How to Bake Quantum into Your Pet Petri Nets and Have Your Net Theory Too

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Abstract. Petri nets have found widespread use among many application domains, not least due to their human-friendly graphical syntax for the composition of interacting distributed and asynchronous processes and services, based in partial-order dependencies and concurrent executions. Petri nets also come with abstract semantics, and mathematical methods for compositional synthesis, structural checks and behavioural analysis. These have led to the use of various kinds of nets for real-time, distributed and parallel programming languages, software and services systems, with a view to their interfaces and interaction protocols. These affordances make Petri nets invaluable for distributed software architecture approaches focused on components, their mutual dependencies and environment-facing interactions.

Quantum computing – and in particular quantum software engineering – is in its infancy and could benefit from the accumulated insights of software architecture research and of net theory, its methods, and its applications.

In this paper, we establish a connection between Petri nets and quantum systems, such that net theory and the component architecture of nets may help in the synthesis and analysis of abstract software models and their interface protocols in hybrid classical-and-quantum programming languages and services systems. We leverage some insights from net formalisms for software specification for a versatile recipe to bake quantum into extant Petri net flavours, and prove universality and compositionality of Petri nets for quantum programming.

Keywords: Component software, Compositionality, Petri nets, Software architecture, Quantum Petri nets, Quantum software engineering, Quantum computing, Model-checking and simulation, Stochastic Petri nets

1 Introduction

Petri nets (PNs) have found widespread use among many application domains. Their graphical syntax is tailored for systems exhibiting concurrency, parallelism and often wide distribution. Their use across different levels and scales from high-level software systems requirements through low-level chip architecture to chemical reactions has assisted their far-flung applications and made PN diagrams a lingua franca for expressing concurrency directly in its interaction with causal partial ordering and mutual exclusion [25,23]. Petri nets empower systems and services analysts, architects and developers alike to engage in informal dialogues with each other and with users, over more or less formal, but accessible, diagrams, about diverse and complex systems issues including extra-functional properties such as liveness, reliability and performance.

Petri nets also come with an abstract semantics, and mathematical methods for composition (gluing nets together in different ways) and for structural and behavioural analysis using the system and services architecture, i.e., its components, their interrelation and interaction with their external environment. The unmarked net structure itself is amenable to analysis and transformation, independent of a specific initialisation in a system net with a selected initial marking. The structure represents the behaviour rules for all possible initial markings; the system net all runs connected with the initial marking and possible in that net structure. The preparation of the initial state remains outside the model. Net behaviour is observer-independent: a run of the net consists of partially ordered occurrences of events tracing, or simulating, the Petri net token game, in which tokens are redistributed from one reachable marking to another. Each marking represents an alternative world or configuration. The events of a run may be sequential, when one depends causally on the result of another, or concurrent and spatially distributed, when they are mutually independent. A set of runs may also reflect choices, which may non-deterministically or probabilistically evolve to different markings. All possible strict sequential event orders that respect their partial order in
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a run are conceivable observations of the given run, whether placed on a timeline or not. Moreover, the system net behaviour can be analysed and transformed both in terms of an algebra of matrices and the marked net structure itself. Thus, an initial marking of the net system provides resource constraints on top of those set by the net structure. This empowers modellers to determine many crucial characteristics of a time-less synchronisation defined solely by the causal dependency and concurrency of underlying net structure. Different logics have been used for model-checking in terms of system Petri nets and their behaviour. Industry-strength model-checkers exist for years capable of handling hundreds of millions of states (cf. e.g., [11, 2]), often using special on-the-fly methods for dealing with the 100s of millions of states without storing transition matrices. The semantics of PNs has led to their use as formal models for real-time, distributed and parallel programming languages, for software systems and services. These affordances make Petri nets invaluable for distributed software and services architecture approaches focused on components, their mutual dependencies and environment-facing interactions.

Quantum computing – and in particular quantum software engineering – is in its infancy and could benefit from the accumulated insights of software architecture research and of net theory, their methods, and their applications. Quantum cryptography is already a viable business; so are niche applications of a number of quantum computing cloud services accessing the first real quantum computers by IBM and Google with a moderate number of qubits [26, 7]. Microsoft and others aim to accelerate the development of quantum software with breakthroughs expected in the application of quantum computers to modelling and simulation of real quantum systems that are currently beyond the reach of supercomputers. These include quantum chemistry and pharmacuetics, advanced materials, quantum neurophysiology and others. Distributed quantum computing is making rapid advances. Research in optical networks and photonics has made the quantum internet [15] feasible. Experimental physics have also demonstrated teleportation of coherent quantum states experimentally, over many tens of kilometres and from a ground station on earth to a satellite in orbit [22]. Networked quantum computing is poised to revolutionise distributed computing and lead to orders of magnitude increases in network speeds and bandwidth.

However, advances in distributed algorithms and software architecture for hybrid, i.e., classical-quantum and hardware-software, systems are far from mainstream software engineering. Currently the field of quantum software engineering requires a blend of physics, applied mathematics and theoretical computer science knowledge. Its models and methods are inaccessible to most practitioners and academics in distributed systems analysis, architectural design, software development and testing. An exposition of quantum principles in reasonably widely applied diagrammatic software models and programming language constructs, like those related to Petri nets, has appeal. For research, teaching and practice, especially in parallel and distributed quantum software engineering, PNs could potentially make a significant difference to practitioners, if quantum were accessible for different kinds of Petri nets. This requires an orthogonal weaving of quantum into PNs with a clear separation of concerns of classical parallelism with its preexisting exponential state space explosion and the extra quantum-specific parallel features, clearly separating concurrency and quantum – while hiding complex vector spaces and their advanced matrix methods.

Overview: This paper establishes a connection between Petri nets and abstract quantum systems. We weave quantumness into selected classes of Petri nets, while separating the concerns for (a) net structure and (b) non-local and acausal quantum characteristics. The paper starts with an informal introduction to Quantum Petri Nets (QPNs) aiming to minimise any vector space knowledge. We then give a formal definition and show how variations in the underlying classical nets can be kept separate from quantum characteristics, yet uniquely extend to QPNs. The main result shows that Quantum Petri nets (QPNs) can represent any universal gate set, in fact any circuit in the circuit model of abstract quantum computation. We also prove a novel compositionality results. (Proofs and other technical material are provided as supplementary material on the web but are here included only for the convenience of the review process.) In a section on related and future work we contrast the novel approach with others, and sketch future research avenues.

2 A Gentle Introduction to Quantum Petri Nets

Before we introduce QPNs formally and connect them with the mathematics of quantum information processing, we briefly look at some simple examples to guide our choices in the design of these models. Beside addressing PN researchers, this introduction is written with a community of net practitioners, software developers and applied informaticians in mind. Many in this community
will only be fleetingly familiar with the mathematics of quantum information processing, if at all.

Fig. 1. Quantum interference in a simplified particle system model of the double-slit experiment. Left: For any positive integer \( N \), the Place-Transition net (PTN) carries \( N \) tokens on place \( G \) only, as its initial marking. Every transition can fire at least once. That means, the net is live (\( L_1 \)-live). Moreover, one of the transitions \( a \) through \( e \) will eventually keep firing (there is no dead marking). When weighting its transitions with classical rates, the PTN becomes a Stochastic Petri net (SPN) of the bullet scattering. With quantum rates, it is a Quantum PTN (QPTN) representing a photon scattering in a simplified double-slit experiment model. Rates not shown default to 1.

Right: The weighted reachability relations for \( N=1 \) are shown as a reachability graph. With edge weights, it becomes the weighted reachability graph of the SPN or QPTN to the left. All PTN states remain reachable in the SPN. For the SPN, markings in \( A,B,D \) and \( E \) are equiprobable at \( 1/6 \). \( C \) attracts tokens from both slits, hence with twice the probability, \( 1/3 \). For the QPN however, the probability of reaching \( C \) is zero, as the complex rates cancel each other. Markings in \( A,B,D \) and \( E \) are equiprobable, here \( 1/4 \). Since \( C \) is not reachable in the QPTN, transition \( c \) is dead (and the QPTN is not \( L_1 \)-live).

Therefore, this section is an attempt to explain the basic principles only in terms of nets and their reachability, wherever possible. We try to tie principles such as superposition, entanglement, tunnelling and teleportation directly to the action of token flow in nets well-known to many in this community. In the words of Petri himself, we aim to “raise the entertainment value from negative to zero” [21] – at least for this gentle introduction. Where they are needed, net-theoretic terminology and notation follow that of Reisig [9] widely used in teaching Petri nets to undergraduate students and practitioners alike. Readers feeling at home in both the “mathematical engine room” of net theory and quantum information theory, may glance at the figures of this section, select relevant text explaining the examples and move straight on to the formalisation of QPNs.

In a nutshell, given a classical PN, the corresponding QPN associates complex-number rates with transition firings, including with their inseparable firing as an ensemble of mutually concurrent transitions.

2.1 Transition Firing with Amplitudes

The system net of Fig. 1 uses \( N \) tokens (\( N \) being a positive integer) and classical rates to model the outcome of firing bullets through two slits. Or it uses quantum rates for modelling photon scattering through the two slits. With classical rates, the resulting Stochastic Petri Net (SPN) describes a gun loaded with \( N \) bullets (in \( G \)). With transitions \( l \) and \( r \), the gun randomly sends a bullet through either the left (\( L \)) or right (\( R \)) slit. For each slit, a scattering (\( a,b \) or \( c \)) occurs to three of five possible detectors (\( A \) through \( E \)). The location of a single bullet can then be found always, by firing the respective transition \( a \) through \( e \). For these final transitions, the number of transition firings per time unit can measure the number of bullets reaching the respective place, if \( N > 1 \).

The probability of a single bullet of \( N \) hitting place \( A,B,D \) or \( E \), respectively, is \( su = sv = 1/6 \), i.e., the product of transitions weights on the respective path from \( G \). \( C \) is reachable either by the firing sequence \( lc \) or \( ra \), i.e., with probability \( sw + su = 1/2 \times 1/3 + 1/2 \times 1/3 = 1/3 \). The token game played on the system Place-Transition net (PTN) and SPN (to the left) and its reachability graph (RG) or weighted RG (to the right) reflect the same reachability relation. As the sum of non-zero probabilities is non-zero for any SPN, all reachable states have non-zero probability, however
small—assuming that transitions have non-zero probability in the first place. In our example, like in the underlying PTN, all transitions $a - e$, including $c$, are enabled at least in some marking. The system is, what is called in net theory, $L_1$-live. Moreover, there is no reachable dead marking, as every token will eventually arrive in one of the detector places and the corresponding transition will then keep firing. Like for its SPN sibling, the quantum firing rates of the Quantum PTN (QPTN) to the left weight its firings and hence its token game. This QPTN abstracts from a simple quantum-physical double-slit experiment. Photons are beamed through two slits and are eventually detected. In the real experiment, unsurprisingly the light shows an interference pattern confirming its wave character for very large numbers of photons ($N$) and any number of runs of the same setup. However surprisingly to physicists about a century ago, for repeated measurements of single photons (here modelled by $N = 1$) the same wave pattern appears in the probabilities of photons arriving in those detector positions, given a sufficiently large number of test runs. The above system QPTN explains a simple cancellation by complex-number rates. Amplitude probabilities exclude $C$ from any marking for all $N \geq 1$. No token will ever be detected in $C$. Many details pertaining to a real physical quantum system are abstracted from our model; for example, in reality, photons bounce back and force. While complex rates cancel, all tokens make their way to one of the remaining four detectors with equal probability.

For a quantum firing rate, one uses a complex number $c = a + bi$ and follows the paths of the net token game, forming products and sums, in a similar way to that for the SPN above. In this paper, we do not wish to go into mathematical physics and wave interpretations of complex rates. Suffice to say, that complex numbers allow compact characterisations of real classical mechanical waves and also of complex waves appearing in quantum mechanics. A complex number is also called amplitude. Its modulus $|c| = \sqrt{a^2 + b^2}$ measures its real magnitude, its modulus squared $|c|^2 = a^2 + b^2$ a real probability, possibly after some normalisation in the context of other complex numbers. So in the example, we have, $su = \frac{-1 + i}{\sqrt{6}}$, $sv = \frac{-1 - i}{\sqrt{6}}$, and $sw = \frac{1}{\sqrt{6}}$. Since amplitudes can cancel, $|su + sv|^2 = 0$. No token can reach $C$ in the system QPTN, whether calculated on the net structure or the weighted reachability steps in its token game and visualised in the RG to the right. Moreover, that is the case, however many experiments are run, and however large $N \in \mathbb{N}$ is chosen to begin with. Hence transition $c$ is dead and the QPTN is not live for any $N$. On the other hand, a short calculation shows that $A, B, D$ and $E$ are equiprobable. We normalise each their four amplitudes with their sum total magnitude $|m| = |su| + |sv| + |sw| = |\sqrt{4/6}|$. Place $A$, for instance, is therefore reached with probability $(|su|/|m|)^2 = |su|^2/|m|^2 = \frac{1}{6}$. 2/6 = 1/4.

2.2 Superposition States and Measurements Over Nets

Let $M_0$ denote the reachability set, i.e., the set of reachable markings, of the underlying PN with initial marking $M_0$. For example, in Fig. 1, $M_0$ is the set of nodes in the RG on the right. A superposition state $a$ (superposition for short) is a function $M_0 \xrightarrow{a} \mathbb{C}$ that assigns a complex number to each marking in $M_0$. The set of all superpositions of the reachability set $M_0$ is also denoted as $a_{\#}$ and called the span of the QPN. We call $a(m)$ the probability amplitude of marking $m \in M_0$ in $a$ and write $a_m$ instead of $a(m)$ for brevity. We also denote $a$ algebraically as a weighted sum of its markings, each placed in a special bracket: $a = a_1|m_1| + \cdots + a_n|m_n|$, omitting terms with weight 0. For convenience in examples, we avoid the brackets, when there is no risk of confusion. For real-valued amplitudes, the superposition represents classical alternative worlds. The trivial superposition $|m\rangle$ (i.e., $a_m = 1$ and other $a_m' = 0$) represents a single marking. We liberally use familiar algebraic manipulating of superpositions (and defer the formal treatment to Sec. 3).

The state of a quantum system is not directly observable. Observation requires a measurement of some sort. A superposition expresses Heisenberg’s uncertainty principle inherent in quantum systems and making measurement outcomes uncertain. Once measured, the subsystem will be in a certain classical state. Physicists speak of the collapse of the wave function. Measurement in a real test setup requires a physical instrument, which is ultimately a quantum system itself, interfering with the system under test (commonly abbreviated SUT in software engineering). For example, a software-defined nanorobotic system may consist of a software-controlled laser measuring and controlling some nanorobotic material in superposition. Light beams sent from the laser change the energy levels and conductivity of particles making up that material. They affect its properties and shape. Any test effect before the ultimate collapse can be regarded as a transition in the SUT from the superposition $a$ prior to the test to another superposition $b$ immediately before the ultimate collapse. That transition is typically forgetful and hence irreversible, because it abstracts from many characteristics of the system not of interest. The ultimate collapse remains unpredictable.
For QPNs, the result of the ultimate collapse is a marking \( m \). That measurement and collapse may be restricted to a part of the system only, not entangled (see below) with the rest of the system. Then collapse may be restricted to the subsystem state. So, having modelled the test setup in terms of its effect on the SUT by a transition from \( a \) to \( b \), the modeller can now inspect the amplitude of a marking \( m \) in \( b \) (in the model) to determine the probability of that outcome (in the actual system) as \( |b_m|^2 \), if \( b \) is normal. A superposition \( a \) is defined as normal if \( a = a/|a| \), where \( |a| \) is the real-valued norm of the superposition defined by \( |a| = \sqrt{\sum_n |a_m|^2} \).

Fig. 2. Convolved enabling and firing.
Left: The marking \( A^4B^6C^3E^2 \) enables all transitions \( a, b \) and \( c \) in the concurrence \( ab^2c \). Does it enable them in the required number? Middle: The net flow multiplicities (arc weights), which define the input and output markings of a single transition, are lifted to input and output markings of a concurrence. These determine the interference-free coupled firing of the multiset. Here the input marking is \( A^3B^7C \). Likewise, the output marking depicted respects multiplicity, here \( D^5E^3 \). Right: Thus the marking \( ABC^2D^5E^5 \) can be reached by firing \( ab^2c: A^4B^6C^3E^2 \overset{ab^2c}{\rightarrow} ABC^2D^5E^5 \). As usual, this joint firing subtracts tokens and adds tokens in a single atomic step. The overall classical effect on the marking is the same as firing subconcurrences in any sequence, no new marking is reachable. However, with entanglement, the transition multiset may fire any way: together, individually or anything in between.

2.3 Entangled Transitions and States

Quantum-mechanically, entanglement requires superposition of multiple interacting subsystems. For example, two or more independent molecules may each be in a superposition of conformations, when “swinging” on a double-bond hinge or “rotating” on a single-bond pivot. These conformations may be frequency-coupled between the molecules, due to the surrounding electronic structure, i.e. the distribution of a number of electrons they share and the uncertainty of their position. In QPNs, entanglement couples the firing of otherwise concurrent transitions in space-time. We call the firing of mutually concurrent transitions a concurrence. Formally, a concurrence is a multiset \( t \) of enabled and mutually independent transitions, i.e., \( t \in \mathbb{N}^T \) (the set of multiset over \( T \)). We think of them as firing together with some given amplitude. Like the transition structure of nets the dual of its place structure, concurrences can be regarded as the dual of markings. However, like single transitions, concurrences define indistinguishable atomic marking updates and must not be confused with historic attempts in net theory to separate the beginning and the ending of transitions. As an abstract example of a concurrence, consider the concurrence \( ab^2c \) in Fig. 2. The shown marking \( A^4B^6C^3E^2 \) has sufficient tokens for an interference-free firing of any pair of subconcurrences partitioning and covering the given concurrence. Hence it can also fire in an atomic single step. This example also shows that concurrences do not have to be maximal.

Thus, for QPNs, concurrences can be entangled by rating the inseparability of any of their proper substeps. In fact, it is possible to acausally force their atomic firing by rating the individual transition firings with amplitude 0, while using amplitude 1 for the joint firing. This is a kind of soft mutual excitation. Inversely, the joint firing could be rated much lower than the individual firing, as a kind of soft mutual inhibition. A marking-dependent rate function \( r \) is a function \( M_0 \times \mathbb{N}^T \overset{r}{\rightarrow} \mathbb{C} \).

1 Physical model-realism may require operations on quantum systems at any scale and hence resulting in superpositions at any scale. This may require re-normalisation.

2 We use the term space-time coupling to avoid the term ‘synchronisation’ which is loaded with temporal meaning, etymologically the old-Greek ‘khronos’ means time and the prefix ‘sun’ together.

3 Concurrences are to transitions what markings are to places.
assigning complex numbers to concurrences. We refer to \( r(m, t) \) by \( r_m(t) \), for brevity, and use \( r_m(t) = 1 \) as the default. For example, in Fig. 3, there are four possible concurrences between the two classical bit PTNs \( P \) and \( Q \). Here each concurrence consists of two transitions highlighted by a coloured line. As rates are not shown explicitly, they default to a coloured line. In contrast, a net is isomorphic to the RG of each single player. Juxtaposition with transition identification loses the individual transition firings. In this example, the two nets juxtaposed with this respective players into mutually dependent moves – players holding hands, so to speak, in their now locally and causally synchronised token game. In this example, the two nets juxtaposed with this particular constraint are behaviourally equivalent to a single classical bit: the RG of the combined net is isomorphic to the RG of each single player. Juxtaposition with transition identification loses the individual transition firings. In contrast, a QPN can fire all transitions of a concurrence together, individually, or anything in between controlled by the rate function.

Formally, an entangled superposition (state) is defined as a superposition that cannot be expressed as a product of the two component superpositions. In Fig. 3, for instance, \( \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle) \) is an entangled state. In contrast, the superposition \( \frac{1}{2} (|i|00\rangle - |i|01\rangle - |10\rangle + |11\rangle) = \frac{1}{2} (|i|P_0Q_0\rangle - i|P_0Q_1\rangle - |P_1Q_0\rangle + |P_1Q_1\rangle) = \frac{1}{2} (|i|P_0\rangle + i|P_1\rangle) \times (i|Q_0\rangle - i|Q_1\rangle) \) is a product of superpositions of the \( P \) and \( Q \) qubit taken by themselves. Therefore this superposition is not entangled. The so-called Bell states\(^4\) of a qubit pair are the four entangled superpositions of the reachability set of Fig. 3(Middle): \( \frac{1}{\sqrt{2}} (|00\rangle \pm |11\rangle) \) and \( \frac{1}{\sqrt{2}} (|01\rangle \pm |10\rangle) \). To stay in \( \frac{1}{\sqrt{2}} (|00\rangle \pm |11\rangle) \), for instance, \( uu \) and \( dd \) have to be rated with probability 1 (or a complex equivalent) with \( u \) and \( d \) rated 0. Informally, rating the individual transitions in the coupling both with amplitude 0 means that the intermediate markings 01 and 10 attract an amplitude of 0 as result of firing the concurrence in a single step.

2.4 Superposition Evolution and Complex Token Game

Complex rates for single transitions and for concurrences allow a QPN to evolve the state from superposition to superposition with entanglement. An evolution process starts from an initial state: any superposition is a valid initial state. The QPN process executes in parallel for all superposed markings and all possible concurrences enabled in any of them. QPN superposition evolution is thus a form of OR-parallelism, well-known from parallel and stochastic process modeling and simulation tools, incl. SPNs. Each step reaches another superposition; a measurement is taken in

\(^4\) named after physicist John S. Bell. These states are maximally entangled.
a distinguished state, for example a final state, or a home state that is both initial and final. The superposition immediately before the collapse reveals the probability of measurement outcomes with a precisely defined uncertainty\(^5\).

Recall like in stochastic variants of Petri nets, QPN rates are marking-dependent. In the RG of an SPN, this permits a modeller to assign different rates \(r_m(t) \neq r_{m'}(t)\) to different enabling markings for the same transition (\(m \rightarrow_{a} m'\), vs. \(m' \rightarrow_{a} m\)). For QPNs, the step \(t\) may be a concurrence. Rating a concurrence with a single transition (\(|t| = 1\)) is trivial and classical. Rating the unit multiset (\(|t| = 0\)), i.e., the NOP process, caters for a resting rate. For example something may change somewhere remote (in another juxtaposed component) and result in redistribution of amplitudes, in particular for non-local entanglements. Any concurrence and its entanglement can now be fully grasped in terms of transition firings in the net. For example, consider the RG (black and coloured) in Fig. 3. Assume we want to compute the amplitude of marking \([11]\) after a direct reachability step starting from a given superposition \(a\). Given the uncertainty expressed in \(a\), there are many steps of length \(1\), that reach \([11]\), i.e. the target node \(11\) in the RG on the right of the figure. To compute the required amplitude (here \(a_{11}\)), one forms the weighted sum over these edges with their source node (marking) amplitudes as the respective weight, plus the weighted resting rate.

\[
\begin{align*}
\text{a}_{00} & := a_{00} \times r_{00}(1) + a_{01} \times r_{01}(d) + a_{10} \times r_{10}(d) + a_{11} \times r_{11}(dd) \\
\text{a}_{01} & := a_{00} \times r_{00}(u) + a_{01} \times r_{01}(1) + a_{10} \times r_{10}(du) + a_{11} \times r_{11}(d) \\
\text{a}_{10} & := a_{00} \times r_{00}(w) + a_{01} \times r_{01}(ud) + a_{10} \times r_{10}(1) + a_{11} \times r_{11}(d) \\
\text{a}_{11} & := a_{00} \times r_{00}(uv) + a_{01} \times r_{01}(w) + a_{10} \times r_{10}(u) + a_{11} \times r_{11}(1)
\end{align*}
\]

\(1\)

Since node \(11\) is reachable only by making a move (a step in one of the first three terms listed) or by resting (fourth term), the normalisation of the rates in Equ. 1 (line 4) results in the sum of their moduli squared equaling 1, provided that \(a\) is normalised to begin with. Philosophically, the required probability sum of 1 (after normalising and converting amplitudes to probabilities) expresses this principle\(^6\): **whether something moves or nothing happens, the system is in a defined state.** In other words, a measurement will collapse the state to a defined outcome.

For each marking amplitude \(a_m\), a corresponding equation in Equ. 1 captures the direct reachability relation reaching marking \(m\). Note that according to Equ. 1 the amplitudes of the next superposition are exactly the result of multiplying row 11 of the adjacency matrix \(A\) (cf. Fig. 3) with \(a\) as a vector of marking amplitudes in the order 00 through 11. Step sequences of different lengths (lengths of paths in RG) and width (cardinality of concurrences) represent partially ordered runs. The net structure of a QPN and various behaviourally equivalent transformations on the classical underlying net \([4]\) may serve transformations of the QPN with different complexity and performance characteristics, yet resulting in the same final measurement up to an error \(\Delta\).

Note, that the rate function does not change the reachability of the underlying classical net. Therefore, QPNs do not add to the classical state space explosion already attributable to concurrency and stochasticity. For example, SPNs already calculate with stochastic uncertainty in their parallel simulations. However, QPNs add concurrence edges to their reachability graph filling the equivalent rate matrix with finely differentiated rates. A secondary and lesser complication arises from the use of complex numbers as rates. Each complex number requires two reals and hence doubles the space and possibly access time compared to SPN implementations. More importantly, adding classical probabilities increases them and multiplying them decreases them. Therefore, rates for classical stochastic nets may converge over increasing numbers of steps, allowing a modelling tool to prune the number of OR-parallel branching. In contrast, complex rates may cancel each other, yet oscillate forever, with no or little chance of reducing the number of processes to follow.

### 2.5 Rate Function Composition and Acausal Computation

In general, any quantum computational function can be expressed using QPNs. The causal characteristics of the computation is captured in the net structure. The acausal characteristics are induced by the firing steps and thus direct reachability, in terms of the overall rate distribution over the net. Below, we show by example (Fig. 3 and 4), how quantum circuit diagrams translate to QPNs. For technical details see Sec. 3.

\(5\) The precision of the mathematics underpinning quantum mechanical predictions is unrivaled and differs from classical stochastic models.

\(6\) in a blend of Einstein and Aristotle
In circuit diagrams, the controlled-not gate, aka CNOT, assigns amplitudes so as to flip qubit \( Q \) if and only if qubit \( P \) is 1, with the rate function CNot induced by the steps of the underlying net of the qubit pair \( P \) and \( Q \). The corresponding QPN amplitude definition (\texttt{defqp}) declares CNot as a rate function on the qubits \( P \) and \( Q \), induced by the steps of the underlying net. The default amplitude is 0 (‘\( @ \) 0’ follows the rate function prototype). The CNot definition body follows the \texttt{with} keyword and defines marking-dependent rules overriding the default for firing steps. With \texttt{P.0} marked the resting amplitude is 1 (‘\( \text{rest} @ 1 \)’, i.e., regardless of the marking of \( Q \). This means CNot\(_{00}(1) = \) CNot\(_{01}(1) = 1 \). With \texttt{P.1} marked, the system is forced to fire one step to a different marking as the resting rate is 0 by default for the remaining markings. In a superposition, the enabling markings have different amplitudes, but for each marking there is only one enabled transition: 10 \( \frac{Q_0}{\sqrt{2}} \) and 11 \( \frac{Q_1}{\sqrt{2}} \). Thus with \texttt{P.1} the rate is CNot\(_{10}(a) = \) CNot\(_{11}(d) = 1 \), thus performing the respective flip with probability 1. Using parentheses, the two transition amplitude rules are contracted here into one rule for \texttt{P.1}.

Similarly, the so-called Hadamard gate, which operates on the single qubit, here \( P \) in Fig. 3, is given by the rate function \texttt{Had} at amplitude \( 1/\sqrt{2} \) for all steps bar \( H_1(1) = -1/\sqrt{2} \).

Each rate function on one or more qubits corresponds to a primitive or composite gate of quantum computing circuits on those qubits. QPNs are not limited to nets representing bits, however. Hence, more generally, each rate function corresponds to a combined causal-and-acausal function of the QPN, in which amplitudes regulate causality, concurrency and choice.

### 2.6 Teleportation Tunnelling and Hybrid Security Protocols

Due to the particle-wave character of entangled quantum systems, their behaviour includes instantaneous synchronisation over large spatial distances, local-point correlations over temporal distance reaching into the past and future, and blends thereof in bounded space-time regions. Quantum-state teleportation experiments have confirmed qubit entanglement over large distances. For example, qubit \( P \) could be located on Earth while qubit \( Q \) is on a satellite in orbit. If the entangled state \( \frac{1}{\sqrt{2}}([00] + [11]) \) were distributed with \( P \) in space and \( Q \) on Earth and a measurement in space resulted in the outcome of \( P_0 \) (and thus a collapse of that state to \( P_0Q_0 = 00 \)), then instantaneously it can be known that the qubit \( Q \) on Earth is in state \( Q_0 \). An analogous argument holds for the alternative outcome \( P_1 \). Furthermore, symmetrically, the measurement could be taken on Earth with the same non-local result. Yet the outcome remains uncertain until a measurement is taken. Superposition does not only work like a perfect quantum oracle. It also implies instantaneous consumption of distributed measurement outcomes. Moreover, any eavesdropping on entangled qubits results in a collapse of the superposition, which can be immediately noticed by the distributed parties. Therefore, quantum protocols are also poised to offer unparalleled security and safety.

It should be noted, however, that the acausal and non-local entanglement is not signalling any information between remote locations. However, it can be used in combination with classical message signalling protocols over such distances to leverage the quantum advantage in protocol security and processing speed. Using the examples above we have the tools to understand the following teleportation protocol, which abstractly captures the common structure of a number of real teleportation protocols that have been conducted over different distances (tunnelling under the Donube in Germany, offshore to onshore US, Tibet to space satellite and others, cf., e.g. [28]).

In this variant of the protocol, Alice and Bob each share one half of an entangled qubit pair (\( A \) and \( B \) say), in the Bell state \( \frac{1}{\sqrt{2}}([00] + [11]) \), which results from evolving \( |00 \rangle \) with \( (A, B) . \text{Bell} \) in...
our QPTN. They both have agreed on the entanglement but neither has knowledge of the specific Bell state or its amplitudes. Alice aims to teleport a third qubit $C$ to Bob. The state of $C$ – also unknown to Alice and Bob – can be represented as the superposition of markings $c(0) + d(1)$. Now juxtapose the QPTNs in the order $C, A$ and $B$ with our convention for marking abbreviations 000 through 111. Alice is located in the space station, Bob on Earth. The entanglement of $A$ and $B$ is prepared in a third place before the experiment using the Bell function above. Next the separate qubits are sent to Alice and Bob taking care not to break the entanglement. This completes the preparation of the initial three-qubit superposition $\frac{1}{\sqrt{2}}(c|000⟩ + c|011⟩ + d|100⟩ + d|111⟩)$. Now:

1. Alice uses $(C,A).\text{CNot} ; C.\text{Had}$ (Fig. 4) transferring the entanglement from $A$ and $B$ to $A$ and $C$. This results in $\frac{1}{2}(c(|000⟩ + |011⟩ + |100⟩ + |111⟩) + d(|010⟩ + |001⟩ − |110⟩ − |101⟩))$ which can be refactored $\frac{1}{2}([|00⟩(c|0⟩ + d|1⟩)) + |01⟩(c|1⟩ + d|0⟩)) + |10⟩(c|0⟩ − d|1⟩)) + |11⟩(c|1⟩ − d|0⟩))$ to show Bob’s qubit as a function of any possible marking of Alice’s qubit pair.
2. Next Alice measures her qubits $(C,A)$ and finds them in one of the four underlying markings, 00, 01, 10 or 11 shown above, and leaving the amplitudes of $C$ hidden in Bob’s formerly entangled qubit. Alice sends the two classical bits of that measured marking to Bob.
3. To reveal $C$, Bob applies one of four functions, depending on the message sent and arrives in superposition $c(0) + d(1)$ for $C$. Note that Alice has lost the initial state of $C$ in the process.

We view tunnelling as a massive entangling with collective teleportation. For example, a long sequence of juxtaposed QPNs of identical system nets can represent a tunnel architecture, with only moderate causal connections between adjacent QPNs. Now the instances of the same transition across different positions can be entangled and teleportation achieved from one end of the tunnel to the other. Causal interconnections in the architecture may reinforce entanglement over the length of the tunnel. Concurrences over instances $t_i$ of the same transition are powers $t^n$ (ignoring the position). Firing rates for these powers may be expressed in terms of the exponent $n$ in one net.

3 Quantum Petri Nets with Variation Points

QPNs have standard Petri nets as underlying classical nets. To avoid ambiguity of similar terminology and notation in nets and quantum computing, we reconcile basic notation first for nets and their matrices. This will also provide variation points for others to “bake in quantum characteristics” to their pet net interpretation, using the machinery laid out in this paper. The fundamental variation points are markings, concurrences and direct reachability. At higher levels there are further variation points in diagram notation and net inscriptions.

Variation points are a familiar concept in software architecture, analysis and design, where they serve the separation of the architectural framework from the more variable architectural elements. For example in the Model-View-Controller framework, a reoccurring pattern of software architecture, the aim is to allow modifications of the view, while minimally, or not at all, affecting the model and controller part of the software. The same goes for changes to the data model or the user and software control of the model. Plugin architectures and feature combinations are further examples. There are many more variation concepts. All have in common that parts of the software are parametrised and varied functionally and as independently as possible.

3.1 Superpositions of Multisets

We begin with a formal account of multisets which are used for markings, concurrences and superpositions in QPNs. Given a set $A$, a multiset over $A$ is a mapping $s : A → \mathbb{N}$. We also write $s ∈ \mathbb{N}^A$ for brevity and abbreviate $s(a)$ by $s_a (a ∈ A)$. Let $s,s' ∈ \mathbb{N}^A$ be two multisets.

The monomial representation of multisets used throughout this paper is one of many common representations of multisets in mathematics, for example, in the representation of the prime factorization of an integer, as a multiset of prime numbers on the one hand, and the corresponding exponent vector $ev(s)$ indexed in the order of prime numbers, on the other. In the monomial representation of $s ∈ \mathbb{N}^A$, the elements $a ∈ s$ are raised to their respective integer multiplicity $s_a$ as their exponent. Multisets are then formed by multiplication (or concatenation) for brevity. For example $ab^2c$ is short for $abbc$ and represents the multiset $\{a ⇒ 1, b ⇒ 2, c ⇒ 1\}$. A superposition $v$ of multisets is a function $\mathbb{N}^A → K$ mapping multisets $s_i$ to coefficients $c_i$ in a field $K$, such as the integers $\mathbb{Z}$, rationals $\mathbb{Q}$, reals $\mathbb{R}$, Gaussian rationals $\mathbb{Q}[i]$ or complex numbers $\mathbb{C}$. $v$ is also written
as the polynomial \( v = e_1 s_1 + \cdots + e_i s_i + \cdots \) with \( e_i = v(s_i) \neq 0 \), i.e., listing only the non-zero terms. Multiplication and addition of monomials and polynomials work with the usual algebraic laws, treating net elements as variable symbols in multivariate polynomials.

In net theory and the simulation of net behaviour, the vector \( ev(s) \) of exponents is often used for efficiently representing a corresponding multiset \( s \). Then multiplication \( ss' \) can be equivalently represented as \( ev(s) + ev(s') \), consistent with \( a^{m+n} = a^m a^n \). We define the partial order \( s < s' \) by comparing the exponents \( s_a < s'_a \) (for all \( a \in A \)) and \( s \leq s' \) if \( s < s' \) or \( s = s' \). For the monomial as a product, \( s \leq s' \) means \( s \) divides \( s' \) and can be cancelled in the division \( \frac{s}{s'} \). Consequently, \( ev(s') - ev(s) + ev(s)' \), as used for transition firings, shows as \( \frac{s}{s'} s' \) and simplifies to a monomial again. Set operations extend to multisets as does some algebraic terminology we need on occasion: The degree \( \text{deg}(s) \) is the largest exponent of \( s \), and the cardinality (aka total degree) \( |s| \) the sum of the exponents. We write \( s = 1 \) iff \( \text{deg}(s) = 0 \). \( s \) is called a proper subset of \( s' \) if \( s < s' \), and a subset iff \( s \leq s' \). Membership \( a \in s \) is defined by \( s_a > 0 \). The intersection (aka greatest common divisor) \( s \cap s' \) is the element-wise minimum of the exponents in \( s \) and \( s' \). The union (aka smallest common multiple) \( s \cup s' \) is the corresponding maximum. The set difference \( s \setminus s' \) is defined by element-wise subtraction of exponents, if the result is non-negative and otherwise 0. If \( f \) is a function \( A \xrightarrow{f} B \) from a set to a multiset, then \( f \) can be lifted naturally to a function \( A^f \xrightarrow{f} B^f \), s.t., for all \( s \in A^A \) we have: \( f(s)_b = s_a \times f(a)_b \) for all \( a \in A \) and \( b \in B \). This was illustrated in Fig. 2.

### 3.2 Classical Petri Nets

Next, we define Petri nets parameterised at two variation points. Various extant net classes can then be derived as variations and restrictions, incl. their quantum variants. Firstly, a generator \( G \) is a function \( Set \xrightarrow{G} Set \), such that \( G[P] \) and \( G[T] \) are disjoint, when \( P \) (the place set) and \( T \) (the transition set) are. This captures a range of net extensions. Secondly, a Boolean function well-formedness, short WF, on \( G[N], N^{[G[N]]} \) and \( N^{[G[N]]} \times N^{[G[N]]} \) captures constraints appearing in the net literature under different names, incl. guards and inhibitors. We define \( \mathbb{P} \) and \( \mathbb{T} \) as the maximal subsets of \( G[P] \) and \( G[T] \) with \( WF(\mathbb{P}) = \text{true} \) and \( WF(\mathbb{T}) = \text{true} \), respectively. \( G[N] \) is called the set of generated net elements. For \( m \in \mathbb{P} \) and \( t \in \mathbb{T} \), we interpret \( WF(m,t) \) as \( m \) may enable \( t \). Also we require strictness of WF on multisets and pairs, i.e., \( WF(m) = \text{false} \) implies \( WF(mm') = \text{false} \), \( WF(m,m') = \text{false} \) and \( WF(m',m) = \text{false} \). Informally, a composite cannot be well-formed, if one of its components is ill-formed. It follows from strictness, that \( WF(1) = \text{true} \).

**Definition 1 (Net structure).** A Petri net structure \( N = (P,T,F) \) (short net) with generator \( G \) and well-formedness \( WF \) is a structure where \( P \) and \( T \) are disjoint sets, called places and transitions. \( F \), which is called flow, is a pair of functions \( \mathbb{P} \xrightarrow{F} T \xleftarrow{F} \mathbb{T} \). \( N = P \cup T \) is also called the set of net elements and \( \mathbb{P} \cup \mathbb{T} \) the set of generated net elements. We call \( F^- (t) \) the input and \( F^+ (t) \) the output of \( t \) and the set of elements \( p \in F^- (t) \) the preset of \( t \) denoted by \( \bullet t \). Analogously, the elements of \( F^+ (t) \) form its postset and are denoted \( \star t \). We require of \( F \) that \( |\star t| + |\bullet t| > 0 \).

For \( G[N] = N \) and \( WF = \text{true} \), we get PTNs. Coloured Petri nets and algebraic nets pair places with data of some sort in \( G[P] \) (see Sec. 4.3).

**Convention 1** For the rest of the paper, let \( N \) be the PN structure with the above components. In the well-known incidence matrix representation of a PTN, \( F^- \) and \( F^+ \) are represented as \( P \times T \)-indexed matrices called the input and output incidence matrix, respectively (c.f., e.g., [19,23]). This generalises to corresponding \( G[P] \times G[T] \)-indexed matrices for the net structures above with a generator \( G \).

**Definition 2 (Enabling and firing).** Let \( m, m' \in \mathbb{P} \) and \( t \in \mathbb{T} \). Then \( m \) is called a marking and \( t \) a concurrence of \( N \). Now, if \( F^- (t) \leq m \) and \( WF(m,t) \), then \( t \) is said to be enabled in \( m \). This is abbreviated by \( m \xrightarrow{t} \). If \( ev(m') = ev(m) - ev(F^- (t)) + ev(F^+ (t)) \), then we say \( m' \) is concurrently (or asynchronously) reachable from \( m \) by firing \( t \). This is abbreviated by \( m \xrightarrow{t} m' \).

We write \( m \xrightarrow{t} m' \) if there is a concurrence \( t \), s.t. \( m \xrightarrow{t} m' \). This binary relation on markings is called direct concurrence reachability. Its transitive closure \( \xrightarrow{t} \) is called concurrence reachability. With the restriction \( |t| = 1 \), we abbreviate \( m \xrightarrow{t} m' \) to \( m \xrightarrow{t} m' \) and \( m \xrightarrow{t} m' \) to \( m \xrightarrow{t} m' \). The binary relation \( m \xrightarrow{1} m' \) is called direct single-transition reachability and its transitive
closure $\rightarrow^+_c$ single-transition reachability. Moreover, if $m \xrightarrow{t} m'$, we call $(m|m',m'=m)$ the effect of $t$. We omit the subscripts $c$ and 1, if there is no risk of confusion in the given context.

Note that the effect of $t$ ignores the intersection of its input and output. Importantly, enabling, firing effect and reachability are defined purely in terms of net structure and WF. Note that $\rightarrow_c$ is reflexive by definition, given that $1$ is a concurrence.

**Definition 3 (Loop-free, reversible, pure and simple).** The net $N$ is loop-free, iff $F^-(t) \neq F^+(t)$ (for all $t \in \mathbb{T}$); reversible, iff for all $t \in \mathbb{T}$ there is a $t' \in \mathbb{T}$, s.t., $F^-(t) = F^+(t')$ and $F^+(t) = F^-(t')$; pure, iff $\text{tr}(t) = \emptyset$ (for all $t \in \mathbb{T}$); and simple, iff for any $t, t' \in \mathbb{T}$: $F^-(t) = F^-(t')$ and $F^+(t) = F^+(t')$ implies $t = t'$.

A loop is thus a transition whose input equals its output, making its effect trivial. Purity means, its inputs and outputs do not share common factors (intersection) in any multiplicity. Simplicity means, the input-output pair uniquely defines the transition. Purity implies loop-freedom. Simplicity does not exclude impurity or loop-freedom. For example, the net in Fig. 1 is simple, but has loops and is impure, while the net in Fig. 3 is simple, pure and loop-free. The definition of purity and simplicity can also be used to define a respective equivalence in order to purify or simplify the net, respectively by forming the quotient, after also removing loops in the case of purification. The resulting net is pure or simple, respectively, by construction.

**Definition 4 (System net, reachability set and graph).** $S = (N,M_0)$ is called a system net with initial marking $M_0 \in \mathbb{N}^p$. The reachability set $M_0$ is defined as the set of all markings reachable from $M_0$ by single-transition reachability. The reachability graph $G_S = (V,E)$ is the multigraph\(^7\) with $V = M_0$ and $E = \{(m,m')\mid m \xrightarrow{t} m', t \in \mathbb{T} \text{ and } m, m' \in M_0\}$. $S$ is called safe iff $\text{deg}(m) \leq 1$ for all $m \in M_0$ and reduced iff for all $t \in \mathbb{T}$, there are markings in $m, m' \in M_0$ with $m \rightarrow m'$.

It is straightforward to verify that the underlying system net of the 2-qubit QPTN of Fig. 3 is loop-free, reversible, pure, simple, safe and reduced.

**Definition 5 (Equivalent shape and behaviour).** Let $S = (N,M_0)$ and $S' = (N',M'_0)$ be two system PNs. Then $S$ and $S'$ are called shape-equivalent under a bijection $f$ between their place sets $P \xrightarrow{f} P'$, if $M_0 \cong M'_0$ and $M_0 \cong M_0'$ under the congruence uniquely induced by $f$ on $\mathbb{N}^P$. They are called behaviour-equivalent if they are shape-equivalent under $f$ and $f$ moreover extends to a bijection $\mathbb{T} \xrightarrow{f} \mathbb{T}'$, s.t. their reachability graphs are isomorphic under $f$: $G_S \cong G_{S'}$.

Shape-equivalent system PNs operate on isomorphic markings but possibly with different transitions and concurrences. With equivalent behaviour, the nets can simulate each other as their direct reachability relations mirror each other under the bijection $f$ between their net elements. Behaviour equivalence implies that $f$ is an isomorphism on their reachability graphs and preserves the direct concurrence reachability. The reverse is not true, because a reachability graph isomorphism may not preserve the enabling of concurrent transitions. For simplicity, henceforth we identify places, markings and reachability set in two nets of equivalent shape, without mentioning $f$.

### 3.3 Baking Quantum into Petri Net Theory

Next, we formalise QPNs and look at the matrix calculus and linear algebra operators they induce based on their underlying nets.

**Definition 6 (Quantum Petri net).** Let $S = (N,M_0)$ be a system PN, then $Q = (S,r)$ is a Quantum Petri net (short QPN) where $r$ is a function $M_0 \times \mathbb{N}^T \rightarrow \mathbb{C}$. We write $r_m(t)$ for $r(m,t)$. A superposition state (short superposition) of $Q$ is any $|M_0\rangle$-dimensional complex vector $v$.

Thus, the underlying net spans an $|M_0\rangle$-dimensional complex Hilbert space of marking superpositions. The canonical basis vectors are $b_m(m \in M_0)$ with all entries $0$ except a single $1$ at index $m$. We conveniently abbreviate $b_m$ by $|m\rangle$. Any superposition $v$ can be written as the linear

\(^7\) In a multigraph a single pair of edges $(u,v)$ may have multiple parallel edges, here represented as triples $(u,k,v)$. A graph with a single unique edge for each pair of vertices is called simple in graph theory.
The inner product of the Hilbert space is a combination of basis vectors. $v$ is also written as $|v\rangle$ to recall it is a column vector.

The inner product of the Hilbert space is $\langle u|v\rangle$, which multiplies the row vector $|u\rangle$, which is the conjugate transpose of $|u\rangle$, with the column vector $|v\rangle$. The inner product lends a geometry to this complex vector space, with the real-valued length $|u\rangle = \langle u|u\rangle$. The distance of two vectors is $||u\rangle - |v\rangle||$ and the angle between them is $\alpha = \arccos \frac{|\langle u|v \rangle|}{|u||v|}$.

**Definition 7 (Rate graph).** Let $Q$ be a QPN as above (Def. 6). The rate graph of $Q$ is the multigraph $G_Q = (V,E)$ with $V = M_0$ and $E = \{(m,t,m')|m \xrightarrow{t} m', t \in \mathbb{N}^2 \text{ and } m, m' \in M_0\}$. $E_{m,m'}$ denotes the set of edges between $m$ and $m'$ and we often simply write $m \xrightarrow{t} m'$ instead of $(m,t,m') \in E_{m,m'}$ given the correspondence between edges and the direct concurrence reachability.

Note that the rate graph of a QPN is defined purely in terms of the underlying system PN, as its concurrence reachability graph. This defines the domain of the rate function, in the sense that any direct concurrence reachability $m \xrightarrow{t} m'$ has a unique edge in the rate graph, for which $r_m(t)$ defines the amplitude, and vice versa. Also note, that $|M_0| = \infty$ is possible in more than one way. Firstly, the generator $G$ may create infinite nets, i.e., $|G[N]| = \infty$. Secondly, even for a very small finite net, the reachability set may be very large (or even infinite). This generative power is well-known for nets and used, for instance, in SPNs, where it is combined with structural (net-theoretic) and behavioural (reachability graph or matrix) methods. However, some numerical difficulties arise for concurrent and stochastic processes when working directly with the reachability graph and therefore, more often than not, we ask whether a given system PN is bounded and therefore $M_0$ is finite. This is solved for the classical underlying PN. We also say a QPN has property $X$ if its underlying system PN has property $X$. For example, $Q$ is simple if $S$ is simple and shape-equivalent with another QPN if their underlying system PNs are. Any $n$-qubit QPN that juxtaposes $n$ qubits is loop-free, reversible, pure, simple, and safe and reduced (cf., e.g., Fig. 3). Therefore its rate graph is a simple graph. All these are decidable in $S$.

**Definition 8 (Rate matrix).** Let $Q$ be a QPN with $G_Q = (V,E)$ and $|V| = n$. Then its rate matrix $R_Q$ is defined as the $n$-dimensional square matrix, satisfying: $R_Q[m',m] = \sum_{t,m \xrightarrow{t} m',r_m} r_m(t)$. The normal rate matrix is defined by normalising the row vectors of $R_Q$.

Let $R$ be a normal rate matrix of a QPN. Then it can be interpreted on the underlying system PN $S$ as follows. $Rx = y$ evolves any superposition $x$ of markings of $S$ in a single-step quantum-parallel evolution to a marking superposition $y$ (cf., e.g., Equ. 1). Since every $n^2$ matrix with complex entries is an operator in the $n$-dimensional complex Hilbert vector space, the following sentence is a consequence of the above definition.

**Corollary 1 (QPN rate matrices are Hilbert space operators).** Let $Q = (S,r)$ be a QPN. Then the rate matrix $R_Q$ and its normal rate matrix are both operators of the complex Hilbert space $\mathcal{H}^n$, with dimension $n = |M_0|$ and state vectors $a \in \mathcal{H}_n$. If the net is reversible, let $t^{-1} \in \mathbb{T}$ be the reverse transition for every $t \in \mathbb{T}$. If the rate function $r$ is conjugate symmetric, i.e., for every $m \xrightarrow{t} m'$, $r_m(t^{-1}) = r_m(t)^*$, then the normal rate matrix is unitary.

**Universality.** Next, we wish to show that QPNs are a universal computation model in the sense of the quantum circuit model for quantum computation. Firstly, we show that the operator matrix of any circuit defines a QPN. Secondly, we represent a specific universal gate set in terms of QPNs. Thirdly, we demonstrate the compositional algebraic nature of QPNs for the construction and analysis of hybrid causal and acausal quantum-parallel processes (cf. proofs in the appendix).

**Theorem 1 (Universality of QPNs).** Any quantum gate circuit defines a QPN $Q$ with $R_Q$ the operator matrix of the circuit.

**Theorem 2 (Clifford+T QPNs).** The universal Clifford+T gate set below of 2-qubit and 1-qubit circuit matrices has a straightforward representation as QPNs:

$$
CNOT = \begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1 \\
0 & 0 & 1
\end{bmatrix}, \quad H = \frac{1}{\sqrt{2}} \begin{bmatrix}
1 & 1 \\
1 & -1
\end{bmatrix}, \quad S = \begin{bmatrix}
1 & 0 \\
0 & i
\end{bmatrix}, \quad T = \begin{bmatrix}
1 & 0 \\
0 & e^{i\pi/4}
\end{bmatrix}
$$

---

8 A system PN is called bounded if there is a bound $b \in \mathbb{N}$ with $deg(m) < b$ for all reachable markings. It is bounded iff its reachability set is finite.

9 ignoring self-loops associated with $r_m(1)$ edges.
For the benefit of interpreting the above universality results, we briefly recall the circuit model of quantum computation and its notion of universal gate set, in order to make this paper somewhat self-contained. For a detailed treatment, the reader is referred to [18]. Circuit diagrams are made from qubits (lines oriented from left to right) and logic gates (typically drawn as boxes or connectors crossing lines vertically). Gates operate on some of the qubits only (cf. e.g., Fig. 4). For a gate, the number of input lines equals that of its outputs. The function of each logic gate on its n qubits is a complex $2^n \times 2^n$ matrix on the corresponding Hilbert subspace $\mathcal{H}^n$ spanned by the $2^n$ canonical basis vectors, i.e., vectors everywhere 0 except for a single position that is 1. The operation of two gates $G$ after $F$ is applied graphically in series from left to right, on the same n qubit lines. It is defined by the matrix-matrix multiplication $GF$ of the corresponding operator matrices. Top to bottom juxtaposition of two gates (incl. NOP as a special case, see below) represents parallel composition, defined by the tensor of the corresponding matrices. The NOP (no operation) gate is simply represented by continuing the n qubit lines it operates on, i.e., without showing the NOP box. Its function is the corresponding $2^n$-squared identity matrix. This leaves the states of these qubits unchanged. Therefore, NOP can be inserted were needed, for example in extending a n-qubit gate to a larger number of qubits using the tensor product with the corresponding identity matrix. A number of finite gate sets (typically very small sets) have been identified as universal, i.e., capable of representing any quantum computation. The Clifford+T gate set above (Th. 2) has been proven to have this property. However, any finite circuit diagram is equivalent to a finite square operator matrix, when, in general, continuous-space-time quantum computations may involve infinite-dimensional Hilbert spaces, i.e., superposition vectors with an infinite number of positions. Therefore, a gate set is defined as universal, more subtly, viz.: if an arbitrarily long but finite sequence of circuits entirely built from this gate set can approximate any quantum computation to any required precision. While this means working with limits, it is not an issue for finite-dimensional Hilbert spaces, which are always complete, i.e., have limits for any converging Cauchy sequence, such as those resulting from arbitrarily long state evolutions from an initial superposition, and converging ever closer to some limit. Completeness guarantees that such limits exist as a superposition in the system.

Hierarchical component architecture. Petri net theory offers a rich set of compositional constructions for the causal, parallel and hierarchical structuring of the underlying system nets of QPNs. For example, foldings are net morphisms that can partition the place set $\mathbb{P}$ lumping together all elements of a single partition into a macro-state and consistently re-interpreting markings and transitions, altogether arriving at a smaller net and generally smaller reachability graph with lower-dimensional matrices. Beyond net compositionality, the relational nature of reachability and the functional character of rates, from single steps to entire QPNs and their rate graphs, lend linear algebra properties to the resulting matrix properties, naturally. However, the linear algebraic compositionality of the target space is present in the QPNs themselves already, as the following compositionality theorem shows. To our knowledge, the generality of this compositionality result is novel and somewhat surprising, although research in stochastic Petri nets has used Kronecker algebra [6,10], however with constraints.

**Theorem 3 (Compositionality of QPNs).** The class of QPNs is closed under the following operations with QPNs $Q = (S, r), Q' = (S', r')$, and complex numbers $c, c' \in \mathbb{C}$:

- zero: $0_Q$, is the QPN over any system PN, with zero rate function defined as $r_m(t) = 0$ for all reachable markings $m$ and concurrences $t$ with $m \rightarrow_c m'$. It follows, that $R_{0_Q}$ is the all-0 matrix.
- unit: $1_Q$, is the QPN over any system PN, with the unit rate function defined as $r_m(1) = 1$ and $r_m(t) = 0$ ($t \neq 1$) for all reachable markings $m$ and concurrences $m \rightarrow_c m'$. It follows, that $R_{1_Q}$ is the identity matrix.
- scaling: $c_Q = (S, c \times r)$, with $(c \times r)(m)(t) = c \times r_m(t)$. It follows that $R_{c_Q} = c \times R_Q$.
- product: $QQ' = (S'', r'')$ is called the monoidal product (aka concatenation) and defined as follows, if $Q$ and $Q'$ are shape equivalent. $QQ'$ has the shape of its components. This means the QPNs have identical places, markings and reachability set (up to isomorphism). We require: for all $m, m', m'' \in M_0$: $E_{m, m''}^r = E_{m, m'}^r \times E_{m', m''}^{r'}$, where $E, E'$ and $E''$ are the respective rate graph edge sets. I.e., for every pair of concurrence edges $m \rightarrow_c m'$ in $E_{m, m'}^r$ and $m' \rightarrow_c m''$ in $E_{m', m''}^{r'}$ we have the contracted edge $m \rightarrow_c m''$ in $E_{m, m''}^r$, and vice versa, with the
rate of the contracted edge \( r^i_{m}(t, t') = r_m(t) \times r_{m'}(t') \). Finally, we define \( T' \) as contraction of singleton concurrences \( t \) and \( t' \) in the respective component, using the contracted concurrence pairs \((t, t'), (1, 1)\) and \((1, t')\) with appropriate \( F^- \) and \( F^+ \) according to the firing sequence \( t' \). It follows that \( R_{Q\otimes Q'} = R_Q R_{Q'} \).

sum: \( Q + Q' = (S'', r'') \) is called the sum and defined as follows, if \( Q \) and \( Q' \) are shape equivalent and all \( t \in T \cap T' \) satisfy \( F^-(t) = F'^-(t) \) and \( F^+(t) = F'^+(t) \). \( Q + Q' \) has the shape of its components. We require \( E'_{m,m'} = E_{m,m'} \cup E'_{m,m'} \) for all \( m, m' \in M_0 \), where \( E' \) and \( E'' \) are the respective rate graph edge sets. The rate function \( r'' \) of the sum is defined s.t. \( r''_{m}(t) = r_m(t) \) for \( (m, t, m') \in E_{m,m'} \cup E'_{m,m'} \). \( r''_{m}(t) = r'_m(t) \) for \( (m, t, m') \in E'_{m,m'} \cup E_{m,m'} \). \( r''_{m}(t) = r_m(t) + r'_{m}(t) \) for \( (m, t, m') \in E_{m,m'} \cap E'_{m,m'} \), and \( r''_{m}(t) = 0 \) otherwise. Finally, we define \( T' \) as singleton concurrences with \( m \xrightarrow{\tau} m' \) in \( E'' \) with their uniquely defined respective input and output markings. It follows that \( R_{Q + Q'} = R_Q + R_{Q'} \).

Kronecker product: \( Q \otimes Q' \) is the disjoint juxtaposition (aka tensor product) of the two QPNs – their isolated parallel composition – in this order. The resulting rate graph satisfies \( G_{Q \otimes Q'} = G_Q \otimes G_{Q'} \) with the usual graph-theoretic Kronecker product of graphs. It follows that the resulting rate matrix satisfies, \( R_{Q \otimes Q'} = R_Q \otimes R_{Q'} \).

Kronecker sum: \( Q \oplus Q' \) is defined as \( Q \otimes 1_Q + 1_Q \otimes Q' \). It follows that the resulting rate matrix \( R_{Q \oplus Q'} \) equals the Kronecker sum of the component rate matrices \( R_Q + R_{Q'} \).

The above compositionality lends linearity properties to quantum Petri net compositions themselves, including hierarchical composition of marked cyclic nets, which are among the hallmarks of classical net architecture. Because stochastic rates are ‘just’ special real-valued rate functions, this result also offers new forms of compositionality to SPNs and similar net classes. In a nutshell, QPN addition is associative and commutative with zero 0. While generally non-commutative, monoidal concatenation, the net equivalent of matrix multiplication, is associative with unit 1 and distributive over addition. Disjoint juxtaposition, with the usual interpretation of concurrent transition firing of isolated subnets, is the free parallel composition. Juxtaposition is associative, but the order matters for the forward reachability and the matrix index sets. Juxtaposition results in the Kronecker product of the rate graphs (graph-theoretically) and of the rate matrices.

As a consequence of the above, we arrive at the following interpretation. If we apply the rate matrix \( R \) of a QPN to a definite marking \( |m\rangle \), i.e., one of the canonical basis vectors, we obtain the vector \( v = R|m\rangle \) identical to the \( m \)-th column of \( R \). If \( v_{m'} > 0 \), then \( m' \) is reachable from \( m \) in the underlying net with amplitude \( v_{m'} \). If \( v_{m'} \neq 0 \), then \( m' \) is neither unreachable in the underlying system from \( m \) in a single step (transition or concurrence). Or else, this underlying reachability step is rated 0 by the rate function of the QPN generating \( R \). So, we can simply read the rated concurrence reachability off the rate matrix.

An n-step evolution of a quantum system can be obtained by matrix-matrix multiplication. For QPNs the rate matrices work in similar way. However rate matrices are forgetful, in that they do not include the concurrency structure inherent in multisets of places and transitions.

In contrast, the product of QPNs is not forgetful of the concurrency structure. Each path with non-zero amplitude in the rate graph allows us to reconstruct a run of the QPN (a kind of PTN occurrence net) of a length defined by the path and a width defined by the maximal cardinality of its concurrence steps. The product \( QQ' \) reflects the OR-parallel quantum execution combinatorially joining up steps and runs through intermediate markings. An n-step superposition evolution of a QPN \( Q \) can then be identified with the direct concurrence reachability in its monoidal power \( Q^n \) (of the same shape as \( Q \)). Similarly, the QPN sum \( Q^{(1 \leq n)} := \sum_{1 \leq i \leq n} Q^i \) characterises such an evolution of at least 1 and up to \( n \geq 1 \) steps; \( Q^0 \) is the identity matrix; and \( Q^{(0 \leq n)} := 1_Q + Q^{(1 \leq n)} \) the evolution of 0 up to \( n \geq 1 \) steps\(^{10}\). Considering the collective OR-parallelism of QPN superposition evolutions as superposed runs, we note that these do not have to follow in lock step. Any mix of possible lengths can be expressed using sums, products and powers of QPNs, as if unwinding the (possibly cyclic) QPNs according to their hierarchical composition.

It should be noted that the concurrences underlying the rate graphs and rate matrices of QPNs, and hence the various interpretations above are independent of a global time and hence independent of a specific observer. The multiple transitions in a concurrence may fire entirely asynchronously. But they can also be entangled in a joint – rhythmical and resonant – firing as a function of the causal net structure, the QPN rates and specific complex amplitudes in initial

\(^{10}\) Cf. the similarity to products and sums of adjacency matrices of graphs – determining the existence of runs of specified lengths
superposition. Because of this, QPNs unify not only classical and quantum computation but also abstract from various time models associated with the corresponding net systems, opening them up for various interpretations, incl. continuous time, discrete time, partial-order event occurrences, stochastic event occurrences etc. Of course, when modeling real physical systems rather than abstract quantum algorithms, any interpretation must be consistent with the quantum mechanical behaviour, ultimately in terms of very specific Hilbert spaces and their operator matrices, whether the generator is a QPN or a quantum circuit diagram.

4 How To Bake Your Pet Net Class with Quantum Flavour

In the literature, many Petri net classes have been defined as extensions of elementary and of place-transition nets. Another approach, taken here, is to parameterise Petri nets and look at specific actual parameters, variation points and restrictions in the spirit of software architecture families and product lines [13,5,29].

For example, we simply define a place-transition net structure (short PTN) as a net structure (see Def. 1) with $G[N] = N$ and WF = true, and, an elementary Petri net, EPN for short, as a PTN with $\deg(F^-(t)) = \deg(F^+(t)) = 1$ for all $t \in T$. A QPN with the corresponding restriction is naturally called Quantum PTN (QPTN) and Quantum EPN (QEPN), respectively.

QPNs that are based, in this way, on our formalisation (Sec. 3) above with specific parameters for the $G$, WF and other variation points, then also induce a well-defined quantum interpretation by virtue of their underlying PN variant generating the relevant reachability relations. Most importantly, the theory (i.e., initially the theorems above) is valid and the bridge to quantum information theory and quantum computation, that we established above, applies to any of those variants.

We briefly sketch a few variations related to extant Petri net classes. This demonstration also aims to enable the reader to apply similar constructions to their own pet Petri net class, without compromising the quantum interpretation of the QPNs that arise from them as their pet underlying PN class.

4.1 Quantum Logical Guards

Many PN extensions associate guards with transitions. A guard is typically a Boolean expression inscribed to, or associated with, a transition. It may have free variables that may be bound to the number of tokens in one or more places related to the transition, or to the token values in coloured nets. Sometimes free variables may be bound to constants, i.e., user-defined parameters, or to variable values in an extended notion of marking, e.g., the values of one or more clocks to represent asynchronous time with several local clocks. Any free variables can be absorbed in the generator $G$ and result in transition schemes $t[x_1,\ldots,x_n]$, with concrete instances $t[v_1,\ldots,v_n]$ for some actual values $v_i$ admissible for the free variables. WF($t[v_1,\ldots,v_n]$) = true then expresses syntactic well-formedness or semantic well-definedness of such transition instances in $\mathbb{T}$. When a guard is false for a given well-formed transition instance $t \in \mathbb{T}$ and marking $m$, the transition is disabled even if $F^-(t) \leq m$. This is represented here by WF($m,t$) = false. According to Def. 2 this implies that the transition is not enabled and hence a corresponding reachability relation is not present in the reachability graph. Clearly the remaining definitions and theorems for QPNs remain well-founded and valid, respectively.

4.2 Quantum Petri Nets with Inhibitors and Phase Transitions

Fig. 5 shows a QPN with initial marking of $A^K$, here with constant $K = 6$. All rates are positive reals and parameterised by a constant $R$. Considering the restriction of rate functions to positive real values and the variation of normalisation to a division by the sum of absolute values (L1-norm) instead of the square root of the moduli squared of the relevant amplitudes, we arrive at Generalized SPNs (GSPNs) as a special case of QPNs. However, there are a few further constructs in GSPNs we need to consider, such as for instance, the inhibitor arc from place $E$ and pointing to transition $c$. This disables $c$ when the marking of $E$ is greater or equal to the arc weight, here 1. For this purpose, the formal definition of GSPNs includes an inhibition function $H$ similar in type to $F^-$, here modelled as $T \xrightarrow{H} \mathbb{N}$. The inhibition action can thus be captured in our formalism by WF($m,t$) = false if $H(t) \leq m$. Immediate transitions, depicted in Fig. 5 by solid black bars, have
GSPNs are a restricted class of QPNs with positive real rates and other restrictions. Left: The underlying PTN illustrates inhibition and immediate transitions with priorities. Transition $e$ has an incoming inhibitor arc from place $E$, graphically represented by a circle head. Immediate transitions are indicated by solid black bars and have associated priorities ($\pi > 0$) with default 1. Rated transitions are drawn as open boxes and have lowest priority 0. Right: Analysis of the underlying system PTN on the left in the GreatSPN toolkit shows that the system is bounded (with bounds shown in places), and (not shown here) that the system has two $S$-invariants ($S$-semiflow eigenvectors) and two $T$-invariants ($T$-semiflow eigenvectors) allowing further reduction using an eigenvector basis in the matrix representation of the underlying net.

an explicit priority $\pi$ associated to them in the net, which defaults to 1 if not specified. When any immediate transitions is enabled, only the immediate transitions of highest priority are enabled. This can be modeled by WF similar to the above conditions, given that all these GSPN firing constraints are expressed in terms of the enabling marking. With successive firings of immediate transitions and acyclic dependencies (which are required for GSPNs) priority levels inductively decrease until only timed transitions, of default priority 0, are enabled. If there is a conflict, a probability distribution (encoded in the rate restrictions for such transitions) resolves that said conflict and chooses one of the conflicting immediate transitions. Any marking that enables an immediate transition is considered vanishing and therefore not part of the reachability set proper that generates the reachability. Typically, one constructs a reachability graph with immediate transitions and then reduces it by contracting all paths consisting of only vanishing markings. This can be done coherently in respect of rates by several PN modelling and simulation tools. We omit the details of the relevant algorithms here and refer to the literature (cf. e.g., [3]). The resulting reduced reachability set can then form the basis for our QPN theory.

Note that GSPNs with the above rate restrictions and those other variations are now a special restricted class of QPNs. In addition, Quantum GSPNs (QGSPNs) with complex-valued rate functions arise from the above transliteration of inhibitors, immediate transitions and priorities. Historically GSPNs cater to the need of modellers to capture significant differences in real rates, especially splitting transitions into those that complete important functions after some duration and those that are orders of magnitude shorter – effectively timeless. Hence immediate transitions are important in this type of net and likely in QPN applications. In practice moreover, for real-time systems modelling, the latter have priorities associated. Amparore et al. write in [3], “a change of state occurs not only because there has been a completion of an activity which takes time, but also because there has been a change of some logical conditions, which may depend on the current state in a rather intricate manner.” Physical systems often exhibit rapid phase transitions and engineered systems rapid mode transitions as a response to critical sensory input or reaching critical reactivity levels etc. Modelling these different types of transitions fully on the basis of Hilbert operators for QPNs, or CTMCs in the case of GSPNs, makes their numerical analysis very complex and sometimes infeasible. Like with real-time systems, we expect that for real-space-time quantum systems, such structuring mechanism will empower modellers similarly, to represent the causal and acausal architecture of quantum systems using both logical and physical dependencies.

4.3 Data-Rich Higher-Level Quantum Petri Nets

Many high-level nets have been studied and a variety of net classes adds data to enrich markings. Among these are Predicate-Transition nets, various kinds of algebraic nets and Coloured Petri
nets. A marking in such a net is generally a multiset of data items for each place. Different net classes add type-checked data types, tuples and various other bells and whistles. We capture such extensions by the generator $G$, which pairs the place set $P$ and data set $D$ and forms $P \times D$ with projections to the respective place and data item. Marking $p \in P$ by multiset $a_1^{n_1} \cdots a_n^{n_n}$ in such a net translates, for our nets, to $(p, a_1)^{n_1} \cdots (p, a_n)^{n_n}$. Similar to the above use of WF, the well-formedness function eliminates ill-formed data pairing with places, or further restrictions on markings such as out-of-bound multiplicities, which are common in some of these higher-level nets.

Likewise, transitions are paired with all the data that can reach them via flow arcs inscribed with data and multiplicity expressions using variables. We can use transition schemes similar to the encoding of guards in WF. Thus $G$ generates a data-rich set of net elements, the flow $F$ between them is generated from the arc inscriptions. $F^-$ and $F^+$ remain input and output multisets like before, for all well-formed and legitimate combinations in the higher-level net. And finally guards on the transitions are transcribed to WF as already shown above.

Algebraic specification of partial functions and predicates mimicking Horn clause logic specification uses a similar construction and has been applied to nets. For example, Predicate-Event nets use many-sorted algebraic specification over nets to generate an ordinary net structure and its markings modulo theory [16,17,24] and enriching net interface descriptions with the power of abstract data types and modules. Analysis methods and executable nets are implemented there based on term rewriting and a compiled functional language. In a partial algebra specification, the free generation and the definedness constraints (here encapsulated\(^\text{11}\) in $G$ and WF) use weak and strong equality in a system of conditional equations. Weak equality satisfies: $t \replace t'$ if $t$ defined, $t'$ defined and $t = t'$. Therefore, we have that $t \replace t$ if $t$ defined. This makes such an equation also useful in a conclusions of a conditional equation, to express conditions for definedness. For strong equality $\equiv$ we have that: $t \equiv t'$ if $t$ defined or $t'$ defined implies $t \replace t'$. That is to say, if one side of the equation is defined, the other must be defined and the two must be equal.

5 Related and Future Work

Ojala’s group [20] used Coloured Petri nets for the analysis of a certain class of quantum cellular automata designs, by example. They achieve a considerable state space reduction compared to the cellular automata. They do not make full use of the asynchronous nature of Petri nets, nor arrive at the kind of universality that characterises QPNs. They model the control structure of the cellular automaton explicitly as a classical PN with complex values as token colours and do not aim at a universal representation of quantum computations. Their encoding achieves a considerable reduction in the state space compared to that of the equivalent quantum cellular automaton. This work was one of the motivations for our approach, in the hope that causal modelling, immediate transitions and other well-known constructions from classical Petri nets can provide a hybrid classical-quantum design with such gains despite offering universality and quantum-only QPNs in the pure quantum case.

Much work exists on classical hybrid and fluid nets, in which causal structuring and stochasticity is mixed with real and integer markings of places [8,12]. Especially their connection with GSPNs has helped us envisage a general approach to superposition and entanglement with its difference to classical stochasticity. For reasons of brevity, we have omitted detailing hybrid quantum nets, in this paper. Suffice it to mention, that one can always partition the set of places into a finite number of place kinds carrying different kinds of tokens, including Boolean, integer, complex integer ($\mathbb{Z}[i]$), real or complex values. Then transitions are classified to form actions on these, including on mixtures of these kinds. This path has been well trodden in Petri net theory and a number of connections can be drawn to QPNs, although, to our knowledge, quantum has never before been combined directly with these nets.

Future work may be fruitful in

1. *graphical calculi* combining QPNs with circuit diagrams such as the ZX calculus [27]. There are well-known theorems relating partial-order semantics of Petri nets with hierarchical message sequence charts and rational algebraic theories of partially ordered event structures, which may benefit quantum calculi. Dually, the circuit diagrams of QPNs may lend themselves for the execution of QPNs on real quantum computers. QPNs and perhaps nets more generally may benefit from the complexity and execution time advantages of quantum computing.\(^\text{11}\) and leaving open how this variation point is actualised
2. **Machine learning and optimisation** of quantum protocols leveraging both the quantum computing speed advantage and advances in classical hardware for machine learning has received much attention recently. Novel approaches such as quantum and classical co-design [14] may be especially applicable to our approach so fundamentally intertwining the two aspects.

3. **Asynchronous quantum automata** have not received much attention. Petri nets have been studied for decades as asynchronously generating and accepting automata for formal languages. A rich set of theorems exists on their decidability and expressive power in comparison to other automata and formal language approaches. A corresponding analysis of quantum automata is still in its infancy. QPNs may assist revisiting these from the perspective of the underlying PNs and their composition.

4. **Open quantum interaction protocols** at the interface of classical and quantum components of QPN systems. Much current focus in quantum hardware is naturally on closed quantum systems. Measurements are typically final, collapse the system as a whole and require the restart of the entire system. With their hybrid causal and acausal structure, QPNs enable a true hybrid between open and closed systems, where the network architecture can increase coherence from the collapse due to partial measurement.

6 Conclusion

This paper introduced a novel diagrammatic model for quantum information processing, Quantum Petri nets (QPNs). It adds to the rich theory of Petri nets new results that are far from straightforward, including the universality of QPNs for quantum computation and their architectural compositional power that reaches from the well-known classical net structure to the operator matrices of Hilbert vector spaces. To our knowledge, these results are *novel and original*. While compositionality is expected for the rate matrices generated by these nets, the matrices are forgetful of the net structure. However, the compositionality we explore here is already inherent in the net structure of the highly parallel quantum processes. QPNs therefore lend themselves for a formal component-based software architecture with well-defined entanglement, teleportation and tunnelling across component boundaries beside the traditional interface protocols, for which nets have been studied in theory and practice. QPNs and their theory are based on the formalism of Petri nets which dates back well before the notion of quantum computation was formulated, to Petri’s 1962 PhD thesis, which itself was developed with reference to principles of relativity and quantum uncertainty [25]. Over the many decades since, nets have become a widely used and standardized notation for concurrent processes in parallel and distributed software modelling and other process-rich domains with several directly and indirectly associated ISO and DIN standards. QPNs are reconnecting with Petri’s original motivation for his nets. Abramsky wrote in [1]

> ...Petri’s thinking was explicitly influenced by physics. To a large extent, and by design, net theory can be seen as a kind of discrete physics: lines are time-like causal flows, cuts are space-like regions, process unfoldings of a marked net are like the solution trajectories of a differential equation. This acquires new significance today, when the consequences of the idea that information is physical are being explored in the rapidly developing field of quantum informatics.

The paper demonstrated that a separation of concerns can be achieved between the classical concurrency structures, typical for Petri nets, and the specific quantum character of entanglement, teleportation and tunnelling. This separation allows modellers to apply Petri net methods and tools to QPNs and leverage them for quantum information processing. Moreover, likely novel results in either field may accelerate advances in the other through a joint focus on the orthogonal connection that QPNs show is possible for the two fields of concurrent and quantum information processes. To this end, this paper included a number of related and future research problems.

> Modern systems architecture requires a dialog between hardware and software platform designers, compiler writers, software library engineers and application software developers, whether for a highly integrated multi-core tablet and single-user workstation, or a high-performance supercomputer. The same will undoubtedly be required of future hybrid quantum and classical systems architectures for networked distributed quantum systems accessible via cloud services and platforms. Such services architectures are currently nascent in commercial offerings. Petri nets have served this dialog in classical distributed systems as a visual user-friendly and at the same time mathematically strong tool alongside other strong representations as a *lingua franca crossing fields*
As part of the formal treatment of quantum processes in the framework of net theory, the paper therefore identified architectural variation points in its formal and informal constructions. We used insights from our prior research in software architecture design and verification. We sketched how the resulting architectural variability can be applied from elementary Petri nets to Generalized Stochastic Petri nets with or without colours. A variety of QPN models, their compositionality and architectures may then be utilised across several classes of Petri nets, contrasted with, and applied to, real quantum software services based on the circuit model of quantum computation.

The paper started by a gentle introduction to quantum computation with QPNs to appeal to the ‘rest of us’: software engineers, practitioners and computer scientists less familiar with the technical details of quantum mechanics and their vector spaces than with diagrammatic models for software programs and their computational processes, in particular state-machine based concurrent processes such as espoused in Petri nets and UML architecture diagrams and dynamic models. The aim was not only to introduce QPNs, but also to recognise and demonstrate – before diving into the requisite formalisation – that a quantum software engineering narrative is needed and possible, with minimal knowledge of complex numbers, some basic familiarity with high-school algebra, and almost no knowledge of vector spaces, at least at the introductory level. The hope is that this diagrammatic approach, or perhaps its combination with other suitable and familiar software models and programming language constructs, may provide a more gradual entrance ramp to the highway of quantum computing, that is bound to become a fast multi-lane freeway. Current on-ramps are steep and access is kept limited to the ‘privileged’ through a mix of physics, applied mathematics and theoretical computer science terminology and theory, yet to be harmonised and standardised, requiring a steep learning curve, and partly mired in unnecessary complexity and, at least in popular science, in myth and hype. Through the architectural compositionality results for QPNs, one might hope, that hybrid classical and quantum software design can be based on a diagram-plus-program approach, with verification in graphs and nets, yet ease of design following principles of modularity, information hiding and separation of concerns. These hallmarks of software engineering may empower domain experts and a future open-source quantum software development community to leverage both classical methods and advances in quantum computing.

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Appendix

The following technical notations and proofs are provided as supplementary material in the arXiv version of the submitted paper, to be filed, and in supplementary material at Springer, should the paper be accepted. They are included here for self-containedness of the submitted paper during the review process. The supplementary material will possibly include code for simulating small QPNs.

6.1 Hilbert Space Notation

Our notation for a Hilbert space $\mathcal{H}$ deserves some comments, as there are different variants for representing inner products and operator matrices, with their usual properties. We use the Dirac notation, i.e., the so-called ‘bra-ket’ notation $\langle u|v \rangle = u^\dagger \cdot v$ to denote the inner product of two vectors $u$ and $v$, where $\dagger$ is the conjugate transpose. The inner product produces a complex number by multiplying a row vector with a column vector. This is useful for a comparison of vectors, for example, to project a vector in the direction of another, to check orthogonality of two vectors and other measurement related calculations. In particular, given two superpositions $|u\rangle$ and $|v\rangle$, the complex amplitude $c$ of a Hilbert space state transition $|u\rangle \rightarrow \rightarrow |v\rangle$ can be computed by $c = \langle u|v \rangle$.

The use of $|u\rangle$ stresses that a Hilbert space vector is a column vector $|u\rangle = [u_1, \ldots, u_n]^T$ and avoids the cumbersome, and in the context of nets ambiguously overloaded, use of $T$ for transposition. $|u\rangle$ is pronounced ‘ket-u’. Any object that uniquely identifies a Hilbert space vector according
to some convention in the given context can be placed inside the ket brackets. For example, a marking \( m \) identifies the canonical basis vector \( |m\rangle = [0, \ldots, 1, \ldots, 0]^T \) that is 0 everywhere, except for a 1 in the position indexed by \( m \). Similarly \( |c_1m_1 + \cdots + c_nm_n\rangle = c_1|m_1\rangle + \cdots + c_n|m_n\rangle \) represents the column vector that is the linear combination of marking basis vectors spanning the Hilbert space over a system Petri net.

The corresponding left part \( \langle u| \) of a bra-ket is pronounced ‘bra-u’. On the one hand \( \langle u| \) represents a conjugate transpose, with \( |u\rangle = |u|^T \) and \( |u\rangle = \langle u|^T \). \( \langle u| \) can therefore be written as the row vector \([u_1^*, \ldots, u_n^*] \). On the other hand, not being a column vector, a bra is not a state vector in \( \mathbf{H} \) but represents the linear function \( \mathbf{H} \xrightarrow{u} \mathbb{C}, \) s.t. \( \langle u|v\rangle = \langle u|v \rangle = \sum u_i^* \times v_i \).

The following are the basic properties of the above inner product in bra-ket notation, with other well-known properties implied by them.

1. conjugate symmetric: \( \langle x|y \rangle = \langle y|x \rangle^* \);
2. positive definite: \( \langle x|x \rangle > 0 \) if \( x \neq 0 \), and \( \langle x|x \rangle = 0 \) if \( x = 0 \);
3. right linear: \( \langle ax + by|z \rangle = a\langle x|z \rangle + b\langle y|z \rangle \); (follows from 2 and 3 above).
4. left antilinear: \( \langle x|ay + bz \rangle = a^*\langle x|z \rangle + b\langle y|z \rangle \).

In particular, we have made use of linearity of a complex Hilbert space, when moving scalars in integrals instead of sums. Hence the notation applies to unbounded nets.

For a tensor product of, say, three qubits \( Q \otimes Q \otimes Q \), conventionally, one also abbreviates a composite (tensor) state to \( |q_1\rangle|q_2\rangle|q_3\rangle \), where a \( q_i \) represents the state of the \( i \)-th qubit, or even shorter to \( |q_1q_2q_3\rangle = |q_1\rangle|q_2\rangle|q_3\rangle \). For example, drawing on such conventions from mathematical physics, we have used \([00]\) to represent the basis vector of the initial marking \( 00 \) of two juxtaposed qubit nets. Taking objects into the kets is versatile as it avoids the exponential combinatorics if used properly. But this convention requires caution, to avoid ambiguity. It also requires careful manipulation in sums and products. In particular recall that, by definition, an entangled superposition is not expressible as a (tensor) product of subsystem states.

### 6.2 Proofs

**Proof (Th. 1).** Let \( C \) be a quantum circuit diagram over \( n \) qubits and \( A \) its \( 2^n \times 2^n \) complex operator matrix. \( A \) represents an operator in the complex Hilbert space \( \mathcal{H}^{2^n} \). By Cor. 1, QPNs are equivalent to complex Hilbert space operators. Therefore, to prove this theorem, we wish to construct a QPN \( Q \) operating on \( \mathcal{H}^{2^n} \) with \( R_Q = A \). Constructing this QPN constitutes a direct proof of Th. 1.

The corresponding QPTN \( Q \) with underlying system PTN \( S \) juxtaposes \( n \) qubits \( P_1, \ldots, P_n \) analogously to the 2 qubits of Fig. 3. The initial marking of this QPN is the combination of the initial markings of the component nets, i.e., \( M_0 = P_{1,0} \cdots P_{n,0} \) or short \( 0 \cdots 0 \) (\( n \) times) by our convention for markings of juxtaposed nets. It is straightforward to show that \( S \) is loop-free, reversible, pure, simple, safe and reduced. These are all properties of the underlying system PN\(^{12} \). Safe markings in \( S \) are thus bit strings of length \( n \). Because of purity and simplicity, the single-transition reachability graph \( G_S \) has a unique edge \( m \xrightarrow{\delta_1} m' \) for all \( m \) with \( m_i = 0 \) and \( m'_i = 1 \), where \( m' \) is identical to \( m \) in all bit positions other than \( i \). Accordingly, there is a unique reverse edge \( m' \xleftarrow{\delta_1} m \) in the other direction. This graph is therefore simple. Consequently, every conceivable safe marking \( \text{deg}(m) \leq 1 \) is reachable from the initial state, and any such marking is reachable from any other in a finite sequence of single-transition steps. Consequently there are \( 2^n \) markings, spanning an \( 2^n \)-dimensional complex vector space with the inner product and other basic operations above. Therefore this vector space is the complex Hilbert space \( \mathcal{H}^{2^n} \). The initial marking \( 0 \cdots 0 \) (\( n \) times) is the basis vector \( |0 \cdots 0\rangle = |0\rangle \cdots |0\rangle \) (\( n \) times). Any pair of different markings \( m \) and \( m' \) has a unique concurrency \( t \) with \( m \rightarrow_{\gamma_t} m' \) (in \( S \)) defined by the bit positions, in which \( m \) and \( m' \) differ. \( t \) is either a single transition, or a concurrency of more than one transition. Therefore, \( G_Q \) is a simple graph, too, with the exception of loops for unit concurrences \( m \rightarrow_{\gamma_1} m \). (Recall that standard graph theory defines simple directed multi-graphs as graphs that are loop-free and have edge multiplicity 1, i.e., unique directed edges, for all pairs of vertices.)

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\(^{12} \)and easily verifiable using standard PN model checkers.
We now read the rate function $r$ for $Q$ off the given circuit matrix $A$: $r_m(t) = A_{m',m}$ for $m \rightarrow_t m'$.

It remains to show that $R_Q = A$. However, this is trivial, because above we already showed that $G_Q$ is simple, except for the unit concurrence self-loops. And the rates associated to these unique edges are exactly those in the diagonal of $A$. Hence the sum in Def. 6 has a single term, viz., $A_{m,m'}$. □

The proof above relies on (a) the interpretation of a complex circuit diagram as a single uniquely defined matrix and (b) universality results for circuits, proven elsewhere. Because of the flattening of the circuit into its matrix, we call the above QPN $Q$ the flattened circuit QPN. The flattened circuit QPN ignores the architecture of the circuit and is only of interest mathematically or in terms of low-level translations. Theorems 2 and 3 are more component-based.

**Proof (Th. 2).** We have already encountered the QPNs for the CNOT and Hadamard gates in Fig. 4. Here we only need to prove that the remaining gates of the universal Clifford+$T$ gate set have corresponding QPNs. This is a straightforward consequence of Theorem 1. Consequently, QPNs can represent the Clifford+$T$ universal gate set. □

We note that standard circuit models include several other commonly used gates, which can all be represented as relatively compact circuits in the Clifford+$T$ gate set and therefore, as QPNs.

The next proof and its Th. 3 guarantee that the composition of QPN nets themselves can capture the stepwise and hierarchical composition of qubit circuits, as a special case of ‘net-plus-transition-rates’ network architecture, describing an overall system by its components, their interdependency via interfaces and their interaction with an environment. For the QPNs this includes classical causal structure because the underlying net is a classical net and rates acausally constraining the independent firing of transitions in concurrences as well as the causal firing. Therefore, this QPN compositionality – applied to just qubit circuit diagrams – does not only cover the compositional structure of the dozen or so of standard gates (via their representation of the equivalent Clifford+$T$ QPNs above) and that of the more complex quantum circuits expressed in several tens of interesting quantum protocols in existence today and characterising the quantum advantage over classical protocols and processes. It also covers the compositionality of hybrid causal and acausal control in terms of system PNs and rate functions in QPNs.

**Proof (Th. 3).** For each of the points, we have to prove firstly, that the corresponding construction results in a well-defined QPN. Secondly, we need to prove the given rate matrix equation for the resulting QPN. The algebraic properties of the different operations on QPNs follow from those on the corresponding matrices, which forgetfully summarise one-step reachability via one or more parallel edges between two different markings. Recall that the diagonal of the rate matrix is directly reduced to transition pairs $(m',m)$ and rate functions in the component nets may differ. Hence their rate matrices differ in general. Therefore, we omit these here, for brevity.

The product $Q'' = QQ'$ constructs $Q'' = (S'',r'')$ with underlying system PN $S'' = (N'',M_0)$. $S''$ shares the place set $P$, place multisets, initial markings and reachability set $M_0$ with the component QPNs, up to isomorphism. For brevity, we treat the corresponding set as equal. The same goes for other compositions, in which shape equivalence of the components is required.

The transitions and concurrences of $S''$ are obtained by contraction of a pair $(t,t')$ with $t$ from $Q$ and $t'$ from $Q'$. Its transition set is defined by single concurrence reachability relations and thus reduced to transition pairs $(t,t')$ where both $t$ and $t'$ can fire in each their component QPNs. The concurrence relation defined for $Q''$ is consistent with the flow definition for single transitions. Likewise the rate function is well-defined. Hence $S''$ is well-defined. Note however, that the net flow and rate functions in the component nets may differ. Hence their rate matrices differ in general.

Now for a fixed pair of markings $m,m'' \in M_0$ (in the shape common to the three QPNs) we have that:

$$R_{QQ'}[m'',m] = R_{Q''}[m'',m] = \sum_{t',m \rightarrow t'm''} r_m(t'') (\text{by rate matrix Def. 8})$$

$$= \sum_{t,t',m \rightarrow t'm''} r_m(t) \times r_{m'}(t') (\text{by def. of product with } t'' = (t,t'))$$

$$= \sum_{m' \in M_0} (\sum_{t,m \rightarrow t'm} r_m(t)) \times (\sum_{t',m' \rightarrow t'm'} r_{m'}(t')) (\text{index rearrangement and distributivity})$$

We have already encountered the QPNs for the CNOT and Hadamard gates in Fig. 4. Here we only need to prove that the remaining gates of the universal Clifford+$T$ gate set have corresponding QPNs. This is a straightforward consequence of Theorem 1. Consequently, QPNs can represent the Clifford+$T$ universal gate set. □

We note that standard circuit models include several other commonly used gates, which can all be represented as relatively compact circuits in the Clifford+$T$ gate set and therefore, as QPNs.
This defines the reachability graph in $Q$ multigraph. If both are simple, then so is $G$. Graphs and matrices reformulate this so as to show the Kronecker product formula, as defined in the literature both for product in terms of reachability graphs and their stochastic rate matrices. The free juxtaposition of two SPNs has been shown to be the Kronecker algebra has been studied intensively in the 1990s (and probably earlier) for the composition of algebras. The Kronecker product of two matrices takes arbitrarily shaped matrices. Because we the tensor product boils down to the Kronecker product an abstract and general construction and applied in many branches of mathematics. For matrices, the Kronecker product of two matrices is in $Q'$ outside of the intersection take their rates from the respective component. This means the sum of QPNs is well-defined.

It is also straightforward to see that the rate matrix sum $R''[m', m] = \sum_{t', m} r''_m(t') = \sum_{t, m} r''_m(t')$, which is a marking union of the nets as graphs: $P'' = P \cup P'$ and $T'' = T \cup T'$ as net elements with the combined function being the union of the two component function, each mapping the corresponding subset of transitions to their input and output in the respective component, as defined there.

Moreover, any combination of component markings $m \in M_0$ and $m' \in M_0'$ is a marking $mm'$ (as multiset product) in $S''$ and by def. of the QPN Kronecker product: $r''_{mm'}(1) = r_m(1) \times r_{mm'}(1)$. In particular the initial marking is such a product marking $M_0'' = M_0 M_0'$. Hence the cardinality of the reachability set, which is also the dimension of the rate square matrix, is given by $|M_0''| = |M_0| \times |M_0'|$. This is what we expect for the Kronecker product of rate matrices too.

The combined single-transition reachability (in $S''$) includes $mm' \xrightarrow{m'} mm''$ if $m \xrightarrow{m'} m''$ in $Q$ and $mm' \xrightarrow{m'} mm''$ if $m' \xrightarrow{m} m''$ in $Q'$, with corresponding single transitions $t$ and $t'$. This defines the reachability graph $G_{S''}$, which is a multigraph if at least one of $G_S$ or $G_{S'}$ is a multigraph. If both are simple, then so is $G_{S''}$.

Next we look at the Kronecker algebra composition operations $\otimes$ and $\oplus$. The tensor product is well-defined. Notice that shared transitions of the two components are required to agree in $F^-$ and $F^+$. This means the intersection of the corresponding rate graph edge sets is well-defined in terms of net structure and reachability. On this intersection, for every pair of reachable markings $m$ and $m'$, the rate function computes the rate matrix sum $E_{m, m'}$ in terms of reachability. On

\[ m \xrightarrow{t, m} m' \] implies by $G_S$ and $G_{S'}$ is a multigraph. If both are simple, then so is $G_{S''}$.

Now as for $G_Q$, we need to consider all concurrences (incl. the unit concurrence 1) implied by $G_{S''}$.

1. A non-unit concurrence $t \neq 1$ with $m_1 \xrightarrow{m_1} m_2$ in $S$ can fire without any firing in $S'$. Hence $m_1 m_2 \xrightarrow{m_1} m_2 m_3$ in $G_{Q''}$ for any reachable marking $m_3$ in $S'$. The rate for the corresponding edge in $G_{Q''}$ is $r''_{m_1 m_3}(t) = r_{m_1}(t) \times r''_{m_3}(1)$.
2. Similarly, a non-unit concurrence \( t' \neq 1 \) with \( \dot{m}_3 \xrightarrow{t'} m_4 \) in \( S' \) can fire without any firing in \( S \). Hence \( m_1 m_3 \xrightarrow{t'} m_1 m_4 \) is in \( G_{Q''} \) for any reachable marking \( m_1 \) in \( S \). The rate for the corresponding edge in \( G_{Q''} \) is \( r''_{m_1 m_3}(t') = r_{m_1}(1) \times r'_{m_3}(t') \).

3. The two concurrences \( t \) and \( t' \) above can fire together as \( m_1 m_3 \xrightarrow{tt'} m_2 m_4 \). This corresponds to an edge in \( G_{Q''} \) with rate \( r''_{m_1 m_3}(tt') = r_{m_1}(t) \times r_{m_3}(t') \).

4. Finally any pair of unit concurrences \( m \xrightarrow{c} m \) and \( m' \xrightarrow{c} m' \) of the respective subnets can be combined, to \( mm' \xrightarrow{c} mm' \) in \( S'' \) and rated \( r''_{mm'}(1) = r_m(1) \times r'_{m'}(1) \).

Again, this is what we expect of the multigraph Kronecker product for our QPN rate graphs, with loop edges \( m \xrightarrow{c} m \) in the rate graphs, as carriers for unit rates \( r_m(1) \). If \( G_{Q''} \) is simple—except for the unit self-loops—, the terms above define exactly the Kronecker product of the corresponding rate matrices. For a multigraph, the corresponding sums of parallel edges have to be formed, in each of the component rate matrices. Then, in the rate matrix of the Kronecker product, the corresponding product of the two sums appears correctly, because in Point (3) above, we have formed all corresponding pairs of edges for a pair of multi-edges, including the degenerate case of the unit concurrence 1.

Hence the rate matrices satisfy: \( R_{Q \otimes Q'} = R_{Q''} = R_Q \otimes R_{Q'} \).

For the Kronecker sum, we first note that the proof is straightforward: all the operations used in the definition of the Kronecker sum, i.e., units 1, + and \( \otimes \), are well-defined as shown above and satisfy their own rate matrix equations. Consequently, the claimed Kronecker sum rate matrix equation \( R_{Q \oplus Q'} = R_Q \oplus R_{Q'} \) is satisfied, too. For, the Kronecker sum of the two QPNs is \( Q \oplus Q' = Q \oplus 1_Q + 1_Q \otimes Q' \), and we can use the rate matrix equations of QPN sum and Kronecker product to arrive at exactly the matrix Kronecker sum shown above.

\( \square \)