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Software for Hydrogenic Atoms and Orbitals Visualization

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ABSTRACT

A program was developed in java for hydrogenic atoms and orbitals visualization. The first 18 atoms in the periodic table were approximated with a hydrogenic wave-function. This simple hydrogenic wave-function allowed quick calculation for real-time interactive visualization. Electron cloud based models were employed and displayed by a ray-tracing technique. One or more orbitals that defined an atom could be selected and displayed. A user could zoom in, zoom out, and rotate the displayed cloud in real time. The approximation method for probability integrals was summation. The intensity of color at each point on the screen directly related to the integrated probability in finding the electron across the viewer's eye path.

Key words: Hydrogenic atom - 3D visualization - Real time ray-tracing

INTRODUCTION

Since 2000, a fundamental science curriculum has been developed by the Institute for the Promotion of Teaching Science and Technology (IPST). The purpose of this curriculum is the revolution of science education in Thailand from the lower education up to the higher one. Thai students will be taught various scientific concepts at an early age (grade 1-6) and be able to think and decide scientifically. One of the chosen topics is quantum states. Quantum states can easily be found in nature such as discrete numbers of various parts of living organisms that are easily visible. However for something small and naturally invisible, such as atoms and electrons, computer models are necessary. The generic 3-D models, such as "ball and stick" used by scientists are not suitable for young students and lead to misunderstanding. The electron cloud based model is more accurately acknowledged but few programs are available. All of them; Atom in a Box, Orbital, Orbital Viewer, Hydrogen Atom Orbital Viewer (1,2,3,4), show quantum states of hydrogenic atoms. They can display electron clouds based on ray-tracing methods in real-time with the ability for user interaction such as rotation and scaling. Atom in a Box and Orbital are available only on the Macintosh platform. Orbital Viewer (4) is PC-compatible while Hydrogen Atom Orbital Viewer is a java applet that can be run from web browsers. Other employed visualization methods are iso-surface and dot-scattering. Normally the iso-surface method, that shows the surface of equal electron density, is employed in textbooks and software for computational chemistry. The dot-scattering method is

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* In memoriy of Dr. Ketsiri Kueseng who tragically passed away on 26 th December 2004

rarely used now. Among these methods, the ray-tracing method provides the best and theoretical-correctly visualization with a limitation of slow rendering. In addition to a single orbital visualization, Atom in a Box and Hydrogen Atom Orbital Viewer can display combinations of orbitals that chemists know as hybridization. However none of these software packages can display the entire atom in real-time, using the ray-tracing method. Therefore, our customized software was developed with an objective to resolve these limitations and make the software suitable for Thai students.

An orbital is represented by various models. Dot-scattering was one of the most popular methods. However, it lead to an incorrect idea that electron density (5) is discrete. So does the iso-surface model. An orbital has no finite boundary; however, the shape of an orbital is generally estimated with the surface having 95% of probability of finding the electron inside its volume. The limitation of this method is that the inside of the atom is invisible. Examples of these models are on the Orbitron homepage (6). Models can never be perfect (7) and their inaccuracies can be good teaching tools.

Many researchers visualize electron density of atoms and molecules with an electron cloud model. For example, Takada and Handa (8) developed two algorithms called Multiple Cross Section Method and Equi-Density Surface Method on a super computer that required less computation power than the ray-tracing method. Four programs mentioned earlier employ the ray-tracing method but implement it in different ways. Orbital viewer did ray-tracing with a more complex calculation. As a result, its visualized graphics were the best, however, real-time rotation or scaling was impossible. Orbital calculated wave-functions in 17×17×17 grid-points in space and multiplied all 17 layers together to obtain the transparency effects. Then bicubic interpolation was used to produce the final image. For the Atom in a Box, the graphics were fastest and the computer code was heavily optimized. It displayed a wave function as a picture of a cloud, uses color as phase, plotted in red-cyan left/right for 3D glasses, and sliced the wave function. Hydrogen Atom Orbital Viewer was similar to Atom in a Box, but the graphics was slower because of java.

METHODS

Model for Atoms and Orbitals

Atoms consist of electrons and a nucleus. The nucleus is small compared to the size of the atom, thus it was neglected and not displayed. Different types of atom have a different number of electrons and protons resulting in a different atomic size. To speed up the rendering, we estimated the orbital with an H-like wave function. The relative size of the first 18 atoms and their orbitals can be roughly compared with this method.

Computational Details

The program developed for this project was written using java for cross-platform compatibility. An H-like wave function was employed which gave its square as the probability. Some (5) may prefer to use the term electron density as total number of electrons in the molecule multiplied by the probability density distribution.

The code displayed the wavefunctions by ray-tracing through the clouds and using a summation integration technique to sum the contributions.

There were 4 steps for graphics computation as shown in **Figure 1**. First, 40×40×40 grid-points were located with the origin at the nucleus. The size and orientation of the grid-points were controlled with parameters from mouse interaction and scaling factor. Secondly, the probability at each point was calculated and integrated across viewer direction. The result was 40×40 grid-points. The integration technique employed was summation and was faster than other methods such as the Simpson's rule integration technique employed in Atom in a Box. However, the accuracy was lower. To be visible on a computer screen, the probability had to be linearly converted to color intensity. The image at this point was at low resolution (40×40 pixels). Thirdly, bilinear image interpolation was performed by a routine method in java to enlarge the image to higher resolution. The computer screen was updated with this final image. Finally, the program waited for input that changed the orientation of the atom or orbitals and the same computational routine was performed. A similar algorithm as in Silicon Graphic's virtual trackball library (in c) was re-written in java for mouse interaction.

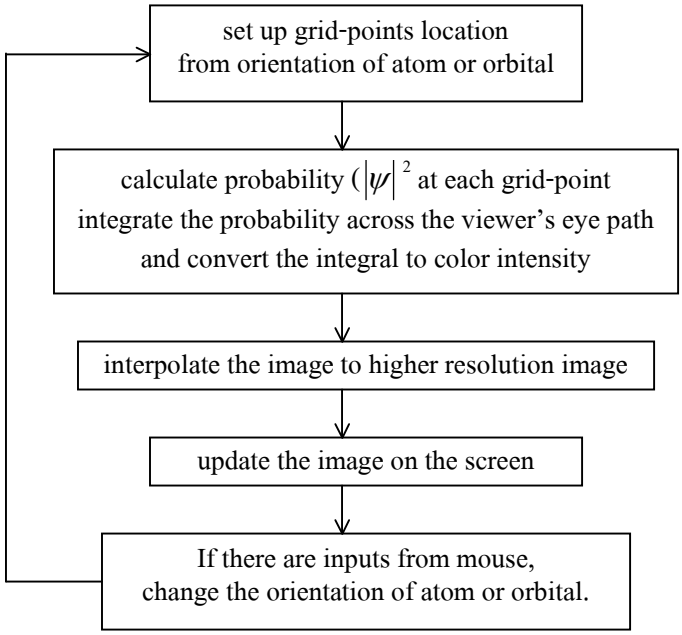

Figure 1. A flowchart showing computational details.

RESULTS

In the classroom, the concept of quantum states of electrons was learnt from our program as follows: When the program started, the program showed the first 18 elements in a table as shown in **Figure 2**. Each element had the atomic number on its upper left. The lower window shows the name of the software and its developers. On the left, the main output shows the electron cloud with control panels on the top and the bottom.

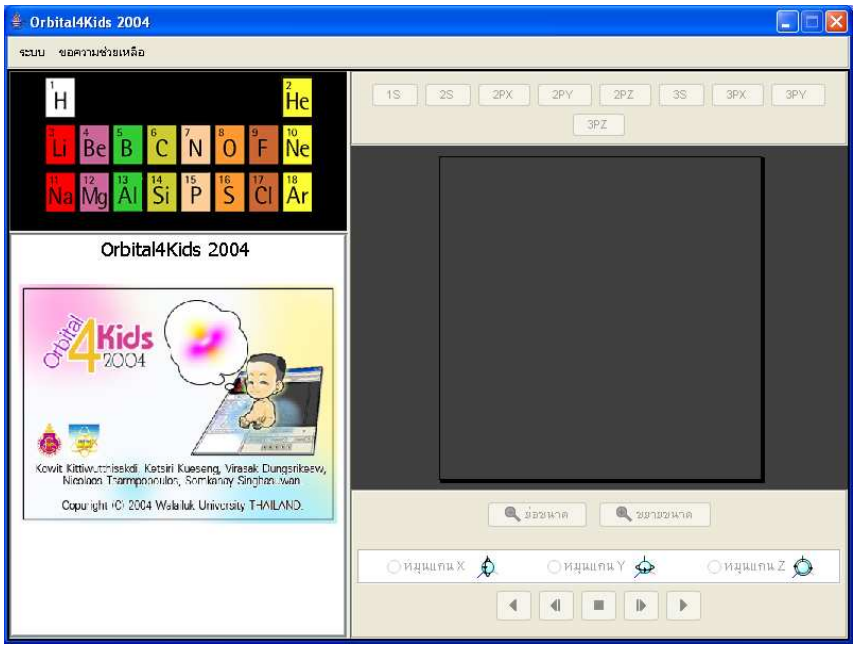

Figure 2. The screenshot of the application's user interface.

For more information about using this program, a help menu is available **(Figure 3)** and the manual in Thai is shown in **Figure 4**.

Figure 3. The screenshot of the help menu.

Figure 4. The screenshot of the help window.

There is also an atomic radius menus in the system menu **(Figure 5)**. It displays trends of atomic radius, boiling and freezing points in the periodic table **(Figure 6)**.

Figure 5. The screenshot of the atomic radius menu.

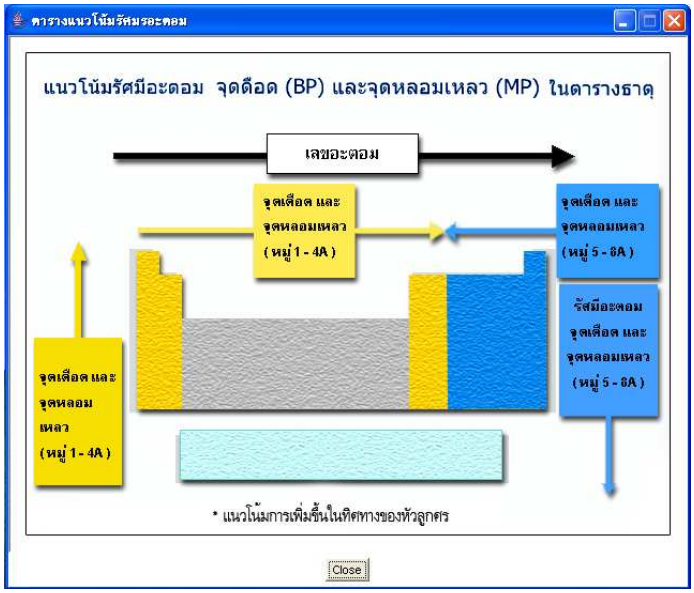

Figure 6. The screenshot of the atomic radius window.

When each element in the table is selected, its general information is shown in the lower left part of the window **(Figure 7)** and its orbitals are available for displaying by clicking at the menu on the upper right part of the window. Example pictures of orbitals are shown in **Figure 8**. The different color for positive and negative phases of the wave function is not implemented. By selecting two or more orbitals, an output of linear combination of selected orbitals can be displayed as shown in **Figure 9**. The outputs look like a donut and a sphere.

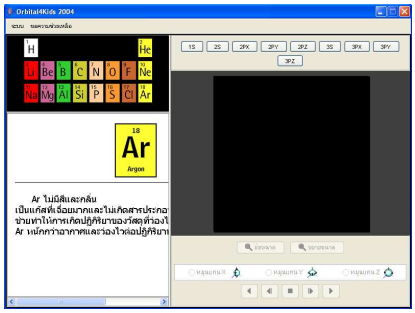

Figure 7. The screenshot of argon general information.

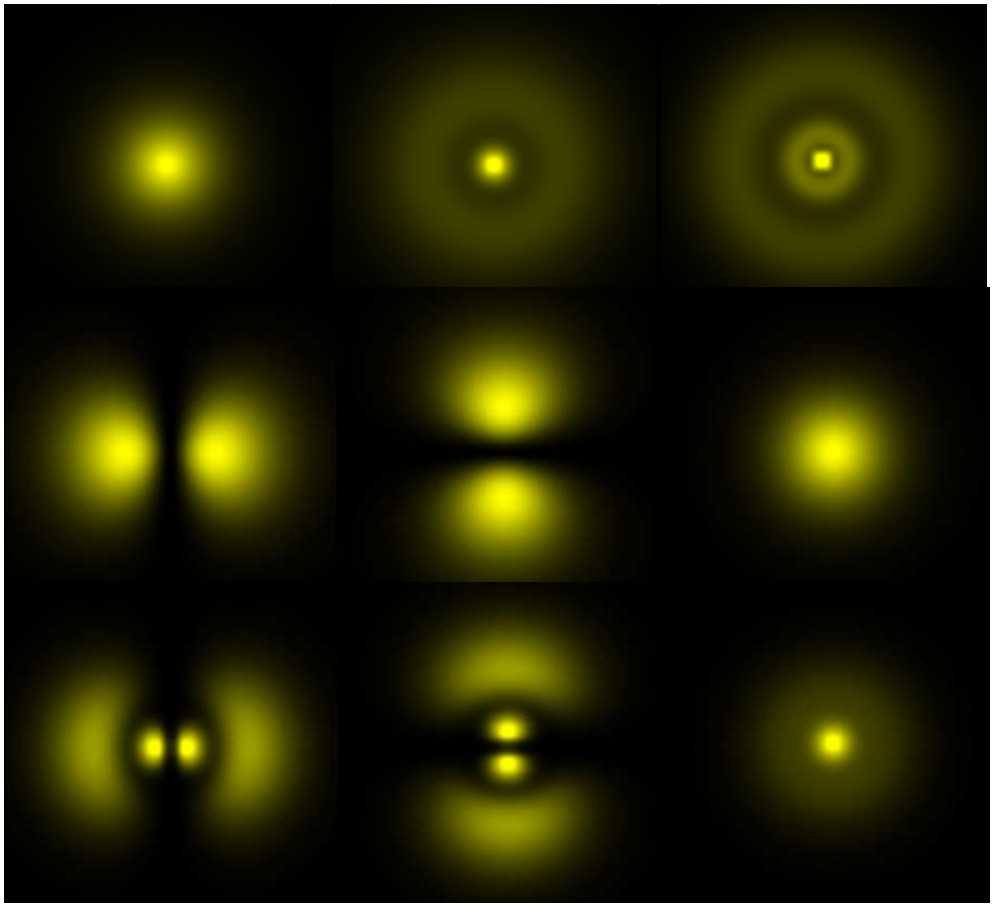

Figure 8. From left to right and top to bottom 1s, 2s, 3s, $2p_x$, $2p_y$, $2p_z$, $3p_x$, $3p_y$, $3p_z$.

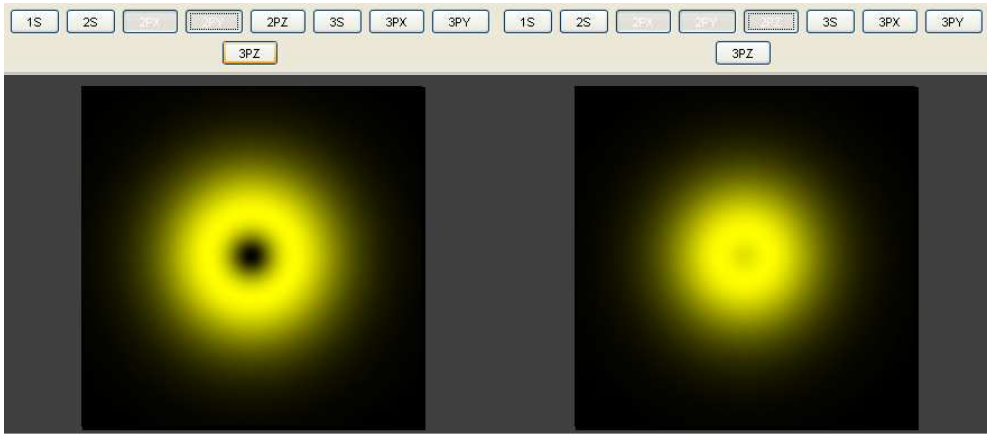

Figure 9. Linear combination of 2p orbitals (a) $2p_x+2p_y$ (b) $2p_x+2p_y+2p_z$.

CONCLUSIONS

In this paper we have presented an application of our program that shows quantum states of an electron in hydrogenic atoms. By employing a real time ray-tracing method, the most theoretically correct picture of an electron cloud can be modeled. This model can be employed in primary school teaching with the new curriculum. We are now working on a project to implement a more accurate wave-function for each atom with better graphics.

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บทคัดย่อ

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โปรแกรมแสดงอะตอมที่เหมือนไฮโดรเจนและออบิทัล

โปรแกรมได้ถูกพัฒนาขึ้นมาด้วยภาษาจาวาเพื่อแสดงอะตอมที่เหมือนไฮโดรเจนและออบิทัลของไฮโดรเจน ธาตุสิบแปดธาตุแรกในตารางธาตุถูกประมาณด้วยฟังก์ชั่นคลื่นแบบไฮโดรเจน ฟังก์ชั่นคลื่นแบบไฮโดรเจนที่ไม่ซับซ้อนนี้ทำให้การคำนวณเป็นไปได้อย่างรวดเร็วเหมาะกับการแสดงผลแบบปัจจุบันและตอบสนองได้ทันที แบบจำลองอิเล็คตรอนแบบเมฆหมอกถูกใช้และแสดงโดยเทคนิค Ray-tracing หนึ่งออบิทัลหรือมากกว่าซึ่งเป็นส่วนประกอบของอะตอมสามารถถูกเลือกและแสดง ผู้ใช้สามารถย่อ ขยาย และหมุนเมฆหมอกที่ถูกแสดงผลในเวลาจริง วิธีการประมาณที่ใช้หาอินติเกรตของความน่าจะเป็นคือการหาผลรวม ความเข้มของสีของจุดบนภาพมีความสัมพันธ์โดยตรงกับค่าอินติเกรตของความน่าจะเป็นในการพบอิเล็กตรอนในบริเวณที่มองผ่าน

สำนักวิชาวิทยาศาสตร์ มหาวิทยาลัยวลัยลักษณ์ อำเภอท่าศาลา จังหวัดนครศรีธรรมราช 80160