Hidden Fields
2012, dance performance from the *danceroom Spectroscopy* project

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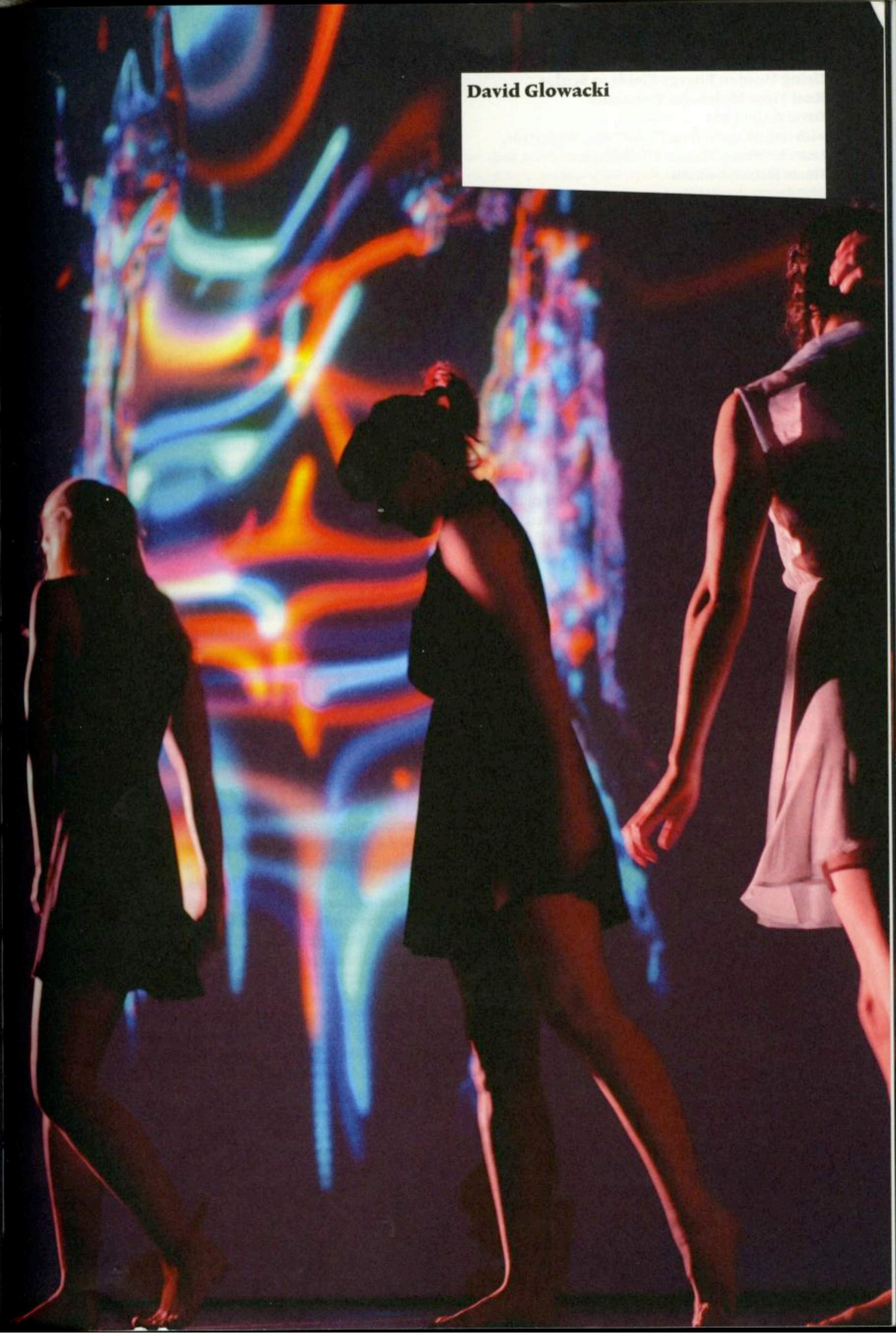

Using Human Energy Fields to Sculpt Real Time Molecular Dynamics

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Time, Equilibrium, and Molecular Structure

Molecules, made from building blocks called atoms, are among the most useful microscopic functional units for understanding the properties and behaviors of the macroscopic world. Despite the fact that the natural world 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.

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 photoreceptors in the cells located in leaf chlorophyll helps us to understand how plants capture light from the sun. Or the highly connected bonding structure of solids like diamond (shown in fig. 1) can help us to understand properties such as hardness and conductivity. In what follows, we refer to the use of static images to understand molecular function as a time-stationary view.

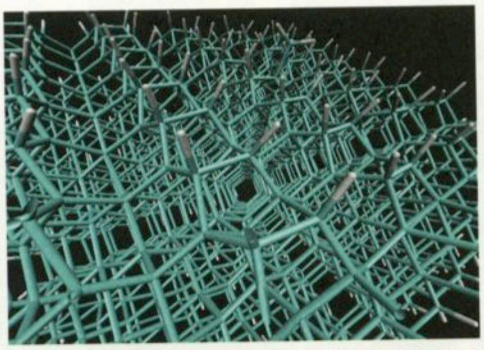


FIG 1 Molecular snapshot of diamond as it might look if our eyes were able to see the nanoscale. This snapshot conceals the time-dependence of the system. In fact, every component is wiggling, jiggling, and vibrating, locked in an interdependent dance, where the motion of each part of the system depends 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 flexible dynamism, 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 changes with time need not be considered. Instead we only need to consider one structure: the average. Indeed, it is these time-averaged equilibrium structures that we are typically shown in snapshots of molecular structures.

Molecules: a Dynamic Perspective

The achievements of equilibrium thermodynamics in modern science cannot be understated – both for improving our fundamental understanding of the natural world, and for allowing us to build a range of sophisticated technological applications. However, detailed studies examining a range of different molecular systems, from gases to liquids to biomolecules, show that the time-stationary, equilibrium view obscures many details of molecular behavior and function. Indeed, time-dependent fluctuations, coupled vibrations, plasticity, and cooperative motions are key to understanding molecules. 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 twenty-first century science.[1]

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. 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 jigglings and wigglings of atoms."[2]

In fact, Heisenberg's uncertainty principle (among the most fundamental principles of quantum mechanics) guarantees microscopic dynamism, and implies that every molecular structure is characterized by perpetual jiggling and wiggling, with vibrational motion and structural fluctuations that span a range of timescales and length scales. 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. 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 resolving.[3]

Molecular Dances, Spectroscopy, and Energy Landscapes

Qualitatively, the vocabulary of molecular dynamism seeps into 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[4] or chemical choreographies.[5] The use of these metaphors is no doubt driven in part by visualizations of time-dependent molecular phenomena using computational methods.[6] For example, visualizing the motion of the diamond structure shown in figure 1 reveals a tightly correlated molecular dance[7], where the vibrational motion of every atom in the system depends on and affects the dance of every other atom in the system.

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. 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 workers across different sub-fields within science. In the field of molecular dynamics, spectroscopy often refers to experimental techniques aimed at identifying the characteristic vibrations that guide molecular dances.

From a theoretical vantage point, 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 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[8], and can be used to rationalize the motion of almost any class of particle, atom, or molecule in the universe. Figure 2 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.

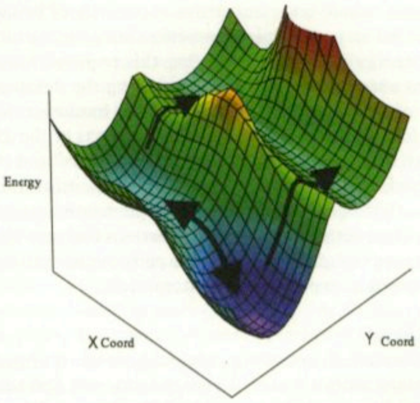


FIG 2 2-D schematic of a generic energy landscape, showing energy as a function of two idealized coordinates, X and Y. The arrows show characteristic paths that atoms might take over this landscape.

The energy landscape shown in figure 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, like waves on the sea, affected by fluctuating external fields and molecular configurations.

danceroom Spectroscopy

In what follows, we describe *danceroom Spectroscopy* (*dS*), which is an attempt to fuse the ideas discussed above – namely, molecular dynamics, spectroscopy, and energy landscapes – in order to generate an immersive audiovisual aesthetic experience. The mathematics and algorithms that drive *dS* are entirely rigorous; this is important because it means that *dS* has potential application to a range of interesting scientific questions beyond the scope of this chapter. However, given that the initial motivation for *dS* arose from artistic and aesthetic considerations, the remainder of this paper 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 the 6th century BCE.[9] More recently, 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.[10] 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 people sculpt molecular vibrational dynamics, and then use that information to generate real time sonic feedback?

Addressing this 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 a molecular dynamics (MD) simulation as an energy landscape. Achieving this required innovations on a number of fronts, including the development of new algorithms, software, and hardware. In what follows, we will describe several aspects of the *dS* project. After a brief outline of the mathematical and algorithmic framework that drives *dS*, we will outline the system that we have designed 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*.

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 figure 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 graphically 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 public installation, and (2) as an artistic tool that knits together the visual, sonic, and choreographic components of a dance performance called *Hidden Fields* (*HF*). Development of *dS* began in January 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 to July 2012, *Hidden Fields* was developed. Recent *dS* and *HF* appearances include: the Arnolfini Art Gallery in July 2012 (Bristol, GB); a 360°, 21-meter projection dome in August 2012 (London 2012 Cultural Olympiad); and the Barbican Arts Centre in November 2012 (London).

FIG 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.

MATHEMATICS AND ALGORITHMS

Interactive Dynamics Framework

In its present form, *dS* carries out an MD simulation involving N atoms, each of which may move in two dimensions (*x* and *y*). The simulation is run with each atom having the physical properties of either carbon, iron, hydrogen, helium, or oxygen (all amongst the most abundant elements in the universe). Within the simulation, each atom has a particular mass and associated set of electrostatic properties. The masses is known exactly, and the electrostatic properties have been previously calculated.[11]

A useful vantage point from which to discuss the simulation begins with Hamilton's equations of motion,[12] commonly used to discuss the dynamics of molecular systems in both classical and quantum frameworks:

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

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:

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

V_{int} is calculated by summing over all possible 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,[13] 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, exploiting the fact that 3-D capture systems 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 2-D energy landscape shown in figure 2. 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 modified in real time to control strongly a particular atom type 'feels' the users' fields, and whether people are attractive or repulsive. Effectively, 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 atom with respect to every other atom, the second term explicitly depends on time, owing to the fact that people are not stationary within the exhibition space.

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 – for example:

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

Substituting (E3) into (E5) gives

$$F(t) = \frac{dV_{int}}{d\mathbf{q}} - \frac{dV_{ext}}{d\mathbf{q}} \qquad \text{(E6)}$$

$$= \mathbf{F}_{int} + \mathbf{F}_{ext}$$

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 approaches, wherein each atom is represented as a point, and the force 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 $\mathbf{F}$ depends on some sort of local average within the force field. To efficiently incorporate this non-locality, we implemented a mixed quantum-classical dynamics strategy based on the so-called frozen Gaussian dynamics approach, which forms the basis of several 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 an integral over a Gaussian function. In two dimensions, the form this function takes is:

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

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.[14] Effectively, λ_i is a sort of measure for how wave-like the atomic particles are.

SYSTEM DESIGN AND SETUP

Image Processing, Physics and Graphics

A simplified schematic of our setup using a single sensor is shown in figure 4. In general, up to eight depth sensors send depth matrices via USB to a custom-built workstation. This occurs at either 30 or 60 Hz, the operational frequencies of our depth sensors. Following a depth matrix grab, the workstation calculates $\mathbf{F}_{int}$ 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.

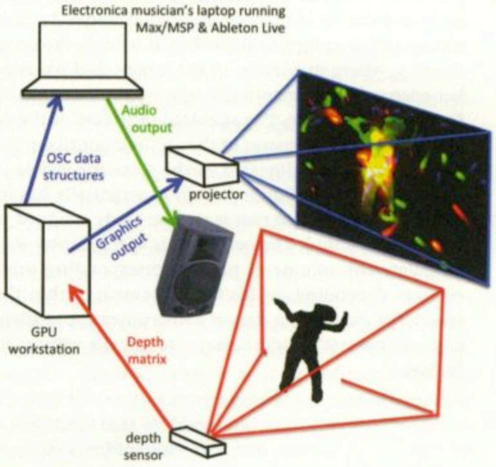


FIG 4

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 '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 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 atom wall and/or atom-atom collision event is tagged with OSC data, triggering an arbitrary sound chosen by the electronica artist.[15] This works fine for small numbers of atoms; 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 use a filter 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.

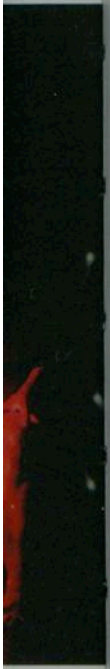
Superparticle Clustering Analysis

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.[16] These clusters we refer to as 'superparticles', since their properties – position, velocity, and size – are similar to those of individual atoms. An illustration of the grouping algorithm at work is shown in figure 5, where 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 figure 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 sonic channel depending on his/her movement within the space. For example, a dancer's instrument goes silent with stillness. With increasing velocity, the volume increases.[17]

FIG 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 vector of atomic velocities at some time step t, and $\mathbf{v}(t_o)$ specify the same vector at some previous time step t_o, the VAC is essentially a time series of size n which measures how $\mathbf{v}(t_o+dt)$, $\mathbf{v}(t_o+2dt)$,... $\mathbf{v}(t_o+ndt)$ project onto $\mathbf{v}(t_o)$, where dt is the dynamics time step. 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.[18]



Hardware

Workstation

Our technical goals have largely been driven by our desire to adapt *dS* to 360° projection environments with a latency no larger than 17 ms (60 Hz). This proved too intensive for a standard desktop or laptop. At present, *dS* runs on a high performance custom-built 64-bit workstation with a hexacore CPU and two top-of-the-range graphical processing units (GPUs), one of which is used solely for graphics rendering over multiple outputs, and one of which is reserved solely for dynamics computations.

Camera Mount

Installing *dS* in 360° requires simultaneous depth matrix capture from at least seven sensors. Our camera mount 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 center 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. 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). 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 cameras' 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. 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, (7) how strongly the thermostat enforces the selected temperature at each dynamics step, and (8) whether different atom types generate OSC data upon collision. Graphics-related variables accessible on the main GUI screen include: (1) whether atoms flash when they collide, (2) the feedback incorporated into the atom rendering (e.g., high feedback results in trails for atomic trajectories), (3) the feedback in the rendering of V_{ext} (high feedback allows human motion to create graphic distortion), (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:

(1) 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.

(2) 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. Among 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 twenty 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 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 – for example, the dancers made gentle orbiting motions across the 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 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.[19]

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*, beyond merely reacting to it, and resulted in a beautiful range of dynamic variance. Such narrative schemes permitted a certain degree of flexibility and spaciousness for facilitating interaction among 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,[20] since the 'dynamics' of dance share a number of important similarities with how scientists describe the 'dynamics' of molecular systems:

(1) Contemporary dance pieces exhibit correlated vibrational and periodic motion, but they also include a certain degree of variability and randomness.

(2) Dance often relies on varying degrees of cooperativity and correlation, which chemists and biologists increasingly recognize as important to molecular dynamics and function.

(3) 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 dynamics and spectroscopy – for example, 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 people a sort of molecular sandbox wherein people can use their fields, either individually or in collaboration with other users, to sculpt the atomic dynamics, 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.[21] Following are a few observations that we have gleaned from non-expert user feedback.

People were simultaneously confused by and attracted to seeing rather abstract energy representations of themselves, compared to the more literal video-game

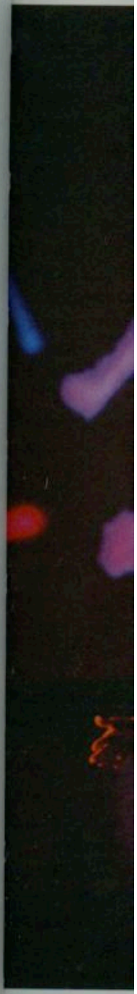


FIG 6 One of the more literal states of *dS*, in which the dancers' energy contours are well-defined, there are relatively few particles, and all sounds are generated from particle-particle collisions.

type representations to which they are accustomed. People seemed 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 figure 6. These simple states offer 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. People 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 people interpret their interactive experience. For example, people found satisfying the fact that the particles they saw being simulated were more than mere abstractions, with properties corresponding to those of real atoms. Also, 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:

"*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 analog 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 atom 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."[22]

OUTLOOK

The relationship between computer science and more traditional fields of science (for example, 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. While the relationship between arts practice and computer science is perhaps less well established, it is rapidly expanding, and arts practice is developing fluency with the algorithmic type thinking and language that dominates the discourse, models, and analogies used in modern science (across fields as diverse as physics, biology, nanotechnology, neuroscience, linguistics, economics, and sociology). So what can art offer science? Within the physical sciences, it is often the case that experiments to facilitate direct visualization of the subjects under investigation are not possible. In this respect, artistic visualizations have much to offer for helping us to effectively imagine phenomena and concepts that are invisible even to the eyes of scientists. And what can science offer art? Challenging the frontiers of how we understand the elegantly woven fabric of nature, science offers fertile conceptual territory for the arts, which is perched on the very horizons of knowledge and always under revision. The time for interaction between art and science is ripe, and it will be exciting to watch what unfolds on this horizon.[23]

CREDITS AND ACKNOWLEDGMENTS

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 molecular dynamics and also holds a master of arts in cultural theory; Philip Tew is a programmer and installation artist with interests in generative processing and physical modeling; 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 focusing on multimedia, dance, telepresence, and interactivity; 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. *Hidden Fields* rehearsals and performances additionally involved five professional modern dancers (Lisa May Thomas, Isabelle Cressy, Kathleen Downie, Emma Harrie, and Kerry Trevaskis), all of whom had three to ten years of professional dance experience/training. Direct funding has been provided by the UK Engineering and Physical Sciences Research Council (grant EP/I017623/1 and *Pathways to Impact* GR4016) and Arts Council England. Indirect funding has been provided by the Pervasive Media Studio (Bristol), the Arnolfini Centre for Contemporary Arts (Bristol), and NVIDIA corporation. We also thank the following individuals: Mike Ashfold, Becca Rose, Lee Malcolm, David McGoran, Paul O'Dowd, Paul Blakemore, Paul Gilbert, Nathan Hughes, Jacob Parish, Tim Gallagher, John Keating, Sarah Warden, Phillipa Bayley, Kate Miller, Maggie Legget, Mel Scaffold, Clare Reddington, David Hotchkiss, Ki Cater, David Coyle, Sri Subramanian

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