have workloads similar to quantum systems since the latter is described by a complex probability amplitude ($\mathbb{C}$ has twice the dimensionality as $\mathbb{R}$). There are also differences in how the results are interpreted, but these details are not germane to the present discussion. Functional and conceptual differences aside, classical

and quantum systems can be represented using state-function based operator notation, so classical systems that can be represented by KvN can be solved on QCP hardware using tools similar to those for the SE. Recent research suggests this is practical and could be highly efficient even for nonlinear dynamics (Joseph 2020), so this is a promising avenue if an associated conceptual picture for ψ can be built up for GW systems. The KvN approach is also more general than HHL since it is able to handle nonlinear and non-Hamiltonian systems, meaning that Richard's equation and coupled/integrated systems simulations (e.g., Hammond et al. 2014; Painter et al. 2016; Kuffour et al. 2020) might even have a path to QCP implementation. What is needed to realize this is to pose GW flow in phase space and map its evolution operators, boundary conditions, and initial conditions onto KvN operators, but doing so seems to be reasonably within grasp.

An Effective Quantum Model

The suggested HHL approach could only address the UQ issue when combined with ensemble simulations, so let us finally consider what a model framework might look like that requires the modeler to evolve *distributions* of properties instead of our current paradigm, for example, one value per cell. Working with distributions directly (or a superposition of distinct states) has direct connections to QM, specifically Heisenberg's uncertainty principle which dictates tradeoffs in the precision with which observables like position and momentum can be known. Abstracting somewhat, consider that when the cell size of a model is defined it now represents an averaging volume where a single mean velocity, for example, is considered, but in reality there should be a distribution of velocities within every cell. Mainstream GW flow models deal in terms of only the average over a cell and the implied assumption is that any distribution within that cell is narrow (small fluctuations about the mean) and/or is Gaussian. However, these are the same reasons why stochastic perturbation approaches are limited to small variance fields and why dispersivities are needed for transport simulations; the sub-grid velocity distribution does not exist in the GW flow model, yet we know the sub-grid variability influences transport and must re-introduce the distribution via spreading operators. Rather than try new "fixes" to our existing flow and transport workflows, the suggested course of action is (1) to build a new kind of GW model framework that works in terms of velocity distributions to embed uncertainty into the problem, and (2) to build it with the target of implementation on QCP hardware from the outset. It may be possible to do much of this within the KvN framework, but here we consider an even more general option that could leverage uniquely quantum aspects of the hardware. Note that quantum annealers, a simpler cousin to general QCPs, have already been used for inverse problems in hydrogeology (O'Malley 2018), but annealers are designed for optimization and are not as well suited to the simulation of distributions.

The mathematical framework laid out by Dirac (1981), and the earlier version of Heisenberg (1925), are generic linear operator frameworks, often called matrix mechanics, and it may be possible to use these tools to define a set of operators to represent GW flow mechanics. These are alternatives that encompass the SE so the core-concept is still the evolution of an abstract state function, ψ, that allows computation of observables (Bohm 1951), but there are some differences in how this ψ is interpreted relative to the same ψ in the KvN framework (Joseph 2020). Requirements for this new method should be developed following lines of reasoning similar to those used to develop QM. At a minimum, the new equations should be required to recover the classical GW flow equations in their "limiting behavior" and should be able to reproduce observations. Regarding the limit, good models for how to achieve this are the correspondence principle (Bohr 1920) and the Ehrenfest theorem (Ehrenfest 1927), which provide the conditions under which the behavior of a QM system adheres to Newton's laws. The point is that the time evolution of the mean of a QM system (i.e., expected position of a particle) does not necessarily follow classical mechanics, but in some important cases, like quadratic potentials or small fluctuations about the mean (Messiah 1962), the classical equations of motion are recovered exactly. Regarding the reproduction of observations, application of measurement operators to the state function ψ should be able to honor all observations to within the precision of the measurement. The uncertainty of the ψ field away from conditioning points would likely yield a map similar to that of prediction variances from kriging, for example, but all the uncertainty of all the properties, measurements, and observations could be embedded in the simulated distribution functions. The distributions represented in these fields would not be restricted to well-behaved (i.e., Gaussian) distributions because the quantum version of superposition allows distinct states to persist when they are combined, and the superposition affects the probabilities of every state. Consider a fractured aquifer made up of small, high K preferential pathways and large volumes of low K aquifer. The classical approach would force us to average these two into a single volume averaged unit but a quantum-like superposition would allow preservation of the bi-modal nature of this system, evolving all the unique distributions over time. Conceptually, this is similar to the method of distributions of Boso and Tartakovsky (2016), but posed using quantum-like mathematics.

A model as suggested here will be more complicated than the GW models commonly seen in the literature but increasing the complexity is sometimes necessary (Hunt et al. 2007), especially if the goal is to embed UQ (e.g., Boso and Tartakovsky 2016) instead of assuming it away. This may seem like a massive increase in complexity but only when comparing to a deterministic model. In reality, stochastic Monte-Carlo methods have similar resource requirements to quantum systems (Joseph 2020). A key difference relative to the development of recent GW

models is that this suggested increase in complexity is solely to describe the uncertainty and not to add more processes or to accelerate current solution methods. Regarding how to build such a model, it seems reasonable to start with a KvN implementation of a GW model. If that does not achieve all the modeling objectives, the KvN model could be used as a stepping stone to develop a "quantum-like effective model." The latter could evolve a discretized version of ψ using matrix mechanics that are naturally suited to QCP hardware. Quantum phenomena like entanglement and tunneling could be used to represent long range correlation effects and statistically rare events, and the indeterminate nature of the model would render it stochastic from the outset. These new QCP-based models would still be similar to a large Monte-Carlo ensemble that includes *all* parameter uncertainties, but the acceleration of truly quantum problems on a QCP is excellent, ranging from polynomial to exponential speedup (Hidary 2019). Contrast this with the requirements for classical Monte-Carlo ensembles on a BDC which are (at best) linear with the number of realizations in the ensemble and consider that the number of realizations needed increases quadratically with the desired accuracy. The potential speedup on QCPs and the potential ability to embed an arbitrary level of uncertainty into GW models makes this kind of effective model an enticing prospect, but the idea has, literally, just been proposed and is in its infancy.

Discussion

Statements about how QCPs might transform science are increasingly common but often lacking are the specifics regarding how this will be achieved for general problems rather than toy problems. This issue paper also lacks detailed specifics, but is at least less vague than previous presentations. The intent is to present some food for thought and stress that the methods of the past need not be those of the future. Throughout, it has been emphasized that translating our current models to QCP hardware is not likely to be an efficient approach and that it is time to try unconventional approaches, even if many of them will not work. As new approaches are tested, the limitations and deficiencies of current generation GW models should be assessed so that the next generation GW models can be conceptual *and* computational advances over those of the past. Indeed, many issues exist in typical proceedures used for GW modeling but the most underrepresented in the literature seems to be robust UQ for predictions. The indeterminate nature of QCPs seems naturally suited to the UQ problem if GW simulations can be posed in the natural language of a QCP. The assessment of (Sposito 2001) may ultimately be correct in that quantum-like methods might not offer any new insights in the field of GW, but QCPs are promising tools for providing new ways of efficiently solving the problems and, perhaps, simultaneously embedding uncertainty or even unresolved heterogeneities in our models (Engdahl 2021). Right now, the most promising approach toward implementing GW models on QCP hardware may be the KvN equation from which the more quantum-like effective model might naturally emerge. Treating GW flow systems at the quantum level (i.e., at the scale of electrons) is obviously impractical, and unnecessary, but aquifers are systems where statistically rare events can have massive impacts on the range of simulated outcomes. With this relatively minor abstraction, aquifers have many properties that are surprisingly similar to QM systems. Preferential flow paths are a classic example that is vaguely reminiscent of quantum tunneling, where an electron passes through a potential barrier that is classically prohibited. Further, what is happening in one area of a model can impact more than the adjacent model cells, which could be represented using a sort of entanglement or correlation. These "effective quantum" ideas are just beginning to be formed, but they could lead to rapid solution schemes beyond anything seen in GW modeling to date where uncertainty is front and center.

The question to resolve going forward is: do we want to keep running the same kinds of GW models we use today in the future or do we want to work with new kinds of models that can overcome some of the limitations of the current workflows and enhance predictions? If the latter is the affirmative, now is the time to start engaging with computer scientists and quantum computing researchers to help them understand the unique needs and challenges presented by GW flow and transport modeling; GW is plagued by uncertainty in ways other fields are not and we should not assume practitioners in other fields understand this. Some disciplines with similarly high levels of uncertainty in specific problems (molecular biology, chemistry, etc . . .) are already turning to quantum tools and QCPs to solve the problems that have been vexing them for decades, but these are truly quantum systems. The missing link for GW is to separate the conceptual pictures of common QM systems from their scales and to then focus on applying the mathematical tools of QM, either to solve our current frameworks or to move beyond them. The skeptical reader might note that indeed QM and GW systems are uncertain but one is aleatoric and one is epistemic, thus their uncertainties are not the same. Yet, the mathematics used to describe QM systems do not require such distinctions. Instead they only require certain properties (granularity, indeterminancy, etc . . .) *relative to the scale of the problem*. At its mathematical core, QM simply requires one to speak in terms of distributions and distinct probabilities rather than the illusion of certainties, which seems to be an appropriate position for the GW modeler to take given the extraordinary uncertainty in GW flow and transport problems. Our current workflows do not make UQ easy to include, but new models could allow us to incorporate uncertainty in new ways if we so choose. QM was designed to be uncertain from the outset and it seems as logical a parallel as any to build next generation GW models for QCPs that are also uncertain from the outset.

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