Curiosity search for non-equilibrium behaviors in a dynamically learned order parameter space

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Exploring the spectrum of novel behaviors a physical system can produce can be a labor-intensive task. Active learning is a collection of iterative sampling techniques developed in response to this challenge. However, these techniques often require a pre-defined metric, such as distance in a space of known order parameters, in order to guide the search for new behaviors. Order parameters are rarely known for non-equilibrium systems a priori, especially when possible behaviors are also unknown, creating a chicken-and-egg problem. Here, we combine active and unsupervised learning for automated exploration of novel behaviors in non-equilibrium systems with unknown order parameters. We iteratively use active learning based on current order parameters to expand the library of known behaviors and then relearn order parameters based on this expanded library. We demonstrate the utility of this approach in Kuramoto models of coupled oscillators of increasing complexity. In addition to reproducing known phases, we also reveal previously unknown behavior and related order parameters.

When handed a new experimental platform, our first instinct is to go exploring - to tune individual experimental parameter knobs and record the resulting behaviors of the system. This scattershot investigation provides a window into the range of behaviors that can be produced. In this way, we build intuition for the right variables to describe the system which in turn can serve as a prelude for more systematic quantitative investigation.

However, as the experimental parameters we have access to grow increasingly high-dimensional (e.g. space- and time-dependent activity or interactions in many-body active systems), and the resulting behaviors grow increasingly complex, it becomes a labor-intensive task to explore the full spectrum of behaviors. Much of the parameter space may be uninteresting, and in the absence of previously built intuition or an analytical theory, it is difficult to know which parts of parameter space might show useful or novel behaviors. Hence we are faced with a twinned challenge: how to efficiently search the space of experimental parameters to reveal novel behaviors, while also learning to characterize the behaviors in terms of order parameters.

Individually, these problems have been recognized and addressed in creative ways. On the parameter side of the challenge, active learning provides iterative methods for efficiently sampling parameter spaces. In these approaches, behaviors collected at previously sampled parameters inform parameter sampling in the future, so as to increase the likelihood of discovering novel behaviors. However, these techniques require a metric in the space of behaviors, which often takes the form of a distance in a space of known order parameters. For most non-equilibrium many-body systems, such order parameters are not known.

However, to find order parameters, one needs to know the range of possible behaviors, thus creating a chicken and egg problem. On the behavior side of the challenge, data-driven dimensionality reduction techniques can reveal a small number of order parameters from a library of known behaviors. But these methods require a sufficiently comprehensive library of behaviors to infer meaningful order parameters.

Here, we will demonstrate how a curiosity-driven search algorithm can efficiently explore non-equilibrium many-body systems, even in the absence of previously known order parameters. We adapt methods that combine the strengths of both active learning and dimensionality reduction. We learn order parameters through unsupervised dimensionality reduction on a library of currently known behaviors; we then use active learning in the space of current order parameters to reveal new behaviors. We expand the library of known behaviors with these newly revealed behaviors, learn order parameters again and iterate. Crucially, we always search in the learned low dimensional latent space of behaviors rather than high dimensional parameter space; in this way, active learning efficiently samples richer parts of parameter space.

We apply our general framework to a paradigmatic class of dynamical systems - the Kuramoto model of oscillators and their variants. We first use curiosity search to recapitulate known results on simple Kuramoto model variants with one or two parameters which are nevertheless capable of producing rich non-equilibrium behaviors. We then explore a 3-population Kuramoto model with 10 adjustable parameters and reveal previously un-characterized behavior and corresponding new order parameters.

Our work establishes a general framework that can be used with other models of complex systems or can directly interface with an experimental system where no model is available.
FIG. 1. Overview of the curiosity-driven search for novel behaviors. We consider a system with a high dimensional parameter space (yellow) whose potential behaviors and order parameters that might describe them are initially unknown. Search is initialized by collecting behaviors corresponding to a uniform sampling of parameter space. These dynamical behaviors are used to train an autoencoder to obtain a low dimensional latent space of behaviors (purple) parameterized by putative order parameters. We then seek a new behavior (‘curiosity’) by randomly sampling the learned latent space (open red circle) rather than sampling parameter space. We map the target new latent space point back to parameter space (solid red circle), evaluate the resulting behavior and thus expand our library of known behaviors. Autoencoder is retrained every K training rounds on a random subset of known behaviors, weighting recent samples, thus improving the learned latent space and order parameters. (Green, mauve, and blue regions of parameter and latent spaces indicate qualitatively distinct behaviors.)

METHOD

The curiosity sampling algorithm has three key components shown in Fig. 1: a potentially high-dimensional parameter space (yellow); a potentially high-dimensional space of raw system behaviors; and a lower-dimensional latent space of behaviors (purple). Our algorithm is as follows: We initialize by randomly sampling parameter space, and compiling the corresponding library of behaviors by integrating the equations of motion for these parameter choices. We then train a dimensionality reduction method on the library of behaviors assembled so far through parameter space exploration, revealing an updated latent space of behaviors and order parameters. Then, crucially, we search for new behaviors in this emergent latent space of behaviors created by dimensionality reduction. The new target behaviors are then mapped back to a new point to sample in parameter space. We evaluate the behavior for this parameter choice by integrating the equations of motion, expand our library of known behaviors, retrain dimensionality reduction and the cycle repeats.

We emphasize that the goal of this algorithm is to construct a space which captures different possible behaviors of the underlying physical system. Intuitively, the latent behavior space is a more efficient space for sampling than parameter space or the full space of behaviors with an arbitrary metric, as the latent space represents the most relevant aspects of behavior. Additionally, sampling in the latent space of behaviors can up-weight behaviors that are rare in parameter space but constitute a significant region of a phase diagram.

Our algorithm, outlined in general above, has several choices in the details of how different steps are implemented. The dynamical behaviors can be processed in standard ways (e.g., mean-centering and binning) to reduce invariances (e.g., global rotations) before dimensionality reduction. For dimensionality reduction, we use a convolutional variational autoencoder (VAE) with relatively simple architecture but also compare other methods. See Supplementary Information for details.

RESULTS

To evaluate the performance of a curiosity-driven search in a well-characterized setting, we turn to the original formulation of the Kuramoto model[17],

\[ \dot{\theta}_i = \omega_i + \frac{K}{N} \sum_{j=1}^{N} \sin(\theta_i - \theta_j), \]  

where the \( \omega_i \) are drawn independently from a distribution \( \mathcal{N}(0,1) \), and the coupling strength \( K > 0 \) is the one tunable parameter. We set \( N = 33 \) for our simulations.

In the limit of infinite \( N \), this model is characterized by a critical coupling strength \( K_c = 0.16 \). For values of \( K < K_c \), the oscillators move independently of each other, creating a desynchronized behavior. For values of \( K > K_c \), the oscillators synchronize and have exactly the same phase \( \theta \).

Let’s pretend that we are approaching this system without prior knowledge about the behaviors that can arise, and where these transitions occur. In other words, the only information we have about the system is that there is one parameter that we can manipulate, which is \( K \). We will make the assumption that interesting behaviors occur in the system when the coupling strength is \( O(1) \) or less. One way to approach exploration of this system would be to randomly sample values of \( K \), and observe the behavior at these sampled values. In this approach, only a small fraction of the observed behaviors would be desynchronized, since \( K_c \) is \( O(1) \). Had we assumed that the coupling strength could be larger than \( O(1) \), the relative frequency of desynchronized samples under random sampling would have been even lower.

Running our curiosity search in the one-dimensional parameter space of coupling strength illustrates the
features of successful system exploration. In the final ensemble of collected parameters, samples are drawn with frequencies weighted towards couplings of $O(1)$, where we expect the infinite-N synchronization to occur (Fig. 2B). We can interpret this weighted sampling as the curiosity search algorithm having learned to distinguish the synchronized and desynchronized phases. The fully-trained latent space also provides evidence for “learning” of the Kuramoto model behaviors, as the final latent space is a thin 1D manifold with the same ordering as the parameter space (Fig. 2B,C). Individual examples of the dynamical behaviors confirm this picture as well (Fig. 2D). Finally, we see that sampling bias towards the desynchronized behavior increases as sampling progresses, indicating that the curiosity search is changing its latent space over time to better reflect the relevant behaviors (Fig. 2E).

To test whether other algorithms could have performed the same task we considered multiple variants of the dimensionality reduction technique, including: PCA, a random autoencoder which was never trained, and a random linear projection. (See Supplementary Information for further detail). In all cases, we quantitatively confirm the relative diversity and richness of samples compared to a random sampling baseline (Fig. 2F). Surprisingly, the random dimensionality reduction techniques outperformed those that were iteratively trained on the collected behaviors. The success of the random methods parallels observations made in the context of timeseries featurization with random convolutions[20]. It also indicates that there was enough structure already present in the raw dynamical systems output such that a random low-dimensional projection was able to separate the various accessible behaviors.

While the uniformly-connected Kuramoto model is an ideal testing ground, the range of dynamical behaviors it can produce is fairly simple. We extend our approach to a Kuramoto model variant whose phase diagram has been equally well-characterized, but is capable of producing a wider range of behaviors, including unintuitive “chimera” states.

Specifically, we investigate a 2-population Kuramoto model with a coupling $K_{11} = K_{22} = \mu$ between all oscillators within the same population, and a coupling $K_{12} = K_{21} = \nu$ between all oscillators in different populations. Subscripts indicate the oscillator population index. We introduce a phase lag $\alpha$ to the coupling between any two oscillators and write the model as:

$$\dot{\theta}_{i}^{\sigma} = \omega + \sum_{\sigma'=1}^{2} K_{\sigma\sigma'} \sum_{j=1}^{N_{\sigma'}} \sin(\theta_{j}^{\sigma'} - \theta_{i}^{\sigma} - \alpha), \quad (2)$$

This model was introduced by Abrams et al[21], where
FIG. 3. Curiosity search efficiently reveals the full phase diagram for a 2-population Kuramoto model. (A) Kuramoto model with two populations of oscillators considered by Abrams et al.[21], with intra-population coupling \( \mu \), inter-population coupling \( \nu \) and shifted phase lag \( \beta \). (B) The curiosity search samples non-uniformly across parameter space, quickly focusing on the small region where rare chimera behaviors occur. Clustering in latent space reveals that this region has the structure of the chimera stability diagram identified by Abrams et al.[21]. Simulations run with \( N = 32 \). (C) Autoencoder latent space at the start and end of curiosity search; in the final latent space, desynchronized states occupy visibly more space relative to synchronized states than in the parameter space. (D) Phase coherence examples from each of the states identified through latent space clustering. (E) As training proceeds, curiosity search increasingly focuses on parameter space where desynchronized states are found. (F) Our curiosity search algorithm works with other dimensionality reduction methods, consistently generating more diversity than random sampling (dashed black line). Each line is computed from 10 replicates.

the parameter space was given by the variables \( \beta = \frac{\pi}{2} - \alpha \) and \( A = \mu - \nu \) (Fig. 3A). Here, we specifically investigate the case \( \omega = 0 \) and total \( N = 32 \), with equal population sizes. We will term this model the “chimera” model, as it was shown to produce chimera states, where two identical populations of oscillators exist with one synchronized and the other desynchronized.

Employing automated diversity sampling in this 2-dimensional parameter space results in a distribution of samples that is concentrated on a narrow strip of the total parameter space, roughly in the area with \( A > 0 \) and \( \theta < .25 \) (Fig. 3B). This is precisely the region of parameter space which is known to support the emergence of chimeric behavior. In fact, the latent space trained through our diversity sampling procedure is able to distinguish between the two types of chimeras originally identified by Abrams et al.[21] (Fig. 3B(inset),C), despite the fact that our analysis is done on a smaller number of oscillators, and those results were derived in an infinite-N limit.

Visualizations of the dynamical behaviors provide additional evidence that automated diversity sampling is capturing a wide variety of behaviors in the chimera model (Fig. 3D), and the temporal changes in sampling indicate that the parameter regions which contain the richest dynamical behaviors are preferentially sampled as the latent space is trained (Fig. 3E).

Finally, we quantitatively confirm the relative diversity and richness of samples compared to a random sampling baseline (Fig. 3F). As in the case for the original Kuramoto model, dimensionality reduction variants, including those that are not trained, continue to outperform random sampling.

Having investigated the utility of automated diversity sampling in a non-trivial but still thoroughly explored model, we now turn to previously unexplored models. We initially define a 10-dimensional variant of the chimera model, with three populations with phase lag (Fig. 4A):

\[
\dot{\theta}_i^\sigma = \omega + \sum_{\sigma' = 1}^{3} \frac{K_{\sigma \sigma'}}{N_{\sigma'}} \sum_{j=1}^{N_{\sigma'}} \sin(\theta_j^\sigma - \theta_i^\sigma - \alpha),
\]

with \( \omega = 0 \) and total \( N = 30 \) divided equally among individual populations. The coupling matrix between the populations is not restricted to be symmetric, though we require all matrix elements to be positive and sum to 1 (lowering the effective number of dimensions to 9).

Due to the 9-dimensional nature of the parameter space, we forego the direct visualization of parameters and instead focus on visualizing our 4-dimensional latent space. We select the two dimension in latent space which
CONTRIBUTE THE MOST TO THE LARGEST PRINCIPAL COMPONENT OF THE TRAINED LATENT SPACE, AND PROJECT OUR DATA ON TO THESE AXES (FIG. 3B). CLUSTERING OF BEHAVIORS IN LATENT SPACE SHOWS THAT THE LATENT SPACE STRUCTURE SIGNIFICANTLY CHANGES BETWEEN INITIAL AND FINAL ROUNDS OF SAMPLING. TO UNDERSTAND THE DYNAMICS IN THIS LATENT SPACE WE CAN VISUALIZE REPRESENTATIVES OF EACH GROUP FOR QUALITATIVE ANALYSIS, PLOTTING BOTH THE OVERALL PHASE COHERENCE, AS WELL AS THE MEAN OF EACH POPULATION’S PHASE COHERENCE (FIG. 3B, RIGHT).

WE FIND A WIDE VARIETY OF VISUALLY INTRIGUING BEHAVIORS (FIG. 4C), MOST OF WHICH CAN BE INTERPRETED IN THE LIGHT OF PREVIOUS BEHAVIORS UNCOVERED IN KURAMOTO MODELS – FULLY SYNCHRONIZED, CHIMERA [21, 22], ChIRAL [23], AND ANTIALIGNED [23] PHASES. FINALLY, TO CONCLUDE OUR AUTOMATED ANALYSIS OF THE 3-PopULATION KURAMOTO MODEL, WE QUANTITATIVELY CONFIRMED THE RELATIVE DIVERSITY AND RICHNESS OF SAMPLES COMPARED TO A RANDOM SAMPLING BASELINE (FIG. 4D).

IN OUR EXPLORATION OF THE 3-PopULATION KURAMOTO MODEL, WE IDENTIFIED A PARTICULAR SET OF PARAMETERS THATLed TO AN UNEXPECTED BEHAVIOR (FIG. 4C10), WHERE THE PHASE COHERENCE OF EACH OSCILLATOR FAMILY WAS SATURATED, BUT THE OVERALL PHASE COHERENCE DISPLAYED PERIODIC VARIABILITY. WE WERE PARTICULARLY INTERESTED IN UNDERSTANDING THIS BEHAVIOR, AS IT DID NOT NEATLY FIT INTO ANY CATEGORIES THAT WE HAD PREVIOUSLY ENCOUNTERED; IT’S CLOSEST PHENOTYPE SEEMED TO BE THAT OF THE TYPE IDENTIFIED AS A CHIRAL PHASE BY FRUCHART ET AL. [23], BUT ONE WITH PERIODIC BREATHING.

WE TOOK A CLOSER LOOK AT THESE “CHIRAL BREATHER” DYNAMICS, AND FOUND THAT THE BEHAVIOR CAME AS A RESULT OF 2 POPULATIONS COMPLETELY SYNCHRONIZING WITH EACH OTHER, WHILE A THIRD POPULATION INTERNALLY SYNCHRONISED BUT MOVED AT A DIFFERENT PERIOD RELATIVE TO THE OTHER POPULATIONS (FIG. 4A).

IN ORDER TO UNDERSTAND THE BEAT-LIKE CHIRAL BREATHER, WE USED THE ANSATZ OF INTERNALLY SYNCHRONIZED FAMILIES WITH AN EXTERNALLY DESYNCHRONIZED PHASE TO IDENTIFY ITS EMERGENCE IN A SIMPLER SYSTEM. WE CHOSE TO INVESTIGATE A 2-PopULATION VERSION OF THE 3-PopULATION MODEL (FIG. 5A), WHICH IS IDENTICAL TO EQ. 2 WITHOUT THE INTER- AND INTRA-PopULATION COUPLING SYMMETRY ASSUMPTIONS.

FOLLOWING THE PROCEDURE OUTLINED FOR THE CHIMERA MODEL BY ABRAMS ET AL. [21], WE DERIVE A SET OF COUPLED DIFFERENTIAL EQUATIONS FOR THE PHASE DIFFERENCE AND COHERENCE OF THE TWO OSCILLATOR POPULATIONS IN THE LIMIT OF INFINITE POPULATION SIZE. USING OUR ANSATZ INSPIRED FROM OUR DATA-DRIVEN EXPLORATION IN FIG. 4, WE COMPUTE THE STEADY-STATE BEHAVIOR OF THE OSCILLATORS AS A FUNCTION OF THE MODEL PARAMETERS (FIG. 5C, LEFT).

TO DERIVE THESE EQUATIONS, WE CAN TAKE AS A STARTING POINT EQ. (9) BY ABRAMS ET AL. [22], WHICH IS:

\[
0 = \dot{a}_1 + \frac{1}{2} a_1^2 (K_{11} a_1^* + K_{12} a_2^*) e^{-i\alpha} - \frac{1}{2} (K_{11} a_1^* + K_{12} a_2^*) e^{i\alpha},
\]  

WITH THE EQUATION FOR \( \dot{a}_2 \) BEING IDENTICAL UNDER THE INTERCHANGE OF SUBSCRIPTS 1 AND 2. THE \( a_i \) ARE THE AMPLITUDES OF THE REMARKABLE OTT-ANTONSSEN ANSATZ [24] FOR THE OSCILLATOR PHASE DENSITY IN THE \( N \rightarrow \infty \) LIMIT. UNLIKE IN ABRAMS ET AL. [21], WE DO NOT MAKE ANY ASSUMPTIONS ON THE \( K_i \).

IN ABRAMS ET AL. [21], THE AMPLITUDES \( a_i \) ARE REWRITTEN IN POLAR FORM, WITH \( a_i = \rho_i e^{-i\phi_i} \). HOWEVER, BECAUSE WE ARE NOT INTERESTED IN THE BEHAVIOR EXHIBITED IN FIG. 4A, WE MAKE A DIFFERENT ANSATZ, AND Assume THAT \( \rho_i = 1 \) FOR BOTH \( i \). IN THIS CASE, EQ. 4 REDUCES TO:
0 = \dot{\phi}_1 + K_{11} \sin \alpha + K_{12} \sin(\alpha + \phi_1 - \phi_2), \quad (5)

with the associated equation for index 2 simply involving the exchange of subscripts for 1 and 2. We can define \( \psi = \phi_1 - \phi_2 \), in which case we have one equation

\[
\dot{\psi} = -[(K_{11} - K_{22}) \sin \alpha + K_{12} \sin(\alpha + \psi) - K_{21} \sin(\alpha - \psi)].
\]  

(6)

Integrating yields

\[
\psi(t) = 2 \tan^{-1} \left[ \frac{D \tan(\frac{K_{11} + c_0}{2} + \alpha) - A}{B} \right]
\]

(7)

where \( c_0 \) is a constant of integration.

We note that there are two behaviors embedded in this solution, depending on whether \( D \) is real. When \( D \) is real, \( \psi \) continues to change over time as \( t \to \infty \). If \( D \) is imaginary, then because of the conversion between \( \tan \) and \( \tanh \), \( \psi \) goes to a constant in the long-time limit.

In the case where \( K_{12} = K_{21} = K_{\text{inter}} \) and we define \( \Delta K_{\text{intra}} = (K_{11} - K_{22})^2 \), the boundary between these two behaviors simplifies to:

\[
\Delta K_{\text{intra}}^2 < 4 K_{\text{inter}}^2 \tan^2 \beta,
\]  

(8)

where \( \beta = \frac{\pi}{2} - \alpha \) is the shifted phase lag.

Indeed, when we simulate specific parameters, we find this transition from chiral breathing to stable chiral behavior, as expected from the infinite-\( N \) analysis (Fig. 5C, right).

**LIMITATIONS AND EXTENSIONS**

While our method is successful in identifying novel phases and order parameters with minimal human effort, there are limitations on the effectiveness of our diversity search as currently implemented. Many of these limitations can be traced to the geometry of the parameter space-to-behavior space map, and can be improved upon in future work.

One set of issues comes from the strength of gradients in behavior as a function of parameters. If the behavior is constant in a region of parameter space, then our choice to sample from locally perturbed of previously explored parameter values can result in search dynamics that is equivalent to diffusion in that region of parameter space. This local diffusion can result in a heavy dependence upon the behaviors initially sampled to seed the diversity search. Furthermore, the problem becomes more acute as the dimension of parameter space increases.

This limitation suggests that “messier” physical systems, away from thermodynamic limits with sharp transitions in behaviors, may be more amenable to methods of diversity search that operate in the space of behaviors. There may be hints of one type of behavior hidden in examples of another behavior, and hence the diversity search can follow a gradient, rather than relying solely on diffusion to randomly find a phase boundary. The tradeoff of being away from a thermodynamic limits is that behaviors might not be as clearly apparent. However, in both the case of diffusive and gradient-following dynamics, we expect that whenever a new behavior is discovered, the diversity search algorithm will sample it with elevated frequency.

A key part of the diversity search framework is the backmapping from behavior space to parameter space.
Our nearest-known-neighbor choice was particularly simple, and as discussed, potentially introduces a decrease in exploration efficiency and an increased dependence on initial conditions when sampling in higher dimensions. One possibility for decreasing the reliance on previously sampled parameters is to translate geometrical information in behavior space back into parameter space. For example, if a target behavior sampled in behavior space lies between two points, we might sample between the two corresponding points in parameter space. However, approaches in this vein assume that the geometry of parameter space and the geometry of behavior space are at the very least diffeomorphic. Another possibility would be to treat the backmapping as a supervised deep learning problem, which would require iterative updates as latent space changed.

Another component of the diversity search framework for which we made a simple choice was the choice of latent space sampling. While our current methodology samples latent space uniformly, it might be more efficient to sample explicitly in regions of latent space which have lower sample densities. Another possibility is to forgo explicit sampling in latent space altogether, and instead select candidate behaviors of interest preferentially based on high reconstruction error following dimensionality reduction. This approach is akin to novelty detection. A final possibility is to construct latent space in a way that more fully takes advantage of the temporal nature of the behavior, for example by using a recurrent autoencoder architecture to predict system evolution, as opposed to the vanilla convolutional VAE used here.

**DISCUSSION**

We have demonstrated that it is feasible to perform active exploration of dynamical systems despite not knowing how to characterize the salient features of their behaviors (e.g., in terms of order parameters). We achieved this exploration by combining the complementary strengths of active learning and dimensionality reduction; dimensionality reduction enables the iterative construction of a low-dimensional latent space of behaviors. Searching in such a behavior space is far more efficient than directly sampling in high-dimensional parameter space, even if the behavior space has to be iteratively improved as new behaviors are discovered.

We applied our method to the well-studied Kuramoto model, reproducing known behaviors in some cases and revealing novel behaviors and related novel order parameters in others. Further, the known behaviors of the canonical Kuramoto model are not thought to transfer immediately to related models such as with excitable oscillators or for different functional forms for oscillator coupling; repeating the years of human effort that went into the canonical equations for these other models would be impractical. Our framework can be used to reveal behaviors for related models that might be of interest as accurate models of natural systems.

While we applied curiosity search to a canonical but in silico model of a complex system, our algorithm can instead directly interface with a physical system by taking control of experimental knobs. This direction will allow for discovering functional behaviors that exploit unmodeled or unexpected effects in experimental systems such as non-linearities or feedbacks. Much like reservoir computing or model-free control, our work here gives a systematic way of revealing behaviors that exploit complex unmodelled effects, rather than discovering them through serendipity. However, questions of time and resource cost of experimental iterations and the effectiveness of our method with only partial observations remain to be explored.

Natural applications along these lines include active matter systems with spatial structure. Recent experimental advances increasingly allow for the control of activity and particle interactions in a space-time dependent manner, allowing for detailed density and orientation dependent motility. These experimental methods have opened up complex high-dimensional spatiotemporal design spaces; since order parameters are typically not available a priori for these systems, the methods in this work might provide exciting opportunities for revealing novel behaviors.

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