Modeling of Harmful Algal Bloom Dynamics and Integrated Web Framework for Inland Waters in Iowa

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Abstract
Harmful algal blooms (HABs) are one of the major environmental concerns, as they have various negative effects on public health, recreational services, ecological balance, wildlife, fisheries, microbiota, water quality, and economics. HABs are caused by many sources, such as water pollution based on agricultural activities, wastewater treatment plant discharges, leakages from sewer systems, natural factors like pH and light levels, and climate change impacts. While many causes of HABs are recognized, it is unknown how toxin-producing algae develop as well as the key processes and components that contribute to their weight due to the distinct algal dynamics of each lake and the variety and unpredictability of the conditions influencing these dynamics. Modeling HABs in a changing climate is essential for achieving sustainable development goals regarding clean water and sanitation. However, the lack of consistent and adequate data on HABs is a significant challenge for all these studies. In this study, we employed the sparse identification nonlinear dynamics (SINDy) technique to model microcystin, an algal toxin, utilizing dissolved oxygen as a water quality metric and evaporation as a meteorological parameter. SINDy is a novel approach that combines sparse regression and machine learning methods to reconstruct the analytical representation of a dynamical system. Moreover, a model-driven and web-based interactive tool was created to disseminate and develop environmental education, raise public awareness on HAB events, and produce more effective solutions to HAB problems through what-if scenarios. This web platform allows tracking the status of HABs in lakes and observing the impact of specific parameters on harmful algae formation. Users can easily share images of HABs in lakes on an interactive and user-friendly platform, allowing others to view the status of the lakes.

Keywords: Harmful algae, microcystin, sparse identification of nonlinear dynamics (SINDy), environmental health, public health, web framework.

1. Introduction

Reduced water clarity, unpleasant odors and tastes, the proliferation of harmful algal blooms (HABs), the loss of aquatic animal populations, increased nutrient concentrations in primary producers, acidification, deoxygenation and shifts in the aquatic food web are all results of eutrophication, which is caused by an influx of nutrients like fertilizers or pollutants (Schindler, 2006; Paerl et al., 2016; Rolim et al., 2023). In recent decades, HABs have been seen as a serious hazard to the environment, according to the consensus of the scientific community (Paerl et al., 2016; Gobler, 2020; Rolim et al., 2023). They have several detrimental effects on the environment (i.e., aquatic ecosystems, animals, water quality) (Graham et al., 2016; Coffey et al., 2019), the public, and economic (i.e., rehabilitation, recreational services, health) (Gobler, 2020; CDC, 2021). Toxins generated by HABs may have adverse consequences on human health, especially in children (Weirich and Miller, 2014).

The impact of climate change on HABs is anticipated to manifest in alterations to their frequency, magnitude, biogeographical distribution, phenology (Bakanoğulları et al., 2022; Yeşilköy and Demir, 2023), and toxicity (Ralston and Moore, 2020). Generally, nutrient pollution from agriculture and industry, water temperature, and water quality parameters are the main drivers of HABs occurrence (Paerl and Huisman, 2008; Paerl and Paul, 2012; Graham et al., 2016). Rapid population development, agricultural expansion, environmental pollution, and climate change have all contributed to a sharp rise in the prevalence of HABs in recent years. The Intergovernmental Panel on Climate Change (IPCC) Special Report on the Ocean and Cryosphere in a Changing Climate (SROCC), which was approved in September 2019, was the first time the connection between HABs and climate change was stated in a formal way.

The monitoring, comprehension, and modeling of HABs are of utmost importance. HAB researchers have endeavored to predict through statistical, process-based, and hybrid models (Ruiz-Villarreal et al., 2016; Ralston and Moore, 2020; Brookfield et al., 2021). Zhou et al. (2022) created a numerical model as an extension of a zero-dimensional model constructed by Zhou et al. (2017b) for modeling the temporal dynamics of diatom and dinoflagellate blooms to simulate the seasonal succession of microalgal blooms using nine state water quality variables. A study was conducted by Kim et al. (2022) to compare the impact of weir removal on algal growth with other factors. Their results show that hydrology emerged as the primary determinant of algal growth, surpassing nutrients, light, and temperature in relative significance. The autoregressive hidden Markov model was employed by Aron et al. (2022) to model dinophysis algae, utilizing historical data. Fang (2020) created a space-time geostatistical modeling framework to estimate HABs and cyanotoxins are not highly linked with algal biomass.

The results of the multiple linear regression analysis indicate that over 70% of the variability in MC can be accounted for by the model. The findings suggest that chl-a, bioavailable nutrients, and water temperature with a lag of two months are significant factors in determining MC production. Díaz et al. (2016) employed a generalized additive model (GAM) that utilized an identity-link function for Gaussian distribution. The model incorporated diverse environmental variables such as sunspot numbers, winter North Atlantic Oscillation (NAO) indices, monthly mean rainfall, air and sea water temperature, salinity, winds and Ekman transport, and phytoplankton data. Gillibrand et al. (2016) built an accompanying hydrodynamic-algal transport model to monitor HABs and examine bloom dynamics. The results have indicated that enhancing the parameterization of growth and mortality's temperature dependence, as well as improving the spatial and temporal hydrodynamic resolution, could lead to more effective modeling of blooms in the future. Using cyanobacteria biomass as an indicator, Moe et al. (2016) used Bayesian network (BN) (Baydaroğlu and Koçak, 2019) to relate future climate change and land-use management scenarios to ecological state.

By integrating various factors such as scenarios, process-based model output, monitoring data, and the national lake assessment system, the BN was utilized to simulate the effects of climate change and management strategies on the biological condition of a lake. These simulations revealed that future warming somewhat offset improved land-use management. Most notably, the BN showed that lake status models need additional biological indicators. In their study, Greene et al. (2021) developed a novel metric for normalizing microcystin congeners, enabling a comparative analysis of water bodies impacted by CyanoHAB. Additionally, they introduced a geometry-based image processing technique that facilitated the integration of aerial images captured by a drone, taken from above the water surface. A significant linear relationship was observed between the concentrations of chlorophyll-a and microcystin in lakes located in Iowa, as evidenced by a correlation coefficient (r) of 62%. The researchers also observed that the feasibility of multispectral imaging for estimating microcystin concentrations may be limited at present, primarily due to the spectral constraints of the multispectral camera.

Some studies reveal that the frequency, volume, biogeography, phenology, and toxicity of HABs are likely to vary as a result of climate change (Hallegraeff, 2010; Anderson et al., 2015; Wells et al., 2015; Zhang et al., 2016; Ralston and Moore, 2020; Treuer et al., 2021; Maniyar et al., 2022). Increased ocean stratification (Townhill et al., 2019; Trainer et al., 2020) brought on by greater glacier melting, higher air temperatures (Gobler et al., 2017; Hou et al., 2022), changing precipitation (Ho and Michalak, 2020; Zhou et al., 2021) and wind patterns (Deng et al., 2016; Liu et al., 2019; Hamilton et al., 2022), changed nutrient availability and composition (Huo et al., 2019), light intensity (Zhou et al., 2022), and ocean acidity all have an impact on HABs (Ralston and Moore, 2020). Furthermore, the dispersion of harmful algal blooms (HABs) can be influenced by wind (Deng et al., 2016), air and lake temperature (Michalak et al., 2013), while precipitation can facilitate the introduction of nutrients into aquatic environments, thereby promoting the development of HABs (Coffrey et al., 2019). Liu et al. (2019) employed turbulence modeling systems in the laboratory to investigate the influence of typhoons on lake ecosystems and, as a result, algal cell size. They anticipated that climate change and typhoon occurrences would have a negative impact on phytoplankton populations. The studies that have been conducted so far to demonstrate associations between climatic change and HABs are based on sparse experimental and observational data that often conflicts with itself (Wells et al., 2015). They are still in their early stages.

There were various efforts to study HAB events, observed in the state of Iowa, which heavily relies on agriculture as its primary economic sector (Islam et al., 2024). In their study, Lee et al. (2020) conducted a collection of 65 water samples from various lake beaches in Iowa to examine the potential relationship between the concentrations of microcystin and the abundances of genes responsible for toxin production. Strong correlations were observed between the abundance estimations of mcyA genes and microcystin concentrations in lake water samples. In a study conducted by Greene et al. (2021), it was discovered that microcystins were present in all 10 lakes that were sampled in Iowa. Furthermore, microcystin was identified as the predominant toxin in 90% of these samples. Villanueva et al. (2023) carried out a study where they collected water samples from 38 lakes in Iowa from 2018 to 2021. They developed three models (neural network, XGBoost, and logistic regression) using nine variables, which included chemical, biological, climatic, and land use factors, to predict cyanobacterial HABs for a one-week period.

The production of microcystins, which are cyanotoxins synthesized by cyanobacterial strains, has emerged as a notable microbial threat to the well-being of both humans and animals. This is primarily attributed to the escalating occurrence and severity of HABs. HABs modeling is a challenging task due to following reasons: (1) it is affected by various and multidimensional factors (Wang et al., 2016; Kim et al., 2021); (2) HABs show complex nonlinear behavior (Yu et al., 2018; Liu and Zhang, 2022); (3) they are not uniform both in time and space (Lee et al., 2015; Hallegraeff et al., 2021); and (4) there is not sufficient and continuous data (Guo et al., 2020; Greene et al., 2021; Wang et al., 2022). Therefore, existing physical models have some difficulties (Janssen et al., 2019) to find relationships between each factor affecting HABs prediction and many variable parameters should be required. It is costly and time-consuming to get around these restrictions.

Sparse Identification of Nonlinear Dynamics (SINDy) (Brunton et al., 2016) employs sparsity methodologies and machine learning algorithms to reveal the differential equations that govern a dynamical system. It exploits the observation that the majority of dynamical systems exhibit a limited number of significant terms. This method utilized in various applications such as deducing biological models (Mangan et al., 2016), simulating and optimizing microalgal and cyanobacterial photo-production processes (Zhang et al., 2020), reconstructing chaotic and stochastic dynamical systems (Nguyen et al., 2020), physics-informed learning (Corbetta, 2020), modeling a biological reactor (Lisci et al., 2021), identifying the governing model of COVID-19 (Ihsan, 2021), predicting blood glucose levels (Joedicke et al., 2022), modeling air pollutants (Rubio-Herrero et al., 2022), identifying digital twin systems (Wang et al., 2023), determining water distribution systems (Moazeni and Khazaei, 2023), and modeling bacterial zinc response (Sandoz et al., 2023).

Moreover, tremendous computational resources are required for calculation (Franks, 2018). To overcome HABs' modeling challenge, SINDy was used to model microcystin, which is one of the main indicators of HABs, using dissolved oxygen and daily total evaporation. The study selected dissolved oxygen as the water quality criterion primarily due to the correlation between the presence of harmful algae and the fluctuation in dissolved oxygen levels. Furthermore, it is the water quality parameter that has the highest amount of accessible data. Another factor included in the study is evaporation, which is a combination of a set of atmospheric variables. This analysis also incorporated other meteorological characteristics, including wind speed, maximum air temperature, lake water mixed layer temperature, and precipitation. Since there is a correlation between all the above meteorological characteristics, it is crucial to incorporate one of these elements into the modeling process to ensure precise modeling. The SINDy allows us to model HAB formation with discrete input dataset (Kaiser et al., 2018) and identify the governing equations that underlie nonlinear natural phenomena (Brunton et al., 2016).

In order to effectively communicate the drivers and impacts of the HAB model, however, it's necessary to integrate such predictive models with web-based technologies. This is evidenced by the recent surge in utilizing such tech in various scientific disciplines, including hydrometeorology and water quality, which have seen a dramatic increase in the use of web technologies in recent years (Ramirez et al., 2022; Mishra et al., 2020; Yeşilköy et al., 2023). Widespread use of these web-based tools for data sharing, scientific visualization, data analytics (Sit et al., 2021), monitoring critical parameters, dissemination of necessary warnings, and decision support (Alabbad and Demir, 2022). The development of these information systems is extremely beneficial for enhancing social awareness (Albano et al., 2015) in terms of scientific communication (Iyengar and Massey, 2019; Sermet and Demir, 2022). As previously mentioned, it has been determined that the state of Iowa has had a severe HAB problem in recent years, and the public's awareness of this significant environmental issue falls short of expectations (Shr and Zhang, 2021). Therefore, it is imperative to disseminate information and enhance public awareness on the issue of HABs in lakes across Iowa (Mount et al., 2023).

To address this requirement, we created a web-based interactive communication tool, which includes the algal toxin, microcystin, model based on SINDy for selected lakes in Iowa. This tool has been developed to share the results, estimate the condition of the lakes according to what-if scenarios, increase awareness about HABs, and help decision-making mechanisms. In addition, it provides an easily accessible mapping environment (e.g., Google Maps API) on the web (Yildirim et al., 2022; Li and Demir, 2022). This web platform may be used not only by water professionals but also by teachers, students and public. When users change any variable, they will be able to see for themselves the change in harmful algae formation in the lake and determine whether the harmful algae value in the lake remains within the safe range for swimming, fishing, etc.

This paper is structured as follows: Section 2 explains the study area, data, SINDy method, and educational framework of HABs in some Iowa lakes. The results of the HAB modeling and its integration into the web-based information system can be found in Section 3. Some suggestions and evaluations were given in Section 4.

2. Materials and Methods

2.1. Study Area

In recent decades, Iowa's lakes have experienced the expansion of cyanoHABs distribution (Greene et al., 2021; Shr and Zhang, 2021). The existing monitoring of cyanoHABs in Iowa is insufficient, resulting in a paucity of data on specific microcystin congeners (Greene et al., 2021). West Okoboji, McIntosh Woods (Clear Lake), Black Hawk, and Geode Lakes that had the most easily obtainable data were chosen as the pilot lakes for the study. These lakes are significant due to their comparatively larger surface area, proximity to rivers, and regular utilization by the public for sports and recreational pursuits, including fishing (with a habitat for over 25 fish species), swimming, camping, and boating.

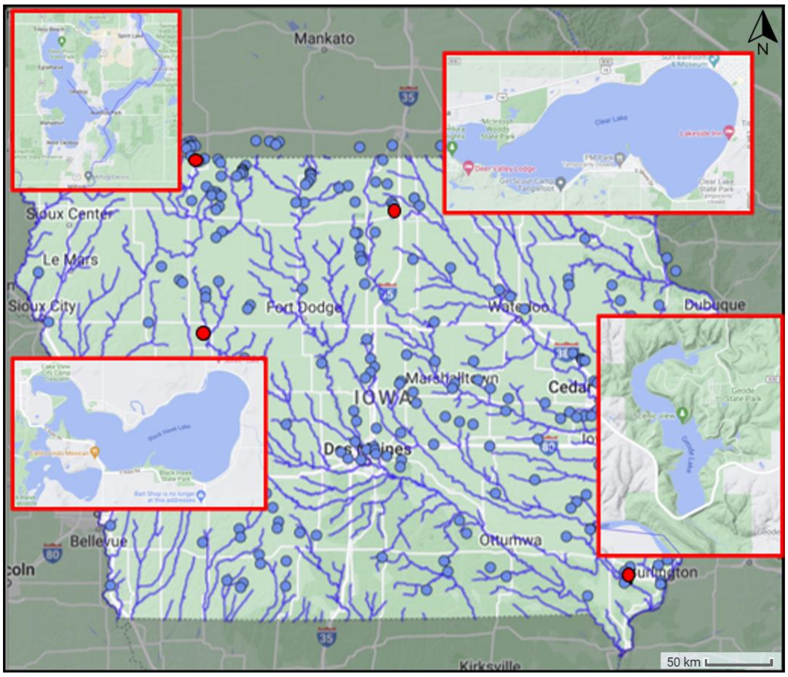

Figure 1. Study Area, which covers the most HAB-experienced lakes in the State of Iowa.

2.2. Case Study

The study analyzed various water quality parameters, including dissolved oxygen, chlorophyll-a, total phosphorus, total nitrogen, microcystin, pH, and turbidity data of the lakes, to identify indicators of harmful algal blooms from the Iowa Department of Natural Resources AQuIA database. After considering the availability and consistency of the data, it was determined that microcystin and dissolved oxygen data would be used.

The time range of algal data is limited to the period from May to September due to certain meteorological and lake water conditions that promote algae development. The primary challenge encountered during the investigation was the acquisition of adequate data at consistent intervals. West Okoboji Lake was designated as the primary lake due to its ample size and form, which allow for data collection from multiple observation sites. The data for West Okoboji was collected from the stations listed in Table 1. Data for additional lakes were obtained at the specific sample site of each corresponding lake. Figure 2 presents the statistical information and graphical representations of the microcystin data.

Table 1. West Okoboji Lake data sources.

Site ID	Site Name
21300001	Gull Point Beach
21300002	Pikes Point Beach
21300003	Triboji Beach
22300009	West Okoboji Lake
14000189	Emerson Bay 1
14000190	Emerson Bay 2
14000191	Emerson Bay 3
14000193	Emmerson T-4

14000410	West Lake Okoboji-Smiths Bay
14000411	West Lake Okoboji-Millers Bay
14000412	West Lake Okoboji-Main Basin North
15300001	Unnamed tributary to Emerson Bay at beach

Mean	0.43
Maximum	1.93
Minimum	0.10
Median	0.26
Mode	0.15
Skewness	1.23
Kurtosis	1.47
Std. Dev.	0.35

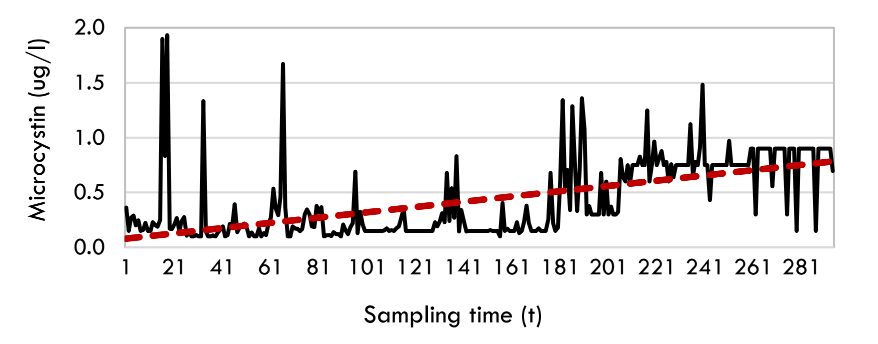

Figure 2. Raw microcystin data and its summary statistics between the years 2006 and 2022 and the months May and September.

In addition, ECMWF Reanalysis hourly ERA5-land data, which are the latest global reanalysis data from 1950 to present with 0.1° spatial horizontal resolution, were used as meteorological data. The meteorological data used in the study were hourly wind speed at 2 m, air temperature, evaporation, lake mixed layer temperature, and precipitation data and converted to daily scale. However, due to the limited quantity of rainfall during the summer months, when HABs occur, a significant portion of the precipitation data consists of zero values and was therefore omitted from the analysis. In addition, other meteorological factors, except evaporation, were eliminated during modeling experiments since they interact with each other, and evaporation allows for the building of the most accurate model.

2.2.1. Data Preprocessing

The phase space was reconstructed and then the attractor of microcystin data was plotted to reveal the characteristics of the microcystin data. In order to reconstruct the phase space, it is necessary to determine the time delay and embedding dimension (Takens, 2006). The study employed the mutual information function (Fraser and Swinney, 1986) to ascertain the time delay. The initial minimal value of average mutual information (AMI) is selected as the optimal time delay. According to Figure 3 (a), time delay (τ) was taken as 13 and the embedding dimension was assumed to be 3. Figure 3 (b) displays the two-dimensional representation of the resulting attractor projection. Given that the maximal Lyapunov exponent of the Microcystin data is negative (-0.54), it can be concluded that the data is not chaotic (Grassberger et al., 1991; Kantz, 1994). However, the presence of a strange attractor in the microcystin data indicates that this data is nonlinear.

Modeling nonlinear data such as microcystin is a challenging task. Furthermore, the presence of measurement mistakes and experimental flaws introduces noise into the data. Deriving the dynamics of a parameter or process from data that is both noisy and nonlinear is an exceedingly intricate undertaking. To ensure accuracy, the microcystin data underwent a sequence of procedures prior to being modeled using the SINDy algorithm (see Fig. 4).

PySINDy (De Silva et al., 2020; Kaptanoglu et al., 2021) was utilized in this study to implement the SINDy application.

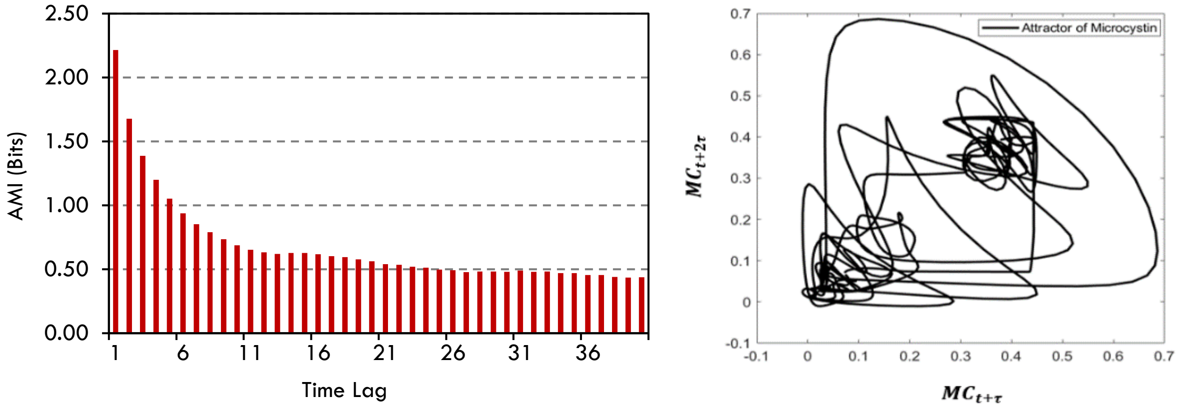

Figure 3 (a) Average mutual information (in Bits) (b) The attractor of microcystin (MC).

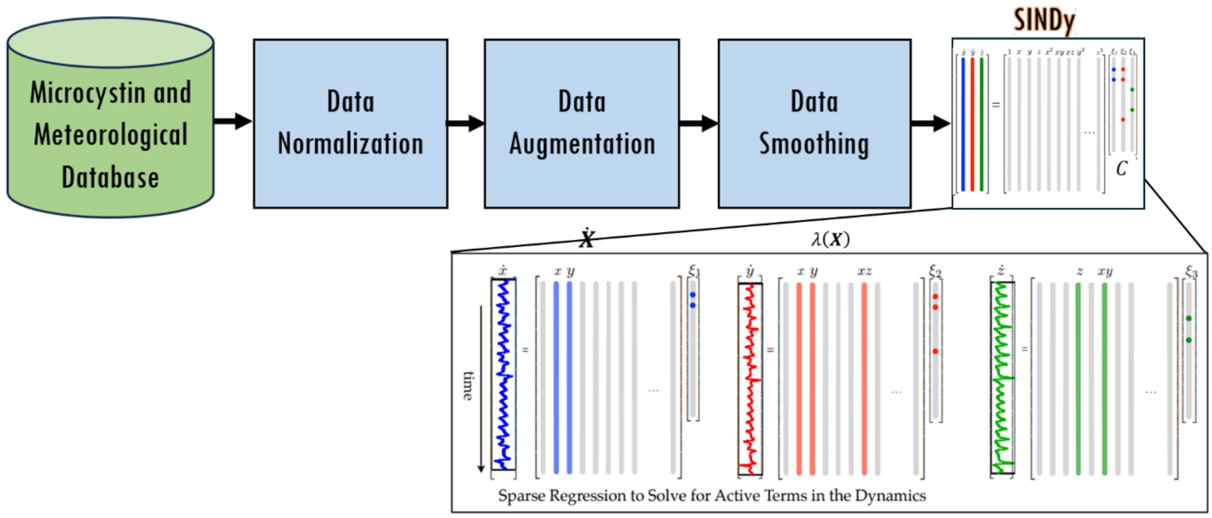

Figure 4. The flow of a sequential process before the application of the SINDy algorithm (Adopted from Brunton et al., 2016).

Data pre-processing techniques, such as standardization and normalization, are used to make variables that have different scales comparable. This helps machine learning algorithms to make more accurate and consistent predictions (Fukami et al., 2021; Rubio-Herrero et al., 2022; Abdullah et al., 2022). Therefore, microcystin, dissolved oxygen and evaporation values were normalized due to their significant differences in scales. The microcystin data given in Figure 2 is raw data. When we take this data simultaneously with dissolved oxygen and evaporation, it is seen that microcystin data number decreases even more as seen in Figure 5.

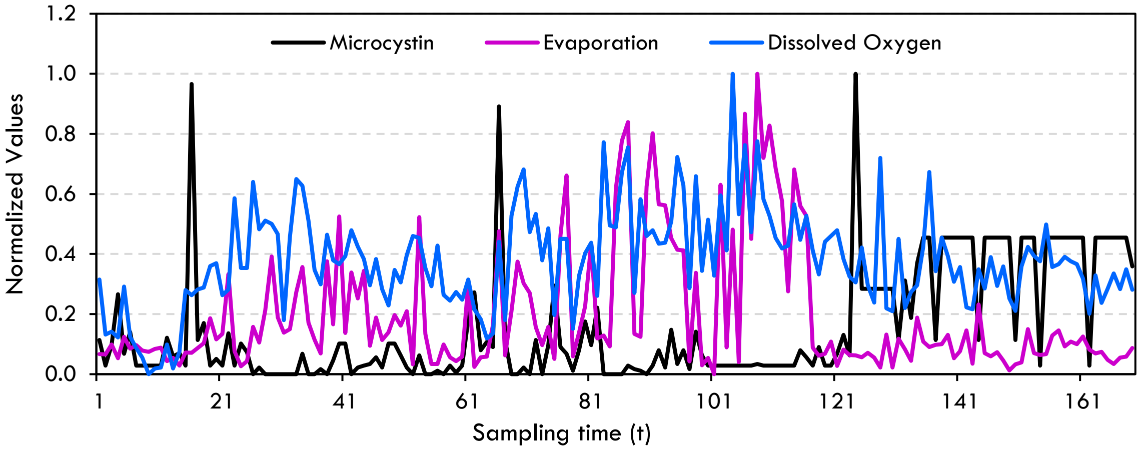

Figure 5. Normalized microcystin, dissolved oxygen and evaporation data

The microcystin data utilized in the study were acquired through weekly sampling. In this work, the modified Akima interpolation technique (MAkima) (Akima, 1970), as utilized by Rubio-Herrero et al. (2022), was employed due to the need for a finer discretization of the time interval when integrating a continuous-time system of ordinary differential equations and for data augmentation. The MAkima approach incorporates MAkima algorithms and is based on shape-preserving piecewise cubic Hermite interpolating polynomial interpolation (PCHIP) (Mohamad et al., 2022). The authors refer to this pre-processing step as data augmentation due to the increase in the quantity of data points. Interpolation is a data augmentation approach utilized in machine learning systems (Baydaroğlu and Demir, 2023). Essentially, the MAkima procedure relies on spline interpolation to determine the values between two given points, resulting in a finer level of discretization. Through this procedure, the quantity of data points for each variable is quadrupled. Figure 6 shows the raw and splined microcystin data after the normalization step. Figure 7 shows augmented microcystin, dissolved oxygen and evaporation data together after MAkima interpolation.

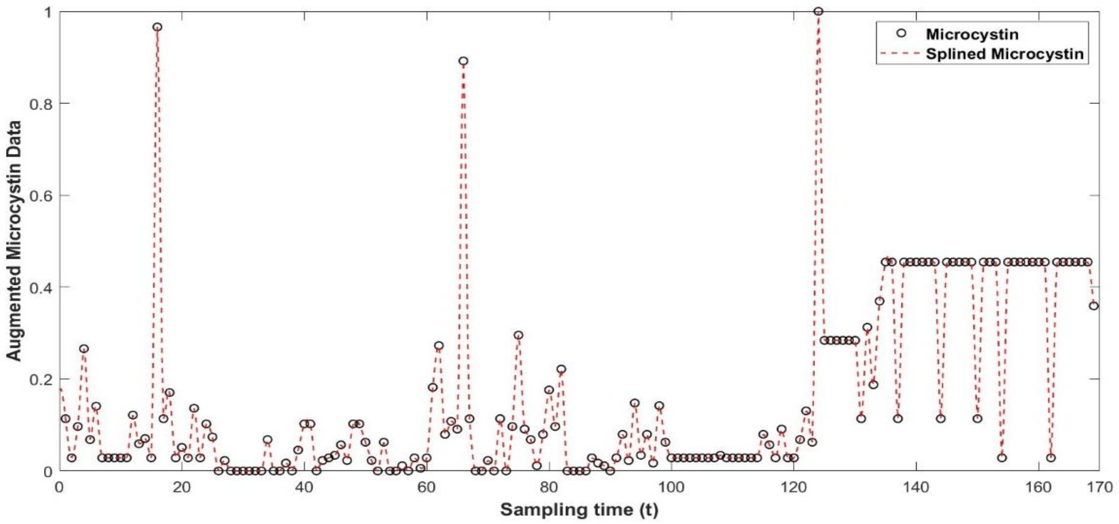

Figure 6. Augmented microcystin data points after modified Akima interpolation.

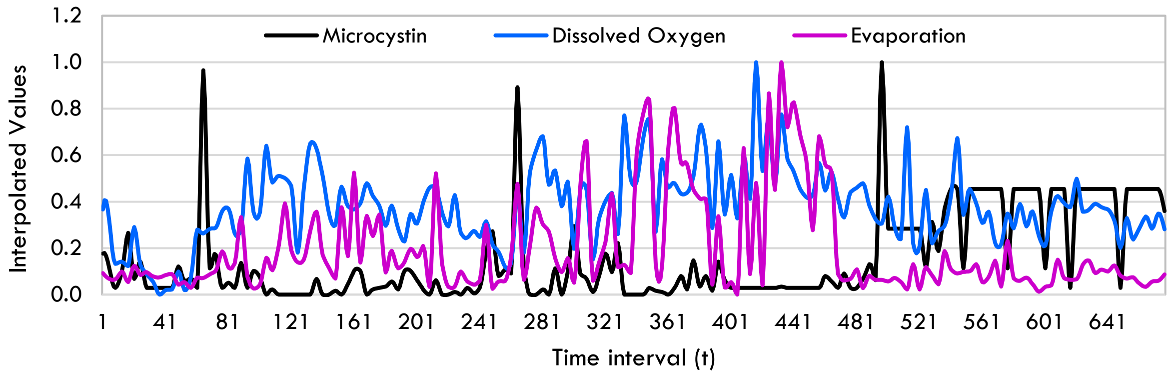

Figure 7. Interpolated microcystin, dissolved oxygen and evaporation data.

The data pre-processing step have a crucial role in facilitating the extraction of valuable information from data (Muste et al., 2017). Applying smoothing and denoising techniques is beneficial for obtaining accurate outcomes when using the SINDy method (Cortiella et al., 2023). In this research, the final stage of data preprocessing involves the process of data smoothing. The Whittaker-Henderson approach (Whittaker, 1922, 1925; Henderson, 1924, 1925) was used to smooth microcystin and meteorological variables. Whittaker-Henderson smoothing is a successful method of smoothing discrete-time data that is based on spline smoothing and is specifically designed for equally spaced data points (Baydaroğlu et al., 2024). Figure 8 displays the normalized and augmented microcystin data with the smoothed version of this data. The R libraries utilized for AMI, Lyapunov exponents' calculations, and Whittaker-Henderson smoothing are 'tseriesChaos', 'nonlinearTseries', and 'pracma', respectively. MatLab was utilized for the implementation of MAkima.

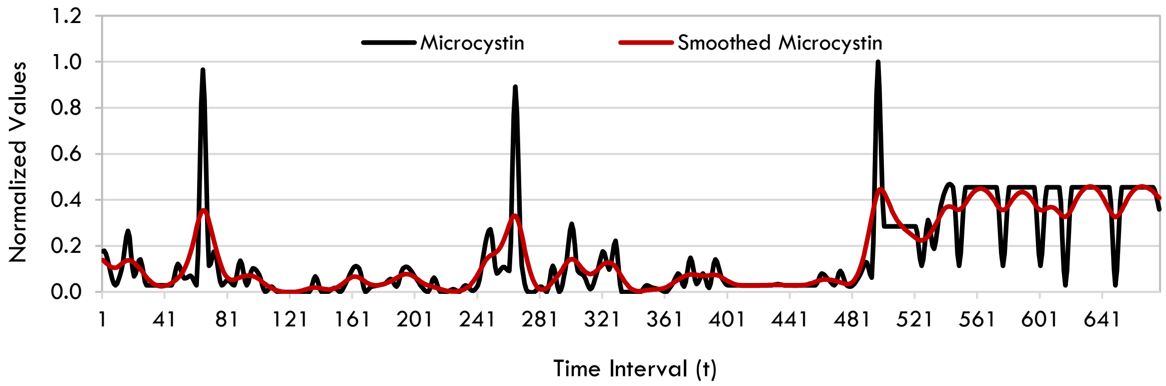

Figure 8. Microcystin and smoothed microcystin data.

2.3. Sparse Identification of Nonlinear Dynamics (SINDy)

Brunton et al. (2016) incorporated sparse regression and machine learning with nonlinear dynamical systems to model nonlinear processes using noisy data. The only model structural assumption is that the dynamics are governed by a few key components, thus the equations are sparse in the space of potential functions. Sparse regression finds the fewest dynamic governing equation terms needed to effectively describe data. To prevent overfitting, parsimonious models balance accuracy and model complexity.

State $\boldsymbol{x}(t)$ in a dynamical system can be taken as $\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}(t))$. In order to ascertain the function from the data, a temporal evolution of the state $\boldsymbol{x}(t)$ is collected and either the derivative $\dot{\boldsymbol{x}}(t)$ is measured, or it is numerically approximated from $\boldsymbol{x}(t)$. After sampling the data numerous times and arranging it into two matrices, a data matrix $\boldsymbol{X}$ and its derivative $\dot{\boldsymbol{X}}$ are as follows:

$$\boldsymbol{X} = \begin{bmatrix} \boldsymbol{x}^T(t_1) \\ \boldsymbol{x}^T(t_2) \\ . \\ . \\ . \\ \boldsymbol{x}^T(t_m) \end{bmatrix} = \begin{bmatrix} x_1(t_1)\; x_2(t_1) \;\dots\; x_n(t_1) \\ x_1(t_2)\; x_2(t_2) \;\dots\; x_n(t_2) \\ \cdots \\ \cdots \\ \cdots \\ x_1(t_m)\; x_2(t_m) \;\dots\; x_n(t_m) \end{bmatrix}, \dot{\boldsymbol{X}} = \begin{bmatrix} \dot{\boldsymbol{x}}^T(t_1) \\ \dot{\boldsymbol{x}}^T(t_2) \\ . \\ . \\ . \\ \dot{\boldsymbol{x}}^T(t_m) \end{bmatrix} = \begin{bmatrix} \dot{x}_1(t_1)\; \dot{x}_2(t_1) \;\dots\; \dot{x}_n(t_1) \\ \dot{x}_1(t_2)\; \dot{x}_2(t_2) \;\dots\; \dot{x}_n(t_2) \\ \cdots \\ \cdots \\ \cdots \\ \dot{x}_1(t_m)\; \dot{x}_2(t_m) \;\dots\; \dot{x}_n(t_m) \end{bmatrix} \quad (1)$$

A library, denoted as $\lambda(\boldsymbol{X})$, is created, which contains potential nonlinear functions of the $\boldsymbol{X}$.

$$\lambda(\boldsymbol{X}) = \begin{bmatrix} |\;|\;|\;| \\ 1\; \boldsymbol{X}\; \boldsymbol{X}^{P_2}\; \boldsymbol{X}^{P_3} \dots \\ |\;|\;|\;| \end{bmatrix} \quad (2)$$

$\boldsymbol{X}^{P_i}$ denotes polynomials of the ith degree. At this point, a sparse regression problem can be formulated to find a coefficient matrix $C = \xi_1, \xi_2, \dots, \xi_n$ that will identify the active nonlinearities in the dynamic system:

$$\dot{\boldsymbol{X}} = \lambda(\boldsymbol{X})C \quad (3)$$

Each column ε_k of C represents a sparse vector of coefficients that determine which terms are active in the right-hand side of one of the row equations $\dot{\boldsymbol{x}}_k = \boldsymbol{f}_k(\boldsymbol{x})$ in $\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}(t))$. After determining the value of C, a model for each row of the governor equations can be developed in the following manner:

$$\dot{\boldsymbol{x}}_k = \boldsymbol{f}_k(\boldsymbol{x}) = \boldsymbol{\lambda}(\boldsymbol{x}^T)\boldsymbol{\xi}_k \quad (4)$$

2.4. HALGIS Web Framework

HALGIS, the Harmful ALGae Information System, was developed as a web-based platform to track the formation of harmful algal blooms in Iowa lakes by monitoring the alterations in microcystin levels, a toxin generated by cyanobacteria. HALGIS aims to offer a one-stop digital platform for accessing data and information about the impacts of HABs on public health, recreational activities, and wildlife. The landing page also provides the causes of HAB, information on data integration, analysis, and visualization, and link to data sources. The main stakeholders for HALGIS are the public, students, and environmental education professionals. Therefore, it is crucial to create an interactive and user-friendly interface that is accessible to individuals with limited technical knowledge and expertise. It can be accessed across multiple platforms such as PCs, smartphones, and tablets. HALGIS was organized into multiple layers, as depicted in Figure 9. HALGIS offers data on lakes and HAB conditions to help users comprehend potential HABs and environmental health risks. Users can contribute photos of hazardous lakes using the HALGIS interface.

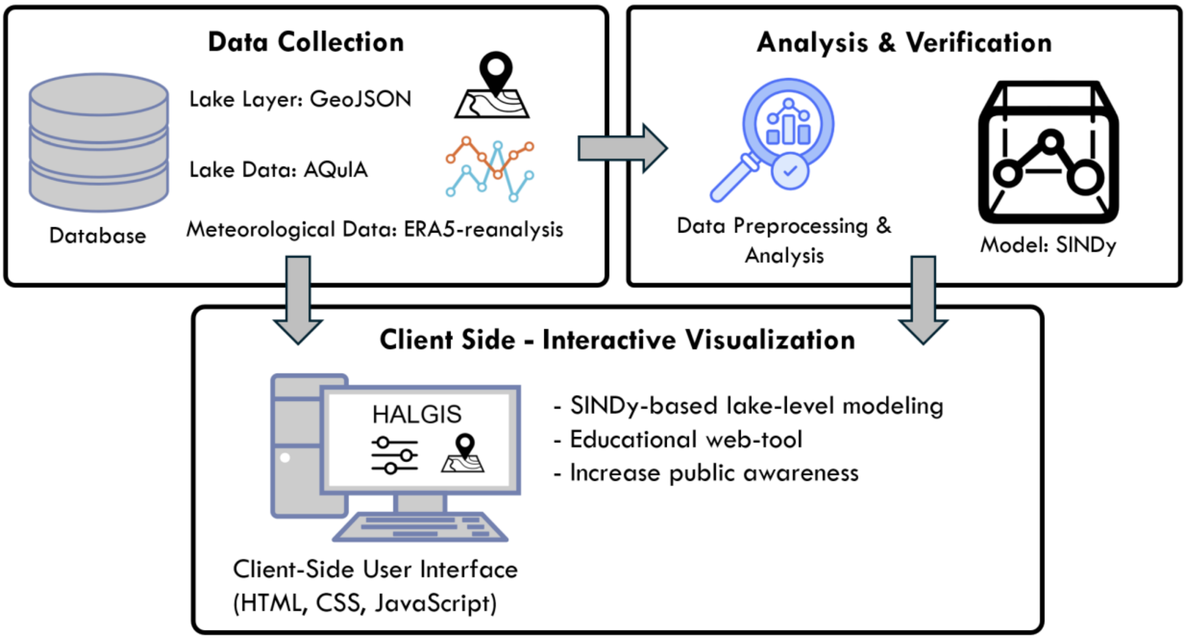

Figure 9. The overall structure and components of web-based framework.

3. Results and Discussions

3.1. SINDy Model

The analyzed data is partitioned into training data, which accounts for 75% of the total, and test data, which accounts for the remaining 25%. Gaussian noise with a standard deviation of 10% of the root mean square error (RMSE) was added to the training data, ensuring that only the most significant terms were retained in the model. The subset of candidate terms in the system was determined using sequential thresholded least squares (STLSQ) as an optimizer since the SINDy algorithm, in its standard form, utilizes the STLSQ method. The algorithm is specifically designed for the least squares formulation and performs effectively, although it lacks the ability to easily incorporate modifications such as extra constraints, resilient formulations, or nonlinear parameter estimates (Champion et al., 2020). The model was fitted to the noisy data, and the coefficients were stored in an array. The performance of the model was assessed using test data. It is crucial to note that as the threshold increases, the model includes fewer terms, making it sparser and reducing the risk of overfitting to noise. Nevertheless, setting the threshold too high can potentially remove crucial dynamics. Hence, the optimal threshold value is being sought for promoting sparsity. Figure 10 illustrates the relationship between RMSE in the test data and threshold values on the testing trajectory of dM/dt where M indicates microcystin. The optimal threshold value is the value that minimizes the RMSE while preserving significant terms. Put simply, the optimal threshold value is the one that effectively captures important dynamics and does not overfit with noise.

West Okoboji, McIntosh Woods, Black Hawk, and Geode Lake were chosen for modeling microcystin using dissolved oxygen and evaporation factors with SINDy. Details of threshold selection and equations for microcystin, dissolved oxygen, and evaporation are provided for the West Okoboji Lake. Only the final microcystin equations are given for the other lakes. The data presented in Figures 11-14, which display the microcystin and predicted microcystin graphs for each lake, were not retrieved prior to pre-processing as they illustrate the rates of change in the microcystin levels. It is evident that performing such a procedure will elevate the error rates.

West Okoboji Lake

The optimal threshold value was determined to be 0.038 for West Okoboji datasets. Figure 10 displays RMSE values plotted against the threshold values for constructing the model using these datasets.

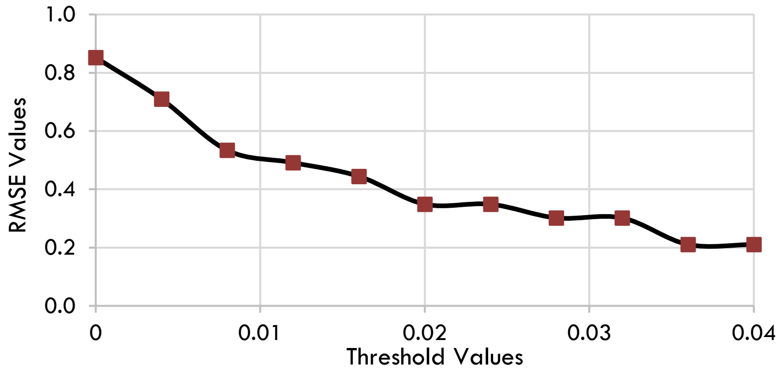

Figure 10. RMSE values vs. threshold values for the model construction for pre-processed data.

The equation system for microcystin (M), dissolved oxygen (D), and evaporation (E), determined using the optimal threshold value, can be represented as follows (Eqs 5-7):

$$\frac{dM}{dt} = 0.984M - 2.352MD - 0.464ME \tag{5}$$

$$\frac{dD}{dt} = 0.121ME \tag{6}$$

$$\frac{dE}{dt} = 0.114M - 0.054D - 0.281MD + 0.099D^2 + 0.069DE - 0.058E^2 \tag{7}$$

The rate of change of microcystin data was calculated by integrating these equations. Figure 11 displays the rate of change of microcystin and the projected microcystin values for West Okoboji Lake.

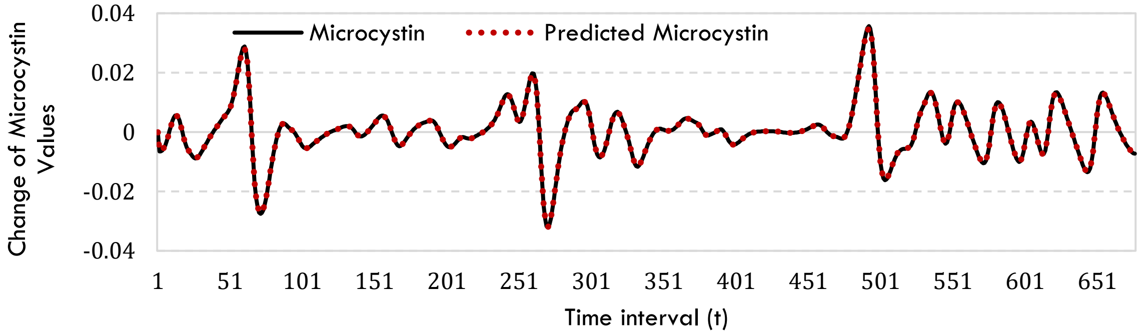

Figure 11. The rate of change of microcystin and predicted microcystin values for West Okoboji Lake.

Figure 11 demonstrates that the SINDy model accurately predicts this change with exceptional accuracy, especially when the microcystin change is very sharp.

<u>McIntosh Woods Lake</u>

SINDy gives rise to the model presented in Eqs 8-10 for McIntosh Woods Lake.

$$\frac{dM}{dt} = 3ME \tag{8}$$

$$\frac{dD}{dt} = -0.065 + 0.539M + 0.337E - 3.105M^2 - 0.356MD - 0.775ME + 0.145D^2 - 0.241DE - 0.328E^2 \tag{9}$$

$$\frac{dE}{dt} = 0.33 + 12.97M - 2.32D + 0.5E - 90.64M^2 - 0.7MD - 24.82ME + 2.74D^2 + 1.23DE - 0.5E^2 \tag{10}$$

The model developed by SINDy identified a significant number of terms, potentially indicating that the approach referenced produces a model of the current system that lacks generalizability. Figure 12 displays the rate of change of microcystin and the projected microcystin values for McIntosh Woods Lake.

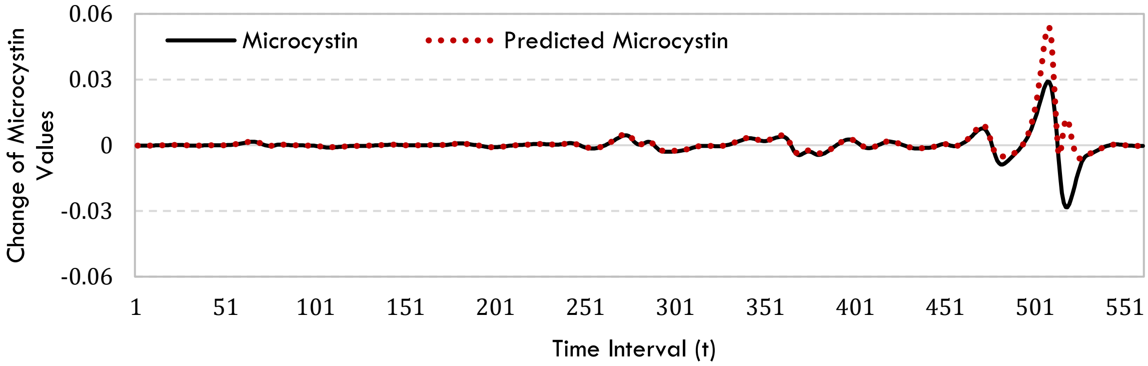

Figure 12. The rate of change of microcystin and predicted microcystin values for McIntosh Woods Lake.

The microcystin change rate in McIntosh Woods Lake has remained constant over an extended period of time. It was observed that this value increased rapidly towards the end of the time period. Although the forecast model accurately predicted this sudden rise, it appears to have overestimated it.

<u>Blackhawk Lake</u>

The model for McIntosh Woods Lake is derived from SINDy and is represented by equations 11-13.

$$\frac{dM}{dt} = 0.9828M - 1.08MD - 1.5732ME \tag{11}$$

$$\frac{dD}{dt} = -0.133M^2 \tag{12}$$

$$\frac{dE}{dt} = -0.097M^2 - 0.124ME \tag{13}$$

Figure 13 depicts the rate of changes in microcystin and the predicted microcystin values for Blackhawk Lake.

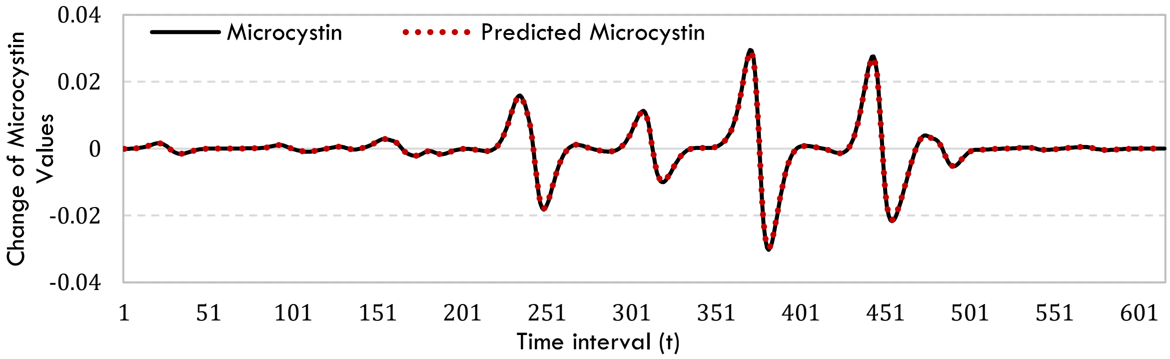

Figure 13. The rate of change of microcystin and predicted microcystin values for Blackhawk Lake.

While accurately predicting variations in change is challenging, the SINDy model effectively captures fluctuations in the rate of change.

Geode Lake

The equation system (Eqs 14-16) for Geode Lake is as follows:

$$\frac{dM}{dt} = 0.952M - 0.356MD - 1.688ME \tag{14}$$

$$\frac{dD}{dt} = 0.072D + 0.029E + 0.301M^2 - 0.257DE - 0.022E^2 \tag{15}$$

$$\frac{dE}{dt} = 0.188M - 0.372ME \tag{16}$$

Figure 14 displays the rate of change of microcystin and the projected microcystin values for Geode Lake.

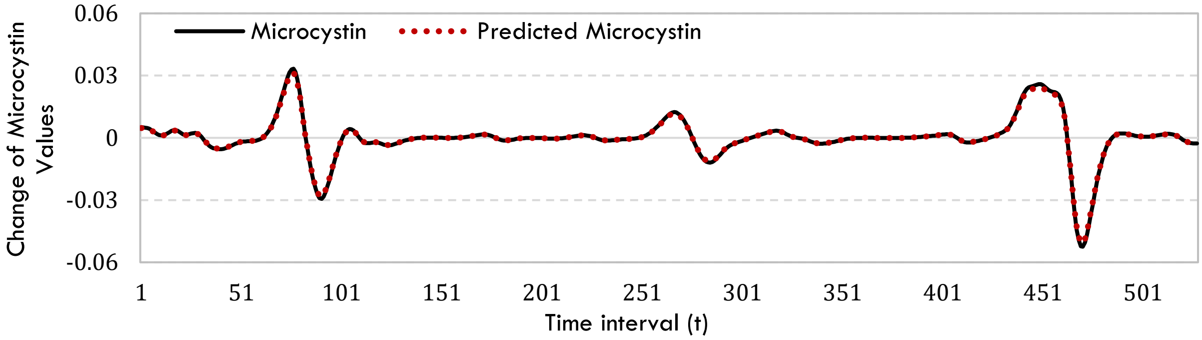

Figure 14. The rate of change of microcystin and predicted microcystin values for Geode Lake.

The estimations for Geode Lake are comparable to those conducted for other lakes. It is seen that the model accurately predicts times of rapid increase or decrease in rate of change values. The prediction outcomes for lakes have demonstrated that the forecasts generated by SINDy are highly effective in predicting the time periods during which harmful algae experience rapid growth or decline. Table 2 shows the prediction model performance results for every lake. Correlation coefficient (r), root mean square error (RMSE) and mean absolute percentage error (MAPE) are used as performance indicators.

Table 2. Model performance criteria for each lake.

Lake	r	RMSE	MAPE
West Okoboji	0.99	0.0001	1.61
McIntosh Woods	0.69	0.0046	11.3
Blackhawk	0.99	0.0001	1.72
Geode	0.99	0.0047	1.95

The correlation coefficients between model findings and observations in lakes other than McIntosh Woods are highly proximate to 1. The reason for this is that SINDy perfectly captured the observed values for all lakes but McIntosh Woods. The prediction findings for McIntosh Woods Lake are satisfactory, albeit its prediction accuracy is lower compared to other lakes. The MAPE results indicate that the SINDY model effectively forecasts the fluctuations in nonlinear microcystin data.

3.2. HALGIS Web Framework

HALGIS is a publicly available informational web platform (Figure 15) that can be accessed freely at https://hydroinformatics.uiowa.edu/lab/halgis. The landing page contains details on the datasets utilized and the analysis available in the system. These harmful algae ML-based prediction results based on SINDy and environmental factors were incorporated into the HALGIS. The data obtained from multiple sources will be temporarily saved in a local database. The web platform incorporates the Google Maps API to display GeoJSON files of the selected lakes in the study area (Figure 16). This allows users to see the size of the lake and which river network and watershed (HUC-8 level) it is connected to. Users are able to open the harmful algae estimator module and change the environmental variables (microcystin, dissolved oxygen, and evaporation) to see the harmful algae trend for the West Okoboji Lake (Figure 17).

HALGIS elevates the understanding of environmental sustainability among different user groups. The general public can utilize it as an informational guide to assess the quality of their nearby lakes, assisting in promoting local ecological awareness and engagement. For educators, it provides a dynamic, interactive tool that promotes in-depth exploration and understanding of aquatic ecosystems and the influence of environmental factors. Students, particularly those involved in environmental science programs, can use HALGIS as a substantial research tool, leveraging authentic data to practice and refine their research skills. The interactivity offered by the platform fosters proactive learning and encourages users to think critically about the interrelatedness of environmental factors and their effect on our water bodies. Thus, HALGIS proves to be a remarkable asset in fostering a more informed and environmentally conscious society.

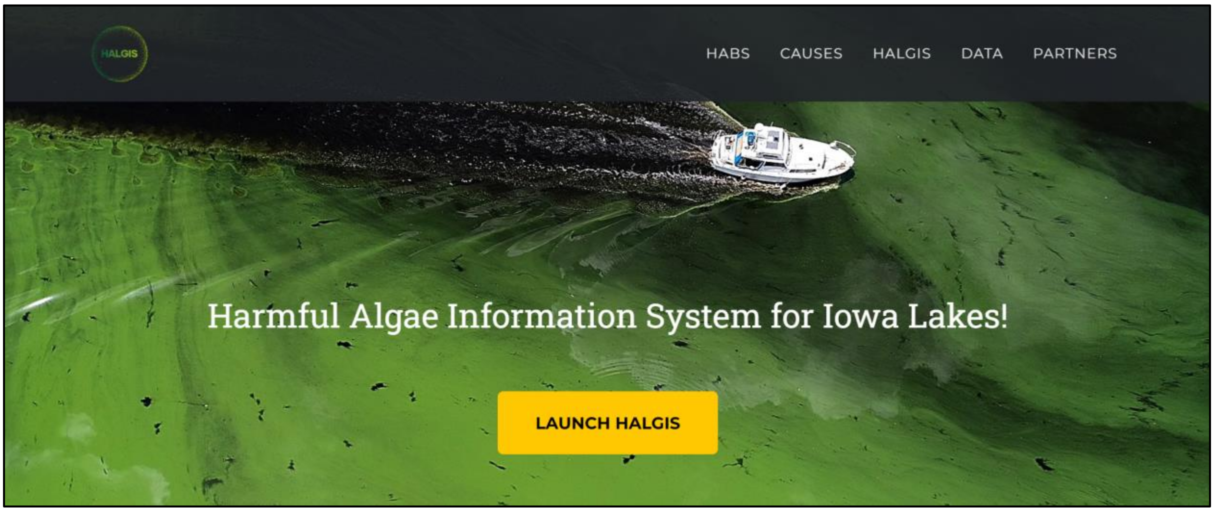

Figure 15. Harmful Algae Information System (HALGIS) landing page.

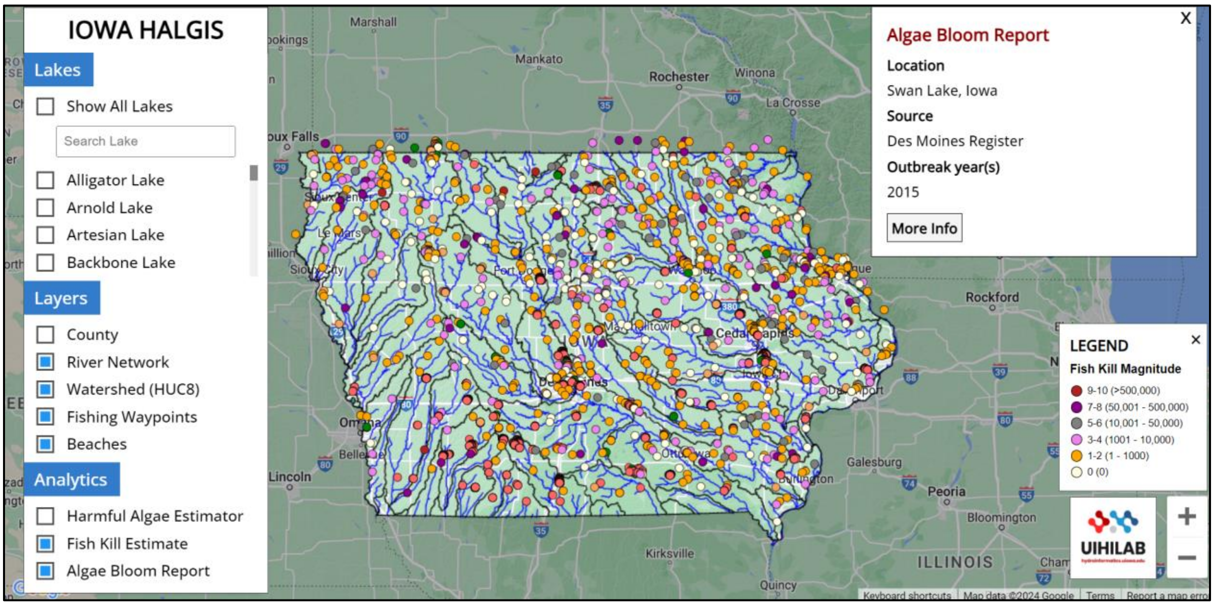

Figure 16. This web framework also allows their users to select different lakes and provides

HAB-related information about beaches, fishing waypoints, fish kill estimates, and algae bloom reports, which were integrated from the Iowa Department of Natural Resources databases.

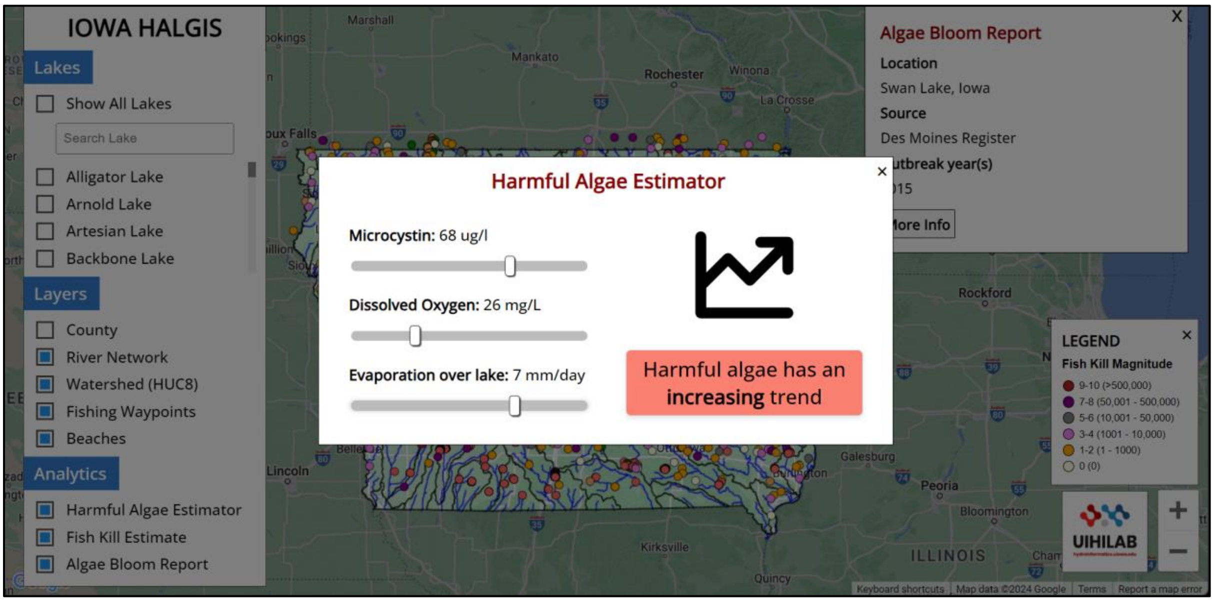

Figure 17. SINDy-based algae trend modeling can be calculated through sliders for the dissolved oxygen and evaporation rate over the lake. Sliders allow users to change the harmful algae-related factors and calculate the harmful algae trends over the lake.

The HAB estimator indicates a positive correlation between the rise in microcystin levels and the occurrence of HAB events in the lake. Furthermore, it is possible to analyze not only the presence of microcystin but also the comprehensive changes in dissolved oxygen and evaporation parameters, as well as the variations in HAB occurrences in the lake. Displaying the interactive HAB trend would enhance users' knowledge of this environmental concern and improve the communication abilities of environmental science students as well as the educators.

4. Conclusion

Environmental contaminants and climate change can lead to the development of harmful algal blooms (HABs) in lakes, affecting ecological balance. These formations in lakes can grow to such an extent that they endanger the survival of other organisms in the environment and pose a risk to public health by contaminating drinking water sources. This study aimed to simulate HABs, a critical aspect for environmental health. For this objective, all water quality parameters linked to HABs, indicators of harmful algal presence in the lake, and pertinent meteorological factors were analyzed. Data availability is the main focus in these assessments. As known, the primary issue in HAB investigations is the insufficient data availability. The second issue that needs to be addressed is synchronizing the data for these parameters. For instance, one water quality measurement could be recorded within an hour, whereas another one could be measured at a different day or time. After identifying various discrepancies, a comprehensive set of data combinations was established, and multi-dimensional time series were generated by aligning them with relevant meteorological data. These time series were used to model HABs with SINDy.

Multiple reasons influenced the selection of SINDy for HAB modeling. The SINDy approach is chosen for its exceptional modeling capability, which remains effective even with limited data. Additionally, it demonstrates robustness in handling data noise features and is well-suited for discrete data. These advantages have been highlighted in research conducted by Kaiser et al. (2018), Champion et al. (2019), Lisci et al. (2021), França et al. (2022), and Moazeni and Khazaei (2023). As a result of modeling experiments, microcystin (a toxic substance produced by harmful algae), dissolved oxygen (a water pollution parameter), and evaporation (a meteorological variable containing temperature and precipitation information) were selected as the three variables that gave the sparsest equation to be used in the study.

The primary lake in the study is West Okoboji Lake which is used actively for various recreational activities such as boating, swimming, and water skiing. The graphs based on the microcystin equations' results derived from SINDy (Figures 10–13) reveal the following about the lake. The equations derived for all lakes did accurately represent the numerical change in microcystin, they precisely described the variations in microcystin values. The high correlation and quite low error values in Table 2 confirm this observation. The SINDy method accurately predicted the nonlinearly varying toxin microcystin, which is produced by cyanobacteria. All models created by SINDy for all lakes share the common characteristic of having a strong capacity to forecast extreme points, in contrast to conventional prediction models.

HALGIS web platform was developed as an information system with integrated data access, analysis, and visualization capabilities. HALGIS is a comprehensive online platform that provides access to harmful algae conditions, HABs-related data, information, and interactive visualizations. HALGIS offers information on monitoring harmful algal blooms and the real-time condition of lakes, while also serving as an educational tool on environmental pollution. Students can acquire insight into future HABs generation by adjusting parameter values and will have the ability to observe the climate change impact on environmental sustainability.

To address the data issue, crucial for future HAB studies, it is essential to standardize data collection by ensuring all measurements are taken simultaneously in a uniform format. Validation with ground-based data is essential for the wider utilization of satellite datasets, highlighting the important nature of the data collection step. Benchmark datasets following FAIR (findability, accessibility, interoperability, and reusability) data principles should be created and shared to tackle the significant threat to environmental health issues posed by HABs. Benchmark datasets may enhance estimation and prediction studies on harmful algae by granting access to the latest data. As research progresses, understanding of climate change and its effects on HABs increases, allowing for more precise planning of preventative and protective actions. Advancements in information systems for lake ecosystems and HABs will allow for real-time monitoring of lake pollutants and environmental health.

Data Availability

The data used in this study is publicly available via the following links:

AQuIA Database (The Iowa Department of Natural Resources Water Quality Monitoring and Assessment): https://programs.iowadnr.gov/aquia/

ERA5-land hourly data: https://doi.org/10.24381/cds.e2161bac.

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