EuroHPC Joint Undertaking (JU) Development Access

**Final Report**

General Information

Type of project granted: Development Access – code development and optimization

Proposal ID

Please fill in the information in the box below.

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Period of access to the EuroHPC JU facilities

Please fill in the information in the box below.

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| Start date of the allocation (DD/MM/YYYY) |  |
| End date of the allocation (DD/MM/YYYY) |  |
| Duration of extension in months (if applicable) |  |

EuroHPC JU system assigned

Please click once in the box to select it, click again to unselect.

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|  | Vega CPU (IZUM) |  | Vega GPU (IZUM) |
|  | MeluXina CPU (LuxProvide) |  | MeluXina GPU (LuxProvide) |
|  | Karolina CPU (IT4Innovations) |  | Karolina GPU (IT4Innovations) |
|  | Discoverer (Sofia Tech Park) |  | Deucalion (MACC) |
|  | LUMI-C (CSC) |  | LUMI-G (CSC) |
|  | Leonardo Booster (CINECA) |  | Leonardo DCGP (CINECA) |
|  | MareNostrum5 GPP (BSC) |  | MareNostrum5 ACC (BSC) |

Principal Investigator

Please fill in the information in the table below.

|  |  |
| --- | --- |
| Title |  |
| First (Given) Name |  |
| Last (Family) Name |  |
| E-mail Address |  |

Project information

Project title

Please fill in the information in the box below.

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Main research field(s)

Please click once in the box to select it, click again to unselect.

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|  | Biochemistry, Bioinformatics and Life sciences (LS1, LS2, LS8, LS9) |  | Fundamental Constituents of Matter (PE2) |
|  | Chemical Sciences and Materials (PE3, PE4, PE5) |  | Linguistics, Cognition and Culture (SH3, SH4, SH5, SH6) |
|  | Earth System Sciences (PE10) |  | Mathematics and Computer Sciences (PE1, PE6) |
|  | Economics, Finance and Management (SH1, SH2) |  | Physiology and Medicine (LS3, LS4, LS5 LS6, LS7) |
|  | Engineering (PE7, PE8) |  | Universe Science (PE9) |

Team members and institutions

Please list all team members and corresponding affiliations that were involved in the project.

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Summary of the project

Please fill in the field with the same text used in the application form (maximum 300 words).

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Main features of the code

Name of the code(s)

Please fill in the information in the box below.

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Type of the code distribution

Please fill in the information in the box below (e.g., open source, commercial, academic, etc.).

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Computational problem executed

Please fill in the information in the box below (e.g., N-body problem, Navier-stokes equation, etc.).

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Computational method

Please fill in the information in the box below (e.g., FEM, FVM, PIC, spectral methods, etc.).

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Kind of parallelism used

Please fill in the information in the box below (e.g., MPI, OpenMP, MPI/OpenMP, pthreads, embarrassingly parallelism, etc.).

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Main libraries used, version and language. Usage of /usr/local libraries.

Please fill in the information in the box below: main libraries (e.g., FFTW, MKL, BLAS, LAPACK, etc.), language (e.g., Fortran, C, C++, etc.).

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Other software used on the EuroHPC JU systems. Usage of post-processing or pre-processing tools.

Please fill in the information in the box below.

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Compilation step

How is the program complied?

Please fill in the information in the box below (e.g., makefile, script, etc.).

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Difficulties met to compile, if any, and how they were tackled

Please fill in the information in the box below.

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Which version of the complier and version of the MPI library was used?

Please fill in the information in the box below.

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Were any tools for studying the behavior of the code used?

Please fill in the information in the box below (e.g., debugger, profiler, etc.).

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Execution step

How is the program launched?

Please fill in the information in the box below.

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Difficulties met to launch the code, if any, and how they were tackled

Please fill in the information in the box below.

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Communication patterns

If you know which are the main communication patterns used in your code configuration, please select the ones from the mentioned below (click once in the box to select it, click again to unselect):

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|  | Many / few / no point-to-point communications |
|  | Many / few / no collective communications |
|  | Barrier |
|  | Reduction |
|  | Broadcast |
|  | Scatter/gather |
|  | All to all |

Scalability testing

Summary of the obtained results from the scalability testing

Please show the scaling behavior of the application. Which progress was achieved? Does it fulfil the set expectations? If not, what were the reasons? (maximum 500 words)

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Images or graphics showing results from the scalability testing

All tables and figures (including photographs, schemas, graphs and diagrams) should be numbered with Arabic numerals (1, 2,...n) and include a descriptive caption. Please attach the images to this form (minimum resolution 300 dpi).

Data to deploy scalability curves

1. **Typical user test cases**

Please include the data for each test case.

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| Number of cores | Wall clock time | Speed-up vs the first one | Number of nodes | Number of processes |
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1. **Strong scaling curve**

Please include the data in order to deploy the scalability curve when the number of processors varies for a fixed total problem size.

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| --- | --- | --- | --- | --- |
| Number of cores | Wall clock time | Speed-up vs the first one | Number of nodes | Number of processes |
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1. **Weak scaling curve**

Please include the data in order to deploy the scalability curve when the number of processors varies for a fixed problem size per processor.

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| Number of cores | Wall clock time | Speed-up vs the first one | Number of nodes | Number of processes |
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Publications or reports regarding the scalability testing

Please use the following format: Author(s). “Title”. Publication, volume, issue, page, month year.

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Development and optimization

Summary of the obtained results from the enabling process

Please describe the spent effort. Which progress was achieved? Please describe in detail which enabling work was performed (porting, work on algorithms, I/O…etc.). List problems encountered, if any (maximum 500 words).

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Used tools for the code analysis, if applicable

Please fill in the information in the box below (e.g., Scalasca, Vampir, etc.) (maximum 500 words).

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Main actions taken for optimization or improvement of codes on the EuroHPC JU systems. Which features were optimized? What were the bottlenecks? Which were the solutions (if any)?

Please fill in the information in the box below (maximum 500 words).

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Publications or reports regarding the development and optimization

Please use the following format: Author(s). “Title”. Publication, volume, issue, page, month year.

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Results on Input/Output

Size of the data and/or the number of files

Please fill in the information in the box below (maximum 300 words).

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Usage of MPI-IO features, if applicable

Please fill in the information in the box below (maximum 300 words).

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Main results

Conclusions about the project

*Please fill in the information in the box below.*

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Usability of the assigned EuroHPC JU system

*Please fill in the information in the box below.*

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Feedback and technical deployment

Feedback on the centers/EuroHPC JU access procedures

Please fill in the information in the box below (maximum 500 words).

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Explanation of how the computer time was used compared with the work plan presented in the proposal. Justification of discrepancies, especially if the computer time was not completely used.

Please fill in the information in the box below (maximum 500 words).

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Willingness to apply to EuroHPC JU Access Modes in the future

Please fill in the information in the box below (maximum 500 words).

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