

HORIZON2020

Deliverable D1.5  
GUI Design and setup



## D1.5

# GUI design and setup

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<sup>1</sup> Acronyms are marked in purple in the text and defined at the end of the document.



## Executive Summary

The present document “GUI design and setup” (Deliverable 1.5) is prepared under the task T1.4. “Graphical User Interface and integration on Marketplace” of Work Package 1 – “IM2D box architecture” of the INTERSECT project. The activity started at M9 of the project and is coordinated by FRA unit in collaboration with EPFL and AMAT.

This report describes the initial design of Graphical User Interface (GUI) that will be developed within INTERSECT, as front-end of the Interoperable Material-To-Device Simulation Box (IM2D). The realization of the IM2D GUI is based on the semantic upscale of the native GUI of the Ginestra™ code, which is one of the main components (for device modelling) of the entire infrastructure. The GUI is conceived to support both the material exploration and device modelling, depending on the user’s need. Two implementations schemes have been considered and discussed in the following Section.

The Ginestra™ GUI has been upscaled for IM2D purposes by including functions for the ‘*material on demand*’ data generation, through the *Ginestra-AiiDA* plugin that allows for the direct communication between Ginestra™ and the DFT engine codes through the AiiDA connection (see also Sec. 4.1 of Deliverable D3.3).

Depending on the user profiles, namely **persona** (see definition in Deliverable D1.1), and their specific computational needs (see “high-level requirements” in Deliverable D1.4), different kinds of access to IM2D have been planned, through local or on cloud installations of the infrastructure. We explored the latter solution by integrating the Ginestra™ GUI within MarketPlace digitalization hub, through SimPhoNy-remote solution.

The rest of the document is organized as follow: Section 1 describes the main objectives and ideas at the basis of the GUI design. Section 2 describes the work plan for the GUI design. Sections 3 and 4 briefly report on the main initial tools we considered for the IM2D GUI preparation and its integration to Marketplace, namely the Ginestra™ GUI and SimPhoNy-remote, respectively. Section 5 presents a first preliminary example of integration of the existing GUI to MarketPlace.

### 1. Objectives, solutions and outlook

INTERSECT main goal is to drive the uptake of materials modelling software in industry (synaptic electronics) and thereby accelerate the process of materials’ selection and device design and deployment by delivering a novel Interoperable Material-To-Device Simulation Box for the exploration of materials and devices. Typically, the target end users of IM2D comprise process engineers and device developers, who are experts in device and material R&D, design and manufacturing, but do not necessarily have nor are expected to exhibit expertise in electronic materials modelling. Vice-versa users can be experts in materials



science without direct expertise in device modelling. These characters identify different kinds of *persona*, to whom will correspond different “high-level requirements” and specific operational workflows (see D1.1. and D1.4).

To facilitate the end user’s interaction, IM2D is provided with a Graphical User Interface (GUI) that removes the underlying complexity of the modelling workflows and enables an end user non-expert in modelling to execute any of the proposed workflows with less intervention: only basic properties of the materials and device need to be prescribed by the user.

Two approaches for the design of the GUI are followed: (i) the IM2D GUI is built on the re-use and upscale of the native interface already provided by GINESTRA™. IM2D integrates the relevant part(s) of this interface using SimPhoNy-remote MarketPlace [1,2] technology into the workflow that includes also materials modelling (i.e., simulation hub) and databases, via AiiDA. This GUI is also used to create complex scripts that involve all relevant tunable materials (e.g. structure, chemical composition, bandgap, dielectric constant, etc.) and device parameters (e.g. effective mass, defect energy distribution, traps states, etc.) that can be either extracted from databases or calculated ‘on demand’. The list of the most important physical quantities has been reported in D1.1 (Table 1). (ii) A simplified interface (pure web) is built on top of complex scripts allowing end users access to specific subset of parameters to change. This allows both complex, fully-fledged IM2D workflows as well as simplified apps to be provided. As an added value, the use of SimPhoNy-remote facilitates readily the integration with MarketPlace. This second solution has some relevant advantages: first, it is natively conceived for integration and development of digital infrastructures and database repositories (e.g. OptiMaDE [3]); second, it best tailors the choice of the operational workflows to the specific profiles (e.g. knowhow and skills) of the user *persona*; last, it allows for a larger autonomy from the Ginestra™ development and its commercial rules. However, this solution would require a much more mature development of the high-level interoperability requirements, including their ontology extension, and a partial reconfiguration of the hierarchical rules that regulate the existing operating modes of single codes (Quantum ESPRESSO [4], SIESTA [5], Ginestra™ [6]) included in IM2D and their interconnection through SymPhoNy [7] and AiiDA [8] (see also Deliverable “Risk assessment and risk-mitigation reports”, D5.2). For these reasons, we decided to start with the implementation of the first approach, and to develop the simplified native GUI in a second step, on the basis of the fully-fledged GUI.

## 1.2 Deviation from Planned work in the DoA

No major deviation, but a shift in focus has resulted as described here: after the start of the project, AMAT was acquired by Applied Materials, a large enterprise in the domain of electronic device design and validation. As a result, the business requirements from AMAT with respect to user interfaces shifted more towards relying first the existing interfaces. Hence, instead of currently focusing on creating a new GUI system, the existing Ginestra™ graphical user interface is upscaled by integrating its relevant parts into the SimPhoNy-



remote framework and consequently into the existing MarketPlace. This reorganization required some initial efforts, unforeseen during the preparation of the project. This affected this task that is currently only in preliminary form. More work is needed to account for the simplified native GUI, a task that is expected to be straightforward based on the integration of the existing relevant parts of the Ginestra™ GUI.

## 2. Workplan

IM2D GUI is designed to be the result of the upscaling of Ginestra™ graphical user interface tailored to support INTERSECT project workflows and semantic requirements. After the decision of reusing the existing industry-ready Ginestra™ GUI, the integration of the relevant parts of the existing GUI components within MarketPlace has been taken as priority activity in Task 1.4.

In this work, the integration of the existing Java Ginestra™ GUI with the MarketPlace via SimPhoNy Remote (S-R) is presented. SimPhoNy Remote is a mature technology developed since 2016 in multiple EU projects (SimPhoNy, FORCE, MarketPlace). It allows creating access for desktop and workstation class applications through a web browser facilitating user access rights. In essence, it can take an existing app and present it to the end user as an app for web. In the present case, it offers the following features:

1. Users can log in to either IM2D standalone app or the MarketPlace and, once acquired a license to IM2D, they are able to access the app;
2. Users can define all parameters of the design supporting all workflows from their web browser;
3. Users can shut down the web browser, re-launch it again, even from another system, and once logged in as in 1, they can continue the session (currently Ginestra™ does not provide such a feature);
4. Users can share their data and perform additional postprocessing on it directly from the app.

Once this route is implemented (work in progress, see Results section for preliminary work) including the curation of the Ginestra™ job file, a simplified web GUI also based on SimPhoNy-Remote will be finalized (i.e. approach 2, see above). This GUI will be based on simple web forms.

## 3. Ginestra™ GUI

Upscaling the relevant parts of the existing Ginestra™ GUI, INTERSECT will easily create a user-friendly front-end for the IM2D platform, which will speed up the validation phase and its final exploitation. Starting from an industrial-validated GUI will allow us also to achieve the highest quality standards in terms of usability and attractiveness (see also Deliverable D3.3).

The Ginestra™ Graphical User Interface is developed in JAVA using the *Swing framework*. It relies on the Visualization ToolKit (VTK) library for the 2D/3D visualization (Figure 1).

The main tools are:

- Device Creation Tool, that allows to design custom devices defining the geometrical and material properties;
- Test Editor Tool, that allows to design electrical tests;
- Output Viewer Tool, that enables the visualization of the 1D, 2D, and 3D outputs (device characteristics and device model structures);
- Simulation Manager, that allows to launch simulation jobs and to manage the simulation queue;
- Material Library Tool, that allows to navigate, load, and save materials to use in the simulation.

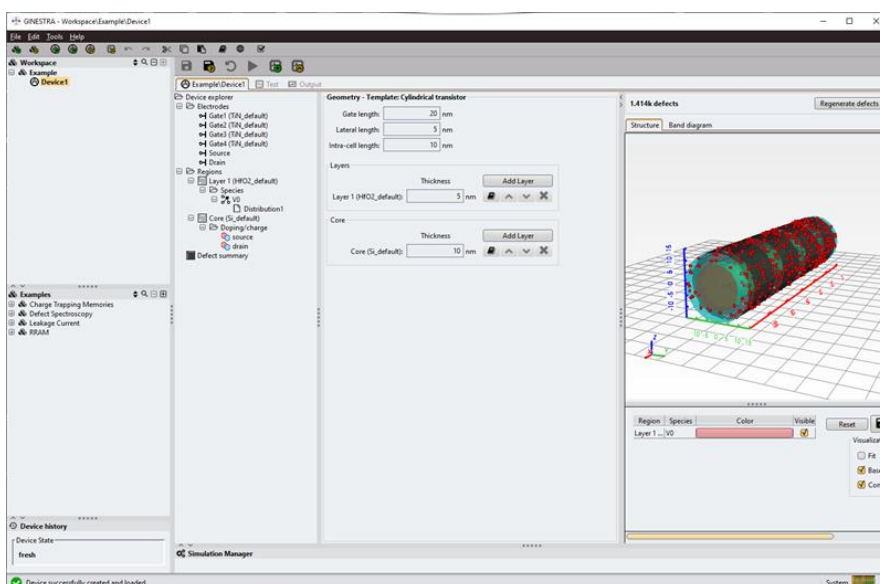


Figure 1 - Ginestra GUI. Visualization Overview.

A successful pilot activity of upscaling Ginestra™ GUI for creating the IM2D front-end has been done during the *Ginestra-AiiDA* plugin development. As described in details in D2.1, the Ginestra™ suite can interact with AiiDA through an extension of its REST API, in order to submit workflows, retrieve data, and query information from an AiiDA database not necessarily installed on the same machine where Ginestra™ is running. The resulting Graphical User Interface provides a simplified interaction with the intercommunication plugin, that allows to search data, submit workflows, monitor the status of the running simulation, and retrieve computed data. An example application of *Ginestra-AiiDA* plugin from the GUI is shown in Figure 2.



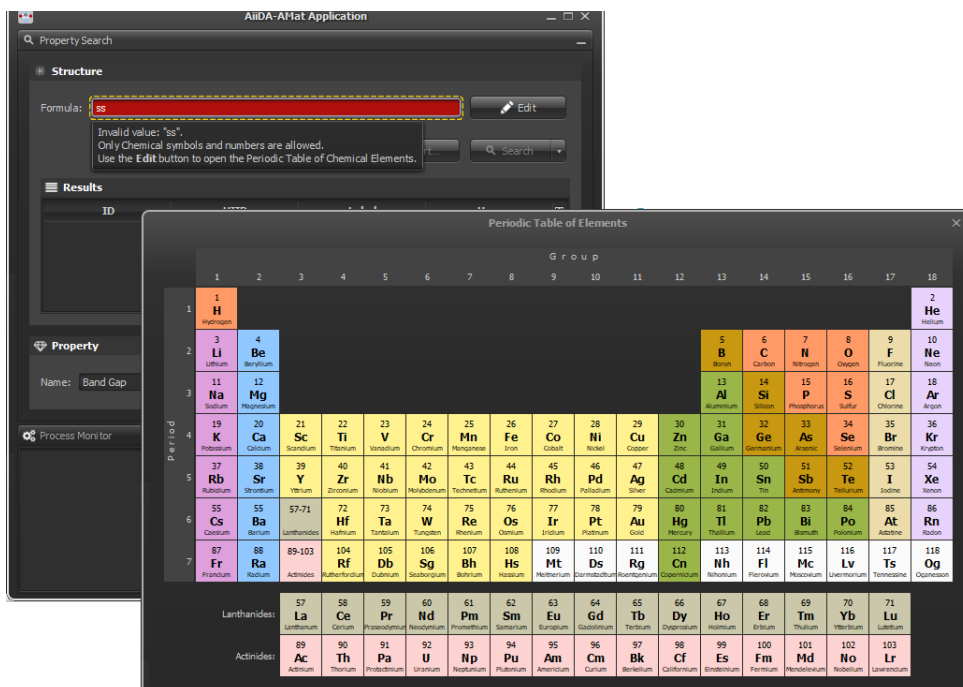


Figure 2 - Ginestra AiiDA Plugin.

Starting from the requirements and the use case described in D.1.1 and D.1.4, the relevant Ginestra™ GUI structures will be selected and distributed to the users. The select users will be able to perform their activities and support validating the IM2D quality requirements (D3.3) such as Functionality and Usability.

#### 4. SimPhoNy-Remote

SimPhoNy-Remote is one of the schemes available for integration of applications in MarketPlace, which has been developed by Enthought (<https://www.enthought.com/>), one of the partners in SimPhoNy project consortium [7]. S-R is a profitable vehicle for cloud deployment of legacy and desktop apps, and enables the user the access applications remotely via a web browser, without caring about tedious installation procedures (Figure 3). Even though the development of S-R is not a prerogative of the INTERSECT project, the understanding of its structure and working mode is necessary prerequisite for the integration of the Ginestra™ GUI into MarketPlace.

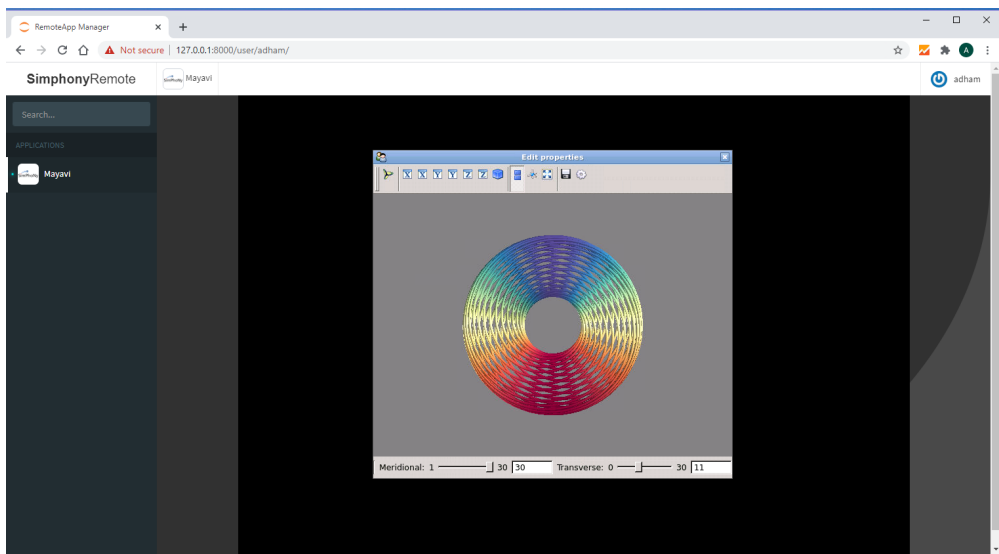


Figure 3 - Symphony-remote example

S-R enables the packaging of any application for the marketplace and other web platforms with a bundle of customized set of tools (Figure 4). It is based on JupyterHub, Docker, noVNC, and NginX frameworks [9]. SymPhoNy-Remote is free and open (BSD Clause 2) and also supports Access rights (secure user login) and Licenses of proprietary codes, as in the case of Ginestra™ GUI.

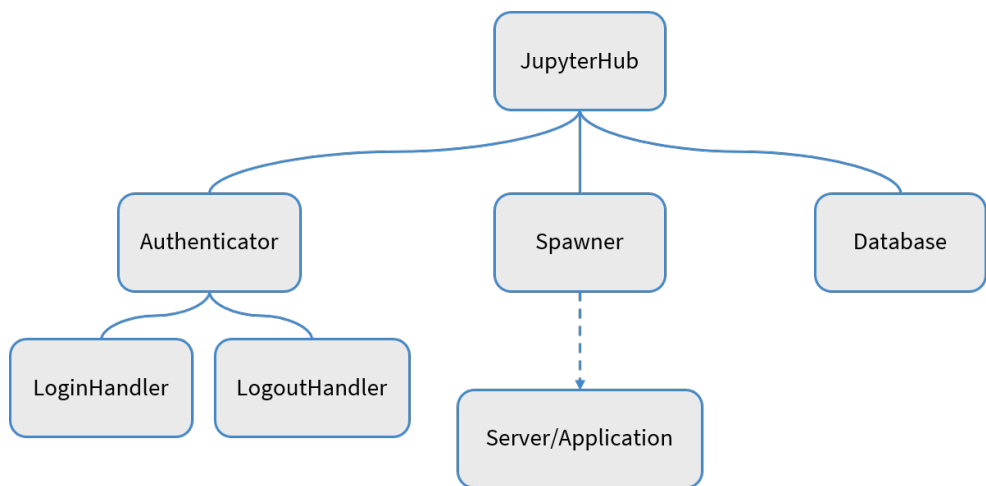


Figure 4 - SimPhoNy-Remote main structure (Credit: MarketPlace H2020 Project [2]).

To access it, the user just needs to create a S-R account and have the application of interest dockerized and integrated within their session. S-R also enables the user to seamlessly share their working sessions with other users via an automatically generated URL, and each account is customized to the user needs (with select applications available).

## 5. Integration to Marketplace

The basic design and setup of an **IM2D GUI** system addressing all requirements needed from both the end user and the workflows have been achieved. However, **Ginestra™** is a licensed proprietary software and its integration into a web infrastructure should be compliant with the Applied Materials Intellectual Properties regulation, such as Copyright and Trademark, for **Ginestra™** access and use. The legal terms for the integration of **Ginestra™** into Marketplace are still under discussion. Thus, in order to have an initial prototype example and to prove the integration of a JAVA based tool by using S-R, we considered the case of *Protégé code* [10], which is an open-source JAVA application for ontology development. The example in Figure 5 confirms its easy feasibility. **SimPhoNy-remote** was shown to offer very good performance and user experience. In the next step the entire **IM2D** will be deployed including **Ginestra™**, **AiiDA** and **SimPhoNy-OSP**.

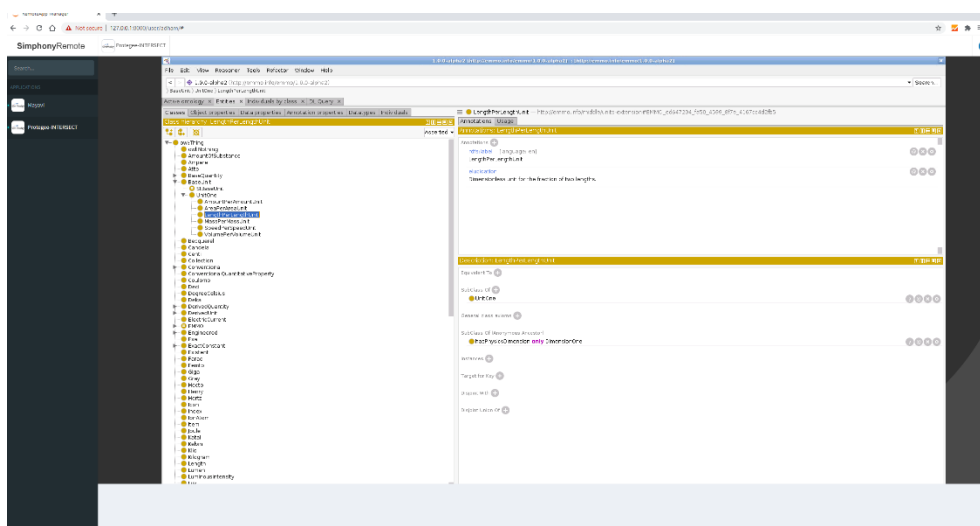


Figure 5 - Protégé integrated with SimPhoNy Remote displaying EMMO

## 6. Conclusion

The realization of use friendly interoperable **GUI** is a relevant and constitutive part of the overall **IM2D** simulation box. The graphical interface will constitute the front-end to access the infrastructure, while its semantic upscaling is intended to remove the underlying complexity of the modelling workflows, for a seamless exploitation by industrial end-users.

We designed the **GUI** development by considering two possible approaches, and we adopted the re-use and upscale the native **GUI** of the **Ginestra™** code as the most promising solution. As a consequence, we prioritized the integration of the **Ginestra™ GUI** within the Marketplace digitalization hub. The second approach, i.e. (pure web) **GUI**, can be pursued in



any case on the basis of the fully-fledged GUI. The actual implementation of GUI started recently and the work is in progress. A proof of concept integration of a JAVA based application in MarketPlace via SimPhoNy-Remote has been presented.



## ACRONYMS

- API** - Application Programming Interface
- EMMO** - European Materials Modelling Ontology
- GUI** - Graphical User Interface
- IM2D** - Interoperable Materials-to-Device
- OSP** - Open Simulation Platform
- S-R** - SimPhoNy-Remote
- VTK** - Visualization ToolKit

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