Hybrid classical-quantum computing: Applications to statistical mechanics of neocortical interactions

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Abstract:
Several commerical quantum computers are now available that offer Hybrid Classical-Quantum computing. Application is made to a classical-quantum model of human neocortex, Statistical Mechanics of Neocortical Interactions (SMNI), which has had its applications published in many papers since 1981. However, this project only uses Classical (super-)computers.
Since 2015, PATHINT, has been used as a numerical algorithm for folding path-integrals. Applications in several systems in several disciplines has generalized been from 1 dimension to N dimensions, and from classical to quantum systems, qPATHINT. Papers have applied qPATHINT to neocortical interactions and financial options.
The classical space described by SMNI applies nonlinear nonequilibrium multivariate statistical mechanics to synaptic neuronal interactions, while the quantum space described by qPATHINT applies synaptic contributions from Ca2+ waves generated by astrocytes at tripartite neuron-astrocyte-neuron sites.
Previous SMNI publications since 2013 have calculated the astrocyte Ca2+ wave synaptic interactions from a closed-form (analytic) expression derived by the author. However, more realistic random shocks to the Ca2+ waves from ions entering and leaving these wave packets should be included using qPATHINT between electroencephalographic (EEG) measurements which decohere the quantum wave packets.
This current project extends calculations to multiple scales of interaction between classical events and expectations over the Ca2+ quantum processes to include these random shocks to fit EEG data to the SMNI model, with previous analytic forms for the quantum processes replaced by qPATHINT. The classical-quantum system is fit using the author's Adaptive Simulated Annealing (ASA) importance-sampling optimization code. Gaussian Quadratures are used for numerical calculation of momenta expectations of the astrocyte processes that contribute to SMNI synaptic interactions.
This project demonstrates how some hybrid classical-quantum systems may be calculated using only classical (super-)computers.
Recent calculations also are reported using the closed-form expression, with and without shocks.

Key words: path integral, quantum systems, neocortical interactions

1 Introduction

1.1 Hybrid computing

Several commercial Classical-Quantum computers now can be accessed via the Cloud, e.g., Rigetti, D-Wave, Microsoft, and IBM (Ingber, 2021a); see

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Additional information may be obtained at https://www.ingber.com.

https://docs.ocean.dwavesys.com/projects/hybrid/en/latest/index.html
https://www.rigetti.com/what
https://azure.microsoft.com/en-us/solutions/hybrid-cloud-app/#overview
https://www.ibm.com/it-infrastructure/z/capabilities/hybrid-cloud

These Classical computers often run optimization program in systems that are described by quantum variables using these companies' Quantum computers (Benedetti *et al.*, 2019), Several studies show Quantum computers still cannot deal with many systems even with classical optimizers (Chakrabarti *et al.*, 2020). Still, Software continues to be developed for quantum systems, e.g., Tensorflow for machine learning also offers Hybrid classical-quantum computing:

https://quantumzeitgeist.com/tensorflow-for-quantum-hits-first-birthday/
https://www.tensorflow.org/quantum

Two previous XSEDE project-codes are merged for this project, "Electroencephalographic field influence on calcium momentum waves" and "Quantum path-integral qPATHTREE and qPATHINT algorithms". These Classical codes on Classical computers define a Hybrid Classical-Quantum system.

Previous fits to electroencephalographic (EEG) data have been published using quantum wave-packets defining a specific class of (re-)generated Ca^{2+} ions at tripartite neuron-astrocyte-neuron sites, which influence synaptic interactions (Ingber, 2018). Since 2011 (Ingber, 2011, 2012a), During tasks requiring short-term memory (STM), classical as well as quantum calculations are consistent with interactions between momenta $\mathbf{p}$ of these wave-packets with a magnetic vector potential $\mathbf{A}$ generated by highly synchronous firings of many thousands of neocortical neurons. An anayltic (closed-form) path-integral calculation of the quantum process, in terms of a wave-function with expectation value $\mathbf{p}$ interacting with $\mathbf{A}$, defines quantum interactions coupled to a macroscopic system (Ingber, 2017a).

It is important to further address this system using these to enable realistic inclusion of shocks to the wave-packet. Due to the regenerative process of the wave-packet, e.g., due to collisions between Ca^{2+} ions in the wave-packet causing some ions to leave the wave-packet during its hundreds of msec lifetime, or as new ions enter from the astrocyte processes, the wave-function is repeatedly projected onto quantum sub-spaces. These may be considered as random processes (Ross, 2012). PATHTREE/qPATHTREE and PATHINT/qPATHINT can include shocks in the evolution of a short-time probability distribution over thousands of foldings (Ingber, 2016a, 2017a,b).

1.2 SMNI

Statistical Mechanics of Neocortical Interactions (SMNI) was developed in the late 1970's (Ingber, 1981, 1982, 1983) and enhanced since by fitting experimental data from short-term memory (STM) and electroencephalography (EEG), including papers on fits to attention data (Ingber, 2018) and affective data (Alakus *et al.*, 2020; Ingber, 2021b).

1.3 PATHINT

The path-integral defines code that numerically propagates short-time conditional probability distributions (Ingber *et al.*, 1991; Wehner & Wolfer, 1983a,b). This was generalized to PATHINT in N dimensions, and applied in several disciplines (Ingber, 2000a; Ingber & Nunez, 1995; Ingber *et al.*, 1996; Ingber & Wilson, 2000), and to PATHTREE (Ingber *et al.*, 2001).

1.4 qPATHINT

PATHTREE and PATHINT were generalized to quantum systems, qPATHTREE and qPATHINT (Ingber, 2016a, 2017b,c).

A companion paper treats "Hybrid classical-quantum computing: Applications to statistical mechanics of financial markets" (Ingber, 2021c).

1.5 Organization of paper

Section 2 further describes SMNI in the context of this project.
Section 3 further describes Adaptive Simulated Annealing (ASA) in the context of this project.
Section 4 further describes qPATHINT in the context of this project.
Section 5 describes how the calculation proceeds between SMNI and qPATHINT.
Section 6 describes performance and scaling issues.
Section 7 gives motivation to this project. Calculations performed on the Ookami supercomputer at StonyBrook.edu test a closed-form derived solution with and without shocks. Shocks clearly lower cost functions.
Section 8 is the Conclusion.

1.6 Caveat

As stated previously in these projects (Ingber, 2018),

> "The theory and codes for ASA and [q]PATHINT have been well tested across many disciplines by multiple users. This particular project most certainly is speculative, but it is testable. As reported here, fitting such models to EEG tests some aspects of this project. This is a somewhat indirect path, but not novel to many physics paradigms that are tested by experiment or computation."

2 SMNI

Statistical Mechanics of Neocortical Interactions (SMNI) has been developed since 1981, in over 30+ papers, scaling aggregate synaptic interactions describing neuronal firings, scaling minicolumnar-macrocolumnar columns of neurons to mesocolumnar dynamics, and scaling columns of neuronal firings to regional (sensory) macroscopic sites identified in EEG studies (Ingber, 1981, 1982, 1983, 1984, 1985a, 1994).

Success of SMNI has been to discover agreement/fits with experimental data from modeled aspects of neocortical interactions, e.g., properties of short-term memory (STM) (Ingber, 2012a), including its capacity (auditory 7 ± 2 and visual 4 ± 2), duration, stability, primacy versus recency rule (Ingber, 1984, 1985a, 1994, 1995, 2000b, 2012a; Ingber & Nunez, 1995), EEG dispersion relations (Ingber, 1985b), as well other phenomenon, e.g., Hick's law (Hick, 1952; Ingber, 1999; Jensen, 1987), nearest-neighbor minicolumnar interactions within macrocolumns calculating rotation of images, etc (Ingber, 1982, 1983, 1984, 1985a, 1994). SMNI was also scaled to include mesocolumns across neocortical regions to fit EEG data (Ingber, 1997, 2012a,b, 2018; Ingber & Nunez, 2010).

2.1 XSEDE EEG Project

The Extreme Science and Engineering Discovery Environment (XSEDE.org) project since February 2013, "Electroencephalographic field influence on calcium momentum waves," has fit SMNI to EEG data, developing ionic Ca^{2+} momentum-wave effects among neuron-astrocyte-neuron tripartite synapses modified parameterization of background SMNI parameters. Both classical and quantum physics support the development of the vector magnetic potential of EEG from highly synchronous firings, e.g., as measured during selective attention, as directly interacting with these momentum-waves, creating feedback between these ionic/quantum and macroscopic scales (Ingber, 2012a,b, 2015, 2016b, 2017b,c, 2018; Ingber *et al.*, 2014; Nunez *et al.*, 2013).

2.1.1 qPATHINT For SMNI

qPATHINT includes quantum regenerative process to Ca^{2+} wave-packets as reasonable shocks to the waves that typically do not damage its coherence properties. A proof of principal has been published (Ingber, 2017b).

2.2 SMNI With A

A model of minicolumns as wires supporting neuronal firings, largely from large neocortical excitatory pyramidal cells in layer V (of I-VI), gives rise to currents, in turn giving rise to electric potentials measured as scalp EEG (Ingber, 2011, 2012a; Nunez *et al.*, 2013). This gives rise to a magnetic vector potential.

$$\mathbf{A} = \frac{\mu}{4\pi} \mathbf{I} \log\left(\frac{r}{r_0}\right) \tag{1}$$

Note the log-insensitive dependence on distance. In neocortex, $\mu \approx \mu_0$, where μ_0 is the magnetic permeability in vacuum $= 4\pi 10^{-7}$ H/m (Henry/meter), where Henry has units of kg-m-C^{-2}, the conversion factor from electrical to mechanical variables. For oscillatory waves, the magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$ and the electric field $\mathbf{E} = (ic/\omega)\nabla \times \nabla \times \mathbf{A}$ do not have this log dependence on distance. Thus, $\mathbf{A}$ fields can contribute collectively over large regions of neocortex (Ingber, 2012a,b, 2015, 2016b, 2017b,c, 2018; Ingber *et al.*, 2014; Nunez *et al.*, 2013). The magnitude current is deermined by experimental data on dipole moments $\mathbf{Q} = |\mathbf{I}|\hat{\mathbf{z}}$ where $\hat{\mathbf{z}}$ is the direction of the current $\mathbf{I}$ with the dipole spread over z. $\mathbf{Q}$ ranges from 1 pA-m $= 10^{-12}$ A-m for a pyramidal neuron (Murakami & Okada, 2006), to 10^{-9} A-m for larger neocortical mass (Nunez & Srinivasan, 2006). Currents give rise to $q\mathbf{A} \approx 10^{-28}$ kg-m/s. The velocity of a Ca^{2+} wave can be ≈20-50 μm/s. In neocortex, a typical Ca^{2+} wave of 1000 ions, with total mass $m = 6.655 \times 10^{-23}$ kg times a speed of ≈20-50 μm/s, gives $\mathbf{p} \approx 10^{-27}$ kg-m/s. This yields $\mathbf{p}$ to be on the same order as $q\mathbf{A}$.

2.2.1 Results Including Quantum Scales

The wave-function ψ_e of the interaction of $\mathbf{A}$ with $\mathbf{p}$ of Ca^{2+} wave-packets was derived in closed form from the Feynman representation of the path integral using path-integral techniques, not including shocks (Schulten, 1999), modified here to include $\mathbf{A}$.

$$\psi_e(t) = \int d\mathbf{r}_0 \; \psi_0 \; \psi_F = \left[\frac{1 - i\hbar t/(m\Delta\mathbf{r}^2)}{1 + i\hbar t/(m\Delta\mathbf{r}^2)}\right]^{1/4} \left[\pi\Delta\mathbf{r}^2\{1 + [\hbar t/(m\Delta\mathbf{r}^2)]^2\}\right]^{-1/4}$$
$$\times \exp\left[-\frac{[\mathbf{r} - (\mathbf{p}_0 + q\mathbf{A})t/m]^2}{2\Delta\mathbf{r}^2}\frac{1 - i\hbar t/(m\Delta\mathbf{r}^2)}{1 + [\hbar t/(m\Delta\mathbf{r}^2)]^2} + i\frac{\mathbf{p}_0 \cdot \mathbf{r}}{\hbar} - i\frac{(\mathbf{p}_0 + q\mathbf{A})^2 t}{2\hbar m}\right] \tag{2}$$

PATHINT also has been used with the SMNI Lagrangian L for STM for both auditory and visual memory (Ericsson & Chase, 1982; Zhang & Simon, 1985), calculating the stability and duration of

STM, the observed 7 ± 2 capacity rule of auditory memory, and the observed 4 ± 2 capacity rule of visual memory (Ingber, 2000a; Ingber & Nunez, 1995).

2.2.2 Results Using $< \mathbf{p} >_{\psi*\psi}$

The author previously used his derived analytic expression for $< \mathbf{p} >_{\psi*\psi}$ in classical-physics SMNI fits to EEG data using ASA (Ingber, 2016b; Ingber *et al.*, 2014). Runs using 1M or 100K generated states gave not much different results. ASA Training with 100K generated states over 12 subjects with and without $\mathbf{A}$, was followed by 1000 generated states with the simplex local code contained with ASA to check precision. XSEDE.org resources took an equivalent of several months of CPU on the XSEDE.org UCSD San Diego Supercomputer (SDSC) platform Comet for Training and Testing runs. Calculations used one additional parameter across all EEG regions to weight the contribution to synaptic background $B^G_{G'}$. $\mathbf{A}$ was proportional to the currents measured by EEG, i.e., firings M^G. The "zero-fit-parameter" SMNI philosophy was enforced, wherein parameters are selected and enforced between experimentally determined ranges (Ingber, 1984).

Sopmetimes Testing cost functions were less than their Training cost functions, a result sometimes found in previous studies using this data. This likely is due to great differences in data, likely from great differences in subjects' contexts, e.g., possibly due to subjects' STM strategies including effects calculated here. ASA optimizations in this project always included "finishing" ASA importance-sampling with the modified Nelder-Mead simplex code included in the ASA code to ensure best precision.

2.2.3 Assumptions for quantum SMNI

Some assumptions made for this quantum enhancement of SMNI can be determined by future experiments.

The quantum wave-function of the Ca^{2+} wave-packet was calculated, adding multiple collisions due to their regenerative processes, and it was demonstrated that overlaps with just-previous wave-functions during the observed long durations of hundreds of ms typical of Ca^{2+} waves (Ingber, 2015, 2016b, 2017b,c, 2018; Ingber *et al.*, 2014) support a Zeno or "bang-bang" effect (Burgarth *et al.*, 2018; Facchi *et al.*, 2004; Facchi & Pascazio, 2008; Giacosa & Pagliara, 2014; Kozlowski *et al.*, 2015; Muller *et al.*, 2016; Patil *et al.*, 2015; Wu *et al.*, 2012) which may promote long coherence times.

Inclusion of repeated random shocks to the above wave-function $\psi_F(t)$ demonstrated only small effects on the projections of the wave-packet after these shocks, i.e., the survival time was calculated (Facchi & Pascazio, 2008; Ingber, 2018).

Of course, the Zeno/"bang-bang" effect may exist only in special contexts, given that decoherence among particles is known to be very fast (Preskill, 2015). Therefore, the constant collisions of Ca^{2+} ions as they enter and leave the Ca^{2+} wave-packet due to the regenerative process that maintains the wave may perpetuate at least part of the wave, permitting the Zeno/"bang-bang" effect. qPATHINT as used here provides an opportunity to explore the coherence stability of the wave due to serial shocks of this process.

2.2.4 Nano-Robotic Applications

t is possible that the above considerations could lead to pharmaceutical products contained in nanosystems that could affect unbuffered Ca^{2+} waves in neocortex (Ingber, 2015). A Ca^{2+}-wave momentum-sensor could act like a piezoelectric device (Ingber, 2018).

The nano-robot would be sensitive to local electric/magnetic fields. Highly synchronous firings during STM processes could be directed by piezoelectric nanosystems to affect background/noise efficacies via control of Ca^{2+} waves. This could affect the influence of of Ca^{2+} waves via the vector potential **A**, etc.

2.2.5 Free Will

Further qPATHINT calculations could give additional support to researching possible quantum influences on highly synchronous neuronal firings relevant to STM, yielding connections to consciousness and "Free Will" (FW).

As described previously (Ingber, 2016a,b), experimental feedback from quantum-level processes of tripartite synaptic interactions with large-scale synchronous neuronal firings, recognized as being highly correlated with STM and states of attention, may be established using the quantum no-clone "Free Will Theorem" (FWT) (Conway & Kochen, 2006, 2009).

Ca^{2+} quantum wave-packets may generate states proven to have not previously existed, since quantum states cannot be cloned. In this context, these quantum states may be influential in large-scale patterns of synchronous neuronal firings, rendering these patterns as truly new. The FWT may consider these patterns as new decisions not solely based on previous decisions. These considerations are quite different and independent of other philosophical considerations, e.g., as in

https://plato.stanford.edu/entries/qt-consciousness/ .

Note that only recently has the core SMNI hypothesis since circa 1980 (Ingber, 1981, 1982, 1983), that highly synchronous patterns of neuronal firings process high-level information, been verified experimentally (Asher, 2012; Salazar *et al.*, 2012).

2.3 qPATHINT For SMNI

A previous project tested applications of qPATHTREE and qPATHINT. The wave-function ψ is numerically propagated from its initial state, growing into a tree of wave-function nodes. At each node, interaction of the of Ca^{2+} wave-packet, via its momentum **p**, with highly synchronous EEG, via its collective magnetic vector potential **A**, determines changes of time-dependent phenomena. Changes occur at microscopic scales, e.g., due to modifications of the regenerative wave-packet as ions leave and contribute to the wave-packet, determining the effect on tripartite contributions to neuron-astrocyte-neuron synaptic activity, affecting both **p** and **A**. Such changes also influence macroscopic scales, e.g., changes due to external and internal stimuli affecting synchronous firings, and thereby **A**. At every time slice, quantum effects on synaptic interactions are determined by expected values of the interactions over probabilities ($\psi^* \psi$) determined by the wave-functions at their nodes.

Due to the form of the quantum Lagrangian/Hamiltonian, a multiplicative Gaussian form (with nonlinear drifts and diffusions) is propagated. This permits a straight-forward use of Gaussian quadratures for numerical integration of the expectation of the momenta of the wave-packet, i.e., of $< \mathbf{p}(t) >_{\psi * \psi}$. E.g., see

https://en.wikipedia.org/wiki/Gaussian_quadrature

2.4 Comparing EEG Testing Data with Training Data

Using EEG data from (Citi *et al.*, 2010; Goldberger *et al.*, 2000)

http://physionet.nlm.nih.gov/pn4/erpbci

As was done previously, fitting SMNI to highly synchronous waves (P300) during attention tasks, for each of 12 subjects, it is possible to find 10 Training runs and 10 Testing runs (Ingber, 2016b). A region of continuous high amplitude of 2561 lines represents times from 17 to 22 secs after the tasks began.

Spline-Laplacian transformations on the EEG potential Φ are proportional to the SMNI M^G firing variables at each electrode site. The electric potential Φ is experimentally measured by EEG, not $\mathbf{A}$, but both are due to the same currents $\mathbf{I}$. Therefore, $\mathbf{A}$ is linearly proportional to Φ with a simple scaling factor as a parameter in fits. Additional parameterization of background synaptic parameters also are included, $B^G_{G'}$ and $B^{\ddagger E}_{E'}$.

2.5 Investigation into Spline-Laplacian Transformation

As is common practice, codes for the Spline-Laplacian transformations were applied to all electrodes measured on the scalp. However, the author thinks that the transformation should be applied to each Region of neocortex separately (e.g., visual, auditory, somatic, abstract, etc.), since each region typically participates in attention differently. This process is further tested in this project.

3 ASA Algorithm

For parameters

$$\alpha^i_k \in [A_i, B_i] \tag{3}$$

sampling with the random variable x^i

$$x^i \in [-1, 1]$$

$$\alpha^i_{k+1} = \alpha^i_k + x^i (B_i - A_i) \tag{4}$$

the default generating function is

$$g_T(x) = \prod_{i=1}^{D} \frac{1}{2 \ln(1 + 1/T_i)(|x^i| + T_i)} \equiv \prod_{i=1}^{D} g^i_T(x^i) \tag{5}$$

in terms of "temperatures" for parameters (Ingber, 1989)

$$T_i = T_{i0} \exp(-c_i k^{1/D}) \tag{6}$$

The default ASA uses the same distribution for the annealing schedule for the acceptance function h used for the generating function g.

The ASA default functions can be substituted with user-defined functions (Ingber, 1993, 2012c).

ASA has been applied to studies of COVID-19, fitting forms like xS^y, for variables S and parameters x and y, in the drifts and covariances of conditional probability distributions (Ingber, 2021d).

With over 150 OPTIONS, ASA permits robust tuning over many classes of nonlinear stochastic systems. These many OPTIONS help ensure that ASA can be used robustly across many classes of systems.

"QUENCHing" OPTIONS are widely used to control Adaptive Simulated Annealing. Fuzzy ASA algorithms additionally offer ways of controlling how QUENCHing OPTIONS are applied across many classes of problems.

For this project in paticular, the ASA_SAVE_BACKUP OPTIONS are useful, periodically saving information (including generated random numbers) sufficient to restart if ASA is interrupted, e.g., typically controlled by ASA_EXIT_ANYTIME OPTIONS, removing file "asa_exit_anytime" which permitting ASA to gracefully exit. E.g., ASA can remove "asa_exit_anytime" each 47 hours.

4 Path-Integral Methodology

4.1 Generic Applications

Many systems are defined by (a) Fokker-Planck/Chapman-Kolmogorov partial-differential equations, (b) Langevin coupled stochastic-differential equations, and (c) Lagrangian or Hamiltonian path-integrals. All three such systems of equations are equivalent mathematically, when limits of discretized variables are taken in the defined induced Riemannian geometry of the system due to nonlinear and time-dependent diffusions (Ingber, 1982, 1983; Langouche *et al.*, 1982; Schulman, 1981).

4.1.1 Path-Integral Algorithm

In classical physics, the path integral of N variables indexed by i, at multiple times indexed by ρ, is defined in terms of its Lagrangian L:

$$P[q_t|q_{t_0}]dq(t) = \int \dots \int Dq \exp\left(-\min \int_{t_0}^{t} dt' L \right) \delta\big(q(t_0) = q_0\big) \delta\big(q(t) = q_t\big)$$

$$Dq = \lim_{u \to \infty} \prod_{\rho=1}^{u+1} g^{1/2} \prod_i (2\pi \Delta t)^{-1/2} dq^i_\rho$$

$$L(\dot{q}^i, q^i, t) = \frac{1}{2} (\dot{q}^i - g^i) g_{ii'} (\dot{q}^{i'} - g^{i'}) + R/6$$

$$g_{ii'} = (g^{ii'})^{-1}, g = \det(g_{ii'}) \tag{7}$$

The diagonal diffusion terms are g^{ii} and the drift terms are g^i. If the diffusions terms are nonconstant, there are additional terms in the drift, and in a Riemannian-curvature potential $R/6$ for dimension > 1 in the midpoint Stratonovich/Feynman discretization (Langouche *et al.*, 1982).

The path-integral approach is useful to give mathematical support to physically intuitive variables in the Lagrangian L,

$$\text{Momentum}: \ \Pi^i = \frac{\partial L}{\partial(\partial q^i/\partial t)}$$

$$\text{Mass}: \ g_{ii'} = \frac{\partial L}{\partial(\partial q^i/\partial t)\partial(\partial q^{i'}/\partial t)}$$

$$\text{Force}: \ \frac{\partial L}{\partial q^i}$$

$$\text{F} = \text{ma}: \ \delta L = 0 = \frac{\partial L}{\partial q^i} - \frac{\partial}{\partial t} \frac{\partial L}{\partial(\partial q^i/\partial t)} \tag{8}$$

Canonical Momenta Indicators (CMI $= \Pi^i$) were used successfully in neuroscience (Ingber, 1996, 1997, 1998), combat analyses (Bowman & Ingber, 1997), and financial markets (Ingber, 1996; Ingber & Mondescu, 2001).

The histogram algorithm numerically approximates sums of rectangles of height P_i and width Δq^i at points q^i. E.g., consider a one-dimensional system. In the prepoint Ito discretization, the path-integral representation is given by the kernel G for each of its intermediate integrals, as

$$P(x; t + \Delta t) = \int dx' [g^{1/2} (2\pi \Delta t)^{-1/2} \exp(-L\, \Delta t)] P(x'; t) = \int dx' G(x, x'; \Delta t) P(x'; t)$$

$$P(x; t) = \sum_{i=1}^{N} \pi(x - x^i) P_i(t)$$

$$\pi(x - x^i) = 1\,,\ (x^i - \frac{1}{2}\Delta x^{i-1}) \le x \le (x^i + \frac{1}{2}\Delta x^i); 0\,,\ \text{otherwise} \tag{9}$$

This yields

$$P_i(t + \Delta t) = T_{ij}(\Delta t) P_j(t)$$

$$T_{ij}(\Delta t) = \frac{2}{\Delta x^{i-1} + \Delta x^i} \int_{x^i - \Delta x^{i-1}/2}^{x^i + \Delta x^i/2} dx \int_{x^j - \Delta x^{j-1}/2}^{x^j + \Delta x^j/2} dx' G(x, x'; \Delta t) \tag{10}$$

T_{ij} is a banded matrix of the Gaussian short-time probability centered about the (possibly time-dependent) drift.

Explicit dependence of L on time t can be included. The mesh Δq^i is strongly dependent on diagonal elements of the diffusion matrix, e.g.,

$$\Delta q^i \approx (\Delta t g^{ii})^{1/2} \tag{11}$$

The covariance of each variable is a (nonlinear) function all variables, presenting a rectangular mesh. Given that integration is a smoothing process (Ingber, 1990), fitting the data with integrals over the short-time probability distribution permits coarser meshes than the corresponding stochastic differential equation(s). The coarser resolution is appropriate for a numerical solution of the time-dependent path integral. Consideration of first and second moments yields conditions on the time and variable meshes (Wehner & Wolfer, 1983a). A scan of the time slice, $\Delta t \le \bar{L}^{-1}$ where $\bar{L}$ is the uniform/static Lagrangian, gives most important contributions to the probability distribution P.

4.1.2 Direct Kernel Evaluation

Several projects have used this algorithm (Ingber & Nunez, 1995; Ingber *et al.*, 1996; Ingber & Wilson, 1999; Wehner & Wolfer, 1983a,b, 1987). 2-dimensional codes were developed for specific projects in Statistical Mechanics of Combat (SMC) (Ingber *et al.*, 1991), SMNI (Ingber & Nunez, 1995), and Statistical Mechanics of Financial Markets (SMFM) (Ingber, 2000a).

The 1-dimensional PATHINT code was generalized by the author to N dimensions. Also, a quantum generalization was made, changing all variables and functions to complex variables, encompassing about 7500 lines of PATHINT code. The N-dimensional code was developed for classical and quantum systems (Ingber, 2016a, 2017a,b).

4.1.3 Monte Carlo vs Kernels

Path-integral numerical applications often use Monte Carlo techniques (O'Callaghan & Miller, 2014). This includes the author's ASA code using ASA_SAMPLE OPTIONS (Ingber, 1993). However, this project is concerned with time-sequential serial random shocks, which is not conveniently treated with Monte-Carlo/importance-sampling algorithms.

4.2 Quantum Path Integral Algorithms

4.2.1 Scaling Issues

qPATHINT has been tested with shocks to Ca^{2+} waves (Ingber, 2017b), using the basic code also used for for quantum options on quantum money (Ingber, 2017a). This has illustrated computational scaling issues, further described in the Performance and Scaling Section.

4.2.2 Imaginary Time

Imaginary-time Wick rotations permit imaginary-time to be transformed into real-time. Unfortunately, numerical calculations, after multiple foldings of the path integral, leaves no audit trail back to imaginary time to extract phase information (private communication with several authors of path-integral papers, including Larry Schulman on 18 Nov 2015) (Schulman, 1981).

5 SMNI With qPATHINT

This defines a process fitting EEG using SMNI with qPATHINT numerically calculating the Quantum path-integral between EEG epochs. At the beginning of each EEG epoch time is reset ($t = 0$); the wave-function is decohered ("collapsed") by any EEG measurement. Until the end of any EEG epoch, there are multiple calls to SMNI functions to calculate the evolution of the Classical distribution. This replaces the author's Quantum path-integral closed-form time-dependent analytic solution.

6 Performance and Scaling

Code from a previous XSEDE grant "Electroencephalographic field influence on calcium momentum waves", is used for SMNI EEG fits. Code from a XSEDE previous XSEDE grant "Quantum path-integral qPATHTREE and qPATHINT algorithm", is used for qPATHINT runs.

6.1 Scaling Estimates

Estimates XSEDE.org's Expanse using 'gcc -O3'. Expanse is described in

https://www.sdsc.edu/support/user_guides/expanse

6.1.1 SMNI

100 ASA-iterations taking 7.12676s yields 0.0712676 sec/ASA-iteration over 2561 EEG epochs. With '-g' the total time is 29.9934s.

The number 2561 of EEG epochs is a region of high amplitude of times from 17 to 22 secs after the tasks began, defining epochs to be about 0.002 sec.

6.1.2 qPATHINT

The qPATHINT code uses a variable mesh covering 1121 points along the diagonal, with a maximum off-diagonal spread of 27. Corners require considerable CPU time to take care of boundaries. Oscillatory wave functions require a large off-diagonal spread (Ingber, 2017b).

$dt = 0.0002$ secs requires 10 foldings of the distribution. This takes the code 0.0002 secs/qIteraction. With '-g' the code takes 0.004s to run.

6.1.3 Projected Hours/Service Units (SUs) for This Project

nSubjects x 2 (switch Train/Test) yields a 24-array set of 1-node jobs.
ASA-iterations x (SMNI_time/ASA-iteration + nEpochs x qIterations x qPATHINT_time/qIteration)

yields 100,000 x (0.07 + 2500 x 10 x 0.0002) = 507,000 sec = 140 hr/run = 6 day/run.
Time for Gaussian quadratures calculations is not appreciable:

https://en.wikipedia.org/wiki/Gaussian_quadrature

Maximum duration of a normal job is 2 days. ASA has built in a simple way of ending jobs with printout required to restart, including sets of random numbers generated.

7 Closed-Form Calculations

Calculations on the Ookami supercomputer at StonyBrook.edu tested the path-integral derived analytic (closed-form) expression (Ingber, 2018) for astrocyte Ca^{2+} wave synaptic interactions

$$< \mathbf{p} >_{\psi*\psi} = m \frac{< \mathbf{r} >_{\psi*\psi}}{t - t_0} = \frac{q\mathbf{A} + \mathbf{p}_0}{m^{1/2}|\Delta\mathbf{r}|} \left(\frac{(\hbar t)^2 + (m\Delta\mathbf{r}^2)^2}{\hbar t + m\Delta\mathbf{r}^2} \right)^{1/2} \tag{12}$$

Shocks were inserted into the mass m of the wave packet of 1000 ions, using a random number generator that contributed up to 1% of the synaptic contribution due to Ca^{2+} wave contributions. I.e., the mass was perturbed as $m = m(1 - R) + Rr$, where $R = 0.1$ and r is a random number between 0 and 1. The results are given in Table 1.

ASA was used with 200000 valid generated states for optimizations, then the modified Nelder-Mead code was used to sometimes gain extra precision with 5000 valid generated states. Training and Testing sets of data were used for 12 subjects, then the Training and Testing sets were exchanged. Runs were done with the added shocks and without these shocks. Each of the 48 runs took about 2 days on the Ookami supercomputer at StonyBrook.edu .

As commented previously (Ingber, 2018), "As with previous studies using this data, results sometimes give Testing cost functions less than the Training cost functions. This reflects on great differences in data, likely from great differences in subjects' contexts, e.g., possibly due to subjects' STM strategies only sometimes including effects calculated here."

8 Conclusion

A numerical path-integral methodology is used by SMNI to fit EEG to test quantum evolution of astrocyte-(re-)generated wave-packets of Ca^{2+} ions that suffer shocks due collisions and regeneration of free ions. SMNI is generalized with quantum variables using qPATHINT.

SMNI has fit experimental data, e.g., STM and EEG recordings under STM experimental paradigms. qPATHINT includes quantum scales in the SMNI model, evolving Ca^{2+} wave-packets

Table 1: Comparison using analytic derivation without and with shocks. The subject numbers are given as sNN, and a "-X" represents exchanging Training and Testing sets of EEG data. Under Results an "I" represents an improvement of a lower cost functions with shocks versus no-shocks. An "N" represents better results with no-shocks versus shocks. These results show 16 "I"s and 8 "N"s, clearly in favor of shocks.

Sub	no-Shocks	Shocks	Results
s01	84.68593	84.34305	I
s01-X	118.8452	118.7469	I
s02	68.48157	68.40058	I
s02-X	49.28883	49.13109	I
s03	59.7605	59.724	I
s03-X	75.0323	74.92172	I
s04	49.99637	50.00408	N
s04-X	63.24503	63.20287	I
s05	66.17184	66.20236	N
s05-X	69.30881	69.54677	N
s06	79.46274	79.65097	N
s06-X	61.53507	61.2894	I
s07	68.26923	68.24647	I
s07-X	75.313	75.19828	I
s08	43.82171	43.74269	I
s08-X	42.6704	42.66051	I
s09	46.90326	46.84606	I
s09-X	24.21445	24.24822	N
s10	53.19396	53.12375	I
s10-X	30.12276	30.04148	I
s11	43.13081	43.17781	N
s11-X	50.20932	50.21808	N
s12	44.24383	44.18135	I
s12-X	44.35697	44.36804	N

with momentum $\mathbf{p}$ serial shocks, interacting with the magnetic vector potential $\mathbf{A}$ due to EEG, via the $(\mathbf{p} + q\mathbf{A})$ interaction at each node at each time slice t, in time with experimental EEG data.

Published pilot studies have given rationales for developing this particular quantum path-integral algorithm, to study serial random shocks that occur in many systems. This quantum version can be used for many quantum systems, which is increasingly important as experimental data is increasing at a rapid pace for many quantum systems.

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Note that in accordance with common practice, standalone website URLs are not necessarily referenced at the end, but often appear within the body of text. E.g., see

https://libanswers.snhu.edu/faq/8627
https://www.scribbr.com/apa-examples/cite-a-website/
https://libguides.css.edu/APA7thEd/Webpages

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