

**EGI-Engage**

Deliverable/Milestone review form

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| **Details of the document being reviewed** | | | |
| *Title:* | **Implementation and evaluation of AMBER and/or GROMACS** | *Document identifier:* | EGI-doc-2774 |
| *Project:* | **EGI-Engage** | *Document url:* | <https://documents.egi.eu/document/2774> |
| *Author(s):* | Antonio Rosato | *Date:* | **18.03.2016** |

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| **Identification of the reviewer** | | | |
| *Reviewer:* | **Mariusz Sterzel** | *Activity:* | **EPOS-CC** |

**General comments on the content**

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| **Comments from Reviewer:** |
| Very good document. I like the analysis CPU vs CPU/GPGPU very much. The tests molecules and simulation types are chosen quite reasonably. Solvent effects included as well.  We have done similar tests on our local cluster with Gromacs and our results actually meet the one presented in the document. One thing I lack here is NAMD package. Especially the version 2.11 has been very well tuned to benefit from GPGPUs and CPUs at the same time. Our tests indicate up to 10x speed-up of the mixed nx(24CPU/2GPGPU) setup. And I would say NAMD is as much popular as Gromacs/Amber.  The other thing I lack here is the EGI Infrastructure reliability. It would be worth to add a short paragraph about it. |
| **Response from Author:** |
| **The research teams involved in the MoBrain CC have providing portals for MD simulations using the AMBER and GROMACS software packages (references 2 and 4). These portals have been operational and accessed by external users, often non-Europeans, for about five years. This endeavour has provided us with considerable experience on what is typically done/desired for such services. On the other hand, none of us is familiar with NAMD, not even for their own “internal” research. Our selection of tools to be benchmarked focused on AMBER and GROMACS since the initial design of the MoBrain activities, explicitly to leverage our long-term experience in using and helping others to use these tools. We now added an explicit reference to NAMD and its optimized performance on GPGPUs, based on published data (REF).**  **The current work exploited mainly the GPGPU test bed that was implemented in Florence in collaboration with the JRA2 accelerated computing task. The reliability of the EGI infrastructure will be addressed in the subsequent deliverable about GPU-enabled portals (D6.12, due in June 2016).** |

**Additional comments**

*(not affecting the document content e.g. recommendations for the future)*

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| **From reviewer:** |
| Please run a spell check over the document. There are several typos in it. |

**Detailed comments on the content**

| **N°** | **Page** | **§** | **Observations** | **Reply from author (correction / reject,  …)** |
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**English and other corrections:**

Note: English and typo corrections can be made directly in the document as comments.