

Barcelona (Spain), September 2009

Dear Volunteers,

With this letter we would like to ask you for more donations towards the GPUGRID project. By January 2009 we would end a grant for one of our two senior researchers as at the moment we do not have the funding to continue it.

In order to maintain the GPUGRID project scientifically and technically, we need you to support us until we have managed to attract new funds. The amount of money necessary for one entire year is approximately 50,000 Euros, but any donation received before the end of the year will contribute towards extending the research contract. The amount is calculated on a base salary of 30,000 Euros, plus taxes and University overheads (20%).

Why should you support us?

Decide a research project!

PS3GRID/GPUGRID was instrumental for the technological break-through of releasing the PlayStation and the graphical devices (GPUs) into BOINC. Hopefully with your support we will be able to continue to do so in the future and provide that technological edge to distributed computing which you are using every day.

We do so because our application, molecular dynamics (MD) simulation, is really computationally intensive. It would not make any sense to run all-atom MD on a single CPU and even on GPUs we will always need more computational power. On the other hand GPUs have allowed us to simulate unprecedented levels of molecular trajectories which are giving us the possibility to quantify molecular interactions and provide important knowledge towards new biomedical approaches and diseases. We have so far worked on proteins related to Alzheimer, heart arrhythmia, HIV and schizophrenia.

We plan to extend these studies and to start new ones with your support.

As this fellow will be supported directly by GPUGRID volunteers, the donor with the highest donation will have the opportunity to decide one disease on which we will try to contribute with our expertise and the top computational infrastructure provided by GPUGRID. This is your opportunity to start your own research. We will report to the volunteers on the progress of this research by providing reports as we would do for other funding bodies. In this way the interaction between volunteers and GPUGRID will be even stronger and could deliver very important outcomes in terms of science and society interactions. Through our studies on molecular dynamics we will seek to provide the highest impact towards the cure of the chosen disease.

How to donate?

You can donate any amount. The amount of funds required is such that it will be impossible to get there with just little donations, so while we encourage everyone to participate we really emphasize that we need some strong support. To donate simply go to: http://www.gpugrid.net/gpugrid_donations.php or contact us at ps3grid@gmail.com.

The highest donors will appear on the front page of gpugrid.net unless they would like to stay anonymous. On the 31st of December 2009 we will communicate with the highest donor to learn whether they wish to specify one of the research themes. As it stands if someone is able to provide the entire support alone, then they are automatically entitled to do so. Please contact ps3grid@gmail.com if you need more information.

Thank you very much!

What have we achieved so far?

Born as PS3GRID, we were the first BOINC project to deliver a client and an application for the Playstation3 using Linux as the host operating system. Our applications are always exploiting the hardware very heavily, with CELLMD, our molecular dynamics application we were able to run on Playstation3 15 times faster than a standard CPU. It is probably fair to say that without PS3GRID, there would not be a version of BOINC for use on the PS3.

The performance of the PS3 was crucial for delivering all-atom molecular simulations and allowed us to use BOINC for simulations which were before only run on supercomputers. We now have the possibility to exploit distributed computing to study molecular processes involved in diseases and possible drugs which could interfere with the causes of the disease. With PS3GRID we have studied methods for computing these interactions efficiently on a membrane pore. The final results have been recently completed and submitted for publications: T. Giorgino and G. De Fabritiis, Convergence of the potential of mean force computed through microsecond-scale bidirectional steered molecular dynamics, (2009).

In August 2008, again our project, by now doubled as GPUGRID, delivered the first application for Nvidia GPUs, again way before any other BOINC project, substantially contributing to the development of BOINC for GPUs with D. Anderson. As always, from the very beginning our application was top optimized achieving on high end GPUs the performance of at least 20 CPUs. The scientific validation of it was available via the scientific paper (so that you can be sure that the flops of your GPUs are sensibly used): M. Harvey, G. Giupponi and G. De Fabritiis, ACEMD: Accelerated molecular dynamics simulations in the microseconds timescale, J. Chem. Theory and Comput. 5, 1632 (2009).

GPUs are a really innovative hardware for scientific applications which will affect the way computational science and for us medical applications are developed: G. Giupponi, M. Harvey and G. De Fabritiis, The impact of accelerator processors for high-throughput molecular modeling and simulation, Drug Discovery Today 13, 1052 (2008). GPUGRID tries to be at the forefront of this new technological wave.

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