Starter Grant Application form – English version

APPLICATIONS ARE PREFERABLY DRAWN UP IN ENGLISH. AN ENGLISH TRANSLATION HAS TO BE ENCLOSED WITH APPLICATIONS SUBMITTED IN DUTCH.

The application form is available in English on the website https://vscentrum.be/.

Name and first name of the applicant:

De Vos Oriana

Institution:

Ghent University

Research group / department:

Center for Molecular Modeling (CMM)

Title / position:

Assistant

e-mail address:

Oriana.DeVos@UGent.be

Disclaimer

Allocated computing time on Tier1 for a Starter Grant is 100 nodedays at most, allocated for a period of 2 months. Total disk storage should not surpass 250 GiB. Allocated time is granted only to the applicant and can never be transferred to anyone else. Used computer time will be free of charge.

1. Motivate your application: why specifically do you want a Starter Grant?

I will start with a study of the oxygen diffusion through cell membranes. For this study, I will use the software CHARMM. I hope that I can use a Starter Grant to learn more about this software.
In CHARMM, I will do molecular dynamics simulations. First of all, the Biosystems need to be equilibrated. Two cell membranes are modelled, both large systems counting thousands of atoms. The one cell membrane is a membrane containing ordered rafts, and the other one a disordered domain. Molecular dynamics trajectories are the simulation output. They allow to follow the position, and thus the mobility, of the oxygen molecules.
CHARMM is software that runs well in parallel, which is the motivation to apply for this starting grant on TIER1.

2. Short description of the computing tasks, the software tools required, expected disk storage and memory usage. Please specify if applicable:

- whether these computing tasks use diversification (OpenMP, MPI, hybrid OpenMP/MPI …)
  The computing tasks will use MPI.
- the estimated memory use of a computing task (maximum 64GiB/node)
  We will run the simulations on a full node (or several full nodes), and the estimated memory use of a computing task will be below 64GiB/node. The memory per node is thus expected to be largely sufficient.
- whether a vSMP system will be used
  There is no need to use a vSMP system.
- the requirements for disk storage (estimated volume in GiB and the total number of files)
  The estimated volume is 1000 GiB. The total number of files should be less than 1000 files over the course of this testing phase.

3. Summary of the software required to perform the computing tasks, and possible installation and compilation instructions. Please clearly provide the following per item in this regard:

- a reference to the software's web page
  http://www.charmm.org/
- the software licence system (open source, GPL, etc.)
  CHARMM has a commercial licence system. CHARMM is already installed on the TIER2.

4. Short abstract

Of the selected proposals the title, the PI and the abstract is published on the VSC website and the website of the Hercules Foundation. Please enclose a short abstract.

Title:
"Study of the oxygen diffusion through cell membranes"

Investigators:
Oriana De Vos & An Ghysels

Abstract:
Everywhere in the human body, there are membranes, for instance around every cell and organelle. Oxygen must be transported through the cell membrane in order to supply energy to the cell. The central question of this project is "how can oxygen diffuse through the membrane?" This project will investigate whether the presence of ordered rafts in the membrane have an influence on oxygen transport. We expect that the transport might be easier in ordered rafts than in disordered domains. In rafts the pathway of oxygen would be (almost) straight, but in disordered domains the pathway would contain more detours and would therefore be longer. Oxygen mobility will be examined using molecular dynamics simulations.

Send the completed Starter Grant application form to the relevant email address below.
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