

# Spatial Clustering Algorithms to Find the Optimal Spatial Resolution for Modelling of PtX Value Chains

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## Abstract:

Although the exact quantities and applications for hydrogen and Power-to-X (PtX) products are still debatable, the general importance of synthetic energy carriers in the future carbon neutral energy system is consent. To further understand and quantify the potential for PtX and align supply and demand, modelling of the process chain can help to understand the sizing and operation of the respective components needed. This is done at Fraunhofer Institute for Solar Energy Systems (ISE) with the inhouse modelling toolbox H2ProSim. With it, techno-economic analysis with high technical, economical, and temporal resolution can be done to optimise the dynamic operation of the PtX value chain.

To further improve the modelling and broaden the application, a spatial resolution is currently implemented in the toolbox. Thereby geographic and infrastructural aspects of the region, where a hydrogen economy shall be implemented, can be analysed and incorporated in the optimization process. This includes available areas for plant construction, renewable energy potentials, transport distances and existing infrastructure. Thereby, besides more realistic results, further questions can be answered via modelling, e.g. if a centralized or decentralized energy system is more reasonable in a specific region.

To integrate spatially resolved data in modelling a specific resolution needs to be chosen to ensure a finite number of possible locations. In energy system models the spatial resolution is often depending on administrative boundaries, for example in Bartholdsen et al. (2019). This is less suitable for technical system analysis like H2ProSim with smaller regions, higher spatial resolution, and a higher focus on single operators like hydrogen producers or applications. A variable spatial resolution with higher respect to technical and geographic conditions is needed. This spatial resolution can be created by using spatial clustering algorithms. Clustering algorithms can identify similarities and dissimilarities in datasets and use these to group data. By choosing the right algorithm and input data, a spatial resolution for a specific region with both respect to the most important characteristics, like hydrogen production, storage, and application potential, and the spatial contiguity can be created. This enables spatial entities with different sizes, like small demand clusters and large homogenous areas with similar renewable potentials.

The scope of this work is to develop a framework to cluster possible PtX regions and further analyse the regions based on the clustering results. The result of the analysis already enables an evaluation of the regions characteristic and potential and is further input for spatial resolved techno-economic optimisation of the hydrogen value chain.

Spatial clustering is already used in energy system context to minimize the effects of administrative boundaries, namely in Siala and Mahfouz (2019) and Fleischer (2020). Despite a different scope and much bigger analysed region, valuable insights and methods can be taken from their work. The max-p algorithm proved to be suitable as it enables flexible region size and numbers and spatial contiguity as well. Therefore, it was chosen as first algorithm in the scope of this work. The algorithm aggregates “n areas into an unknown maximum number of homogeneous regions, while ensuring that each region satisfies a minimum threshold value imposed on a predefined spatially extensive attribute” (Duque et al. (2012)). Converted to the PtX region problem, max-p can find the optimal number of regions with similar conditions like hydrogen application and production potential fulfilling a threshold such as minimal total hydrogen demand. The input data and first results for the clustering of the Upper Rhine Region (URR) with the max-p algorithm based on renewable energy potential (a) and possible hydrogen application (b) can be seen in Figure 1. It is already visible that, mainly urban, regions with a concentrated hydrogen demand like cluster 12 and 13 fulfil the threshold in smaller area and are therefore especially interesting for hydrogen applications, because of high amounts and short internal transportation distances.

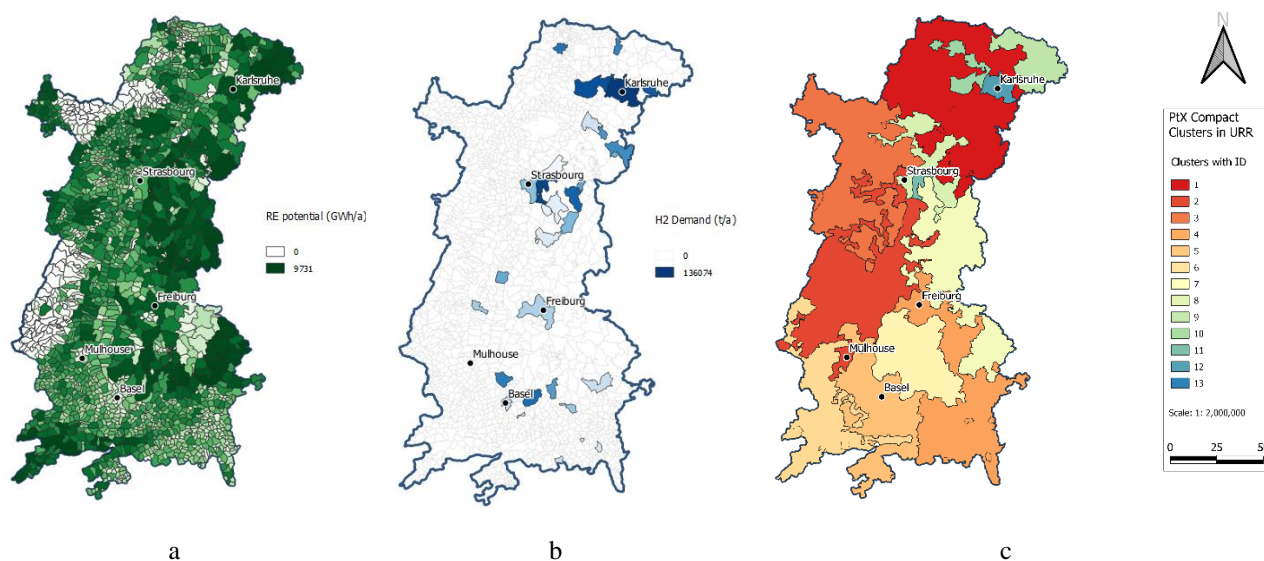


Figure 1: Spatially resolved renewable energy potential (a) and hydrogen demand (b) as input data and first clustering results (c) in the example Upper Rhine Region

The region is further analysed based on the clustering results to create additional spatial data. The results can be grouped in intra and inter cluster data, describing conditions inside and in between clusters, respectively. The first category includes results based on spatial data like possible area and capacities for plants, connections to existing or possible grids, applications for hydrogen, oxygen, or excess heat and the weighted cluster centre based on different possible criteria. The second set of results includes transport distances, times, and costs or capacities of existing grid connections in between the clusters. With this data, the suitability of areas for PtX applications can be assessed and unsuited regions can already be filtered out and therefore excluded from the list of optimal solutions. Furthermore, the data enables the spatially resolved analysis and optimisation of PtX regions with optimal resolution as described in the beginning.

The presented methodology is extended in current work. Different clustering algorithms, different input parameters and analysed regions shall be compared to improve and validate the methodology. Further data will be used in clustering and the following analysis to broaden the application and give further results. Ultimately, the methodology will be automated and combined with the H2ProSim modelling toolbox to enable flexible, objective, and fast spatially resolved techno-economic analysis and optimization.

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