

DCSC policy seen from the “small users” side

Grant holders in DCSC can roughly be divided into two groups. The first group consists of large research groups with continuous super computing (SC) needs, which have resources to maintain their own highly specialized installations and which can allocate the man-power needed for support and program development. The second group consists of smaller research groups or research groups with only occasional needs for SC, which do not want or do not have the resources to allocate man-power for development and maintenance of their own installations.

The current DCSC setup favors the first group with large grants for hardware installations and hardly any support for human resources. No doubt, this is the most rewarding arrangement with regards to SC output; however, it also makes it very difficult for smaller groups or newcomers to SC to get into the field. The authors of the present script all belong to the group of small users and they welcome the new initiatives on addition of technical/academic user support as well as addition of how-to-courses brought forward in the “Scientific Computing and Grid Infrastructure” application (submitted to “den national pulje for forskningsinfrastruktur” 4/9-2007). However, we find that the resources set aside for these initiatives (1Mkr/year for how-to courses and 1.5Mkr/year for support only in phase 2, 2009-2010) are way too low compared to the total budget (5Mkr out of 90Mkr) when considering that users and hardware centers are distributed all over Denmark.

At present, new users of DCSC facilities get a letter stating that they have gained access to some of the DCSC facilities. Apart from some technical support the new user is “on his own”. He has to figure out what software is installed on the system, whether his preferred software can be installed on the available system, he may need to purchase his own expensive software licenses since there exist no central list of software, he needs a lot of help to get in-house software ported to the system and he needs a lot of help to install out-of-house research software that may only have been tested and compiled on other platforms. When all the initial troubles have been overcome, maybe he finds out that his kind of problems do not parallelize well on the system architecture he has access to. It is our impression that many researchers have experienced this once and hence do not want to waste anymore time on SC.

We are not advocating that large parts of the DCSC grant must be set aside for human resources, however, it must be possible to develop a centralized facility for SC technical/academic support which will help to attract more users to the area. In the last issue of “Scientific Computing World”, Issue 96, Oct./Nov., 2007, there is an article on the HPC-European programme “A new power base in Europe”. Here it is stated that “each visitor is given two contacts at the center – a specialist in high performance computing and a specialist in their field of research”. While the latter may not be possible within the limits of DCSC, it should at least be possible to have access to a specialist in high performance computing. Ways to obtain these goals could also be a more active role of the DCSC administration in organizing user groups, user meetings, discussion forums and centralized software administration/negotiation. It may also be an option to refer users to similar computing facilities in other countries for qualified help.

From talking with colleagues and other small DCSC grant holders we have learned that above described obstacles have prevented and are preventing many researchers in entering the SC community.

We find it imperative that initiatives, as mentioned here, are taken in order not to lose newcomers and smaller groups in Danish scientific computing. This will require more initiatives and a higher funding than the 5Mkr reserved for these purposes in the grant proposal.

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Mathias Stolpe, Jens Honore Walther, Mads Peter Sørensen and Ole Sigmund

In the following we briefly outline some individual experiences and needs by the authors of this script:

Associate Professor Mathias Stolpe from Department of Mathematics, DTU:

Our experience with DCSC is based on a three year grant for solving optimization problems with parallel methods. Our main need has been assistance in installing/compiling and updating the relevant optimization packages and the related linear algebra packages which are needed. The open source initiatives we use are rapidly improving both in terms of functionality and robustness. However, they are often only tested on a limited number of combinations of platforms, operating systems, and compilers. Hence, significant knowledge of the architecture and installed libraries and compilers is absolutely necessary to get these packages to work properly.

The second need is availability and easy access to updated written documentation and guides on how to use the available parallel computers and the installed software libraries.

The third need is courses on Ph.D. and other levels on Scientific Computing and related topics in general and on the use of this on the local installations in particular.

DCSC could support in the last two areas by taking initiatives to documentation and course development projects.

Associate Professor Jens Honore Walther from Department of Mechanical Engineering, DTU:

Our software has been developed on UNIX/Linux platforms using FORTRAN 90 and explicit message passing (MPI), and ported to Sun, SGI, IBM (e.g., Blue Gene/L), and NEC and is currently running on IBM and Linux Intel/AMD platforms at www.cscs.ch and www.csc.fi. These national computing centers (here Switzerland and Finland) offer professional hardware and software maintenance, data archiving, and currently access to more than 500 processing units – a service not available in Denmark. Symptomatically, Denmark does not appear on the Top 500 ranking of HPC installations (www.top500.org July 2007) whereas Switzerland rank 39, 60 (www.cscs.ch), 91, 96, and 115, and Finland 109, and 118. In my view this situation is detrimental for HPC related research in Denmark, and it is imperative that the country installs and operates a national computing center. I propose to *gather* rather than *scatter* the resources of DCSC, to allow state-of-the art hardware lines: currently Shared Memory Processor (SMP) and MPP platforms, and a slim, agile administration and task force for user support. The user support should include installation of commercial and open source software,

and furthermore guide optimization of user software, and data visualization. In my view, the “gridification” and/or “grid-computing” proposed by DCSC is not an alternative to a national computing center, as it does not enable MPP based HPC.

Professor Ole Sigmund from the Department of Mechanical Engineering, DTU.

Our current experience with DCSC is based on a three year grant. During this period we have used the High Performance Computing facilities (HPC) at DTU for running in-house parallel implementations in FORTRAN and the commercial code COMSOL.

Despite of many efforts (and good help from Bernd Dammann at DTU/HPC) we have not managed to obtain good efficiency for our problems. This may partly be attributed to wrong and slow platform, partly due to problems with installing out-of-house software, partly due to limited amount of software available for the SUN platform and partly due to lack of experience and academic support on solving large scale linear and non-linear problems. In conclusion, we have learned a lot about scientific computing but we have not gained what we expected from being part of HPC at DTU.

Our group is rather small and hence we can not afford to dedicate one person to SC tasks. Also, we believe that it is un-economical in a bigger picture that every user of DCSC facilities has to build up his own knowledge base. Hence, we are missing steady support on both the software side, help in the choice of the appropriate platform, system architecture etc.; and ideally also on the theoretical side, for solving ill-conditioned matrix problems efficiently using parallel solution strategies. Part of the support by DCSC could be to take initiatives and forming user groups on topics that must be common for many groups, e.g. efficient solution of large and ill-conditioned systems of linear equations.