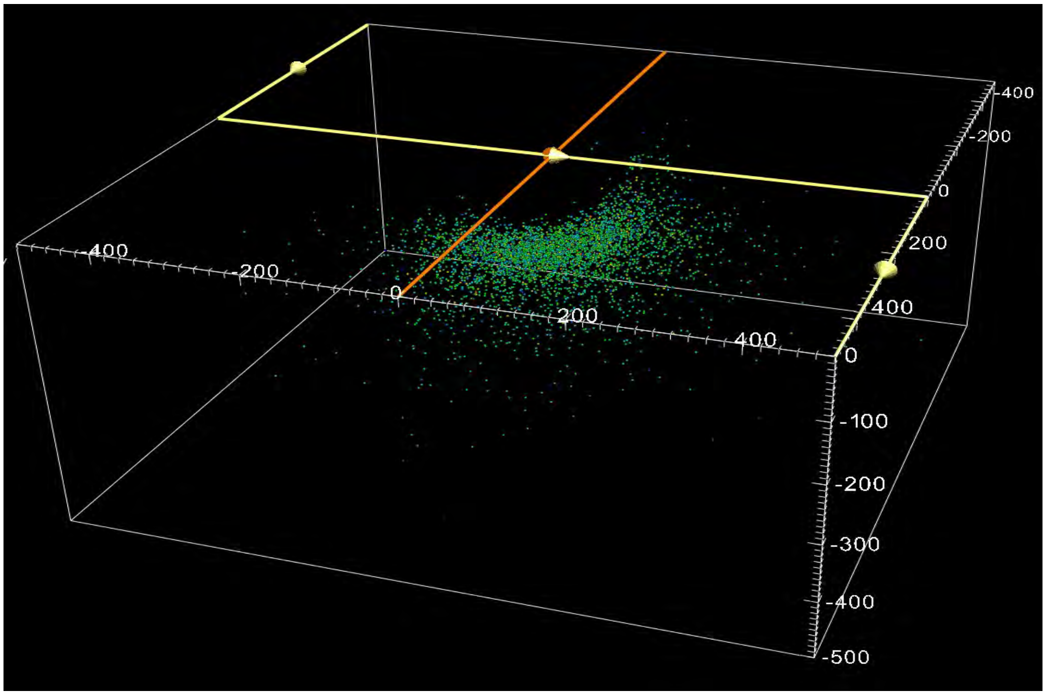
Atom Interferometer Modeling Tool
Final Report

August 8, 2011



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Abstract

Over phase II of this STTR, we developed a flexible and powerful tool, called **LiveAtom**, for designing and modeling experiments with cold and ultra-cold atoms. The tool was developed using a flexible development methodology that allowed us to build on our successes in phase I of the contract, and to quickly incorporate feedback from a variety of different research groups that were using the tool. In this report, we describe the resulting product and show different examples of the two and three dimensional visualizations the tool provides. We discuss the major computational features of the tool, and describe the motivation for their development. Finally, we discuss the reception of the tool by our users and in the larger cold atom research community. LiveAtom is a reliable and valuable tool for groups working with atom chips, has been validated against real world experiments, and is currently in use at several different laboratories across the country.

Table of Contents

Introduction to LiveAtom

The Need For a Tool

In our phase II proposal, we described the motivation for developing LiveAtom:

> From the time of the original demonstration of Bose-Einstein condensation (BEC) in 1995, ultracold matter experiments have become increasingly sophisticated in their use of magnetic, electric, radio-frequency, and optical fields to affect atoms. Atom chip work, for example, utilizes circuits of tiny lithographically patterned conductors to manipulate atoms on a small scale. Eventually, such chips may incorporate several atom based functions on a single substrate. On another front, interfering light beams are used to produce optical lattices, i.e., light structures that confine atoms to periodic potentials, which can be used to emulate a condensed matter system. In the future, technology advances may permit the combination of optical and magnetic control of atoms on a chip. Generally speaking, as the degree of spatial control over atoms has grown over time, so has the complexity of designing and modeling the effects of various control schemes.
>
> Every research group with which we are familiar has developed rudimentary CAD/CAM tools to facilitate experimental design. The tools frequently utilize standard computational packages such as Matlab and Mathematica to carry out relatively simple (but computationally intensive) first-principle calculations of the field resulting from electric or magnetic structures, using simple geometrical approximations entered by hand. These home-grown efforts provide a subsistence level of capability, but they are woefully short of the power and flexibility that can be offered by specialized software. By now it is clear that ultracold matter research can be greatly facilitated by a set of professionally developed CAD/CAM tools specifically targeting the design, computational, and visual needs of the community. Such software will almost certainly play an essential engineering role as ultracold matter technology transitions from the academic research labs into the military, commercial, and industrial labs.

Thus, our goal was to develop a specialized CAD/CAM tool that would offer cold atom researchers the ability to design and understand the small, complex structures found on an atom chip. This software will provide more detail, more flexibility, and a better understanding of the problem than homegrown software, and thus should provide significant benefit across the community. In order to facilitate adoption, we wanted our users to be able to see the value our tool provides within 15 minutes of starting to use it. This mandated a simple and intuitive user interface, clear and easy to understand visualizations of the results, and a simple install process that would work on a standard desktop computer.

We have achieved these goals with a software product called LiveAtom.

LiveAtom: A Modeling Tool For Cold and Ultra-Cold Atom Physics

LiveAtom is a computer aided design and modeling tool designed specifically to meet the needs of cold atom researchers – to aid in the development of atom chips and the design of cold atom experiments. Specifically, given a conductor geometry of coils, thin wires, or thicker, lithographed wires, and a description of currents flowing through those conductors, LiveAtom will provide the user with a visualization of the resulting magnetic field, find magnetic field traps, and model atomic interactions in the resulting potential.

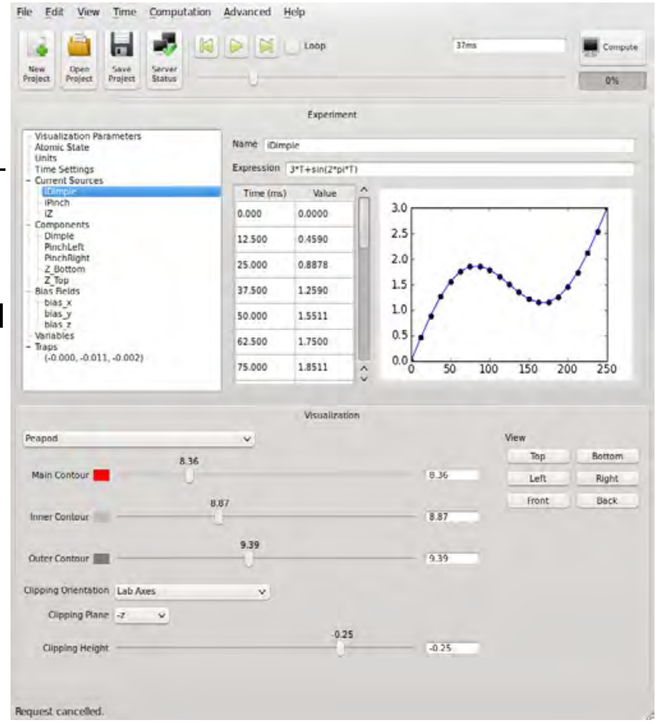

Figure 1: The LiveAtom interface has a full-featured expression parsing interface that provides visual feedback.

The software was developed through a partnership with Professor Dana Anderson's group at the University of Colorado. Researchers at the university have validated both the results and the utility of the software in a broad variety of experiments over the last two years. In fact, LiveAtom has become one of the primary design tools for Dana Anderson's group.

Simple Experimental Design

One of our primary goals for LiveAtom was that it should be easy to learn and use, yet provide useful and detailed results to complex problems. Achieving this goal begins with providing our users with a means to specify their experiment that is both intuitive and flexible.

LiveAtom users can design experiments in two ways. Using infinitely thin wires allows for fast prototyping of designs and is sufficiently accurate for many experiments, while using two-dimensional wires specified in an external CAD system allows for detailed modeling of the extremely complicated geometries.

In both cases, LiveAtom provides immediate visual feedback to the user as the design in being specified. This rapid feedback loop allows a user that is familiar with the field of cold atom physics to learn how the application works simply by using it, without needing external training.

Advanced Visualizations

LiveAtom allows users to visualize the magnetic fields that result from their experimental setup in three dimensions, offering a quick and intuitive way to see all of the relevant features. Lower dimensional plots provide insight only into the regions that are plotted, and can be misleading when features do not remain in one plane. All of LiveAtom's visualizations are interactive, allowing users to better see the subtleties of the magnetic field by rotating, zooming, and moving plots through the region of interest.

Integrated Physics

LiveAtom is more than just a visualization tool; it will perform a variety of physics calculations and simulations. The tool will find any traps resulting from the conductor geometry and the values of their key properties -- trap frequency, depth, axes, etc.. The tool will model the loading of these traps with atoms in a static equilibrium, or, if the system is designed to vary over time LiveAtom will simulate how thermal atoms will behave using Monte Carlo simulation methods.

A Tour of LiveAtom

Experimental Specification

In this report, we will explore the features of LiveAtom in the same way that a user would see them: starting with experimental layout, then specifying currents and bias fields in order to generate a visualization of the resulting magnetic field, and finally examining the more advanced physics capabilities of the tool.

LiveAtom offers two different ways to specify the conductor geometry that defines the experiment.

The first method is to use thin lines to represent wires, which allows for fast specification and computation. Users specify these wires by entering a series of points in three dimensional space, which allows for the construction of arbitrarily complex conductors and coils. In the case where the atoms will be trapped at a distance below the chip that is far greater than the width of the wires and the size of the features on the chip, this model provides sufficient detail.

The second method of experiment definition is to import conductor geometry from an outside CAD tool such as AutoCAD. This allows users to specify the more complex layouts using a fully-featured tool of their choice, while significantly reducing the complexity of LiveAtom. Furthermore, most groups have already been using a 2D CAD package to define the layout of their atom chips for fabrication, and this allows us to use their library of existing designs without requiring any additional work from the user.

The LiveAtom user interface provides visual feedback for every action a user performs while specifying an experimental layout. This gives users instant feedback on each action they perform, making it easy for a new user to learn the program and for an experienced user to quickly find and correct mistakes.

To assist in designing complex geometries, LiveAtom provides a full-featured expression parser which allows for variable definition and provides a number of commonly used functions. Both conductor layouts and current sources use this expression language. Thus, if a user wants to see the effects of using coils of differing diameters, he would specify the coils position in space in terms of a variable, *radius,* say. He could then simulate variations in the radius of the coil by changing only one value. Further, this allows users to specify experiment geometries that change over time allowing us to represent, for example, a moving coil.

Once the wires are laid out, users specify where and how they would like currents to flow through the wires. In LiveAtom, this is done by specifying where the current sources are attached to the experiment, and providing a current schedule. This schedule can be defined by a function, using the LiveAtom expression language, or by using a table to specify a specific value at each timestep. LiveAtom will reflect the specified current sources in the visualization through a plot that is brighter at areas where there is the most current.

In addition to conductors and current sources, users can specify a uniform external bias field. This specification also the expression language, allowing bias fields to change over time or in response to another variable. In this fashion, bias field can be tied to current to allow users to change the current flowing through the wires while maintaining some trap properties (e.g., position).

Now that the experiment has been defined, LiveAtom can compute the resulting magnetic field.

Advanced Visualizations of the Magnetic Field

One of the most compelling features of LiveAtom, when compared to home grown software, is its sophisticated three dimensional visualization. As soon as a user begins specifying conductor geometry LiveAtom offers the user a 3D visualization of their experiment. Once the experiment is fully specified, computing the magnetic field generally takes only a few seconds.

Figures 2 - 5 show the different visualizations that LiveAtom provides. Each of these visualizations are interactive: users can adjust the position of the contours or slices, zoom in and out, translate the camera in the x or y direction, and rotate the camera about any axis. The interactivity has proven to be incredibly valuable in understanding the geometry of a complex problem. One can gain much more information by watching an animation of a two-dimensional slice move through three-dimensional space than by simply seeing a static image of the same slice.

Because LiveAtom's magnetic field computations are performed quickly, interactive design is also possible with LiveAtom. In this scenario, a user may have a specific trap geometry or manipulation in mind but not know exactly how to create it. With LiveAtom, it is easy to evaluate several different ideas quickly, and then “fine tune” one of them by making small changes to the layout, currents, or bias field and recomputing the results. The sophisticated visualizations make it easy to see the effects of small changes to the experimental parameters.

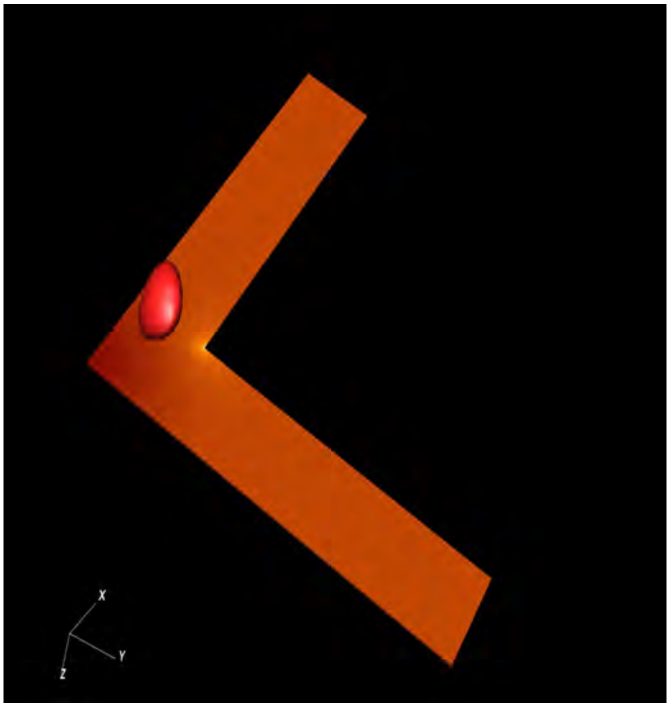

Figure 2: The first visualization: a hard shell contour (in red). The contour can be changed by moving a slider in the user interface window.

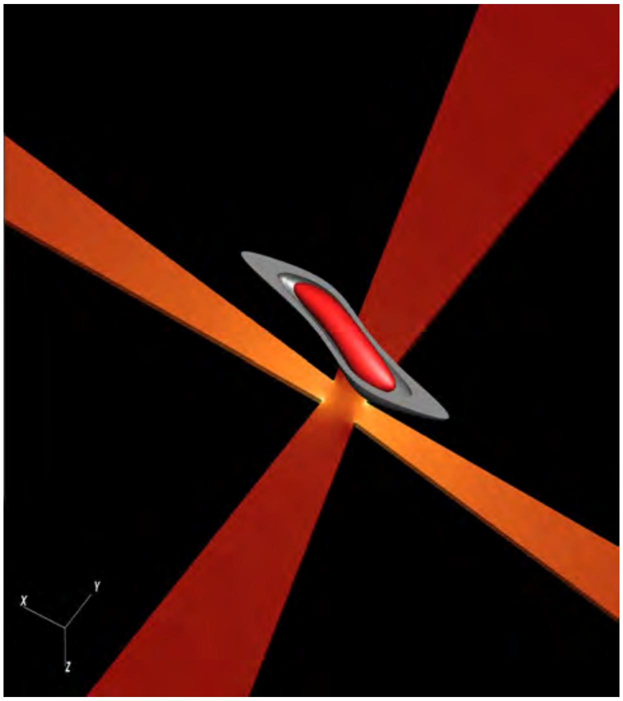

Figure 3: Peapod (1 hard shell in red, 2 more in gray, cut). This view provides insight into where the trap is and how the field changes around it.

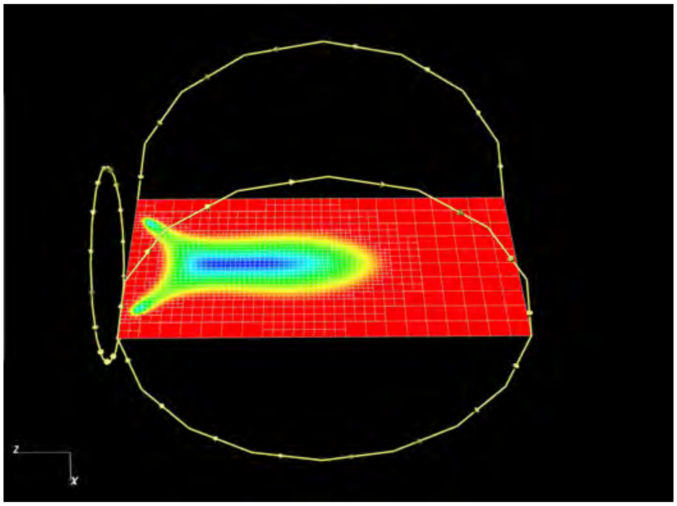

Figure 4: Slice visualization - this view can be seen in two or three dimensions, and the slices can be moved using a slider in the UI.

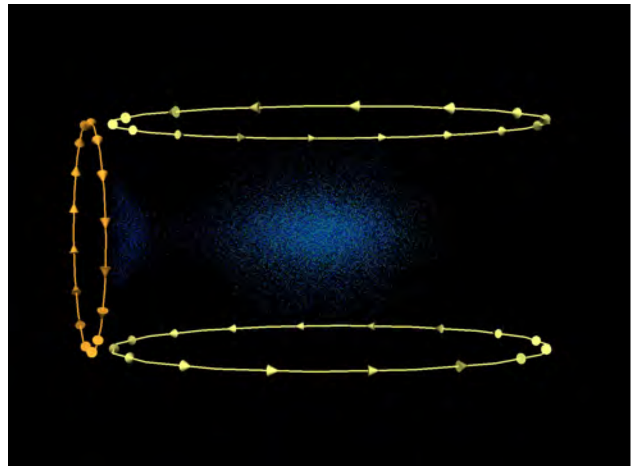

Figure 5: Monte Carlo Simulation: Atom Cloud View - LiveAtom will model the behavior of thermal atoms in the presence of magnetic potentials.

Desktop Client / Network Server

Another of our goals for LiveAtom is that it be easy to install and use. It is critical that potential users can see the value in the tool quickly, without investing a lot of time or effort. However, the computational requirements of the software are beyond what a standard desktop computer can perform in a reasonable amount of time, and many of the tools that we use in the numerical computation module are Linux specific. As a result, we decided to host a computation server "in the cloud."

LiveAtom now provides all of the power and speed of cluster computing, while still running on an ordinary desktop or laptop computer.

Atomic Physics in LiveAtom

Calculation of the Magnetic Field

LiveAtom begins the process of solving for the magnetic field by determining the current distribution through the conductors. In the case of one dimensional conductors, this is trivial. However, for the thicker, two dimensional conductors, we use finite element analysis to determine the current distribution through the wire.

In the normal case, we have long wires with relatively uniform current for most of their length, with only short sections where the current is changing rapidly. We take advantage of that configuration by using adaptive mesh refinement to focus on only the parts of the wire where the current is changing rapidly. The result is that we can solve a finite element problem in two-dimensional conductor in only a few seconds, while still providing an accurate result.

Once we have determined the current distribution, we use direct integration (Biot-Savart law) to determine the magnetic field. Again, we employ mesh refinement in the areas where the field values are the lowest, to provide a high level of detail near the trap without incurring a time penalty for computing the field in places where a detailed picture is not needed.

Automated Trap Finding and Analysis

Once LiveAtom has solved for the magnetic field, it performs an automated trap detection algorithm, and computes the most frequently used trap parameters: trap location, orientation, frequency, and depth. These parameters can then be used to provide standard plots and three-dimensional visualizations oriented with the trap, rather than the lab axes.

Because many of these values depend on the isotope and state of atom that is being trapped, we ask our users to pick from a table of known isotopes. At present, LiveAtom supports the alkali metals from Lithium to Cesium. LiveAtom will also show where atoms in the equilibrium state will sit if a trap is loaded with the specified atom at a given temperature, for both thermal atoms and condensates.

Trap Optimization

If the researcher has a specific trap or potential in mind, LiveAtom can help her determine the appropriate geometry or current schedule to achieve that goal. LiveAtom has a built-in optimizer that asks a user to specify certain trap parameters (location, frequency, depth) and to select current sources, bias fields, or variables (which, in turn, can define layouts, currents, or bias fields) to optimize to achieve the desired results.

LiveAtom uses an optimization technique known as Particle Swarm Optimization, or PSO. PSO is a metaheuristic optimizer – that is, it avoids making assumptions about the problem, and does not use the gradient to reach a solution. This allows us to optimize across a broad range of different variables, and adapt to the different types of effects that a change to each variable might have. PSO also handles multivariate optimization well – there is no upper limit on the number of parameters that can be optimized at one time.

t should be noted that while these optimization techniques can be a powerful aid to the user, they only work well within a narrow range of parameters. It is possible for a user to either under- or over-specify the optimization conditions, such that no solution or many different solutions to the problem exist, leading to inconsistent solutions.

Monte Carlo Modeling

Once atoms are trapped, cold atom researchers want to manipulate them. This, invariably, involves placing them in a non-equilibrium state. While the static visualizations provided by LiveAtom are no longer adequate in this situation, we provide a tool that will provide good results for thermal atoms.

Using the Direct Simulation Monte Carlo (DSMC) modeling feature, users can simulate the behavior of cold, thermal atoms in a dynamic magnetic potential. This could be used, for example, to understand and optimize trap loading or atom transport. Each Monte Carlo simulation requires between 20 minutes and one hour to run (though future work could reduce this time significantly), and provides the user with statistics describing the loss rate, change in temperature and distribution, and phase space density of the atom cloud.

Using the DSMC simulator, a user can understand if her current schedule for trap loading is adiabatic or not, and measure the effects of ramping the currents faster or slower.

In addition to providing plots of the calculated statistics above, LiveAtom provides an animation of particles representing the atom cloud. With this animation, users can see atoms falling out of a trap if, for example, they are moved too quickly or there is a mode mismatch during transfer.

Reception By The Cold Atom Research Community

We began a Beta program in the late fall of 2010, making the software available to a limited group of users. Through the Beta program, we have found six different groups that were interested in using the software, in addition to the University of Colorado. The feedback that we received from these groups helped to guide us through a major rework of the user interface in the last months of the contract.

Overwhelmingly, the community seems impressed with the visualizations, the speed, and the ease of use of the software. During the beta program, we found that users were able to learn how to use the tool productively very quickly, and that a simple tutorial was sufficient to get started. One user said, “I had it finally installed last week and had a chance to look at a few simple examples. I really like its capabilities! It was able to give immediate answers for things that took weeks to implement in COMSOL.”

In the summer of 2011 we debuted the software at DAMOP, presenting it to a much larger audience. There was a substantial amount of interest in the tool, and we received a significant amount of feedback. It seems that the tool is heading in the right direction. People were impressed with the interactive three-dimensional visualizations, and liked the idea of getting results quickly. Those groups that were working exclusively in far field situations liked the idea of the tool, but said that they would likely not see sufficient value in it to justify a significant purchase price. Groups working with atom chips, on the other hand, uniformly said that they would consider purchasing the tool before designing a new chip. Further strengthening LiveAtom's presence at the show, Violetta Prieto from the Army Research Lab referenced the software on a poster she gave at the show.

Table 1, below, lists the different groups that are currently using LiveAtom.

Organization	Head of Group	Researchers	Area of research
University of Colorado at Boulder	Dana Anderson	Steve Segal, Evan Salim, Kai Huduk, more	Atom interferometry, atomtronics
ColdQuanta	Dana Anderson / Rainer Kunz	Danial Farkas, Evan Salim	General atom chip work
ARL	Mike Golding	Violetta Prieto	Atom interferometry
AFRL	Steve Miller	Jim Stickney, Matt Squires, Spencer Olson	Atom interferometry
NIST Boulder		Jeramy Hughes	Atom chip setup
Harvard University	Lene Hau	Danny Kim	Atom chips / Rb87
University of Oklahoma	Jim Shaffer	Jon Sedlacek	Atom chips

Changes Since Last Milestone

Since the last report (Milestone 7), we released a resigned and rewritten user interface. This new interface provides a much more “professional” appearance to the software, increases its usability, and addressed a list of frustrations with the old interface.

Our new user interface is depicted in Figure 1. Significant improvements over the old interface include:

- The addition of a tree widget to contain all of the components of the experiment. Prior designs had a separate tab for each item, which made it more difficult to see the big picture and forced users to change between tabs frequently to accomplish a single task.
- An updated interface to the visualization engine. The previous implementation would cause the user interface to block or “lock up” for a fraction of a second while the visualization was being redrawn. This lead to “clunky” feeling sliders and widgets. The new interface addresses these issues by changing the way we connect to the visualization engine. We now offer proper acceleration on the sliders (that is, if a slider is moved quickly, the rate at which the object in the visualization changes is increased).
- An improved network interface, server status dialog, and estimated time of completion. While most of our tasks complete quickly, providing frequent and accurate feedback to the user is a crucial task – this way the user knows that everything is continuing to work correctly. The new interface provides a server console that allows users to monitor what is happening on the network server.
- Right click to clone, move, rotate, and delete components. These actions are consistent with what users expect when they use a computer.

While some users have found the floating visualization window can be source of confusion, many have requested that we retain that feature. It allows users with dual monitor systems to split the visualization and the control in an ideal way.

Through the Beta program, we received exclusively positive feedback on the user interface changes, and have found that they were on-target and well received.

During this time period, we also spent time working on the commercialization strategy for LiveAtom, created promotional literature and videos, and demonstrated the software at the APS DAMOP conference.

Next Steps

At the DAMOP conference there was significant excitement about the software, and a number of people expressed interest in extending its capabilities. The two most frequent requests were:

1. The addition of optical potentials. Many people suggested that a simple model of a detuned Gaussian beam would be sufficient, while others had more complex needs.
2. Time averaged potentials.

We are continuing to explore different commercialization options and avenues for further funding, and we hope to be able to add these new capabilities and more in the future.

Significant Purchases

There were no significant purchases made during this reporting period in support of this contract.

Personnel

During this reporting period, there was no shift in the personnel staffing the contract.

Meetings, Travel, and Conferences

During this reporting period, we attended the APS DAMOP conference as an exhibitor.

Areas of Concern

At present there are no major areas of concern.