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Deeper understanding of client needs

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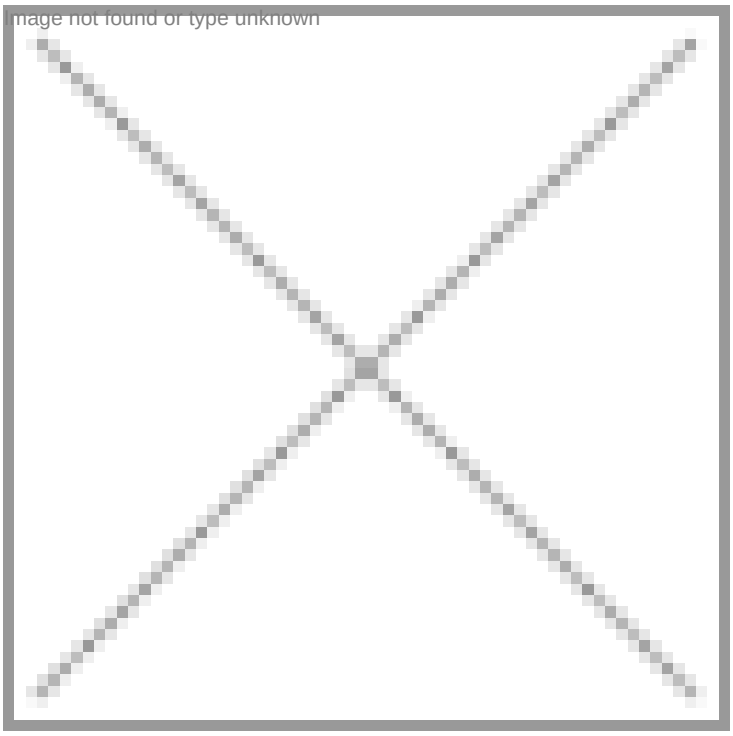

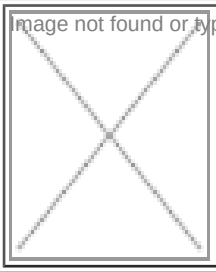

Mr Pankaj Sharma
CEO and co-founder, LeadInvent Technologies

The author is a biotechnologist and a computer scientist. He worked at IIT Delhi, where he developed simulation algorithms for biological systems. He is the CEO and co-founder of LeadInvent Technologies that was awarded the Asia Pacific Emerging Company of the Year 2011 Award by BioSpectrum.

Biotechnology in particular, and life sciences studies in general, provide an ideal field for ground breaking innovation and discoveries because much less is known about biology when compared with some of our other mature scientific pursuits. Biology seems to be far ahead than our current understanding of it. After all, life has more than three billion years' of head start over us. And it is in this attempt of understanding and interaction with biological systems lies our greatest promise. One such long-standing quest has been in the area of understanding diseases at the cellular level and trying to come up with solutions to fix them.

A disease is nothing but an end point observation of multiple small events that go wrong inside the body. The only way to deal with such a situation is to deconstruct a disease into a meaningful scientific quest. There are multiple approaches that could enable us to do this. One such approach is popularly known as computational biology that literally translates to computer simulations of biological systems.

At the core of this discipline is our ability to study protein molecules and their interaction with small molecules. Computational

biology receives a somewhat mixed reaction. One school of thought completely ridicules its usage with generalization that computers don't give drugs. The other, somewhat curious, attempted the logic between computer simulation and their correlation to experimental results. The accuracy of such simulation predictions versus experimental results has always been debated.

Both disciplines have made considerable progress over the last two decades. Our experimental techniques have advanced with newer methods: from PCRs for reading whole genome to micro arrays. Miniaturization and automation of assays have allowed experimentalists to evaluate millions of compounds with unmatched ease and accuracy.

The newer advances have also created challenges of their own. Our genomics' scientists are able to read terabytes of data within a short span of time, but are grappling with challenges of assembling such huge data and interpreting key insights. Techniques using ultra fast X-ray spectroscopy hold the promise to truly understand different conformations of protein molecule samples but remains in development. Our Förster resonance energy transfer (FRET)-based assays are allowing accurate understanding of interacting molecules but requires more standardizations than those, which are currently available in the market.

Computer hardware has consistently caught up with Moor's law leading to doubling computational capabilities of chips every 18 months. We are now at a point where the fastest supercomputer in the world can compute more than eight quadrillion calculations per second (petaflop/s). This is serious computing by any dimension and reminds me of how far the computate capabilities have reached from the early days of 2002 when our team was building the first dedicated supercomputer for computational biology at IIT Delhi. The challenge, however, is for computational biologists to capitalize this opportunity and make use of such compute power.

One of the key advantages that simulations provide is the ability to understand our biological system at the atomic level. The world seems to operate on two fundamental levels. One that is beautifully and intuitively explained through Newton's equations, popularly known as classical mechanics or molecular mechanics, and the other more fundamental, known as quantum mechanics.

The challenge for computational techniques is to walk the fine line between these two worlds and balance the approximations within the details of the study. The most
important step in understanding a problem is formulation of the right question. This should be followed by setting up simulation protocol within the framework of available compute resources and simulation technology capabilities.

The right start in this direction stems from collaboration between the experimental team and the computational team. At LeadInvent, our greatest learning curve has been working with experimentalists. In our observation, when simulation answers start guiding experimental effort, that's when the true realization of molecule simulations effort is felt.

Edge over others

LeadInvent has gone through a transition as a company. The company was started purely as a bioinformatics company with a business plan to package its simulation technologies as products and eventually sell them as standalone application in the drug discovery market. We quickly realized that the targeted industry's challenges were far deeper in demands of drug discovery than unavailability of appropriate bioinformatics tools. LeadInvent metamorphosed and we started working more closely with experimental teams on our client side. Framing the right simulation questions and providing simulation feedback were key to our engagement with clients. This gave LeadInvent the market edge over others.

Meanwhile, we collaborated extensively with top notch academic centers, such as the All India Institute of Medical Sciences, Delhi University, the Indian Institutes of Technology, Tata Institute of Fundamental Research and Harvard Medical School for broadening our overall knowledge and capabilities in experimental science for specific projects. We generated support from the Department of Biotechnology under the small business innovation research Initiative programs and invested in upgrading missing links in technology and ensuring that the technology was in tune with experimentalist requirements.

The benefit has been felt on both the sides. While our partners have had access to LeadInvent's team, technology and computational platform as one billable resource, LeadInvent got the opportunity to re-evaluate how best to apply its simulation technologies in drug discovery pursuit. The question again appears before us. Is it safe to say that the recent development in computational biology coupled with newer computing platform is ushering renewed interest in simulation results? And, are we close to making an opinion for the selected few who generalize that computer's don't give drugs?

I guess the greater knowledge is in our understanding that computational biology plays a pivotal role when coupled with experimental team in pursuit of right questions. There is definitely no single technology that could alone give rise to drugs. Why than generalize it for computational biology? After all, more than 55 drug candidates were recently reported in a review

to have benefited from computational biology approaches. It’s not the technology that is at the heart of drug discovery, it’s the team. After all it’s not the rocket that puts a man on the moon, it’s the people.

The challenges for any computational biology company are many. The underlying technology is definitely a place to start with, followed by constant revaluation in this era of computing growth and experiment.