

CLAIX / Lichtenberg2 Projects

High Performance Computing at NHR4CES

Reporting period: December 01, 2021 - November 30, 2022

Please return this report at latest 12 weeks after the project period. The content of this report will be published online. Please let us know if you do not agree to that and also provide us with the copyright of all pictures and figures (if applicable).

1 Project title

For example:

Investigation of Spray Combustion of Oxymethylenethers and Oxymethylenether/Diesel Blends using Large Eddy Simulations

2 Project ID

For example: p0029999

3 DFG classification

Please use the old DFG classification (2016-2019):

<https://help.itc.rwth-aachen.de/en/service/rhr4fjuttff/article/dcddb5af9e6463a9e1c5b0abd03d254>

For example: 201, Life Sciences, Basic Biological and Medical Research

4 (List of) Involved people

Format: function, name, institute, organization, country

Function is one of: Principal Investigator (PM) (supervisor of the project), Project Manager (PM), Researcher (R)

For example:

PI, Petra Mueller, Department of Mathematics, University of Namur, Belgium
PM, Hans Meyer, Solid State Physics, RWTH Aachen, Germany

5 Project report

Please, give a short report, generally understandable, without using formulas or discipline specific abbreviations with the following subsections, and without references. This report should emphasize the motivation, tasks and special challenges (why do you need a High Performance Computer (HPC)?). Your report should contain at least 450 words. Please make sure that your report does not exceed 900 words in total. Please stick to the following form:

1. Introduction: Short introduction, which motivates the research topic and the use of HPC.
2. Methods: Short description of the used methods.
3. Results: Results of the project (if the project is running for more than one year, please clarify which results you achieved in which phase of the project).
4. Discussion: Please discuss your results and give a short outlook.
5. Keywords: Please, give 2-5 keywords.
6. Software: Please list the software that you mainly used for your project.

6 Pictures

Please send pictures that can be used for publication in a separate file in high quality (vector graphics or high-resolution images with at least 1500x1500 pixels). Make sure that you yourself hold the copyright to these pictures.

7 Awards, cooperations, publications

7.1 Selected honors, prizes, awards (up to ten) related to your project.

Format: name, title, description

For example:

Petra Mueller, Scientist Award 2020, RWTH Aachen, Germany

7.2 Selected conference participations (e.g. invited keynote lectures or online conferences) during 2021 related to your project.

Format: name, theme, title, location incl. country, date

For example:

Petra Mueller, Quantum mechanically guided design of borides or experimentally guided quantum mechanical calculations, International Supercomputing Conference / ISC, Frankfurt, Germany, June 10-14, 2020

7.3 Selected national and international cooperations (up to five) related to your project

Format: name, institute/company, city, country

For example:

Petra Mueller, Los Alamos National Lab, UC Santa Barbara, USA

7.4 Publications related to your project

Format: Author/co-author, title, place and year of publication, reference

7.5 Thesis (bachelor, master, PhD) related to your project

Format: Author, title, place and year of publication, reference

8 Support by NHR4CES

Have you used the support (mail, phone, personal conversation) NHR4CES support services at RWTH Aachen University or TU Darmstadt for HPC-related inquiries within the last 12 months or participated in training organized by NHR4CES (e.g. Simulation and Data Lab, Cross-Sectional Group, PPCES, aiXcelerate, SX-Aurora, HPC Intro, etc)?

By sending this information, I agree to its publication by RWTH Aachen and TU Darmstadt for the purpose to report on the scientific use of NHR4CES infrastructure, in print and online.