Digital Single Market

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Linking supercomputers to simulate the sun, the climate and the human body

European scientists can simulate the fusion taking place in the sun, create new climate models and will eventually build a biologically-correct virtual human thanks in large part to EU-funded research that has developed a European infrastructure for supercomputing.

 [1]

These results were made possible through the efforts of the 'Distributed European infrastructure for supercomputing applications' [2] (DEISA), which has now completed two phases spanning seven years. Its work has delivered one of the most advanced distributed 'High performance computing' (HPC) facilities in the world.

This infrastructure has, over several decades, provided a major boost to European simulation science. And this strong position looks set to continue as Europe plans to invest nearly EUR 500 million in the domain over the next five years.

The first phase of the project initially linked together Europe's most advanced supercomputing centres in Germany, Spain, France, Italy, the Netherlands, Finland and the UK, ultimately connecting 11 supercomputing centres in all. Physical links were established by using the GÉANT and the 'National research and education networks' (NRENs) infrastructure.

GÉANT is the high-bandwidth, academic internet serving Europe's research and education community.

It connects over 40 million researchers in 40 European countries and links to a number of other world regions. It offers bandwidth reaching 40 Gigabits per second (Gbps). Meanwhile, the NRENs provide data communications networking facilities to the national research and education communities.

DEISA scientists went much further than simply creating high-speed connections between computers. 'Before you had different supercomputers, using different software and different file structure, and it was a nightmare to go from working on one supercomputer to another,' explains Hermann Lederer, from the coordination team of the DEISA2 project. 'DEISA harmonised the infrastructure and made it much easier for scientists to get the most out of their computing time.'

DEISA1 started the harmonising process, while DEISA2 consolidated and extended it, and solidified the Application Support Task Force. 'We got together specialists on each of the supercomputing systems within the consortium, so we [can] match research programmes to the best supercomputer for the job and offer them expertise that can get the very best performance out of that system. We even provided application support that would optimise software for a particular research task,' Dr Lederer remarks.

The project also established the 'DEISA extreme computing initiative' (DECI). DECI was launched in May 2005 by the DEISA consortium to enhance the project's impact on science and technology. Its main purpose was to provide enormous computing resources to tackle 'grand challenge' applications in all areas of science and technology.

The programme has been hugely successful and was massively oversubscribed in its sixth call, with researchers in 121 proposals looking for half a billion processor-core-hours, which is a measure of supercomputer resource consumption. There were just 91 million processor-core-hours available, less than a sixth of the demand, and 56 projects were chosen.

'We select science research topics based on a two-fold review process. Peer review establishes the scientific merit of the proposed research, while a technical review decides whether it is a feasible or appropriate supercomputing application,' Dr Lederer says.

Once a research project is chosen, DEISA secures the best supercomputer for the job and supplies scientists with technical support to optimise applications for each research goal. DEISA has dramatically augmented and supplemented national supercomputing services, not only providing the best supercomputer for the job, but also speeding up the rate of scientific progress.

Research gap

'Some projects that we approve might also work at the researcher's national supercomputing facility, but there might be a long waiting list, heavy oversubscription, or not so suitable architecture,' says Dr Lederer. 'In competitive science domains relying on big simulations that could be a serious problem, so the researcher can submit a proposal to DECI.'

And because the DEISA consortium includes Europe's largest supercomputing centres, researchers know that the most advanced computers are available at one of the partners. This is a vital point, because computing power increases rapidly, quickly making supercomputers obsolete.

The technology is advancing so fast that a research gap is beginning to emerge. Processors have reached speeds of 3 gigahertz, but energy constraints mean that they cannot get much faster. Multi-core processors provide an alternative upgrade path which, allied to parallelisation, offers another route to faster data processing. But fundamental research into a substantial increase in application parallelisation is lacking.

'We could really use research funding focused on new, highly parallelisable algorithms to attract the brightest mathematicians, computer and computational science specialists to attack this challenge,' says Dr Lederer. 'If there is not a focus on the issue now, it will become a problem in a few years time,' he cautions.

DEISA2 completed its work in April this year and now the 'Partnership for advanced computing in Europe' (PRACE) will take over. PRACE will maintain a pan-European HPC service consisting of up to six top-of-the-line leadership systems (Tier-0) integrated into the European HPC ecosystem established by DEISA.

Tier-0 leadership systems are those supercomputers that are first among the top 500 supercomputers in the world, and PRACE has already put into operation two of these systems, the 1 petaflop/s IBM Blue Gene/P system at the Julich supercomputer centre in Germany and the 1.6 petaflop/s BULL system called CURIE at the new Trés Grand Centre de Calcul (TGCC) in France.

PRACE has secured EUR 400 million in national funding for Tier-0 systems over the next five years, and the European Commission will provide an additional funding total of EUR 70 million over the lifetime of the PRACE family of projects (PRACE, PRACE 1IP, PRACE 2IP).

'DECI will continue, indeed it is still running now with the DEISA team keeping the programme running voluntarily until PRACE 2IP takes over in September,' reveals Dr Lederer, 'But now it will be known as the Distributed European Computing Initiative. The term "extreme" will be reserved for the Tier-0 supercomputers.'

Supercomputing research and investment like DEISA is particularly valuable because it serves several functions. Firstly, it advances computational science directly, tackling fundamental problems in application development, networking, informatics and mathematics.

Secondly, it has enabled and continues to enable leading-edge research in every conceivable scientific discipline, particularly in relation to the most challenging and urgent problems in science.

And finally, it paves the way for PRACE, a hugely ambitious, continent-wide programme to maintain and enhance European supercomputing leadership.

This is the first of a series of features on the contributions of DEISA2 towards important but computationally demanding research, such as the work of the RNAHIV project on the molecular mechanics of the HIV virus, the MillCli project's study of complex climate models, and the Cylinder project's research on the effects of turbulence on maritime structures.

DEISA2 was funded to the tune of EUR 10.24 million (of EUR 18.65 million total project budget) under the EU's Seventh Framework Programme for research, 'e-Science grid infrastructures' sub-programme.

- Distributed European infrastructure for supercomputing applications [2]
- DEISA2 project data record on CORDIS [3]
- e-Infrastructures programme / projects [4]

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