# Designing targeted interactive software for chemical education for multiple educational environments

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What is the Next Big Step for Using Computers to Teach Chemistry?
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http://quantumconcepts.bu.edu/dissem/DesigningTargetedSoftware.pdf
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About muggles and wizards: anyone who is not a wizard or witch is a muggle. Muggles are not allowed to see magic according to the Ministry of Magic. Their enforcers are very effective and use memory charms when a slip occurs. Witches and wizards have pictures and paintings just as we do, however they move. Characters move between paintings. More to the point, a wizard photograph will show someone waving to you, or winking, and generally in motion (though repetitive). It's what our books will have when LCDs are paper thin and cheap and the chip that goes with it will show students what we now see on big bulky computers. Then the oscillations we now see will appear in textbooks. Of course, they already appear in Harry Potter's General Chemistry text.

Peter Garik, 2004.

### Abstract

The challenge in packaging sophisticated computations of chemical properties is to make their output accessible in a controlled way, thereby exposing only those details that are appropriate to the target educational objectives. *Pedagogica*™, created at the Concord Consortium, is an authoring environment that provides a framework within which selected computational features of Java components (isosurface visualization, bond energies, dipole computations, etc.) are exposed. We are using *Pedagogica*™ in conjunction with quantum chemical computations to design activities from which students can learn quantum concepts in a context of interactive inquiry and puzzle solving. Visually these explorations are a mixture of graphical displays, controllers (buttons, sliders, numeric inputs, etc.) for interaction with the computational engines, text to direct student progress through the activity, and buttons and text windows to monitor student achievement. We are creating and studying the use of these inquiry activities for learning of fundamental quantum concepts by individuals, and in classroom and PLTL workshop environments. One significant advantage of *Pedagogica*™ for instruction is its automatic logging and seamless archiving of student progress for subsequent assessment and project evaluation. We will report on strategies for creating and implementing activities with *Pedagogica*™ to support student learning in varied learning contexts.

### Our Sponsor

This project is funded by the Fund for the Improvement of Postsecondary Education (FIPSE) Grant P116B020856, *Exploring Quantum Concepts in Chemistry: Active Discovery by Students in the General Chemistry Course*, http://quantumconcepts.bu.edu.

### The Exploring Quantum Concepts Project

The context for our presentation today is the teaching of quantum concepts in the undergraduate curriculum. The computer based materials we are designing are appropriate for use in general chemistry, physical chemistry, and potentially in organic chemistry.

Quantum concepts have traditionally been difficult to teach, although they are at the heart of our understanding of modern chemistry, materials science, and emerging quantum technologies such as quantum computing.

The teaching of quantum concepts in chemistry cries out for using computer programs. By means of the computer we can make graphical and dynamic what otherwise is mathematical and static.

## Designing software

Since 1996, we have been designing software to teach quantum concepts. The Quantum Science Across Disciplines project, http://qsad.bu.edu, developed a suite of applications. These applications gave the user broad options on how to investigate the properties of atoms and molecules.

However, once the applications were completed, we needed to write separate worksheets to guide the student. Use of worksheets can be very successful (e.g., Virtual ChemLab and Contemporary Laboratory Experiences in Astronomy). However we decided that students could get greater benefit if we used the computer to guide the way students interacted with the applications.

## Precision guided software using Pedagogica™

Our needs:

- Control what the students sees, and when the student sees it.
- Control the student’s progress through the activity based on performance.
- Early assessment of student performance. This feedback is critical for formative development of our programs. It is also very useful for instructors to know how their class is responding to the instruction.

Pedagogica is an authoring environment developed at the Concord Consortium, http://concord.org. With Pedagogica:

- The interactive environment is built from Java components.
- The programmer can specify which affordances of the components students can access.
- There is automatic logging of student responses to questions.

## Software Example: Using spectroscopy to discover the Bohr-Einstein energy relationship, $h\nu = |E_{final} - E_{initial}|$

Students in their first semester of general chemistry have just completed this activity, after several weeks of introduction to quantum aspects of light, matter, and electrons in atoms (http://quantum.bu.edu/notes/GeneralChemistry/index.html#quantumAtoms) . One student sent the following message after completing the activity:

> What is confusing is that [in] the spectroscopy assignment we didn't really care about wavefunctions or probability density. The results jump out of, and [are] verified by, the spectral lines alone.

> Beyond that, once we assumed there is one electron, we didn't mention electrons again; we deal with this *atomic* energy level vs. that *atomic* energy level, the light quanta comes out of the *atom*, we are "blind" to the fact that there is one electron there, we just deal with those spectral line[s] that come off of the entire atom, for all we know. It is confusing because in class we are on the "wavefunction study path" and the spectroscopy assignment doesn't seem to me to be on it.

> BTW, Did Bohr know about wavefunctions when he came out with his formulas?

This student has wonderfully grasped the power of experiment to elucidate the structure of atoms. For the student to have achieved such a sophisticated insight exemplifies the power and promise the precision guided software approach made possible using Pedagogica.

In this case, if we had provided the student with a standard application depicting energy levels *a priori* and also connected with wavefunctions (as our own Atomic Explorer did, http://qsad.bu.edu), the student would never have recognized that the energy level concept can be developed independently of the wavefunction, and that that is what happened historically. If all the tools are available at all times, students will make their own connections which may not be in the causal net we hope to induce through proper instruction.

### Software example: Using wavefunctions and probability densities to discover the Bohr-Einstein energy relationship, $h\,\nu = |E_{\text{final}} - E_{\text{initial}}|$

Time dependence of wavefunctions is difficult to teach without animation software (though the flippets in Max Born's text *The Restless Universe* are a neat exception, telling authored by an architect of quantum mechanics). Yet this time dependence is essential to understand the resonant interaction of light with matter—the Bohr-Einstein relationship. We are building an activity to explore these ideas. Our goal is for students to discover, for hydrogen atom electron wavefunctions:

- Wavefunctions oscillate but the corresponding probability densities do not (stationary state idea).

- The relative frequency of oscillation depends only on the principal quantum number, and not on orbital momentum or magnetic quantum number (subshell degeneracy).

- The relative frequency of oscillation is invesely proportional to the square of the principle quantum number, and so energy determines the oscillation frequency (phase $e^{-i E_n t/\hbar}$).

- Neither the 1s not the 2p oscillation frequency correspond to the 1s→2p transition frequency—a puzzle!

- In order for a density to oscillate, it must be *a mixture* of wavefunctions *of different principal quantum numbers*. Mixing 1s and 2p give a probability density that oscillates with precisely the 1s→2p transition frequency—puzzle resolved by $\nu = (E_{2\,p} - E_{1\,s})/h$.

In this way we hope student can achieve a dynamical model of the interaction of light with matter.

### Multiple Educational Environments

The materials that we are developing can be used to support teaching of students in several circumstances.

- Individual students can be asked to log in an use the Exploring Quantum Concepts software.

- In a Peer Led Team Learning (PLTL) setting, groups of students can work on an activity. This may require some tuning of activity scripts.

- These materials can also be used by groups engaged in interactive inquiry without a team leader as in Process Oriented Group Inquiry Learning (POGIL).

### Where to view and get our work

We look forward to providing you with access to all of our materials. Our software is available at http://quantumconcepts.bu.edu. However, because of the rapid rate of development, this public site sometimes falls behind the software available. For access to all of our software (including Light and Matter and to Spectroscopy) as it is being developed, please write to us for a Pedagogica account, to either Dan Dill, dan@bu.edu, who is your presenter today, or to Peter Garik, garik@bu.edu, to request a password.