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Nuclear Reaction Network Unveils Novel Reaction Patterns and Nuclei Stability

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Despite the advances in discovering new nuclei, modeling microscopic nuclear structure, nuclear reactors, and stellar nucleosynthesis, we lack a systemic tool, in the form of a network framework, to understand the structure and dynamics of 70 thousands reactions discovered until now. We assemble here a nuclear reaction network in which a node represents a nuclide, and a link represents a direct reaction between nuclides. Interestingly, the degree distribution of nuclear network exhibits a bimodal distribution that significantly deviates from the power-law distribution of scale-free networks and Poisson distribution of random networks. The distribution is universal for reactions with a rate below the threshold, $\lambda < e^{-T^\gamma}$, where T is the temperature and $\gamma \approx 1.05$. We discovered three rules that govern the structure pattern of nuclear reaction network: (i) reaction-type is determined by linking choices, (ii) spatial distances between the reacting nuclides are short, and (iii) each node in- and out- degrees are close to each other. By incorporating these three rules, our model unveils the underlying nuclear reaction patterns hidden in a large and dense nuclear reaction network. It enables us to predict missing links that represent possible new nuclear reactions not yet discovered.

Introduction

Since the birth of the universe in the Big Bang about 15 billion years ago, its evolution was accompanied and often driven by nuclear reactions. The birth, life and death of stars, Earth and their occupants, either animate or inanimate are all the products of these processes, evolved from the nucleosynthesis of the lightest elements (hydrogen, helium and lithium) ^{1,2}. Furthermore, the discoveries in nuclear science have also led to modern innovation and technology advances that have improved our lives by enabling, for example, the sustainable clean energy ^{3,4}, the introduction and use of radioisotopes for medical diagnosis and therapeutic purposes ⁵⁻⁸, and advances in material science ^{9,10} by use of the nuclear reaction microanalysis.

During 1870s, the Russian chemist, Dmitri Mendeleev, discovered the periodic patterns of chemical reactions among elements and created the famous periodic Table ^{11,12}. The prediction of new elements became possible based on the empty positions in this Table. Accordingly, some unknown elements in Mendeleev's time have been predicted, and indeed, were later discovered ¹³. Until now, new elements are still emerging and filling their missing places in the Table ¹⁴. At the time of discovery, nobody understood what caused the regularities observed by Mendeleev but they were widely used in chemistry. It took physics over 50 years to catch up and explain them. The periodic Table is a powerful tool, but from the network science point of view, it is a regular lattice capable to reveal very simple and realistic patterns. It is neither able to differentiate between the isotopes of the same elements nor depict the reactions from one isotope to another. Therefore, nuclear reaction networks were proposed in which each element had been represented by set of

nuclei of its isotopes together with nuclear reactions among them. They are used to describe the nuclear energy generation or the evolution of entire composition of nuclei in different astrophysical scenarios^{15–24}. The current state-of-the-art is that the existing nuclear reaction networks are limited to several nuclei, which can be modeled by a set of ordinary differential equations. The difficulty with this approach is that it relies on full knowledge of three correlated layers, each of which is only partially known: (1) all the nuclei in our universe; (2) all the possible direct reactions between nuclei; (3) the exact reaction rates. Consequently, this approach is forced to use a set of dynamical equations to model an incomplete graph, which may lead to a completely wrong parameter estimation or prediction of each nuclide abundance. Currently, progress has been possible only for few closed systems with several dozens or hundreds of nuclei^{19,22,24}, where all three layers are assumed to be fully known. Examples are the explosive nucleosynthesis in supernovae¹⁷, core-collapse supernovae^{20,21}, novae^{15,16,23}, or X-ray bursts^{18,19,22,24}. Thus, the existing approach can only represent closed systems that include all the nuclei. Consequently, it cannot be used for predicting new nuclides or reactions, and we are far from understanding the full range of nuclear reactions in our universe. Despite some pioneering conceptual work in both nuclear physics^{25–30} and network science³¹, we still lack a systematic network framework for predicting new nuclei and nuclear reactions analogous to the famous periodic Table of elements. Here, for the first time, we apply network tools into nuclear physics and develop a framework, which enables modeling the global structure of the nuclear reaction network without considering their dynamical equations. This approach opens novel ways to discover new reactions.

We find some intriguing regularities, such as binomial degree distribution, symmetry of in

and out degree, which are not yet explained by the current theory of nucleus dynamics and stability. We also show that our nuclei network framework guided by machine learning techniques and network science enable us to model the properties of isotopes as dependent on their positions in the network. Our main contribution is the discovery of hidden patterns in a large and dense nuclear reaction network by applying network framework approach. We hope in future work to address the open questions which arise from our current framework, like what physical properties of nuclei can cause the existence of the discovered patterns.

Results

Spatially Embedded Nuclear Reaction Network

Many complex systems, such as transportation networks, power grids, Internet, and neural networks, are organized as spatial networks with nodes and edges embedded in some kind of geometric space³². In these networks, there is a cost associated with the length of edges that, in turn, dramatically affects network topology. As shown in Fig. 1b, the reaction network defines an affinity relation from one nuclide to another, such that a pair of nuclides are connected if there is a direct nuclear reaction (see Fig. 1a). The reaction network, in essence, is analogous to a spatially embedded grid network in a two-dimensional Euclidean space. As demonstrated in Figs. 1c and d, each nuclide is characterized by its neutron and proton numbers, that can be represented as a lattice grid point in the nuclear chart, where the x coordinate value is defined by the number of neutrons

N , and the y coordinate value is defined by the number of protons Z . All isotopes of an element are placed on the same row in the lattice. The spatial network brings stability into our consideration, and provides another benefit to distinguish the one-hop neighbors according to the statistics N and Z . Fig. 1a illustrates a reaction chain from $^{63}_{29}\text{Cu}$ to $^{60}_{28}\text{Ni}$. It shows two primary direct reactions: (i) $n + ^{63}_{29}\text{Cu} \rightarrow ^4_2\text{He} + ^{60}_{27}\text{Co}$, which is an α decay, and (ii) $p + ^{60}_{27}\text{Co} \rightarrow n + ^{60}_{28}\text{Ni}$, which is a charge exchange reaction (p, n). These three nuclides ($^{63}_{29}\text{Cu}$, $^{60}_{27}\text{Co}$ and $^{60}_{28}\text{Ni}$) and two reactions form a network shown in Fig. 1d, which is part of a large network (Fig. 1b) with 8,042 nuclei and 77,293 direct nuclear reactions³³ (see Section S1 B for detailed description). The topology of the entire nuclear reaction network indicates obvious spatial constraints (Fig. 1b) and strong in-out degree correlations (Fig. 1f), which, however, significantly differs from traditional two-dimensional lattice model or other spatial networks³². Fig. 1c illustrates a sub-network of $^{235}_{92}\text{U}$, showing all the possible direct reactions from and to $^{235}_{92}\text{U}$. The in-degree of $^{235}_{92}\text{U}$ is 5, including two charge exchange reactions of the type (n, p) and (p, n), two photon-disintegration reactions of the type (γ, n) and (γ, α), and one neutron capture (n, γ) reaction, as shown in Fig. 1e. The in-degree of a nuclide measures number of other nuclides that can produce this nuclide, and the out-degree denotes the number of nuclides that one nuclide can produce.

The degree distribution is an essential characteristics of the model and real-world networks^{34,35}, determining their robustness³⁶, controllability³⁷ and resilience³⁸. The degree distribution of nuclear reaction networks enables us to discover the reaction patterns as well as promoting novel prediction approaches for new reactions. As demonstrated in Fig. 1e, the nuclear reaction network exhibits an interesting bimodal degree distribution, which is very different from the common scale-

free ³⁹ or Poisson distribution ⁴⁰. In the nuclear reaction network, the degree of a nuclide indicates the number of all one-hop neighbors of the nuclide, which is strongly related to the stability of the nuclide. Generally speaking, a nuclide with balanced neutrons and protons tends to be more stable than those with excess of neutrons or protons. There is an implicit limit on N and Z numbers that a nuclide can hold, forming the nuclear chart's boundaries, where the nuclei tend to have fewer direct nuclear reactions. Such spatial constraint and the spatial distribution of nuclei strongly affect the degree distribution, deserve close attention. For the nuclides containing the same number of protons (i.e., associated to the same element) in one row of the nuclear chart, we notice that the degree generally reaches a peak between the stable nuclides and the ones on the boundaries (i.e., nuclides with minimum or maximum number of protons), as shown in Fig. S1d. For different elements, the degree also presents a significant difference between the heavy elements with $Z > 82$ denoted as *upper region* and the light ones with $Z \leq 82$ denoted as *lower region*. Despite the vast differences in degrees exhibited in different regions of the spatial space, surprisingly, we still observe a strong correlation between the in- and out-degree of the individual nuclide as shown in Fig. 1f.

For the nuclides with degree between 7 and 10, such correlation is not as strong as for other nuclides, as indicated by the size of the circle. We suggest two possible reasons for this feature: (i) there is no sufficient number of nuclides in this region; (ii) most of the nuclides in this region are located on the boundaries of the nuclide chart, where spatial constraints limit the reaction types that can happen there (see Fig. S1).

Impacts of Temperatures and Reaction Rates

The nuclear reaction network in astrophysics is a system composed of N ordinary differential equations ²⁴, where N denotes the number of nuclides and each variable represents the abundance of the species. The Jacobian matrix of the system, when it reaches a steady state, represents the topological interactions between nuclides, forming a weighted nuclear reaction network. The nonzero entries in the matrix represent the coupling strength between nuclides ¹⁹, which can be defined as a function of the stellar temperature T and parameters specific for each reaction given in Gigakelvins ⁴¹. Specifically,

$$\lambda = \exp \left[a_0 + \sum_{i=1}^5 a_i T^{\frac{2i-5}{3}} + a_6 \ln T \right], \quad (1)$$

where $a_0, a_1, \dots, a_6$ are the parameters associated with each individual reaction collected in JINA REACLIB ³³. Note that we correct the inverse reaction rates for the astrophysical context using partition functions (see Section S6). Thus, Eq. (1) enables us to construct a weighted nuclear reaction network for a given temperature. As shown in Fig. S6, the reaction rate distributions vary with temperature, promoting us to explore the topology of the nuclear reaction network response to the temperature.

For a given temperature and a reaction rate threshold, λ_θ , we generate a subnetwork by removing the edges whose reaction rates are below the threshold. When $\lambda_\theta = 0$, we always observe the complete nuclear reaction network for any given temperature. However, as we increase the threshold, more and more reactions with low rates disappear from the network. Therefore, both the temperature and the rate threshold, λ_θ , determine the connectivity of the network, see Fig. 2a.

As the temperature increases from left to right horizontally, and λ_θ stays the same, the nuclear reaction network increases its connectivity. This trend arises because some nuclides stable at lower temperatures become unstable at higher temperatures. In contrast, for a fixed temperature, as λ_θ increases (from bottom to top vertically), reactions disappear, making the nuclear reaction network sparser.

To summarize, we discover that the number of connected nuclides and reactions increases with temperature and decreases with λ_θ . Thus, at high temperatures and low thresholds, the system develops the richest community structures, and we illustrate these communities with different colors both in the scaled-down reaction networks and the nuclide chart (see the inset in Fig. 2 and Fig. S7). Surprisingly, we discover that the stable nuclides (shown in red in the nuclide chart) play an essential role in bridging the two communities, shown in the right and bottom of Fig. 2a. Furthermore, we observe the modality of the degree distribution of the subnetworks (Fig. 2b-d) based on Gaussian kernel density estimation and peak detection (see Methods). The degree distribution exhibits a modality shift from a bimodal degree distribution (left subfigure in Fig. 2b) as observed in the full reaction network to a unimodal degree distribution as the reaction rate exceeds the critical point λ_c (right two subfigures in Fig. 2b). In Figs. 2c and d, we demonstrate that such modality shifts with the detected most frequent degrees. The red and blue bars in Fig. 2b divide the degrees into two distinct clusters, each of which has a characteristic degree. Finally, we find the critical reaction rate threshold λ_c of the modality shift and it shows a universal law as a function of the temperature (see Fig. 2e)

$$\lambda_c = \exp[-T^\gamma]. \quad (2)$$

Empirically, we get $\gamma \cong 1.05$ for reaction networks at temperatures $0.1 \leq T \leq 1.5$.

Nuclear Network Model

In spatial network models, such as random geometric graphs, two nodes are connected with high probability if their Euclidean distance is short, which are usually modeled as undirected networks with bidirectional links. The bidirectional topology, however, does not hold (Fig. S1) in our nuclear network, prompting us to use a directed spatially embedded model ⁴².

On the two-dimensional spatial grid described in Section , we find that the spatial distribution strongly associates with the position of the nuclides on the grid and the reaction modes. There are neutron-rich or proton-rich regions, also known as drip lines on the nuclide chart ¹⁴. The boundaries of the nuclide chart limit the possible nuclear reactions, and the nuclides lying close to the boundaries are short-lived radioactive nuclides having small degrees in the reaction network. The radioactive nuclei tends to decay to stable nuclei while the amount of radioactivity of reaction products always decreases. However, fewer reactions occur on short-lived radioactive nuclei when compared with the stable or long-lived ones. The 253 stable nuclides shape a valley of stability between the boundaries ⁴³, which have an abundant number of in-coming and out-going reactions. For nuclides of different elements (i.e., containing different numbers of protons), there is a clear separation line between the high and low degrees nuclides, and it also delineates the limit of the valley of stability. Up to Lead (i.e., $Z = 82$), each element has at least one stable isotope; for the elements above Lead, no stable isotopes exist, and these heavy elements have few edges in

comparison with elements at the bottom of stability valley.

Motivated by the fact that the degree of a nuclide depends on its spatial location in the nuclide chart, we incorporate both the stability valley and the boundaries, that is the distance d_s to the nearest stable nuclide and the distance d_b to the nearest chart boundary, and propose a simple degree model $K(d_b, d_s; \Theta)$, where Θ is a vector of parameters. The nuclide degree for the given element increases for both large d_s and d_b . Note that there are various forms of $K(d_b, d_s; \Theta)$, and we consider two specific implementations in our analysis, see Methods and Section S2 for their explicit forms and the approach to learn the parameters.

Our model predicts the degree of each nuclide, i.e., the number of possible reaction modes, as shown in the Supplementary Movie. With these predictions, we reconstruct the nuclear reaction network. Instead of randomly connecting a pair of stubs as presented in the configuration network model^{44–47}, we reconstruct the network based on three rules: (i) *reaction type is determined by linking choices*, (ii) *distances between the reacting nuclides are short* and (iii) *each node in- and out- degrees are close to each other*. For details of these assumptions, and the detailed reconstruction procedure, see Methods.

We compare the reconstructed networks with the real network from different perspectives, including the global degree distribution and the local degree differences between elements and different regions. This comparison demonstrates that our network model can capture the essential characteristics of nuclear reactions, especially the bimodal degree distribution. Moreover, it is theoretically proved that the bimodality can be captured with the proposed network model on an

approximated triangular nuclear chart (see Section S4 for detailed derivation). We choose a random network model as a baseline, which considers the constraint of *reaction-type being determined by linking choices* and each edge is assigned to one of the 15 reaction modes. For convenience, hereinafter, the random model is denoted as **rand**, and the other two models are denoted as **min** and **prod** respectively.

As shown in Fig. 4, both **min** and **prod** models reproduce the degree distribution of the real nuclear network accurately, much beyond preserving only the overall bimodality. Most importantly, the locally relative ordering of degrees is preserved. Also, the error bars in Fig. 4 indicate the robust performance of our model. Overall, the **min** implementation achieves better agreement with the real degree distribution. In marked contrast, the baseline random model produces a Poisson degree distribution, deviating significantly from the real bimodal degree distribution, and show high variance from the real network. These indicate the importance of restricting reacting nuclides distances and strong correlation of in- and out- degrees for generating the bimodal distribution characteristic of nuclear reaction network degree distribution. As shown in Figs. 1e-f with this distribution, only a tiny fraction of nuclides have degree $k_{out} = \{0, 7, 8, 10, 11, 16\}$, and therefore the predicted degrees have large fluctuations due to limited data points. Meanwhile, a remarkably close agreement between the reconstructed degrees and the ground truth can be found for $k_{out} = 12$, which contains nearly 25% of the nuclides, and for $k_{out} = 15$ with 17% of the nuclides, further validating the outstanding performance of our model.

Next, we employ four metrics to evaluate the performance of our model – precision, recall,

and Jaccard index for both in-degree and out-degree of each nuclide, and the clustering coefficient (see Methods for specific definitions). As shown in Fig. 3, we consider the directions of edges and obtain the average performance on the element level (Figs. 3a-g) and network level (Fig. 3i). For the degree distribution, one can see a valley between the two peaks, which is eroded by nuclides with 8 to 11 reactions. Their geographic positions relative to the boundaries and their number of protons are shown in Fig. S1b. As demonstrated in Fig. 3h, the reconstructed models identify the patterns in d_b with remarkable 80% similarity to the original network, but less than 60% similarity w.r.t the distribution of the number of protons. Yet, the **rand** implementation is very far from the other two, except for recalls (see Figs. 3b,e) in the upper region $Z > 82$. The reason is that nuclides in this region have only 3 to 6 edges and the **rand** implementation gives predictions of at least 8, which increases the recall values. In summary, our network model, described by the three mechanisms, retains the essential real properties of the nuclear reactions, and captures the spatial attributes, offering a better and new understanding of the nuclear reaction network.

Nuclide Chart Expansions

Scientists still continue to discover new elements and nuclides ¹⁴, and thus the boundaries of the nuclide chart are expanding as well. To examine the predictive power of our model, we ask the fundamental question: can we predict new reactions across the entire network extracted from the JINA REACLIB database using the experimentally validated subnetwork? Until the end of 2017, scientists have discovered 3,196 nuclides and 32,184 reactions in nature or in the laboratories ^{43,48},

forming a validated subnetwork (the red region in Fig. 5a). Based on this subnetwork, we use our parametric degree model to predict the probability of occurrence of directed reactions between 4,846 new nuclides. Our approach is significantly different from the current state-of-the-art models for nuclear reaction discovery. These models primarily probe the microscopic physical or chemical properties of isotopes, e.g., energetic possibilities⁴⁸. There exists evidence^{48–50} that the newly discovered nuclides are always close to the existing nuclides in the nuclide chart.

Our network approach can precisely predict novel reactions that have not yet been discovered in nature or in the laboratories as shown in Fig. 5. As the size of the nuclide chart increases, the overall quality of agreement with the ground truth (i.e., the real reaction network) does not fluctuate too much except for the last expansion, which shows a decline on each measure relative to other steps (Fig. 5). The nuclides discovered during previous expansions are densely connected, but the ones included in the fifth expansion, especially the heavy radioactive nuclides that lately join the network, have much fewer connections.

Interestingly, analogous heterogeneity in the links for different regions has been observed in city development⁵¹. As formulated in the core-periphery model⁵² in the emergence of an urban system, the constructions of the core and the periphery regions are very unbalanced. In our case, the previously discovered nuclides are in this core, and those found later belong to the periphery region, and nuclides in the core region have more connections than those in the periphery region.

Reaction Prediction

Our degree model predicts the number of potential reactions for each nuclide, and many nuclides may have less connections than that predicted. The difference implies missing nuclear reactions. To predict the missing nuclear reactions, we propose a simple matching algorithm. It is straightforward, and does not have any spatial preference over the choice of nuclear reactions. Therefore, we are able to study reactions beyond specific nuclides, reaction modes⁵³, or regions in the nuclide chart^{54,55} and make new discoveries.

We search all eligible out-going and in-coming edges for each nuclide by excluding all existing nuclear reactions. An eligible reaction first should belong to one of the 15 most common modes of nuclear reactions, then the nuclide must have missing connections. Also, an eligible connection $u \rightarrow v$ must be eligible for both u and v . We iteratively match pairs of nodes with eligible edges, remove the illegible ones and drop nodes without missing connections based on the predictions, until no eligible connection can be found. As illustrated in Fig. 6, we predict all potential new reactions with nuclide u as the target. There are 8 feasible reaction modes from u , and 4 of them (red edges) have been discovered. According to our degree model, nuclide u is predicted to have 6 connections, i.e., $k_u = 6$. Therefore, it still has 2 missing links from the possible choices $\{u \rightarrow 1, u \rightarrow 2, u \rightarrow 3, u \rightarrow 4\}$. The prediction will be made based on the states of the possible production nuclides $\{1, 2, 3, 4\}$. According to the degree prediction, node 1 should have $k_1 = 4$ in-coming connections, excluding 4 already discovered reactions, there is no space for extra reactions. Therefore, the edges $u \rightarrow 1$ can be discarded (dashed). Node 2 is checked similarly. It has

$k_2 = 6$ stubs, but only 5 feasible reaction modes, and 4 of them have been discovered. Therefore, node 2 must choose u , and $u \rightarrow 2$ must be kept. But it may be not the only choice for node u , which can have other choices. Node 3 has to choose from the remaining undetermined edges to build 1 or at most 2 connections. We examine node 4, which still misses 2 possible reaction modes. Suppose the degree model is accurate, and no nuclide has more connections than that predicted, the prediction becomes the general *b-matching* problem ⁵⁶.

Conclusions

We lack an effective representative “Table” for nuclides that is analogous to the well-known Periodic Table for elements. The organization of such a “Table” should be both microscopic, because a nuclear reaction involves interaction between atomic nuclei; and also global, because otherwise one might miss the big picture of the interplay between the structure and the dynamics of nuclear reactions. In the present article, we fill this gap by developing a network framework for nuclear reactions, which encodes the existing discovered nuclides as nodes and linking the nuclides that are involved in the same direct nuclear reaction. With a wealth of techniques established in network science, we analyze the network reaction network, and develop a predictive degree model $K(d_b, d_s; \Theta)$ that captures the impact of spatial properties of nuclides on the number of the reactions in which a nuclide participates. Also, we develop a growth model to explore the evolution of nuclear reactions and understand how the characteristic bimodal degree distribution emerges.

All the reactions associated with one nuclide represent different reaction modes, and a reaction mode can be identified with the spatial information (i.e., N and Z) encoded in all involved nuclide nodes of the direct reactions. The spatial information is implicitly encoded in the reactions or the edges of the reaction network. But, the reaction network is still unweighted without an explicit weighting scheme over the edges. From an unweighted reaction network, we discover the characteristic bimodal degree distribution and three recurring patterns. As we explicitly weigh the connections using the reaction rates, we make an additional contribution in studying the modality transition in the degree distribution of the weighted nuclear reaction network. We find that the network topology changes with the temperature of the reactions, and the bimodal distribution is universal for reactions with a rate below the threshold, $\lambda < e^{-T^\gamma}$, where T is the temperature in Gigakelvin and $\gamma \approx 1.05$.

There are several important problems uncovered by the research presented in this article, including (i) improving the overall reconstruction performance by incorporating the correction among different reaction modes (Fig. S2) to our current reconstruction procedure, (ii) developing a dynamical model over the proposed spatially embedded network to predict nuclide abundances, and (iii) identifying the most economical path to produce medically useful isotopes^{57,58}. We leave detailed investigations of these questions for future work.

Methods

Model of Nuclear Reaction Network

Degree Model. To demonstrate the ability of our degree model to capture the spatial degree distribution, we introduce two specific implementations:

1. define $K_{\text{prod}}(d_b, d_s; \Theta) = c(d_b^\alpha + b)(d_s^\beta + a)$, where $\alpha, \beta, c \in \mathbf{R}^+, a, b \in \mathbf{R}$
2. define $K_{\text{min}}(d_b, d_s; \Theta) = \min \{c_1 d_b^\alpha + b, c_2 d_s^\beta + a\}$, where $\alpha, \beta, c_1, c_2 \in \mathbf{R}^+, a, b \in \mathbf{R}$

Both have the exponent parameters α and β that represent the strength of d_b and d_s . The bias terms a, b , the coefficients c, c_1 and c_2 are included to improve the fit of the predicted degree with the degrees of known nuclides in the nuclide chart. These two implementations yield the accurate degree distribution, although they are structurally different. For example, K_{prod} is a continuous function of d_b and d_s , but K_{min} is a discontinuous function. For K_{min} , even if two nodes are predicted with the same degree, the sources of this prediction may be different, some come from the impact of stable nodes, $c_2 d_s^\beta + a$, others from the chart boundary, $c_1 d_b^\alpha + b$. Also, there exists obvious difference in the distribution of the degree between nodes at the two sides of the stable nodes. Hence, in order to reflect this difference, we introduce two different bias terms b_1 and b_2 for nodes located at the left and the right side of the stable nodes, respectively.

Both K_{min} and K_{prod} are parametric models, and each has several parameters to calibrate.

To have a good prediction of the node degrees, and to fit the degree distribution of the entire network, we adopt a mixed optimization approach to search for optimal parameters. We apply the gradient-based optimization method BFGS⁵⁹ in the initial searching stage, then make further calibration with the derivative-free Bayesian optimization method⁶⁰, which is widely used in machine learning. The optimal parameters and associated prediction accuracy are summarized in Table S3.

The degree implementations yield continuous predictions, however the true degrees are integers. To be realistic, in the estimation of the prediction accuracy, all predictions are rounded to their nearest integers in our analysis.

Network Reconstruction Model. Both the configuration model and the hidden parameter model are able to generate networks with arbitrary degree distribution. The configuration model assigns each node a predefined degree as stubs, then randomly chooses a pair of stubs in two nearby nuclides and connects them. But this procedure is likely to produce multi-links, which are forbidden in many real networks, including the nuclear reaction network. The hidden parameter model assigns a hidden parameter to each node, and randomly selects two nodes with probability proportional to their hidden parameters, respectively. Both nodes are discarded if they are already connected, otherwise a new link is created. This method can avoid parallel-links, but it still suffers the same problem as the configuration model, i.e., producing many long-distance links, which do not exist in reactions.

To reproduce the nuclear reaction network, we need to resolve the aforementioned issues encountered by both network models. To this end, we put additional constraints on the network

generation procedure:

(i) *Reaction type is determined by linking choices:* According to the categories of the reactions presented in Table S2, nuclides are linked primarily through 15 reaction modes which constitute an eligible reaction space to generate the network. The linking choices for nodes are limited to be dominant reaction modes.

(ii) *Distances between the reacting nuclides are short:* Another critical aspect of the model is the preference for short Euclidean distances in the chart between reacting nuclides, so that connections are chosen with different priorities. In general, the nuclides close to each other in the chart are connected with higher priority than those located further away from each other.

(iii) *Each node in- and out- degrees are close to each other.* This constraint enforces the correct degree distribution illustrated in Fig. 1f, that the in- and out-degrees of each node are strongly correlated. Most of the nodes have in- and out- degrees close to each other. Therefore, a simplification is made in our generation procedure, by assuming that the number of out-going edges from a node is the same as the number of edges in-coming to it.

Another important aspect is the maximum number of eligible edges, which is predicted with the *degree model*. Accompanied by the aforementioned three assumptions, we propose the following procedure to reconstruct the nuclear reaction network from isolated nodes, expecting to achieve moderate accuracy.

Step 1. Search the nearest stable nuclides and the nuclide boundaries for each element, and set them as the references.

Step 2. Compute the distance d_s to the nearest stable nodes, and the distance d_b to the nearest boundary for each node.

Step 3. Predict the degree of each node with the degree model, and the predicted degree is the capacity of eligible edges that can be attached to the node.

Step 4. Select an eligible outbound edge according to the associated spatial priority, then update the vacancy of the related nodes with the predicted degree and the eligible edges.

Step 5. If a node has no vacancy to fill, it will be removed in the next round.

Step 6. The procedure is terminated once all nodes have their vacancies filled, and a new network is constructed.

It is possible that the procedure fails to generate a network with enough edges, hence a network with the same number of edges as the original nuclear reaction network is not guaranteed. To produce such a network, an additional aggregation step is carried out after the initial reconstruction. It works as follows. We repeat the reconstruction for multiple times, say 100, and produce 100 link-deficient networks. Then, we count the times that an edge appears in these networks, and wire the nuclides with the m most popular edges for a link-sufficient network.

The quality of predictive ability of the degree model directly affects the reconstruction performance, since too high or too low degree predictions both cause the deviations from the ground truth degrees. To ensure a reconstruction model of high-quality, we must first design accurate degree models. Here, two variants of degree models with high prediction accuracy have been developed, and tested in our experiments. Actually, in future work we plan to try and design better degree models that assume other forms. To improve the reconstruction accuracy, the degree correlation can provide additional useful information, as shown in Fig. S2.

Nuclide Chart Expansion

The evolution of the nuclide chart from recently discovered nuclides is represented as the spatial expansion of the boundary of the nuclear chart.

Step 1. We start from the seed subnetwork that consists of 3,196 nuclides and the incident 32,184 reactions (see Fig. 5a). Then, we expand the nuclide chart by adding extra 1,000 nuclides in each of the subsequent steps. These additional nuclides come from the boundaries of the current nuclide chart. We train a degree model from the current subnetwork and recalculate the degree of all the nuclides in the newly formed nuclide chart. Based on the network model proposed in Methods Section, we reproduce the nuclear reaction network, and evaluate the performance of our network model in terms of several commonly used metrics (see Section for the definitions in detail).

Step 2. Additional 1,000 nuclides from the boundaries of the current nuclide chart are randomly chosen and included. Following the same procedure as in Step 1, the pre-trained degree model is applied to calculate the degrees for new members.

Step 3. Repeat Step 2 until all nuclides in the JINA REACLIB have been added.

Our evolution process gives five expansions. During the first four expansions, 1000 nuclides have been added each time, and the fifth expansion includes other 846 new members and finally defines a chart of 8042 nuclides. Hence, we have five nuclear reaction networks to record the entire expansion history, as illustrated in Fig. 5.

Reconstruction Performance Metrics

Let $G = (V, E)$ be the input nuclear reaction network, $G' = (V, E')$ be the reconstructed network. Both are directed networks on the same set of nodes with the same number of edges, i.e. $|E'| = |E|$. In our case, $|V| = 8,042$ and $|E| = 77,293$. To measure the reconstruction performance, several common metrics are used.

Precision and Recall. Borrowing an idea from Information Retrieval⁶¹, the reconstruction procedure is considered as the retrieval of the edges. Let $E_{v,out}$ be all outgoing edges from node $v \in V$, and $E'_{v,out}$ be the reconstructed edges outgoing from v . Precision on v is defined as the percentage of correct edges among the reconstructed ones, i.e. $\text{POS}_v = |E_{v,out} \cap E'_{v,out}| / |E'_{v,out}|$. Recall on v is the

percentage of correct ones in all real outgoing edges, i.e. $\text{ROS}_v = |E_{v,out} \cap E'_{v,out}|/|E_{v,out}|$. Similarly, we define precision and recall on the incoming edges as:

$$\text{PIS}_v = \frac{|E_{v,in} \cap E'_{v,in}|}{|E'_{v,in}|}, \quad \text{RIS}_v = \frac{|E_{v,in} \cap E'_{v,in}|}{|E_{v,in}|}.$$

Suppose node v has three incoming edges $\{e_1, e_2, e_3\}$. If the reconstruction model gives two incoming edges $\{e_1, e_4\}$ for v , then, $\text{PIS}_v = 1/2$ and $\text{RIS}_v = 1/3$.

Jaccard Index. Jaccard index is introduced to measure the similarity between two networks in terms of neighborhood:

$$\text{JOS}_v = \frac{|E_{v,out} \cap E'_{v,out}|}{|E_{v,out} \cup E'_{v,out}|}, \quad \text{JIS}_v = \frac{|E_{v,in} \cap E'_{v,in}|}{|E_{v,in} \cup E'_{v,in}|}.$$

Clustering Coefficient. Clustering coefficient^{47,62} is a measure of the degree to which nodes in a graph tend to cluster together. Node v 's clustering coefficient is defined as the fraction of its neighbors that are also connected to each other (triplets of nodes)

$$\text{CS}_v = \frac{|\{e_{uw} : u, w \in N_v, e_{uw} \in E\}|}{k_v(k_v - 1)},$$

where N_v is the neighborhood of v , and $k_v = |N_v|$ is the number of nearest neighbors, irrespective of the direction of the edges.

All these metrics are applied at node level. To estimate the overall reconstruction performance, we stack all nodes' performance scores w.r.t a metric $\mathcal{M}$ into vectors $\mathbf{x}_{\mathcal{M}}$ and $\mathbf{x}'_{\mathcal{M}}$ for G and G' respectively, then compute the cosine similarity between $\mathbf{x}_{\mathcal{M}}$ and $\mathbf{x}'_{\mathcal{M}}$. The overall performance is positive and less than 1, and the higher is better.

KDE for Peak Detection

Degree distribution is a crucial characteristic of networks' topology. However, the common histogram plot, if not given sufficient data points, is often unable to reveal the number of peaks in modality analysis. To address this difficulty, we apply the *kernel density estimation* (KDE) ⁶³ to smooth the histograms to ease identification of peaks.

KDE is proposed to estimate the shape of some unknown probability density function f , from n independent and identically distributed samples $\{x_1, x_2, \dots, x_n\}$ that are supposed to be drawn from f . A kernel density estimator

$$\hat{f}_h(x) = \frac{1}{n} \sum_{i=1}^n K_h(x - x_i) = \frac{1}{n} \sum_{i=1}^n \frac{1}{h} K\left(\frac{x - x_i}{h}\right),$$

is used for this purpose. Here, K is the kernel function, and the *bandwidth* $h > 0$ is a smoothing parameter, controlling the tradeoff between bias and variance in the result. There are many different choices of K . The most common one is the Gaussian kernel function $K(x) = \frac{1}{\sqrt{2\pi}} \exp(-x^2/2)$, which is also used in our analysis. Bandwidth selection is crucial in KDE and greatly affects the result. It can be selected in many ways, either a “rule of thumb”, cross-validation, or “plug-in methods”. We use the build-in bandwidth selection algorithm in scikit-learn ⁶⁴ to run KDE.

A peak or local maximum is defined as a point whose two direct neighbors have a smaller amplitude. A simple detection approach for all peaks (or local maxima) is to compare all neighboring density values (see Fig. S8). However, the procedure is very vulnerable to noise. Therefore, some sort of smoothing is necessary, and KDE can meet such need. In our analysis, the SciPy

package (<http://www.scipy.org/>) is used to detect peaks.

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Figure 1: **Nuclear reaction network.** (a) Neutron (n) bombardment of the nucleus Cu63 with the subsequent emission of the alpha particles (He4) and the nucleus Co60, which itself is then bombarded by protons (p) and produces the neutrons and Ni60. (b-d) Force-directed drawing of the nuclear reaction network from JINA REACLIB database. (b) The full reaction network contains 8,042 nodes and 77,293 directed edges. The nodes can be roughly separated into two categories, one (d, edges in gray) has much more connections than another (c). (d) A mapping from a set of reactions shown in (a) to a tiny nuclear reaction network of size 3. Each node represents a nuclide, and each edge is a nuclear reaction associated with two nuclides (*excluding* the subatomic particles and γ rays). If the nuclear reaction between two nuclei is reversible, the corresponding edge becomes bidirectional. (e) Bimodal degree distribution of the reaction network with the largest degree being 16. (f) Positive correlation between the in- and out-degrees. For most nuclides the numbers of in-coming and out-going edges are close to each other.

Figure 2: **Temperatures, reaction rates and topologies of reaction networks.** (a) Subnetworks of reactions $\langle \gamma, n \rangle$ with reaction rates exceeding the thresholds $\log \lambda_\theta \in [-100, -10]$ (y-axis) at certain temperatures $T \in [0.1, 1.0]$ (x-axis). N and L represent the number of nodes and the number of edges in the corresponding subnetwork. For large values of T , communities appear and are illustrated with different colors in both reaction networks and the nuclide chart (inset). (b) Degree distributions and their Gaussian density estimations (red regions) for the reaction networks corresponding to position of the threshold before, at and above the critical point λ_c . (c,d) Modality curves of the degree distribution affected by λ_θ at (c) $T = 0.1$ and (d) $T = 1.0$. Red line shows the large, and green line depicts the low degrees in the bimodal degree distribution. After exceeding λ_c (dashed line), the two merge into a blue line, and the bimodality disappears. (e) Critical points of the degree modality versus temperature.

Figure 3: **Reconstruction performance of min, prod and rand.** (a,d) Precision, (b,e) Recall, (c,f) Jaccard index, and (g) Clustering coefficient. (h) Similarities between the reconstructed networks and the real nuclear reaction network in the valley region between the two degree peaks. The left three bars show the distributions of d_b , the following three bars show the number of protons. (i) Average performance over the entire network in terms of Precision, Recall, Jaccard index and Clustering coefficient.

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Figure 5: **Predict the theoretically obtained reactions using the discovered reactions.** (a) Boundary of the spatial expansions describing the evolution of the nuclide chart. (b) Degree distributions of the evolved nuclide charts with 3196, 4196, 5196, 6196, 7196 and 8042 nuclei, respectively. The currently discovered 3,196 nuclides are the seed from which the nuclide chart experiences five expansions. Four expansions of the five added 1,000 nuclides each, and the fifth expansion includes additional 846 nuclides included. Each expansion starts from the boundaries of the nuclide chart in preceding expansion, and the five expansions shape the chart of 8,042 nuclides. During the evolution, the overall bimodality in the degree distribution is preserved. (c) Reconstruction performance of the reaction networks based on the degree model derived from the base nuclide chart in dark red presented in (a).

Figure 6: **Prediction of new reactions based on the degree model.** (a) Predicted reactions with the nuclides in red as the reaction targets. (b) Prediction mechanism.

Figures

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