Using Human Energy Fields to Sculpt Real-Time Molecular Dynamics

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ABSTRACT

Chemistry has historically placed a great deal of emphasis on "structure function" relationships, where a molecule's function and associated properties are understood with reference to how its atoms are arranged. However, the way we imagine molecules is evolving toward a dynamic and time dependent perspective, where molecular function is increasingly recognized to depend on how molecules change. Within this framework, molecular systems are characterized by dynamical complexity, involving chaotic fluctuations, coupled vibrations, and instability.

In this article, we describe danceroom Spectroscopy (dS) – a recent attempt to construct a system that allows people to interactively manipulate a molecular dynamics simulation. Adapted from algorithms commonly used to simulate molecular dynamics (MD), dS interprets people's movements as perturbations within a virtual energy field, and embeds them within a real-time molecular simulation, where their movement sculpts the atomic dynamics. Using methods from molecular vibrational spectroscopy, dS is able to detect whether human motion gives rise to coherent structure within the atomic dynamics, and turn this into real-time soundscapes. The result is a real-time immersive and interactive audiovisual molecular dynamics experience for an arbitrary number of users, which doubles as both a scientific simulation, and an aesthetic tool.

Time, Equilibrium, and Molecular Structure

Molecules, made from building blocks called atoms, are amongst the most useful microscopic functional units for understanding the properties and behaviors of the macroscopic world around us. Despite the fact that the natural world and our experience of it is characterized by perpetual change and fluctuation, neither the word 'molecular' nor the word 'atom' are famous for conjuring up images of dynamism and change. Rather, both of these words are usually associated with static images – namely, snapshots that are effectively architectural blueprints showing how atoms are arranged in molecular structures.[1] For example, iconic molecular images include the famous DNA double helix, or C_{60} (Buckminster-fullerene), the carbon structure which looks like the skeleton of a soccer ball.

To date, much of the emphasis in chemistry has been on so-called "structure function" relationships, where a molecule's function and associated properties are understood with reference to its underlying atomic connectivity. For example, the orientation of molecular photo-receptors in the cells located in leaf chlorophyll helps us to understand the efficiency with which plants can capture light from the sun. Or the highly connected bonding structure of solids like diamond (shown in Figure 1) can help us to understand properties like hardness and conductivity. Or the shape of a cavity inside a biomolecule can help us to understand the efficiency with which it can carry out shape-recognition and interact with other molecules. In what follows, we refer to the use of static images to understand molecular function as a "time-stationary" view.

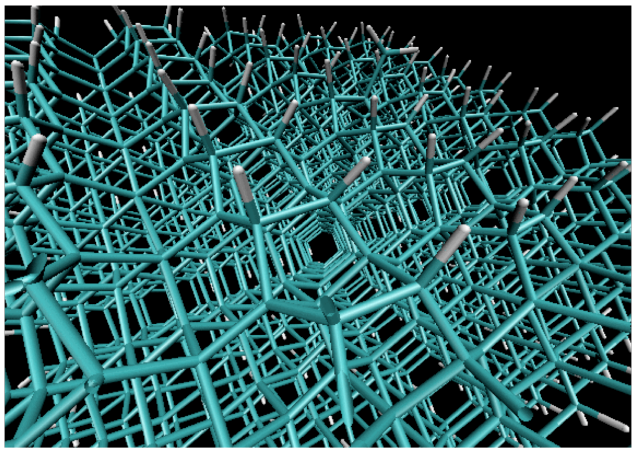

Figure 1: molecular snapshot of diamond as it might look if our eyes were able to 'see' the nanoscale. This snapshot conceals the time-dependence of the system. In fact, every component is wiggling, jiggling, and vibrating, locked in an interdependent "dance", where the motion of each part of the system depends on the motion of every other part of the system.

The 'time-stationary' view is strongly linked to equilibrium thermodynamics, which is perhaps the dominant conceptual framework that has guided mathematical modeling of systems within chemistry and physics for the last few hundred years. A large part of the success and beauty of

the equilibrium framework lies in its simplicity: whereas the motion of real molecular systems is characterized by complexity, involving chaotic fluctuations, coupled vibrations, and instability, the equilibrium picture permits us to understand and predict molecular properties and behavior in terms of their time-averaged properties. This means that the precise details of how a system moves as from time t to time $t + \Delta t$ need not be considered. Instead we need only consider one structure – namely, the average. Indeed, it is these time-averaged equilibrium structures that we are typically looking at when we see snapshots of molecular structures.

The achievements of equilibrium thermodynamics in modern science cannot be understated – both for improving our fundamental microscopic understanding of the natural world, and in allowing us to build a range of sophisticated technological applications. However, a number of detailed studies examining a range of different molecular systems, from gases to liquids to biochemistry, produce results that cannot be explained within the equilibrium framework. These studies show that the time-stationary, equilibrium view obscures many details of molecular behavior and function, and that time-dependent fluctuations, coupled vibrations, and cooperative motions are key to understanding a range of physical systems. This recognition is leading to somewhat of a paradigm shift: understanding how physical processes *far from equilibrium* impact systems within physics, chemistry, and biology is now recognized as a 'grand challenge' facing 21st century science.[1]

Molecules: A dynamical perspective

Within chemistry, the limits of the time-stationary view of molecules are becoming increasingly obvious. For example, a number of studies show that molecular function involves a certain degree of plasticity. Molecules do not adopt a single structure, but can instead adopt any of an ensemble of interrelated structures. With advances in technology and computation, chemistry is increasingly attempting to go beyond the equilibrium view of molecules and develop methods that let us 'see' how fundamental physical laws drive molecular change as a function of time, in an effort to identify the fluctuations, vibrations, and motions that guide molecular function. This heralds an important new way of thinking about molecules: whereas *structure* previously dominated the way we think about molecular function, *dynamics* is emerging as an equally important consideration. Richard Feynman hinted at the fundamental role of the dynamic molecular world in his now-famous claim that "everything that living things do can be understood in terms of the wigglings and jigglings of atoms."[2]

In fact, Heisenberg's uncertainty principle, amongst the most fundamental principles of quantum mechanics, guarantees microscopic dynamism. So far as molecules are concerned, it tells us that every molecular structure is characterized by perpetual jiggling and wiggling, with vibrational motion and structural fluctuations that span a range of timescales and corresponding lengthscales. However, this dynamism is not always so obvious. A good example is diamond, amongst the hardest substances we know, whose structure is shown in Figure 1. Hardness is generally associated with rigidity; so it seems rather counterintuitive to imagine that, at a molecular level, diamond is actually a dynamic and vibrating system. However, "seeing" this fundamental molecular dynamism requires time resolution on the order of nanoseconds, and spatial resolution on the order of nanometers, far beyond what our eyes are capable of. It is this gap between scientific observations and our everyday intuition that underpin Richard Feynman's famous statement: "it's very hard to imagine all the crazy things that things really are like."

It's important to point out that the wiggling and jiggling of molecules is one particular level at which matter exhibits dynamic phenomena. More generally, we live in a dynamic and vibratory universe.[3] At the tiniest level, string theorists postulate that different particles found in nature arise from the vibrational dynamics of tiny stringlike objects. At a larger level, quantum mechanics tells us that matter actually exhibits wave-like behavior with specific vibrations, energies, and frequencies. Microscopic living systems such as cells exhibit vibrations that last anywhere from milliseconds to seconds. And on the largest scale of all, cosmologists think that the entire universe is still vibrating at frequencies excited in the big bang.

Molecular Dances, Spectroscopy, and Energy Landscapes

Modern science is often faced with the task of identifying points where one conceptual framework breaks down, and another takes over.[4] Often, these interfacial regions are amongst the most interesting territory for scientific investigation. Perhaps the best-known example of this sort of discontinuity is that of classical versus quantum mechanics, where continuum models of physical systems fail, requiring discretized wave-like models. Similarly, the transition between the time-stationary, equilibrium view of molecular structure versus the time-dependent dynamic view is another point of discontinuity, and has consequently provoked a range of debates and questions. A particularly difficult challenge involves the development of analytical mathematical frameworks for reliably predicting the point at which the equilibrium frameworks are inadequate and dynamic frameworks are required.

Qualitatively, ideas of molecular dynamism are beginning to infiltrate chemistry in interesting ways. For example, it seems increasingly common to hear chemists and biochemists invoke choreographic and dance analogies to describe the dynamics of molecular systems – referring to molecular 'dancefloors'[5] or chemical 'choreographies'.[6,7] The use of these metaphors is no doubt driven in part by visualizations of time-dependent molecular phenomena using computational methods.[8] For example, visualizing the motion of the diamond structure shown in Figure 1 reveals a tightly correlated molecular "dance",[9] where the motion of every atom in the system depends on and affects the "dance" of every other atom in the system.

Experimentally mapping the real-time motion of every component of a molecular system is a complicated task that is practically impossible for all but the smallest systems. And even if it were possible, the quantity of data obtained from carrying out such an analysis would be overwhelming. Consequently, we require strategies for characterizing the most important components of the overall dynamical structure. In this respect, 'spectroscopy' is a key tool within chemistry. The Oxford English Dictionary

defines spectroscopy as "the branch of science concerned with the investigation and measurement of spectra produced when matter interacts with or emits electromagnetic radiation". Practically however, 'spectroscopy' has come to mean a range of things to a range of workers across different sub-fields within science. In the field of molecular dynamics, spectroscopy often refers to experimental techniques aimed at identifying the characteristic vibrational fingerprints of molecular 'dances'.

Theoretically, chemists and physicists frequently invoke the idea of an 'energy landscape' to: (1) understand how the atoms within a molecule "dance", and (2) interpret the vibrational information provided by spectroscopy experiments. An 'energy landscape' is effectively a topological map of the forces that an atom feels in different atomic arrangements. Indeed, the "energy landscape" metaphor has become prevalent within the discourses of chemistry, physics, and biology,[10] and can be used to rationalize the motion of almost any class of particle, atom, or molecule in the universe. Figure 3 shows a simple schematic of an idealized, two-dimensional energy landscape, where the energy is a function of arbitrary X and Y coordinates. In general, atoms move across energy landscapes in ways that are similar to humans: they prefer going downhill rather than uphill; they sail over wide-open spaces; and they move chaotically through denser topologies.

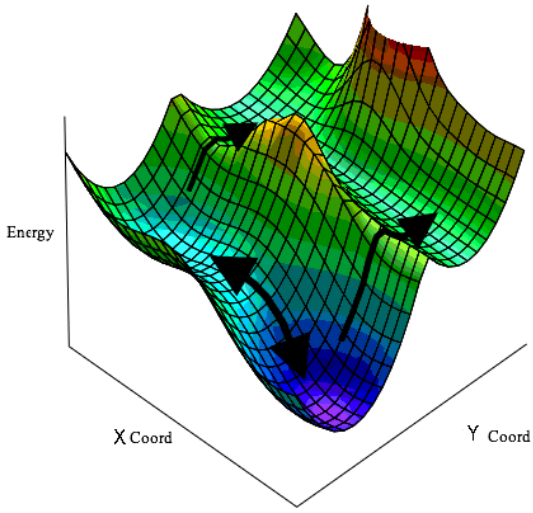

Figure 2: 2d schematic of a generic energy landscape, showing energy as a function of two idealized coordinates, X and Y. The arrows show characteristic paths that atoms might take over this landscape.

The energy landscape shown in Fig 2 is simplified compared to more realistic models in two important respects: (1) real energy landscapes generally have a significantly higher dimensionality than two, since they depend on the interaction between any given particle with every other particle, and (2) real energy landscapes are not static. Rather, they are time-dependent, affected by fluctuating external fields and molecular configurations.

Interactive Molecular Dynamics systems

Using a range of physics-based mathematical models that span both classical and quantum mechanics, accurate predictions of how molecules behave are increasingly formulated using numerical algorithms run on computers. These computational approaches allow us to construct detailed representations and animations of molecular structures. In general, these visualizations are only possible 'offline' or 'after-the-fact'.[11] Generating a molecular visualization typically works in a three-stage process, as follows:

(1) Run a numerical simulation, solving the equations of motion for a particular molecular system;
(2) Load the data generated from the numerical simulation into a visualization program;
(3) Within the visualization program, choose how the molecule will be rendered, and subsequently generate molecular snapshots and/or movies.

With developments in computational power and interactive technologies, effort has been made to develop systems wherein the simulation is integrated with the visualization, so that a user can see 'on-the-fly' how a molecule fluctuates and vibrates during the solution of its equations of motion. These 'on-the-fly' systems have paved the way for attempts at making MD interactive.[12] In general, there are three levels at which interactivity has been introduced within MD simulations:

(1) Allowing the user control over the visual representation of the molecular system being simulated, or the perspective from which it is seen. This may be accomplished using a range of interactive techniques, including face tracking, stereoscopic displays, and virtual reality gloves.[13]
(2) Giving the user real-time control over parameters that affect the numerical solution of the equations of motion: e.g., temperature, inter-atomic forces, atomic number, atomic size, etc.[12]
(3) Allowing the user to exert external forces on particular atoms, changing the energy landscape, and 'steering' what the molecule does. The tool of choice here has been haptic devices, given their relatively low cost, portability, and ability to generate tangible force-feedback.[14,15]

So far, efforts to make interactive MD systems are aimed at augmenting them so that users can more quickly gain insight into the microscopic motion that characterizes molecular systems.[16] Beyond this, interactive MD systems are valuable from an educational perspective, in order to help non-specialists and students quickly grasp otherwise difficult molecular concepts.[17]

danceroom Spectroscopy

Compared to the interactive dynamics systems discussed above, danceroom Spectroscopy (dS) was motivated more with artistic and aesthetic questions in mind. The rigor of the mathematics and algorithms that drive dS is clearly important: because it is driven by research-grade methods used within computational chemistry, it has potential application to a range of interesting scientific questions beyond the scope of this chapter. However, in what follows, we will focus on dS as a platform for graphic and sonic generative art.

Musical tones arise from vibrational structure and wave mechanics, a discovery going back to Pythagoras. Legend has it that he showed the connection between string lengths and pleasurable sounds as early as 600 BCE.[3] More re-

cently, those interested in cymatics have devoted a great deal of effort to visualizing the wave structures that emerge when a range of materials are subject to sonic impulses.[18,19] With this sonic vibrational framework in mind, one of the principle questions motivating dS was as follows: *Using tricks from molecular vibrational spectroscopy, can we measure how arbitrarily large groups of users 'sculpt' molecular vibrational dynamics, and then use that information to generate real-time sonic feedback?*

Previous systems for steered interactive MD have been designed solely for single users, with feedback derived exclusively from graphics and haptics, with no sonic component. Hence, addressing the above question turned out to be rather involved, requiring us to develop a brand new framework in which arbitrarily large user groups could have the real-time, whole-body immersive experience of being embedded in an MD simulation as an 'energy landscape'. It required innovations on a number of fronts: *First*, we had to investigate a rigorous algorithmic and mathematical framework for modeling human bodies and energy fields and allowing them to interact with an MD simulation. This required us to apply mathematics from chemical physics to depth image processing – an area in which it has never before been investigated. *Second*, we had to develop an algorithmic framework for effectively sonifying molecular dynamics. *Third*, running our system required a new, flexible software interface, along with a suite of algorithms capable of exploiting modern high-performance computational hardware frameworks. *Fourth*, we built some portable new hardware that allowed us to carry out 360º depth capture in large spaces. Finally, to determine whether or not dS fueled a pleasant aesthetic experience, we had to test it out with users in a of range installation and performance formats.

In what follows, we will describe several aspects of the dS project. After providing a brief overview and the background of the collaborators involved, we will briefly outline the mathematical and algorithmic framework that drives dS. Following this, we will outline the software and hardware that we have developed and implemented to run dS. We close with a number of observations that provide qualitative insight into how both performance artists and the public experience and interpret dS. There are several components of the dS system which (so far as we know) are novel, and perhaps merit a more detailed technical discussion than what is provided herein. Thus, it is important to note that this chapter provides a broad overview, with a focus on the artistic and aesthetic aspects of dS. We are presently preparing a number of follow-up publications to detail various components of the system related to scientific visualization, sonification, graphics, image processing, and physics algorithms.

dS in brief

Briefly stated, *dS* interprets people's movements as perturbations within a virtual energy field, and embeds them within a real-time molecular dynamics simulation in order to facilitate both graphic and sonic interactivity, as shown in Fig 3. Graphically, on a large projection screen, users see their energy fields along with the real-time waves, ripples and vibrations created as their motion perturbs a virtual simulation of atomic dynamics. Simultaneously, the dS software detects transient structures and vibrations amidst the apparent chaos of the atomic dynamics, and transforms them into sound which is fed back to users. This feedback cycle (users affect atomic dynamics, and atomic dynamics affect sound) gives users a textured visual and sonic experience, letting them experience the effect that their real-time field perturbations have within a dynamic atomic system.

dS has so far been deployed in two different capacities: (1) as an interactive installation for the public, and (2) as an artistic tool that knits together the visual, sonic, and choreographic components of a 30-minute dance performance called *Hidden Fields* (HF). Development of dS began in March 2011, when the original prototype code was written. Subsequent development was facilitated by a series of workshops and public installations held during the summer and autumn of 2011. In a second series of workshops held during March – July 2012, HF was developed. Recent dS and HF appearances include: the Arnolfini Art Gallery in July 2012 (Bristol, UK); a 360°, 21-meter projection dome in August 2012 (London 2012 Cultural Olympiad); and the Barbican Arts Centre in November 2012 (London, UK).

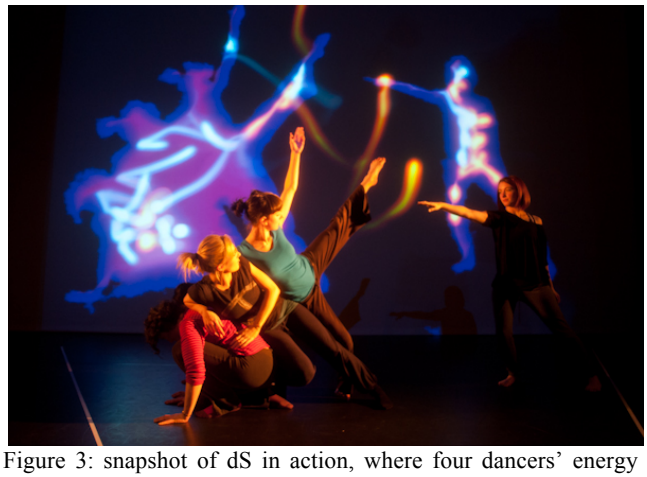

Figure 3: snapshot of dS in action, where four dancers' energy fields are being used to sculpt a molecular dynamics simulation. The photo shows the silhouettes of the dancers fields. Simulated atoms reside within and react to the fields.

COLLABORATORS

dS's eclectic mix of physics, chemistry, mathematics, high-performance computing, interactive technology, digital art, electronic music, and dance is reflected in the diverse backgrounds of a core group of collaborators: David R. Glowacki, the project leader and conceptual architect, is a theoretical chemical physicist and programmer who carries out research in classical and quantum dynamics and also holds a master of arts in cultural theory; Tom Mitchell is a lecturer in music technology with interests in adaptive sound design and interactive musical composition; Joseph Hyde is a professor, musician and electronic sound artist whose work focuses on multimedia, dance, telepresence, and interactivity; Philip Tew is a programmer and installation artist with interests in creating artworks that utilize generative processing and physical modeling; Simon McIntosh-Smith and James Price are computer scientists with expertise in high performance computing hardware and software; and Laura Kriefman is a choreographer who experiments with a range of interactive technology, with a mission statement to "find the dances in everyday life".

Hidden Fields rehearsals and performances additionally involved five professional modern dancers, all of whom had 3 – 10 years of professional dance experience/training.

MATHEMATICS AND ALGORITHMS

Interactive Dynamics Framework

3d capture systems typically return depth, z, as a function of pixel position within a two dimensional matrix indexed by x and y. This has a close correspondence with the 2d energy landscape in Fig 2. The biggest difference between Fig 2 and the output from a depth sensing camera is that the former represents space as a continuum, whereas the latter is discretized – i.e., space is partitioned into pixels, each of which have a finite extent. Nevertheless, the correspondence between Fig 2 and a depth matrix is close enough that we decided to represent people's energy fields using a depth matrix.

In its present form, dS carries out an MD simulation involving N atoms, each of which may move in two dimensions (x and y). For reasons discussed later, we have decided to constrain the simulation so that each atom has the properties of either Carbon, Iron, Hydrogen, Helium, or Oxygen (each of which is amongst the most abundant elements in the universe). Each atom has a particular mass and associated set of electrostatic properties. The masses are known exactly, and the electrostatics have been previously parameterized for use in molecular dynamics simulations.[20]

A useful vantage point from which to discuss the simulation begins with Hamilton's equations of motion, commonly used to discuss the dynamics of molecular systems in both classical and quantum frameworks.[21] Hamilton's equations are as follows:

$$\begin{aligned} d\mathbf{p}/dt &= -dH/d\mathbf{q} \\ d\mathbf{q}/dt &= dH/d\mathbf{p} \end{aligned} \qquad \text{(E1)}$$

where $\mathbf{p}$ and $\mathbf{q}$ are vectors characterizing the x, y momentum and coordinates of each atom in the simulation. H is the so-called Hamiltonian function describing the total system energy, defined as:

$$H = \sum_{i=1}^{N} \frac{m_i v_i^{\,2}}{2} + V \qquad \text{(E2)}$$

where i is an index that runs over a collection of N total atoms, m is the mass of an atom, and v is its velocity. The first term in (E2) describes the total kinetic energy of the system while the second, V, describes the total potential energy. Within our system:

$$V = V_{int} + V_{ext} \qquad \text{(E3)}$$

where the total potential energy, V, is calculated as the sum of two terms, V_{int} and V_{ext}, which correspond to the potential energy owing to internal and external interactions, respectively:

$$\begin{aligned} V_{int} &= \sum_{i=1}^{N} \sum_{j=i+1}^{N} V(r_{ij}) \\ V_{ext} &= C_a \sum_{i=1}^{N} V_{ext}(x_i, y_i, t) \end{aligned} \qquad \text{(E4)}$$

V_{int} is calculated by summing over all possible pairwise atomic interactions, $V(r_{ij})$, where r_{ij} is the distance between atoms i and j. Mostly for computational efficiency, this term is presently calculated using a so-called "Lennard-Jones" interaction model,[21] which includes attractive interactions at long-range and repulsive interactions at short range. V_{ext} is calculated as the difference between a raw depth matrix at time t, and an averaged background depth image. In practice, V_{ext} is calculated as a sum over $V_{ext}(x_i, y_i, t)$, which is the energy field that a particular atom located at (x_i, y_i) 'feels' as a consequence of people's motion. C_a is a scaling constant that can be interactively controlled to tune in real-time how strongly a particular atom type 'feels' forces from the users' fields, and whether people are 'attractive' or 'repulsive'. C_a is responsible for coupling human motion to the atomic dynamics, allowing them to warp the potential energy "landscape" felt by each atom, and thereby sculpt the system dynamics. Unlike the first term, which depends only on the relative position of each particle with respect to every other particle, the second term explicitly depends on time, owing to the fact that people are not stationary within the exhibition space.

In Hamiltonian mechanics, the energy function, H, should remain constant for any closed dynamical system, in line with the conservation of energy required by the first law of thermodynamics.[21] The (E2) Hamiltonian is not, however, subject to this constraint because of the V_{ext} term, which effectively makes the system open rather than closed. With fluctuations in the depth data that arise as a consequence of digital noise, or human motion, energy effectively flows into and out of the system. This introduces significant instabilities into standard numerical algorithms for propagating the time-dependent system dynamics. In our initial experience, it led to frequent system crashes. To alleviate these difficulties and improve numerical stability, dS utilizes a system thermostat which enforces a user-specified energy distribution on the atomic dynamics. A number of thermostatting approaches are available within the physics literature, and we found a modified Berendsen thermostat[21] to give a good comprise between computational efficiency and system stability.

In general, the vector of forces acting on a set of atoms, $\mathbf{F}(t)$, can be written in terms of the system's potential energy–i.e.:

$$\mathbf{F}(t) = -dH/d\mathbf{q} = -dV/d\mathbf{q} \qquad \text{(E5)}$$

Substituting (E3) into (E5) gives

$$\begin{aligned} F(t) &= -\frac{dV_{int}}{d\mathbf{q}} - \frac{dV_{ext}}{d\mathbf{q}} \\ &= \mathbf{F}_{int} + \mathbf{F}_{ext} \end{aligned} \qquad \text{(E6)}$$

where $\mathbf{F}_{int}$ and $\mathbf{F}_{ext}$ are the force vectors arising from the internal energy and the external field, respectively.

Mixing Quantum and Classical Mechanics For Smooth interactivity

A significant utility of Hamiltonian mechanics is that it can be applied to both classical and quantum equations of motion. Initially, our intention was to propagate the system dynamics using (E1) and forces calculated using standard classical atomic mechanics. In this approach, each atom is represented as a point, and the force which it 'feels' corresponds to the force field acting at that point. However, we found that this approach resulted in choppy atomic motion and unsatisfactory interactivity. This arose because noisy variations in the matrices returned from the depth sensors gave fluctuations in V_{ext} that rivaled the effect of human energy landscapes.

Achieving more fluid dynamics and improved interactivity therefore required that we introduce some sort of non-locality into our dynamics propagation strategy, so that **F** depends on some sort of local average within the force field. To incorporate this non-locality in an efficient manner, we implemented a mixed quantum-classical dynamics strategy. The so-called 'frozen Gaussian' dynamics method forms the basis for a number of more sophisticated approaches that approximately model the quantum dynamics of molecular systems. Within this approach, $V_{ext}(x_i,y_i,t)$, the effective potential energy felt by an atom centered at the coordinates (x_i, y_i) is described using a Gaussian function. In two dimensions, the form this function takes is:

$$V_{ext}(x_i,y_i,t) = \int\int dxdyV_{ext}(x,y,t)e^{\left(\frac{(x-x_i)^2+(y-y_i)^2}{2\lambda_i^2}\right)} \quad \text{(E7)}$$

where λ is Gaussian width parameter that tells us how 'blurry' the atom is. Within dS, λ_i is chosen to satisfy the quantum thermal width predicted by Heisenberg's uncertainty principle.[22,23] Effectively, λ_i is a sort of measure for how wave-like the atomic particles are. Implementing (E7) is approximately twenty times more expensive than a purely classical approach, meaning that we are able to simulate fewer atoms. But it gives atomic dynamics which react smoothly to human motion, making for substantially improved interactivity.

SYSTEM DESIGN AND SETUP

Image Processing, Physics and Graphics

A simplified schematic of our setup using a single sensor is shown in Fig 4. In general, up to seven depth sensors send depth matrices via USB to a custom-built workstation. This grab occurs at either 30 or 60 Hz, the operational frequencies of our depth sensors. Following a depth matrix grab, the workstation is able to calculate $\mathbf{F}_{int}$ and $\mathbf{F}_{ext}$, the internal and external forces acting on the atomic ensemble. Using these forces, the atomic dynamics are propagated forward a step using the frozen Gaussian equations of motion. The atom positions as well as V_{ext} are then rendered at 60 Hz using a range of graphics parameters (discussed below) that may be specified on-the-fly to achieve a desired aesthetic effect. The graphics data is then sent out to a projector for users to see.

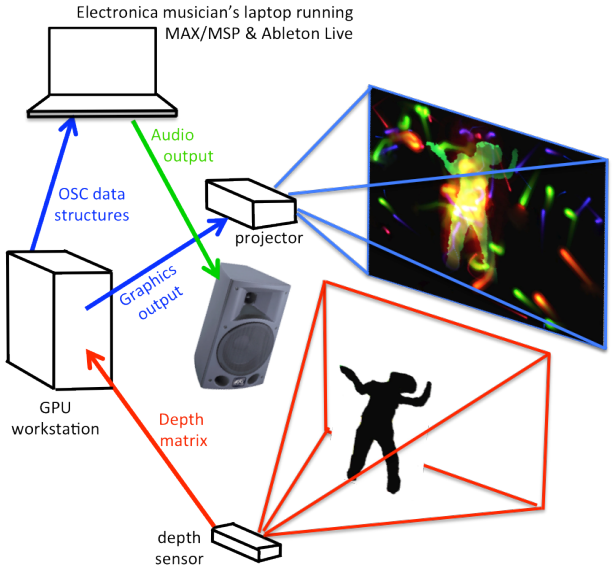

Figure 4: Schematic of the dS setup with a single depth sensor.

Sonics

As discussed above, one of the principal motivations for dS was to measure how arbitrarily large groups of users 'sculpt' molecular vibrational dynamics, and subsequently feed this data back to users in sonic form. dS includes three different means for sonifying the atomic dynamics. All of the sonics derive from analysis of the atomic ensemble dynamics, and subsequent encapsulation of this data in an appropriate open sound control (OSC) data structure for Ethernet transfer to an electronica artist's laptop. As shown in Figure 4, the OSC data structures may then be processed by Max/MSP and sonified directly or forwarded on to music programs like Ableton Live to generate real-time sonic feedbacks for users within the installation space. Each of the sonic structures detailed below has its own characteristic fluctuation timescale, combining to give a textured sonic experience: collisional data fluctuates on very fast timescales, superparticles on intermediate timescales, and vibrational dynamics on the slowest timescales.

Collisional Analysis

The simplest form of sonic feedback is to run a collision detection algorithm. The net result is that every particle-wall and/or particle-particle collision event is tagged with OSC data, triggering an arbitrary sound chosen by the electronica artist.[24] This works fine for small numbers of particles; however, it can quickly grow cacophonous when the ensemble has no more than a few users and less than ~250 atoms. It is possible to limit the maximum number of sonified collisions per frame, but this diminishes user perception of interactivity. There are always a certain number of background collisions, and it is difficult to guarantee that only those which arise from user motion pass through the filter.

Superparticle Clustering Analysis

To harvest meaningful data for sonification when there are a large number of atoms, we have developed a grouping algorithm which detects the transient formation of atomic clusters.[24] These clusters we refer to as 'superparticles', since they have properties similar to those of individual atoms: position, velocity, and size. An illustration of the grouping algorithm at work is shown in Fig 5. The dancer in the foreground has used her energy field to manipulate the atomic dynamics to form a superparticle. The standard deviation of the average x and y coordinates of the atoms comprising the superparticle are delineated by the rectangle visible in the background of Fig 5. Each superparticle has its own sonic channel, so that it may be easily assigned to a particular sound. The net result is that a dancer may modulate the volume of his/her corresponding sound depending on his/her movement within the space. For example, a dancer's instrument goes silent with stillness. With increasing velocity, the volume increases.[24]

Figure 5: An illustration of the superparticle algorithm. The dancer shown in the foreground has used her field to manipulate the atomic dynamics and form a superparticle. The average x and y boundaries of the superparticle are outlined by the rectangle visible in the background.

Vibrational Analysis

The algorithm we use to determine whether there is any vibrational structure within the atomic dynamics is inspired by methods typically used to analyze vibrational spectroscopy experiments of molecular systems. By maintaining a moving time history of a vector containing all the atomic velocities, we calculate the so-called 'velocity autocorrelation function' (VAC). Letting $\mathbf{v}(t)$ specify the ensemble velocity vector at some timestep t, and $\mathbf{v}(t_0)$ specify the ensemble velocity vector at some previous timestep t_0, the VAC is essentially a time series of size n which measures how $\mathbf{v}(t_0+dt)$, $\mathbf{v}(t_0+2dt)$, … $\mathbf{v}(t_0+ndt)$ project onto $\mathbf{v}(t_0)$, where dt is the dynamics timestep. Fast Fourier Transform (FFT) of the VAC gives a spectrum whose peaks show any characteristic vibrational frequencies within the ensemble dynamics. A dynamic peak-picking algorithm identifies these peaks and packages their amplitude and frequency into an OSC data structure. If the dancers' movements create periodic vibrational motion within the on-screen atomic dynamics, appropriate peaks in the FFT vibrational spectrum undergo a characteristic beating motion perfectly in phase with the dancers' motion. This leads to sounds that are similarly aligned with the dancers' vibrational motion.[24]

Hardware

Workstation

Our technical goals have largely been driven by our desire to adapt dS to 360° projection environments. Following from this, we set out to accomplish the following tasks with a target latency of less than 17 ms (60 Hz):

(a) stable dynamics and graphics rendering for anywhere from 0 – 10,000 atoms;
(b) image capture and processing for up to seven 3d sensors to calculate V_{ext};
(c) real-time analysis of the ensemble dynamics to obtain sonification data to ship out to an electronica artist;
(d) rendering of particles and V_{ext} on up to five graphics outputs for typical 360° projection setups.

The goals outlined above proved too intensive for a standard desktop or laptop. At present, dS runs on a high performance custom-built 64-bit workstation with a hexa-core CPU and two dual-graphical processing units (GPUs): (1) an NVIDIA GTX 590 GPU with 1024 cores; and (2) a Sapphire Radeon HD6990 dual GPU with five graphics outputs and 3072 cores. We significantly optimized our computational performance by profiling our code and moving the most intensive computational algorithms to the NVIDIA GPU, increasing our computational efficiency to the extent that we were able to simulate the dynamics of 8,000 – 10,000 atoms at 60 Hz, compared to no more than 3000 prior to GPU acceleration. The Sapphire HD6990 GPU was used solely for graphics rendering over multiple outputs.

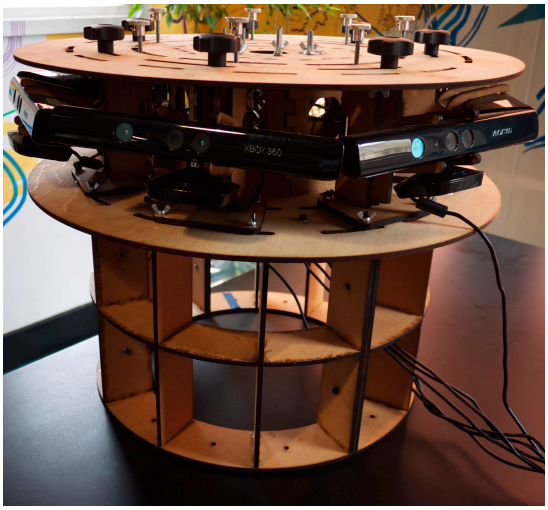

Figure 6: Our custom-built 360° optical mount which houses seven depth sensors in a circular arrangement.

Camera Mount

Installing dS in 360° required simultaneous depth matrix capture from at least seven sensors. Consequently, we re-

quired a relatively robust sensor mounting solution: lightweight enough to carry, sturdy enough to withstand transport and bumps, and quick to set up. It needed to allow sensitive camera alignment, and also to be useful in non-360° setups, where we typically run with 2-3 sensors. The camera mounting solution we designed is shown in Figure 6. It consists of seven cradles arranged around a central axis. Each cradle fits snugly around a depth sensor's outer casing, and is mounted in a fashion that allows us to control the pitch and roll of each sensor as well as the distance of each sensor's focal point from the centre of the circle. Following alignment, the cameras are fixed using a set of fasteners.

Software

dS is written in ~50,000 lines of C# code built on Windows 7 in Visual Studio 2010. The code interface to the depth sensors utilized the OpenNI C# wrappers. Graphics rendering was carried out using DirectX 11. Code ported to the GPUs for accelerated compute operations utilized the OpenCL programming language. We devoted considerable effort to making the code general, flexible, and user-friendly for use by musicians, dancers, and choreographers without requiring a programming specialist. All aspects of the system can be controlled via a multi-tab graphical user interface (GUI), an example screen grab of which is shown in Figure 7.

Figure 7: primary interface screen of the 7-tab dS GUI. The sliders and buttons allow control over a range of physics and graphics parameters. The graphs on the bottom relate to the real-time vibrational spectrum of the atomic dynamics, and the rows of numbers at the top allow the dS operator to rapidly save and access a range of dS states

Each of the different tabs in the GUI allows the system operator to interactively control a different component of the dS system: (1) depth matrix capture and background calibration; (2) graphics rendering of both the atoms and V_{ext}; (3) relative orientation and position of each camera's depth matrix within the composite field that makes up V_{ext}; (4) edge blending between depth images; (5) behavior of the superparticle clustering algorithm; (6) parameters controlling the collision analysis and detection algorithm; (7) the vibrational analysis and peak picking algorithm; and (8) the OSC output.

When using dS to make *Hidden Fields* and also during public installations, we found that certain physics and graphics variables significantly impacted the aesthetic feel. Access to these variables for real-time modification is provided on the main screen of the dS GUI in the form of sliders and buttons, as shown in Fig 7. Physics-related variables accessible on this screen include: (1) the number of atoms; (2) the size of the atoms; (3) the temperature of the system; (4) the on-screen position where new atoms should be initialized; (5) how strongly the atoms "feel" V_{ext}; (6) whether each atom type "feels" V_{ext} as attractive or repulsive; (6) how strongly the thermostat enforces the selected temperature at each dynamics step; and (7) whether different particle types generate OSC data upon collision. Graphics-related variables accessible on the main GUI screen include: (1) whether particles flash when they collide; (2) the 'feedback' incorporated into the particle rendering (e.g., high feedback results in trails); (3) the 'feedback' in the rendering of V_{ext} (high feedback results in graphic distortion from human motion); (4) the extent to which users are able to see V_{ext}; (5) the color of users' fields; and (6) a range of variables related to a graphical effect we named the 'warp grid'. The 'warp grid' is a grid which can be distorted by V_{ext}, resulting in a range of interesting and subtle graphics effects that very much give the atomic dynamics a sort of liquid feel. It was inspired by asking, "how might we imagine people's energy fields if we could see them?" Different physics and graphics parameter combinations result in an enormous number of distinctly different states, a few examples of which are shown in the photos accompanying this chapter.

AESTHETICS

In what follows, we offer some qualitative thoughts on the sort of aesthetic experience made possible with the dS system. Our observations are broken down into two broad categories. First, we consider the artistic interaction that arose during the making of Hidden Fields, where dS serves as an artistic tool and the collaborative glue facilitating interaction between a musician, a choreographer, a digital artist, and five professional dancers. Second, we consider user feedback from those who participated in public dS installations and/or watched the *Hidden Fields* performance. Whereas the former group could be considered 'experts' insofar as they had received in-depth explanations of the ideas and technology driving dS, this was not necessarily true for the latter group.

Observations From the Creative Artistic Process

Aesthetic Moods and Variability

Everything that a user might experience within dS emerges from a single rule – namely, the frozen Gaussian equations of motion outlined above. This raises some interesting questions: Are different system states capable of producing a range of aesthetic moods? What are effective strategies for weaving together different states to produce a performance?

One way to address these questions is to examine the creative process which culminated in *Hidden Fields*. Using sliders and buttons on the dS GUI, nearly every physics, graphics, and sonic parameter can be modified in real-time by the system operator and/or the artists. This means that the number of possible parameter combinations is enormous. Amongst the most challenging and fun aspects of dS

is exploring this enormous parameter space to discover aesthetically satisfying combinations, which we henceforth refer to as system 'states'. The initial workshops that inspired the ideas behind *Hidden Fields* were organized in a fashion that allowed plenty of freedom for testing out and playing with different choreographic, visual, and sonic arrangements – either separately or as an integrated whole. During this exploratory process, we would stumble upon states that we liked, and were able to save the parameter combinations that had produced that state using a single click within the dS GUI. This allowed dS to fit smoothly within an organic artistic process, rather than be a distraction.

The *Hidden Fields* performance is composed of approximately 20 different states, with names like 'Swaying,' 'Puddle Jumping', 'Firation', 'Ghosts in the Grass', 'Butterflies', 'Heartbeats', 'Super-Terrific Mega-Trip', 'Earth from Space', 'Intergalactic Space Man', or 'Jupiter's Memories'. The name of each state was usually coined by one of the artists involved, to reflect a particular idea or feel which related to some aspect of the choreography, graphics, and sonics. In many cases, the name initially referred to only one of the three aspects listed above; however, we found that the names subsequently provided a concise thematic vision that helped to guide our efforts to refine and weave together the other aspects. A good example of this is the process leading to the "Jupiter's Memories" scene. In its initial stages, this name mostly referred to the choreography and movement – i.e., the dancers made gentle orbiting motions across the mapped stage space, reminiscent of planetary motion. As rehearsals wore on, this name helped us to refine the visual state (cool blue sparkling atoms) as we imagined how to represent what Jupiter might encounter hurtling on a lonely journey through space. This name also helped us to refine the associated sonics: for this scene, the dancers' interactions with the simulation modulate the sonification of NASA data recordings taken during Voyager's flyby of Jupiter's moon, Ganymede.[25]

Determinism and Chaos

HF raised interesting issues concerning the relationship between determinism and chaos. Choreography and dance often tend to follow structures that are rather linear and deterministic (of course there are exceptions, but we are speaking generally here). dS, however, is characterized by a certain amount of noise rather than deterministic certainty. This arises from well-known chaotic instabilities that inevitably arise in the numerical simulation of dynamical systems, often described as the 'butterfly effect'. Hovering somewhere between chaos and determinism, the interactive experience enabled by dS may approximately be described as 'stochastic'. We can never predict exactly how the dS system will react to the motion of human energy fields; however, over a large number of system instantiations, we can confidently build up an intuitive picture of its average response. This "blurriness" distinguishes dS from other interactive art tools, which are often more obviously deterministic. Consequently, we found ourselves exploring how to build choreographic, sonic, and graphical frameworks which could harness and accommodate dS's inherent blurriness to make emergent beauty.

Effective utilization of dS required all of the artists to understand and appreciate that the system was not deterministic nor should it be expected to behave as such. This recognition led to a shift in emphasis: rather than focus our creative attention on tightly coupled choreography and musical accompaniment arranged in linear sequences, our approach took on much more of a jazz feel. Each dS system state was built around a particular combination of graphical, sonic, and choreographic phrases. Hence, we tended to focus on how best to interweave these phrases to highlight the feel, ambience, and ideas which led us to discover the state in the first place.

The fact that both the visual and sonic effects are generated from the dancers' motions meant that specific timings between the graphics, sonics, and choreography were not emphasized nearly as much as they may have otherwise been. Particularly important in this respect was crafting a choreographic narrative for the dancers. This provided them with an intrinsic rhythm to drive dS, rather than only 'reacting' to it, and resulted in a beautiful range of dynamic variance. This permitted a certain degree of flexibility and spaciousness for facilitating interaction between the dancers, musicians, programmer, and choreographer, but it also introduced a certain degree of uncertainty. For example, Joseph Hyde, who was the principle architect for the sonic contours of *Hidden Fields*, once said "Every time I perform this piece, I'm always slightly scared, cause there's always a certain amount of variability that I know I can't control, and it might not work."

Vocabularies

HF development relied on interaction between an interdisciplinary group with dS forming a sort of creative hub. Given the diverse backgrounds of this group, and in an attempt to facilitate artistic interaction rather than hinder it, much of our time together was devoted to exploring effective metaphors and vocabulary that allowed us to merge physics concepts with dance ideas, musical analogies, and interactive high-performance computing. Dance is perhaps particularly well-suited to this sort of cross-fertilization with the sciences,[26,27] since the "dynamics" of dance share a number of important similarities with how scientists describe the "dynamics" of molecular systems. First, contemporary dance pieces exhibit correlated vibrational and periodic motion, but they also include a certain degree of variability and randomness. Second, dance often relies on varying degrees of cooperativity and correlation, which chemists and biologists increasingly recognize as important to molecular dynamics and function. Third, dancers and choreographers frequently use metaphors that suggest a manipulation of time, space, and energy – three concepts which form the foundations of modern scientific thinking. The scientific language of MD and spectroscopy – i.e., energy transfer, vibrational frequencies, coupled motion, field strengths, attractive and repulsive interactions, etc. – was remarkably easy to communicate to dance artists involved in *Hidden Fields*.

Observations From Public Participants

Presently, dS offers users a sort of molecular 'sandbox' wherein people can use their fields, either individually or in collaboration with other users, to sculpt the atomic dy-

namics, creating emergent graphic and sonic structure. The net result is that the individual and collective motion of arbitrarily large groups of people are able to create transient graphical and sonic 'sculptures'.[28] In general, the feedback has been excellent. Perhaps one of the most interesting aspects of the dS and HF feedback process arises from the fact that the science and associated theoretical frameworks are largely decontextualized from the spaces and discourses they normally inhabit. Under these circumstances, all bets are off, and the interpretative frameworks that participants use to understand what dS is showing them are fascinating. There is a certain respect in which dS has this in common with any other art installation. However, what distinguishes dS from a range of other art installations is probably the fact that its theoretical foundations are so rigorously and precisely defined, as outlined in this chapter. Hence, there is perhaps a starker relational contrast between the actual scientific origins and user interpretation. I cannot claim that we yet understand the origins, mechanics, and consequences of these varied interpretive acts, but the feedback process has increased my own interest in what might be referred to as 'paradigm hermeneutics' – i.e., the frameworks that we use to interpret conceptual paradigms outside those that normally guide our day-to-day thinking. Following are a few lessons that we have gleaned from non-expert user feedback, including user questionnaires, written feedback, and conversations.

Figure 8: one of the more literal states of dS, in which the dancer's energy contours are well-defined, there are relatively few particles, and all sounds are generated from particle-particle collisions

People were simultaneously confused by and attracted to seeing rather abstract 'energy' representations of themselves, compared to the more literal "video-game" type representations to which they are accustomed. In explaining dS, referring to people's 'energy avatars' proved much less confusing than referring to their 'energy fields'. Users seem to have had the least confusing and most engaging experiences when their initial encounters with dS presented them extremely literal, "person-shaped" energy fields embedded in a system comprised of only a few atoms with easy-to-interpret collision sounds, as shown in Fig 8. These simple states offer the user a well-defined and literal relationship with the system's interactive graphic and sonic properties, accelerating understanding of the system, and increasing their interest in more abstract visual and sonic states. Participants who had seen *Hidden Fields* prior to interacting with dS tended to embrace more abstract representations of themselves, presumably having a better understanding of the system from watching the dancers.

The fact that dS is built on rigorous scientific principles had noticeable consequences for how users interpret their interactive experience. For example, early on in dS deployment, people frequently asked us if the atoms were real. Initially we responded along the lines of, "No, they're purely virtual." In a few instances, people non-verbally registered their dissatisfaction and promptly left the installation. However, when we responded along the lines of "Yes, they're representations of five of the most abundant elements in the universe – Oxygen, Hydrogen, Helium, Carbon, and Iron," we found they were satisfied. Because of the more positive response we received from this latter answer, we actually altered the electrostatic properties of the atoms to match their measured properties, as discussed above.

People generally reported increased satisfaction with their dS experience if they had some sort of explanation of how the system works and the scientific ideas from which it derives. The scientific link added significant depth to how people interpreted their interactive experience. For example, the introduction to *Hidden Fields* contains a brief explanation of the system. And users who experienced dS having seen *Hidden Fields* had a distinctly metaphysical tone to their feedback compared to those who had not. They often hinted at how it left them with a sense of interconnectedness to nature and others, beyond the limits of their material body. Many of these feelings are beautifully encapsulated in a written review following the first ever *Hidden Fields* performance in Bristol:[29]

"[Hidden Fields] followed a vague narrative scheme of birth, the exploration and discovery of the self and its connection with the world, interaction and connection with others, and eventual death and dissipation. It was fascinating and a little bedazzling to have to flicker the focus of your perceptions between the dancers and the motions they created on the screen. It must have been strange for the dancers to not be the sole object of attention during the performance, and indeed to have no following lights drawing the eye to their movements. But the essence of the piece lay in the interaction between the human element and its computer-projected analogue on the screen, and it was necessary somehow to be aware of both. The images on screen were often abstract and strikingly beautiful. Waves of color would ripple across, or oscillating pulses of light

would waver back and forth. Particulate clusters in roughly human form would merge with one another and then bifurcate with the appearance of fluid cellular division. Joseph Hyde provided electronic music which drew on the visuals, reacting to them in real time, and gave them sonic contours. He began with the hum and hiss of white noise, the aural analogue of the chaos of the untuned TV screen with which was what the projections initially resembled. As forms began to emerge, along with the dancers, the music too began to resolve into individual notes and tones. Thick, angular particle trails slowly drew lines across the screen before ricocheting off the edges, accompanied by oddly mammalian squeaks and cries of surprise. One of the dancers played a game of interrupting or evading these firefly atomic contrails, the first tentative exploration of how the self could affect the world through which it moved. Towards the end, the human shape became a container for shimmering colonies of pointillistic atoms. The dancers began to lose their energy, and their partners cradled their dying forms and lay them gently down onto the ground. Their atomic clusters lost coherence, and slowly dissipated out into the general particulate matter which drifted all around them. It was a mystical image of essential indivisibility, of a certain continuity of being, and of the connection of all things which was in keeping with the spiritual tenor of the piece as a whole. The projected visuals, with their semi-abstract and vibrantly colored but still somehow recognizably human forms, gave the impression of a technologically-enabled emanation of some inherent essence of spirit, and iridescent imprint of the soul. It all ended with the music crackling and humming with the background noise of the universe. The screen was a frosty white, etched with the black craquelure of shattered safety glass. The last of the dancers slowly made her way to the wings, her movements creating a ghost which passed across the patterned screen like a watery shadow beneath thick ice, like life spiriting away in the face of the heat death of the universe. The whole was a fantastically beautiful and at times very moving meeting of science and art, human grace and technological ingenuity, rationalism and mysticism, dispassionate programming and emotional engagement. After the dancers had left, the floor was open once more, and the audience were free to project their own stories and selves onto the screen, to make sport and play in the Atomic World."

OUTLOOK

The relationship between computer science and more traditional fields of science (e.g., physics, chemistry, and biology) has a long and rich history, with many of the early developments in computer science driven by attempts to solve scientific questions. Computational methods have now developed to the point that they have become staples in a number of scientific fields, allowing the solution of previously insoluble problems. While the relationship between arts practice and computer science is perhaps less well established, it is rapidly expanding. As arts practice comes to increasingly utilize and gain familiarity with interactive technology and tools from computer science, it necessarily develops fluency with the algorithmic type thinking and language that dominates the discourse, models, and analogies used in modern science (e.g., across fields as diverse as physics, biology, nanotechnology, neuroscience, linguistics, economics, and sociology). Consequently, the time for interaction between art and science is ripe, and it will be exciting to watch what unfolds on this horizon.[30,31]

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