Early Warning Systems for Shellfish Safety: The Pivotal Role of Computational Science

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Abstract. Toxins from harmful algae and certain food pathogens (*Escherichia coli* and Norovirus) found in shellfish can cause significant health problems to the public and have a negative impact on the economy. For the most part, these outbreaks cannot be prevented but, with the right technology and know-how, they can be predicted. These Early Warning Systems (EWS) require reliable data from multiple sources: satellite imagery, *in situ* data and numerical tools. The data is processed and analyzed and a short-term forecast is produced. Computational science is at the heart of any EWS. Current models and forecast systems are becoming increasingly sophisticated as more is known about the dynamics of an outbreak. This paper discusses the need, main components and future challenges of EWS.

Keywords: Shellfish safety · Early warning systems · Aquaculture

1 Introduction

Shellfish harvesting and production in aquaculture has been steadily growing over the past few years, both in quantity and value, a pattern mostly driven by the constant increase in human needs of fish protein. In 2013, for instance, shellfish amounted up to almost 25% (≈4.9 kg per capita) of fish consumption

Supported by the Interreg Atlantic Area Operational programme, Grant Agreement No.: EAPA_182/2016. A. Silva supported by Grant IPMA-BCC-2016-35.

J. M. F. Rodrigues et al. (Eds.): ICCS 2019, LNCS 11539, pp. 361–375, 2019.
https://doi.org/10.1007/978-3-030-22747-0_28

worldwide [1]. The response of the aquaculture sector to this gradual increase in demand has been the intensification in production, which has been rewarded with a growing willingness to pay by the consumer and the consequent escalating financial revenue for the sector (see Fig. 1). However, several natural and human-related factors hinder these efforts, with impacts to both the economy and human health. Besides the many polluting sources (e.g. heavy-metals, hydrocarbons, etc.), a number of biological agents, which may or may not be associated to human activities, pose increasing risks to human health and to the seafood industry worldwide. Harmful algal blooms (HABs), enteric bacteria such as *Escherichia coli* (*E. coli*) and marine viruses (e.g. norovius, NoV) are currently seen as the major threats to shellfish production and safety [2].

The presence of these agents in the water and in shellfish has been the reason for persistent closures in production areas, sometimes for long periods, resulting in heavy monetary losses. In the EU, the annual cost of HAB events is estimated to be more than 850 million USD [3]. Also, the consumption of contaminated shellfish has caused health problems, occasionally leading to human death. For this reason, governments, management agencies and producers are seriously committed to address this problem and find a set of adequate tools to prevent exposure to these agents. So far, the best options rely on monitoring and early warning systems (EWS) providing timely information for the industry to prevent or minimize exposure and, failing at this, to mitigate the impacts.

Limited knowledge about natural mechanisms triggering toxic HABs or the processes involved in outbreaks of microbiological events poses serious problems to scientists and engineers involved in developing such warning systems. Besides, these efforts rely on a significant variety of computational systems and methodologies, ranging from traditional data loggers used in monitoring programs, to more sophisticated computational approaches such as the processing of satellite remote sensing imagery and complex computational models.

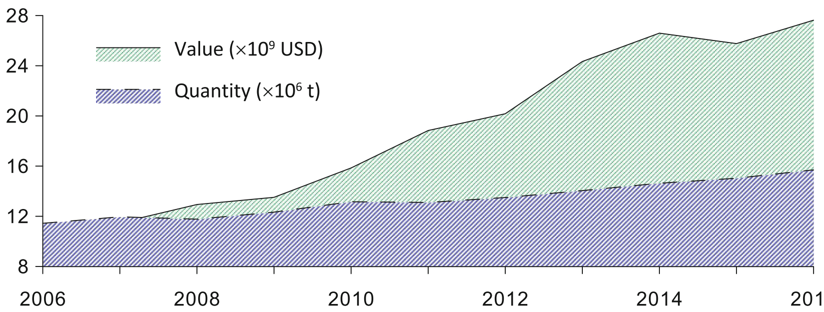

Fig. 1. Shellfish aquaculture in quantity and value for brackish and marine waters worldwide (2006–2016). Values for abalones, winkles, conchs, clams, cockles, arkshells, mussels, oysters, scallops and pectens. Data source: FAO - Fisheries and Aquaculture Information and Statistics Branch - 20/02/2019.

Over the past few years some forecast systems have been proposed, such as the experimental HAB forecast system in Lake Erie by the National Oceanic and Atmospheric Administration (NOAA) in the US, or the forecasting of the onset of HABs in the coastal waters surrounding Charlotte County, Florida [4]. EWS prototypes were recently developed and other systems already in place were matured during project ASIMUTH (supported by the EU FP7 Programme, Space Theme, Grant Agreement No. 261860) for some European countries in the Atlantic Arc (France, Ireland, Portugal, Scotland and Spain) [5,6]. Many other countries are pursuing similar systems [7]. However, only recently a few have focused on shellfish safety and try to tackle the negative impacts of microbiological contaminants or viruses. Some of these systems are currently providing warnings including such additional elements in their forecast.

This paper addresses some of the benefits of EWS for the shellfish aquaculture sector, and how computational science is central in their development. As such, this work engages EWS from a computational perspective mostly, briefly addressing some of the essential steps from harvesting field data, up to the delivery of information (early warnings) to end-users, tackling issues such as data gathering, algorithms, modeling approaches, forecast systems and platforms to integrate data. The work described here is being developed by an international consortium, as part of the work plan of the project PRIMROSE – Predicting Risk and Impact of Harmful Events on the Aquaculture Sector (information available at www.shellfish-safety.eu).

2 Aims of Early Warning Systems

Anticipating risks for public health is essential to communicate, promote and regulate public health measures. The huge amount of data collected by monitoring programs, remote sensing and ocean models is essential in this identification, but the very nature of the amount and type of data requires integrative computational tools to merge, process, interpret and transform data into something useful, minimizing human intervention in the process. EWS for impending threats to shellfish safety aim at such demanding task; they provide a short window of opportunity for producers and regulating entities to take preventive actions against impending threats, safekeeping the financial revenue of the sector and human health. For that, they must necessarily address the threats that may lead to major impacts on health and the economy: harmful algae, bacteria and viruses. Their major causes and impacts are briefly described.

2.1 Algal Toxicity

Algal blooms, the excessive growth of phytoplankton species triggered by optimal environmental conditions in the water, are natural phenomena and a frequent occurrence in the ocean, but mostly in coastal areas, upwelling systems, estuaries, bays and coastal lagoons. The main mechanisms triggering algal blooms are well known (light, nutrients and water column stability) and the conditions favoring different taxa understood [8]. However, predicting which species will bloom, and where, is still elusive. This might be due to the lack of accurate information about the environmental conditions resulting in the bloom (both in terms of conditions and temporal evolution of the conditions), but also to a fundamental unpredictability due to competition between species and chaotic effects [9]. In addition, under certain circumstances which are not yet well understood, some species flourish and produce toxins, giving rise to harmful algal blooms with ecotoxicological consequences [10].

The main syndromes usually associated with the ingestion of shellfish contaminated with the toxins produced by some HAB species include ciguatera poisoning, paralytic shellfish poisoning (PSP), neurotoxic shellfish poisoning (NSP), amnesic shellfish poisoning (ASP), and diarrhetic shellfish poisoning (DSP) [11]. Death is also a possible outcome of the exposure to such toxins. Other symptoms associated with contact with toxic algae include gastroenteritis, respiratory problems, skin irritation and liver failure [12]. Besides the impacts on human health, HABs also negatively affect the marine ecosystems through hypoxia/anoxia events, decreased water clarity, and altered feeding behavior and toxicosis of marine fauna [13], leading to mortality of sea birds, marine mammals, fish and sea turtles [14]. Consequently, HABs are associated with detrimental effects on marine biota and to significant economic damage to the aquaculture industry by making shellfish unsafe to eat and, ultimately, challenging to commercialize.

2.2 Microbiological Contamination

Most shellfish harvesting grounds for human consumption are located on inshore coastal areas. Due to their proximity to land and frequently by being within range of heavily occupied coastal strips, these shellfish producing areas are subjected to human fecal pollution from a number of point and diffusive sources. Significant quantities of fecal pathogens are introduced into the marine environment by the discharges of wastewater treatment plants, by septic tanks and pits, and by the overflows from such systems. Also, fecal pollution may reach shellfish waters by land runoff or by watercourses contaminated higher in the catchment.

The control of shellfish-borne disease related to microbiological agents has traditionally been based on the classification of production areas by the monitoring of fecal indicator bacteria, mostly *E. coli* [15]. *E. coli* may cause diseases in gastrointestinal, urinary, or central nervous systems, with symptoms such as nausea, abdominal pain, vomiting, diarrhea and cramps. *E. coli* outbreaks are mainly produced by poor management of water quality. Regulatory and market requirements for supply of safe shellfish products to consumers imposes serious restrictions on contaminated shellfish growing waters (e.g., Regulation (EC) No 854/2004 of the European Parliament and of the Council of 29 April 2004). In addition, the risk of illness associated with the ingestion of shellfish exposed to fecal pollution raises concern to the aquaculture industry and food authorities.

2.3 Viruses Infections

Shellfish accumulates NoV in a similar way to fecal pathogens, and may cause outbreaks with substantial impacts on human health. However, shellfish require a longer period to purge NoV than fecal indicator bacteria, when transferred to uncontaminated waters. NoV outbreaks are one of the leading causes of acute gastroenteritis and responsible for substantial morbidity and mortality. NoV poses the major viral risk to human health associated with shellfish consumption, though Hepatitis A virus (HAV) is also a threat. NoV outbreak symptoms are usually expressed in the form of diarrhea, nausea, vomiting, and abdominal cramps [16]. Secondary transmission from person to person is also likely to occur.

NoV are frequently present in oysters growing in contaminated waters, especially after heavy rainfall, which often results in contaminated overland run-off, combined sewer overflow, or hydraulic overload in sewage treatment plants [17], the same input routes as for *E. coli.* These infections lead to obvious healthcare costs. In the U.S. alone, a total of $184 million has been estimated as the annual cost of illness attributed to seafood contamination with NoV [18]. In Australia, for instance, 525 NoV cases were identified in March 2013, originating from consumption of contaminated oysters [19]. Given the threat to human health, the presence of NoV in oyster production areas may lead to the closure of the harvesting waters and costly oyster recalls, resulting in serious financial losses.

3 Main Components of the System

An EWS is typically set in a threefold structure or steps (see Fig. 2) combining multiple computational resources and methodologies (e.g. computational models, algorithms to process remote sensing data, machine learning approaches, etc.). The first step usually involves the gathering of information, or input data that can be potentially used by the system. The second steps deals with both the interpretation of data and its selection to run predictive models (when applicable). The last step is for the final assembly of the forecast (e.g. web services, apps, bulletins, etc.) and its dissemination to end users. Some steps can be partly or fully automatized, and are repeated according to the desired frequency of the bulletin and/or warnings.

3.1 Data Acquisition

EWS are primarily information systems: acquiring available information on the state of the ocean, meteorological conditions, health reports, etc., and processing it to generate specific information to assist end users in the decision-making process. As such, they rely on data and on many retrieval approaches including satellite imagery (remote sensing), field observations (monitoring programs) and numerical tools (computer models) (see Fig. 3). Data format and size varies significantly depending on their source and acquisition method (see Table 1).

The EWS starts with the collection of data from remote sensing and ongoing monitoring programs, some from long term coastal surveillance stations that monitor phytoplankton communities and other physical, chemical and biological parameters. Data usually relate to phytoplankton biomass and composition at study sites, and the presence of toxins in the water and shellfish. Automatic download and processing of satellite images or use of processed data services frequently take place at this stage (e.g. Copernicus, https://www.copernicus.eu/en). If the EWS include models that are not part of an operational modeling forecast system, the necessary data to force those models (e.g. meteo data) can also be gathered at this stage. Data sources for specific parameters used in the preparation of EWS are summarized in Table 2.

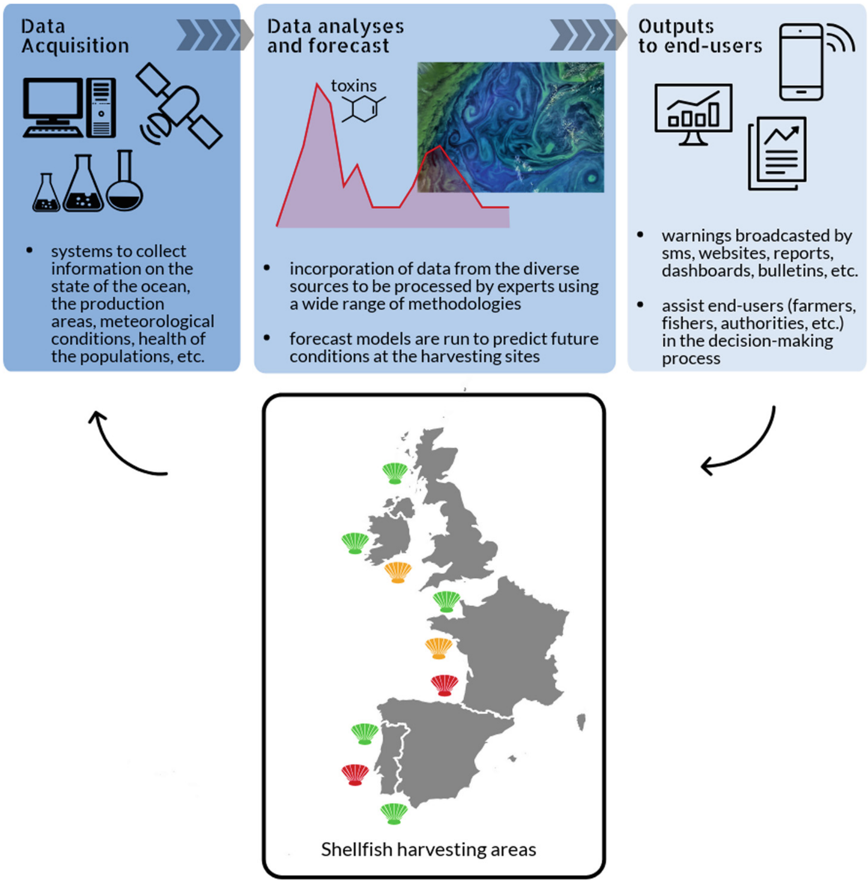

Fig. 2. Production pipeline of an EWS for shellfish harvesting areas. The outcome of the EWS can range from a simple traffic light system to classify particular areas according to shellfish safety (illustrated in the picture), to more elaborate bulletins with detailed information.

Monitoring Programs. Monitoring is an essential part of the implementation of the body of laws and directives that drive/force management strategies of natural resources. Monitoring programs can be defined as the establishment and operation of appropriate devices, methods, systems and procedures necessary to monitor, compile, and analyze data on the condition of a target systems. As such, monitoring can range from simple systematic observation and recording of current and changing conditions of a few parameters at a local scale, to a wide range of parameters over a significant wide area. These programs usually include the assessment of data leading to an evaluation on the state and evolution of the target systems, thus supporting the decision-making and planning processes.

Well designed and executed monitoring and assessment programs are a critical components in water resources management and protection. They allow to establish a baseline in the monitored systems condition and function, detect change, assess value, and characterize trends over time. Monitoring programs must ensure appropriate field sampling techniques, to obtain accurate data for HAB species such as *Dinophysis* spp. that can cause shellfish poisoning even when they comprise a small percentage of the microplankton community [20].

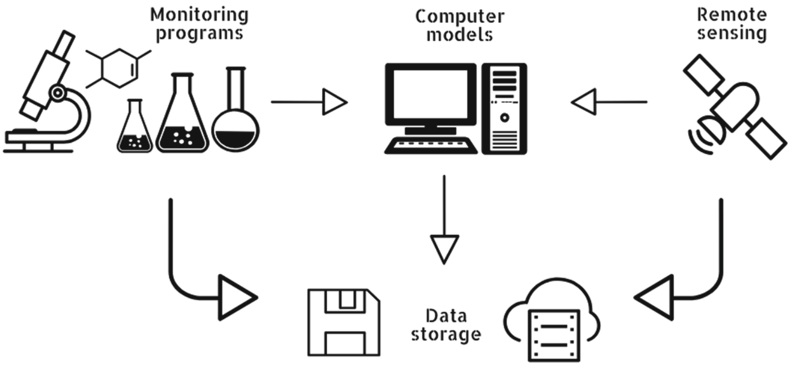

Fig. 3. Data sources for early warning system. Data from field observations and satellite imagery are also used by computer models to generate new layers of information.

Remote Sensing. Remote sensing, or data acquisition by satellite Earth observation (EO) technology, provides the capacity to monitor several parameters with reasonable accuracy, for significant expanses of territory. The strength of remote sensing techniques lies in their ability to provide both spatial and temporal views of surface water quality and atmospheric parameters that is typically not possible from *in situ* measurements. EO can observe microalgae blooms due to their coloring of the sea when in high concentrations [21,22]. Although not all plankton species that produce water discoloration are toxic (e.g. *Mesodinium rubrum*), some can be harmful to the ecosystems due to high biomass related effects and can be harmful also for the mariculture industry [23]. Consequently,

Table 1. Summary description of the characteristics of data according to its origin.

	Monitoring programs	Remote sensing	Computer models
Parameters/variables	Meteorological data, oceanographic physical and biogeochemical parameters, pathogens, pollutants, etc	Salinity, sea surface temperature, chlorophyll, ocean color	Several physical and biogeochemical param-eters, and some pollu-tants
Spatial coverage	One sampling point to several sampling stations over a vast area	Global	Local (areas of a few km^2) to regional (ocean basin scale)
Spatial representation	1-D (point samples) and 2-D (profiles)	2-D (ocean top layer)	3-D
Temporal resolution	Instant (e.g. water sam-ples) to continuous monitoring (e.g. fixed probes)	Depending on the revisiting frequency of a satellite sensor for a specific location	Continuous outputs with temporal resolutions from a few minutes to days
Data types	Time series, profiles	Surface maps	3-D plots, surface maps, profiles, sections, time-series, etc.
Data formats	Text files (.txt, .dat), spreadsheets (.csv, etc.)	NetCDF, raster, raw	NetCDF, HDF, data files
Data size	KB to MB	MB to GB	GB to TB
Computational requirements	Low: data loggers, computers to visualize and treat data, conventional software	High: high-performance computers, complex algorithms, tailored programs	Parallel computing, computational clusters, complex code, high storage requirements
Required skills	Elementary knowledge on generic software (e.g. excel); basic programing skills	Proficient users: good programing skills (e.g. python)	Advanced programing skills (several computer languages)

satellite-related technologies may be integrated in monitoring programs defined by national or local authorities. As such, remote sensing is central in the development, implementation and control of management strategies.

Currently there are several sources of remote sensing data, covering a wide range of products available to be accessed or downloaded. The Copernicus Services (https://www.copernicus.eu/en) is the most relevant EO data provider for European seas, incorporating a range of sensors and temporal and spatial resolutions. A significant number of these products are freely available for registered users, and additional products can be available for national governments or local authorities. Novel Copernicus Climate Change Service (C3S) products will also provide indicators for future scenarios (https://climate.copernicus.eu/), including indicators relevant to aquaculture.

Computer Models. Computational models offer unparalleled capabilities for studying the ocean by simulating its physical, biogeochemical and ecological processes. Their unique contribution to EWS is the ability to forecast ocean conditions from a known state, usually characterized by data retrieved from monitoring programs and remote sensing. In this sense, numerical models integrate data from field observations and satellite imagery and initial and forcing conditions for the simulations, but also for calibration and validation, contributing to produce additional layers of information that would be impossible to achieve by any other means [5].

Numerical modeling approaches comprise a significant range of methodologies, algorithms and computational tools [24]. They can be purely hydrodynamic and simulate the physical structures of the ocean to describe them in the form of tridimensional velocity fields and thermal distribution. Such models can be coupled to Lagrangian models to simulate the passive transport of particles, without necessarily incorporating any biological processes. In the modeling of HABs, for instance, this approach is commonly used when physical processes dominate over biological ones [25]. During ASIMUTH, HAB forecasts based on hydrodynamic and particle tracking models showed skill in predicting and characterizing transports of HABs alongshore and in and out of harvesting areas in Ireland, Portugal, Galicia and Scotland [26,27]. In a more complex approach, ocean models can also couple physical and ecological algorithms, typically Eulerian in nature, calculating biogeochemical properties, with these variables being subject to physical (advection, diffusion) and biological processes (growth, mortality, mineralization, etc.).

Statistically based models are also used to identify potential relationships between variables and processes, such as phytoplankton abundance and potentially causative environmental conditions for NoV outbreaks and patterns of human health. Finally, there are also risk assessment models that are empirical in nature and, from a computational perspective, significantly simpler than the modeling approaches previously mentioned. These models infer cause and effect relationships between HABs or NoV outbreaks and environment parameters, identifying possible trigger thresholds.

3.2 Data Analyses and Forecasts

This stage involves the incorporation of data from the diverse sources and may include current synoptic, recent trends (past month) and historical patterns (10 years) from phytoplankton and shellfish toxin monitoring programmes, satellite temperature and chlorophyll, results from 3D primitive equation coastal hydrodynamic models and particle tracking models. These data are processed by experts using a wide range of methodologies:

Table 2. Data sources for specific parameters used in the preparation of EWS.

	Monitoring programs	Remote sensing	Computer models
Algal biomass, composition and toxins	Yes	Ocean color (algorithms to estimate algal biomass from chlorophyll *a* pigments)	Yes, models can simulate several phytoplank-ton groups but only a few include toxins
Microbiological agents	Yes	—	Yes
Viruses	No	—	—
Temperature	Yes	Sea surface temperature	Yes (thermal structure)
Currents	Yes	—	Yes (2-D, 3-D)
Nutrients	Yes	—	Yes
Diss. oxygen	Yes	—	Yes

(1) Processing software to extract temporal and spatial variations of remote sensing-based variables over the study area. Remotely sensed data provide insight into the possible locations and extent of the blooms. For instance, remote sensing data in near real-time from Medium Resolution Imaging Spectrometer (MERIS) and Moderate Resolution Imaging Spectroradiometer (MODIS) like sensors has been used to detect and trace HABs [28,29]. Satellite images are also used to assess thermal patterns at the surface, enabling the identification of phenomena that may be related with the occurrence of HABs (e.g. upwelling episodes and fronts);

(2) Numerical models to identify oceanographic structures and conditions associated with the onset of HABs [30]. Numerical models can also simulate biogeochemical processes and include several functional groups of phytoplankton and may predict the timing and place of the formation of HABs. Another modeling approach that is frequently used consists in the use of particle tracers to simulate the transport patterns of HAB, once they have been identified by monitoring or remote sensing. While the development of operational biological models of HAB dynamics remains a major challenge, physical models to simulate the Lagrangian transport of detected HABs have proven to be a useful tool for HAB early warning [25–27];

(3) Statistical approaches that are characterized by having an explicit underlying probability model, which provides a probability of the outcome, rather than simply forecast without uncertainty [31]. The Probabilistic Graphical Models (PGMs) paradigm, based on probability theory and graph theory, can be used. PGMs include Bayesian networks, which are suitable to deal with uncertainty. Their intuitive properties and the explicit consideration of uncertainty enhance experts' confidence on forecasts [32,33].

3.3 Outputs to End-Users

At the final stage of the process, experts select the graphics, sometimes relying on automated routines, to produce the short term forecast. Frequently a short text is also prepared, highlighting some aspects found relevant by the experts. If a bulletin is produced, it is usually sent to producers and regulators via email or uploaded to a designated site (usually from local or national authorities), becoming accessible to the general public. The actual content of the EWS depends on the site characteristics, type of shellfish production, used methodologies and data, specific threats, etc. As such, EWS do not have a specific template, and can either be quite simplistic (using a simple traffic light system to classify production areas, for instance) or highly complex, with elements such as current and sea surface forecasts, historical trend analyses for the presence of toxins or site closures, plots for hydrodynamic patterns, etc. Either way, EWS aim to be relevant and effective and provide simple answers regarding shellfish safety, however sophisticated their methodologies.

4 Current and Future Challenges

4.1 Computational Tools and the New Possibilities

Computational science is at the core of EWS. In that respect, significant developments are expected to occur in the hardware and software, ultimately leading to improved performance of both machines and algorithms. The implications to EWS of these continuous developments are significant: new approaches to gather and process data may arise, and more computational power may become available to face the ever increasing complexity of forecast ocean models [30].

While HABs and microbiological agents such as *E. coli* impacts in shellfish areas have been the focus of intense research (even though their dynamics are not entirely understood), the study of NoV is comparatively recent. Consequently, one of the main challenges at the moment lies in addressing the dynamics of NoV and its inclusion in EWS for shellfish safety. Computational tools are also playing a major role here, with considerable effort applied to better understand the epidemiology and control of NoV, especially in the development of mathematical models to describe their transmission dynamics [34,35]. These models range from purely statistical [36], to more sophisticated approaches, such as probability based Artificial Neural Network models to predict NoV outbreaks in oyster cultures [37]. Such models can be combined with other approaches to provide the necessary time frame for a timely intervention and/or appropriate management decisions to reduce or even prevent norovirus related risks.

4.2 Knowledge Gaps

The need to continue optimizing early warning systems for shellfish safety is an ongoing challenge, not just to scientists, but also to the shellfish industry and regulators. Although knowledge has increased considerably in recent years, and algorithms, models and computational systems keep developing, further research and technical developments are required to address the following:

(1) Predicting the onset of algal blooms from identified conditions has become possible by using new algorithms to analyze remote sensing data and model forecasts. However, predicting the presence of toxins in such blooms is still elusive, as many of the underlying mechanisms inducing toxicity are still unknown;
(2) While modeling the dynamics of generic types of phytoplankton (diatoms, flagellates, picoalgae, etc.) has become a rather straightforward task, as seen by the myriad of models available today, achieving the same goal for harmful groups (e.g., toxin-producing species) has proved to be significantly more challenging;
(3) Development of effective NoV monitoring programs for commercial production areas to better understand contamination patterns and improve understanding on the hydrographical relationships between NoV inputs and consequential impacts on shellfisheries to better model risk [38];
(4) Monitoring data for phytoplankton composition and biomass, or even toxicity levels, and fecal contamination have an abundant spatial-temporal coverage, whereas NoV data are relatively limited [39,40];
(5) Exchange of data among different national monitoring programs is required for accurate HAB forecast when transnational alongshore transport takes place [6]. For example, early warning for the risk of autumn toxic dinoflagellate blooms in the Galician Rías is only feasible if the system is combined with a similar system for the Portuguese waters [27].

4.3 Climate Change

Expected changes in climate conditions poses additional challenges to the shellfish aquaculture industry, as key environmental parameters are expected to shift from their mean values. Water temperature, that strongly regulates the metabolism of organisms, is one of these parameters. The increased frequency of warm water events in recent decades has been reported [41]. Besides affecting the shellfish metabolic rates, these shifts may also change phytoplankton productivity and composition in coastal waters, potentially promoting the formation, and even the dominance of HAB species [42]. Under this scenario, an increased impact of HABs on shellfish can be expected. Furthermore, ocean acidification can exacerbate the impact on shellfish species [43].

Climate change may also bring new challenges associated with fecal pollution. More frequent flood events and rainwater discharge will increase the exposure of shellfish to *E. coli* and NoV (and other potentially harmful agents), imposing adaptive strategies in design and capacity of wastewater treatment plants in shellfish production areas. Considering that there is a recognized link between winter seasonality and NoV outbreaks, climate change has the potential to influence the transmissibility, host susceptibility and virus resistance to environmental conditions [44]. Climate change will drive developments in EWS but, at the same time, will also provide the opportunity to prove their value. If these systems maintain their links to the latest knowledge and state-of-the-art computation, they will surely become critical or even mandatory forecast tools, in the management of shellfish harvesting areas.

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