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Paving the way for the integration of synthesis, assessment, and design tools within an ontological framework

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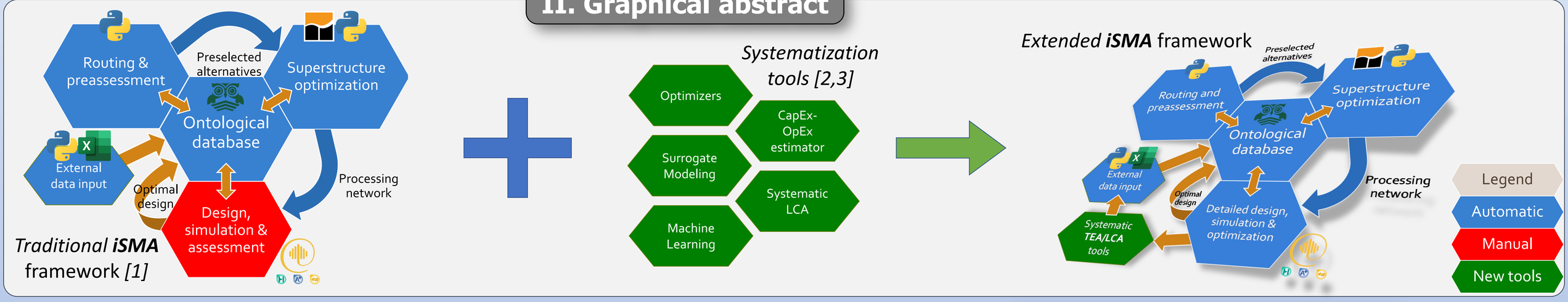
I. Highlights

- **Ontological framework** integrating various tools for **W2R process synthesis**
- **Modularity** provides expandability for further **automation & systematization**

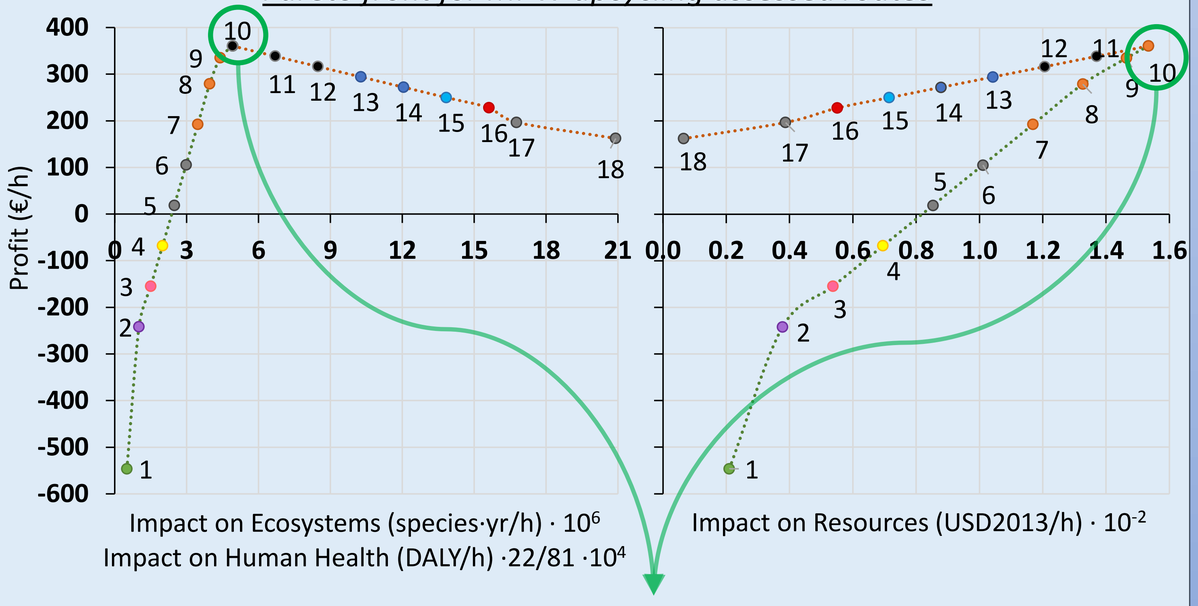
II. Graphical abstract



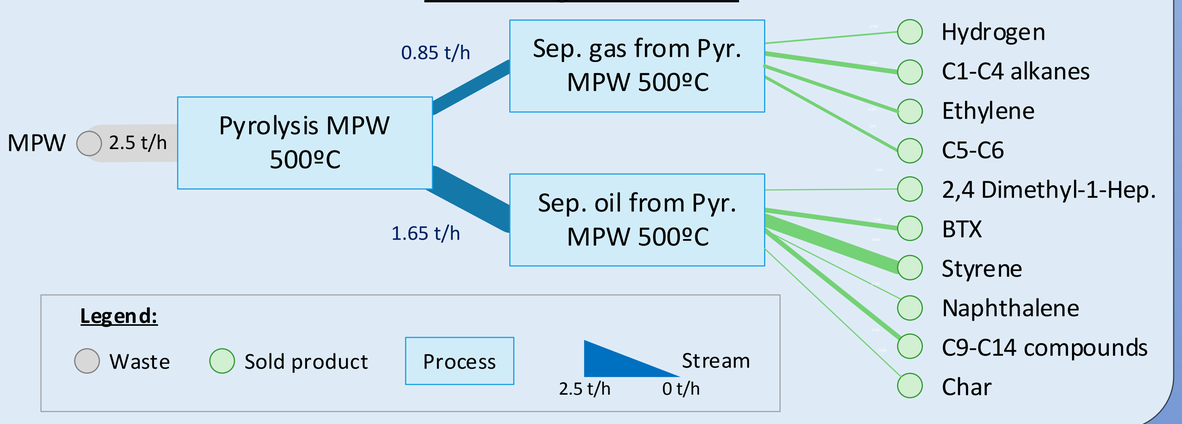
III. Methodology & Results

- **Waste-to-resource** alternatives are needed for the Circular Economy. A framework to assist **decision-making** to assess and find best alternatives was developed (aka *iSMA*)*[1]*. However, it relies on **manual** procedures that may hindrance its application.
- Thus, a need for tools to **increase automation** and reduce human intervention was envisaged. Especially in preliminary economic (**TEA**) and life-cycle (**LCA**) assessments and process **simulation**. Thanks to its modularity it is easy to be expanded.
- Framework's economic assessment automated with integration of ***CORO*** (CapEx OpEx Robust Optimizer)*[2].* **LCA automation** being developed with the same premise. **Surrogate Modeling** (SM) has also been envisaged for simulation of the process*[3].*
- Application of extended ***iSMA*** to case study of **MPW upcycling** (adding new instances e.g. gasiforming™*[4]*). *iSMA* synthesized and assessed 18 alternative routes using **multiple objectives**.
- **Pyrolysis** still shows better performance against new included routes due to their low TRL (high **CapEx**) and high electric energy consumption (high **OpEx**). Results are shown in the **Pareto** front (Points represent assessed processing routes) along with the optimal network for the economic objective (**route nº 10**).

Pareto front for MPW upcycling assessed routes



Processing route nº 10



IV. Conclusions

- Framework's **modularity** provides effortless expandability, increasing its automation & **systematization** capabilities.
- CORO has been implemented for **TEA automation** and **standardization**, LCA automation is under development.
- **SM & ML** (Machine Learning) are envisaged to systematize process simulation and perform a sensitivity analysis of the framework.
- Some **identified challenges** have been approached with the inclusion of new tools. Some extra performance improvement was identified: inclusion of **carbon credits** & **CCU** technologies.
- **Future work:** Auto-LCA & TIRESIAS *[3]* development & implementation; & ontology broadening.

V. References

[1] Pacheco-López, et al., 2023

[2] Prifti et al., 2022

[3] Galeazzi et al., 2023

[4] Prifti et al., 2021

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