

Enterprise Case Study: Using Cloud in the Chemistry Lab

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Summary

Catalyst

Bristol, UK-based Interactive Scientific (iSci) helps universities and pharmaceutical firms to accelerate their molecular research through molecular visualization. Beyond the research world, the firm is also looking to encourage more pupils to become passionate about chemistry by incorporating its software into chemistry teaching at secondary schools.

Interactive Scientific did initial development work on its own internal servers but as interest in the firm's application grew, it knew it would need to support its application with a more robust and scalable solution. The company moved to cloud infrastructure and chose to use Oracle Bare Metal Cloud Services. Furthermore, iSci was selected to participate in the Oracle Global Startup Ecosystem, the vendor's initiative to support and mentor emerging companies in exploiting the power of cloud services.

Ovum view

As software businesses scale, their infrastructure needs to grow accordingly, and new firms can falter quickly if their promising application fails to support customers' workloads. This has led to demand for infrastructure-as-a-service (IaaS) platforms such as Oracle's Bare Metal Cloud Services that can provide the flexibility that a growing firm such as iSci requires.

Interactive Scientific was founded in 2013 by Dr David Glowacki and Phill Tew, with Dr Becky Sage joining as CEO in 2014. The company is looking to transform molecular research and student chemistry classes through the use of interactive technology. Instead of reading textbooks and using the occasional video, Interactive's Nano Simbox is a software platform that enables researchers and students to visualize and manipulate molecules in real time, currently via an app and later this year also in virtual reality.

Interactive Scientific already has a track record of success. After graduating from the xEdu Education Accelerator in Finland, it had its education technology showcased in the Great British Classroom at the 2018 British/China Business Summit in Shanghai, and is one of the first five companies to be inaugurated into Oracle's global startup program.

Key messages

- .With the inclusion of new technologies such as virtual reality, the Nano Simbox service should enliven lessons and encourage more students to extend their studies.
- .Growing demand for iSci's educational tools meant the firm had to reconsider its technical infrastructure and decided to move its workloads to Oracle's Bare Metal Cloud Service.
- .Being chosen for Oracle's global startup program has given iSci access to Oracle's R&D teams, enabling it to bring products to market sooner.
- .Working with Oracle's sales and marketing teams brings iSci new opportunities within the vendor's large global customer base.

- .iSci's commercial opportunity is to offer "Simulation as a Service", helping clients to accelerate scientific research and avoid the need for each to run their own high-performance computing facility.

Recommendations

Recommendations for enterprises

Oracle's Bare Metal Cloud Services ensure that each client's workloads are running on their own dedicated machines. In so doing, clients have an on-demand resource that not only provides a secure environment for running sensitive applications but also provides much more predictability around network performance, which leads to predictable pricing for end users.

Prior to working with Oracle, iSci used on-premises servers, but knew that a cloud infrastructure would be required to support the growth of its business. Oracle Bare Metal Cloud Services deliver the bandwidth to support academia and pharmaceutical clients in running their molecular visualizations. The key benefits for iSci are the guaranteed uptime and low latency that mean that it can confidently price usage for its simulations.

This raw power enables iSci to demonstrate that it can deliver simulations on the cloud, but perhaps more importantly, by working with Oracle it can also provide secure containers for the workloads. The adoption of Oracle Bare Metal Services means that iSci can deliver both the scalability and flexibility a project requires.

Recommendations for vendors

Offering a startup program helps vendors to grow the ecosystem for their IaaS and PaaS services, plus the opportunity to work alongside small innovative companies. But for the program to work well for both parties, several factors need to be considered when setting up the initiative.

The program should be clear in its benefits for participants, with a simple application process that is not too time-consuming. A successful applicant needs to have a point of contact who can help them to identify the relevant individuals and teams they need to engage with and facilitate introductions. Vendors should also create an alumni program that enables new participants to share experiences.

Oracle has recently unified its different programs and transitioned into a single resource called Oracle Global Startup Ecosystem, designed to provide startups with personalized journeys through Oracle's vast ecosystem, mapping each selected startup to a tailored journey based on their unique business objectives and goals. Selected startups begin from a technical and architectural standpoint, receiving advice on how best to position them to meet their priorities and goals via cloud technologies. Their journeys also include additional resources and opportunities to help further boost their business, incorporating peer-to-peer interaction and mentoring, engagement opportunities with 430,000+ customers, and marketing and PR, as well as an alumni program.

A key differentiator for Oracle's program is that participants have the opportunity to connect with Oracle's R&D teams and, via the sales organization, make introductions to the company's extensive customer base. The startup is therefore no longer on its own but has access to a wealth of technical expertise to tap into as well as marketing support to help build opportunities.

iSci has benefited from all aspects of the program, especially the opportunity to work alongside Oracle's engineers to understand costings and pricing for its molecular simulation services. It has also been able to develop useful contacts in the pharmaceuticals, higher education, and more recently, the oil and gas sectors.

Using cloud infrastructure for predictable service delivery

Developing a cloud service to inspire the next generation of researchers

The Nano Simbox platform helps students, teachers and researchers to visualize atoms and molecules. For corporate researchers, the platform enables them to perform complex simulations in a secure environment, with the platform currently being trialed by several research groups around the world.

For students, the platform brings chemistry to life because behind the scenes the platform draws on data from science labs from across the globe and augments textbook-based learning. Similar to other SaaS products, pricing for using the Nano Simbox platform is on an annual subscription basis, based on the size of the institution. iSci estimates that it costs £1 per student per year.

The company's first educational product was an app, Molecules and Me, which was demonstrated on Promethean screens (the interactive displays often used for immersive learning in the classroom) during the aforementioned China visit. The app, which can be downloaded on any Android or iOS device, enables students to visualize, observe, and interact with molecules, and includes 24 walkthrough stories. To be released later this year, the Nano Simbox VR system will provide students with an immersive experience, with students wearing HTC VIVE headsets.

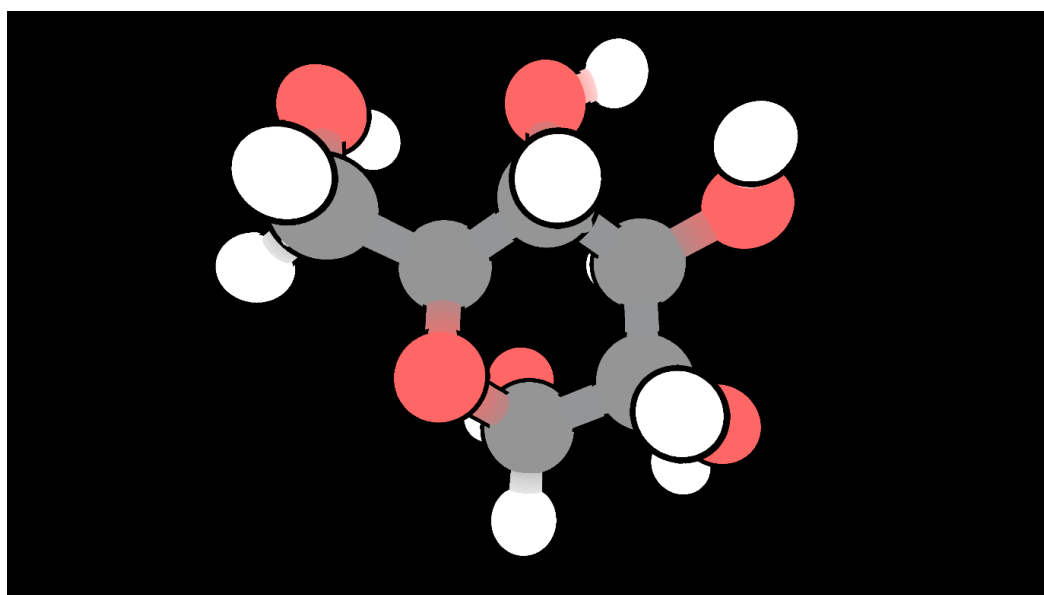
Interactive Scientific's solution brings molecules to life

With advancements in virtual reality, the students will be able to display and work with the molecules in three dimensions which will help them identify and understand patterns. Mimicking the design from computer games, users can move around independently and customize their virtual world.

iSci will need to work with education authorities and teaching bodies to incorporate Nano Simbox into lesson plans and make training available for teachers. Schools will need to ensure that they have sufficient network bandwidth for situations when multiple classes are using the platform.

There are similar considerations for adoption in the higher education and corporate sectors. To get buy in, latency will need to be minimized while uptime is maximized, and iSci has already published a paper in conjunction with the University of Bristol and Oracle on the efficacy of using Nano Simbox in research. In these research domains, iSci wants to offer clients what the company terms "Simulation as a Service". The virtual reality interface will be similar, but the onus will be on supporting research processes rather than fueling users' curiosity.

Figure 1: An example molecular simulation

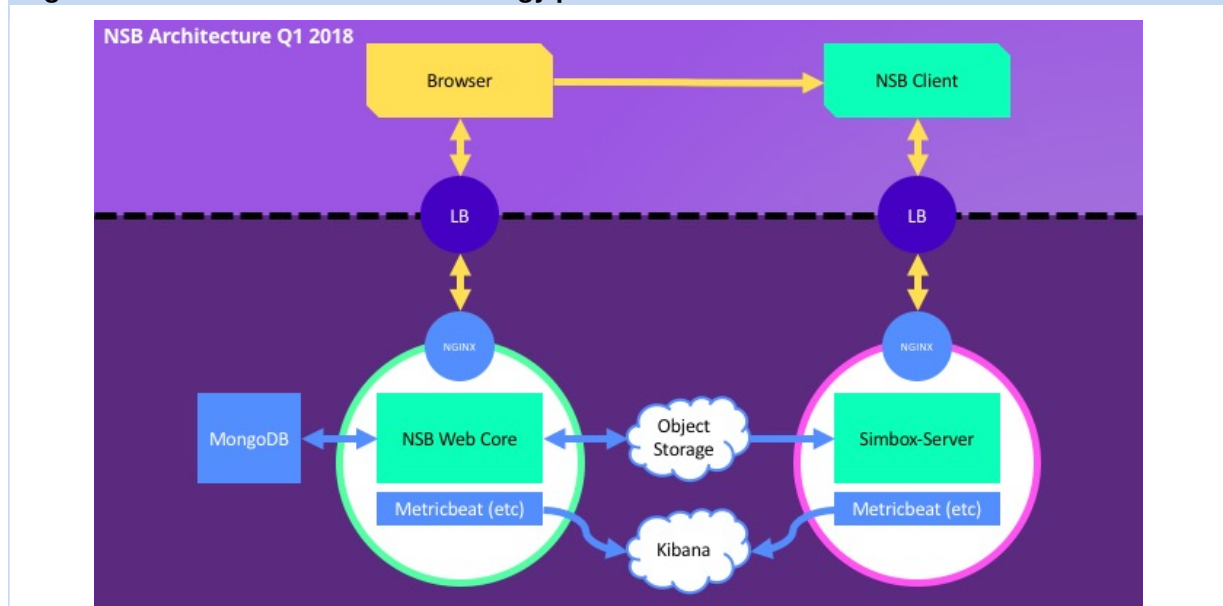


Source: Interactive Scientific

Designing a predictable, scalable architecture on the Oracle cloud

When designing the underlying infrastructure for iSci's simulations, Oracle's engineers worked alongside iSci to design scalable architectures. This was welcomed by iSci because the company had no previous cloud experience. Key priorities for iSci were to deliver consistent performance at a predictable cost, with enterprise-grade security. The high-level architecture for iSci's solution is shown in Figure 2.

Oracle's Bare Metal Cloud Services are designed and deployed with at least three fault-independent availability domains in each region, with a low-latency, high-bandwidth network interconnect enabling a range of high-availability application architectures. Resources are virtualized and provisioned at the network layer, enabling on-demand bare metal compute instances that offer extremely high peak and predictable performance to the tune of millions of IOPS per instance. Network virtualization also gives customers the maximum flexibility over the stack they use and allows for a zero-trust relationship between the customer and the provider as well as between the host and the network. Finally, every workload runs in a private overlay network that isolates workloads from each other and increases security.

Figure 2: Interactive Scientific technology platform

Source: Interactive Scientific

Everything on or below the dotted line in Figure 2 is hosted on Oracle's cloud infrastructure, including load balancers that Oracle provides on either bare-metal instances or virtual machines. With assistance from Oracle, iSci has designed the application as a set of microservices and has used containerization for each of the solution components. Some components, such as web APIs, can happily run on a virtual machine, but for the more demanding requirements of the simulation components, bare-metal instances are used.

Some cloud providers oversubscribe their virtual machines, so performance can vary from moment to moment. Because Oracle prevents this oversubscription, it means that iSci can guarantee the network performance and so simulations work well even over 4G connections, providing a good customer experience for iSci's pharma clients and those conducting scientific research. Furthermore, the Nano Simbox client works equally well on laptops or smartphones.

This predictable network performance means that iSci can offer clients predictable subscription pricing rates for simulations, so that customers can easily calculate their costs for each job. This would not be possible if network performance levels fluctuated significantly. The cloud accelerator program gave iSci the opportunity to thoroughly trial its applications on Oracle's infrastructure and identify bottlenecks before bringing the service to market.

Benefiting from Oracle's global startup program

The key benefits of the Oracle Global Startup Ecosystem for companies such as iSci include Oracle office space or co-working facilities (the UK program is based at the Engine Shed innovation and technology center in Bristol), interaction and advice from Oracle technical and product teams, and Oracle Cloud credits based on each startup's personalized journey. Unlike some incubator programs, Oracle does not take equity in the participating companies, but sees this as a mutually beneficial opportunity to foster innovation and engagement with its customer base of more than 400,000 customers.

According to iSci CEO Becky Sage, “Oracle opens up new opportunities for us. With compute power and accessibility via cloud, we are able to scale up this really complex science technology and help solve problems in education, research, and beyond.”

The global startup program begins with an application and selection process, with successful startups mapped to a personalized journey based on their unique priorities, needs, and objectives. There are then two parallel tracks for technical engagement and customer engagement. The latter includes mentoring and advice on refining the startup’s strategy and go-to-market approach. After the completion of a journey, there is also an alumni track that continues the connection into the Oracle customer ecosystem, with support for PR and marketing, access to business mentors, and further help with exploiting cloud technology.

iSci says the program has not only helped it to develop its technology proposition and architecture but has also raised the company’s profile internationally with website traffic from overseas growing exponentially, with interest from academia and large enterprises in the company’s solutions.

Lessons learned

Cloud services can compete head on with High Performance Computing

iSci’s use of cloud technology shows that it is a viable alternative to on-premise high-performance computing (HPC) facilities for many compute-intensive applications, and that organizations, such as higher education institutions, pharmaceutical firms, and oil and gas companies, undertaking this type of research might no longer need to invest in their own HPC facilities. Cloud services such as Oracle Bare Metal Cloud Services are now sufficiently performant to accommodate the demanding workload requirements of research projects. These services can now underpin services from small companies such as iSci and allows them to concentrate on developing compelling solutions built on a solid technology foundation.

Partnering with a global vendor such as Oracle offers rapid acceleration from business and technology perspectives

Incubator programs such as Oracle’s global startup program are a great boon to early-stage and scaleup technology companies, providing the resources, advice, and market introductions that would otherwise take a protracted effort to develop. Many vendors will offer some free or discounted access to cloud resources for startups, but competition to join premier programs is stiff, and admission to the process can itself bring a raft of good publicity. Startups should ensure however that they keep their options open from both business and technology perspectives. iSci has designed its architecture to be technology-agnostic, so that it can deploy workloads on other cloud environments should the need arise.

Interactive molecular simulation will enlighten both research and education

Other companies are looking to tap into the potential for VR in the classroom with MEL Science, the creator of online chemistry sets, launching a VR subscription service aligned with schools' curriculums. iSci hopes to fend off competition by building a reputation as the core resource both in secondary and higher education, and it is looking to roll out its education solution internationally later this year, having formed partnerships with universities as well as pharmaceutical firms.

The opportunities for iSci in higher education are twofold. The first opportunity is similar to secondary schools in that Nano Simbox helps students' understanding of molecules, and the inclusion of virtual reality provides a powerful tool to help them manipulate the 3D images. The second is to aid research-intensive universities by offering a platform for them to run scientific trials.

In the commercial field, where pharmaceuticals and oil and gas are two of the opportunities, the performance, low-latency, and enterprise-grade security provided by Oracle's Bare Metal Cloud Services means that iSci can compete head on with far bigger firms to run molecular simulations. The next step is to build a roster of clients and case studies to showcase the potential.

Appendix

Methodology

Ovum Enterprise Case Studies use in-depth interviews with key enterprise stakeholders as well as a review of any available documentation such as strategic planning, RFP, implementation, and program evaluation documents.

Further reading

"Bare metal becomes a key part of the Oracle IaaS cloud story," IT0014-003222 (January 2017)

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