Cloud computing

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Introduction

According to Gartner's Hype Cycle Special Report for 2009, "technologies at the 'Peak of Inflated Expectations' during 2009 include cloud computing, e-books… and Internet TV, while social software and microblogging sites…have tipped over the peak and will soon experience disillusionment among enterprise users". Is cloud computing also heading for the trough of disillusionment?

The Internet is often represented as a cloud and the term "cloud computing" arises from that analogy. Accenture defines cloud computing as the dynamic provisioning of IT capabilities (hardware, software, or services) from third parties over a network. McKinsey says that clouds are hardware-based services offering compute, network and storage capacity where: hardware management is highly abstracted from the buyer; buyers incur infrastructure costs as variable OPEX [operating expenditures]; and infrastructure capacity is highly elastic (up or down).[1] The cloud model differs from traditional outsourcing in that customers do not hand over their own IT resources to be managed. Instead they plug into the cloud, treating it as they would an internal data center or computer providing the same functions.

Large companies can afford to build and expand their own data centers but small- to medium-sized enterprises often choose to house their IT infrastructure in someone else's facility. A colocation center is a type of data center where multiple customers locate network, server and storage assets, and interconnect to a variety of telecommunications and other network service providers with a minimum of cost and complexity. A selection of companies in the collocation and cloud arena is presented in Table 1.

Amazon has a head start but well known companies such as Microsoft, Google, and Apple have joined the fray.[2]

Although not all the companies selected for Table 1 would agree on the definitions given in this article, it is generally supposed that there are three basic types of cloud computing: Infrastructure as a Service (IaaS), Platform as a Service (PaaS) and Software as a Service (SaaS). In IaaS, cpu, grids or clusters, virtualized servers, memory, networks, storage and systems software are delivered as a service. Perhaps the best known example is Amazon's Elastic Compute Cloud (EC2) and Simple Storage Service (S3), but traditional IT vendors such as IBM, and telecoms providers such as AT&T and Verizon are also offering solutions. Services are typically charged by usage and can be scaled dynamically, i.e. capacity can be increased or decreased more or less on demand.

PaaS provides virtualized servers on which users can run applications, or develop new ones, without having to worry about maintaining the operating systems, server hardware, load balancing or computing capacity. Well known examples include Microsoft's Azure and Salesforce's Force.com. Microsoft Azure provides database and platform services starting at $0.12 per hour for compute infrastructure; $0.15 per gigabyte for storage; and $0.10 per 10,000 transactions. For SQL Azure, a cloud database, Microsoft is charging $9.99 for a Web Edition, which comprises up to a 1 gigabyte relational database; and $99.99 for a Business Edition, which holds up to a 10 gigabyte relational database. For .NET Services, a set of Web-based developer tools for building cloud-based applications, Microsoft is charging $0.15 per 100,000 message operations.

SaaS is software that is developed and hosted by the SaaS vendor and which the end user accesses over the Internet. Unlike traditional applications that users install on their computers or servers, SaaS software is owned by the vendor and runs on computers in the vendor's data center (or a colocation facility). Broadly speaking, all customers of a SaaS vendor use the same software: these are one-size-fits-all solutions. Well known examples are Salesforce.com, Google's Gmail and Apps, instant messaging from AOL, Yahoo and Google, and Voice-over Internet Protocol (VoIP) from Vonage and Skype.

Pros and Cons of Cloud Computing

The great advantage of cloud computing is "elasticity": the ability to add capacity or applications almost at a moment's notice. Companies buy exactly the amount of storage, computing power, security and other IT functions that they need from specialists in data-center computing. They get sophisticated data center services on demand, in only the amount they need and can pay for, at service levels set with the vendor, with capabilities that can be added or subtracted at will.

The metered cost, pay-as-you-go approach appeals to small- and medium-sized enterprises; little or no capital investment and maintenance cost is needed. IT is remotely managed and maintained, typically for a monthly fee, and the company can let go of "plumbing concerns". Since the vendor has many customers, it can lower the per-unit cost to each customer. Larger companies may find it easier to manage collaborations in the cloud, rather than having to make holes in their firewalls for contract research organizations. SaaS deployments usually take less time than in-house ones, upgrades are

easier, and users are always using the most recent version of the application. There may be fewer bugs because having only one version of the software reduces complexity.

This may all sound very appealing but there are downsides. In the cloud you may not have the kind of control over your data or the performance of your applications that you need, or the ability to audit or change the processes and policies under which users must work. Different parts of an application might be in many places in the cloud. Complying with federal regulations such a Sarbanes Oxley, or FDA audit, is extremely difficult. Monitoring and maintenance tools are immature. It is hard to get metrics out of the cloud and general management of the work is not simple.[3] There *are* systems management tools for the cloud environment but they may not integrate with existing system management tools, so you are likely to need two systems. Nevertheless, cloud computing may provide enough benefits to compensate for the inconvenience of two tools.

Cloud customers may risk losing data by having them locked into proprietary formats and may lose control of data because tools to see who is using them or who can view them are inadequate. Data loss is a real risk. In October 2009 1 million US users of the T-Mobile Sidekick mobile phone and emailing device lost data as a result of server failure at Danger, a company recently acquired by Microsoft.[4] Bear in mind, though, that it is easy to underestimate risks associated with the current environment while overestimating the risk of a new one. Cloud computing is not risky for *every* system. Potential users need to evaluate security measures such as firewalls, and encryption techniques and make sure that they will have access to data and the software or source code if the service provider goes out of business.

It may not be easy to tailor service-level agreements (SLAs) to the specific needs of a business. Compensation for downtime may be inadequate and SLAs are unlikely to cover concomitant damages, but not all applications have stringent uptime requirements. It is sensible to balance the cost of guaranteeing internal uptime against the advantages of opting for the cloud. It could be that your own IT organization is not as sophisticated as it might seem.

Calculating cost savings is also not straightforward. Having little or no capital investment may actually have tax disadvantages. SaaS deployments are cheaper initially than in-house installations and future costs are predictable; after 3-5 years of monthly fees, however, SaaS may prove more expensive overall. Large instances of EC2 are fairly expensive, but it is important to do the mathematics correctly and make a fair estimate of the cost of an “on-premises” (i.e., in-house) operation.

Standards are immature and things change very rapidly in the cloud. All IaaS and SaaS providers use different technologies and different standards. The storage infrastructure behind Amazon is different from that of the typical data center (e.g., big Unix file systems). The Azure storage engine does not use a standard relational database; Google’s App Engine does not support an SQL database. So you cannot just move applications to the cloud and expect them to run. At least as much work is involved in moving an application to the cloud as is involved in moving it from an existing server to a new one. There is also the issue of employee skills: staff may need retraining and they may resent a change to the cloud and fear job losses.

Last but not least, there are latency and performance issues. The Internet connection may add to latency or limit bandwidth. (Latency, in general, is the period of time that one component in a system is wasting time waiting for another component. In networking, it is the amount of time it takes a packet to travel from source to destination.) In future, programming models exploiting multithreading may hide latency.[5] Nevertheless, the service provider, not the scientist, controls the hardware, so unanticipated sharing and reallocation of machines may affect run times. Interoperability is limited. In general, SaaS solutions work best for non-strategic, non-mission-critical processes that are simple and standard and not highly integrated with other business systems. Customized applications may demand an in-house solution, but SaaS makes sense for applications that have become commoditized, such as reservation systems in the travel industry.

Virtualization and Private Clouds

Virtualization of computers or operating systems hides the physical characteristics of a computing platform from users; instead it shows another abstract computing platform. A hypervisor is a piece of virtualization software that allows multiple operating systems to run on a host computer concurrently. Virtualization providers include VMware, Microsoft, and Citrix Systems (see Table 1). Virtualization is an enabler of cloud computing.

Recently some vendors have described solutions that emulate cloud computing on private networks, referring to these as “private” or “internal” clouds (where “public” or “external” cloud describes cloud computing in the traditional mainstream sense). Private cloud products claim to deliver some of the benefits of cloud computing without the pitfalls. Hybrid solutions are also possible: building internal clouds and connecting customer data centers to those of external cloud providers. It has been reported that Eli Lilly wants to benefit from both internal and external clouds[3] and that Amylin[6] is looking at private cloud VMware as a complement to EC2. Other experts, however, are skeptical: one has even gone as far as to describe private clouds as absolute rubbish.[7]

Platform Computing has recently launched a cloud management system, Platform ISF, enabling customers to manage workload across both virtual and physical environments and support multiple hypervisors and operating systems from a single interface. VMware, the market leader in virtualization technology, is moving into cloud technologies in a big way, with vSphere 4. The company is building a huge partner network of service providers and is also releasing a “vCloud API”. VMware wants customers to build a series of “virtual data centers”, each tailored to meet different requirements, and then have the ability to move workloads in the virtual data centers to the infrastructure provided by cloud vendors.

Cisco, EMC and VMware have formed a new venture called Acadia. Its strategy for private cloud computing is based on Cisco’s servers and networking, VMware’s server virtualization and EMC’s storage. (Note, by the way, that EMC owns nearly 85% of VMware.) Other vendors, such as Google, disagree with VMware’s emphasis on private clouds; in return VMware says Google’s online applications are not ready for the enterprise.

Applicability

Not everyone agrees, but McKinsey has concluded[1] as follows. “Clouds already make sense for many small and medium-size businesses, but technical, operational and financial hurdles will need to be overcome before clouds will be used extensively by large public and private enterprises. Rather than create unrealizable expectations for “internal clouds”, CIOs should focus now on the immediate benefits of virtualizing server storage, network operations, and other critical building blocks”. They recommend that users should develop an overall strategy based on solid business cases not “cloud for the sake of cloud”; use modular design in all new software to minimize costs when it comes time to migrate to the cloud; and set up a Cloud CIO Council to advise industry.

Applications in the Pharmaceutical Industry

In the pharmaceutical sector, where large amounts of sensitive data are currently kept behind protective firewalls, security is a real concern, as is policing individual researchers’ access to the cloud. Nevertheless, cheminformatics vendors are starting to look at cloud options, especially in terms of Software as a Service (SaaS) and hosted informatics. In bioinformatics and number-crunching, the cloud has distinct advantages. EC2 billing is typically hours times number of cpus, so, as an over-generalization, the cost for 1 cpu for 1000 hours is the same as the cost of 1000 cpus for 1 hour. This makes cloud computing appealing for speedy answers to complex calculations. Over the past two years, new DNA sequencing technology has emerged allowing a much more comprehensive view of biological systems at the genetic level. This so-called next-generation sequencing has increased by orders of magnitude the already daunting deluge of laboratory data, resulting in an immense IT challenge. Could the cloud provide a solution?

An unnamed pharmaceutical company found that processing BLAST databases and query jobs was time consuming on its internal grid and approached Cycle Computing[8] about running BLAST and other applications in the cloud. After the customer had approved Cycle’s security model, Cycle built a processing pipeline for BLAST that provides more than 7000 public databases from the National Center for Biotechnology Information (NCBI), Ensembl, and the Information Sciences Institute of the University of Southern California (ISI) that are updated weekly. The CycleCloud BLAST service is now publicly available to all users.

Pfizer, Eli Lilly, Johnson & Johnson, and Genentech are already experimenting with cloud computing.[9] Lilly has demonstrated the viability of cloud computing by launching a 64-machine cluster computer working on bioinformatics sequence information, completing the work, and shutting down in 20 minutes, using Amazon’s EC2, at a cost of only $6.40, and a saving of 12 weeks’ processing. Pfizer’s Biotherapeutics & Bioinnovation Center has used Amazon cloud services to develop and refine models in antibody-antigen docking runs, shortening the process to two to three hours from two to three days.[9]

Porting applications to the cloud, however, is not straightforward. Cloud service providers such as Amazon provide Infrastructure as a Service (IaaS) but users need help in scheduling and using the infrastructure. A cloud provider manages the security of its physical computer infrastructure, but users are responsible for data encryption, data access control, and other security measures. Some of the

companies listed in Table 1 supply such business application and security management services for cloud computing. Pfizer is working with the BioTeam, a consulting firm, while Lilly is using software and services from Cycle Computing and RightScale to access Amazon's network and manage the transfer of data onto and off of the cloud.[9] Johnson and Johnson (J&J) is also a Cycle Computing customer.[8] Lilly has tried cloud applications in genomics, including BLAST; pharmacokinetics using NONMEM; statistics through R; and simulations of clinical trial data.[8] J&J has also experimented with NONMEM applications, using Amazon Web Services (AWS) scripts.[3]

Molecular Modeling

Schrödinger is another company working with Cycle Computing. The two partners are offering cloud solutions to run Schrödinger's chemical simulation and molecular modeling software on elastic resources in the US and Europe. Schrödinger argues as follows. Computation is central to drug discovery but too often it is rate-limiting. Local computational resources, though they may be adequate on a time-averaged basis, are often insufficient to perform the massive burst-mode computations needed to bring a project forward in a timely fashion. Schrödinger believes that the combination of its own software and CycleCloud offers a way to perform large computational experiments quickly, robustly and securely, even when local resources are inadequate. Schrödinger plans eventually to make all its applications available on the cloud, staging them in an order dictated by customer demand. The company is working with interested customers on a case-by-case basis at this point, rather than pushing out a "cloud product". Schrödinger already has commercial customers running Glide on the cloud, and has in-house experience with additional applications.

A spokesman for Schrödinger's competitor Accelrys, says that Accelrys is pulling together its strategy with regard to cloud computing, hosted informatics and SaaS. Some customers are experimenting with the cloud to see whether it meets security standards, and whether the pricing model has benefits. There *are* security guidelines. "It's all about trust; it's all about value", says the spokesman. Amazon, Google and Microsoft will gain trust. It *is* possible to build a mission-critical application that is cloud-based. Admittedly, customization is a challenge; there is a balance between customization and configuration. Accelrys must provide a solution that meets market demand. This issue is not unique to pharma. Accelrys wants to make sure that its solutions meet customers' demands and expectations.

Symyx Technologies

Symyx sees cloud computing and hosted solutions as very different. A spokesman says that the cloud is awesome, for instance, for calculation or data look-up services where users want to overcome bottlenecks that may be placed by high demand on single servers. Symyx customers are already doing big QSAR calculations and homology modeling using EC2, but they have barriers that prevent them from making full use of the cloud right now. They cannot accept the concept of grabbing at any available service in the cloud, provided by a number of resources or servers from almost an undetermined source. Pharmaceutical industry users often require audit trails and, in the cloud, following the audit trail can be difficult. In "true SaaS" this can still be an issue if the system being used is multi-tenant and has no audit trails for specific tenants. A hosted system can obviously be deployed and fine tuned to meet specific

audit and security needs. Security is essential for registration and electronic laboratory notebook (ELN) applications in the pharmaceutical industry.

Symyx has extensive experience with hosting DiscoveryGate, its integrated platform for delivering content from the primary and secondary literature, and tertiary reference information. The architecture and data for Symyx' DiscoveryGate Web service are hosted in a bullet-proof, secure environment with 24*7*365 service. The system runs on dedicated hardware hosting multiple VMware servers delivering the Web service. The hardware can scale up to 300 VMware servers if needed, allowing Symyx to cope with high demand. Added technology allows Symyx to load share requests between VMware servers ensuring that all customers get a good service. The same environment will now be used to deliver Symyx' hosted ELN solution. Based on their business needs and security concerns, customers can choose to have a "no frills", multi-tenancy ELN, or choose a custom hosting solution for their ELN where they have designated VMware servers, or just designated Oracle instances, as requested in some cases.

The hosted informatics infrastructure provided by Symyx is supported by Switch Communications Group, an information storage and protection specialist. Switch provides highly secure, mission-critical, interconnectivity, and disaster-avoidance colocation services, within guaranteed reliable, lowest risk (so-called Tier 4+) facilities. The secure Switch facility where Symyx hosts the ELN service is compliant with SAS 70, Type II auditing standards and specifications supporting disaster recovery and business continuity plans. Third-party, offsite data backup, archiving and recovery services are also provided.

Hosted informatics provides cost benefits over the traditional software model because its shared resources environment offers significant economies of scale, but moving to a hosted informatics model is not just to cut costs: the primary goal is to improve operational agility.[10] For example, partnering is a key issue when it comes to hosting. A hole in an in-house firewall is costly to manage but a hosted system streamlines outsourcing by enabling R&D organizations to turn on and turn off third-party collaborators quickly and efficiently. Vendor, customers and collaborators can then concentrate on their core competencies.

CambridgeSoft

Symyx' competitor, CambridgeSoft has recently announced ChemBioOffice Cloud, an integrated informatics suite available over the Internet, also allowing customers to focus on the science while CambridgeSoft takes care of the science IT. CambridgeSoft believes that staffing and running an IT department is not core to the research activities for a growing number of today's life science companies. To meet its customers' needs, CambridgeSoft offers professional, standard, basic and customized hosting services. All hosting models cover database maintenance, application maintenance, hardware and software maintenance, monitoring, support and help desk for CambridgeSoft E-Notebook, Inventory, Registration, BioAssay and BioSAR. A special team is dedicated solely to customer hosted solutions. The team involves hardware and operating system specialists, Oracle DBA's, and application and support specialists and project managers strategically positioned worldwide to provide 24*7 support. Like Symyx, CambridgeSoft offers high standards of security and reliability in its colocation

facilities. Rather than repeat the complexities of industry standards and jargon, we refer the reader to a detailed white paper on the company's Web site.[11]

ChemAxon and Partners

In response to increasing demand for software as a service and hosted cheminformatics solutions, DeltaSoft and ChemAxon have teamed up to provide a suite of fully hosted applications, including compound registration, inventory, bioassay, and structure activity searching and reporting.[12] DeltaSoft already had a suite of Web applications based on chemical cartridge technology and ChemAxon has a cartridge and a suite of tools. Several joint customers had internal and virtualized servers with the ChemCart suite and the ChemAxon cartridge, so further collaboration made sense.

DeltaSoft currently offers the ChemCart suite hosted internally, externally, or in the cloud. For the cloud, the company uses Amazon EC2. Oracle explicitly supports Amazon Web Services. EC2 provides ready-made "machine images" (AMIs), which include both operating systems (Linux or Windows) and Oracle images. This makes the installation very quick and easy; DeltaSoft simply installs its components on top of these machine images. ChemCart is already a Web based product, so DeltaSoft was able to take advantage quickly of this new platform without any code changes.

The ChemCart modules currently offered using Amazon on the backend are Compound Registration, Electronic Laboratory Notebook, Reagent Inventory, Sample Inventory, BioAssay, and Structure Activity Browser; further cloud offerings are planned in the future. In addition to these SaaS offerings, DeltaSoft also offers the basic ChemCart product as a Platform as a Service (PaaS) offering, allowing users to develop custom Web applications quickly and easily in the cloud. DeltaSoft has licensing agreements with both ChemAxon and Oracle to provide the underlying chemistry cartridge and other components in its chemistry solutions, so it can offer a complete package to customers. Other chemistry cartridges are also supported, but they would be licensed separately.

Contur Software is another partner of ChemAxon's. Contur has added chemistry functionality[12] in iLabber, the company's recently launched ELN system available as an online service. Using a software as a service (SaaS) model, Contur Software is making iLabber available to individual researchers and smaller R&D organisations that previously have not been able to use high-end ELN systems due to the cost of hardware, licences and maintenance. The added functionality gives users of iLabber access to chemistry drawing, chemical structure and reaction searching, stoichiometric calculations (reaction planning), and iLabber's reagent and reactant databases. All chemistry searching in iLabber is powered by JChem Cartridge. In addition, MarvinSketch is provided to premium users at no extra cost. To use iLabber, scientists download a desktop client; operation, maintenance and data storage is managed by Contur Software. The service is available to individual researchers and smaller research groups (recommended up to 15 users). Individual researchers use iLabber for free, while there is a fee of $60 per month and user for commercial organisations. Academic institutions pay half of that fee.

Conclusion

Trevor Heritage, CEO of Symyx, claims that pharma's concerns about data and operations security are largely alleviated by today's mature scalable and redundant multitier architectures, and shared resources environments.[10] Third-party data centers offer facilities to isolate customer data, perform regular backups, and minimize failure through redundancy. Detailed service level agreements spell out responsibilities. There are standards for disaster recovery and business continuity to protect SaaS customers. His arguments are persuasive for hosted informatics but it is obvious that big pharma is unlikely to risk its intellectual property in the public cloud at large, as the technology currently stands.

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Table 1. Selected Technologies

Company/technology	Web site	Comments
Amazon Web Services	http://aws.amazon.com/	Amazon Elastic Compute Cloud (Amazon EC2) Amazon SimpleDB Amazon Simple Storage Service (Amazon S3) Amazon CloudFront Amazon Simple Queue Service (Amazon SQS) Amazon Elastic MapReduce Amazon Relational Database Service (Amazon RDS) AWS Premium Support
Cirrhus9	http://www.cirrhus9.com/	IT infrastructure. C9 Cloud computing integration services
Citrix Systems	http://www.citrix.com/English/ps2/products/product.asp?contentID=1681633	Citrix Cloud Center (C3) virtualization and networking products
Cycle Computing	http://www.cyclecomputing.com/	CycleServer: administration for managing and using Condor pools CycleCloud: secure, on-demand grids via CycleCloud, built on Amazon Web Services Cloud FS file system for building storage cloud
Google App Engine	http://code.google.com/appengine/	Development stack for building and hosting Web applications
IBM	http://www.ibm.com/ibm/cloud/	Dynamic infrastructure. Service management for cloud computing. IBM software in a cloud environment using Amazon Machine Images
Isilon	http://www.isilon.com/	Scalable Network Attached Storage (NAS) solution
Microsoft Windows Azure	http://www.microsoft.com/windowsazure/	Windows Azure: operating system as a service. Microsoft SQL Azure: relational database in the cloud
Nirvanix	http://www.nirvanix.com/solutions/index.aspx	Cloud storage solutions
Nirvanix	http://www.nirvanix.com/solutions/index.aspx	Nirvanix Storage Delivery

		Network: cloud storage for the enterprise
ParaScale	http://www.parascale.com/	Software-only solution to create, manage and power cloud storage
Platform Computing	http://www.platform.com/	Cluster, grid and cloud management software
RightScale	http://www.rightscale.com/	RightScale cloud management platform
Salesforce	http://www.salesforce.com	Cloud infrastructure. Force.com platform including database, security, workflow, user interface, and other tools. Customer Relationship Management applications
Sun Cloud Computing	http://www.sun.com/solutions/cloudcomputing/index.jsp	Developer tools. Sun Cloud Partner Initiative Scalable infrastructure
Switch Communications Group	http://www.switchnap.com/	Highly secure, mission-critical interconnectivity and disaster-avoidance colocation services
Univa UD	http://www.univaud.com/	Infrastructure products for private cloud, hybrid cloud and intelligent cloud
VMware	http://www.vmware.com/	vSphere data center virtualization. vCloud Express for VMware Virtualized infrastructure. Private cloud

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