Semiclassical modeling of multiparticle quantum systems using high-performance clustering and visualization on the Macintosh

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Abstract

We have developed, and implemented on the Macintosh platform, a method that recasts the time-propagation of dynamic, mutually interacting quantum-mechanical wavefunctions principally as the time-evolution of many classical particles. The computations modeling up to 128 interacting quantum particles, represented by millions of classical paths, were developed and performed entirely using Macintosh-based clusters. The compilers used in the research included Absoft Fortran, IBM xlf, and Metrowerks CodeWarrior, while the internode message passing used both the BSD sockets and Open Transport versions of MacMPI as well as LAM/MPI. Debugging and optimization were assisted with message-passing visualization diagnostics using the Macintosh GUI. These calculations, including data post-processing, were highly numerically-intensive and tightly-coupled, therefore demanding the computational power and networking capabilities of clusters of Macintoshes.

The Carbon libraries and QuickTime were utilized directly to visualize the time-dependent quantum-mechanical wavefunction data. Complex quantum data was represented using a color mapping algorithm and drawn as successive frames for compression into QuickTime movies. Later, real and imaginary components of the wavefunction were encoded as stereo sound in these QuickTime movies for wavefunction sonification, leading to insights that ultimately made possible the high accuracy of this quantum model when compared to quantum theory.

The modeling approach utilizes an approximation of Feynman path integrals, known as the semiclassical method, to reduce the path integral to only the "classical" paths connecting the wavefunction at one time step to the next. Tracing these classical paths through phase space provides the necessary data to evolve quantum wavefunctions in time. Particle techniques implemented on massively parallel computers for plasma modeling were used to propagate quantum systems using this alternative method. Potential applications include the solar interior, protein folding, semiconductor surfaces, and other situations were quantum effects become important.

The Idea

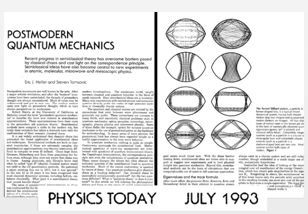
Traditional methods

Is the Schrödinger Equation enough? It poses challenges for computational approaches to solve many-body systems.

$$\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x,t)\,\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t)$$

Something new?

Semiclassical methods reveal a way to represent a quantum wavefunction using many classical paths, which we knew we could do with plasma codes.



Theory

Start with all possible paths

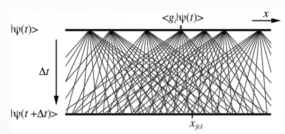
Deriving from Feynman path integrals using semiclassical methods reveals an explicit description how to sample classical paths.

$$|\psi(t+\Delta t)\rangle = \frac{1}{N_{p_0}}\sum_{p_0}\sum_{g_i}|p_{fcl}\rangle\exp(-ip_{fcl}x_{fcl}/\hbar)\frac{\exp(iS_{cl}(p_0,g_i,\Delta t)/\hbar)}{\sqrt{h\det(p_0,g_i,\Delta t)}}\langle g_i|\psi(t)\rangle$$

where $S_{cl}(p_0,g_i,\Delta t) \equiv \int_t^{t+\Delta t} L(x,\dot{x},t')dt'$, an integral on the classical path from g_i with p_0 to x_{fcl} with p_{fcl}.

Virtual classical particles

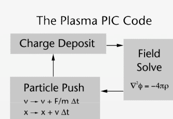
Rather than have us calculate all possible paths, the derivation prescribes an judicious sampling: just the classical paths. Like virtual particles of Quantum Field Theory, *virtual classical particles* are said to trace these paths.



Implementation

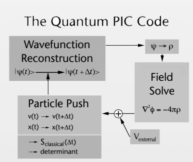
Flow chart of the classical plasma PIC code

We began with a plasma PIC code designed for massively parallel computers.



Flow chart of the quantum PIC code

We converted the plasma code into a quantum code, extending to the particle push and adding a wavefunction reconstruction routine.

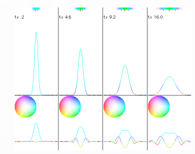


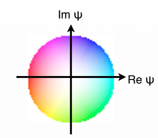
Visualization and Sonification

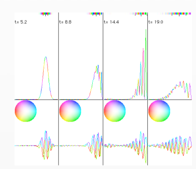
Color and sound

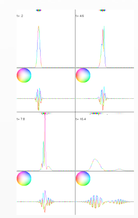
Quantum wavefunctions in the position-space representation can be written as an array of complex numbers. To visualize this data in a meaningful way, we display the phase of the wavefunction as hue (since both are cyclic) and its magnitude as intensity.

To sonify the complex data, the real part of the wavefunction was sent to the left stereo channel and the imaginary part sent to the right channel. The signal was then looped like how an digitized instrument would be played. This technique made the momentum characteristics of the wavefunction audible, leading to insights both into the numerical technique and quantum physics.









Macintosh technologies

Numerous technologies on the Macintosh platform were used to produce these results. They include:

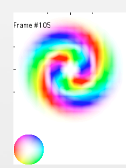
- QuickDraw
- Palette Manager
- Sound Manager
- QuickTime
- Open Transport

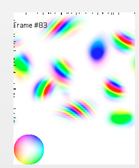
Also, certain products available on the Macintosh platform were employed in this work:

- Metrowerks CodeWarrrior
- Absoft Fortran
- IBM xlf
- Adobe Photoshop
- Canvas

Higher dimensions

A two-dimensional version of the quantum PIC has successfully been created, making possible more accurate simulations of semiconductor substrates and similar scenarios. Our latest effort is to extend the technique to three dimensions.



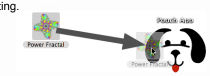


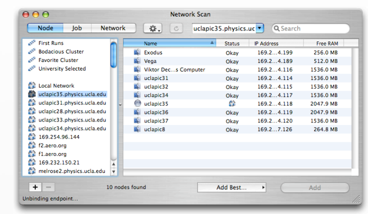
Inventing the Mac Cluster

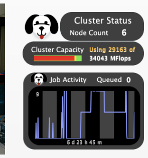
Plug-and-play cluster computing

Our group was the first to build a cluster using Macintosh hardware and operating system. Starting in 1998, we wrote MacMPI, the first Message-Passing Interface implementation for the Macintosh, which enabled parallel codes that ran on the largest supercomputers to run on the Mac.

Since that time, we evolved the technology to use TCP/IP and Mac OS X, even clustering Intel-based and PowerPC-based Macs. The latest incarnation of the latest interface is the Pooch Application, featuring the only modern, easy-to-use, drag-and-drop interface to parallel computing.







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We wish to thank the late John M. Dawson for the insight, vision, discussion, and support he gave for this work. His contribution was critical for this project. The original development of the quantum PIC was supported by LLNL ISCR 99-012 and was performed as part of the doctoral dissertation of D. Dauger. Further work has been performed with the support of a grant from NSF.