

A two-step cascade modelling between EnergyScope Pathway-BO and PyPSA-BO for energy transition planning. Part B: Geo-spatial characterization and effects

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ABSTRACT

As the transition of energy systems becomes more urgent worldwide, countries and communities are searching for pathways toward sustainable energy systems, which involves developing long-term energy plans and deciding on the key resources and technologies required to meet their future energy needs. In this context, bottom-up models are commonly used to analyze scenarios that assess the development of energy systems. Nevertheless, the technical, temporal, and spatial detail levels vary as systems and cases become more complex.

Various modelling tools are currently available, each tackling issues using distinct approaches or addressing specific aspects of the system's behaviour. Thus, considering a common objective and structure, redundancies among models could be used to check consistency across models and provide an additional validation layer. Alternatively, models can be enriched by including inputs or supplementary information from other tools, considering the aspects each tool focuses on.

This study is one of a two-part study and addresses the coupling coupling, synergies and complementarities of two models to tackle the issue of planning the development of an energy system in the long term. The first part, focuses on optimizing the investment strategy path from 2021 to 2050 (EnergyScope Pathway), while the second, detailed in this article, concentrates on a detailed characterization of the electrical network and dispatch (PyPSA-Earth). This paper (Part B) analyses the electric system development of Bolivia taking into account the geo-spatial factor, which until this point has been simplified by disregarding the complexities of the transmission system. For the future scenario, the model makes use of the electrical demands expected in 2050 calculated by EnergyScope-Bolivia (Part A of this study).

In this sense, alternative clustering levels are explored between 2 and 62, using the k-means clustering method available in PyPSA-Earth to aggregate network components. An analysis is conducted across over 25 alternative node configurations where total installed capacities, generation, transmission capabilities, and computational runtime are considered. The analysis of optimization runtime and number of nodes considered confirms that a power-law relation exists between these variables, justifying the necessity of defining an cost-optimal configuration of a modelled network. A Pareto analysis comparing the expansion for solar technologies and the number of nodes shows that a 22 node configuration, would suffice to accumulate over 80% of the deviations compared to the maximum resolution possible, with only a 3% divergence for this technology. Finally, general results from PyPSA-BO are consistent with those from EnergyScope-Bolivia, as both tools provide a titular role to solar PV in the transition of the system. However, discrepancies can be found in the total installed capacities and the inclusion of storage technologies required. These differences open the door for future work where a feedback loop is implemented in the coupling of both tools, providing inputs from PyPSA-BO to EnergyScope-Bolivia.

1 INTRODUCTION

Since the 70s, several models started to appear and be used to analyze energy systems, their characteristics, and behavior. However, the modelling of energy systems poses a complex task given that it requires the representation of real objects into simplified versions that facilitate their understanding and study. In this sense, energy system models started differentiating from each other based on their methodological approach, structure, or time horizon, among others (Bhattacharyya and Timilsina, [2010\)](#page-10-0). Currently, only accounting open-source modelling tools, it is possible to find over 80 different tools available according to the repository from the Open Energy Modelling Initiative (Openmod, [2024\)](#page-11-0).

From this group, ESOMs (Energy System Optimization Models) are a popular sub-type of models given their approach used to find optimal solutions for problems linked to energy systems, such as how to adequately operate energy dispatch, plan expansions, limit environmental impacts, or simply minimize overall costs in a system (Plazas-Niño et al., [2022\)](#page-11-1). Nevertheless, while the representation of a system can be somewhat achieved based on a series of functions and restrictions, its complexity and data requirements can become exponentially larger as more variables are considered. In this sense, while some overlapping is always present, ESOM tools have been designed to balance these requirements and focus on particular aspects of the system, depending on the objectives of the tool. For instance, ESOM tools like PyPSA differentiate by considering physical effects like power transmission (Brown et al., [2018\)](#page-10-1), while OSeMOSYS focuses on flexible representations to analyze development pathways (Howells et al., [2011\)](#page-11-2), or EnergyScope which provides additional details in the representation of the energy demand and its final usage (Limpens et al., [2019\)](#page-11-3).

Among the most studied variables in energy systems, time aggregation is one of the most relevant, as its adequate characterization allows the exploration of alternative characteristics of the system. A time frame between seconds to hours can be used to represent the operational behavior of plants, while a range between years and decades can be used to explore the evolution and expansion of the system (Fernandez Vazquez, Vansighen, et al., [2024\)](#page-10-2).

In a similar fashion, the spatial aspect becomes a relevant factor as well, as it can provide additional inputs regarding how energy is produced, consumed, and exchanged among different regions. This is a particularly relevant variable when large systems are studied, as the network resolution can have relevant impacts on the characterization of electric systems by providing important constraints like grid bottlenecks for power transmission or improving the availability of resources in specific regions (Frysztacki, Hörsch, et al., [2021\)](#page-10-3). However, the simplification of spatial aggregation is a much more common practice given that it allows modelling efforts to reduce computational requirements and data gathering (Frysztacki, [2023\)](#page-10-4). Within this context, the question regarding how to achieve an adequate spatial aggregation for a system arises, given that a compromise has to be made between accuracy and complexity.

Models such as Calliope, ETM, Oemof, OSeMOSYS, or PyPSA are some of the open-source tools that currently consider the geographical aspect of energy systems and provide flexibility regarding the spatial resolution, albeit with different levels of detail (Martínez-Gordón et al., [2021\)](#page-11-4). While some of them allow the manual definition of subsystems, others can apply clusterization methods to characterize them. In this context, PyPSA-Earth, an open-source model developed and based on PyPSA, appears as an alternative to create country- and region-wise models with a significant focus on data handling to customize the model to the requirements of the user (Parzen et al., [2022\)](#page-11-5).

In this paper, we propose a methodology to evaluate the effects of spatial aggregation (number of clusters) in an ESOM in order to find a cost-effective configuration regarding model size (node-configuration) and optimization results (deviations between cases). For this purpose, the PyPSA-BO model is used, a country-specific version of PyPSA-Earth developed for Bolivia where an expansion scenario for 2050 (based on results from part A) is run with several alternative node configurations.

2 METHODOLOGY

As mentioned before, working in energy system modelling implies a much-needed compromise between accuracy and complexity for the representation of a system, tackling either the model size, the problem class, or the connectivity between variables (Kotzur et al., [2021\)](#page-11-6). Particularly in terms of spatial aggregation, the topic has become more relevant in the last years and some studies and methodologies are now being developed and explored in order to tackle and improve the clusterization process (Hörsch and Brown, [2017\)](#page-11-7), and focusing mostly in the algorithms or heuristics used for solving the clusterization process (Biener and Garcia Rosas, [2020\)](#page-10-5).

While several methods are available and can provide alternative results depending on the components of interest for the study (like electrical components characteristics or renewable resources distribution), one of the most common clusterization techniques is the k-means method (Frysztacki, Recht, et al., [2022\)](#page-10-6). This method works by finding clusters of components with low variance regarding a specific variable (usually distance with respect to each other) and is implemented in established models like PyPSA-Eur and PyPSA-Earth.

With this in mind, the methodology in Figure [1](#page-2-0) presents a flowchart of the main stages for the study, which should be applicable to any other ESOM, as well as particular considerations followed for this case. This method tries to provide a simple and comprehensible way to evaluate the effects of aggregation in energy systems and define an adequate node configuration that allows an accurate representation of the system without exponentially increasing the demand for computational resources.

Figure 1: Base steps followed for the analysis of aggregation effects

3 CASE STUDY

3.1 PyPSA-BO model

The PyPSA-BO model is a customized version of the PyPSA-Earth model that uses its setup and workflow to generate an electric model of the Bolivian case study. Its main difference from the PyPSA-Earth repository is the pre-configuration of parameters across scripts, adapted for the particular case of the country, and the introduction of curated information. Figure [2](#page-3-0) shows the different stages in the workflow that have been adapted either by modifying sections of the script or by introducing particular sets of information instead, or on top of, the predefined data.

The PyPSA-BO model has been developed periodically, and several stages of its development, intermediate results, and configurations are available online in an open-source repository on GitHub, [Pypsa-earth-BO.](#page-0-0) Nevertheless, a compiled and more user-friendly version of the model will be made available in the open repository [\(github.com/CIE-UMSS.\)](#page-0-0) from the University Research Center of Energies from UMSS-Bolivia (CUIE), along with all data sets used.

Currently, the PyPSA-BO model is capable of representing the Bolivian National Interconnected System (SIN) and creating alternative versions of it based on the configuration desired. To achieve this,

Figure 2: PyPSA-BO's adaptations over PyPSA-Earth's base workflow

adaptations were made in the predefined workflow of PyPSA-Earth to tackle specific issues, mostly linked to data availability for the Bolivian system. Figure [2](#page-3-0) highlights the sections/scripts that were either adapted or customized with additional information such as Line information (GeoBolivia, [2021\)](#page-10-7), Poweplants (CNDC, [2021\)](#page-10-8), Demand profiles (CNDC, [2024\)](#page-10-9), Inflow information for hydro units (Huallpara et al., [2023\)](#page-11-8), or Expansion limits (Lahsen, [2015;](#page-11-9) Morato et al., [2019\)](#page-11-10).

Currently, the model continues to be developed as it improves its configuration and data sources, but previous implementations and usage of the PyPSA-BO model have already been presented at scientific conferences. In the first instance, the exploration of PyPSA-Earth and its application for Bolivia was presented (Fernandez et al., [2023\)](#page-10-10). In the second case, the study tackles some issues of data availability and achieves a simplified representation of the National Interconnected System (SIN) in Bolivia, allowing the exploration of potential development scenarios focused on the impact of water availability over the development of the system (Fernandez Vazquez, Hannotte, et al., [2024\)](#page-10-11).

Finally, by tackling the Bolivian case, the model has also been used to contribute to the main repository of PyPSA-Earth to improve the usage of the tool, particularly the implementation of complementary information. Currently, PyPSA-Earth covers close to 99% of the countries in the world, facilitating the creation and analysis of energy systems at a global scale (Fioriti et al., [2023\)](#page-10-12).

3.2 Baseline model

With all these changes, a 4-node configuration has been used to represent the Bolivian SIN (Fernandez et al., [2023\)](#page-10-10), defined by how entities in the electric sector consider the system, as composed of 4 major regions, North, South, Central, and Oriental (Transmision, [2022\)](#page-11-11). Results of the simulation of the Bolivian system with this configuration show relatively similar values when compared to historical values.

When simulating the characteristics of a historical year (2020), total installed capacities (3,253.87 MW) and energy production (9,212.90 GWh) match historical values, as both consider the same powerplants

and expected energy demands. Differences are found during the operation of the system, where the energy produced by thermal plants in the model is done exclusively by Combined Cycle Gas Turbines (CCGT), compared to reality, where fractions of the generation are covered by Open Cycle Gas Turbines (OCGT), Biomass, and Oil Plants. This is explained by the subsidized price of natural gas for the electrical sector in Bolivia (1.3\$/btu) (Hidrocarburos y Energia, [2012\)](#page-11-12), the large overcapacity available as the current peak demand is close to 1600 MW (CNDC, [2024\)](#page-10-9), and that the model disregards other social or political reasons for which powerplants should operate even if their efficiencies or costs are higher than others.

Another relevant difference is linked to the expected production from wind power plants, which is only a fraction of what can be expected in real conditions. This is a result of the generalized average to low availability factors expected for wind resources in Bolivia (Hidrocarburos y Energías, [2021\)](#page-11-13), with the exception of very particular zones like Qollpana (Corani, [2024\)](#page-10-13). Nevertheless, and with these considerations in mind, the model behaves as expected, showing minor differences between the usage of fossil thermal units (3.73% higher in real conditions) and renewable units (5.98% lower in real conditions).

With this context, the framework for future scenarios is done by implementing some additional considerations: Expected costs will follow reductions trends for each technology (Schröder et al., [2013\)](#page-11-14); planned and under-construction plants are included if they are expected to be finished before 2050 according to national reports (Electricidad y Energías Alternativas, [2014\)](#page-10-14) and ENDE's webpage (the main energy company in Bolivia) (ENDE, [2023\)](#page-10-15); older powerplants that have completed their lifespan before 2050 are taken out/decommissioned from the available set of generation units; future hydro powerplants are limited to consider only projects that have been identified and that at least went through under pre-investment analysis (Energetica, [2020\)](#page-10-16), as several of them have been put on hold due to social or environmental issues (Fundacion Solon, [2020\)](#page-10-17); the total electrical demand expected by 2050 assumes the results of Part A of this study (95.80 TWh), based on transition scenarios that push for the electrification of energy demands.

4 RESULTS AND DISCUSSION

4.1 Effects and limits of spatial aggregation over expansion analysis

The current version of PyPSA-BO allows the creation of alternative node configurations of the SIN in Bolivia, however, the representation of the system is restricted to a minimum of 2 nodes due to the characteristics of the model and its components, e.g. lines or links require two buses for their characterization and function and connect both components. On the other hand, the maximum representation possible with the current configuration is 62 nodes. This limit is defined mostly by the amount of data available regarding electrical components (generators, lines and substations) and the tolerance limits for grouping buses close to each other (5 km for this case).

Within these limits, results from alternative node configurations are run and used to exemplify the aggregation effects over the expansion of the energy system. Figure [3](#page-5-0) presents a compilation of the spatial distribution of installed capacities and transmission lines with alternative node numbers and displays how the location of components will change the characteristics of the system.

The most noticeable effect is that the generation mix will face an extreme transformation compared to its state in 2020. This is a result of the decommissioning of a large fraction of the older powerplants (mostly fossil fuel based), but mostly because of the growth expected from the system under transition conditions. As shown in Part A of this study, it is expected that the search for net-zero scenarios will imply the electrification of most of the energy demands and therefore the increment of electricity demand and renewable energies to cover it. A more detailed look on the expansion of generation capacities is available in Figure [4,](#page-5-1) where it is possible to compare how powerplants are expected to grow in the future in 25 different node configurations. Results show that, total capacities in the system remain somewhat stable compared to the magnitude of growth that the system has to undergo, however some particularities can be found.

Figure 3: Capacity distribution of powerplants and transmission lines for alternative configurations of the Bolivian energy in 2050

Figure 4: Capacity expansions expected in 2050 defined by number of nodes and technology

In every case, flexible powerplants (biomass, geothermal and hydro) are expanded to their maximum availability given the expected energy demand in the 2050 scenario. For hydro, the future capacity is defined by potential projects identified for exportation purposes to Brazil (Electricidad y Energías Alternativas, [2014\)](#page-10-14), however, we assume that the available potential will be used initially to cover the large increase in local demand and that exports would be outside of the scope of this study. For geothermal, generation potential was estimated between 600 and 1200 MW (Lahsen, [2015\)](#page-11-9), reason for which we used an average value (a maximum of 880MW on top of already planned powerplants). For biomass, the limit of systems was set based on the use of agroindustrial waste, which before 2020 was estimated to be 847 MW (Morato et al., [2019\)](#page-11-10) and we assume will at least double until 2050 if growth trends in population and industry are continued.

However, while significant growth is expected in these technologies, the biggest player to be considered regarding the expansion of the system is solar, with an average value of over 18 GW across simulations. This expansion is the result of the restriction on the usage of non-emitting technologies under the scope of a net-zero scenario (Part A), the abundance of solar irradiation in the south-west region in the country (Hidrocarburos y Energías, [2021\)](#page-11-13), and the low prices of the technology. These are the same reasons why wind resources are not expanded significantly in the future, given its average low availability in most of the country and higher investment prices compared to solar.

When evaluating the energy produced by source, some additional effects of the spatial aggregation can be identified. While energy is almost constant in all runs (particularly for flexible powerplants that are used at their maximum capabilities), it is possible to observe increases in the energy produced by solar and even wind generation as the number of nodes becomes higher, as shown in Figure [5.](#page-6-0) This effect is the result of the averaging process done during clusterization, as more and smaller regions can reduce averaging conditions and provide zones with higher capacity factors. This is consistent with results from similar studies done for Europe and at a much larger scale (Frysztacki, Hörsch, et al., [2021\)](#page-10-3). While changes in solar capacity production are mild compared to their capacity and overall production, results behave as expected, as the country has a high and uniform capacity factor. For wind generation, it is possible to see that a threshold of 35 nodes has to be overcome so that averaging effects stop limiting the deployment of the technology. While this increase in capacity is minor compared to other technologies, it is highly noticeable for wind resources as they were disregarded for the most part at fewer node configurations.

Figure 5: Expected energy production for solar (PV) and wind (onshore) powerplants

Another noticeable effect of the large increase in the energy demand is the introduction of regulation technologies such as batteries and hydrogen. Both storage technologies behave similarly to solar growth and dispatch, mainly due to their complementarity, and serve as a short-term storage to improve flexibility in the system. During the middle of the day, when solar capacity is at its peak, energy produced is stored in batteries or as hydrogen, to be later used in the afternoon, during hours of peak demand. While total generation and dispatch values might vary between cases, the overall behavior in the system is kept, for which Figure [6](#page-6-1) provides a referential case of how dispatch is procured in 2050 at a 20-node aggregation.

Figure 6: Aggregated dispatch simulation for the first week of June in a 20-node configuration of the Bolivian energy system in 2050

Finally, the expansion of transmission capacities depicted in Figure [7](#page-7-0) shows that node configurations lower than 12 would expect large concentrated increases in the transmission system (up to 1105MW for a single line in the south). This is a direct effect of the large installed capacities clumped in a few nodes and the need to create connections between them to facilitate the energy flow between regions. In other words, the representation of the transmission system and the constraints that it implies for the model are only noticed after a certain aggregation threshold that avoids oversimplifications in the model, which is consistent with what other authors reported (Frysztacki, [2023\)](#page-10-4).

Figure 7: Average and total expansion expected per node for the transmission system

Any additional number of nodes (higher than 17) would result in the reduction of the average expansion per line but with a larger total capacity expansion for the transmission system, as seen in Figure [7.](#page-7-0) In this sense, it is shown that an adequate node resolution, even at relatively small quantities, could have significant effects on the accuracy and development expectations of the transmission system, as stated by other authors (Priesmann et al., [2019\)](#page-11-15).

4.2 Trade-offs between computational resources and system representation

As mentioned before, the more complex or detailed the representation of a system is desired, the more complex the models will become. For this particular case, a compilation of the optimization time required to solve each alternative version of the model was done, considering that all simulations were run on the same computer with a CPU AMD Ryzen 7 5700U and the Gurobi Optimizer version 10.0.1. Results show that as the model considers a higher spatial resolution, the complexity evolves as time required to find and optimal solution increases, as shown in Figure [8.](#page-8-0) While simplified versions, under 5 nodes, would require less than a minute to find an optimal solution, solving the model with the highest resolution would require over 50 minutes of optimization. While these values are still within the margins of what most users could run in commercial equipment, larger or more detailed versions would require dedicated equipment due to the power-law relation between the node-configuration size and optimization times.

Nevertheless, while an accurate representation of the system is important, the definition of an adequate configuration is also relevant, as systems can become exponentially more complex by including additional variables and information or changing certain parameters. In this sense, defining an objective of analysis would be a good practice to find an adequate node configuration. For this case, a Pareto analysis was made focused on the capacity expansions expected for Solar powerplants, as the most relevant technology in the scenarios. Differences between the expected installed capacity for each node configuration and the current maximum representation of the system (62 nodes) were made to make the analysis.

Results, available in Figure [9,](#page-8-1) show that analyzing a system with a total of 22 nodes would be sufficient to accumulate over 80% of divergences in all the cases considered. Additionally, results show that the 22-node version would have a difference of only 3% compared to the capacity found at 62 nodes. Aside from certain outliers where simulations provided capacity expansions close to the most desegregated version (5-node configuration), this analysis serves as a way to define a cost-effective configuration, as

Figure 8: Optimization time require to solve the model at different node configurations

by compromising the representation of the system, a large cut can be made regarding computational resources (4.8 times less optimization time than in the 62-node version).

Figure 9: Pareto analysis for capacity divergences in solar generation and number of nodes

Finally, while this approach provides relevant inputs regarding how to limit the complexity of the model, it is important to consider that the actual sizing of the model (its spatial resolution) will be dependent on the variable of interest. Because of this, complementary analysis could be made by considering other relevant factors and analyzing them in tandem.

4.3 Soft-linking and synergies between models

Results from the study show that expansion of the system requires a total installed capacity of 27 GW (excluding storage charge and discharge capacities), which would represent a transcendental change in the Bolivian energy system under the conditions defined for the 2050 scenario in Part A. This growth is mainly derived from a big electrification process of fossil fuel demands, as showed in Part A, and is consistent with other studies that have sized for the transition of the Bolivian system (Fernandez Vazquez, Vansighen, et al., [2024\)](#page-10-2).

This capacity expansion for Bolivia is significantly larger compared to what is expected for Europe (Crespo Del Granado et al., [2020;](#page-10-18) Hainsch et al., [2022\)](#page-10-19) or European countries (Hansen et al., [2019\)](#page-11-16), which estimate an increase closer to doubling the capacities from 2020 by 2050. In these cases, electricity consumption already represents a significant share of energy demands (close to 23%), electricity consumption and growth have stagnated, and the deployment of technologies such as hydrogen is expected to compete/replace certain fossil-based energy demands. All these conditions are completely different for Bolivia, where electricity represents only 12% of energy consumed, demands are expected to double as they are still coupled with population growth, and non-conventional technologies have much higher costs, niche applications, and technology readiness (Part A).

Because of these results, it is clear that models that can focus on demand-side analysis, such as EnergyScope Bolivia, are required to properly size the challenge linked to the energy transition, as a model like PyPSA-BO currently cannot do this. In contrast, while the assessment of which technology would become the biggest player in the transition of the system (solar) found by EnergyScope is consistent, by considering a system without transmission restrictions and a reduced time resolution, the expansion and dispatch are much more permissive regarding the flexibility of the technology, installing higher capacities and little to no storage capacities. In this sense, PyPSA-BO provides a much-needed adjustment given that, even with a small number of nodes considered, transmission limits will constrain the operation of the system. This is done by either incrementing transmission capacities between nodes, adding storage capacities to provide the system with flexibility, or both. In this sense, while PyPSA-BO also considers solar as the biggest player for the expansion of the system in 2050, its implementation is more discrete, and is only possible thanks to the massive deployment of short-term storage capacities, close to 8 GW of power distributed evenly between batteries (dischargers) and hydrogen (fuel cells).

5 CONCLUSIONS AND FUTURE WORK

This paper (Part B) focuses on exploring the role that spatial aggregation can play in the representation and development of an energy system, and for this particular case, the Bolivian energy system transition until 2050 as presented in Part A. While a wide array of modelling tools are currently available to tackle this issue, we focus on the use of an adapted version of the model PyPSA-Earth for the Bolivian case, which uses a k-means clustering algorithm for clustering the system based on its electrical components.

An analysis of the capacity expansion under alternative spatial resolutions shows that in every case the system will incur in major changes regarding its installed capacity, expecting a total of over 27 GW. The change on the generation mix is attributed to the substantial increase of energy demands and the introduction of renewable powerplants (planned and not planned), where solar plays a pivotal role.

Nevertheless, while all cases show relatively similar outcomes, the spatial resolution of the system plays a relevant role in the behavior of the system. A high aggregation (few nodes) can lead to the misrepresentation of the transmission lines as well as underestimating and concentrating expansion requirements. As more nodes are considered (over 12), transmission lines start playing a more constraining role in the system, distributing the expansion capacities more evenly across the country. In a similar way, as more nodes are considered, variables such as solar and wind capacity factors can be better represented, favoring the deployment of these technologies in specific zones and improving their yields.

While a case can be made to consider conditions as close as possible to reality to improve the accuracy of the simulations, it is important to consider the trade-offs between the model's complexity and the computational resources. An analysis made for the optimization times of over 25 node configurations between 2 and 62 nodes shows that there is a clear power-law scaling between the optimization time and the spatial resolution. In this sense, to find a cost-optimum configuration of the system, a Pareto analysis is done for the expansion divergences of the solar capacities. Results show that using a node configuration of 22 nodes would suffice to cover over 80% of the aggregated divergences and would require less than a fourth of the optimization time while having only a 3% difference compared to the 62-node version.

Finally, it is important to mention that the work done in Part B is highly synergistic with Part A, as models like EnergyScope Pathway-Bolivia, which have a higher level of detail and representation on technologies and demand characterizations, can provide a key input for PyPSA-BO in the form of the expected demand in the system for future scenarios. In contrast, the higher spatial and temporal resolution used by PyPSA-BO can provide both a consistency check on results from EnergyScope, as well as potential feedback, additional constraints, expansion limits, and technological requirements to improve its results. In this sense, future work will focus on expanding this feedback process and developing a proper soft-linking methodology for both tools in order to better exploit the presented synergies and achieve convergent results that can provide a robust development plan for the transition of the Bolivian energy system.

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