



An experimentally-validated multi-scale materials, process and device modelling & design platform enabling non-expert access to open innovation in the Organic and Large Area Electronics Industry (MUSICODE)

Grand Agreement: 953187

Project Start Date: 01/01/2021

Project Duration: 48 months

Deliverable 4.4

HPC Integration and Remote Execution

Date: 03-01-2023



This project has received funding from the European Union's Horizon 2020 Research and Innovation Programme under the Call

DT-NMBP-11-2020 "Open Innovation Platform for Materials Modelling"

Project co-funded by the European Commission within Horizon 2020 Research and Innovation Programme		
Dissemination Level		
PU	Public	
PP	Restricted to other programme participants (including the Commission Service)	
RE	Restricted to a group specified by the consortium (including the Commission Services)	
CO	Confidential, only for members of the consortium (excluding the Commission Services)	x

Deliverable author(s): Borek Patzak (CVUT)

Contributors: Stanislav Šulc (CVUT), Aron Kneer, Klaus Reimann (Tinnit), Konstantinos Kaklamanis (UOI)

Draft Revisions:

- v1.0, 02/12/2022, Borek Patzak (CVUT)
- v1.1, 10/12/2022, Konstantinos Kaklamanis (UOI), Added MDAPI demo
- v1.2, 12/12/2022, Aron Kneer, Klaus Reimann (Tinnit), Added material processing demo
- v1.3, 27/12/2022, Borek Patzak (CVUT), Final editing
- v1.4, 28/12/2022, Review by Aron Kneer (Tinnit), Elefterios Lidorikis (Uoi)
- v2.0, 03/01/2023 approved by coordinator

Copyright

@ Copyright 2021-2024 The MUSICODE Consortium

Consisting of Coordinator:	University of Ioannina (Uoi)	Greece
Partners:	Karlsruhe Institute of Technology (KIT)	Germany
	University of Surrey (SURREY)	UK
	Aristotle University of Thessaloniki (AUTH)	Greece
	Czech Technical University in Prague (CVUT)	Czechia
	Fluxim AG (FLUXIM)	Switzerland
	TinniT Technologies GmbH (TINNIT)	Germany
	Granta design LTD (GRANTA)	UK
	Esteco SPA (ESTECO)	Italy
	Organic Electronic Technologies (OET)	Greece
	Apeva SE (APEVA)	Germany
	ANSYS UK (ANSYS)	UK
	AIXTRON (AIXTRON)	Germany

This document may not be copied, reproduced, or modified in whole or in part for any purpose without written permission from the MUSICODE Consortium. In addition to such written permission to copy, reproduce, or modify this document in whole or part, an acknowledgment of the authors of the document and all applicable portions of the copyright notice must be clearly referenced.

All Rights reserved.



This project has received funding from the European Union's Horizon 2020 Research and Innovation Programme under the Call

DT-NMBP-11-2020 "Open Innovation Platform for Materials Modelling"

"The European Commission support for the production of this publication does not constitute an endorsement of the contents which reflects the views only of the authors, and the Commission cannot be held responsible for any use which may be made of the information contained therein."

Contents

Contents	3
Publishable summary	4
Glossary	5
1. Introduction.....	6
1.1 Objectives of WP4 Task 4.1	6
1.2 Purpose of this Document	7
2.MUSICODE Simulation platform.....	8
3. Remote execution and HPC integration	9
4. Documented examples of remote execution and HPC integration	12
4.1 MD workflow	12
4.2 Modelling of material processing.....	14
4. Conclusions.....	18
Bibliography.....	18

Publishable summary

MUSICODE is an ambitious project that develops a novel Open Innovation Materials Modelling Platform to enable the Organic and Large Area Electronics Industry to expediate accurate and knowledgeable business decisions on materials design and processing for optimization of the efficiency and quality of OLAE device manufacture. Modelling the processing of materials requires hierarchical workflows spanning the micro- to macro-scales and thus spanning across different disciplines: chemistry, physics, engineering. The efficient support of remote computing resources (including HPCs) is necessary. This deliverable describes the MUSICODE remote execution and HPC capabilities. These capabilities are documented on selected examples.