

GTA4: Enabler of Life Sciences Research?

By Salvatore Salamone

May 29, 2008 | Life sciences researchers should be thrilled. Earlier this month, the highly anticipated video game "Grand Theft Auto IV" (GTA4) was released and brought in more than \$500 million in global sales in its first week. That's about \$200 million more than the blockbuster "Indiana Jones and the Kingdom of the Crystal Skull" made internationally in its first week out.

So what does the popularity of a new video game have to do with helping life scientists?

The success of a game like GTA4 will spur on the chip manufacturers and systems vendors to push the envelope to deliver better graphics and faster and smoother animation in the future. And while this processing power is being used by video games to deliver cool animation and graphics, it also is increasingly being tapped to conduct life sciences R&D.

For years, while CPUs kept pace with Moore's Law to increase the computing power of servers and desktop computers, so too did the GPUs (graphics processing units), which are used to improve and accelerate rendering and animation. In fact, some argue that over the last few years GPU performance has outpaced that of CPUs.

Recent examples give a hint to the gains that can be made by tapping gaming processing power.

At last month's Bio-IT World Expo in Boston, [SimBioSys](#) demonstrated a version of its eHiTS (Electronic High Throughput Screening) Lightning ligand docking software running on the Sony PlayStation 3 game console. Specifically, SimBioSys ported the software to run on the PS3's guts, which is the microprocessor architecture called the Cell Broadband Engine (Cell/B.E.). The Cell/B.E. was jointly developed by Sony, Toshiba, and IBM. It enables the PS3 to speed up physics simulations so that they can catch up with the 3D graphics rendering speeds of the system's GPUs.

Essentially, by exploiting the parallel computer architecture of the Cell/B.E., SimBioSys dramatically speeds up the process of virtual screening and docking. In demonstrations, the eHiTS Lightning software application has been able to make throughput 30x faster than the application running on a traditional processor configuration.

Those who don't own a PS3 can take advantage of similar speed benefits using an IBM BladeCenter QS21 blade server based on the same Cell/B.E. processor.

In their presentation at the Expo during the "Best of Show" judging, SimBioSys noted that a job that would take a 400 CPU cluster can be done on four IBM Cell blades or 10 PS3s.

One point to note: This isn't the first venture into life sciences for the PS3. Starting in March 2007, users could download and run [Folding@home](#) software on their systems to help assist the Stanford University's distributed computing protein-folding project.

Tapping Another Type of Gaming Power

Efforts like Folding@home and others have demonstrated the benefits of getting people to volunteer their idle

computer cycles to help screen molecules and fold proteins. And many life sciences companies are tapping the same power of their desktop computers.

But even with the advances in high-performance computing and the additional computing power volunteers and office workers' computers deliver, there are still many life sciences problems that require much more processing power.

To tackle just one problem – the folding of very large proteins – researchers at the University of Washington (UW) decided on a new strategy: Put the gamers to work.

In 2005, researchers at the university developed [Rosetta@home](#), folding software that users downloaded to help find new proteins to fight diseases such as HIV, malaria, cancer, and Alzheimer's. The software works well for smaller proteins, but large proteins have too many variations in the way they can fold and thus require enormous amounts of computing power to simulate.

"There are too many possibilities for the computer to go through every possible one," said David Baker, Rosetta@home developer and a UW professor of biochemistry and Howard Hughes Medical Institute investigator. "An approach like Rosetta@home does well on small proteins, but as the protein gets bigger and bigger it gets harder and harder, and the computers often fail. People, using their intuition, might be able to home in on the right answer much more quickly."

With that idea in mind, researchers developed [Foldit](#), a game where after about 20 minutes of training, users play along and use mouse clicks to help fold proteins.

Foldit is the first protein-folding project that asks volunteers for something other than unused processor cycles on their computers or PlayStation machines. It also differs from other interactive games that use a human's ability to recognize images or interpret text. Instead, Foldit capitalizes on people's natural 3-D problem-solving skills.

The intuitive skills that make someone good at playing Foldit are not necessarily the ones that make a top biologist. Baker says his 13-year-old son is faster at folding proteins than he is.

With such efforts, perhaps the great interest in gaming and the success of popular games like GTA4 can be leveraged by the life sciences community to get more processing power for their simulations and more eyeballs to help refine 3D protein-folding puzzle solutions.

Do you use any distributed software applications that take advantage of your company's unused computing cycles? What obstacles do you see in using such an approach? Are you looking into using the GPU processing power of your desktop computers? Drop me a note at s.salamone@att.net and share your thoughts on the subject.

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