SCIENTIFIC COMPUTING WORLD

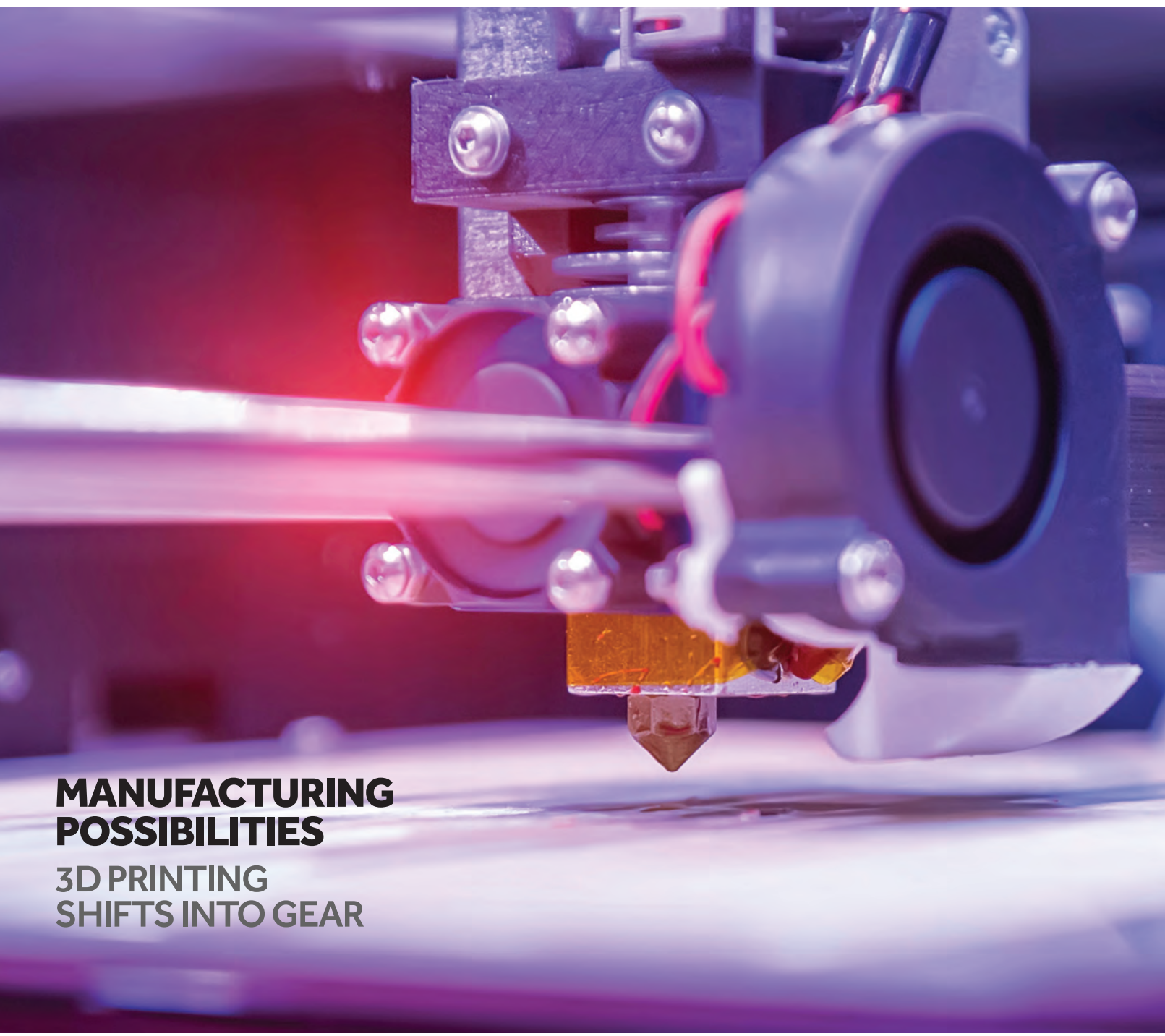
Computing solutions for scientists and engineers

Spring 2022
Issue #179

High performance computing
Exascale prototypes

Laboratory informatics
Active automation

Modelling and simulation
Realistic robots



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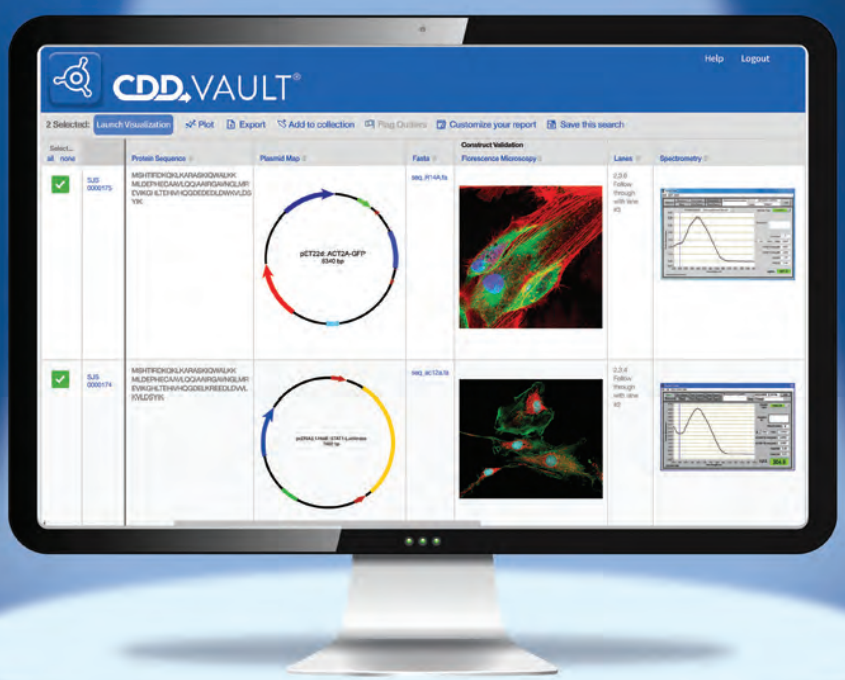

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Oligo

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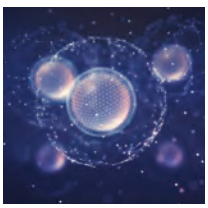

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Scientific Computing World is published by Europa Science Ltd, 4 Signet Court, Cambridge, CB5 8LA ● ISSN 1744-8026
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Web: www.researchinformation.info

Subscriptions: Free registration is available to qualifying individuals. Register online at www.scientific-computing.com Subscriptions £180 a year for six issues to readers outside registration requirements. Single issue £20. Orders to ESL, SCW Circulation, 4 Signet Court, Swann Road, Cambridge, CB5 8LA, UK. Tel: +44 (0)1223 221 030. Fax: +44 (0)1223 213 385.

US copies: Scientific Computing World (ISSN 1356-7853/USPS No 018-753) is published bi-monthly for £180 per year by Europa Science Ltd, and distributed in the USA by DSW, 75 Aberdeen Rd, Emigsville PA 17318-0437. Periodicals postage paid at Emigsville PA. Postmaster: Send address corrections to Scientific Computing World PO Box 437, Emigsville, PA 17318-0437.

Cover: Shutterstock.com

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Robert Roe
Editor

Research possibilities

In this issue of *Scientific Computing World*, there are a number of articles looking at how computing technology is shaping new avenues for research. From exascale to AI and cloud or automation, computing is driving new method of research and enabling scientists to solve challenges that were previously impossible.

On page 4 coverage of the high-performance computing industry begins with an article looking at the development of exascale computing systems. This article highlights more than 10 years of development leading to the creation of new hardware to support exascale class computing systems. On page 8 there is an interview from Professor Dieter Kranzlmüller of Leibniz Supercomputing Centre. Professor Kranzlmüller highlights the work done at the facility and how this HPC centre supports its user base.

Next, there are two tech focus articles which look at computing tools for storage and networking technologies (page 10 and page 12 respectively).

On page 16, there is an article looking at the development of engineering software in the cloud. Cloud computing technologies are being used to give engineers more access and freedom to access their data. Cloud technologies have now attained a level of maturity that has made them appealing to HPC users across an increasing range of disciplines including engineering.

Laboratory Informatics coverage begins on page 18 as Sophia Ktori takes a look at automation in the laboratory. This article looks at the importance of automation, robotics and digital transformation and how these technologies will be critical to the journey towards Lab 4.0.

On page 26 we take a look at the role of additive manufacturing software in helping engineers to develop new manufacturing methods and to design new components with higher performance than was previously possible.

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Some high-performance computing (HPC) providers promise you the world, but leave you high and dry while you attempt to learn a foreign language. At DUG, our reliable, green, cost-effective HPC solutions come with a team of experts. Experts that are fluent in HPC and always on hand to help you optimise your software, onboard your code, and make your project successful. Now that's worth shouting about!

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Innovation at scale

ROBERT ROE EXPLORE'S ADVANCES IN CPU, ACCELERATOR AND NETWORKING HARDWARE THAT IS BEING DESIGNED TO SUPPORT EXASCALE.

Creating the technology stack for exascale has taken years of innovation beyond simple iterative improvement of technology. In many cases, new computing architectures, networking systems, accelerators and processors are being constructed and optimised to deliver efficient exascale computing.

The drive towards exascale has often focused on delivering the highest possible raw computational power. The standard measure of exascale has generally been an exaflop or the ability to generate 10^{18} floating-point operations per second. But this really just scratches the surface of what is required to support an exascale system Scientists require sustained application performance on real scientific codes.

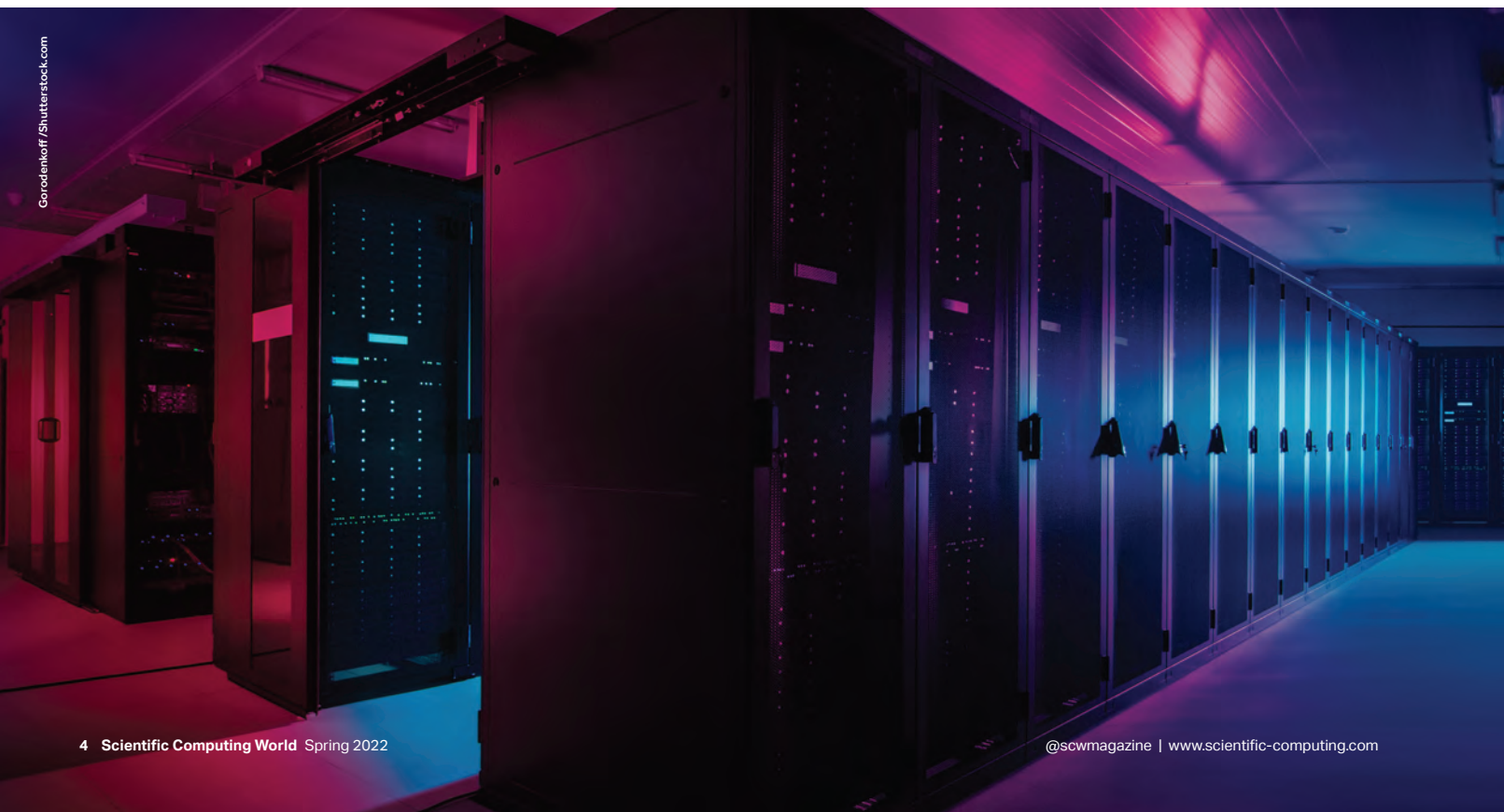
Driving application performance at exascale requires a combination of computational power, I/O and memory bandwidth, and increases in energy efficiency that can make these future systems viable.

The European Processor Initiative (EPI) is an ongoing project funded by the European Commission, whose aim is to design and implement a roadmap for a new family of low-power European processors for extreme-scale computing that includes high-performance big-data and a range of emerging applications.

The EPI technology stack includes a General Purpose Processor (GPP) research stream and an accelerator stream which supports the development of multiple accelerator technologies. This is being co-developed to deliver a European-based HPC platform for exascale computing.

The GPP is based on the Arm ISA while the accelerator is based on RISC-V. Etienne Walter, Atos, EPI Phase 2 General Manager commented: 'The continuation of phase one, but more clearly it's about finishing the work initiated in phase one with the first generation of processors. It's about improving global performance, and also the security of the chips. It's rather similar also for the accelerator. We have several improvements in mind, we are changing the foundry technology, and we will have some denser and more complete chips for the accelerator.'

The decision to codevelop both the GPP and accelerator technologies in the same project hugely increases the complexity, but also provides a range of potential benefits. For example, EPI organisers have full control over the design specification of this hardware stack and can thus optimise both components around



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their given objectives. This means that each technology is optimised together. This could potentially provide better performance and efficiency as components have been designed in tandem to support the same goals.

Walter noted that this gives certain advantages that support the European Commission's objectives: 'It was really a benefit because we can see in the competitive landscape, we need very general-purpose processors, we need the accelerator to have the computing power that is needed for many application today and a growing number in the future. It makes sense to work on having both and trying to make them work together as well as possible.'

'It would certainly have been simpler to address only one because of course you would have less discussion and probably a simpler consortium,' Walter continued. 'But I expect a long-term benefit from working on both aspects. For instance, the GPP stream is based on the Arm ISA. That's one fundamental choice. The accelerator work is more based on RISC-V ISA. We expect that, in the future, we will have more RISC-V in the GPP. So we have the kind of cross-fertilisation for the GPP stream and that is just one benefit of working together.'

Walter was also careful to state that there is no single choice or architectural design that can support the entire HPC ecosystem. There has to be a careful selection of tradeoffs. In the case of EPI they have chosen a platform where the GPP stream focuses on developing a stable CPU that can support legacy X86 applications. On the accelerator side, they are proposing multiple different types of acceleration technology that can then be used to maximise the benefit for a certain subset of applications.

'There is no optimal solution for all applications, it's really not possible. So we have to consider different combinations and so this is why we really work on one side to ensure legacy and consistency with the Arm ISA and ecosystem,' stated Walter. 'Here, we can benefit from ecosystems that already exist. We can see the Fugaku system in Japan, for instance. We have quite significant systems running the Arm ISA.

The EPI project builds on the existing Arm ecosystem for HPC but also on previous European research projects such as the series of Mont-Blanc projects which investigated the use of Arm for HPC starting in 2011. 'We have the experience from the work done within the Mont-Blanc project working on the Arm ISA. It has proved really easy to port, some X86 applications onto the arm ISA. Of course, you need to recompile the code, but, in general, we have had very little trouble doing that. So it's quite a limited effort when compared to taking a new programming model into account. It's not the same level,' added Walter.

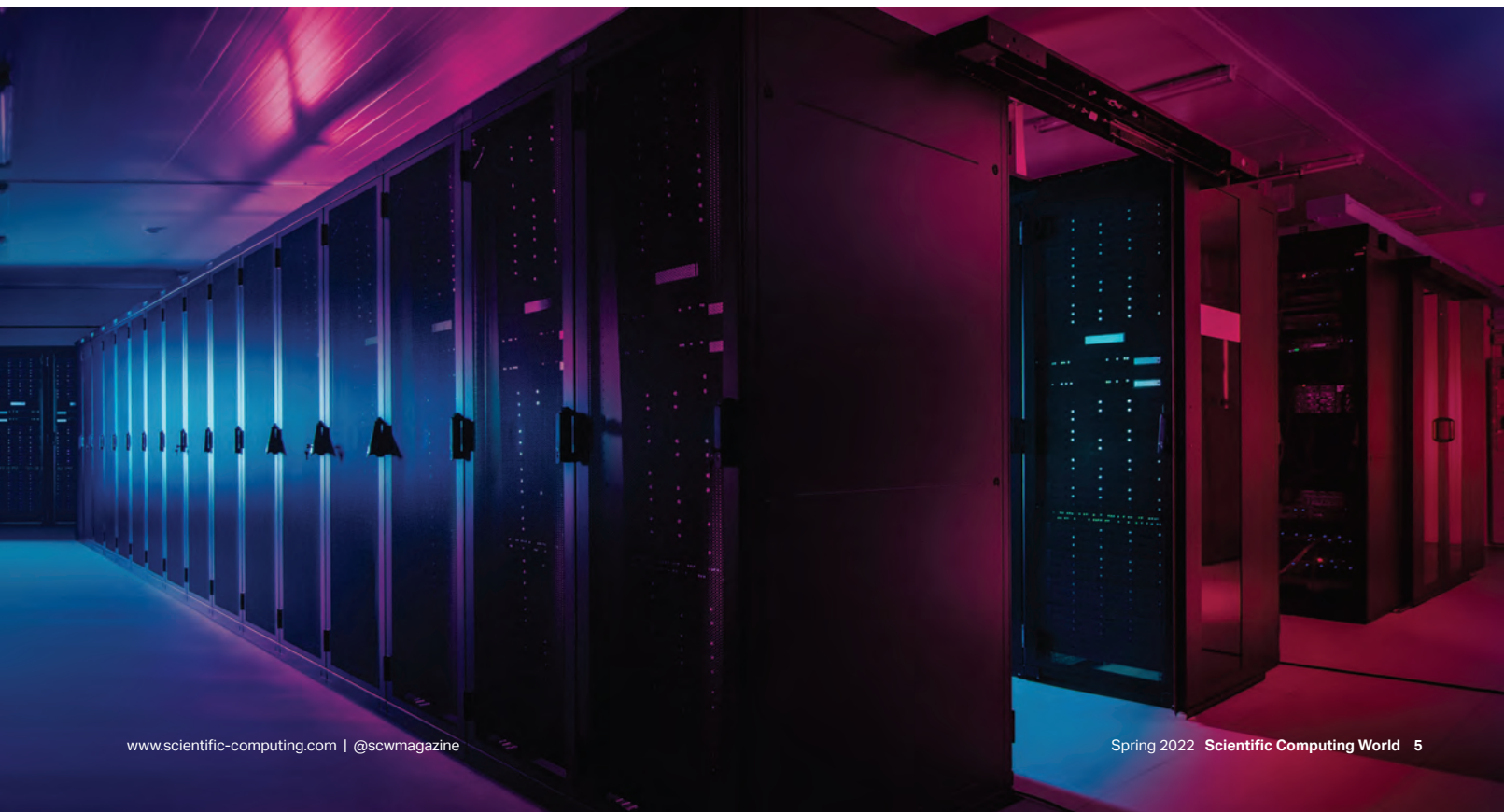
Exascale networking

CPU and accelerator technologies are just one aspect of the exascale puzzle. As the parallelism in exascale systems will be vastly larger than anything seen today it will be a significant challenge to deliver the I/O bandwidth needed to support application performance. But this is not just a challenge for exascale HPC but other markets including AI and also traditional datacentre applications.

> **"It's about improving global performance, and also the security of the chips"**

Hewlett Packard Enterprise and Ayar Labs recently signed a multi-year strategic collaboration to accelerate the networking performance of computing systems and data centres by developing silicon photonics solutions based on optical I/O technology. This was soon followed by news that Ayar Labs had secured $130m in additional funding from Boardman Bay Capital Management, Hewlett Packard Enterprise (HPE) and Nvidia, as well as multiple new and existing financial investors which include GlobalFoundries and Intel Capital.

Silicon photonics will be used to enhance the networking capabilities and support future requirements for high performance computing (HPC), artificial intelligence (AI), and cloud computing architectures. The technology also has the potential to reduce the amount of →



→ energy used in data centres and large computing systems.

Hugo Saleh, Ayar Labs senior vice president of commercial operations, stated: 'Within the press release, we talked about a few things. One is a future design of HPE Slingshot architecture, which has its genesis back at Cray. Today it is their high-end, Ethernet-like, networking solution that is targeted for HPC. We're also working with HPE on advanced architectures where we're talking about the composability of disaggregated resources, with an intelligent software stack.'

Solving problems for extreme-scale HPC

The silicon photonics designed by Ayar Labs could be used to create architectural designs that can support different configurations of hardware. 'When we talk about the different markets we serve, we like to think of this whole cloud space and the focus there mostly is on disaggregated architectures or pooled and composable resources,' Saleh said. 'The reality is that it also applies to HPC. For AI and HPC, the focus is on glueless fabrics and memory semantic fabrics. AI especially is on the glueless side,' Saleh continued. 'So think about systems that may want to interconnect 64, 128 or 256 CPUs, seamlessly. We're not talking about traditional, large, Xeon class CPUs, these could be smaller accelerators, or AI engines, where you want to be able to create a mesh.

'In the AI space, I like to simplify it as: we're trying to replicate the human brain. You've got a bunch of nodes, maybe each node doesn't compute a lot, but it does a very specialised function. Then you have a lot of connections, the synapses between all those different nodes. And you need those nodes to be firing at high bandwidth, very low latency and low power to be able to create and solve these large AI problems,' Saleh added.

The partnership between HPE and Ayar Labs aims to develop capabilities that leverage optical I/O, which is a silicon photonics-based technology that uses light instead of electricity to transmit data, to integrate with HPE Slingshot or other future networking products.

'Whether you're talking about HPC, or disaggregated computing, there is a real limiter on I/O.' said Saleh. 'In HPC, it's usually referred to as a memory bottleneck. It's not a memory capacity issue, it's the ability to move the data out of memory DIMMs into the CPU and back. The other bottleneck that's been seen and talked about quite a bit is the bottleneck on the GPU. Between the CPU and GPU transferring the data and then again, between the GPU itself and the memory.'

4 PM production/Shutterstock.com

These bottlenecks are a growing concern for scientists and researchers using HPC and AI systems as they have the potential to limit application performance.

'What we do at Ayar Labs is an attempt to change the physical domain that data is transmitted,' noted Saleh. 'Going from electricity, voltages and currents, to photons. And we do that coming straight out of the socket. So it's not a transceiver at the back of the server, it's not a mid-board optics. We design chiplets that sit inside of the package, that are nearly abutted to the CPU, memory, GPU or accelerator. We're agnostic to the host ASIC. Then we transmit photons and light outside of the package for your high speed, low power I/O.'

Ayar Labs first demonstrated this technology at Supercomputing 2019, the US conference and exhibition held annually in the US. 'We have a full test rig. We first demonstrated our technology to the HPC community at supercomputing 2019 in Denver. Since then we've made two public announcements that are the projects we're doing with Intel. So Intel has themselves demonstrated an FPGA with our photonics inside of it, transmitting massive amounts of data at much lower power,' stated Saleh.

This technology could massively increase the memory bandwidth for future HPC and AI systems. Each chiplet delivers the equivalent of 64 PCIe Gen 5 lanes, which provides up to two terabits per second of I/O performance. The system uses standard silicon fabrication techniques along with disaggregated multi-wavelength lasers to achieve high-speed, high-density chip-to-chip communication with power consumption at a picojoule range.

Ayar Labs developed its technology alongside GlobalFoundries as part of its monolithic silicon photonics platform.

'We worked with the Global Foundries on developing a monolithic process, one that lets you put electronics and optics on the same chip,' Saleh said. 'A lot of traditional optics are separate; we have it all combined into one and that simplifies our customer's life when they're packaging all these components – it reduces power, it reduces costs and reduces latency.'

GF Fotonix is Global Foundries' next-generation, monolithic platform, which is the first in the industry to combine its 300mm photonics features and 300GHz-class RF-CMOS on a silicon wafer. The process has been designed to deliver performance at scale and will be used to develop photonic compute and sensing applications. Ayar Labs also helped GF develop an advanced electro-optic PDK that will be released in Q2 2022 and will be integrated into electronic design automation (EDA) vendor design tools.

Case study: NTU scientists boosting traffic control AI by 200 per cent

A team of scientists at NTU has adopted Gigabyte's G242-P32 server and the Nvidia Arm HPC Developer Kit to incubate a 'high-precision traffic flow model'– a smart traffic solution that can be used to test autonomous vehicles and identify accident-prone road sections for immediate redress.

The Nvidia – Arm-based solution gives the project a 200 per cent boost in efficiency, thanks to the cloud-native processor architecture that 'speaks' the same coding language as the roadside sensors, the high number of CPU cores that excel at parallel computing, the synergy with GPUs that enable heterogeneous computing and the ISO certifications, which make the resulting model easily deployable for automakers and government regulators alike.

Dr Chi-Sheng Shih, professor and director at the Graduate Institute of Networking and Multimedia at Taiwan University (NTU), is leading a team of scientists to develop a 'high-precision traffic flow model' of Taiwan's roads and highways. The benefits of such a model are twofold. One, developers of autonomous vehicles and ADAS can conduct simulations to test their creations, while government regulators can run safety checks before greenlighting a new product.

Two, existing 'accident-prone road sections'– locations which exhibit a higher frequency and greater severity of vehicular accidents – can be quickly identified, so steps can be taken to prevent more accidents and save lives. The model is already being tested on roads in northern and central Taiwan. The team is in talks with Tier IV, a deep-tech startup based in Japan, about incorporating the finished product into Autoware, the world's leading open-source software project for autonomous driving; this will pave the way for broader adoption and the possibility of commercialisation.

How are Dr Shih and his team developing the model? First, three or four sensor packets, each composed of a lidar and three cameras, are installed along a stretch of road around a hundred to two hundred meters long. During each batch of testing, the sensors gather data from the traffic flow for a duration of around two hours. Data points include the number of vehicles, vehicular speed, the distance between each vehicle, etc. Then, the data is taken back to the computer lab to be processed. The end result is a highly precise computer model that shows intricate details about the traffic flow; it is a kind of digital twin that can be used for mobility simulation and modelling, which is a key component of a smart traffic solution.

'Our goal is to serve as the Qianliyan and Shunfeng'er of autonomous vehicles,' says Dr Shih, citing two deities from Chinese mythology known for their far-seeing eyes and all-hearing ears. Not only can the computer model improve the positioning accuracy and safety of self-driving cars, it can also be used to analyse and fine-tune traffic flow, which is beneficial for all vehicles, autonomous or otherwise.

In 2021, Dr Shih's team welcomed a valuable new member: Nvidia's Arm HPC Developer Kit, an integrated hardware and software platform for creating, evaluating, and benchmarking HPC, AI, and scientific computing applications. At the core of this comprehensive solution is Gigabyte Technology's G242-P32, a G-Series GPU Server powered by a single ARM-based Ampere Altra Processor.

Its contribution to the research project has been remarkable. By Dr Shih's estimates, development time has been reduced by at least half, which is an efficiency boost of 200 per cent. The scientists have taken to calling Gigabyte's Nvidia-ARM-based solution a 'machine learning multicooker'—an all-in-solution that can train the AI, develop the computer model, transfer the data, and more. It is a real boon to the advancement of the traffic flow model, and it has made the team's work considerably easier.

How has Gigabyte's G242-P32 and the Nvidia Arm HPC DevKit been able to accomplish all this? The four main benefits can be summarised as follows:

1. Arm processors are 'cloud-native', meaning they follow the same RISC architecture as the computer chips used in roadside devices.
2. The Ampere Altra CPU has an immense number of cores–up to 80 in a single processor, making it eminently suitable for parallel computing.
3. The DevKit is outfitted with dual Nvidia A100 GPUs, which complement the CPU through a process known as heterogeneous computing. What's more, the 8-channel 512G DDR4 memory provides the necessary bandwidth to handle the high data transfer rate.
4. The Arm solution observes the ISO 26262 safety standards, which means computer models developed with Arm can be easily deployed by companies and institutes in the auto industry.

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Holistic and complementary

PROF DIETER KRANZLMÜLLER OF LEIBNIZ SUPERCOMPUTING CENTRE (LRZ) OUTLINES THE WORK OF THE FACILITY

Can you tell me about your background and qualifications?
I'd describe myself as a 100 per cent computer scientist by heart and by my training, but with strong interests in interdisciplinarity to other scientific domains. I've got a fair amount of experience in the IT industry, which proves very valuable for my management role at LRZ.

I am chairman of the board of directors at the Leibniz Supercomputing Centre (LRZ), and a full professor of computer science at the Ludwig-Maximilians-Universität Munich (LMU). I studied computer science at Johannes Kepler University in Linz, Austria, which is where I obtained my PhD and habilitation. In addition, I spent times at the universities of Reading (UK), TU Dresden (Germany) and École Normale Supérieure Lyon (France). I also served as deputy director of the EGEE project at CERN in Geneva (Switzerland) before joining LRZ and LMU Munich in 2008.

How does your 'HPC centre/research centre/lab' use computing for research?
The three centres that comprise the Gauss Centre for Supercomputing (GCS) focus on leading-edge, high-performance computing capabilities – that is, how can we best support and enable HPC capabilities for science at the front line?

The users of our HPC resources are always at the centre of our strategy. Hence, GCS is not only about providing the 'bare metal' – we have built up an extensive support and education programme over the years, and recently established a mentoring programme across all three sites.

Our computational X/or support teams are usually made up of computer scientists and domain scientists to understand and support researchers' requirements as best as we can. Each GCS centre has different characteristics and caters to the needs of different domain sciences. At LRZ in particular we do not only offer HPC resources, but also a holistic approach as a partner for digitalisation in science.

Can you outline the type(s) of projects undertaken at your facility: how do researchers access computing resources?
Access to computing resources is through a peer-review process within GCS. Proposals by scientists have to be solid both in terms of the computer science aspect and the domain science work to be carried out. Excellent research then gets access to the most suitable of the various GCS-systems; at LRZ, we focus for example on environmental science and energy efficiency.

How do requirements vary between your different users?
The set-up of GCS with its three complementary centres ensures the broad science community can be supported. As such, we see many different requirements from our diverse communities.

As an example, we have HPC experts, optimising their codes for the bare iron, but also 'clickers', who want to work on our systems through GUIs and web portals. At LRZ, we have astrophysicists, who work on the largest simulations of our galaxy, or geophysicists researching tsunamis and earthquakes, through to biomedical scientists, who work within the cells of our body.

What are the computing trends you see happening in your area of research?
It is expected that future systems will be much more heterogeneous. The GCS approach, with three different systems, proves useful, as we will see different systems with different characteristics. Our current SuperMUC-NG is a pure X86-based system, but with Phase 2 (coming later this year), we will be introducing GPU accelerators.

For the upcoming generation – an exascale system – we are evaluating different technologies, among them quantum accelerators.

Prof Dieter Kranzlmüller

What are the main computing challenges you face in your research?
For exascale, it's the supply of electricity! Also, the slow down or end of Moore's law requires new approaches to accelerate computing: in the short term, GPUs; in the mid-term, AI acceleration; and in the long term, quantum; and ideally a combination of all approaches, always dependent on what suits best the respective applications.

How could you further increase the speed or efficiency of your research in the future?
Time to science is always critical to us. Currently, we're working on the integration of the technologies above. To achieve this, a team effort is required and we need to make sure our people are engaged and that new and innovative ideas are introduced.

Finally, do you have any fascinating hobbies, facts or pastimes you'd like to tell us about?
As an Austrian, I'm a passionate skier. I love running and listening to the latest tech podcasts, or riding my motorbike through the mountains of my home country.

Interview by Tim Gillett

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Tech Focus: Storage

A ROUND-UP OF THE LATEST STORAGE PRODUCTS AND TECHNOLOGY AVAILABLE FOR SCIENTISTS USING HPC

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While storage volumes continue to increase dramatically, storage providers are trying to meet demand by increasing performance and introducing more efficient methods of managing data across large multi-petabyte storage platforms.

Choosing the right system for a particular workflow is critical. Traditional products associated with parallel file systems still persist, but now there is increasing competition from cloud and all-flash storage arrays, which are becoming increasingly attractive to users at opposite ends of the hardware spectrum.

Ultimately, choosing the right storage architecture means understanding the application portfolio being run on your system and choosing a technology to best support the operations that are critical to sustained performance.

Storage products

Atipa Capella storage solutions with Lustre – the scalable storage solution that is affordable, reliable and high performance. The Capella LZE series is Atipa's flagship Lustre appliance for enterprises, including high-availability and advanced monitoring features. The starting configuration consists of one Lustre metadata/management module and one Lustre object storage module.

BullSequana Xstor – A single family of storage appliances from Atos. Today, machine learning (ML) and data analytics are creating many of the most challenging HPC workloads. Atos actively participates in initiatives to strengthen the industrial control of digital simulation and big data technologies.

BeeGFS is a parallel file system, developed and optimised for high-performance computing (HPC). BeeGFS includes a distributed metadata architecture for scalability and flexibility, and is available free of charge for end users. For enterprise systems, professional commercial support is available.

Caringo's Swarm software-defined object storage provides a complete platform for data protection, management, organisation and search at massive scale for all of your unstructured data (for example, photos, videos and files). Users no longer need to migrate data into separate solutions for long-term preservation, delivery and analysis.

ClusterVision has 16 years of knowledge and expertise working with different storage solutions. We have designed straightforward to very complex installations and can offer classic NAS systems, (hybrid) cloud solutions, parallel HPC storage installations with BeeGFS, IBM Spectrum Scale, or Lustre, and many more.

DDN provides high-performance storage solutions, and was voted number one in high-performance storage for AI and HPC computing in 2020 (HPCwire Readers' and Editors' Choice Awards). With DDN A3I and EXAScaler Data Management Solutions, organisations can analyse petascale datasets, with capacities up to 500+ PB, and throughput up to 2 TB/second.

Excelero's NVMesh software-defined storage deploys distributed data protection over public cloud instances with ephemeral NVMe drives. Excelero delivers low-latency distributed block storage for web-scale applications. NVMesh enables shared NVMe across any network and supports any local or distributed file system.

HPC using fungible solutions eliminates the lengthy delays and lost output typically related to legacy HPC clusters. Elastic, high-performance configurations supporting practically unrestricted scalability allow you to grow and contract your infrastructure as required.

HPE provides HPC storage solutions that span the whole storage hierarchy to accelerate time-to-insights

while managing and protecting the data in your parallel file systems. The Cray ClusterStor E1000 Storage System from HPE embeds Lustre and is ideal for attachment with HPE Slingshot, InfiniBand HDR and 100/200 GbE to HPC Cray EX supercomputers and large clusters of HPE Apollo systems.

IBM Spectrum Scale meets these challenges as a parallel, high-performance solution with global file and object data access for managing data at scale with the ability to perform archive and analytics in place.

MemoScale specialises in developing compression and erasure coding software for data storage solutions. The team has extensive experience in software and hardware optimisations as well as coding theory.

MooseFS allows the combination of data storage and data processing in a single unit using commodity hardware. The company provides professional services and expert advisory for storage solutions, as well as implementation and support.

NEC provides a variety of storage disk array solutions, or its award-winning distributed grid storage platform, enabling long-term data retention through performance scalability, maximised capacity and large-scale storage consolidation.

NEC Storage HS Series platform enables long-term data retention through scalability of performance and maximised capacity, without the complexity and limitations of legacy storage solutions.

NetApp has simple, smart, trusted storage for shared NAS and SAN environments, to arrays built for dedicated, high-bandwidth applications like data analytics and disk-based backup.

Open-E DSS V7 is a fully featured NAS (Network Attached Storage) and SAN (Storage Area Network) software platform. NAS offers support for multiple file protocols, enabling cross-platform solutions, and SAN offers iSCSI Target and Fibre Channel Target functionalities.

Open-E DSS V7 enables organisations of all sizes to create storage solutions to meet and adapt to the simplest or the most complex data management needs.

Panasas supports global industry and research innovation with PanFS Dynamic Data Acceleration, which automatically adapts to evolving workloads to deliver a consistently fast, total-performance HPC storage solution. PanFS is delivered on the ActiveStor Ultra turnkey appliance.

Pure Storage FlashArray//C delivers NVMe performance, hyper-consolidation and simplified management. FlashArray//X is designed for entry-level to enterprise applications.

QCT HPC/DL solution integrates with open source software and features a modularised architecture that can be tailored to meet customer demands.

QNAP NAS is a fast storage solution in post-production workflows. TVS-473e transfers high-volume files and provides large storage for high-resolution 3D scanning.

Qualstar magnetic tape and data storage solutions are known throughout the world for their high quality, ease of use and reliability. Tape has long been used as a digital data storage medium, but it is the expansion of big data that has really made its value proposition apparent.

Qumulo – Qumulo Core is a high-performance file data platform designed to help you store, manage and build workflows and applications with data in its native file form at massive scale, across on-prem and cloud environments.

Quobyte is a software storage system that delivers unlimited performance and consistent low latency to applications and users through scale-out without limits, managing hundreds of petabytes with demanding users and many applications.

Scality helps scientists manage file and object data from cloud-to-core-to-edge. Scality Ring is a scale-out file and object storage while Scality Artesca provides lightweight, cloud-native object storage.

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SoftIron's HyperDrive Performance+ leverages the AMD EPYC 3000 processor, the new Performance+ family debuts the company's first x86 CPU and NVMe SSD-based designs to be introduced in its HyperDrive series of storage appliances.

Spectra Logic deliver disk, object storage, tape and data management software for archive, backup and cloud. Spectra Logic builds some of the world's largest storage systems.

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Weka offers a modern storage architecture that can handle the most demanding I/O intensive workloads and latency-sensitive applications at Exabyte scale, on-premises or in the cloud, or across both.

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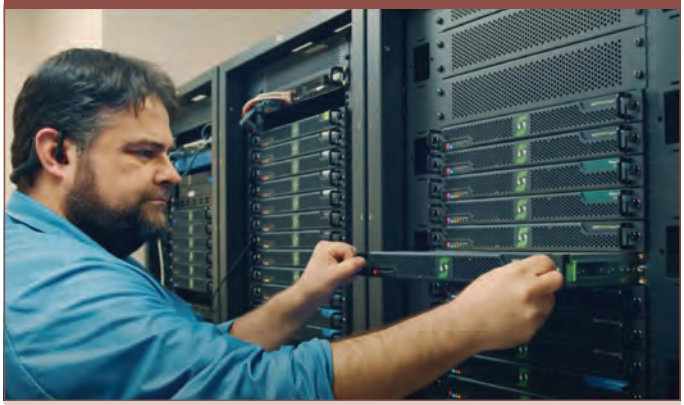

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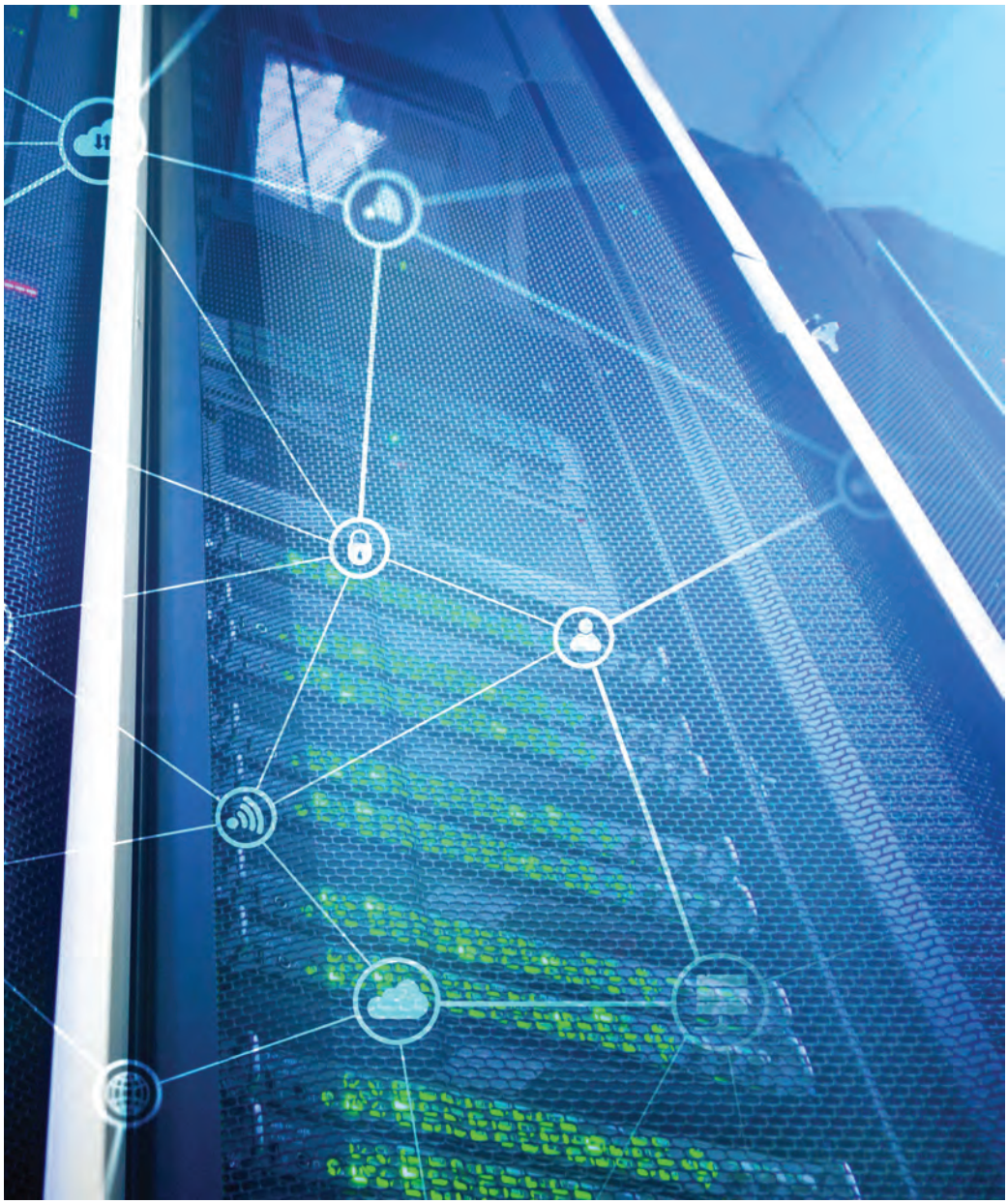
Visit: softiron.ltd/HyperDriveTechFocus

Tech Focus: Networking

A ROUND-UP OF THE LATEST PRODUCTS FOR SCIENTISTS USING NETWORKING TECHNOLOGIES



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In recent years, the movement of data – rather than the sheer speed of computation – has become a major bottleneck to large scale or particularly data-intensive HPC applications. This has driven bandwidth increases in interconnect technology, effectively widening the pipe that data uses to travel across the network.

With increasingly complex challenges in science and engineering, researchers are looking to larger computing systems that require fast networking to deliver the data they need for their experiments and research projects.

The choice to develop a bespoke system or use an end-to-end solution to support scientific research projects depends on workloads, scale and budget. There are many ways to solve these challenges, but the answer for each organisation will depend on the scale of the challenge and the demand for latency, which inevitably drives the cost of deployment.

As the demand for better performance leads to more highly parallel solutions and data-intensive computing systems, networking technology is becoming increasingly important in supporting sustained application performance.

Networking companies provide high-speed access to data, which can support high throughput workloads. While the main networking technologies used in HPC are based on either Ethernet or InfinBand, there are also other technologies that use PCI-Express to develop networking fabrics to support other ultra-low latency, high-bandwidth workloads. This is generally based on the use of high-speed, real-time systems, clustered databases, general networking, web services and industrial embedded applications.

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Other products

Ayar Labs is disrupting the traditional performance, cost and efficiency curves of the semiconductor and computing industries by delivering up to a 1,000x improvement in interconnect bandwidth density at one-10th the power. They use standard CMOS processing to develop high-speed, high-density, low-power optical interconnect 'chiplets' and lasers to replace traditional electrical I/O.

Cisco UCS helps change the way IT organisations do business. It combines industry-standard, x86-architecture servers with networking and storage access into a single unified system. UCS brings increased productivity, reduced total cost of ownership and scalability into your data centre.

DustPhotonics helps hyperscale data players move to more optical lanes and complexity with a uniquely simple yet strategic, reliable and efficient Electro-Optic Coupling technology.

The **DustPhotonics** QSFP-DD-SR8 is a hot, pluggable transceiver designed for 400GB/s optical links of up to 100 meters over OM3/4/5 multi-mode fiber. The transceiver is IEEE 802.3bs 400GBASE-SR8 and QSFP-DD MSA compliant for use in data centres, high performance computing (HPC), and enterprise applications.

Eoptolink is dedicated to researching, developing and manufacturing, and markets a diverse portfolio of high-performance, optical transceiver modules and optical components for various ICT applications, such as data centre, telecom networks (FTTx, LTE and transmission), security monitoring and smart grid.

Extoll is a company that delivers products to the high-performance interconnect IP market. The company believes in digital-centric design for physical IP, for example, its high-speed, multi-rate, multi-protocol SerDes is based mainly on digital logic. Complemented by advanced verification and modelling methodology, Extoll can offer robust and flexible solutions to customer's interconnect challenges.

GigaIO is a cloud-class, enterprise-class and open standards composable infrastructure solution. GigaIO is committed to open standards and a contributing member to Linux, to the PCIe standard, and to the CXL consortium.

You can pick and choose the orchestration software that best fits your needs, and build your solution using your preferred vendor and model for servers, GPUS, FPGAs, storage, and for any other PCIe resource in your rack.

With the pervasive use of AI across industries, enterprise data centres carry a large number of vital services. **Huawei CloudFabric 2.0** solution provides customers with a next-generation data centre network that delivers super capacity, intelligent experience and autonomous driving, helping enterprises mine intelligence from data, accelerate digital transformation and promote the development of the digital economy.

LDA Technologies is a provider of high-end FPGA-oriented solutions optimised for ultra-low latency operation, targeted for data processing acceleration, high-performance computing, low-latency networking, and high-frequency trading.

LDA products range from small add-on cards to 4U HPC devices. In addition, LDA offers a broad set of specialised industry-oriented solutions and standalone, ultra-low latency networking IP cores that can be used as part of users' FPGA logic. LDA also offers consultancy services.

Mellanox InfiniBand solutions incorporate In-Network Computing technology that performs data algorithms within the network devices, delivering 10 times higher performance and enabling the era of 'data-centric' data centres. By delivering the fastest data speed, lowest latency, smart accelerations and highest efficiency and resiliency, InfiniBand is the best choice to connect the world's top HPC and artificial intelligence supercomputers.

Dolphin Interconnect Solutions products are used to connect multiple computers and IO systems together to create high performance computing platforms for demanding applications. Application clusters created using Dolphin's interconnect products provide significant improvements in response time and transaction throughput compared to using alternative interconnect technologies.

The Ethernet Alliance is a global, non-profit industry consortium of member organisations that are dedicated to the continued success and advancement of Ethernet technologies.

To help advance the industry as a whole, the Ethernet Alliance also provides the industry with a forum for the open exchange of ideas and dialogue and a platform for consensus-building. We follow strict impartiality guidelines to encourage productive discourse and idea-sharing. This in turn increases growth, advancement and adoption of Ethernet technology around the world.

HPE Slingshot is a high-performance network for HPE Cray supercomputers designed for exascale era supercomputing of diverse simulation, modelling, AI and analytics workloads on one system. Ethernet compatible, HPE Slingshot enables straightforward execution of cloudlike and converged workloads in a supercomputing environment.

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Engineering discipline progresses to find its rightful place in the cloud

Increasingly, engineering organisations are discovering the benefits of cloud-based technologies

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Cloud technologies have now attained a level of maturity that has made them appealing to HPC users across an increasing range of disciplines; increasingly, this includes engineering.

Whether using public or hybrid cloud, these technologies offer unprecedented flexibility for scientists who can create nodes with specific architectural requirements, use cloud bursting to increase the capacity of their in-house infrastructure – or it can increase the agility of a company that shares data over multiple sites. Engineering has traditionally lagged behind other industries such as media, sales and commerce in its use of the cloud – partly because of more complex user requirements – but there are positive signs this situation is changing.

For smaller organisations in particular, there are huge benefits to the cloud. It enables businesses or laboratories to carry out work that may have moved beyond their financial reach just a few years earlier; they no longer have to spend large amounts of money on equipment and have the flexibility to use only the resources they need at a particular time.

"Organisations now have the flexibility to use only the resources they need at a particular time"

Therefore, the use of the cloud allows businesses to adapt and scale their use of computing virtually on a week-by-week basis according to their particular needs, their financial constraints, and as their organisation grows.

Flexibility is key

Over the last couple of years, the Covid pandemic has exacerbated a trend towards mobile working – and, even though operations are returning to a more normal state in many parts of the world, flexibility is increasingly being demanded by workers and businesses have been following the trend by allowing their employees to work remotely on an increasing basis. Cloud is further facilitating this trend, by enabling engineering teams to access software and data wherever they are, on different devices, while still working effectively as a group.

Of course, engineering companies also have many other business needs, including accounting, logistics and so on – all of which can be enhanced and made more efficient through use of the cloud. Of course, these efficiencies can bring financial benefits to organisations that deploy them – and they also mean researchers are less distracted by non-engineering or non-research tasks, such as retrieving files, setting up infrastructures and so on. Organisations that can help researchers focus their time on R&D have been shown to be more than twice as likely to achieve project goals consistently.

As reported in *Scientific Computing World*, over the last two years – spurred on by the pandemic – cloud companies have been offering tools, services and funding initiatives to help scientists and researchers.

It's clear that cloud computing brings accelerated innovation and speeds up the process of taking new products to market. Not only does this increase an organisation's competitiveness in the present, it promises flexibility and agility as needs change in today's fast-moving industrial markets.

Going mainstream

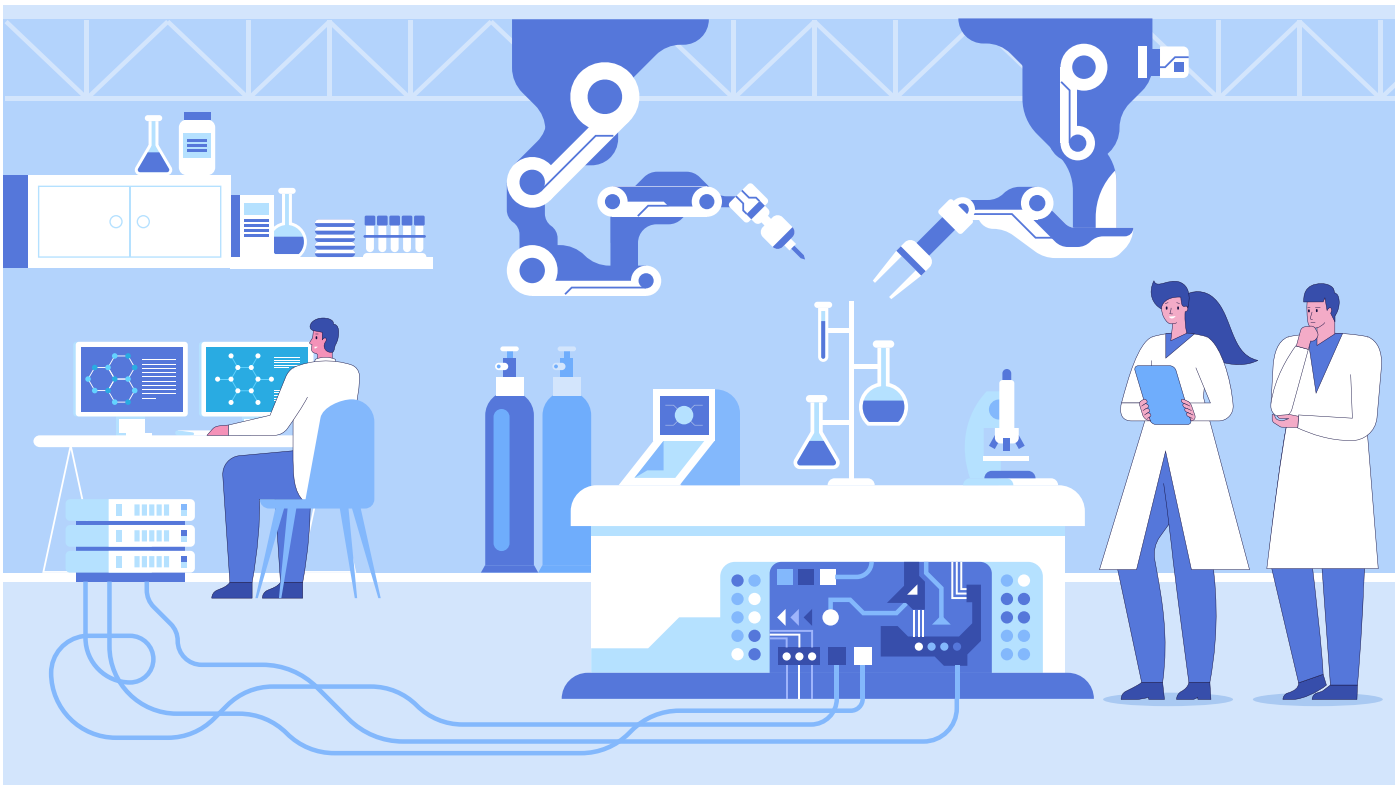
Computational science and engineering is now mainstream, with adoption in every major industry and a transition to the cloud in full swing. For many organisations, navigating this cloud transition will require new skills and automation tools to manage technology, spend, security and compliance.

We have also seen that the transition to the cloud drives significant business impact. Organisations that are able to give engineers easy access to compute at scale are having more successful and on-budget projects. As cloud scale and ease of use become increasingly available in more organisations, we will undoubtedly see continued acceleration in science and engineering innovation.

"Cloud computing brings accelerated innovation and speeds up the process of taking new products to market"

Most organisations realise the benefits of cloud HPC implementation, but many are unsure of how to achieve effective implementation. Rigorous course planning is required for cloud HPC success; companies must evaluate and establish an effective governance and security plan, remain cognisant of application requirements for workload placement, and ensure seamless integration between on-premises and cloud environments for effective operation.

Open automation



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SOPHIA KTORI DISCUSSES THE IMPORTANCE OF INTEGRATION AND OPEN SYSTEMS IN SUPPORTING LABORATORY AUTOMATION

Automation, robotics and digital transformation will be critical to the journey towards Lab 4.0. This vision of seamless, hands-off routine lab tasks, experiments and data handling is motivating investment in hardware and software that will increase lab efficiency, flexibility and throughput, while reducing costs and failures.

However, achieving integration of all of this lab equipment, and getting systems to communicate with each other remains a struggle. Even highly automated labs are today faced with managing islands of language-barriered hardware, and carrying out workflows that are interrupted by the requirement for error-prone, time-consuming manual tasks.

At a foundational level this punctuation results in part, because vendors of lab equipment have traditionally paired their systems with proprietary software that was not designed to talk to that of other suppliers, suggested Pantea Razzaghi, head of design at Automata. And this has been 'oftentimes intentional,' she suggested. 'Some of the larger players had a monopoly within the industry,' and it may not have been in their interest to make instrumentation that communicated easily with systems outside of their brand. Ease of integration would smooth the way for customers to switch to competing systems at upgrade, or when expanding or diversifying their labs.

This lack of interconnectivity means labs often have to maintain software that doesn't fit with the evolving lab environment, and retain equipment that generates data requiring manual housekeeping for downstream utility, Razzaghi pointed out. Labs may even decide to sideline equipment that works perfectly well and does a great job, because it remains disconnected with the lab setup.

Whatever the outcome, this disconnect is likely to be costly, time-consuming and result in interrupted workflows and the need for repetitive manual tasks. It's also likely the format of the data 'doesn't fit well' with that required by the next instrument using that data. You may then have silos of data that are not standardised or optimised, and so there's no way to maximise its utility, she noted. 'We may then need a middle layer of translation before that data can be used to its full benefit.'

Think about at which point lab functionality is most reliant on human intervention, and somewhere near the top of the list will possibly be the requirement to manually pull data out of devices and transfer that data to the next stage. 'It's almost comical how manual this process commonly still is,' Razzaghi commented. 'We see people literally →

walking up to an instrument, inserting a USB stick, downloading the data, walking over to a computer and uploading it into that system.'

The lab today thus fosters equipment that has a level of 'intelligence', lets say, that is analogous to that of the early era of digital cameras, she further suggested. 'To use these early digital cameras we had to insert a memory card into the camera, take the photo, then take out the memory card, put it into a reader, connect it to a computer, pull the images out of it, and store them on that computer. But today we can just snap a photo on a smartphone and send it directly to someone else, wirelessly and in an instant… ' It's this sort of ability that we need to bring into the lab space. 'It's not just about making scientists more efficient, but removing punctuation in processes and the requirement for manual data input, retrieval and transfer will save scientists from having to engage in multiple, repeated manual steps as part of everyday experiments.'

Progressive changes

Fortunately, the philosophy in the vendor space is changing, Razzaghi suggested. An increasing number of what she described as 'more progressive' companies are developing systems designed with an open architecture that can more easily be configured to interconnect and communicate. Vendors are also recognising that culture and expectations are changing within labs themselves.

Scientists and lab technicians are increasingly becoming more interested in engaging with the different layers of a system's software, to help it 'play together'. As she explained: 'Automation scientists may come from a scientific background or an engineering background, but today are interested in extending the utility of how they relate with a device. And that means they're actively looking for new ways to modify a system – whether that's through drivers or API's – to orchestrate different instruments to connect and communicate together.'

This cultural change is also driving a shift in expectations. 'Similar to consumer markets in other industries, the move within the lab sector is to diversify options on the market, and particularly to give users far greater flexibility,' she said. This means that suppliers and developers are evolving their own mindset. 'They're realising that to survive in this space they have to make sure they offer this flexibility – think open API – and develop systems that offer a set of drivers, or advanced tools that give more advanced users within a lab space the option to interact with that software,' she added.

This interaction may be the responsibility of the organisation's automation engineer, or automation scientist – 'who may be few in number and in great demand,' Razzaghi noted. 'These are the people who the lab will call on when they want to scale up an assay or experiment, or transition from manual tasks to a partially or even fully automated task.' But even with open APIs and inbuilt tools, there's still a great deal of work that needs to happen to enable that progress to automation.'

Not every organisation will have its own library of drivers, or automation tools, so even with a more open system, enabling that connectivity and communication device to device can be a major task. 'It's still very early in the process for most labs, and it's going to take time for them to have a robust, reusable library of software tools – a fact which itself opens up another interesting question,' she pointed out. 'Should every lab have to do that? Should each lab have to develop its own library of tools and drivers to enable that lab integration?'

As consumers we now expect our technology to be plug and play, and to work with whatever else we've got on our home or office networks. We no longer have to download drivers or other integration tools when we set new systems up. So why has the pharma industry lagged behind? It's partly down to the already mentioned complexity of the lab environment, and also the diversity of automation and robotics systems now available in the lab sector, Razzaghi commented. And while 'democratisation is now happening within this space', these closed systems are still commonplace in labs.

Thinking to the future, system developers in both the R&D and the manufacturing space realise the imperative to reduce the risk of market entry, and that making systems more 'amenable' to integration will help to attract potential customers. Interestingly, Razzaghi said the lab is becoming a much more stimulating space from the perspective of user experience and interface designers. 'Whereas there has historically been a huge focus on developing consumer-oriented tools in fields such as gaming design or application design, the lab space is offering great opportunities for designers to help make the world a better place.'

Coming back to that cultural shift within the lab, and we can also see that, with scientists today having a far greater understanding of how software works, the imperative is again there for vendors to open up their system's configurability. 'Compared with scientists who were graduating 10-15 years ago, scientists these days are far more knowledgeable about software tools, and how to configure them. Their personal toolset is very different. It's far more common for scientists who graduate today to be Python-savvy, for example.'

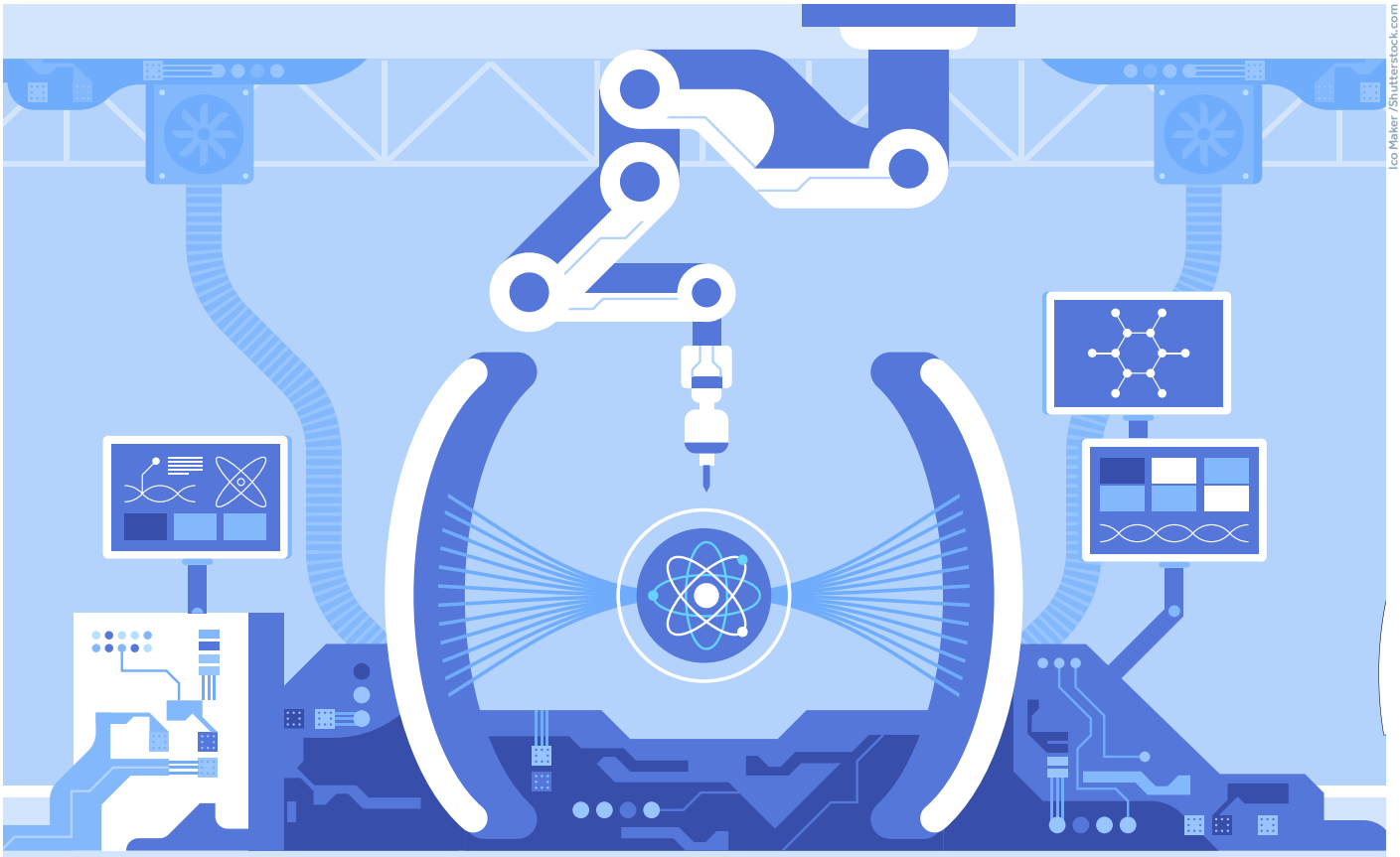
> "We may then need a middle layer of translation before that data can be used to its full benefit"

Scientists want to demonstrate more value out of their workflow, and to be able to use their time more productively, formulating new projects or writing up papers, for example, rather than having to spend time doing repetitive, manual tasks. 'So if they can access a tool that has an open API, they are more likely to try to work it to get the system to do what they want.' This is also generally a more cost-effective option than having to hire someone in, and will also likely be much faster with respect to upstream and downstream connectivity, because the scientists are the ones who know how the lab functions, and what is required to optimise that functionality.

Further challenges

However, Razzaghi acknowledged, the caveat to all this is that it's never a case of walking into a lab and immediately being able to undertake a single automation project that will connect everything. And that gap between expectation and reality can, in itself, present as a significant problem when labs are looking to undertake some sort of digital transformation or automation exercise. 'A lab may, for example, have a manual protocol or experimental workflow they want to translate to an automated format. What they may not realise is that transformation may not be possible as a single step. Here at Automata we understand this gap between expectation and reality, and so we work hard to educate as well as provide the software solutions to get that integration in place.'

Part of Razzaghi's role is also to teach scientists about how to 'think in an automated manner,' she explained.



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→ 'When you are doing something manually it's a linear process. You may have restrictions, for example, waiting for a thermal cycler to finish before you can move to the next step. Or you may only have one liquid handler and it can only be used for a certain task. But labs going through an automation transformation may be able to achieve greater parallelisation of tasks.' It can thus be possible to save hours of work by optimising processes, and this is reliant on the communication channels and integration between instrumentation.

Factor in tools such as scheduling software, and the lab then becomes even more efficient. 'You can then schedule your lab resources and leverage applications to calculate your workforce and instrument capacity.' Supporting automation and interconnectivity thus makes it possible to adapt workflows and processes to maximise efficiency. 'It gives you a way to adapt that journey map to understand how, by moving different steps, or blocks, around, you're going to achieve a certain task or workflow more efficiently, whether that efficiency is how much of a reagent is used, the time it takes for the experiment to complete, or when and how many of the lab instruments are required to complete that task.' Then, of course, it may be possible to calculate the cost benefits associated with each alternative iteration of that task or workflow. 'And that's one of the greatest bits of value we can bring to the table,' Razzaghi stated. 'Our aim is to really help labs leverage the key instrumentation they already have, as well as implement new robotics hardware, through software.'

> "They're realising that to survive in this space they have to make sure they offer this flexibility"

As well as offering both hardware and software to aid lab integration and automation, Automata has the industry insight and expertise that is helping labs make a smoother transition. 'So, we provide the robotic lab bench system that has different actuation devices. This can be thought of as the device framework. Then to that robotic platform customers can integrate their own devices, or we can help them through the process of putting together and purchasing a bundle of instrumentation, and then leverage software so they can write the workflow protocols and do the day-to-day runs and data collection.'

Automata partners with the scientists running the experiments, so that everyone in the lab and other stakeholders understand how systems and software work together, and what they are capable of, Razzaghi noted. 'Importantly, the lab bench system is very much vendor agnostic, so it can fit with a variety of different instruments, and this really helps to connect them together. We have an existing library of drivers and can develop custom drivers to enable that integration.

'Our software also offers a workflow design tool, which makes it possible to interact with the protocols developed for each individual instrument, and facilitate communication so that you can program flexibility into your procedures,' Razzaghi continued. 'It's then possible to run the workflow through a simulator to help identify where there may be errors, and help to optimise experiments and workflows to make the most of time and generate the best quality outcome.'

So, how might these developments impact on lab function within the next few years? Razzaghi suggested: 'In five to 10 years, we can imagine labs no longer having to rely heavily on service integrators for a bespoke solution, instead [having] the ability to independently build out their own automation platform using Automata and cutting-edge instruments from the vendor of their choice.'

Case study: Global Analytical Services Group: enabling lab automation and data harmonisation

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The Global Analytical Services group of Merck KGaA, Darmstadt, Germany comprises 21 labs worldwide offering a wide range of critical services, supporting more than 220 analytical methods and processing 100,000+ samples per year. This 'one-stop shop' is unique in the breadth and depth of the customised analytical chemistry methods, consulting and other independent services they provide across all business entities within the company.

The group's workflow was complicated by numerous manual steps. Samples arrived in batches, representing multiple orders and requiring various analytical methods. Each sample required the work order to be downloaded from the laboratory information management system (LIMS) and printed out.

Next, the analyst consulted a database for the correct preparation procedure, which could involve various methods for the same sample, and either printed out or manually transcribed the instructions. Sample prep required quantification and documentation of various parameters, usually by hand. The next step was generating a barcode label of essential sample information and placing it on the correct tube. Daughter samples prepared from a mother sample for different measurements that had to be mutually logically linked took considerable extra effort.

Samples were fed into analytical instruments. Each sample required manual entry of the sample ID, programming of the desired method and choice of the correct experimental parameters for each instrument. Transforming the raw data generated into the result could require manual calculations, print screens and annotations. The scientist transferred important results into the lab notebook or Excel and generated a report by matching results obtained from various daughter samples and methods to the mother sample. Finally, reports were uploaded – usually manually – to the LIMS.

These processes were not just time consuming but error-prone. The typical rate of data entry errors in each step of manual transcription is 3.6 per cent. In the average lab, the conveyance of data from its original source to the final result takes multiple manual steps, performed by different users over a period of time. Irreproducibility attributable to manual error during experimentation and data reporting is estimated to exceed 35 per cent, and the costs of repeated experimental work caused by these errors are about $28bn per year.

These facts prompted Global Analytical Services to ask themselves:

- Why do we document our data on paper when we have them all in electronic form?
- Why do we type information into analytical instruments when the barcode label can deliver it automatically?
- How can we achieve interoperability and connectivity between different systems?
- How can we link datasets for parent-child samples across multiple process steps and measurement techniques?

The solution: go paperless by automating the complete data lifecycle using Data Management Solutions software.

The Lab Automation Project aimed to create interoperable, bi-directional information exchange among all Global Analytical Services systems and instruments. All analytical and biological data would be captured at the point of origin, organised and made accessible where needed. The biggest stumbling block to this was lack of standardisation: most lab instruments can't communicate with one another due to their vendor-proprietary software formats.

Our software is built on the open source Analytical Information Markup Language (AnIML) data standard; we harmonise experimental data from disparate formats into this single standard via software APIs and data converters. Doing so contextualises results with relevant metadata and enables visualisation in external systems for superb data management across all measurement techniques.

Our instrument connectors are the linchpin of this process. They link instruments, where data originate, to a central storage database. Also extracted and stored are valuable metadata of all kinds. This fully automates data flow, report generation and LIMS upload, laying the foundation of a well-organised data structure. Meanwhile, data standardisation also addresses the challenge of long-term, vendor-agnostic data archival.

We created a toolbox for Global Analytical Services from our library of 300+ instrument connectors. These, and our converters, let individual workflows be created on the fly, tailored to scientists' needs, guaranteeing a seamless data workflow. Customised interfaces and a preselected range of information let the lab group work more efficiently with their data.

One year later, the Lab Automation Project had successfully streamlined the data ecosystem of three different labs in this group, embracing 20+ instruments, four leading systems and 11 measurement interfaces. The project also implemented a central data store with Hub, and universal data analysis and visualisation with Workbench. Benefits to Global Analytical Services were:

- 423 working days saved by FTEs
- 20 per cent annual increase in samples processed
- €400K estimated ROI

In addition, the group's confidence in their data integrity and reporting capabilities was boosted, which meant more satisfied customers in the long run.

Find out more at:
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Expectation of sophistication

WE CAUGHT UP WITH DAVID FOX, CHIEF BUSINESS OFFICER AT MODALITY. AI, FOR A QUICK CHAT ABOUT BIOTECH SOFTWARE TRENDS

Can you tell me about how your organisation is involved with biotechnology?
We provide research data on digital biomarkers and assessment for neurological disorders and psychiatric conditions through multimodal analysis of speech and facial gestures.

Our results have been published in several scientific publications and presented at major scientific convenings, including Interspeech and the American Academy of Neurology. See **www.modality.ai/publications** for references.

How does your software help scientists? How has this changed over time?
Our software helps clinical researchers conduct remote patient monitoring of neurological and psychiatric disorders, including Parkinson's, ALS, schizophrenia and depression. We have clients in the United States, as well as Germany and the Netherlands.

There's also our focus on following standard of care methods, starting with protocols that clinicians are familiar with, such as audio/video recordings that can be reviewed, measurements that can be confirmed by reviewing recordings, and so on (versus the 'black box' approach of divining from a short audio-only sample).

Finally, we provide privacy with a fully opt-in, test-based system, which was designed first for the user's data privacy.

What are the trends you see happening in your area of research?
We see integration and consolidation of audio and visual modalities to unlock important insights. In line with this approach, we are pioneering a platform, multimodal approach that offers utility across multiple conditions. This will better support clinicians as well as patients.

What are the new requirements coming from your user base?
While not a requirement for use in clinical trials, we have found an expectation of an FDA stamp of approval. We expect to receive FDA Class I device approval shortly as a requirement for clinical use and will see Class II approval later in 2022.

> "We see integration and consolidation of audio and visual modalities to unlock important insights"

How might the market you are working in change over the next few years?
We expect development of even more sophisticated technologies for remote assessment of physical and mental conditions, resulting in accelerated development of drugs to treat these conditions. We also expect the most successful biotech companies to take a broader approach to health research by incorporating a wide range of biomarkers for related medical and psychiatric conditions.

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The chemistry of real-time analytics

AHEAD OF HIS KEYNOTE SPEECH AT APRIL'S PAPERLESS LAB ACADEMY EVENT, LLOYD COLEGROVE HIGHLIGHTED EXPERIENCES FROM HIS 30 YEARS IN CHEMICAL MANUFACTURING

Lloyd Colegrove

I hold a doctorate in chemical physics from Texas A&M University, where I was fortunate to work in an R&D group that required synthetic, spectroscopic and quantum mechanics (read 'computational') skills at a time when this was not the norm. I spent almost 30 years at the Dow Chemical Company, starting in R&D before entering the maw that is chemical manufacturing.

Within six months I discovered an ugly truth – engineers and operators didn't know how to handle data or data uncertainty and because of this were making poor decisions, based solely on the next data point. Many of the quality labs were almost screaming at operations that a problem was looming, but the engineers and operators didn't believe them. There was general frustration all round. Eventually data and how to use it became my primary interest, giving me 22 years of rewarding work.

Before I got into real-time data, one of the first unique things I did was invite a young colleague in on a project. He was a chemical engineer with a doctorate in data science. We applied, for the first time, a chemometric model (today known as artificial intelligence (AI)), to a batch plant that allowed for multivariate discernment in the lab data. This revealed random yet systemic problems in the batch production. While it took two years to solve this mystery, which had existed for decades unnoticed, we used the model to protect our customers from receiving batches of material 'within specification' from a univariate approach (the normal way of looking at the data), but was way out of normal from a multivariate view (something no one had done in the chemical industry before). We published our first paper on this in 2007, which greatly increased the lab's ability to support the plant and gave their measurement process much greater credibility.

As teams I developed gained speed within the business, I was given greater resources to go after another problem – one that I will demonstrate in the PLA talk. The problem is data, and too much of it. No human being can manage all the data a plant generates. There is value in all that data, but much of it is overlooked because of the sheer volume of minute and shift data. The only time engineers might look at a broader data set is after a problem has slowed or shut the plant down. I reasoned that if you can tell after the fact you had a problem, and understand it just by looking at more data, you should also be able (with AI) to predict/anticipate the problem.

I went to my friends at Northwest Analytics and we collaborated on developing their FOCUS Enterprise Manufacturing Intelligence suite. For the first time, plants were able to look at a much larger grouping of data, and see – real time – how the data was behaving in the plant. This led to improvements in plant operation, and there was clear value created – less fouling, elimination of 'surprise' events, and experts from around the globe could look in very quickly at how a plant was running and make a phone call if they saw something that concerned them). The list goes on.

> "Real-time analytics helped my global labs, plant engineers and operators bolster their understanding"

One of my sites very enterprisingly installed FOCUS EMI as a monitoring system for the plant labs. Their idea: if you can monitor a plant while it's running, why not monitor the lab instruments real time in the same way? A lab technologist comes in from a weekend away and can – in seconds – ascertain the health of their measurement systems and plan their day or week. And, they can troubleshoot at home from their smart phone if necessary. The tool is used to track and monitor calibrations as well as process measures. It makes the lab more efficient and less costly to run.

The irony of AI in the chemical industry is that it hasn't changed as much as I would like over the last 30 years. The issue lies in the fact that AI was already present in the industry doing a task that chemical engineers assigned it – that of supporting open- and closed-loop process control and use in online or at-line analysers. The mathematics of AI was not used for problem solving and problem avoidance – which should have been the next step. The chemical industry started down this road in the '80s and has only grudgingly expanded the use of the mathematics to go beyond the control and online sensor arena. At Dow I became the 'personality' that pushed for the additional capabilities I first employed with the invaluable help of others. The implementation of AI is a challenge. For those who say that chemical plants will be run by AI, I say, 'not so fast'. There is not a data set complete enough to show that an algorithm can run a plant without human monitoring and intervention. It is for humans to learn to use AI to help them run plants, not the other way around.

Where the industry has changed dramatically is real-time analytics and anticipating and planning for problems that are to come, rather than doing a post-mortem after a problem caused the plant to fail. This is a key difference in chemical production today. Real-time analytics helped my global labs, plant engineers and operators bolster their understanding of the plants and the data, and increased the credibility of the information coming out of the labs. It's a fight – changing habits and perspective on data visualisation and manipulation is very difficult in the engineering and plant operation community, but the industry continues to move forward, which has positive impacts on people, the environment and our customers.

Lloyd Colegrove recently retired as director of data services and fundamental problem solving within manufacturing and engineering. He was also the analytics platform director for Dow's Manufacturing and Engineering's Industry 4.0 programme.

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SCIENTIFIC COMPUTING WORLD

Advancing additive manufacturing

ROBERT ROE TAKES A LOOK AT HOW SOFTWARE IS HELPING TO IMPROVE THE EFFICIENCY AND EFFECTIVENESS OF 3D PRINTING

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Additive manufacturing (AM) is opening up new possibilities for engineers to create components and subsystems enabling rapid prototyping and novel designs that can help to accelerate innovation. Software plays a key role in the maturation of this market with rapid increases in the complexity of parts and the materials and methods used to create new components with AM.

Increasingly, the market is seeing validation and quality control tools that can help designers and engineers to ensure that time and resources are not wasted on unnecccsary design iterations. Software is also driving the use of new methods and materials such as the application of AM techniques to the production of solid rocket energetics or the use of machine learning to print AM designs more accurately.

Quality-control software for additive manufacturing

Aerospace, automotive, consumer products, medical devices, national defence and other sectors that use additive manufacturing (AM) and 3D printing technologies can benefit from quality-control software that is being commercialised by Araqev, a Purdue University-spin out company.

Araqev's software helps end-users print products in only a few design iterations, leading to less scrap material and machining time, eliminating the frustrations with 3D printing, and improving satisfaction with the final printed products.

Araqev creates software solutions for closed-loop, smart control in additive manufacturing and 3D printing based on machine learning (ML). Araqev's patented ML algorithms enable users to learn in fractions of a second how to print more accurately across new shapes and processes, resulting in less wasted scrap and machining time.

Arman Sabbaghi, associate professor in Purdue's Department of Statistics in the College of Science, is Araqev's CEO and president. 'We estimate that the quality-control issue with additive manufacturing can lead to nearly $2bn in global losses annually based on a model for the production costs of metal additive manufacturing systems that was developed by Baumers, Dickens, Tuck and Hague in their 2016 paper published in the peer-reviewed journal Technological Forecasting and Social Change,' Sabbaghi said.

To use Araqev's software, customers upload their nominal design files and scanned point cloud data from their printed products.

'Our software uses these inputs to fit machine learning models that can simulate shape deviations for future printed products,' noted Sabbaghi. 'Furthermore, the machine learning models enable our software to derive modifications to the nominal designs, known as compensation plans, so that when the modified designs are printed, they will exhibit fewer shape deviations compared to the case when the original designs are printed.'

Araqev's algorithms also enable the transfer of knowledge encoded via machine learning models across different materials, printers and shapes in an additive manufacturing system.'This means that our software enables a comprehensive platform for a customer to improve quality of their entire system,' Sabbaghi added.

'The power and cost-effectiveness of our algorithms were most recently demonstrated via two validation experiments for the Markforged Metal X 3D printer involving 17-4 PH stainless steel products,' Sabbaghi said. 'Our algorithms reduced shape inaccuracies by 30 per cent to 60 per cent, depending on the geometry in at most two iterations, with three training shapes and one or two test shapes for a specific geometry involved across the iterations.'

Araqev is establishing direct partnerships with 3D printing manufacturers and companies using 3D printers that Sabbaghi said will enable the company to scale quickly.

'We will establish licensing contracts after demonstrating to the companies the savings and benefits that we can offer for their processes,' Sabbaghi said. 'These partners will incorporate our software into their systems and sell them to their customers, which provides us with a significant customer channel.'

Araqev licensed the software from the Purdue Research Foundation Office of Technology Commercialisation. The research to create the software received funding from the NSF's Cyber-Physical Systems program and CMMI EAGER program, and the Purdue Research Foundation Office of Technology Commercialization's Trask Innovation Fund. Araqev received funds from Elevate Ventures' Regional Pre-Seed Competition, Purdue's Regional NSF I-Corps program, the MKE Tech Hub Coalition Challenge and the Purdue Foundry Boost program.

Velo3D's software deployed at Lockheed Martin

Velo3D, a metal additive manufacturing technology company for mission-critical parts, delivers an end-to-end additive manufacturing solution that has been selected by Lockheed Martin for its Additive Design and Manufacturing Center. This research centre pilots new additive manufacturing technologies for production deployments in Lockheed Martin's Space division.

> "Our software uses these inputs to fit machine learning models that can simulate shape deviations for future printed products"

Velo3D was selected for its advanced quality assurance capabilities made possible through its Assure software, which provides layer-by-layer traceability of machine health, part integrity, and build reporting.

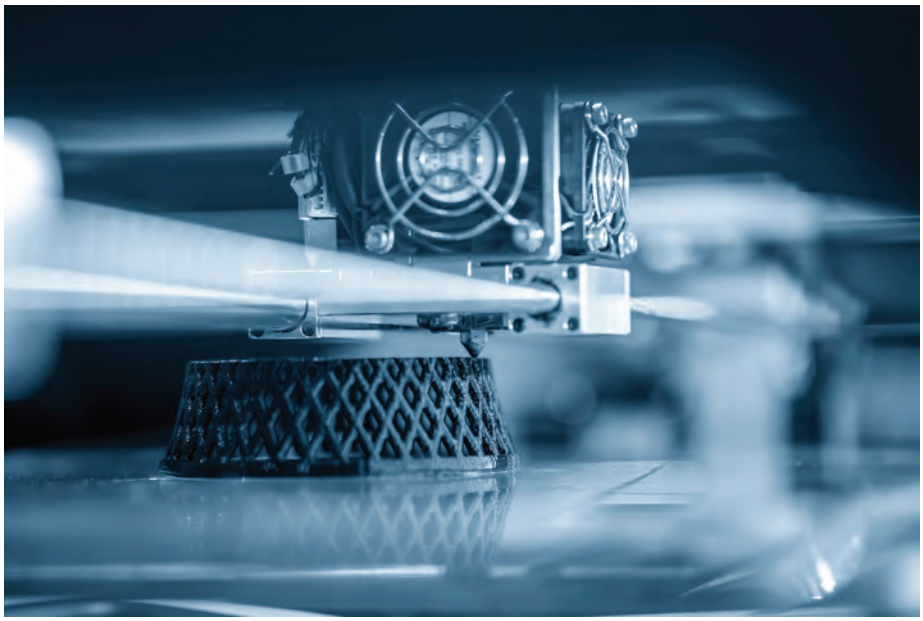
Benny Buller, Velo3D CEO and founder commented: 'The past few years have uncovered weaknesses in the global supply chain, which is causing many companies to evaluate new technologies to feed production of their mission-critical parts and hardware, and distribute their manufacturing processes.'

'An additive manufacturing solution that can print identical parts anywhere you have a printer can not only help solve some very specific, complex challenges in our global supply chain, it can also lower production costs and lead times, and enable the manufacturing of parts in closer proximity to where they are needed,' Buller added.

The solution Velo3D has delivered to Lockheed Martin includes a Sapphire printer, Velo3D's Flow print preparation software, its Assure quality assurance and control software, and its underlying Intelligent Fusion manufacturing process, which optimises the additives manufacturing process by combining process simulation, geometry-based detection, and build process monitoring during print execution.

This end-to-end solution gives customers the confidence that the mission-critical parts printed using Velo3D's additive manufacturing technology preserve design intent. It also provides customers with the ability to produce identical parts across any Velo3D Sapphire printer, so as production needs increase, customers can merely add additional printers to their production facilities anywhere in the world or utilize Velo3D's network of contract →

"This means that our software enables a comprehensive platform for a customer to improve quality of their entire system"



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→ manufacturers.

The company's latest Sapphire XC system enables higher productivity and lower production costs for Velo3D customers. It also enables the printing of parts that are 600 mm in diameter and up to 550 mm in height – 500 per cent larger than the previous Sapphire system.

Lockheed Martin also recently invested in another AM startup, X-Bow Systems. X-Bow Systems, a US-based space technology company applying additive manufacturing techniques to the production of solid rocket energetics, announced it had closed a $27 million Series A investment round.

The round closes ahead of X-Bow's static fire test of its 32" diameter 'Ballesta' solid rocket motor and subsequent launch at White Sands Missile Range, New Mexico. This will be the first large-diameter scale motor designed and tested by a non-legacy systems integrator supplier in over 30 years, bringing innovation to the sector from a modern technology competitor.

The Series A round was co-led by Crosslink Capital and Razor's Edge Ventures, with additional participation from Lockheed Martin Ventures and Broom Ventures.

X-Bow's capital raise team was led by its co-founder and CRO, Maureen Gannon. The capital raise comes at a time of significant growth for X-Bow as the company advances its patent-pending additive manufacturing technology for solid rocket energetics and expands its solid rocket motor product portfolio. X-Bow plans to release affordable large-scale motor designs and modular boost vehicle architectures, which are already in development with customers across the US national security, defence and space communities.

Jason Hundley, X-Bow CEO and founder commented: 'We are proud of the support we have received from our investors and appreciate the confidence they signal in X-Bow's team, breakthrough technology and innovative approach to solid rocket motor development. Raising a strong round with these high calibre investors allows us to increase our rapid growth and accelerate our plans to disrupt a critical industry.'

'I am also very fortunate to work with an outstanding team here at X-Bow that is making groundbreaking achievements in the sector,' Hundley added.

Matt Bigge, Crosslink Capital Partner added: 'X-Bow has a great combination of experienced leadership and a truly innovative additive manufacturing technology for energetics. They are the much-needed changemaker poised to disrupt the energetics market with its disruptive technologies. Crosslink invested in X-Bow because of its ability to catalyze a critical evolution in the national security, defense and commercial space technology markets.'

Improving the validation of critical components

Markforged, the creator of the integrated metal and carbon fibre additive manufacturing platform, The Digital Forge, recently announced the acquisition of Teton Simulation Software, whose SmartSlice technology automates validation and optimises part performance for additive manufacturing applications.

Markforged will integrate Teton's technology with its 3D printing software solution, Eiger, as a subscription add-on that will offer all manufacturing customers, including small- and medium-sized businesses, a streamlined workflow spanning part design, testing, optimisation, validation and printing at the point of need, all on a single, cloud-based platform.

The integration of cloud-native simulation software into Markforged's digital forge platform will enable manufacturers to validate advanced composite parts for the most demanding production applications.

Shai Terem, president and CEO of Markforged states: 'Software is the core of Markforged's solution and our competitive edge. The acquisition of Teton Simulation advances our industry leadership in using software to increase process automation and offers our customers an easy way to validate their parts on the same platform they use to print them.'

'Adding this functionality enables our customers to utilise The Digital Forge deeper into their manufacturing operations,' Terem continued. 'I am excited to welcome the Teton team to Markforged, as we share the vision of leading the future of distributed manufacturing. Together, we continue to strengthen our team and enable our customers to produce mission-critical, end-use parts.'

The acquisition adds strategic functionality to the Digital Forge to give Markforged's thousands of users confidence that printed parts will perform as intended, enabling them to replace even more end-use metal parts with validated Continuous Fiber Reinforcement (CFR). This addition to Markforged's software offerings will help customers take the guesswork out of configuring slicing parameters for end-use requirements, knowing they can estimate part performance without the wasteful and slow process of physical testing.

Teton's SmartSlice product integrates with slicer programs and replaces the typical print-break-repeat prototyping cycle which speeds up development and reduces the time and cost of production-quality parts.

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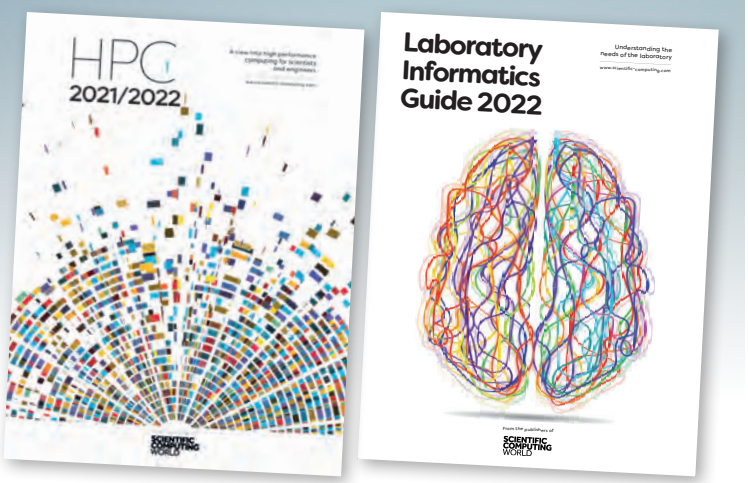

The latest news stories in scientific computing

HIGH PERFORMANCE COMPUTING

DOE announces $20m for extreme-scale science

The US Department of Energy (DOE) announced $20m in basic research to explore potentially high-impact approaches in extreme-scale science and scientific computing.

The research is focused on developing enabling technologies for artificial intelligence, quantum information science, high-productivity programming and discrete event simulation.

Barbara Helland, DOE associate director of science for Advanced Scientific Computing Research, said: 'Disruptive technology changes, due to advances in high-end computing coupled with the creation of massive data sets for use with scientific machine learning, are impacting science applications, algorithms, computer architectures and ecosystems.

'We need new, innovative ideas to develop effective approaches and enable technologies to realise the full potential of scientific heterogeneous computing from these emerging technologies,' Helland added.

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The two-year, multi-institutional team proposals are open to universities and colleges, non-profit organisations, for-profit organisations, DOE/NNSA laboratories, and other federal agencies. Applicants are encouraged to implement DOE diversity, equity, and inclusion guidelines. The total planned funding is up to $20 million in 2022.

MODELLING AND SIMULATION

Partnership aims to make autonomous driving more realistic

Simulation software provider dSPACE is working with cogniBIT to integrate its AI-based driver model and the unpredictable behaviour of human drivers to make traffic scenarios for the development and testing of autonomous vehicles even more realistic.

In the first stage, dSPACE is pairing its simulation environment Automotive Simulation Models (ASM) with driveBOT, cogniBIT's AI-based driver model. In the future, behaviour models from road users, such as pedestrians or motorcyclists, will be successively integrated into simulations.

Dr Lukas Brostek, co-founder and CEO of cogniBIT, said: 'dSPACE provides a powerful and widely used tool in the industry for developing functions for automated and autonomous driving. We at cogniBIT are pleased to complement ASM's already-high fidelity in areas such as vehicle dynamics, sensor and environment modelling with a valid driver and road user model.'

Traffic situations are influenced by the behaviour of individual road users. This includes emotions such as fear, surprise and happiness, but also limitations such as the road user's impaired view. Highly automated and autonomous driving will become safer in practice only once all of these aspects are realistically integrated into the simulation. driveBOT, the AI-based driver model from cogniBIT, lets users replicate human-like behaviour in the simulation and reproduce realistic traffic scenarios.

Realistic driver models play an important part in ADAS/AD development because, the functions for autonomous driving are designed for the operational design domains (ODD). The automated-driving systems have to function in these defined fields of operation. The system will request the driver to take control if the vehicle leaves this field.

To make the assistance systems more realistic in the next stage, further factors can be included using cogniBIT's AI-based driver models, for example, a nervous new driver or a stressed driver behind the wheel.

The AI-based driver models from cogniBIT can be used in the ASM simulation to simulate more realistic surrounding traffic, not only for the ego-vehicle, but also in multi-agent simulation for the surrounding traffic participants (fellows). The realistic movement of the fellows allows simulated traffic scenarios to be varied efficiently, to identify corner cases, and therefore, to define the limits of a driving function.

Christopher Wiegand, strategic product manager of the dSPACE Automated Driving and Software Solutions business unit, added: 'Driving function for SAE Levels 2-5 must be carefully validated with regard to safe interaction with road users. The involvement of neuroscientists and sensorimotor findings leads to valid and meaningful simulation results and will make driving functions safer.'

HIGH PERFORMANCE COMPUTING

Fraunhofer IPMS part of project to develop first German quantum computer

Together with 24 German research institutions and companies, the Fraunhofer Institute for Photonic Microsystems (IPMS) is working on a quantum computer with improved error rates in the collaborative project QSolid, coordinated by Forschungszentrum Jülich.

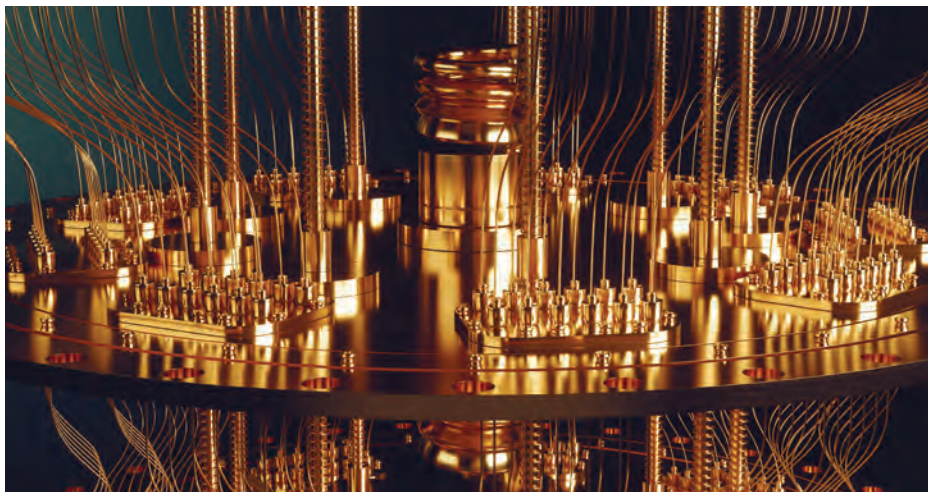
The goal is to make Germany a leader in the field of quantum technology and thus to maintain its independence and open up numerous new applications in science and industry. The Federal Ministry of Education and Research has allocated €76.3m in funding for the next five years.

Dr Benjamin Lilienthal-Uhlig, business unit manager for Next Generation Computing at Fraunhofer IPMS, stated: 'We intend to use our know-how and infrastructure to enable scalable quantum processors that build on the achievements and advantages of silicon-based semiconductor manufacturing.

'This concerns, for example, manufacturing processes like deposition and nanopatterning, or wafer-scale electrical characterisation. Together with Globalfoundries and Fraunhofer IZM-ASSID, an interposer technology will be developed focusing on high-density superconducting interconnects and thermal decoupling through advanced packaging,' added Lilienthal-Uhlig.

Fraunhofer IPMS is part of the newly launched German-funded project, QSolid (Quantum Computer in the solid state). The project centres on quantum bits – or qubits for short – of very high quality, that is, with a low error rate. The quantum computer will be integrated into Forschungszentrum Jülich's supercomputing infrastructure at an early stage and will contain several next-generation superconducting quantum processors, including a 'moonshot' system that has been proven to exceed the computing power of conventional computers. The first demonstrator will go into operation in mid-2024 and will make it possible to test applications as well as benchmarks for industry standards.

Fraunhofer IPMS' Center Nanelectronic Technologies contributes a 4000 m² clean room and its expertise in state-of-the-art, industry-compatible CMOS semiconductor fabrication on 300 mm wafer standard. 'Additionally, cryogenic characterisation of Globalfoundries' CMOS technology for scalable control will be studied,' explained Lilienthal-Uhlig.



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LABORATORY INFORMATICS

Partnership aims to use AI to identify novel cMET inhibitors for lung cancer

Arctoris, a tech-enabled biopharma company, and Evariste Technologies, an AI-drug discovery company, have announced a joint venture to identify novel small molecule kinase inhibitors for the treatment of patients with Non-Small Cell Lung Cancer (NSCLC). The partnership brings together two highly synergistic approaches for AI-guided and robotics-powered molecule design, to significantly accelerate the DMTA (Design, Make, Test, Analyse) cycle.

Dr Nicholas Firth, CEO of Evariste Technologies, stated: 'We are really excited to be working with Arctoris on this project. There is a huge need for next generation cMET inhibitors for NSCLC. This is a cancer that affects millions globally, and we hope we can bring meaningful benefit to some of these lives in the near future.'

Current treatment options for NSCLC are limited, especially in advanced stages. It has been shown that the proto-oncogene cMet is mutated or upregulated in approximately 5% of all NSCLC cases. While cMET has been successfully targeted by two recently approved drugs (Tepotinib, Capmatinib), rapid development of resistance has been reported and there is a clear need for improved second-generation cMET inhibitors to overcome resistance.

The two companies are combining their platforms for AI-guided and robotics-powered drug discovery to develop a set of novel kinase inhibitors against cMET. The partnership will bring together two highly synergistic approaches – quantitative decision-making and state-of-the-art generative chemistry, combined with real-time biological and biochemical profiling and data generation, to significantly accelerate the design-make-test-analyze cycle. The two companies will also use their strong links to leading centres for NSCLC treatment to leverage clinical insights, inform their discovery and development efforts and directly address clinically relevant liabilities limiting the effectiveness of currently available therapies.

Arctoris CEO Martin-Immanuel Bittner MD DPhil FRSA, commented on the joint venture: 'Together with our partners at Evariste, we are developing novel treatment options in NSCLC against a fully validated target, where first generation inhibitors can be improved in a clinically meaningful way. Combining patient-derived insights on resistance and toxicity patterns with AI-powered molecule design and our robotic platform, Ulysses, we aim to develop superior next-generation inhibitors within a significantly accelerated time frame.'

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The collaboration between Arctoris and Evariste is already underway and has identified novel, active chemical matter. 'We look forward to keeping our community updated about the progress we are making within the joint venture between Evariste Technologies and Arctoris. We have had an incredible start already, and we look forward to continuing our work to develop better treatment options for patients worldwide,' added Bittner.

LABORATORY INFORMATICS

CliniSys acquires ApolloLIMS

CliniSys has announced it has acquired ApolloLIMS, a provider of laboratory information management systems based in Nashville, Tennessee, with specialist expertise in clinical, public health, toxicology and molecular diagnostics.

The ApolloLIMS team will join CliniSys, bringing their industry expertise, knowledge and proven technology offering. The announcement confirms a significant step toward fulfilling CliniSys' vision to enable a new wave of digital diagnostics and community laboratories, spanning environmental, water quality, public health, toxicology and agriculture laboratory testing markets.

CliniSys' CEO Michael Simpson commented: 'ApolloLIMS and its team bring tremendous expertise to CliniSys. Not only will they help expand our knowledge of diagnostics within and beyond the clinical laboratory, but they share our deep belief that the future of digital diagnostics lies in the cloud. With the addition of ApolloLIMS, we are now poised to seize new opportunities to quickly expand our offerings in community and public health diagnostics, and to help better track and prevent disease.'

All current ApolloLIMS customers will continue to be supported as normal. Overtime, the ApolloLIMS solution will be integrated into the CliniSys product family as the business accelerates the roadmap for its next-generation SaaS product strategy.

Eric Dingfelder, SVP and general manager, Horizon and ApolloLIMS (CliniSysGroup companies), added: 'ApolloLIMS diverse expertise helps us push the boundaries of the diagnostics market and enable organisations and governments to better fight the spread of disease. Modern laboratories need the very best technology platforms to streamline their workflows and improve disease monitoring. JoiningCliniSys ensures ApolloLIMS' customers of that future.'

MODELLING AND SIMULATION

Siemens collaborates with Pasqal to research quantum applications

Pasqal has announced a multi-year research collaboration with Siemens Digital Industries Software to advance quantum computational multiphysics simulation.

Pasqal's proprietary quantum methods are used to solve complex nonlinear differential equations and could be applied to enhance the performance of Siemens' software solutions, which are used for computer-aided product design and testing in the automotive, electronics, energy and aerospace sectors.

The first phase of the collaboration will last 3.5 years and will involve researchers from both companies and from Exeter University, Pasqal's academic partner. The project is fully funded by Siemens and includes a sponsored academic working in the research group of theoretical physics, professor Oleksandr Kyriienko.

Georges-Olivier Reymond, CEO and founder of Pasqal, commented: 'Our collaboration with Siemens will explore how quantum computing can benefit Siemens' customers, who are looking for more accurate "digital-twin" prototyping, which can reduce the need for costly and time-consuming physical prototyping in sectors like automotive, electronics, energy and aerospace. We're proud to collaborate with Siemens, a technology giant and innovator, to apply and expand our quantum solutions to solve real-world problems with significant business impact.'

The project builds on Pasqal's research, including its methods for solving nonlinear differential equations. For years, it was uncertain whether quantum computers were able to outperform classical computers in this field, but Pasqal's recent progress makes these methods promising candidates for near-term quantum advantage – especially since researchers developed a novel digital-analogue implementation tailored for its neutral-atoms quantum processors, which makes these 30 times more efficient than superconducting quantum processors.

The collaboration allows Siemens to leverage Pasqal's quantum solutions and expertise to fast-track the development of quantum-enhanced solutions for its customers. For Pasqal, this collaboration builds on the company's momentum since its merger with Qu&Co earlier this year, which formed a full-stack quantum computing company with a strong focus on industrial applications and a stellar line-up of industrial clients, including Johnson & Johnson, LG, Airbus, BMW Group, EDF, Thales, MBDA and Credit Agricole CIB.

'We look forward to seeing how quantum computing can yield a significant near-term benefit for our clients,' said Jean Claude Ercolanelli, senior vice president of simulation and test solutions at Siemens Digital Industries Software. 'Pasqal's algorithms for solving differential equations and its neutral atom quantum processors are ideally suited to solve the [most relevant and challenging] computational problems, and we look forward to working with Pasqal to advance this field.'

Pasqal's quantum computing technology controls neutral atoms (atoms possessing an equal number of electrons and protons) with optical 'tweezers', using laser light to engineer full-stack processors with high scalability, unprecedented connectivity and long coherence times. Its software-agnostic quantum processing units can operate at room temperature with lower energy, allowing the company to address complex problems more efficiently than classical computers.

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