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(54) **DECENTRALIZED GRAPH CLUSTERING USING THE SCHRODINGER EQUATION**

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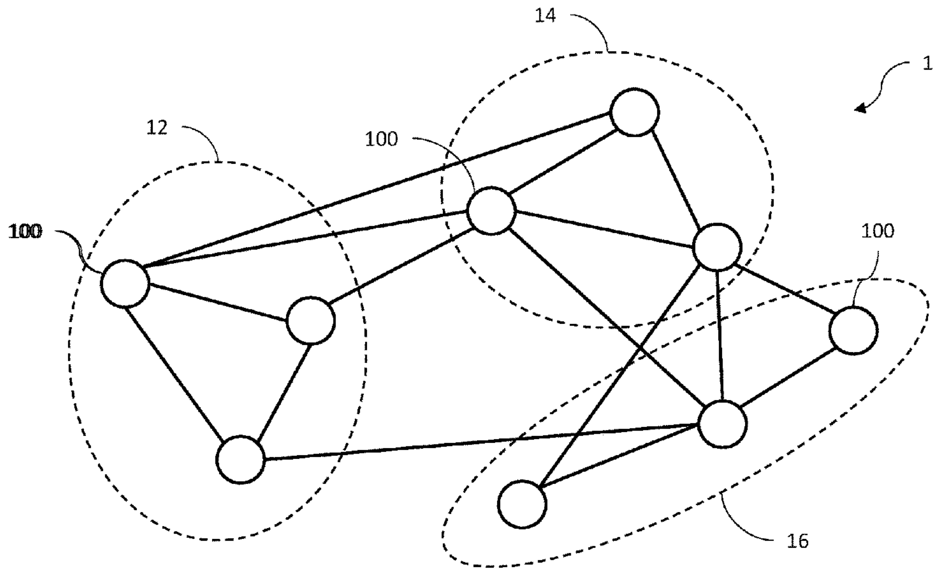
(57) **ABSTRACT**

A method for node cluster assignment in a graph includes identifying neighboring nodes of a first node in the graph, calculating one or more elements of a graph Laplacian of the graph, the one or more elements of the graph Laplacian corresponding to the first node and the neighboring nodes, initializing a first wavefunction associated with the first node with an initial value, evolving the first wavefunction associated with the first node over time based on the initial value, the one or more elements of the graph Laplacian, and previous states of wavefunctions of the neighboring nodes to generate a time-evolved wavefunction vector, and identifying a cluster assignment of the first node based on the time-evolved wavefunction vector.

20 Claims, 5 Drawing Sheets



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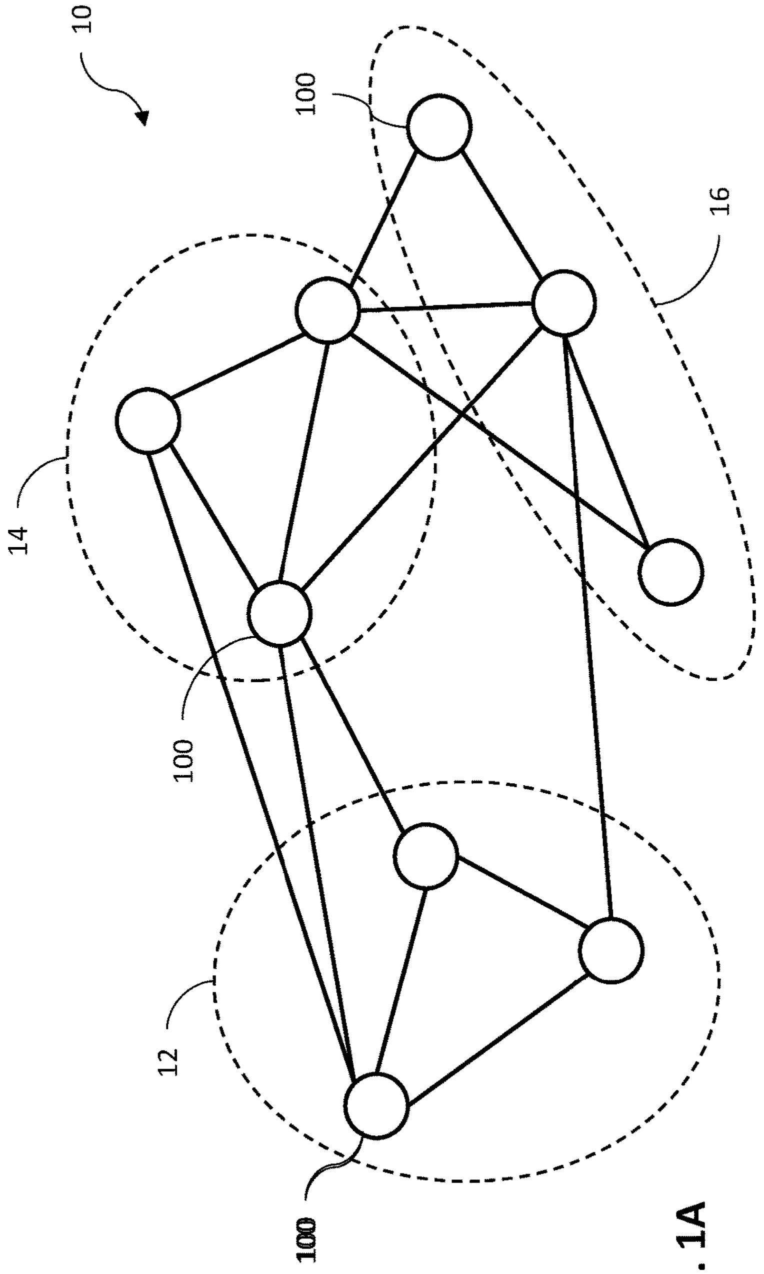
10
100
16
14
100
12
100

FIG. 1A

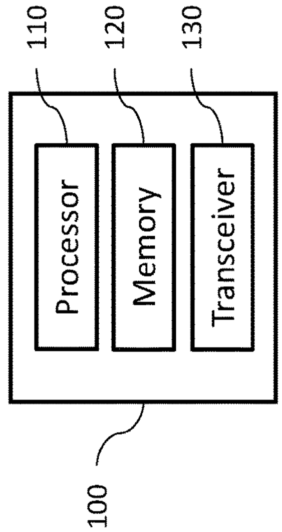
110
120
130
Processor
Memory
Transceiver
100

FIG. 1B

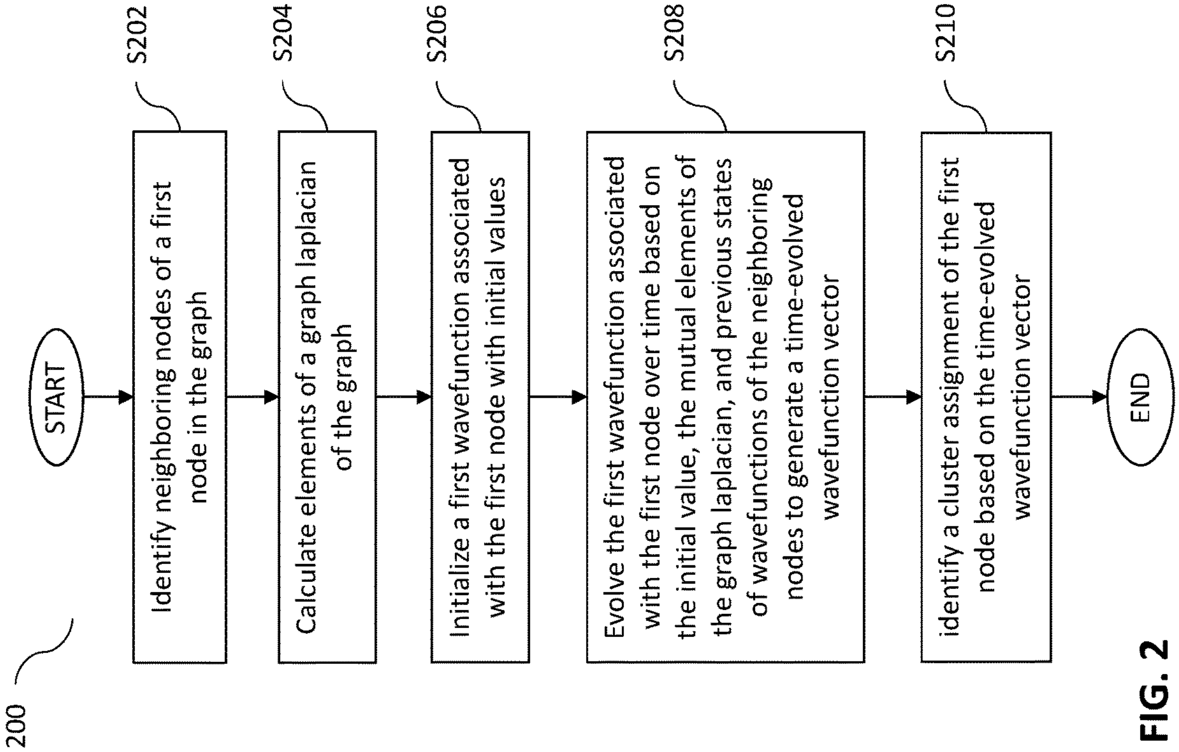
200
START
S202
Identify neighboring nodes of a first node in the graph
S204
Calculate elements of a graph laplacian of the graph
S206
Initialize a first wavefunction associated with the first node with initial values
S208
Evolve the first wavefunction associated with the first node over time based on the initial value, the mutual elements of the graph laplacian, and previous states of wavefunctions of the neighboring nodes to generate a time-evolved wavefunction vector
S210
identify a cluster assignment of the first node based on the time-evolved wavefunction vector
END

FIG. 2

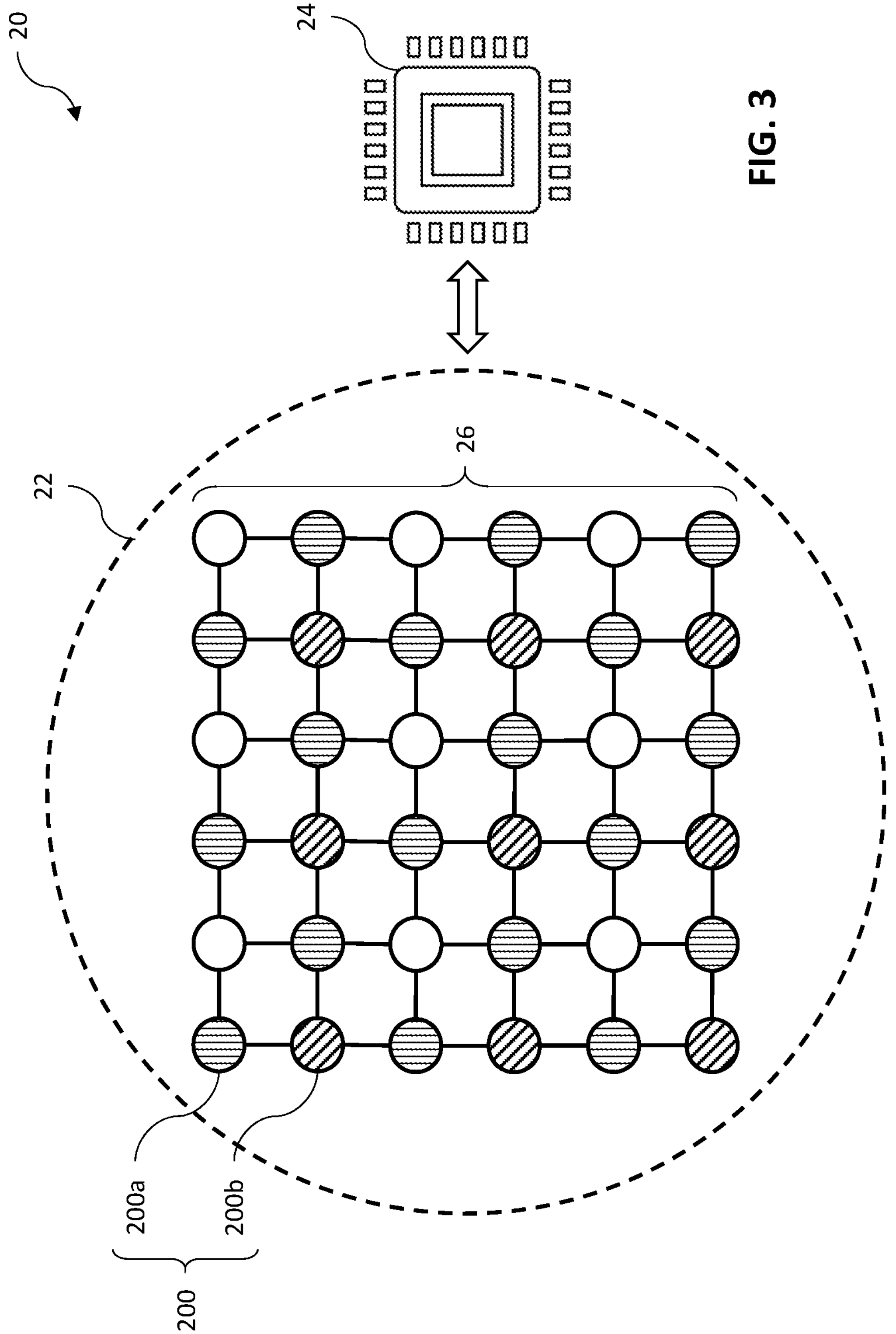

FIG. 3

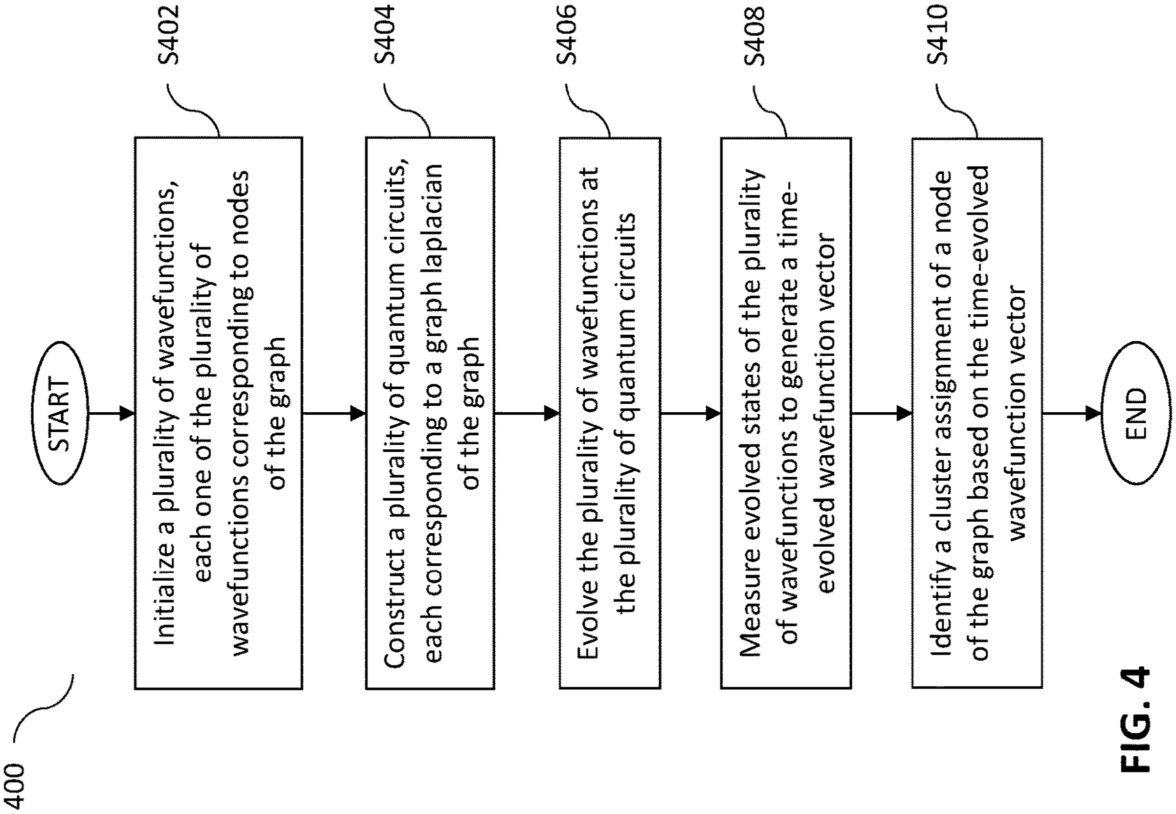
400
START
S402
Initialize a plurality of wavefunctions, each one of the plurality of wavefunctions corresponding to nodes of the graph
S404
Construct a plurality of quantum circuits, each corresponding to a graph laplacian of the graph
S406
Evolve the plurality of wavefunctions at the plurality of quantum circuits
S408
Measure evolved states of the plurality of wavefunctions to generate a time-evolved wavefunction vector
S410
Identify a cluster assignment of a node of the graph based on the time-evolved wavefunction vector
END

FIG. 4

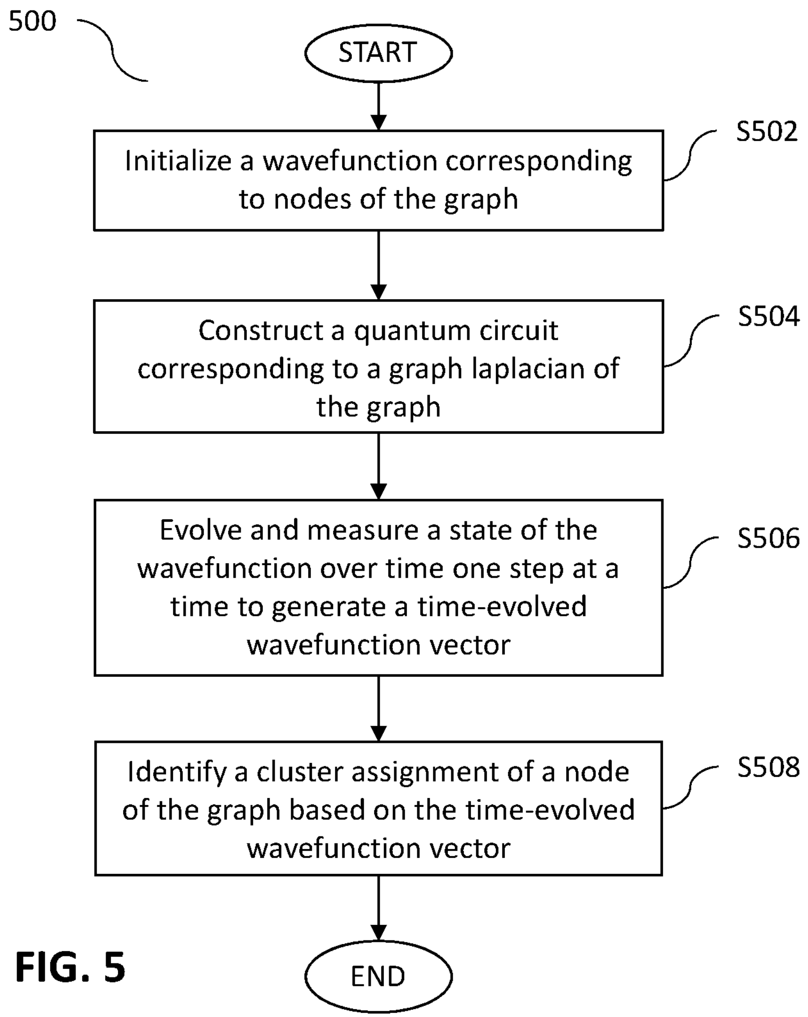
500
START
Initialize a wavefunction corresponding to nodes of the graph
S502
Construct a quantum circuit corresponding to a graph laplacian of the graph
S504
Evolve and measure a state of the wavefunction over time one step at a time to generate a time-evolved wavefunction vector
S506
Identify a cluster assignment of a node of the graph based on the time-evolved wavefunction vector
S508
END

FIG. 5

DECENTRALIZED GRAPH CLUSTERING USING THE SCHRODINGER EQUATION

FIELD

Embodiments of the present invention relate to the field of graph clustering.

BACKGROUND

Algorithms for graph analysis have a wide variety of applications such as routing, pattern recognition, database searches, network layout, and internet page ranking. Although some of the problems in these area can be solved efficiently on present day computing devices, several graph analysis problems are computationally intractable. For example, the problem of partitioning graphs into equal size clusters while minimizing the weights of cut edges arises in a range of settings such as social anthropology, gene networks, protein sequences, sensor networks, computer graphics, and internet routing algorithms. To avoid unbalanced cuts, size restrictions are typically placed on the clusters; instead of minimizing inter-connection strength, if one minimizes the ratio of the inter-connection strength to the size of individual clusters, the problem becomes NP-complete. In fact, the approximation problem is also NP-complete.

The above information disclosed in this Background section is only for enhancement of understanding of the background of the invention and therefore it may contain information that does not form the prior art that is already known to a person of ordinary skill in the art.

SUMMARY

Aspects of some embodiments of the present invention are directed to a distributed computing system for performing node cluster assignment in undirected graphs and a method of using the same. In some embodiments, the distributed computing system includes a distributed set of node processors each of which utilize the Schrödinger wave equation to identify their corresponding cluster assignment based on their interaction with nearby nodes. That is, each node processor may identify the cluster assignment of the corresponding node with only localized knowledge of nearby nodes, and without knowledge of the entire graph.

According to embodiments of the present invention, there is provided a method for node cluster assignment in a graph, the method including: identifying neighboring nodes of a first node in the graph; calculating one or more elements of a graph Laplacian of the graph, the one or more elements of the graph Laplacian corresponding to the first node and the neighboring nodes; initializing a first wavefunction associated with the first node with an initial value; evolving the first wavefunction associated with the first node over time based on the initial value, the one or more elements of the graph Laplacian, and previous states of wavefunctions of the neighboring nodes to generate a time-evolved wavefunction vector; and identifying a cluster assignment of the first node based on the spectrum of the time-evolved wavefunction vector.

In some embodiments, the calculating the one or more elements of the graph Laplacian includes: calculating one or more elements of an adjacency matrix of the graph; calculating one or more elements of a diagonal degree matrix of the graph; and calculating the one or more elements of the

graph Laplacian based on the one or more elements of the adjacency matrix and the one or more elements of the diagonal degree matrix.

In some embodiments, the initializing the first wavefunction associated with the first node with the initial value includes: generating a random value as the initial value; and assigning the initial value to a corresponding element of the first wavefunction at time zero.

In some embodiments, the method further includes: receiving, from the neighboring nodes, the previous states of the wavefunctions of the neighboring nodes.

In some embodiments, the evolving the first wavefunction over time is further based on an evolution parameter.

In some embodiments, the evolving the first wavefunction over time includes: calculating the first wavefunction at a second time t_2 via the following expression: $\psi(t_2, j)=\psi(t_1, j)+\sum_{k\in N(j)}^{\square} i\beta L_{jk}\psi(t_1, k)$ where $\psi(t_2, j)$ and $\psi(t_1, j)$ represent the first wavefunction at the second time t_2 and first time t_1, respectively, N(j) represents a set of nodes neighboring the first node j, β represents an evolution parameter, and L_{jk} represents an element of the graph Laplacian corresponding to the first node j and a neighboring node k, and the second time t_2 is one time step Δt greater than the first time t_1.

In some embodiments, the time-evolved wavefunction vector is expressed as $[\psi(0, j), \psi(\Delta t, j), \psi(2\Delta t, j) \ldots \psi(\text{Tmax}, j)]$ where ψ(t,j) represents a value of the first wavefunction of the first node j at time t, Δt represents an evolution time step, and Tmax represents a maximum evolution time.

In some embodiments, the identifying the cluster assignment of the first node includes: estimating eigenvalues and one or more scaled components of eigenvectors of the graph Laplacian based on the time-evolved wavefunction vector; and determining the number of clusters and the cluster assignment of the first node based on the eigenvalues and the one or more scaled components of eigenvectors of the graph Laplacian respectively.

In some embodiments, the estimating the eigenvalues and the one or more scaled components of the eigenvectors of the graph Laplacian includes: performing a Fourier transform of the time-evolved wavefunction vector to generate a frequency domain wavefunction; identifying frequencies of peaks of the frequency domain wavefunction; estimating the eigenvalues as corresponding to the frequencies of the peaks; and calculating the one or more scaled components of the eigenvectors based on coefficients of the frequencies of the peaks.

In some embodiments, the determining the cluster assignment of the first node includes: identifying a number of clusters of the graph based on the eigenvalues of the graph Laplacian; and assigning the first node to one of the clusters based on the eigenvectors of the graph Laplacian.

In some embodiments, the graph represents a distributed computational system, and each of the first node and the neighboring nodes includes an independent processor of the distributed computational system and a communication device.

According to embodiments of the present invention, there is provided a distributed computing system including: a plurality of computational nodes interconnected as a graph, a first node of the plurality of computational nodes including: a processor; and a processor memory local to the processor, the processor memory has stored thereon instructions that, when executed by the processor, cause the processor to perform: identifying neighboring nodes of a first node from among the plurality of computational nodes;

calculating one or more elements of a graph Laplacian of the graph, the one or more elements of the graph Laplacian corresponding to the first node and the neighboring nodes; initializing a first wavefunction associated with the first node with an initial value; evolving the first wavefunction associated with the first node over time based on the initial value, the one or more elements of the graph Laplacian, and previous states of wavefunctions of the neighboring nodes to generate a time-evolved wavefunction vector; and identifying a cluster assignment of the first node based on the spectrum of the time-evolved wavefunction vector.

In some embodiments, the calculating the one or more elements of the graph Laplacian includes: calculating one or more elements of an adjacency matrix of the graph; calculating one or more elements of a diagonal degree matrix of the graph; and calculating the one or more elements of the graph Laplacian based on the one or more elements of the adjacency matrix and the one or more of the diagonal degree matrix.

In some embodiments, the initializing the first wavefunction associated with the first node with the initial value includes: generating a random value as the initial value; and assigning the initial value to a corresponding element of the first wavefunction at time zero.

In some embodiments, the distributed computing system further includes:

receiving, from the neighboring nodes, the previous states of the wavefunctions of the neighboring nodes.

In some embodiments, the evolving the first wavefunction over time is further based on an evolution parameter.

In some embodiments, the evolving the first wavefunction over time includes: calculating the first wavefunction at a second time t_2 via the following expression: $\psi(t_2, j)=\psi(t_1, j)+\sum_{k\in N(j)}^{\square} i\beta L_{jk}\psi(t_1, k)$ where $\psi(t_2, j)$ and $\psi(t_1, j)$ represent the first wavefunction at the second time t_2 and first time t_1, respectively, N(j) represents a set of nodes neighboring the first node j, β represents an evolution parameter, and L_{jk} represents an element of the graph Laplacian corresponding to the first node j and a neighboring node k, and the second time t_2 is one time step Δt greater than the first time t_1.

In some embodiments, the time-evolved wavefunction vector is expressed as [ψ(0, j), ψ(2Δt, j) . . . ψ(Tmax, j)] where ψ(t,j) represents a value of the first wavefunction of the first node j at time t, Δt represents an evolution time step, and Tmax represents a maximum evolution time.

In some embodiments, the identifying the cluster assignment of the first node includes: estimating eigenvalues and one or more scaled components of eigenvectors of the graph Laplacian based on the time-evolved wavefunction vector; and determining the number of clusters and the cluster assignment of the first node based on the eigenvalues and the one or more scaled components of the eigenvectors of the graph Laplacian, respectively.

In some embodiments, the graph represents a distributed computational system, and each of the first node and the neighboring nodes includes an independent processor of the distributed computational system and a communication device.

BRIEF DESCRIPTION OF THE DRAWINGS

The accompanying drawings, together with the specification, illustrate example embodiments of the present invention, and, together with the description, serve to explain the principles of the present invention.

FIG. **1**A illustrates a schematic diagram of a distributed computing system including a plurality of interconnected nodes that are grouped into a number of clusters, according to some embodiments of the present disclosure.

FIG. **1**B illustrates a schematic diagram of a node of the distributed computing system, according to some embodiments of the present disclosure.

FIG. **2** illustrates a process of node cluster assignment in a graph, according to some embodiments of the present disclosure.

FIG. **3** illustrates a schematic diagram of a quantum computing system, according to some embodiments of the present disclosure.

FIG. **4** illustrates a process of performing node cluster assignment in parallel by a quantum computing system, according to some embodiments of the present disclosure.

FIG. **5** illustrates a process of serially performing node cluster assignment by a quantum computing system, according to some embodiments of the present disclosure.

DETAILED DESCRIPTION

In the following detailed description, only certain exemplary embodiments of the present invention are shown and described, by way of illustration. As those skilled in the art would recognize, the invention may be embodied in many different forms and should not be construed as being limited to the embodiments set forth herein. Descriptions of features or aspects within each exemplary embodiment should typically be considered as available for other similar features or aspects in other exemplary embodiments. Like reference numerals designate like elements throughout the specification.

Data or graph clustering is a widely used technique for exploratory data analysis and has a wide range of applications from statistics and computer science to social sciences. The goal of clustering is to determine patterns (i.e., groups) in the data or graph. However, as the size of the data/graph grows, clustering can quickly become an intractable problem when using traditional approaches.

The systems and methods according to some embodiments of the present disclosure utilize the Schrödinger equation and its connection with the Laplacian of a graph for clustering large graphs and datasets, and significantly improve upon the clustering algorithms of the related art.

FIG. **1**A illustrates a schematic diagram of a distributed computing system including a plurality of interconnected nodes that are grouped into a number of clusters, according to some embodiments of the present disclosure. FIG. **1**B illustrates a schematic diagram of a node of the distributed computing system, according to some embodiments of the present disclosure.

Referring to FIGS. **1**A-**1**B, in some embodiments, distributed computing system **10** includes a distributed network of interconnected nodes **100** that together represent a graph. Each node may interact with (e.g., be connected to and communicate with a number of neighboring nodes. Some or all of the nodes may not have any knowledge about the entire network. For example, each node **100** may only be aware of (e.g., have any information about) other nodes **100** that it interacts with (e.g., its neighboring nodes **100**), and have no knowledge of remaining nodes in the system **10**. Each node **100** may include a processor **110** to perform data processing, a memory **120** for storing data and instructions performed by the processor **110**, and a communication device (e.g., a transceiver) **130** for communicating with one or more other nodes **100**.

The nodes **100** may be organized (e.g., grouped) into a number of clusters (e.g., 12/14/16) based on the interaction strength between connected nodes, size of the clusters, etc. For example, nodes in a one cluster may have strong interaction with one another (i.e., strong intra-connection), while having weak interaction with nodes in other clusters (i.e., weak inter-connections). According to some embodiments, each node of the distributed computing system **10** is capable of independently determining its cluster assignment without knowledge of the entire network/graph and without the aid of a central computer with knowledge of the entire system **10**.

In some examples, the distributed computed system **10** may be a constellation (i.e., graph) of satellites (i.e., nodes), each of which is in communication with a number of neighboring satellites. Teaming/grouping the satellites may aid in object (e.g., missile or meteor) tracking. In other examples, the distributed computed system **10** may be a swarm/network (i.e., graph) of unmanned aerial vehicle (UAV; e.g., drones) for which teaming/grouping may aid in rapid decision making in time evolving scenarios. The strength of the interaction between the satellites/UAVs may be the signal strength of the communication between interacting satellites/UAVs, the distance between interacting satellites/UAVs, or the like.

Graph decomposition may be performed via spectral clustering whereby nodes are assigned to clusters based on the signs of elements of the eigenvectors of the Laplacian matrix corresponding to increasing eigenvalues. The Laplacian of a graph may be derived based on an adjacency matrix that embodies how strongly each pair of nodes in the graph interact with one another. The interaction between two nodes of the system may be visually represented by an edge touching both nodes, and the interaction strength may be represented by the weight of the edge.

As in a distributed system **10**, each node **110** may not have full knowledge of the system, one or more nodes **100** in the system **10** may not possess knowledge of the full Laplacian matrix of the graph. The decentralized graph clustering method according to some embodiments of the present disclosure utilizes spectral clustering, while exploiting the Laplace-Beltrami operator in the Schrödinger equation and its connection to the graph Laplacian, to allow nodes in a distributed system to independently identify their cluster assignments without full knowledge of the entire graph Laplacian.

The Schrödinger equation may be expressed as

$$i\hbar\frac{\partial\psi}{\partial t}=\left[-\frac{\hbar^2}{2m}\Delta+V\right]\psi, \qquad \text{Eq. (1)}$$

where ψ represents the wavefunction, V represents potential energy, m represents mass, $\hbar$ is the reduced planck constant, and Δ is the Laplace-Beltrami operator, which when discretized on the graph gives the graph Laplacian

$$L=I-D^{-1}A \qquad \text{Eq. (2)}$$

In the graph Laplacian definition, A is the adjacency matrix of the graph where each element of the adjacency matrix indicates the interaction strength of the two corresponding nodes, D is the diagonal degree matrix where diagonal elements of the matrix are each the sum of the weight of all edges touching a node, and I is the identity matrix. Here, for an N node graph, the wavefunction ψ is an N-dimensional vector at time t.

Using Equation 1, the discretized Schrödinger update equation on the graph may be expressed as,

$$i\hbar[\psi(t+1)-\psi(t)]=\left[-\frac{\hbar^2}{2m}L+V\right]\psi(t), \qquad \text{Eq. (3)}$$

$$\psi(t+1)=\left[I+i\frac{\hbar}{2m}L-\frac{i}{\hbar}V\right]\psi(t)$$

The above update equation (Equation 3) corresponds to a local update equation at any node j on the graph,

$$\psi(t+1,j)=\psi(t,j)+\sum_{k\in N(j)}^{\square}i\left(\frac{\hbar}{2m}L_{jk}-\frac{1}{\hbar}V_{jk}\right)\psi(t,k), \qquad \text{Eq. (4)}$$

Where k and j are positive integers, $\mathcal{N}$ (j) are neighbors of node j (i.e., nodes that interact with/are connected to node j). Appropriate selection of potential energy can simplify this equation further. In some embodiments, the potential energy V is chosen to be real-valued (and not a complex value) such that it is proportional to L. The potential energy V may be expressed as,

$$V=\alpha\hbar L \qquad \text{Eq. (5)}$$

where

$$\alpha=\frac{\hbar}{2m}-\beta \qquad \text{Eq. (6)}$$

Here, β is an evolution parameter whose value can be suitably chosen given a particular application. Using Equations 5 and 6, Equation 4 may be reduced to:

$$\psi(t+1,j)=\psi(t,j)+\sum\nolimits_{k\in N(j)}^{\square}\ i\beta L_{jk}\psi(t,k), \qquad \text{Eq. (7)}$$

Here, β because node j has knowledge of the interaction strength between it and its neighbors, L_{jk} is known to node j; therefore, the wavefunction ψ for node j can be evolved over time to obtain the time-evolved wavefunction vector [ψ(0), . . . , ψ(T)] for node j. Performing a fast Fourier transform (FFT) operation on the time-evolved wavefunction vector [ψ(0), . . . , ψ(T)] yields spectral components whose peak frequencies that can be used to estimate the eigenvalues of the Laplacian and the corresponding coefficients of the peak frequencies can be used to determine the (scaled) components of the eigenvectors. Using spectral clustering, node j may determine the total number of clusters and its cluster assignment based on the eigenvalues and the j-th (scaled) components (e.g., the signs of such components) of the eigenvectors, respectively. Spectral clustering is described in further detail in Von Luxburg, Ulrike. “A tutorial on spectral clustering.” Statistics and computing 17.4 (2007): 395-416, which is incorporated herein in its entirety.

As will be recognized by a person of ordinary skill in the art, because the computation of the Koopman operator effectively provides the same function as the FFT, anytime the disclosure herein references performing an FFT, such an operation may be substituted by the computation of the Koopman operator and its spectra.

The reason why performing FFT on the on the time-evolved wavefunction vector [ψ(0), . . . , ψ(T)] can yield the desired eigenvalues and eigenvectors can be demonstrated using the analysis below.

Using the assumptions of Equations 5 and 6, the discretized Schrödinger update formulation of Equation (3) can be reduced to:

$$\psi(t+1)=[I+i\beta L]\psi(t) \qquad \text{Eq. (8)}$$

The initial wavefunction ψ(0), which is an N-dimensional vector at time zero, may be expanded in terms of the eigenvectors of the Laplacian L in the form of

$$\psi(0)=C_1v_1+C_2v_2+\ldots+C_nv_N \qquad \text{Eq. (9)}$$

where v_1 to V_N are the eigenvectors of the Laplacian, and C_1 to C_n are the corresponding coefficients. This expansion is possible because the eigenvectors of L form a basis through which any vector (hence ψ(0)) may be expressed. With that as the initial wavefunction, and knowing that $Lv_j=\lambda_jv_j$, the solution of Equation 8 may be expressed using the eigenvalues λ_j of L as

$$\psi(t+1)=\Sigma_{j=1}{}^{N}C_j[1+i\beta\lambda_{j]}{}^{t+1}v_j \qquad \text{Eq. (10)}$$

Generally, $0=\lambda_1\leq\ldots\leq\lambda_N\leq 2$ and v_1 is an N-dimensional vector equal to $[1\ 1\ 1\ \ldots\ 1]^T$. Using Euler's formula,

$$1+i\beta\lambda_j=\sqrt{1+(\beta\lambda_j)^2}(\cos(\omega_j)+i\ \sin(\omega_j)) \qquad \text{Eq. (11)}$$

where

$$\omega_j=\tan^{-1}(\beta\lambda_j) \qquad \text{Eq. (12)}$$

As a result, the solution of Equation 10 may be reformulated as

$$\psi(t+1)=\sum_{j=1}^{N}C_j\left[1+(\beta\lambda_j)^2\right]^{\frac{t+1}{2}}((\cos(t+1)\omega_j)+i\sin((t+1)\omega_j))v_j \qquad \text{Eq. (13)}$$

Using this equation, one may generate the time-evolved wavefunction vector [ψ(0), . . . , ψ(T)]. Performing FFT on this vector provides spectral components, and the frequencies ω_j of the peaks can be used to determine the eigenvalues λ_j based on Equation 12. As the coefficients of the FFT spectral components may be expressed as $C_j(1+(\beta\lambda_j)^2)v_j$, the (scaled) eigenvectors v_j may be calculated based on the eigenvalues μ_j and the magnitude of the corresponding peak at frequency ω_j. Thus, performing FFT on the time-evolved wavefunction vector can yield the eigenvalues and scaled components of the eigenvectors of the graph Laplacian. In some examples, the increase in magnitude of the various frequencies may also be used to estimate the eigenvalues.

As shown in Equation 8, for evolution parameters β greater than 1, the amplitude of the wavefunction only grows over time. To prevent this value from growing too large, which could complicate numerical computations, it is desirable to set evolution parameters β to be as small as possible, while maintaining a detectable signature of the Laplacian in Equation 8 to allow for accurate estimation of the eigenvalues and scaled components (e.g., signs of the scaled components) of the eigenvectors of the Laplacian.

While the above description was based on a real-valued potential energy V, embodiments of the present disclosure are not limited thereto, and by allowing the potential energy to have a complex value(e.g., if $V=i\alpha\hbar L$), the update equation may not increase the magnitude of the signal as in Equations 7 and 8, which may simplify the computation of signal values.

FIG. **2** illustrates a process **200** of node cluster assignment in a graph, according to some embodiments of the present disclosure.

In some embodiments, a first node (e.g., node j) **100** of the graph **10** perform quantum-based cluster assignment by first identifying neighboring nodes of a first node in the graph (S**202**). These may be nodes that interact with (e.g., communicate with) the first node. The interaction of the first node with the neighboring nodes may be facilitated by the communication device **130** of the nodes **100**.

The first node **100** calculates the elements L_{jk} (where k E N(j)) of the graph Laplacian L of the graph **10**, which correspond to the first node and the neighboring nodes (N(j); S**204**). The elements L_{jk} may be calculated by first calculating the corresponding elements A_{jk} and D_{jk} of the adjacency matrix A and the diagonal degree matrix D and using Equation 2. However, embodiments of the present disclosure are not limited thereto, and the elements L_{jk} may be provided to the first node **100**. Here, each node in the graph constructs their own "row" of the adjacency matrix A and the diagonal degree matrix D, but these matrices may not be fully constructed by any node.

The first node **100** then initializes a corresponding element (i.e., a j-th element) of a first wavefunction (which is an N-dimensional vector) with an initial value (S**206**). In so doing, the first node **100** assigns a random value to the corresponding element ψ(0, j) of the N-dimensional vector ψ(0) at time zero.

Once the first wavefunction is initialized, the first node **100** evolves the first wavefunction over time based on the initial value of the first wavefunction ψ(0, j), the elements L_{jk} of the graph Laplacian corresponding to the first node and its neighboring nodes, an evolution parameter, and previous states of wavefunctions of the neighboring nodes to generate a time-evolved wavefunction vector (S**208**). The evolution may occur at discretized time steps of Δt (also referred to as evolution time step). For example, at time t_2 the first wavefunction may be calculated as

$$\psi(t_2,i)=\psi(t_1,j)+\sum\nolimits^{\square}_{k\in \mathrm{N}(j)}\ i\beta L_{jk}\psi(t_1,k) \qquad \text{Eq. (14)}$$

where $\psi(t_2, j)$ and $\psi(t_1, j)$ represent the first wavefunction at the second time t_2 and first time t_1. Here, the second time t_2 may be one time step Δt greater than the first time t_1. The first node may receive the previous states of the wavefunctions $\psi(t_1, K)$ from its neighboring nodes.

The time-evolved wavefunction vector at node j may be expressed as

$$[\psi(0,j),\psi(\Delta t,j),\psi(2\Delta t,j)\ \ldots\ \psi(T\max,j)] \qquad \text{Eq. (15)}$$

where ψ(t,j) represents a value of the first wavefunction of the first node j at time t and Tmax represents a maximum evolution time.

The first node **100** then identifies the cluster assignment of the first node based on the time-evolved wavefunction vector (S**210**). The cluster assignment includes estimating eigenvalues and the j-th scaled components of the eigenvectors of the graph Laplacian based on the spectrum of the time-evolved wavefunction vector (e.g., based on the coefficients of the Fourier transform); and determining the number of clusters and the cluster assignment of the first node based on the eigenvalues and the signs of the j-th scaled components of the eigenvectors of the graph Laplacian, respectively.

Estimating the eigenvalues and the j-th scaled components of the eigenvectors of the graph Laplacian may be done by performing a Fourier transform (e.g., FFT) of the time-evolved wavefunction vector to generate a frequency domain wavefunction, identifying frequencies ψ_j of peaks of the frequency domain wavefunction, estimating the eigenvalues λ_j based on the frequencies of the peaks (e.g., using

Equation 12), and calculating the scaled components of the eigenvectors v_j based on the coefficients of the frequencies that correspond to the eigenvalues

The first node may then determine its cluster assignment by identifying the total number of clusters in the graph based on the eigenvalues of the graph Laplacian, and assigning the first node to one of the clusters based on its locally estimated scaled components (e.g., signs of such components) of the eigenvectors of the graph Laplacian.

The decentralized graph clustering method according to some embodiments of the present disclosure may have a time to convergence that is orders of magnitude faster than the approaches of the related art. Further, the Schrödinger update equation has a lower overhead when compared to update equations of the related art, which confers a computational advantage to the quantum-based cluster assignment of the present disclosure and makes it particularly useful in decentralized clustering of networks (e.g., sensor networks) that are resource limited. Further, the decentralized nature of the quantum-based clustering provides scalability which enables the clustering of large graphs and datasets.

Aspects of embodiments of the present disclosure are directed to a quantum-based clustering method for clustering on fault tolerant quantum computers. Further aspects are directed to a quantum-based method for noisy intermediate scale quantum (NISQ) systems using the quantum approximate optimization algorithm (QAOA) approach.

FIG. **3** illustrates a schematic diagram of a quantum computing system **20**, according to some embodiments of the present disclosure.

According to some embodiments, the quantum computing system **20** includes a quantum computational device **22** and a classical computer (e.g., a classical processor) **24**, which are in communication with one another. For example, the classical computer **24** may provide the input data to the quantum computational device **22** for processing, and may receive the results of the quantum computations from the quantum computational device **22** as output data. For example, some portions of data processing may be performed by the quantum computational device **22** while other portions may be performed by the classical computer in a hybrid implementation. The quantum computational device **22** may include one or more quantum circuits **26**, each of which may include a plurality of quantum bits (or qubits) **200** that may be arranged in a two-dimensional (2D) array or three-dimensional (3D) matrix. Each qubit **200** may communicate with its neighboring qubits and can be prepared in a specific state or be measured with readout ports. In some examples, the qubits **200** may include ancilla qubits **200***a* and computation qubits **200***b*.

According to some embodiments, the quantum-based clustering approach is implemented on a quantum device **22**, in which one or more qubits **200** may be used to represent a node of a graph. However, embodiments of the present disclosure are not limited thereto, and an abstraction layer may define the relationship between nodes and qubits **200**.

The Schrödinger equation in Hamiltonian form may be expressed as

$$i\hbar\frac{\partial\psi}{\partial t}=H\psi, \qquad \text{Eq. (16)}$$

By choosing the Hamiltonian as H=βL, the solution to the above equation is,

$$\psi(t)=e^{-i\beta Lt}\psi(0) \qquad \text{Eq. (17)}$$

which expanding ψ(0) in terms of the eigenvectors of the graph Laplacian L (as expressed in Equation 9) gives,

$$\psi(t)=\Sigma_{j=1}{}^{N}C_je^{i\beta\lambda_j t}v_j=\Sigma_{j=1}{}^{N}C_jv_j(\cos(\beta\lambda_jt)+i\ \sin(\beta\lambda_jt)) \qquad \text{Eq. (18)}$$

Thus, as noted about with reference to Equation 13, the evolution of the wavefunction depends on the eigenvalues and eigenvectors of the graph Laplacian L. In particular, the frequencies depend on the eigenvalues and the coefficients on the entries of the eigenvectors. Here, the evolution parameter is a design parameter that may be tweaked as desired for a given application.

FIG. **4** illustrates a process **400** of performing node cluster assignment in parallel by a quantum computing system **20**, according to some embodiments of the present disclosure.

In some embodiments, the quantum computing system **20** (e.g., the classical processor **24**) initializes M independent wavefunctions (M being an integer greater than 1) such that each one of the wavefunctions is a vector whose dimension is equal to the number of nodes in the graph (**S402**). For a graph of N nodes (N being an integer greater than 1), each one of the wavefunctions includes a vector of N elements, which are each a function of time. In some embodiments, the wavefunctions are initialized to a same vector of random-valued elements $\psi_j(0)$ at time zero ($1\leq j\leq M$).

The quantum computing system **20** (e.g., the quantum computational device **22**) constructs a plurality of quantum circuits **26**, each of which correspond to a graph Laplacian L of the graph (**S404**). This may involve creating, for each quantum circuit **26**, a plurality of quantum gates that are configured to perform coherent quantum operations corresponding to the graph Laplacian L on quantum data (e.g., qubits **100**). The quantum circuits **26** may be identically constructed.

The quantum computing system **20** then evolves (e.g., concurrently or simultaneously evolves) the independent wavefunctions ψ_j at the quantum circuits **26**, such that each one of wavefunction is evolved to a different time than other ones of the wavefunctions (**S406**). In some embodiments, the j-th wavefunction ψ_j is evolved for j time steps Δt. For example, the first wavefunction is evolved by one time step to arrive at $\psi_1(\Delta t)$, the second wavefunction is evolved by two time steps to arrive at $\psi_2(2\Delta t)$, and the Mth wavefunction is evolved by M time steps to arrive at $\psi_M(M\Delta t)$. Here, MΔt represents the maximum evolution time Tmax.

Once each wavefunction is evolved, the quantum computing system **20** measures the evolved states of the wavefunctions (i.e., $\psi_1(\Delta t)$, $\psi_2(2\Delta t)$, . . . , $\psi_M(M\Delta t)$) to generate a time-evolved wavefunction vector (**S408**). It may do so by performing quantum state tomography on the quantum circuits **26** to detect values of the plurality of the wavefunctions and to generate the time-evolved wavefunction vector. The time-evolved wavefunction vector may be expressed as [ψ(Δt), ψ(2Δt) . . . ψ(Tmax)]. As each wavefunction is an N-dimensional wavefunction, with each element corresponding to a different node, the time-evolved wavefunction vector includes N node-specific vectors, of which the jth vector corresponding to the j-th node can be expressed as [ψ(Δt, j), ψ(2Δt, j) . . . ψ(Tmax, j)]. This information may be passed on to the classical computer **24** for further processing.

With this information, the quantum computing system **20** (e.g., the classical computer **24**) may identify the cluster assignment of each node of the graph based on the time-evolved wavefunction vector (**S410**). Using spectral clustering, the classical computer **24** may estimate the eigenvalues and the j-th scaled components of the eigenvectors of the graph Laplacian based on the time-evolved wavefunction vector, and determine the cluster assignment of the node based on the eigenvalues and the j-th scaled components (e.g., signs of such components) of the eigenvectors of the graph Laplacian L. The quantum computing system **20** may perform an FFT on the time-evolved wavefunction vector corresponding to each of the nodes (e.g., [ψ(Δt, j), ψ(2Δt, j) . . . ψ(Tmax, j)]) to generate frequency domain wavefunctions for each node, may identify frequencies of the peaks of the resulting frequency domain wavefunctions, may estimate the eigenvalues as corresponding to the frequencies of the peaks, and calculate the scaled components of the eigenvectors based on the coefficients of the frequencies. The eigenvalues determine the number of clusters, and the signs of the scaled j-th components of the eigenvectors determine the cluster assignment of the j-th node.

As the process **400** of FIG. **4** relies on performing evolutions on M quantum circuits **26** (e.g., concurrently or simultaneously), a large number of qubits may be employed. Thus, while the parallel process may be performed quickly, this comes at the cost of system complexity.

Thus, according to some embodiments, the time-evolution and measurements of the quantum-based clustering approach are performed serially, rather than in parallel. While serial processing may produce slower results, it does result in a significant reduction on the number of qubits used in the quantum circuit **26**, which may be desirable in some applications.

FIG. **5** illustrates a process **500** of serially performing node cluster assignment by a quantum computing system **20**, according to some embodiments of the present disclosure.

In some embodiments, the quantum computing system **20** (e.g., the classical processor **24**) initializes a wavefunction corresponding to nodes of the graph (S**502**). For a graph of N nodes (N being an integer greater than 1), the wavefunction includes a vector of N elements, which are each a function of time. In some embodiments, the wavefunction is initialized to a vector of random-valued elements ψ(0) at time zero.

The quantum computing system **20** (e.g., the quantum computational device **22**) constructs a quantum circuit **26** that corresponds to a graph Laplacian L of the graph (S**504**). This may involve creating a plurality of quantum gates that are configured to perform coherent quantum operations corresponding to the graph Laplacian L on quantum data (e.g., qubits **100**). Such a quantum circuit fora graph Laplacian can be constructed by encoding the vertices of the graph in binary and performing logical operations on the bits that correspond to moving between vertices (that the Laplacian encodes). For example, if the graph is a two-vertex graph with an edge between them, then the bit-flip gate encodes the adjacency matrix of this graph. This can be used to create the Laplacian.

The quantum computing system **20** then evolves and measures the state of the wavefunction ψ at the quantum circuit **26**, one time step Δt at a time, for a total evolution time Tmax to generate a time-evolved wavefunction vector (S**506**). This evolution time Tmax may be an integer multiple of the time steps (e.g., Tmax=MΔt, where M is an integer greater than 1). The evolving and measuring the state of the wavefunction may include repeatedly performing the following: step-evolving the wavefunction p by one time step Δt; determining an evolved state of the wavefunction (e.g., using quantum tomography as described above with respect to FIG. **4**) to generate an element of the time-evolved wavefunction vector (e.g., to generate an element of the vector ψ(jΔt)); and reinitializing the wavefunction to the evolved state (e.g., setting ψ(0) of the reinitialized wavefunction to the values of the N-dimensional vector ψ(jΔt) at step j). This process may be repeated M times (i.e., until the evolution time reaches Tmax), and the measurement results at each steps may be stored (e.g., at the classical computer **24**) to generate the time-evolved wavefunction vector [ψ(Δt), ψ(2Δt) . . . ψ(Tmax)]. As each wavefunction is an N-dimensional wavefunction, with each element corresponding to a different node, the time-evolved wavefunction vector includes N node-specific vectors, of which the j-th vector corresponding to the j-th node can be expressed as [ψ(Δt, j), ψ(2Δt, j) . . . ψ(Tmax, j)].

With this information, the quantum computing system **20** (e.g., the classical computer **24**) may identify the cluster assignment of each node of the graph based on the time-evolved wavefunction vector (S**508**). As noted above, using spectral clustering, the classical computer **24** may estimate the eigenvalues and eigenvectors of the graph Laplacian based on the time-evolved wavefunction vector, and determine the number of clusters and the cluster assignment of the node based on the eigenvalues and the eigenvectors of the graph Laplacian L, respectively.

Given that the process **500** relies on one quantum circuit (which is repeatedly reinitialized), rather than the M quantum circuits of process **400**, far fewer qubits are utilized in serially performing the quantum-based node clustering. Further, as the quantum computer natively evolves the Hamiltonian, the process outlined above may be performed significantly faster than it would be on a classical computer, which performs the evolution numerically using digital circuits.

While the processes **400** and **500** that are described above rely on fault tolerant quantum computers that employ redundant qubits to correct errors (e.g., resulting from cross talk or environmental noise), embodiments of the present disclosure are not limited thereto. In some embodiments, spectral clustering may be performed using quantum approximate optimization algorithm (QAOA), which can produce approximate solutions for combinatorial optimization problems.

Let A be the adjacency matrix and D be the diagonal matrix with row sums of A i.e $D_{ii}=\Sigma A_{i,j}$ and $D_{ij}=0$, i≠j. The row normalized adjacency matrix is $W=D^{-1}A$. The row normalized adjacency matrix W has one eigenvalue at $\lambda_1=1$ with eigenvector $v_1=\sqrt{N}[11\ldots 1]^T$. By Gershgorin's theorem, all eigenvalues lie within $-1\leq\lambda\leq 1$ and are real for undirected graphs. For purpose of spectral clustering, the second eigenvalue λ_2, which is closest to $\lambda_1=1$, and its corresponding eigenvector are of particular interest. Thus, consider the modified matrix,

$$W_p=W-v_1v_1^T \qquad \text{Eq. (19)}$$

The above matrix removes the spectral basis vector corresponding to the eigenvalue 1. Now the optimization problem becomes,

$$\max\langle y|W_p|y\rangle \qquad \text{Eq. (20)}$$

where y=2z−1 (mapping from binary to {−Li}). Here y is a bit string and the above mapping gives z which corresponds to a string consisting of 1 or −1. Since y is not being relaxed to real values, the above maximization becomes

$$\max\ 4z^TW_pz-2W_pz-2z^TW_p+A \qquad \text{Eq. (21)}$$

which when expressed in quadratic form becomes

$$\max\ z^TQz. \qquad \text{Eq. (22)}$$

QAOA may then be applied to obtain an estimate of the above quantity in Equation 22.

While one or more exemplary embodiments have been described with reference to the figures, it will be understood by those of ordinary skill in the art that various suitable changes in form and details may be made therein without departing from the spirit and scope as defined by the following claims, and equivalents thereof.

It will be understood that, although the terms “first”, “second”, “third”, etc., may be used herein to describe various elements, components, and/or nodes, these elements, components, and/or nodes should not be limited by these terms. These terms are used to distinguish one element, component, or node from another element, component, or node. Thus, a first element, component, or node discussed below could be termed a second element, component, or node, without departing from the spirit and scope of the inventive concept.

The terminology used herein is for the purpose of describing particular embodiments and is not intended to be limiting of the inventive concept. As used herein, the singular forms “a” and “an” are intended to include the plural forms as well, unless the context clearly indicates otherwise. It will be further understood that the terms “include,” “including,” “comprises,” and/or “comprising,” when used in this specification, specify the presence of stated features, integers, steps, operations, elements, and/or components, but do not preclude the presence or addition of one or more other features, integers, steps, operations, elements, components, and/or groups thereof. As used herein, the term “and/or” includes any and all combinations of one or more of the associated listed items. Further, the use of “may” when describing embodiments of the inventive concept refers to “one or more embodiments of the inventive concept.” Also, the term “exemplary” is intended to refer to an example or illustration.

It will be understood that when an element, component, or layer is referred to as being “connected to” or “coupled to” another element or layer, it can be directly connected to or coupled to the other element or layer, or one or more intervening elements, components, or layers may be present. When an element or layer is referred to as being “directly on,” “directly connected to” or “directly coupled to” another element, component, or layer, there are no intervening elements, component, or layers present.

As used herein, the terms “use,” “using,” and “used” may be considered synonymous with the terms “utilize,” “utilizing,” and “utilized,” respectively.

The node, node processor, the quantum computing system, and classical computer (hereinafter collectively referred to as “processing devices”), and/or any other relevant devices or components according to embodiments of the present invention described herein may be implemented utilizing any suitable hardware, firmware (e.g. an application-specific integrated circuit, field programmable gate arrays, and/or the like), software, or a suitable combination of software, firmware, and hardware. For example, the various components of each of the processing devices may be formed on one integrated circuit (IC) chip or on separate IC chips. Further, the various components of each of the processing devices may be implemented on a flexible printed circuit film, a tape carrier package (TCP), a printed circuit board (PCB), or formed on a same substrate. Further, the various components of each of the processing devices may be a process or thread, running on one or more processors, in one or more computing devices, executing computer program instructions and interacting with other system components for performing the various functionalities described herein. The computer program instructions are stored in a memory which may be implemented in a computing device using a standard memory device, such as, for example, a random access memory (RAM). The computer program instructions may also be stored in other non-transitory computer readable media such as, for example, a CD-ROM, flash drive, or the like. Also, a person of skill in the art should recognize that the functionality of various computing devices may be combined or integrated into a single computing device, or the functionality of a particular computing device may be distributed across one or more other computing devices without departing from the scope of the exemplary embodiments of the present invention.

What is claimed is:

1. A method for node cluster assignment in a graph, the method comprising:

identifying neighboring nodes of a first node in the graph;

calculating one or more elements of a graph Laplacian of the graph, the one or more elements of the graph Laplacian corresponding to the first node and the neighboring nodes;

initializing a first wavefunction associated with the first node with an initial value;

evolving the first wavefunction associated with the first node over time based on the initial value, the one or more elements of the graph Laplacian, and previous states of wavefunctions of the neighboring nodes to generate a time-evolved wavefunction vector; and

identifying a cluster assignment of the first node based on a spectrum of the time-evolved wavefunction vector and eigenvalues of eigenvectors of the graph Laplacian, by removing the spectral basis vector corresponding to a first eigenvalue of an adjacency matrix of the graph.

2. The method of claim **1**, wherein the calculating the one or more elements of the graph Laplacian comprises:

calculating one or more elements of the adjacency matrix of the graph;

calculating one or more elements of a diagonal degree matrix of the graph; and

calculating the one or more elements of the graph Laplacian based on the one or more elements of the adjacency matrix and the one or more elements of the diagonal degree matrix.

3. The method of claim **1**, wherein the initializing the first wavefunction associated with the first node with the initial value comprises:

generating a random value as the initial value; and

assigning the initial value to a corresponding element of the first wavefunction at time zero.

4. The method of claim **1**, further comprising:

receiving, from the neighboring nodes, the previous states of the wavefunctions of the neighboring nodes.

5. The method of claim **1**, wherein the evolving the first wavefunction over time is further based on an evolution parameter.

6. The method of claim **1**, wherein the evolving the first wavefunction over time comprises:

calculating the first wavefunction at a second time t_2 via the following expression:

$$\psi(t_2,j)=\psi(t_1,j)+\ \sum_{k\in\mathbf{N}(j)}^{\square}\ i\beta L_{jk}\psi(t_1,k)$$

where $\psi(t_2, j)$ and $w(t_1, j)$ represent the first wavefunction at the second time t_2 and first time t_1, respectively, N(j) represents a set of nodes neighboring the first node j, β represents an evolution parameter, and L_{jk} represents an element of the graph Laplacian corresponding to the first node j and a neighboring node k, and wherein the second time t_2 is one time step Δt greater than the first time t_1.

7. The method of claim **1**, wherein the time-evolved wavefunction vector is expressed as

$$[\psi(0,j),\psi(\Delta t,j),\psi(2\Delta t,j)\ldots\psi(T\max,j)]$$

where ψ(t,j) represents a value of the first wavefunction of the first node j at time t, Δt represents an evolution time step, and Tmax represents a maximum evolution time.

8. The method of claim **1**, wherein the identifying the cluster assignment of the first node comprises:

estimating the eigenvalues and one or more scaled components of eigenvectors of the graph Laplacian based on the time-evolved wavefunction vector; and

determining the cluster assignment of the first node based on the eigenvalues and the one or more scaled components of eigenvectors of the graph Laplacian.

9. The method of claim **8**, wherein the estimating the eigenvalues and the one or more scaled components of the eigenvectors of the graph Laplacian comprises:

performing a Fourier transform of the time-evolved wavefunction vector to generate a frequency domain wavefunction;

identifying frequencies of peaks of the frequency domain wavefunction;

estimating the eigenvalues as corresponding to the frequencies of the peaks; and

calculating the one or more scaled components of the eigenvectors based on coefficients of the frequencies of the peaks.

10. The method of claim **8**, wherein the determining the cluster assignment of the first node comprises:

identifying a number of clusters of the graph based on the eigenvalues of the graph Laplacian; and

assigning the first node to one of the clusters based on the one or more scaled components of the eigenvectors of the graph Laplacian.

11. The method of claim **1**, wherein the graph represents a distributed computational system, and

wherein each of the first node and the neighboring nodes comprises an independent processor of the distributed computational system and a communication device.

12. A distributed computing system comprising:

a plurality of computational nodes interconnected as a graph, a first node of the plurality of computational nodes comprising:

a processor; and

a processor memory local to the processor, wherein the processor memory has stored thereon instructions that, when executed by the processor, cause the processor to perform:

identifying neighboring nodes of a first node from among the plurality of computational nodes;

calculating one or more elements of a graph Laplacian of the graph, the one or more elements of the graph Laplacian corresponding to the first node and the neighboring nodes;

initializing a first wavefunction associated with the first node with an initial value;

evolving the first wavefunction associated with the first node over time based on the initial value, the one or more elements of the graph Laplacian, and previous states of wavefunctions of the neighboring nodes to generate a time-evolved wavefunction vector; and

identifying a cluster assignment of the first node based on a spectrum of the time-evolved wavefunction vector and eigenvalues of eigenvectors of the graph Laplacian, by removing the spectral basis vector corresponding to a first eigenvalue of an adjacency matrix of the graph.

13. The distributed computing system of claim **12**, wherein the calculating the one or more elements of the graph Laplacian comprises:

calculating one or more elements of the adjacency matrix of the graph;

calculating one or more elements of a diagonal degree matrix of the graph; and

calculating the one or more elements of the graph Laplacian based on the one or more elements of the adjacency matrix and the one or more of the diagonal degree matrix.

14. The distributed computing system of claim **12**, wherein the initializing the first wavefunction associated with the first node with the initial value comprises:

generating a random value as the initial value; and

assigning the initial value to a corresponding element of the first wavefunction at time zero.

15. The distributed computing system of claim **12**, further comprising:

receiving, from the neighboring nodes, the previous states of the wavefunctions of the neighboring nodes.

16. The distributed computing system of claim **12**, wherein the evolving the first wavefunction over time is further based on an evolution parameter.

17. The distributed computing system of claim **12**, wherein the evolving the first wavefunction over time comprises:

calculating the first wavefunction at a second time t_2 via the following expression:

$$\psi(t_2,j)=\psi(t_1,j)+\ \sum_{k\in N(j)}^{\square}\ i\beta L_{jk}\psi(t_1,k)$$

where $\psi(t_2,j)$ and $\psi(t_1,j)$ represent the first wavefunction at the second time t_2 and first time t_1, respectively, N(j) represents a set of nodes neighboring the first node j, β represents an evolution parameter, and L_{jk} represents an element of the graph Laplacian corresponding to the first node j and a neighboring node k, and

wherein the second time t_2 is one time step Δt greater than the first time t_1.

18. The distributed computing system of claim **12**, wherein the time-evolved wavefunction vector is expressed as

$$[\psi(0,j),\psi(\Delta t,j),\psi(2\Delta t,j)\ldots\psi(T\max,j)]$$

where ψ(t,j) represents a value of the first wavefunction of the first node j at time t, Δt represents an evolution time step, and Tmax represents a maximum evolution time.

19. The distributed computing system of claim **12**, wherein the identifying the cluster assignment of the first node comprises:

estimating the eigenvalues and one or more scaled components of eigenvectors of the graph Laplacian based on the time-evolved wavefunction vector; and

determining the cluster assignment of the first node based on the eigenvalues and the one or more scaled components of the eigenvectors of the graph Laplacian.

20. The distributed computing system of claim **12**, wherein the graph represents a distributed computational system, and

wherein each of the first node and the neighboring nodes comprises an independent processor of the distributed computational system and a communication device.

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