

# ***Dissemination Plan***

WP5 - Dissemination

Deliverable D5.1

## **Project description**

Molecular modelling – and notably the conformational sampling and docking procedures – are in principle able to provide help for understanding the interaction mechanisms between (macro) molecules involved in physiological processes. Beyond the obvious interest in computationally predicting the binding modes of partners involved in supramolecular complexes participating in regulatory processes within the living cell, such approach may equally be used for “In Silico” research for means to interfere with the normal or pathological process (rational drug design). However, the processes to simulate are of a combinatorial complexity (molecule size, number of degrees of freedom) that represents an important challenge for the currently available computing power, hence the three imperative research directions in present day’s molecular modelling: (1) the search for mathematical models of maximum simplicity that nevertheless provide a relevant description of molecular behaviour, (2) the development of powerful distributed optimization algorithms (genetic algorithms, local search, hybrid algorithms) for sampling the molecular energy surface for stable, populated conformations, and (3) deploying those intrinsic distributed algorithms on computational Grids. This approach will be generalized to include intermolecular degrees of freedom, turning it into a flexible docking procedure.

Docking of (virtual) molecules into active sites of interesting biological targets will then be performed. A direct application could be flexible docking of organic molecules into the *Mammalian* and *Plasmodium* tubulin binding sites, in order to detect compounds with potential anti-cancer or anti-malaria effects.

## **Objectives**

The purpose of this Dissemination Plan is to ensure that the project:

- Communicates project results to widest possible audience
- Targets specific audiences that will benefit from the results: publishers, researchers, and users of our methodologies and software
- Uses a variety of techniques which are appropriated to deliver the content and to reach the target audience.

## **Target Audience**

Docking@Grid is a collaborative project associating teams coming from various scientific origins and developing approaches which take place both on a theoretical level and on an applied level. We want to reach a large community, in academia and in industry, in terms of scientists, developers and users. The target audience is wide, coming from computer science, chemistry, biology, chemoinformatics, and bioinformatics.

## **Channels and Methods**

We use these following channels:

- Reports are for internal circulation within Docking@Grid; they document the work done.
- Presentations at conferences will stimulate interest in Docking@Grid and in the project results.
- Workshops allow a more detailed discussion of results and feedback
- Publications communicate the detailed research results and conclusions, together with supporting data and methodology
- Web site serves as a source of information for external parties that are interested in the work done as well as a tool for internal communication

## 1. Internal Reports

Reports are for internal circulation within the project. They can be of different types:

Synthesis of intermediate results, Open issues, Docking application documentation (External specifications, Design, Development, etc ...), Report meetings...

Their objectives are to:

- Fully document all data collected by the project
- Ensure that all members of the project have access to the collected data
- Provide sufficient analysis that the data can be understood and trends can be identified
- Register the main points of each project meeting
- Allow to keep the history of the project

To save on printing and distribution, most reports will be posted on the Docking@Grid web site, at least in a "Members only" section.

## 2. Conferences and Presentations

Conferences would be used to:

- Stimulate interest in Docking@Grid methodologies, its software realised implementation and its results
- Reach wide and varied audiences: librarians, publishers, and researchers in relevant disciplines (computer science, biology, chemistry, bioinformatics and chemoinformatics, drug-design and screening communities )
- Stimulate discussion and feedback.

Performing Docking@Grid related presentations is a task that might be carried out by every Docking@Grid partner , for own exploitation and publicity. Nevertheless there are some minor restrictions:

- Presentations should always make clear reference to the Docking@Grid project
- Existing presentations can (and should) be reused, after publicly notifying their creators and obtaining approval for any modifications
- Making publicly a presentation on other's work (i.e work not produced or owned or assisted) by a partner should always follow approval or interested parties. Stated in another way, public presentations' material should generally be approved by the partners that are involved in the work being presented

Participants of the project are planning to present papers at major national and international conferences. Up to now (January 2007), we have presented (or submitted) papers to the following conferences:

- IPDPS Conference,USA, March 2007.

## **Workshops**

As for conferences, workshops are an opportunity to share results and stimulate discussion. However, the format allows more detailed presentation of results, more interactive discussion, and a greater opportunity to explore implications.

Nevertheless, the above-mentioned conference restrictions are also applicable.

We plan a few days workshop for project members whenever we need to work closely on a specific question. We also plan a one-day conference/workshop for project participants at the end of the project. If funds allow, this conference/workshop will be opened up to a wider audience.

## **3. Publications**

Publications will be the main way that the project communicates results and conclusions to the outside world. The objective of publications would be to:

- Communicate project results widely
- Reach specific audiences that will benefit from the results (researchers, software developers, docking users)

Publication could include peer reviewed journals (print or electronic), key magazines, conference proceedings, and books. Docking@Grid does not pose restrictions on scientific publications because of the well known applied ethical rules that do apply to

such cases (regarding references, authors, unpublished work, owned work, proofs ...). All of these will be safeguarded within Docking@Grid dissemination activities.

In addition, as general guidelines:

- An optional request is submitted to other interested parties for collaboration
- A version of the document is presented to the whole project for approval, 2 weeks prior to the final submission
- All publications should refer to Docking@Grid project in the acknowledgement section.

It is planned to submit papers to international and national journals, on technical topics as well as on topics based on the research itself. Up to now, published (or submitted) papers are:

- A-A. Tantar, N. Melab and E-G. Talbi, B. Parent and D. Horvath, "A Parallel Hybrid Genetic Algorithm for Protein Structure Prediction on the Computational Grid", *Elsevier Science Publishers B. V.*, 2006.
- Alexandru-Adrian Tantar and Nouredine Melab and El-Ghazali Talbi and Bernard Toursel, «Solving the Protein Folding Problem with a Bicriterion Genetic Algorithm on the Grid», CCGRID '06: Proceedings of the Sixth IEEE International Symposium on Cluster Computing and the Grid, *IEEE Computer Society*, 2006.
- Chapter in a book "GRIDs for bioinformatics and computational biology", Wiley, 2007.
- Submitted paper to the journal FGCS "Future Generation Computer systems", 2007

## Web site

Docking@Grid has developed a website, <http://dockinggrid.gforge.inria.fr/>. This site provides public access to general information on the project (objectives, partners, scope, etc ...) and to its public deliverables and presentations. It is planned to add also a restricted part for exchanging internal project information between the partners.

Structure and configuration of the website are modified upon recommendation by partners, or as needed by the webmaster team (currently IFL Team). Every modification is notified by email to all the partners to inform them so that they can check the content and ask for corrections if needed.

In the future, a platform could be chosen to allow easy contribution from all partners of the project. Nevertheless modification or addition of content will not be uncontrolled. The platform will provide appropriate mechanism to support controlled editing and publishing of the content and limited structural management.