

# PROTEIN POWER

Biophysics institute works up to 80 per cent faster to map proteins, using HPC blade solution with Intel Xeon Processors



Unlocking the secrets of proteins is essential to understanding how organisms work. In the future, this could help scientists develop ground-breaking new medicines or industrial applications. However, proteins are made up of thousands of atoms and studying them involves lengthy and complex computations. This poses a challenge for researchers, who depend on high-performance computing (HPC) but often lack datacentre space at publicly funded universities and research centres.

#### SOLUTIONS:

- GREEN IT
- HPC



#### CUSTOMER PROFILE

**COMPANY:** Max Planck Institute of Biophysics  
**INDUSTRY:** Biotechnology & Science  
**COUNTRY:** Germany  
**FOUNDED:** 1937  
**EMPLOYEES:** 187  
**WEBSITE:** [www.biophys.mpg.de](http://www.biophys.mpg.de)

#### CHALLENGE

Computational researchers at the Max Planck Institute of Biophysics needed to expand their high-performance computing cluster. With limited datacentre space and cooling capacity, the expansion had to be compact and energy efficient.

#### SOLUTION

The IT team chose a cluster of Dell blade servers supported by a Dell storage array. The team uses Dell ProSupport for IT with the Mission Critical option to help it maintain maximum uptime.

#### BENEFITS

##### Get IT Faster

- Solution implemented in one month, to plan and within budget

##### Run IT Better

- Power and cooling minimised
- Research accomplished up to 80 per cent faster with Intel® Xeon® Processors
- Expanded infrastructure managed without extra staff resources

##### Grow IT Smarter

- Compact solution accommodates 45 per cent future expansion

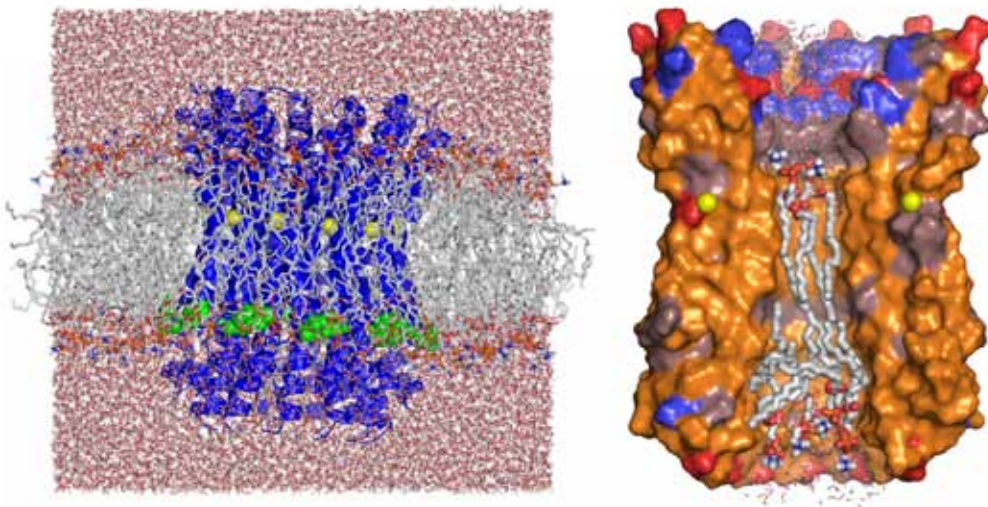


At the Max Planck Institute of Biophysics in Frankfurt, two research groups use computations to map the function of proteins based on their structure and dynamics. They hope this understanding might one day help biomedical scientists work out ways to correct proteins that are malfunctioning, or lead to the development of new biotechnological applications. The two groups launched their research with a Dell HPC cluster, based on 47 Dell™ PowerEdge™ 1950 rack servers with Intel® Xeon® quad-core Processors, supported by a Dell PowerVault™ MD1000 direct attached storage array. But when the scope of their work widened, the groups needed more processing power.

This change in requirements coincided with blade technology coming onto the market. Max Planck Research Group leader José Faraldo-Gómez quickly saw that compact high-performance blades would let him and his colleague Lucy Forrest significantly expand the HPC cluster, while staying within Max Planck Institute's limited datacentre space. At the same time, blades were highly energy efficient, minimising the power required to run the expanded cluster and avoiding the need for expensive alterations to the cooling system.

Faraldo-Gómez decided to continue working with Dell whose HPC cluster had supported the research groups well so far. Following advice from Dell consultants, Faraldo-Gómez and his colleague selected a high-density, energy-efficient 96-node cluster of Dell PowerEdge M600 servers with quad-core Intel Xeon Processors 5440, mounted in six compact PowerEdge M1000e enclosures. They chose to support the cluster with a reliable and scalable Dell PowerVault MD1000 direct attached storage array and connected the solution with a cost-efficient Dell PowerConnect™ 2748 gigabit Ethernet switch.

The solution was implemented by Dell consultants in a month, to plan and within budget. The Max Planck Institute ensured maximum uptime with Dell ProSupport for IT with Mission Critical four-hour on-site repairs.



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José Faraldo-Gómez, Max Planck Research Group leader, Max Planck Institute of Biophysics

“Dell worked with us every step of the way to optimise our HPC solution. As a computational research scientist, I know my tools, but I was impressed with the level of expertise shown by Dell’s consultants. Knowing that you are in good hands with your IT partner is more than reassuring – it’s priceless,” says Faraldo-Gómez.

#### RESEARCHERS WORK UP TO 80 PER CENT FASTER WITH MULTI-CORE PROCESSOR BLADES

Faraldo-Gómez and his colleagues chose Dell PowerEdge M600 blade servers, because they come with Intel Xeon Processors. They were convinced that Intel offered the best price-performance ratio. “To understand protein function, we need to study the movement of

thousands of individual atoms, which involves many independent computations. The more processing cores we have, the more we can accomplish. Our Dell PowerEdge blades with Intel Xeon quad-core Processors let us work up to 80 per cent faster than with dual-core Processors,” says Faraldo-Gómez.

#### DATA CENTRE CAN ACCOMMODATE 45 PER CENT INFRASTRUCTURE EXPANSION

With space at a premium at the busy Max Planck Institute, the research groups needed the most compact HPC infrastructure possible. Dell PowerEdge M1000e modular blade enclosures, each holding 16 Dell PowerEdge M600 blade servers, provided the perfect answer.

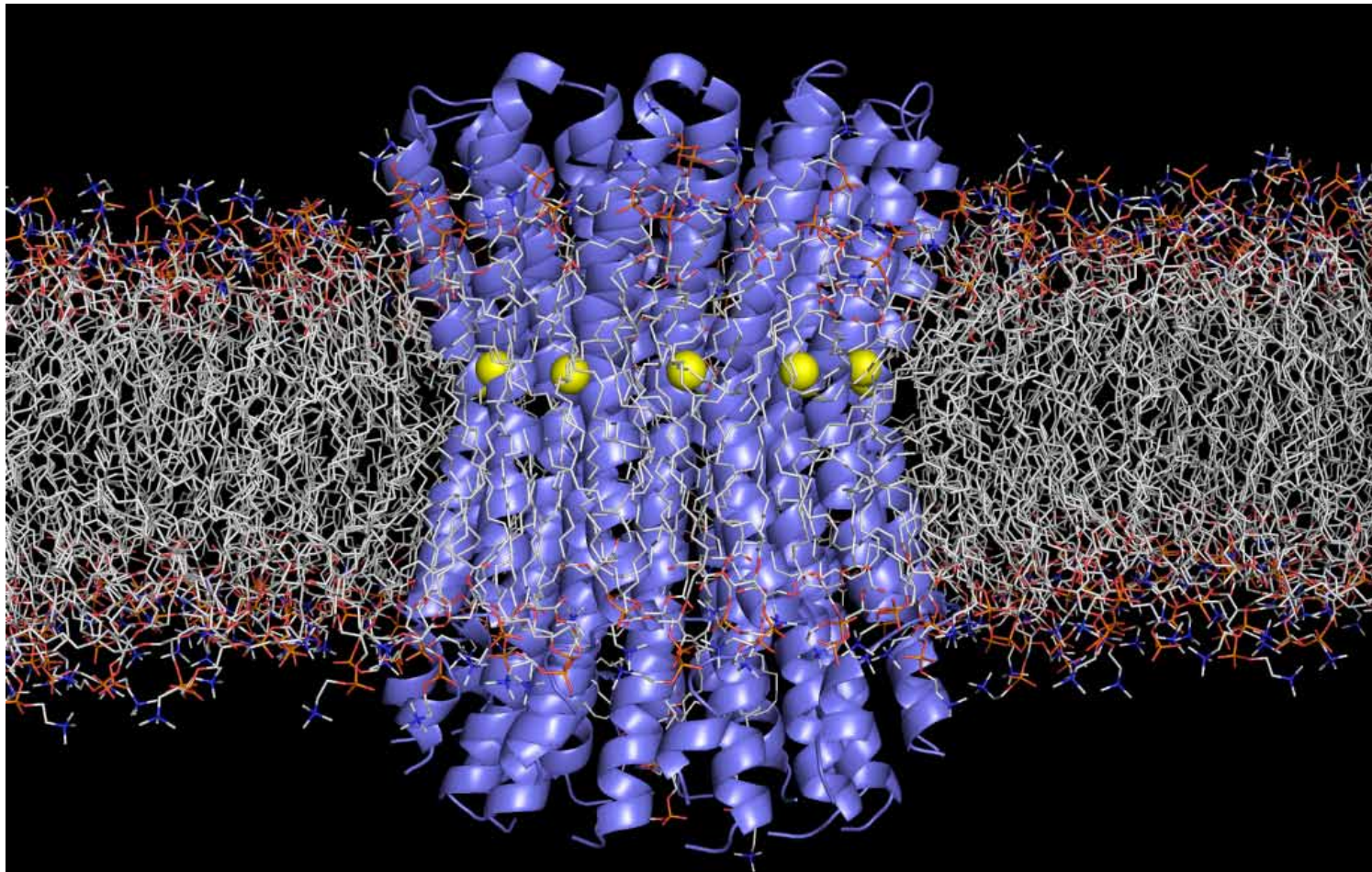
### HOW IT WORKS

#### HARDWARE

- Dell™ PowerEdge™ M600 blade servers with Intel Xeon Processors 5440
- Dell PowerEdge M1000e modular blade enclosures
- Dell PowerVault™ MD1000 direct attached storage array
- Dell PowerConnect™ 2748 gigabit Ethernet switch

#### SERVICES

- Dell ProConsult
- Dell ProSupport for IT
  - Mission Critical option
  - Next Business Day On-site Service



**“BECAUSE WE COMPUTE 24/7, OUR ELECTRICITY BILL COULD ADD UP VERY EASILY, BUT OUR DELL POWEREDGE M600 BLADES KEEP IT TO A MINIMUM. AS PUBLICLY FUNDED RESEARCH GROUPS, THIS IS IMPORTANT BECAUSE IT HELPS US DEMONSTRATE THAT WE ARE AS COST AND ENERGY EFFICIENT AS WE CAN POSSIBLY BE.”**

José Faraldo-Gómez, Max Planck Research Group leader, Max Planck Institute of Biophysics

M1000e enclosures are built from the ground up to combat server sprawl and optimise manageability, and M600 blades offer a 60 per cent greater density than traditional 1U rack servers<sup>1</sup>. “We were running out of space, but, thanks to our compact Dell PowerEdge blade solution, we have tripled our HPC cluster node-count and still have more room to spare. Now, if we need to, we can expand our solution by another four blade enclosures, or 45 per cent, without having to extend our datacentre,” says Faraldo-Gómez.

#### **POWER CONSUMPTION MINIMISED**

The Dell HPC solution is highly energy efficient, which helps the Max Planck research groups keep their cooling requirement and power consumption low. “Because we compute 24/7, our electricity bill could add up very easily, but our Dell PowerEdge M600 blades keep it to a minimum. As publicly funded research groups, this is important because it helps us

demonstrate that we are as cost and energy efficient as we can possibly be,” says Faraldo-Gómez.

The Dell PowerEdge M600 blade servers and M1000e modular blade enclosures are highly power efficient. Designed to deliver a high performance-to-watt ratio, they also minimise the requirement for cooling. For example, the M1000e enclosure takes advantage of thermal design efficiencies, such as ultra-efficient power supplies and dynamic power-efficient fans with optimised airflow design that help cool the chassis. This meant that the research groups tripled their HPC cluster without redesigning their datacentre cooling system.

#### **EXPANDED INFRASTRUCTURE MANAGED WITH SAME RESOURCES**

Due to the specialist nature of their work, the computational research groups at the Max Planck Institute use a proprietary system

management solution. However, because the blade expansion integrated seamlessly with the institute’s existing HPC cluster and is easy to manage, the research groups did not need to upgrade the management software, upload a new operating system, install a new network or pay for more manpower to run the infrastructure. This keeps costs low, which helps the research groups optimise their financial resources.

#### **RELIABLE STORAGE KEEPS VITAL RESEARCH DATA SAFE**

Faraldo-Gómez was looking for a storage solution that would be reliable and flexible as well as cost-effective. He chose a second Dell PowerVault MD1000 direct attached storage array because this product had worked well with the existing cluster.

1. [www.dell.com/content/products/productdetails.aspx/pedge\\_m600?c=us&l=en&s=bsd&cs=04](http://www.dell.com/content/products/productdetails.aspx/pedge_m600?c=us&l=en&s=bsd&cs=04)

**“IT WAS IMPORTANT FOR ME TO SECURE  
MAXIMUM AVAILABILITY FOR THE CLUSTER AND  
TO KNOW THAT IF A SERIOUS PROBLEM ARISES  
SOMEONE WILL COME ON-SITE WITHIN FOUR  
HOURS TO FIX IT. PROSUPPORT FOR IT MISSION  
CRITICAL GIVES ME THAT PEACE OF MIND.”**

José Faraldo-Gómez, Max Planck Research Group leader,  
Max Planck Institute of Biophysics

Faraldo-Gómez says: “Our computations take months, and afterwards we need to write up the results for scientific journals, so the data must be available for interactive work for a year or more. With our reliable Dell PowerVault MD1000 direct attached storage array, we can be sure that is the case.”

The MD1000 storage array is designed to work optimally with Dell PowerEdge blade servers. It lets the Max Planck Institute computational research groups mix serial attached SCSI (SAS) and serial advanced technology attachment (SATA) drives within a single enclosure, which means that they can choose the most cost-efficient storage solution to meet their requirements at any one time. And, thanks to its modular design, they can expand the storage array from 15 to 45 drives per RAID port, which further increases the flexibility of the groups.

**PEACE OF MIND WITH DELL  
PROSUPPORT FOR IT MISSION  
CRITICAL OPTION**

The Max Planck Institute computational research groups depend 100 per cent on their HPC cluster. If the system goes down, the researchers are unable to work. The fast response offered by Dell ProSupport for IT was an important factor in the decision to work with Dell. Another significant factor was the flexible modular structure of Dell ProSupport, which allowed the research

groups to design the support solution to suit their specific needs. They chose ProSupport for IT Mission Critical with four-hour on-site repairs to maximise uptime for the PowerEdge blade cluster’s head node as well as the PowerVault MD1000 storage array and PowerConnect 2748 switch. For the less critical part of the infrastructure, they selected ProSupport for IT with the Next Business Day On-site Service. “It was important for me to secure maximum availability for the cluster and to know that if a serious problem arises someone will come on-site within four hours to fix it. ProSupport for IT Mission Critical gives me that peace of mind,” says Faraldo-Gómez.

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