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## CMBI recalculates protein structures using VMware-based HPC cloud

For the recalculation of protein structures the Centre for Molecular and Biomolecular Informatics (CMBI) at the UMC Academic Medical Centre St. Radboud in Nijmegen needs vast computing power that can be deployed simply and flexibly. Additional computing power must be immediately available as demand arises. The CMBI addresses this need with a VMware-based 'High Performance Computing Cloud', delivered by a vCloud Powered Partner.

Proteins are extremely complicated molecules. A protein's structure is a three-dimensional model, as it were, showing the location in space of each of its atoms. From a scientific point of view, having an accurate picture of as many proteins as possible is vitally important. A clear understanding helps in the development of new medicines, for instance. At the moment, about 89,000 protein structures are known, 10,000 of which have been resolved by a physical phenomenon called Nuclear Magnetic Resonance (NMR). The research of the Centre for Molecular and Biomolecular Informatics is aimed at this latter group. About half of the structures resolved with NMR is a candidate for recalculation, which yields an even better insight into the structures. "The technology to calculate structures has made great strides over the last few years", said researcher Wouter Touw, a PhD student working for the CMBI. "Now we can calculate more in a single day than we could ten years ago in a whole month."

### CHALLENGE

Proteins are extremely complicated molecules. For the recalculation of protein structures the CMBI primarily needs ample computing power that can be scaled up indefinitely without the need for scheduling. Another CMBI requirement is that computational power is simple, flexible and quickly available.

### SOLUTION

The type of CMBI project is very well suited to a High Performance Computing cloud platform. The cloud platform is aimed at maximum performance and maximum reliability. VMware vCloud Director enables 'horizontal' as well as 'vertical' scaling.

### RESULTS

With the High Performance Computing cloud platform the CMBI has the flexibility to get started quickly calculating protein structures and scaling up indefinitely. Additional computing power is simple and immediately available. This saves the CMBI much time and money.

### Embarrassingly parallel

For the recalculation of protein structures the CMBI primarily needs ample computing power that can be scaled up indefinitely without the need for scheduling. Another CMBI requirement is that computational power is simple, flexible and quickly available. Cloud computing fits the research institute's requirements best.

"Our issues are really embarrassingly parallel", says professor Gert Vriend, leading the research group 'Protein Structure Bioinformatics' in the CMBI. "For every protein structure we want to recalculate we follow the same steps in a set order and one core runs somewhere between 1 and 24 hours. We do not need a lot of memory for our project; it is especially the 'supercycles' that have to be available quickly as soon as we need them. The cloud fits the bill exactly."

### The VMware-based cloud platform

The CMBI, through the national HPC center SARA (now called SURFsara), eventually decided on a vCloud Powered Partner by VMware. The type of CMBI project and this partner's High Performance Computing cloud platform quickly proved to complement each other perfectly. For instance, the platform is geared towards embarrassingly parallel calculations, enabling them to make heavy calculations in a short time.

The cloud platform is aimed at maximum performance and maximum reliability. VMware vCloud Director enables 'horizontal' as well as 'vertical' scaling. In 'vertical scaling', a maximum of cpu and memory always remain in the blades. In 'horizontal scaling', this restriction is lifted, enabling seamless upscaling. CMBI uses horizontal scaling: doubling the number of resources really means doubling of the speed.

## VMWARE CASE STUDY

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***“Five years ago we would have needed servers across Europe for our calculations, but now this cloud platform suits our needs very well”.***

Professor Gert Vriend, Centre for Molecular and Biomolecular Informatics

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### VMWARE IN PRACTICE

- vSphere
- vCenter
- vCloud Director
- vShield
- ChargeBack
- vCenter Operations
- vCenter Orchestrator

### 100,000 cpu hours

The CMBI has now recalculated about 3400 structures on the cloud platform. In total 100,000 cpu hours were used in about a week. “This would take almost three years on a normal four-core pc”, says Touw.

The CMBI is understandably very excited. Touw: “Capacity is always available when we need it. So we can always keep calculating, period. And if there are any small problems, the partner has proven very helpful indeed.”

“Five years ago we would have needed servers across Europe for our calculations, but now this cloud platform suits our needs very well”, is Vriend’s conclusion. “It enables us to do science we all benefit from.”

### Results

With the High Performance Computing cloud platform the CMBI has the flexibility to get started quickly calculating protein structures and scaling up indefinitely. Additional computing power is simple and immediately available. This saves the CMBI much time and money.

