



plan4res : Synergistic Approach of Multi-Energy Models for an European Optimal Energy System Management Tool

Deliverable D6.1 Specification for the plan4res Platform Implementation

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PLAN4RES: Specification
for the
plan4res Platform Implementation



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Glossary of terms used in this document

CDO Core Data Object

CLI Command Line Interface

HPC High-Performance Compute

HTC High-Throughput Compute

MILP Mixed-Integer Linear Program

MKL MarketLab

MPI Message-Passing Interface

PID Persistent Identifier

URN Uniform Resource Name

VM Virtual Machine



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Executive Summary

This document provides a specification for the Plan4res platform, a software environment

- suitable to be used on all partner site's compute infrastructure,
- suitable to be used on a wide range of hardware performance classes,
- usable to obtain repeatable results over time,
- able to communicate with the MARKETLAB data repository,
- suitable to run the necessary data transformations and optimization codes,
- permitting exchange of data and code as well as executables between partners.

In appendices it also contains a description of the Universal Data Junction software (UDJ), as well as reference manuals for the first releases of UDJ, (Deliverable D6.2), the SMS++ library and the data format used by it (Deliverable D6.3).



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- [1] G. M. Kurtzer, V. Sochat, and M. W. Bauer. Singularity: Scientific containers for mobility of compute. *PLoS ONE*, 12(5):e0177459, 2017.
- [2] Cray EMEA Research Lab. UDJ-0.4.1 – universal data junction. A high performance transport-independent data movement library, March 2019.
- [3] J. M. Wozniak, T. G. Armstrong, M. Wilde, D. S. Katz, E. Lusk, and I. T. Foster. Swift/t: Large-scale application composition via distributed-memory dataflow processing. In *2013 13th IEEE/ACM International Symposium on Cluster, Cloud, and Grid Computing*, pages 95–102, May 2013.