White Paper

Immersive Visualization in Pharmaceutical Development

Improving Drug Discovery with SGI® Reality Center™ Facilities

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1.0 Business Challenges in the Pharmaceutical Industry

Successfully developing a new drug and delivering it to market is a huge undertaking that requires an enormous investment in manpower, time, and capital. Recent studies suggest that on average the development and clinical trial process for a single drug takes from 8 to 10 years, with costs greater than $500 million (E&Y Biotech Industry Report 1998, Anderson). Drugs that fail to make it to market also further contribute to research and development costs in the pharmaceutical industry.

In recent years, the genomics revolution has both enhanced and complicated the drug development process, by providing a wealth of new information that creates potentially enormous opportunities for enhanced product development. At the same time, *in silico* techniques for modeling chemicals and proteins have become reliable and have been integrated as key components in the drug discovery process. While these technologies have clearly demonstrated value, they are extremely costly and have added data management, analysis, and decision-making complexities to pharmaceutical research. In today's post-genomic research environment, companies are struggling to obtain predictable value from vast amounts of data so they can leverage that information for improved product development and, ultimately, a competitive advantage.

To remain viable in the competitive pharmaceutical and biotechnology environment, an organization must focus on the effective and efficient use of resources. Scientists trained in fields such as bioinformatics, chemical and protein modeling, quantum chemistry, and crystallography are essential in bringing value to genomic and chemical data. Providing the infrastructure to allow scientists to collaborate and interact in real time is a critical element of success; they can then use their collective knowledge to make quick and definitive decisions based on the latest data.

To meet these challenges, many companies are utilizing immersive visualization with SGI Reality Center facilities. A Reality Center facility provides a high-resolution visual environment that helps researchers make sense of complex data, ranging from sequence information to detailed molecular structures. Using a Reality Center facility, researchers can share critical information visually, improving the quality and timeliness of decisions and fostering collaboration.

This paper discusses the use and benefits of SGI Reality Center facilities for bioinformatics, molecular modeling, and drug design, emphasizing the efficiency that results from the use of an immersive visual environment—improved efficiency that ultimately contributes to decreased time to market and increased competitiveness.

2.0 SGI Reality Center Facilities—Ideal Visual Environments for Drug Development

Over the past several years SGI Reality Center facilities have proved their value in a variety of industries, including automobile manufacturing and oil exploration. More recently a number of pharmaceutical companies have begun to discover the advantages of these facilities. A Reality Center facility combines the advanced computation and visualization capabilities of SGI® systems such as SGI® Onyx® 300 and SGI® Onyx® 3000 series visualization systems with immersive display technologies including large, floor-standing desk displays, cylindrical or spherically curved wall displays, or screened rooms in which outputs can be projected on multiple surfaces. These elements create an environment in which individuals or teams can gather to absorb themselves in the data so they can quickly comprehend the results of simulations such as models of proteins or small chemical compounds.

An SGI Reality Center facility powered by an SGI® Onyx® family supercomputer is ideal for use in drug research. The combined solution delivers both the compute and visualization capabilities required for accurate and real-time molecular simulations. The visualization environment provides a high degree of detail, allowing high-resolution molecular data to be visualized and manipulated in real time. As an additional benefit, Onyx family systems can be configured as computational supercomputers, allowing researchers to perform complex data analyses on the same system when visualization is not required. This combination of visual realism, large-scale images, and high-end computational power has proven to be a powerful catalyst to unleash creativity and insight.

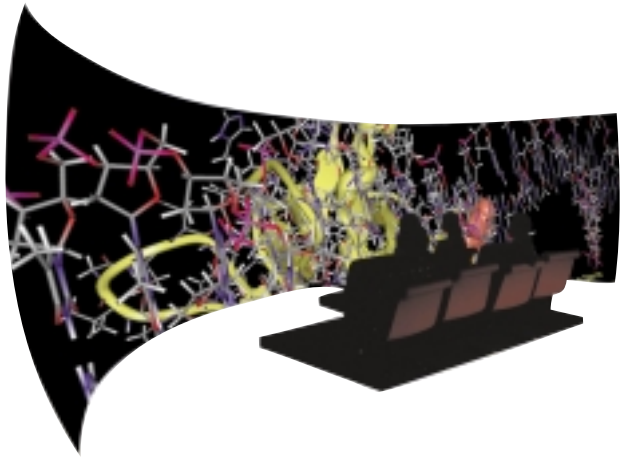

Fig. 1. A SGI Reality Center facility

3.0 Improving the Drug Discovery Process

A primary goal of drug discovery is to bring drugs to market faster while increasing the overall efficiency and economy of the process. The key to achieving this objective is improving the quality and timeliness of decision making, thereby ensuring that a company is focusing its resources on the best new drug candidates while eliminating programs with low potential for success.

A Reality Center facility offers an ideal environment for facilitating data-driven decision making. Groups of specialists from a department or from different disciplines can use a Reality Center facility to review all relevant data, fostering understanding and increasing cooperation between groups. High-resolution, real-time visualization of molecular models, simulations, and other important data help researchers quickly identify the best opportunities and decide on a course of action. In addition to creating an infrastructure that fosters collaborative efforts, another benefit of the Reality Center environment is that it discourages small groups of people from gathering together around a computer monitor and making decisions without input from the rest of their colleagues. The Reality Center environment reduces the building of these sub-team "fiefdoms," which can be very disruptive to the product development cycle. An estimate of the ROI associated with Reality Center deployment is provided on page 4.

Janssen Pharmaceutica uses an SGI Reality Center environment at its research facility in Belgium to act as a catalyst in the generation of new ideas in drug design, to empower project teamwork, and to stimulate discussions among different groups.

According to Hans De Winter, senior scientist at Janssen, Janssen Pharmaceutica researchers from pharmacology, biology, chemistry, and molecular modeling departments typically interact with the Reality Center environment in small, flexible teams of up to 10 people. "The most significant benefit of the Reality Center facility is the way researchers interact with the system," says De Winter. "Because SGI visualization technology enables the projection of large, realistic, and human-sized images of drugs located in protein pockets, researchers are able to become completely immersed within the target protein and, as such, obtain a realistic feeling about the important molecular functionalities and how to elaborate further on them."

Using the SGI Reality Center environment to facilitate ultra efficient screening, Janssen Pharmaceutica researchers who are looking for molecules with a desired therapeutic profile are now able to conduct extensive tests on up to 100,000 chemical compounds per day. Powerful computer algorithms simulate binding between drugs and target proteins. Thus Janssen takes full advantage of both the compute and visualization capabilities of its SGI Reality Center facility throughout the drug discovery process.

4.0 Facilitating Collaboration

The need to maintain competitiveness and ensure strong drug discovery pipelines has fueled a wave of mergers and acquisitions in the pharmaceutical industry, and that trend shows no sign of stopping. As a result, many companies now have multiple research centers, often located at great distances from one another. This development makes communication and cooperation between researchers more important than ever, but more difficult as well.

As discussed in the preceding section, a Reality Center facility is an important step towards fostering the cooperation that is so important to effective drug development. In a single campus environment, researchers can meet regularly to review the latest information using immersive visualization.

Bringing collaborators together from remote locations, however, still requires expensive and time-consuming travel. To overcome these difficulties, customers are beginning to add additional Reality Center facilities at multiple research sites, giving researchers at both sites the same visual tools for analyzing and reviewing data. AstraZeneca recently added a second Reality Center facility for this purpose.

"Following the purchases of an SGI Reality Center facility for our research and development site in Mölndal, Sweden and another in Wilmington, Delaware, our Södertälje lab asked SGI to propose a solution for an additional visualization facility, and we worked together on an assessment study," said AstraZeneca project leader Sven Hellberg. "The SGI Reality Center facility offers a high level of interactivity with very large visual data sets, such as large molecules, and will greatly enhance the speed of the decision-making process between our cross-collaborative scientific teams."

Immersive Visualization for Drug Discovery

Estimating the Benefits and Return on Investment (ROI)

As yet, no drug company has reported concrete calculations of ROI for Reality Center deployment. Given the long product development path and the natural tendency towards confidentiality, this is not surprising. However, some estimates can be made based on what is known about the typical costs of drug development. The conservative estimates provided in these analyses demonstrate the significant financial and process benefits that can be achieved by adding a Reality Center facility to a drug discovery institution's infrastructure. Clearly, the financial benefits will be different for each institution and this analysis is presented as an example to provide a framework to help with individual analysis:

Average total development time	10 years
Duration of drug discovery phase	2 years
Average annual costs during discovery	$100 million per year
Revenue for moderately successful drug	$500 million per year

A very conservative estimate would be that the advantages of using a Reality Center facility as detailed in this paper would reduce the total time spent on discovery by 2%. Assuming 250 working days per year, this works out to 5 days per year or 10 days saved during a typical two-year discovery period. Based on the projected revenue and average annual cost figures shown, the return on investment for including collaborative visualization in the development process is calculated as follows:

Daily cost of development	= $100 million/250 days per year	= $0.4 million per day
Daily revenue for a drug	= $500 million/250 days per year	= $2 million
Number of days saved	= 2% X 250 days per year X 2 years	= 10 days

Revenue from earlier time to market

Daily revenue	$2 million
X number of days	X 10 days
	$20 million

Reduced development expense

Daily cost of development	$0.4 million
X number of days	X 10 days
	$4 million

Total ROI

Earlier time to market (10 days)	$20 million in increased revenue
Reduced development expense	$4 million in reduced expenses
Total ROI for a single drug	$24 million

While this conservative estimate alone demonstrates a considerable return on investment, it completely ignores the financial benefits of getting a drug to market ahead of competitors and does not account for such things as fixed costs, amortization, etc. Still, the benefits that accrue from using a Reality Center facility for a single drug offer a substantial return over the initial cost of the facility.

Additional benefits result from improved decision making regarding projects that are not destined to result in viable drugs. Assuming that nonviable projects would be canceled an average of one month sooner results in substantial savings:

Monthly development costs	$100 million/12 months = $8.3 million

Savings from terminating a project one month ealy	$8.3 million
Number of projects terminated annually	X 10
Potential annual savings from earlier termination of nonviable projects	$83 million

Ultimately, companies with multiple SGI Reality Center facilities will link those facilities together, sharing the same visual information from a single database and a single supercomputer using Visual Area Networking (VAN). SGI's flagship VAN product, OpenGL Vizserver™, allows a single visualization server to render an image on both local and remote Reality Center (or other) displays over local or wide-area connections. Users at each site see exactly the same view and share control of the application. Changes made in one location are automatically seen everywhere. This technology will make it possible for researchers in multiple locations to collaborate while sharing the same high-resolution visual information without copying data, while eliminating expensive and time-consuming travel. Clearly, the ROI of this solution is significant, as it maintains and extends the virtues of collaboration while saving on travel costs and the downtime associated with travel.

5.0 Conclusion

In today's highly competitive pharmaceutical industry, effective drug discovery is critical to ongoing success. Companies that can best leverage critical data to make important decisions gain a strategic advantage by reducing development costs and decreasing time to market for valuable products. An SGI Reality Center facility is an important visualization tool that can be used throughout the drug development process to foster cooperation between researchers, resulting in better and timelier decisions, as well as a substantial return on investment.

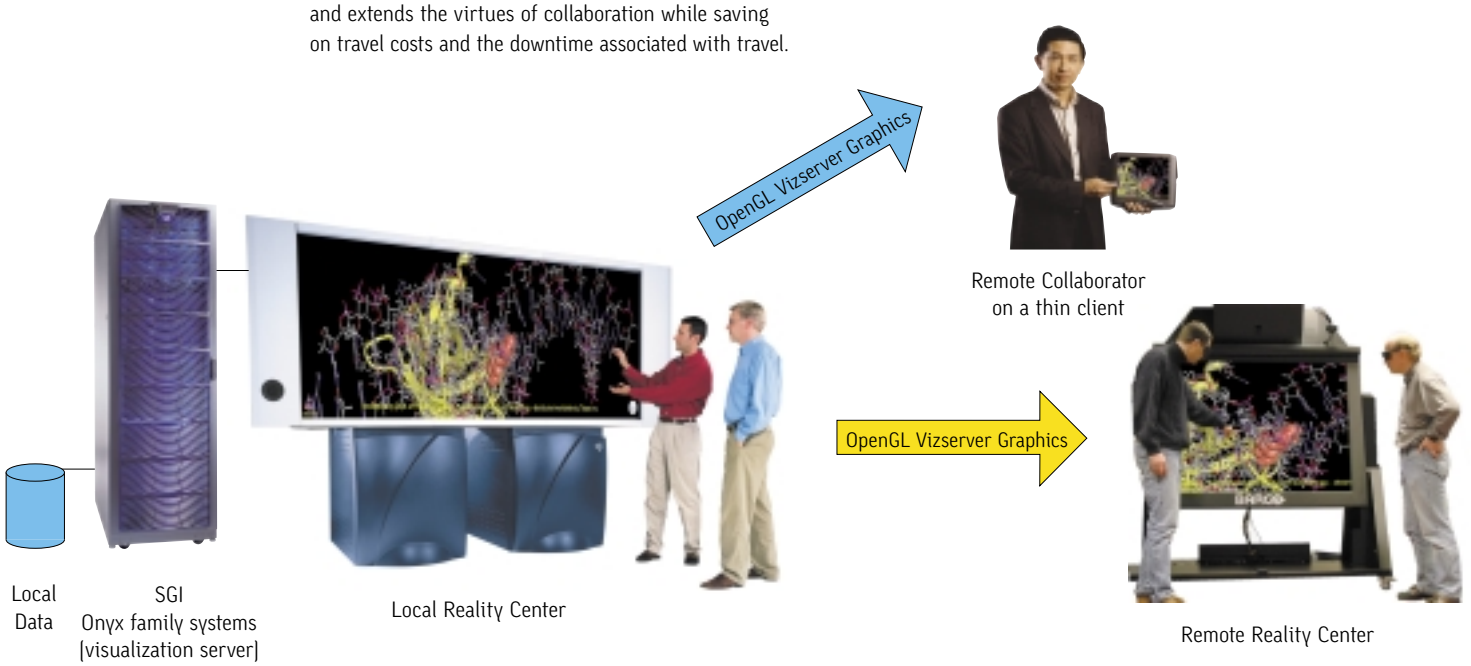

Fig. 2. SGI's flagship Visual Area Networking (VAN) product, OpenGL Vizserver™, allows a single visualization server to render an image on both local and remote Reality Center (or other) displays over local or wide-area connections. Users at each site see exactly the same view and share control of the application.

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