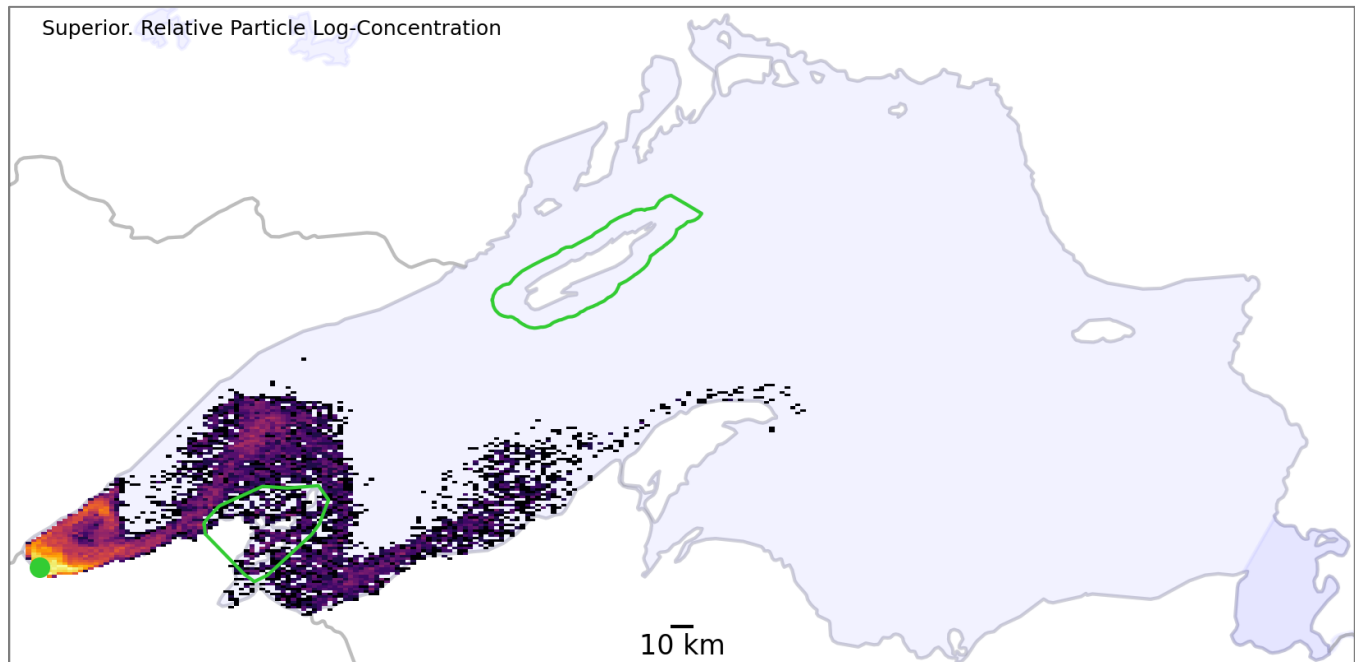




Demonstrating a Lake Superior Particle Tracking Model for Research and Management Applications



Simulated plume of particles released from the St. Louis River and allowed to drift for 7 weeks.

NPS / DANIEL SANDBORN / JAY AUSTIN / BRENDA LAFRANCOIS

Demonstrating a Lake Superior Particle Tracking Model for Research and Management Applications

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Abstract

A particle tracking model was deployed in a preliminary study of Lake Superior particle dynamics. It was driven by the Great Lakes Operational Forecast System (GLOFS) hydrodynamic model output and run using OceanTracker, an open-source particle tracking software package. This report details the results of several experiments applying this particle tracking program to aquatic invasive species transport, harmful algal bloom dynamics, and pollution transport in and around Lake Superior, with particular emphasis on two national park units (Apostle Islands National Lakeshore and Isle Royale National Park). The first experiment found particle transport times on the scale of days between the park regions and major tributaries known to host Dreissenid mussels, illustrating a potential intra-lake vector of invasion. The second experiment highlighted hotspots of pelagic and nearshore accumulation of particles, demonstrating the potential for larval or pollutant aggregation and deposition. The third experiment sought to backtrack observed harmful algal blooms to infer bloom drivers and found an association between advective transport of water from the St. Louis River estuary to remote locations and blooms. While further development of particle tracking experiment methods is needed to refine the experiments detailed in this work, the model demonstrated potential for extension to other Laurentian Great Lakes and application to important questions in limnology and water resources.

List of Acronyms

AIS: Aquatic Invasive Species

APIS: Apostle Islands National Lakeshore

FVCOM: Finite Volume Community Ocean Model

HAB: Harmful Algal Bloom

ISRO: Isle Royale National Park

LSOFS: Lake Superior Operational Forecast System

Introduction

Hydrodynamic processes have implications for lake thermal structure, chemistry, and mixing, biological community structure, ecological processes, and physical transport of materials (Lerman et al. 1995). In Lake Superior, prevailing circulation patterns are generally cyclonic or counter-clockwise, but there is substantial spatial, seasonal, and interannual variation in current behavior due to wind direction, thermal gradients, and bathymetry (Beletsky et al. 1999; Bennington et al. 2010). Summer circulation patterns are organized and seasonally-persistent, with strong currents existing along shorelines. Increasingly sophisticated and high-resolution models of lake hydrodynamics have developed in the Great Lakes region in recent years, including a Finite Volume Community Ocean Model (FVCOM; Chen et al. 2003) in 2022, allowing for more elaborate modeling exercises and insights.

The importance of hydrodynamic processes in shaping the physical and biological landscapes of the Laurentian Great Lakes (hereafter: Great Lakes) has been underscored by recent studies of tributary plume movement (McKinney et al. 2018), microplastics transport (Weber et al. 2020), and invasive species spread (e.g., Sieracki et al. 2014). Lake Superior managers and scientists have noted a need for more attention to the interaction of lake hydrodynamics with emerging management concerns such as *Dreissena* mussel establishment, harmful algal bloom (HAB) development, and pollutant transport (EPA 2023), particularly in light of anticipated climate change and effects on air-surface temperature gradients, biogeochemistry, and currents (Bennington et al. 2010; Phillips et al. 2015; Xue et al. 2022).

With respect to *Dreissena* mussels (zebra mussels, *Dreissena polymorpha*, and quagga mussels, *Dreissena bugensis*), Trebitz et al. (2019) and Larson et al. (2022) provided evidence of transport of larval dreissenids (veligers) from existing populations in Duluth-Superior/Twin Ports to the Apostle Islands via longshore currents, suggesting that veliger transport can help explain the uneven distribution of adult dreissenids within the Apostle Islands (Lafrancois et al. 2022). Sterner et al. (2020) noted that although recent algal bloom events are partially explained by large scale temperature and precipitation changes, hydrodynamic entrainment of river plumes and/or concentration of algal blooms may be important in shaping local bloom intensity. The National Park Service protects unique shoreline habitats and has long been interested in understanding their vulnerability to potential spills and microplastic pollution due to local and long-range transport (Egan et al. 2014; Minor et al. 2020). Given recent development of new hydrodynamic data resources and tools, more focused attention to the role of hydrodynamics in key lake management questions is warranted.

One tool for exploring the intersection of hydrodynamic processes and emerging management issues is Lagrangian particle tracking, a numerical method by which simulated particles are transported through a virtual environment described by hydrodynamic model output. It can be applied to model the transport of chemical tracers, sediments, pollutants, drifting objects, invasive species, or anything else that could be conceptualized as an infinitesimal point. Particle tracking models are enabled by the combination of sufficiently detailed simulations of fields from high-resolution hydrodynamic

models and physical equations describing the interactions between fields and particles. While a detailed treatment of the developing field of Lagrangian particle tracking in environmental fluids (e.g., Lynch et al. 2015) is beyond the scope of this work, the numerical method can be summarized as integration of velocity fields (interpolated to a particle's position) simulating advection superimposed upon a random walk simulating dispersion. This may be performed in concert with hydrodynamic modelling (online) or using model output (offline). Previous particle tracking efforts in the Great Lakes have yielded insights into harmful algal bloom structure and transport (Rowe et al. 2016; Zhou et al. 2023), chlorophyll distribution and productivity (Xue et al. 2017), and invasive alewife transport (Rowe et al. 2022).

Here we present an effort to couple offline hydrodynamic model fields and ocean particle tracking software to produce fast and user-friendly simulations of particle transport in Lake Superior, focusing on several applications relevant to adjacent National Park Service lands. This report details three experiments developed to explore the capabilities of the model and provide a proof-of-concept upon which future work can build:

1. **Characteristics of aquatic invasive species (AIS) transport in Lake Superior**—Riverine delivery and plume transport of particles were simulated in order to model AIS species transport in Lake Superior. Two *Dreissena* veliger source locations (the St. Louis and Nipigon Rivers) and two destinations (Apostle Islands National Lakeshore / APIS and Isle Royale National Park / ISRO) were considered. Populations of *Dreissena* mussels have been established in the St. Louis River Estuary since the 1980s but have established more recently in Nipigon Bay. Managers are interested in understanding the transport of veligers from these source locations to high value national park habitats and fish spawning reefs. Connection between sources and destinations was demonstrated and quantified via time-to-arrival and transport efficiency metrics.
2. **Hotspots of particle accumulation**—Particles transported through Lake Superior exhibit accumulative and dispersive behaviors that create heterogeneity in particle concentrations. This heterogeneity may have consequences for dispersal of AIS, microplastics, or other contaminants by creating uneven delivery of particles in pelagic and onshore environments. Similar “hotspots” of particle accumulation have been observed in oceans and inland seas, in which persistent eddies, up/downwelling phenomena, and settling behaviors tend to concentrate particles. Lake Superior experiences a range of physical circulation phenomena which may create particle hotspots, including Coriolis-driven eddy formation and associated up/downwelling, seasonally to annually persistent currents, and nearshore environments that may present opportunities for settling and resuspension. This experiment illustrates particle hotspots in pelagic and nearshore environments and suggests directions for observational and management work.
3. **Backtracking harmful algal blooms**—Lake Superior algal blooms are often reported as sudden, short-lived observations (Benesh et al. 2023), but may develop over time in waters far from their observation points, accumulating in some locations due to wind and current action (Sterner et al. 2020). Managers seek insights to where particles associated with surface

bloom observations may have originated in order to help target nutrient reduction or other management actions. Particles from several documented Lake Superior bloom observations in 2023 (Lafrancois and Reint 2024) were simulated backwards in time to illustrate potential factors of algal bloom formation. Particles were deposited at sites and/or times of algal blooms, and their potential sources were outlined by the distributions of particle sources produced by backtracking simulation.

Methods

The particle tracking model was composed of three modules: hydrodynamic model output, a particle tracking package, and a wrapper program written to integrate the pieces of the particle tracking model and generate output. Each of the experiments described in the following sections relied on these modules to describe water physics, translate water physics to particle transport, and interpret particle transport in the context of the experiment.

Hydrodynamic Model Output

The Lake Superior Observational Forecast System (LSOFS 2022) has provided high-resolution model output fields describing water movement and conditions in Lake Superior since October 2022, when the Finite Volume Community Ocean Model (FVCOM) was implemented to replace the earlier lower-resolution Princeton Ocean Model (Peng et al. 2023). The other Laurentian Great Lakes received FVCOM models earlier, and all lakes continue to be described by nowcast and up to six hours of forecast fields continually released and freely available. Previous research utilizing the detailed physical descriptions of the Great Lakes provided by FVCOM output have confirmed its agreement with observations of hydrodynamic conditions and physical mixing phenomena (Gronewold et al. 2019; Huang et al. 2019; Kelley et al. 2022). Model output used for the experiments described below was accessed via the National Centers for Environmental Information website (NOAA 2017) and downloaded with the highest (hourly) time resolution and all hydrodynamic variables necessary to run OceanTracker software. Further details on model output access methods, including variable subsets, can be found in the Github repository described below.

Particle Tracking Package

OceanTracker is a Lagrangian particle-tracking software package offering fast, user-friendly, and extensible offline simulations in unstructured grids (Vennell et al. 2021). It is written in Python (an open-source, high-level coding language) and freely available on Github (Vennell and Steidle 2025). OceanTracker proved particularly well-suited for rapid simulation and statistical analysis of nearshore particle transport and has previously been used to model transport of larval organisms (Atalah et al. 2022). The speed of its simulations stems mainly from an implementation of a “short triangle walk” which enables more rapid computation of particle movement, along with reuse of interpolation weights between time steps. The speed of OceanTracker, paired with its open-source accessibility and inbuilt statistical capabilities, recommend it for deployment in large lake environments.

Among the factors contributing to OceanTracker’s flexibility are the model parameters and particle properties, which enable the “tuning” particle transport to resemble the behavior of an experiment’s subject. These parameters include buoyancy, resuspension, tidal stranding, horizontal and vertical dispersion rates, other properties affecting transport behavior, and the ability to create arbitrary particle properties representing biological or biogeochemical characteristics. One pitfall of such flexibility is the need to adjust these settings to constrain simulation results to realistic outcomes. In this work, particle and model parameters were specified with reference to literature values (as with the range of resuspension values considered in Experiment 2), restricted (as for the surface-

constrained particles in Experiment 3), obviated (tidal stranding), or left at reasonable default values aligning with physical transport principles (vertical and horizontal diffusivity). Unless otherwise noted, default OceanTracker simulation settings were used, including hard surface, bottom, and lateral boundary conditions and neutral buoyancy of particles. For details on the implementation of particle transport as a function of hydrodynamic parameters, the interested reader should consult previously-referenced works by Vennell et al. To the extent that tuning model and particle parameters may alter model outcomes, ground-truthing as considered in the discussion may aid in constraining their values.

Wrapper

A series of scripts were produced as a wrapper over OceanTracker, aggregating LSOFS fields and creating particle simulations in Lake Superior. A demonstration of the wrapper is available at the Github repository (Sandborn 2024). A family of scripts (Table 1) tied the various model components together with the intent of flexible reuse and extension to experiments in any of the Laurentian Great Lakes.

Table 1. Description of various files in the Lake Superior particle tracking model (Sandborn 2024).

File Name	Description
experiments/...	Python scripts defining experiment's geographic bounds, particle properties, input/output file handling, performance of basic post-processing (graphic), and initializing simulation.
nc_compressor.py; fields/...	Downloads and manages the sizeable (c. 1 TB/yr after subsetting and compression) inventory of LSOFS model output necessary to describe water physics. This is done only once and the fields stored locally, as the nature of large files and host server bandwidth makes on-demand access of FVCOM fields over the internet unreliable and impractical.
utils/...	Various scripts called by the experiments for graphical output and data processing.
.sh and serial_output/...	This model is run on high performance computing (HPC) resources via the Minnesota Supercomputing Institute (MSI); shell (.sh) scripts and corresponding reports in the serial_output folder form the interface with this mode of computing. While OceanTracker is designed to not need a supercomputer (at least for small runtimes/particle numbers), the stability and storage of HPC resources is a boon to robust and repeatable scientific computing.
output/...	Particle tracking simulation output is stored in a directory containing OceanTracker diagnostic outputs, processed graphics, and particle tracks/heatmaps/statistical summaries as NETCDF4 files.
oceantracker/...	The OceanTracker package defines functions that accept FVCOM model fields and simulation parameters and return simulation results. This subdirectory is not included in the demonstration repository and may be obtained from the OceanTracker repository.

Experiment 1: Time-To Arrival and Efficiency of AIS Transport

Summary

AIS vectors may be transported to sites of interest by advection from sources. This experiment was designed to examine transport of veligers (pelagic larvae) of *Dreisseina* mussels through Lake Superior. The open waters of Lake Superior are generally considered hostile to *Dreisseina* settlement and prohibit colonization in all but a few nearshore sites for reasons including cold water, low calcium and ionic concentrations, and low food concentrations. Transport from source populations (tributaries) to potential colonization sites must span tens to hundreds of kilometers on a scale of days to weeks to deliver viable veligers to national park sites. We present two transport characteristics which may affect the success of *Dreissena* establishment:

1. **Transport efficiency.** The fraction of *Dreissena* veligers that arrive at a specified location within a specified time. Mean circulation patterns direct tributary plumes, which may or may not overlap with a site of interest, and deliver veligers with relatively high efficiency. A “cutoff time” is defined to limit the model to tracking relatively direct particle transport from source to destination. Particle concentration becomes homogeneous in Lake Superior on the scale of months depending on release date and location.
2. **Transport period.** A statistic describing how long veligers take to arrive. In this work, the minimum of the distribution of particle arrival times (the soonest-arriving particle) is reported, as other statistics (e.g., mean, median) are functions of the model cutoff time (Jönsson and Watson 2016).

Particle transport periods on the scale of days were observed between two sets of closely connected source and destination locations in Lake Superior, well within likely periods of *Dreissena* veliger viability. Significant sub-seasonal variability tied to stochastic weather events was a significant driver of transport period and efficiency. These results indicated periods of relatively rapid transport of particles which may be important modes of *Dreissena* spread.

Setup

Two particle source locations were specified: the mouth of the Nipigon River (N 48.94°, W 88.19°) and the mouth of the St. Louis River (N 47.71°, W 92.00°). These tributaries of Lake Superior are known to host reproducing *Dreissena* populations among other AIS and pollutants. Two destination areas were defined as polygons described by the boundaries of APIS and ISRO (Figures 1 and 2). A particle that crossed either polygonal boundary was considered to have “arrived,” regardless of its depth or settling/suspension, as these are poorly constrained behaviors that depend on particle buoyancy, morphometry, and vertical diffusivity.

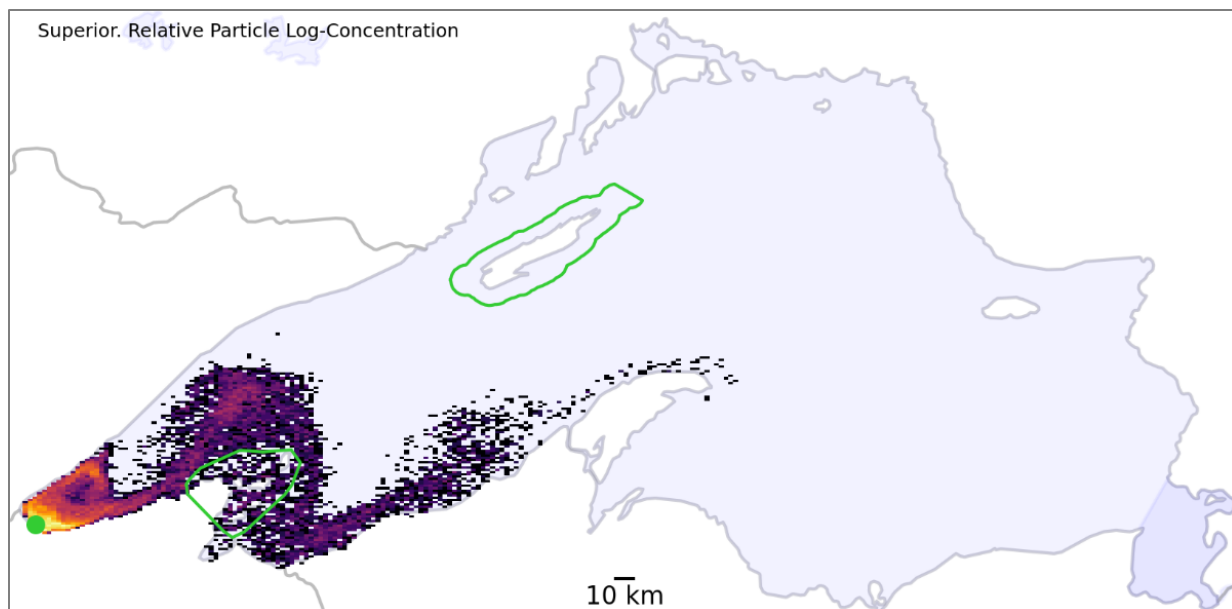


Figure 1. Heatmap of particles released from St. Louis River (green dot), captured on the final day of the simulation. Heatmap colors indicate the natural logarithm-transformed concentration of particles per rectilinear grid square integrated over the water column. Isle Royale National Park and Apostle Islands National Lakeshore are circled in green.

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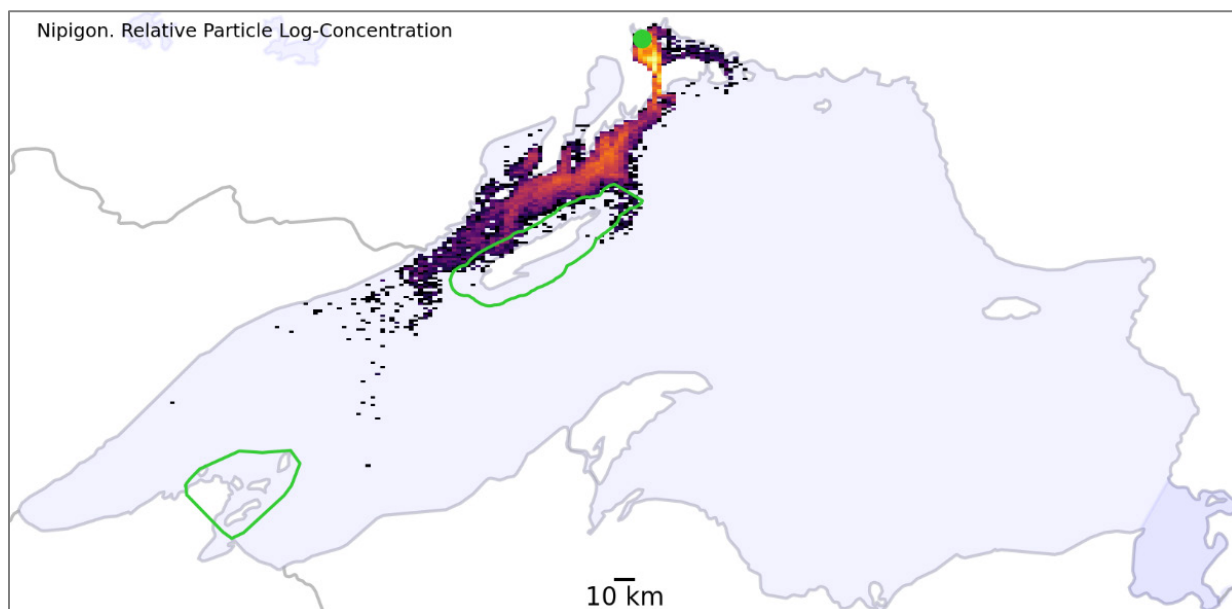


Figure 2. Heatmap of particles released from Nipigon River (green dot), captured on the final day of the simulation. Heatmap colors indicate the natural logarithm-transformed concentration of particles per rectilinear grid square integrated over the water column. Isle Royale National Park and Apostle Islands National Lakeshore are circled in green.

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Simulated particles were released at the surface from source locations daily for the period 21 October 2022–31 October 2023 in pulses of 512 particles (model parameters in powers of two were found to lead to faster simulation, likely due to reduced memory demands). Their movements were tracked in three spatial dimensions every 1,024 seconds (ca. 17 min) before being removed from the simulation after approximately 49 days (2^{22} sec). This runtime was chosen as a compromise between veliger viability timescales (days to weeks) and the timescales at which particles become well-mixed throughout the lake (months to a year). The arrival time of each particle was recorded, as well as the fraction of particles from each day’s pulse that arrived within either polygon.

Results

Relatively strong connectivity of sources and destinations, as measured by particle transport efficiency, were observed between the St. Louis River and APIS, as well as between the Nipigon River and ISRO (Tables 2 and 4). These connections are in agreement with previous observations of mean water circulation patterns in Lake Superior (Bennington et al. 2010). Transport periods between strongly connected sources and destinations varied significantly over time (Figures 3 and 4), displaying an annual average of 12.7 ± 7.8 days ($\pm$ s.d.) between the St. Louis River and APIS, and 18 ± 11 days ($\pm$ s.d.) between the Nipigon River and ISRO. In general, the most rapid transport was observed in March–April and June–August (Tables 3 and 5). The fastest simulated particle advection from the St. Louis River to APIS was 46 hours on 1–2 March 2023, while the fastest simulated particle advection from the Nipigon River to ISRO was 52 hours on 4–6 April 2023. In straight-line distances over open water, both periods correspond to average travel speeds of about 50 cm/sec, which corresponds to approximately the upper decile of mean global ocean surface current speeds (Cheng et al. 2023).

Table 2. Monthly and annual mean transport efficiency from the St. Louis River (%). Transport efficiency is reported as the percentage of particles from pulses during the indicated time period that reached the indicated destination. Months with no particle arrivals are labeled “N/A.” Not all particles released in October 2023 received the full advection period due to constraints on model field availability.

Park	Nov 2022	Dec	Jan 2023	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	All
APIS	30.0	20.0	24.0	41.0	37.0	12.0	31.0	39.0	36.0	38.0	36.0	7.3	30.0
ISRO	N/A	N/A	N/A	1.7	2.8	<1	<1	<1	<1	<1	N/A	N/A	<1

Table 3. Monthly and annual mean transport period from the St. Louis River (days). Transport period is reported as the minimum time to arrival of a particle in a daily pulse. Months with no particle arrivals are labeled “N/A.” Not all particles released in October 2023 received the full advection period due to constraints on model field availability.

Park	Nov 2022	Dec	Jan 2023	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	All
APIS	5.6	7.8	13.0	2.8	1.9	2.0	6.1	2.1	2.1	2.8	4.9	13.0	12.7
ISRO	N/A	N/A	N/A	30.0	12.0	11.0	24.0	17.0	16.0	37.0	N/A	N/A	18.0

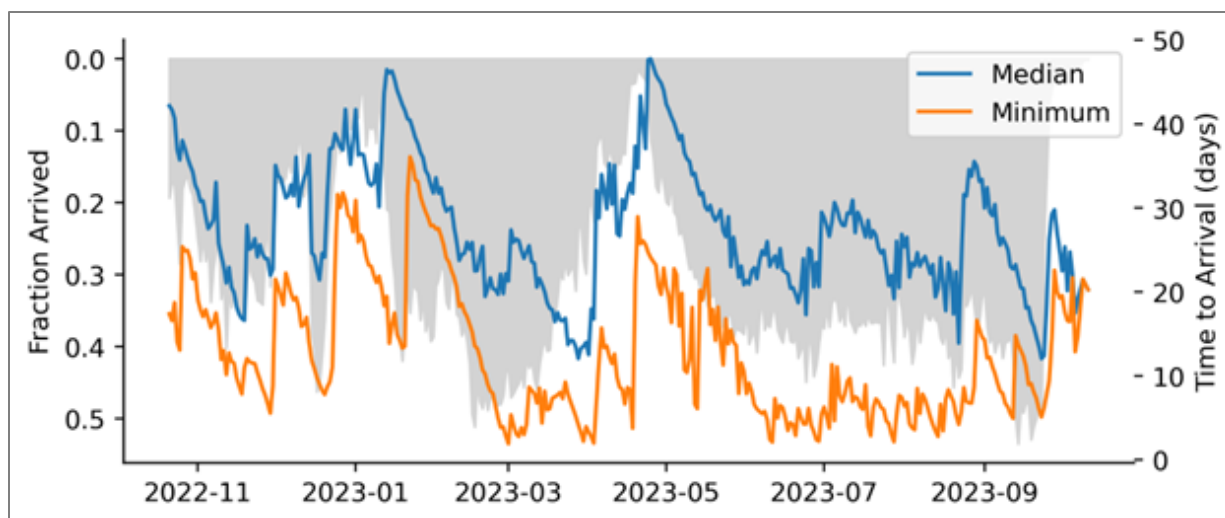


Figure 3. Particle transport statistics for St. Louis River to APIS. Transport period (orange) is indicated as the minimum advection time for each day's pulse of particles. The median advection time (blue) is also given for comparison. The median advection time was greater than the minimum by 15 ± 6 days on average ($\pm$ s.d.). Arrival fraction is indicated in grey; note reversed axis.

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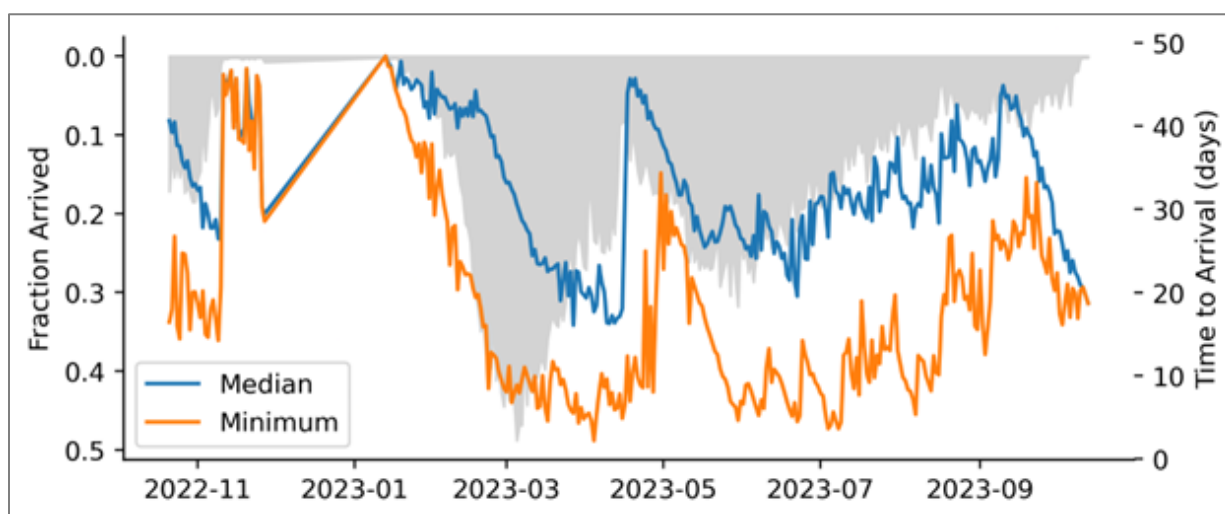


Figure 4. Particle transport statistics for Nipigon River to ISRO. Transport period (orange) is indicated as the minimum advection time for each day's pulse of particles. The median advection time (blue) is also given for comparison. The median advection time was greater than the minimum by 15 ± 8 days on average ($\pm$ s.d.). Arrival fraction is indicated in grey; note reversed axis. No particles departing during December 2023 arrived in the ISRO polygon within the allotted advection period.

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Table 4. Monthly and annual mean transport efficiency from the Nipigon River (%). Transport efficiency is reported as the fraction of particles from pulses during the indicated time period that reached the indicated destination. Months with no particle arrivals are labeled “N/A.” Not all particles released in October 2023 received the full advection period due to constraints on model field availability.

Park	Nov 2022	Dec	Jan 2023	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	All
APIS	N/A	N/A	N/A	<1	<1	N/A	<1	<1	<1	<1	<1	N/A	<1
ISRO	3.0	N/A	1.5	23.0	37.0	17.0	25.0	22.0	13.0	7.9	6.2	7.0	16.0

Table 5. Monthly and annual mean transport period from the Nipigon River (days). Transport period is reported as the minimum time to arrival of a particle in a daily pulse. Months with no particle arrivals are labeled “N/A.” Not all particles released in October 2023 received the full advection period due to constraints on model field availability.

Park	Nov 2022	Dec	Jan 2023	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	All
APIS	N/A	N/A	N/A	40.0	29.0	N/A	32.0	25.0	27.0	48.0	36.0	N/A	39.0
ISRO	14.0	N/A	31.	8.4	4.3	2.2	4.6	4.5	3.6	5.3	12.0	14.0	18.0

The transport period (as the minimum of the distribution of arrival times) was on average 15 days faster than the median of the distribution of arrival times for both St. Louis River to APIS and Nipigon River to ISRO (illustrated in Figures 3 and 4), demonstrating a range of individual particle transport behaviors introduced by the superposition of advective and dispersive drivers. The difference between minimum arrival time and median arrival time appeared to be greatest during prolonged periods of relatively rapid transport in March–June and July–August in both systems. These periods may have been characterized by high rates of dispersion relative to advection, which would broaden the distribution of particle arrival times. These results may be biased by OceanTracker’s failure to comprehend ice cover as a driver of particle transport. While the LSOFS hydrodynamic model is coupled with an ice cover model (Anderson et al. 2018), the direct effects of ice cover on particle transport in Lake Superior remain unclear.

Strong sub-seasonal variability was visible in the timeseries of transport periods as “sawtooth” behavior, whereby transport periods increased while transport efficiency decreased suddenly (on the scale of days) followed by a gradual return to former conditions (on the scale of days to weeks). Visual comparison of Figures 3 and 4 indicates some connection of these saw-toothed spikes, most visible in mid-April 2023. This spike co-occurred with a major flood stage reading on the St. Louis River in Scanlon, Minnesota, on 16 April 2023, indicating that water circulation and particle transport in Lake Superior may interact with regional weather and hydrologic phenomena.

Patterns of arrival location within the polygonal park boundaries were not considered in this experiment; Experiment 3, described later in this work, indicates that particle arrival is likely to be uneven in space and time. These dimensions are particularly important for future particle models of

Dreissena veliger transport to consider, as the timing and locations of spawning season (mid-summer into autumn as a function of water temperature; Trebitz et al. 2019), stratification, and flooding all interact with veliger transport. This transport simulation lays the foundation for further model experiments exploring AIS invasion routes, point-source pollution transport, and physical properties of circulation in Lake Superior. Expanding this work to other Laurentian Great Lakes and connected water bodies such as the St. Louis River Estuary may broaden the scope of possibilities for this avenue of research and expand its potential impact on sensitive ecosystems and communities around the Great Lakes region.

Experiment 2: Hotspots of Particle Accumulation

Summary

In the previous section we demonstrated transport of particles representing *Dreissena* mussel veligers within biologically relevant timescales between two defined start- and endpoints. This experiment expands on that work by exploring variability in particle accumulation on a lake-wide scale. The distribution of particles in a large body of water is influenced by sources (rivers, atmosphere, resuspension), transport (advection, dispersion), and sinks (decomposition, burial, outflow). This model does not attempt to offer a comprehensive simulation of all these mechanisms driving particle fate and transport, but rather an illustration of the interaction of inert infinitesimal particles and a subset of physical drivers. This limited description is useful for inferring properties of particle transport and the modeled representation of physical limnology.

The primary goal of this experiment was to identify sites and times of relatively high particle accumulation in and around Lake Superior. Simulated neutrally buoyant particles were introduced to the surface of Lake Superior and allowed to drift, experiencing advection, diffusion, deposition, and resuspension, which concentrated or dispersed particles, illustrating regions and periods of relatively high particle density. These were termed “hotspots” of particle accumulation. The spatiotemporal distribution of these hotspots indicated that particle delivery and settlement in nearshore sediments was highly uneven, with particle densities (defined as the number of particles per two-dimensional area) spanning two orders of magnitude. The case for offshore or pelagic particle accumulation was harder to interpret, as high pelagic particle densities were correlated with total water column depth. These phenomena illustrated by particle tracking modeling may inform observational and management campaigns seeking to understand and predict delivery of particle-like objects including larval AIS, turbidity, point-source pollutants, and microplastics.

Setup

Particle simulations were conducted for the period 21 October 2022 to 31 October 2023. One million neutrally buoyant simulated particles were released randomly over the surface of Lake Superior at the beginning of the modeled period and allowed to circulate for 28 days. At the end of this period, gridded two-dimensional heatmaps were produced depicting relative particle densities in waters deeper than 5 m (“pelagic”) and on the lake bottom in waters shallower than 5 m (“nearshore”). While particles were neutrally buoyant and experienced no internal vertical forcing which might approximate sinking or floating behaviors of real-world particles, two model behaviors affected vertical transport and sediment grounding: up- and downwelling currents and the vertical component of the random walk. The latter is parameterized in OceanTracker just as for the horizontal direction: as a random walk scaled to the default diffusivity. While OceanTracker default diffusivities assume reasonable magnitudes, their spatial and temporal invariance may not realistically inform the random walk component, potentially contributing to the model artifacts described in the Summary above and Results below.

Resuspension behavior was also captured by this model; near-bed resuspension critical friction velocities (τ_{crit}) were simulated with values of 25, 50, 75, 100, 125, and 150 cm/s. Current velocities

of 150 cm/s have been found to inhibit *Dreissena* veliger settlement (Mackie and Claudi 2009), but that value refers to a bulk water velocity rather than a near-bed friction velocity, which is usually smaller due to water-sediment roughness and turbulence (Wiberg and Sherwood 2008). For this reason, we believe resuspension with respect to *Dreissena* veligers could be underestimated by the model using a 150 cm/s τ_{crit} , but it is unclear which (if any) of the smaller simulated τ_{crit} values may better represent resuspension of veligers. This latter uncertainty motivated the secondary goal of simulating a range of τ_{crit} values in this experiment.

Results

This experiment produced two depictions of particle accumulation in two contrasting environments: pelagic waters of Lake Superior and its nearshore sediment environment. Although produced from the same simulation, they offer distinct insights on the variability of particle accumulation in and around Lake Superior. Heatmaps depicting relative particle concentrations were colored on a linear scale corresponding to two orders of magnitude (standardized among all figures associated with this experiment) to aid comparison of particle accumulation across figures.

Nearshore Accumulation

Nearshore sites were defined as regions with total water column depth less than 5 m, at which only “grounded” particles (which have descended to the lakebed) were counted. A broad spectrum of particle accumulation densities was observed in nearshore environments around Lake Superior, with many locations devoid of particles throughout the year, and other regions accumulating the majority of released particles. In general, enclosed bays (e.g., Nipigon), islands (e.g., Apostles, Caribou), and south and east shorelines received the majority of particles. We expect slower currents inhibited resuspension and combined with prevailing southward and eastward winds to drive particles to these locations. The locations of nearshore particle accumulation sites were relatively invariant over time. Comparison of nearshore accumulation heatmaps produced on 23 September 2023 assuming varying τ_{crit} did not appear to indicate variability in particle accumulation sites nor concentration over the span of τ_{crit} values simulated, so the remainder of this experiment treats the case of $\tau_{crit} = 125$ cm/s, chosen as a midpoint among τ_{crit} values considered in this study while maintaining biological relevance. More detailed exploration of particle resuspension as a factor of settling and accumulation should be a target of further study.

Few differences in nearshore hotspot locations were observed over the year-long span of the simulation, which produced 13 heatmaps, of which 12 are shown (Figures 5–7). Small-scale differences in particle concentrations (as indicated by color) were apparent: the western Keweenaw Peninsula received greater concentrations of particles in June–August than any other period, while the Apostle Islands and nearby Bayfield Peninsula received fewer particles in April and May compared to a steady accumulation in other months. The extent to which this phenomenon represented short-term wind and current events versus seasonal changes in water circulation is unclear and merits more detailed study.

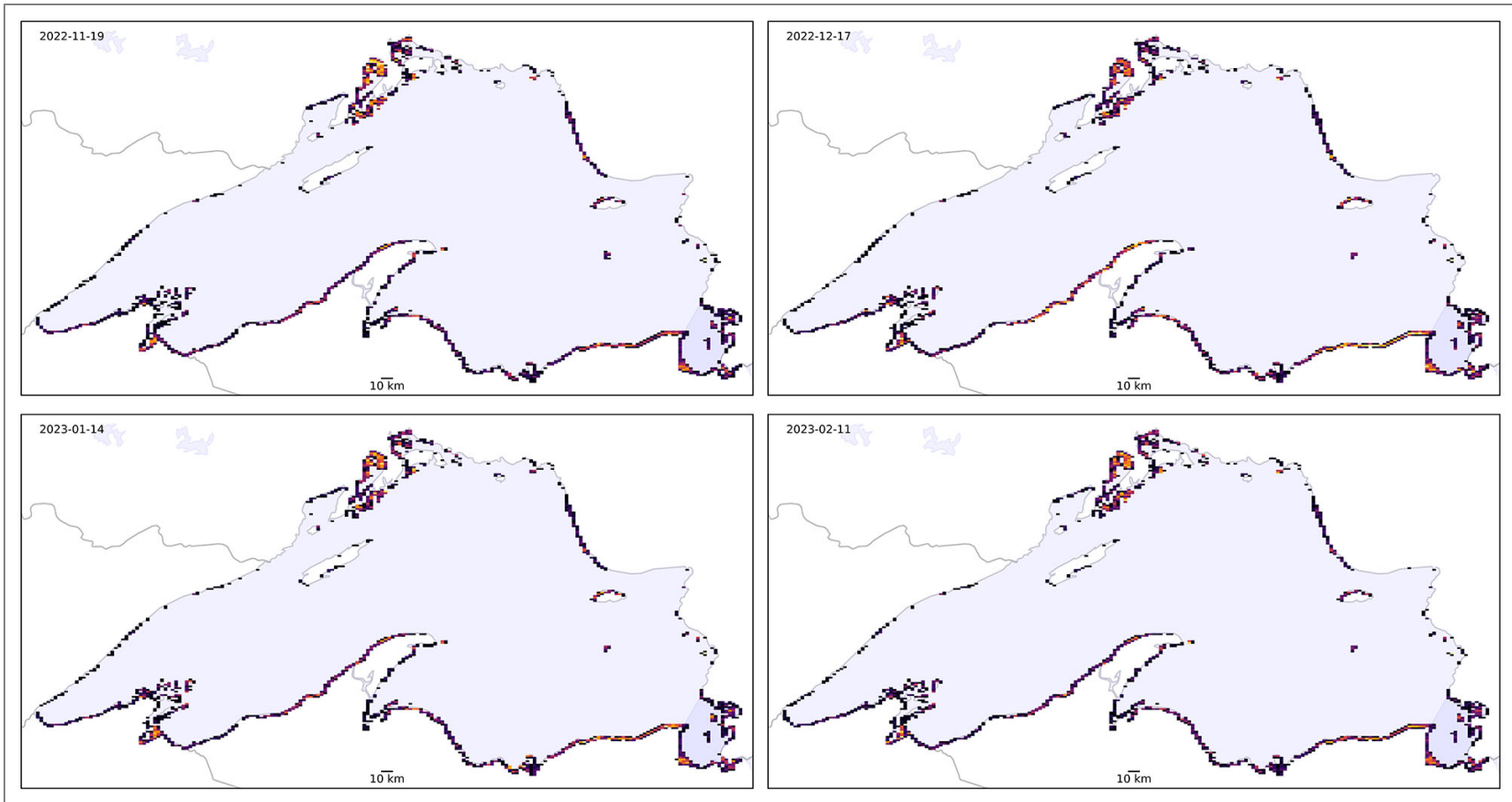


Figure 5. Heatmaps of nearshore particle accumulation at the conclusion of 28-day pulse of particles on the dates indicated, spanning November to February, assuming $T_{crit} = 125$ cm/s.

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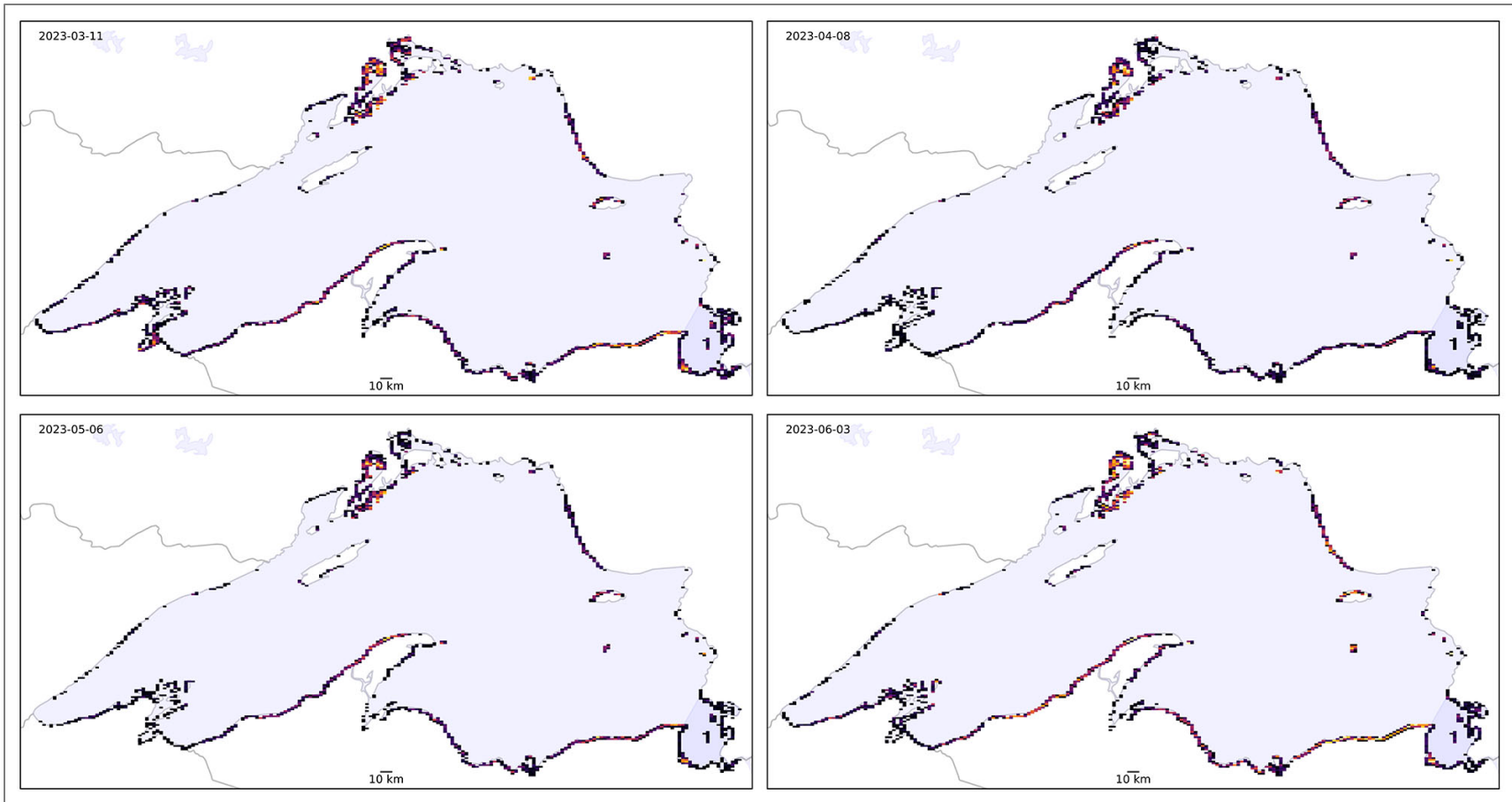


Figure 6. Heatmaps of nearshore particle accumulation at the conclusion of 28-day pulse of particles on the dates indicated, spanning March to June, assuming $T_{crit} = 125$ cm/s.

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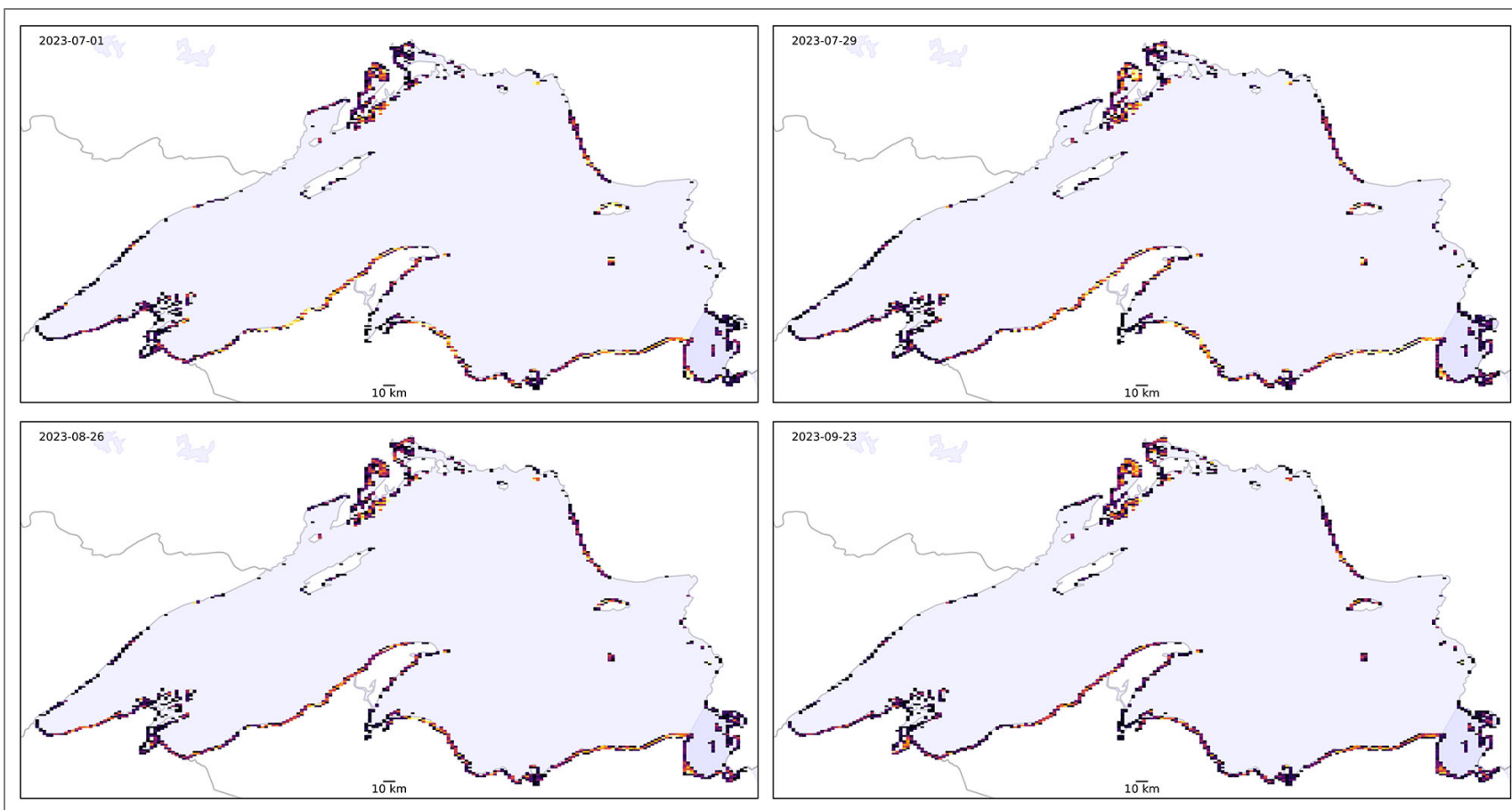


Figure 7. Heatmaps of nearshore particle accumulation at the conclusion of 28-day pulse of particles on the dates indicated, spanning July to September, assuming $T_{crit} = 125$ cm/s.

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Pelagic Accumulation

Heatmaps of particle concentrations were produced for four depth-delimited sections of the water column, over which particles were integrated to provide a three-dimensional concentration: the surface to 50 m (Figures 8–10), 50 m to 100 m (Figures 11–13), 100 m to 150 m (Figures 14–16), and 150 m to 200 m (Figures 17–19). Spatial heterogeneity was observed in particle distributions in all four depth sections, which unexpectedly appeared to correlate with the bathymetry of Lake Superior despite being normalized over the 50 m depth sections represented. While these concentrations could be once again normalized over total water column depth, we elected not to over-interpret what may be a model artifact. We hypothesize that at locations with greater total water column depth, the finite number of vertical layers in the hydrodynamic model (20) are extended, effectively extending the area of greater vertical turbulence associated with the surface mixed layer, resulting in greater vertical particle movement.

Assuming the correlation of pelagic particle density with bathymetry is an artifact of the model, this result hinders analysis of the spatial distribution of pelagic particle hotspots; however, the temporal variability in particle concentrations shown in Figures 8–19 indicates some differences in particle concentrations over time. Comparison of particle concentrations in April with those in January indicates fewer particles in pelagic waters in April, perhaps due to enhanced mixing associated with unstratified waters in January.

Particles released at the surface of Lake Superior mixed throughout the entire water column in every simulated period, regardless of stratification state. This was another unexpected result, as the strength of stratification in Lake Superior was expected to act as a barrier to whole-column mixing of neutrally buoyant particles during stratified periods (generally mid-summer to December and January to March). It is possible that the default constant vertical diffusivity utilized by OceanTracker was unsuited to the spatial and temporal variability of diffusivity in Lake Superior. Despite the previously-noted seasonal differences in onshore and pelagic particle concentrations, the observed seasonal variability in particle transport was less than anticipated.

This analysis of particle accumulation was focused on the lake-wide picture as a first step towards more detailed modeling studies. Focusing on regions of interest in the Laurentian Great Lakes may yield more detailed descriptions of the dynamics of particle transport and accumulation on smaller spatial and temporal scales. The pelagic and nearshore hotspots identified in this work (including the Apostle Islands, Nipigon Bay, Whitefish Bay, the Keweenaw Peninsula, and elsewhere) should be candidates for more detailed analysis interfacing with a wider array of research and management concerns such as pollutant spills, transport of cyanobacterial toxins, or riverine sediment delivery.

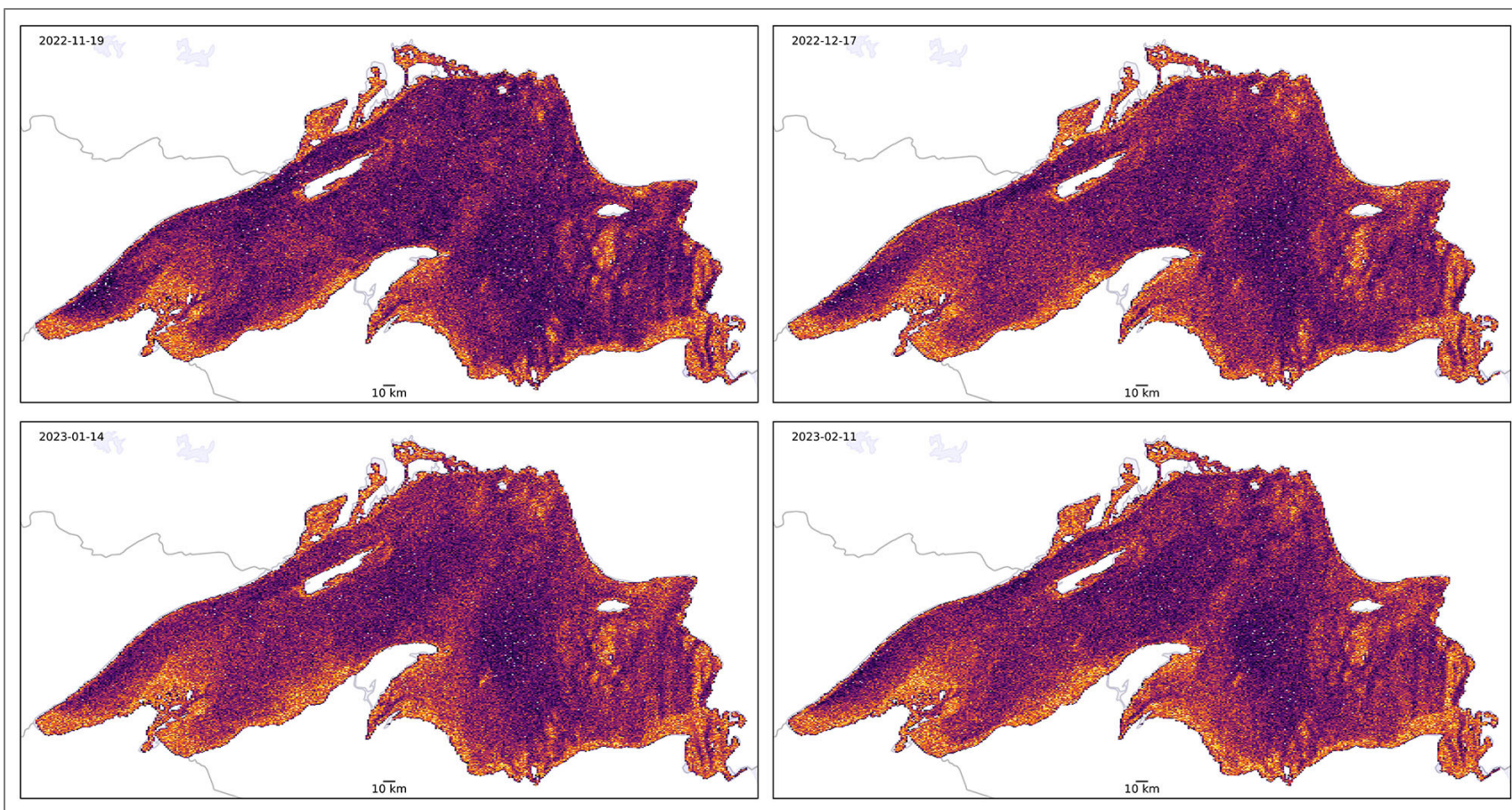


Figure 8. Array of monthly snapshots of particle concentrations integrated over the surface to 50-m depth section on the indicated dates in November to February.

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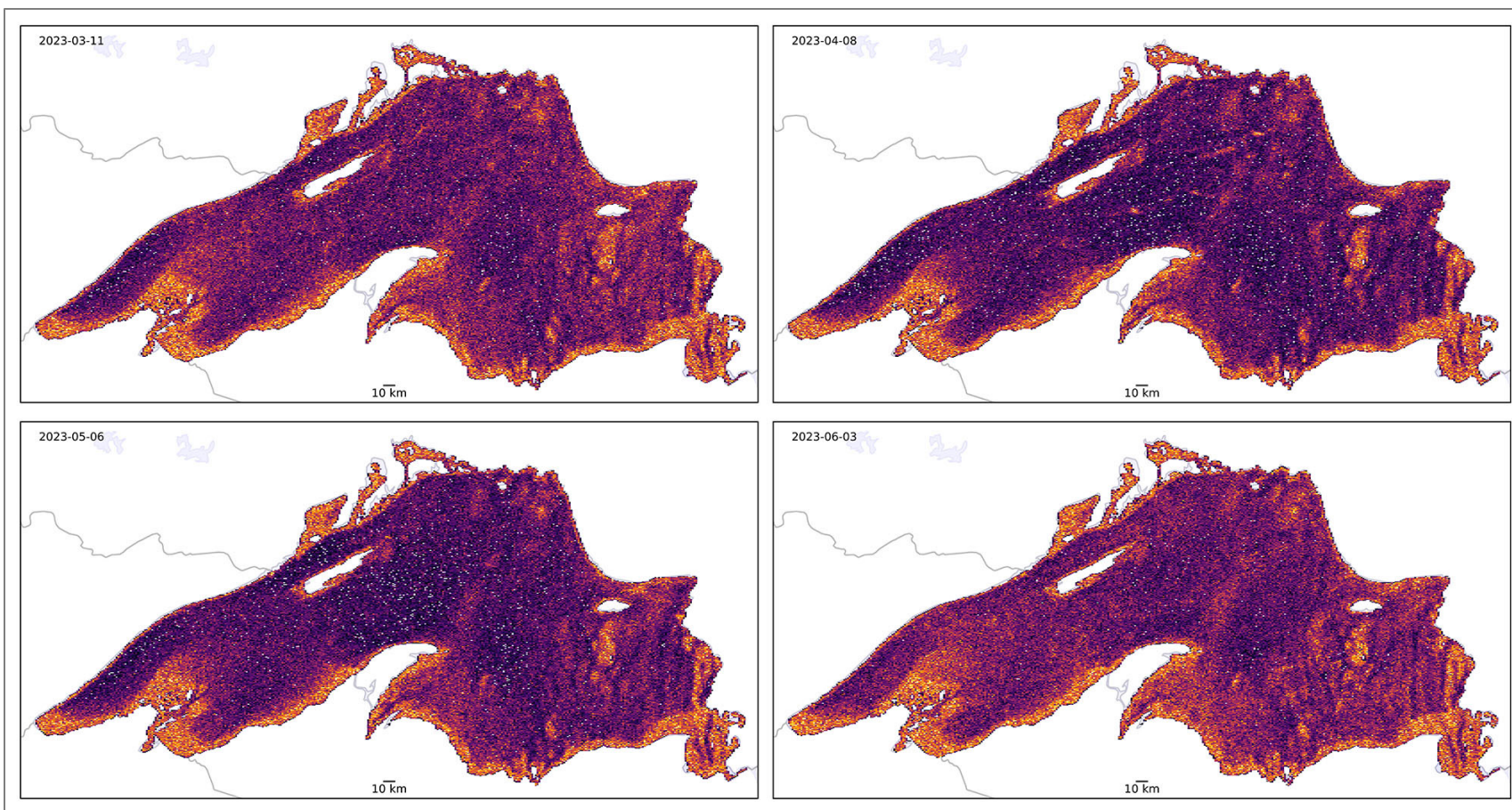


Figure 9. Array of monthly snapshots of particle concentrations integrated over the surface to 50-m depth section on the indicated dates in March to June.

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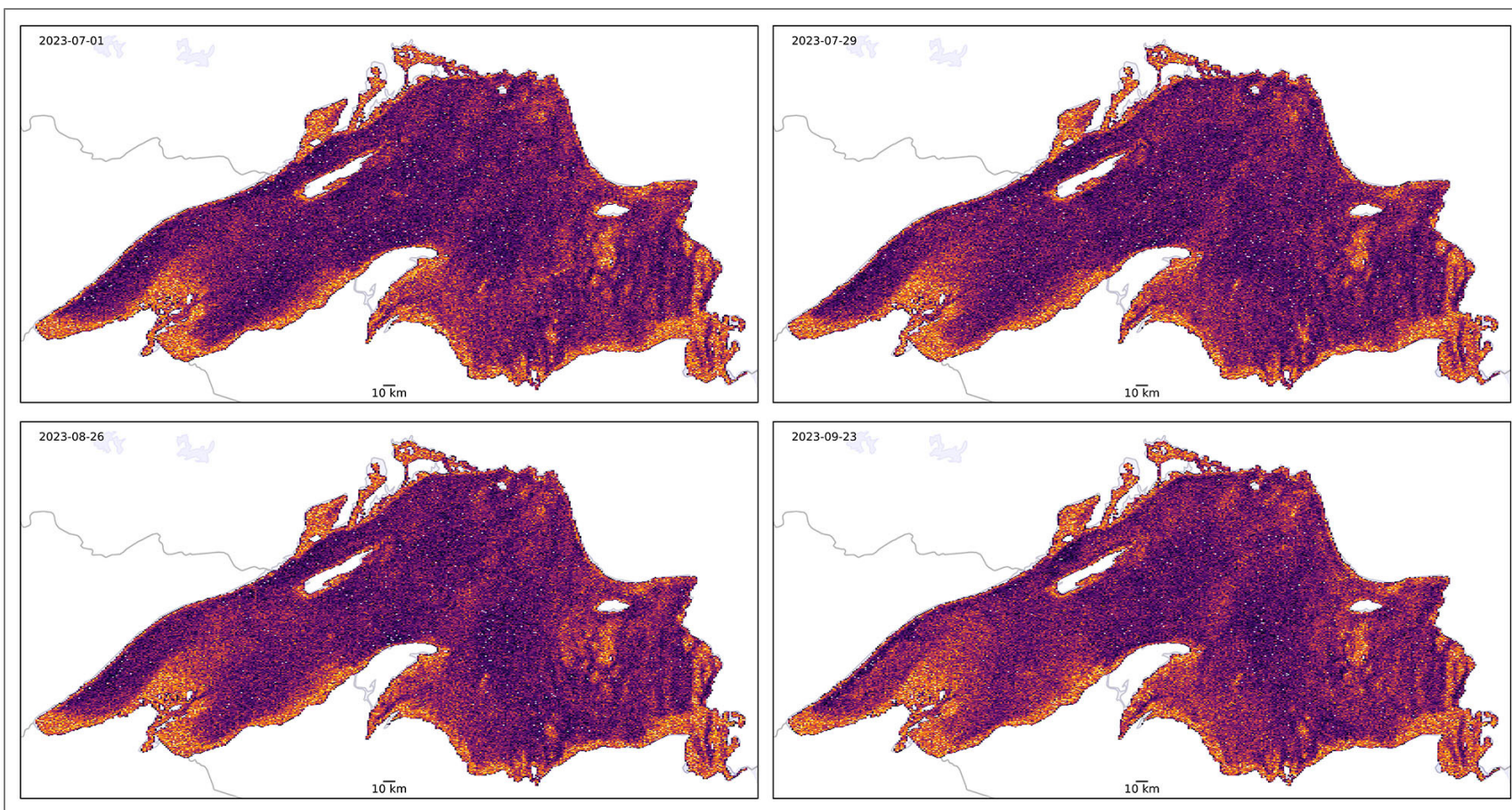


Figure 10. Array of monthly snapshots of particle concentrations integrated over the surface to 50-m depth section on the indicated dates in July to September.

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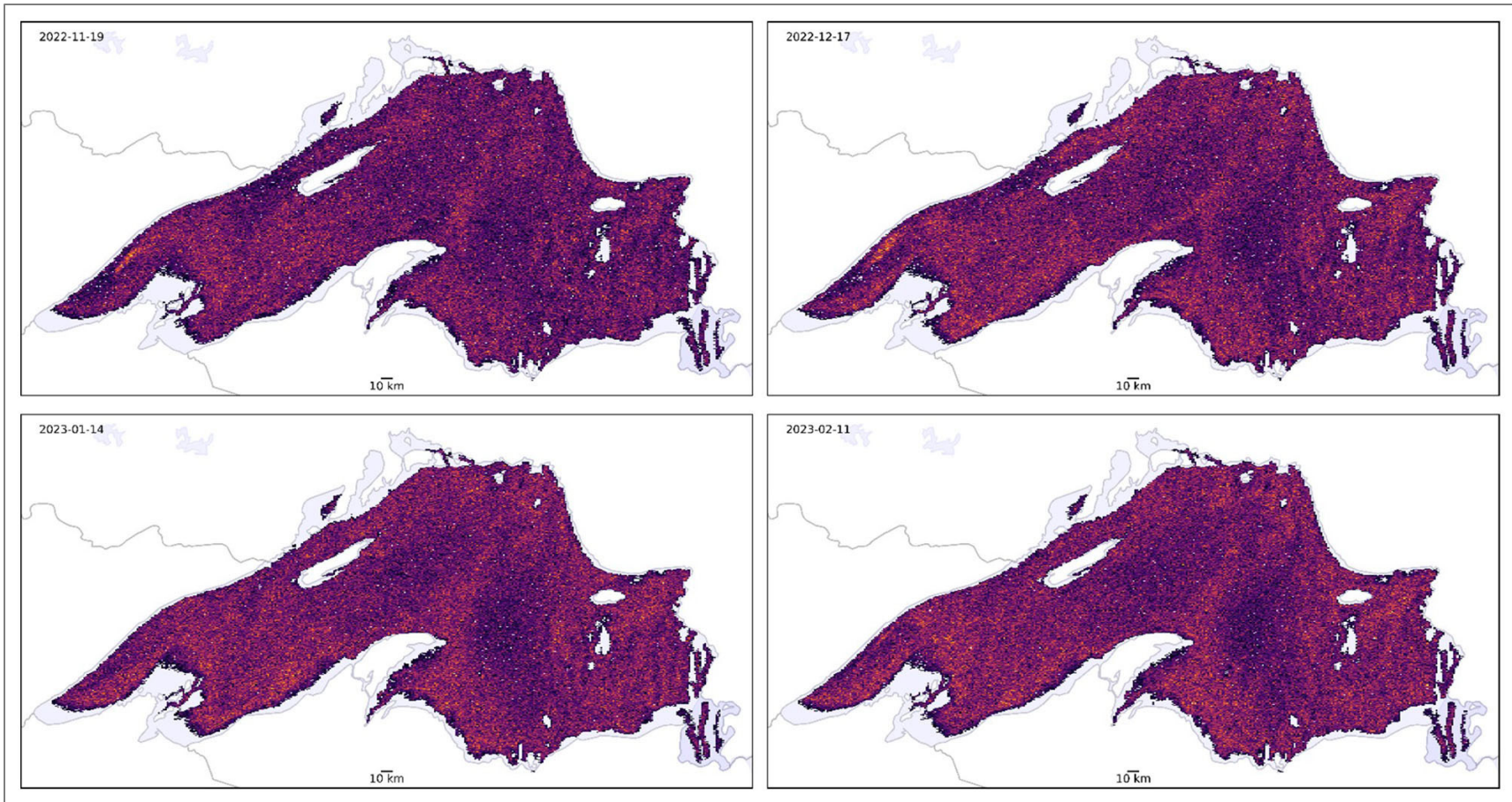


Figure 11. Array of monthly snapshots of particle concentrations integrated over the 50- to 100-m depth section on the indicated dates in November to February.

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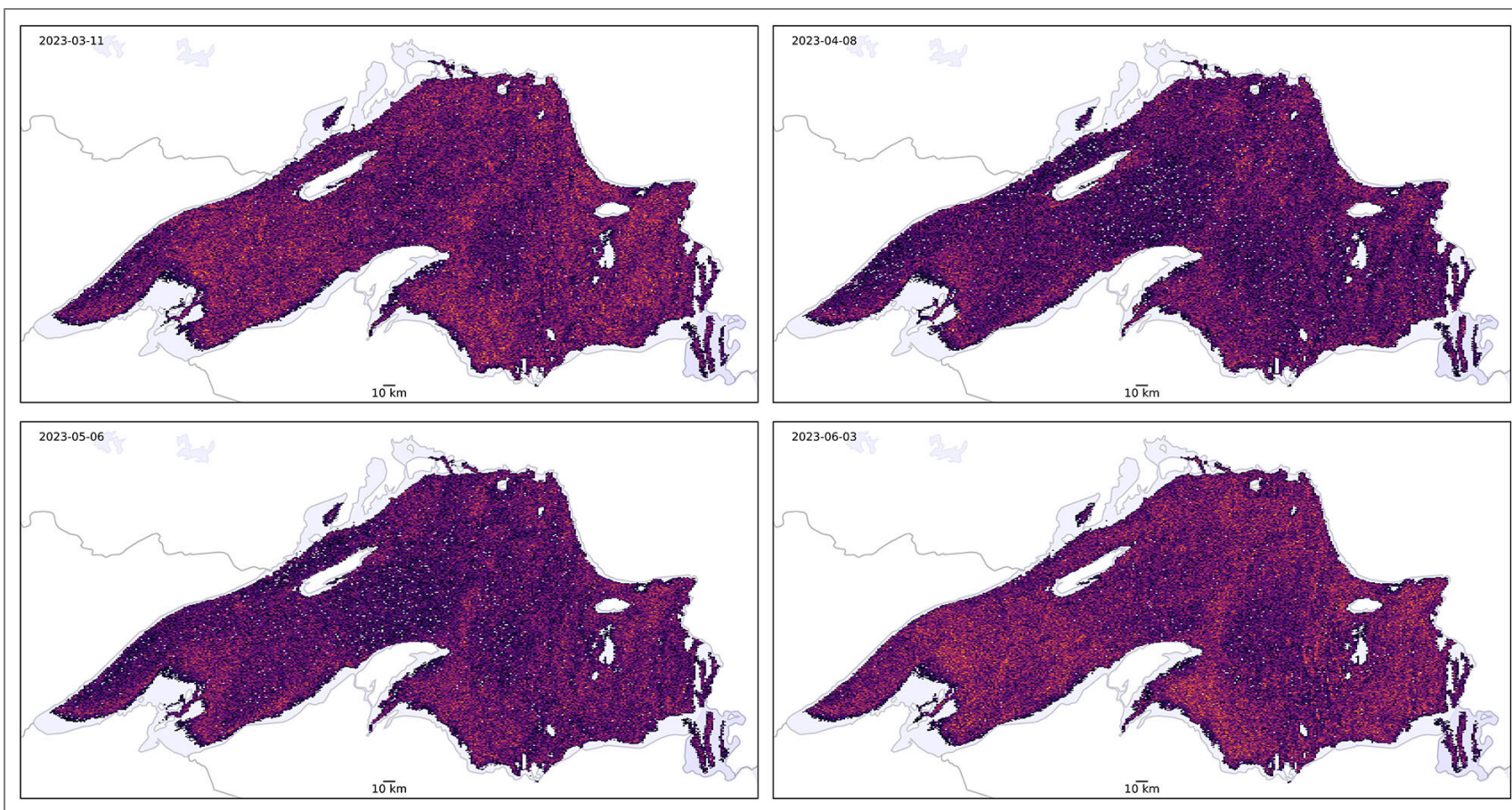


Figure 12. Array of monthly snapshots of particle concentrations integrated over the 50- to 100-m depth section on the indicated dates in March to June.

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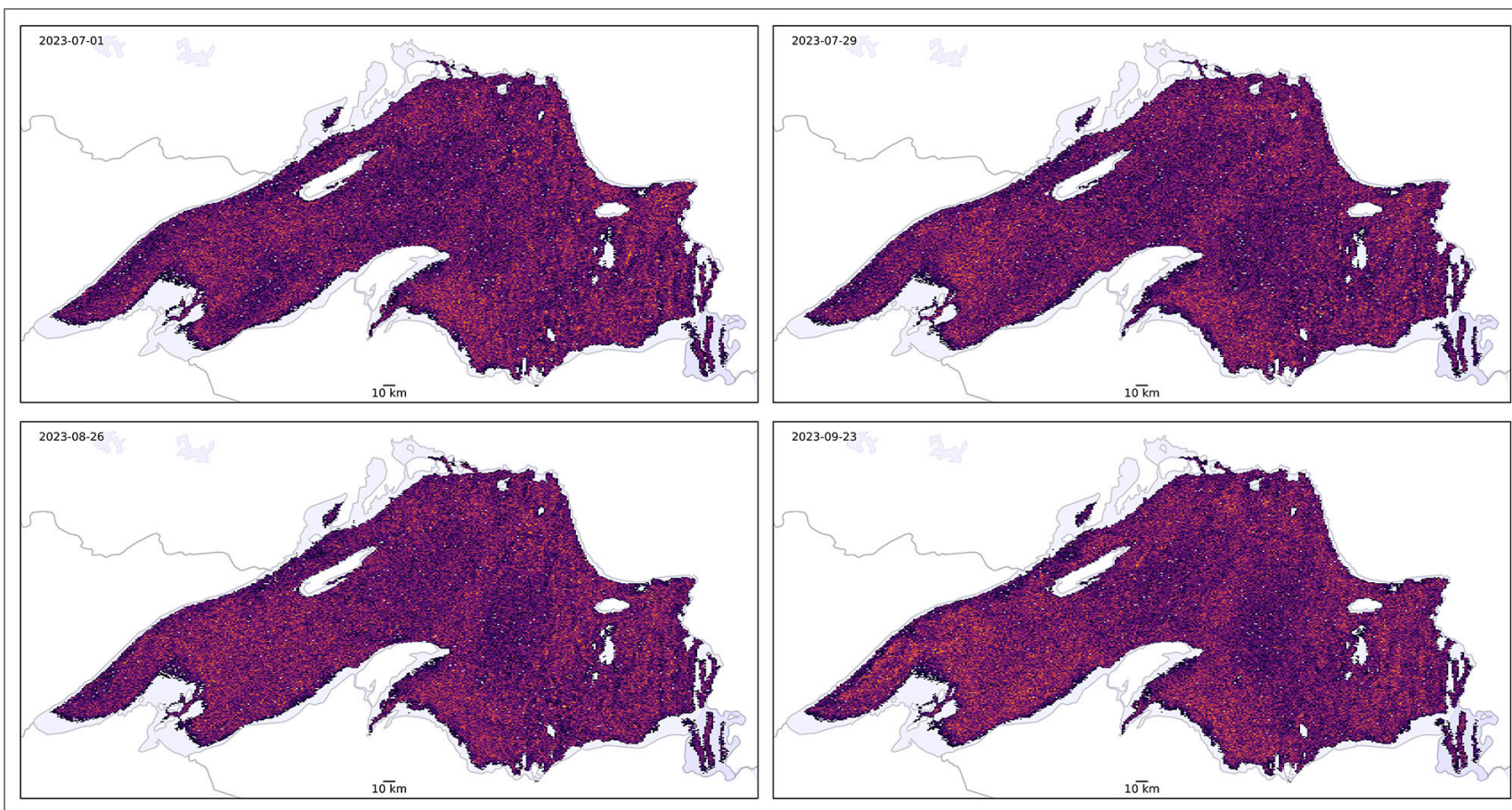


Figure 13. Array of monthly snapshots of particle concentrations integrated over the 50- to 100-m depth section on the indicated dates in July to September.

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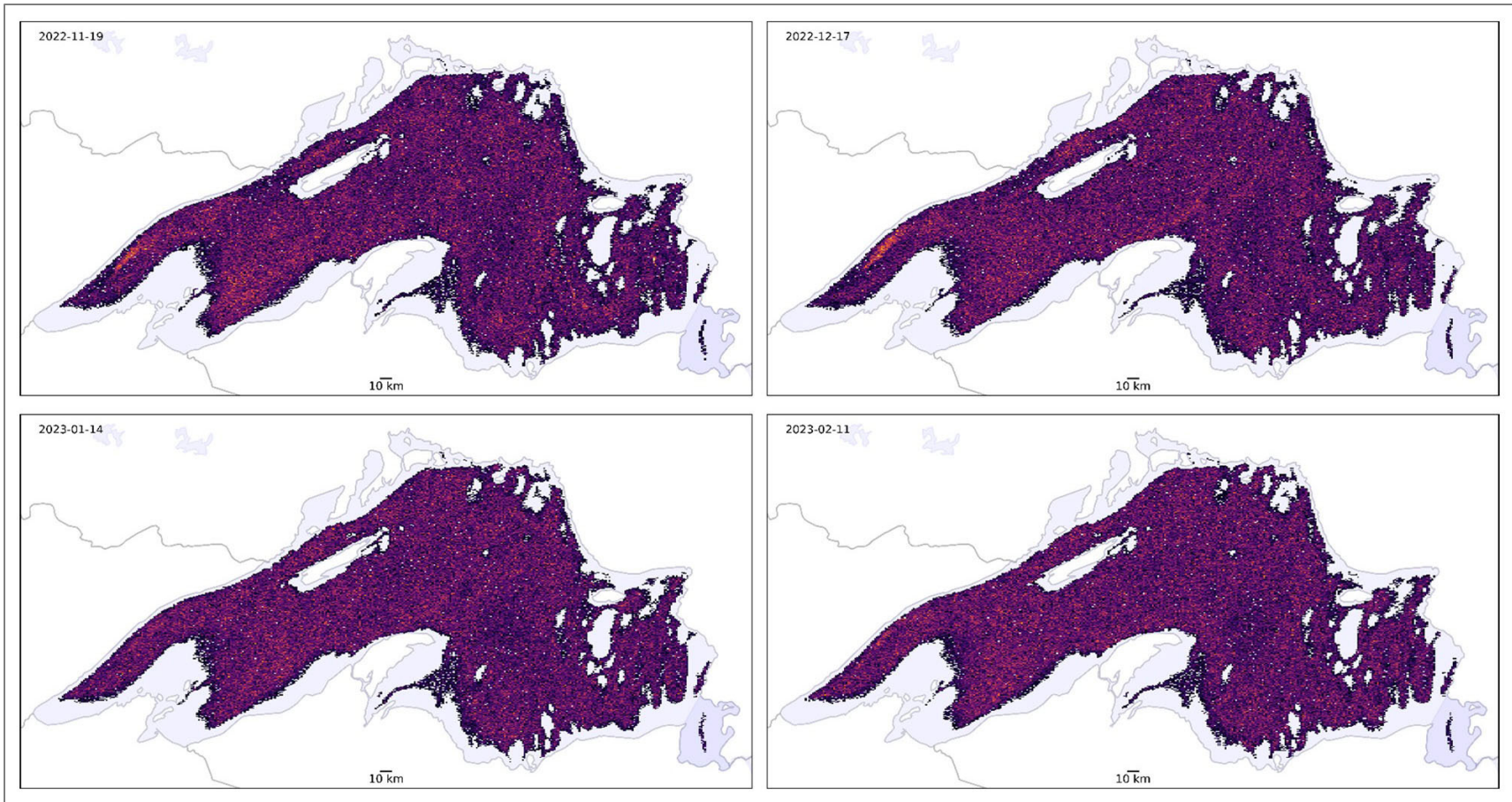


Figure 14. Array of monthly snapshots of particle concentrations integrated over the 100- to 150-m depth section on the indicated dates in November to February.

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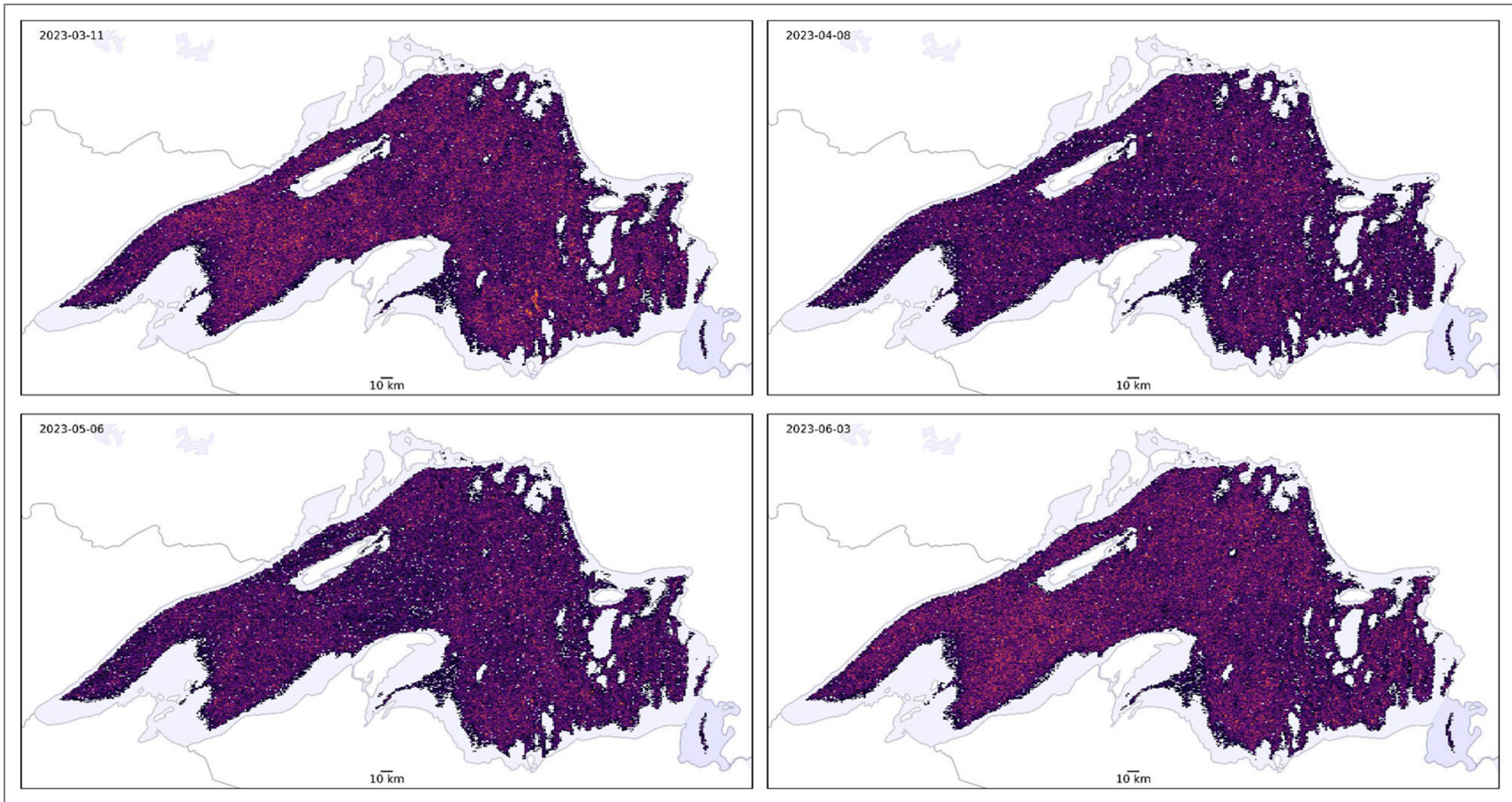


Figure 15. Array of monthly snapshots of particle concentrations integrated over the 100- to 150-m depth section on the indicated dates in March to June.

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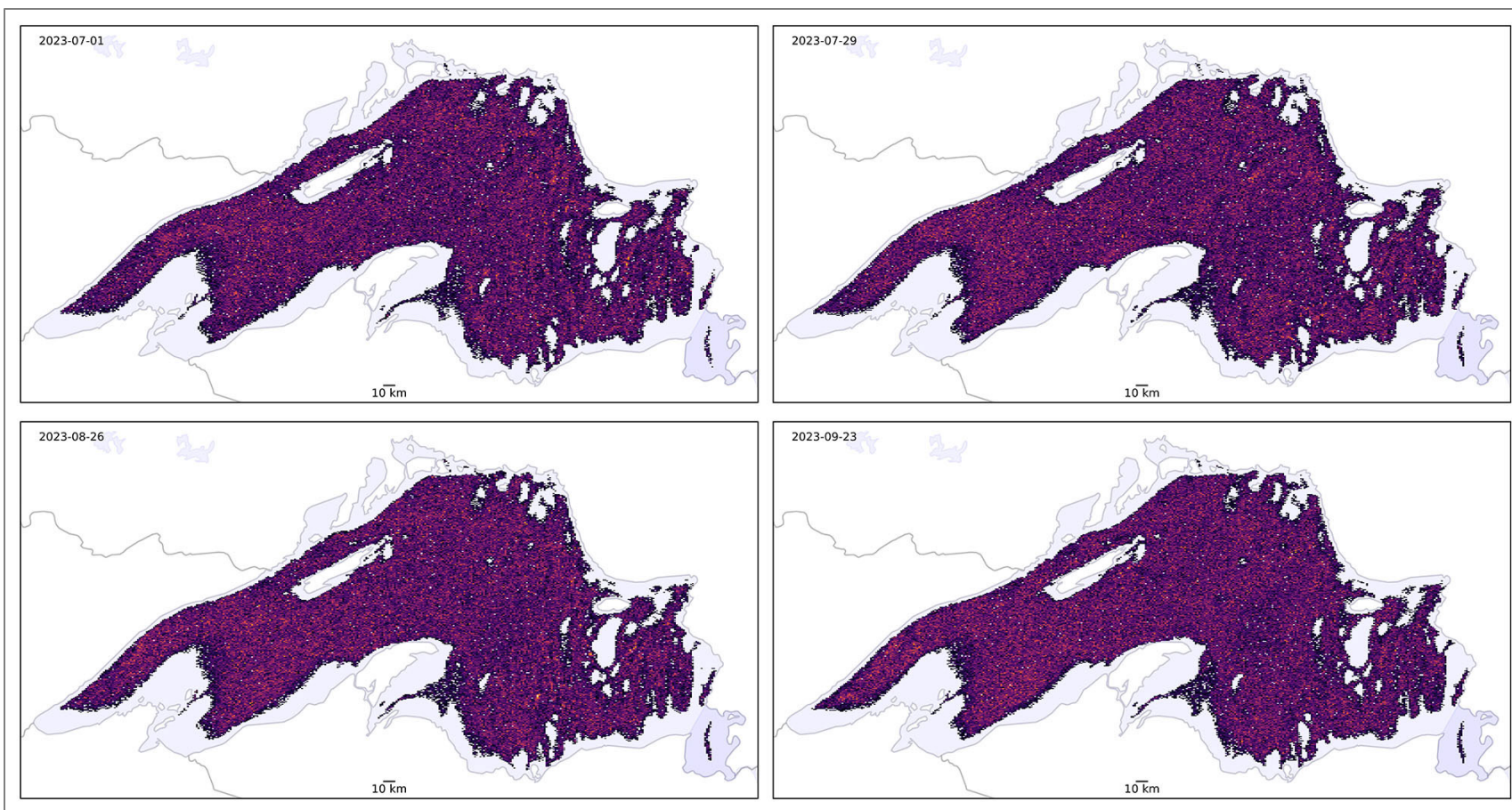


Figure 16. Array of monthly snapshots of particle concentrations integrated over the 100- to 150-m depth section on the indicated dates in July to September.

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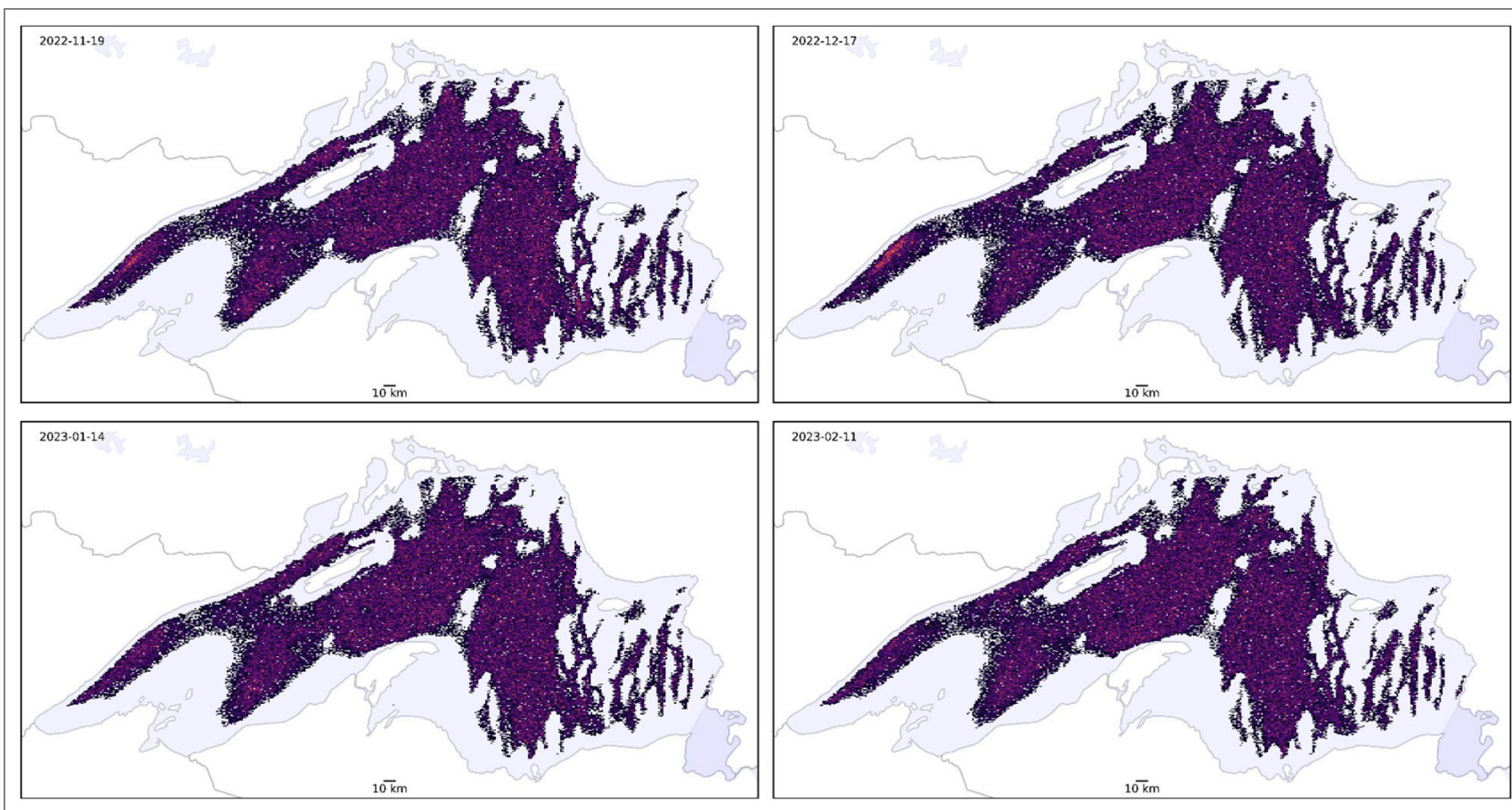


Figure 17. Array of monthly snapshots of particle concentrations integrated over the 150- to 200-m depth section on the indicated dates in November to February.

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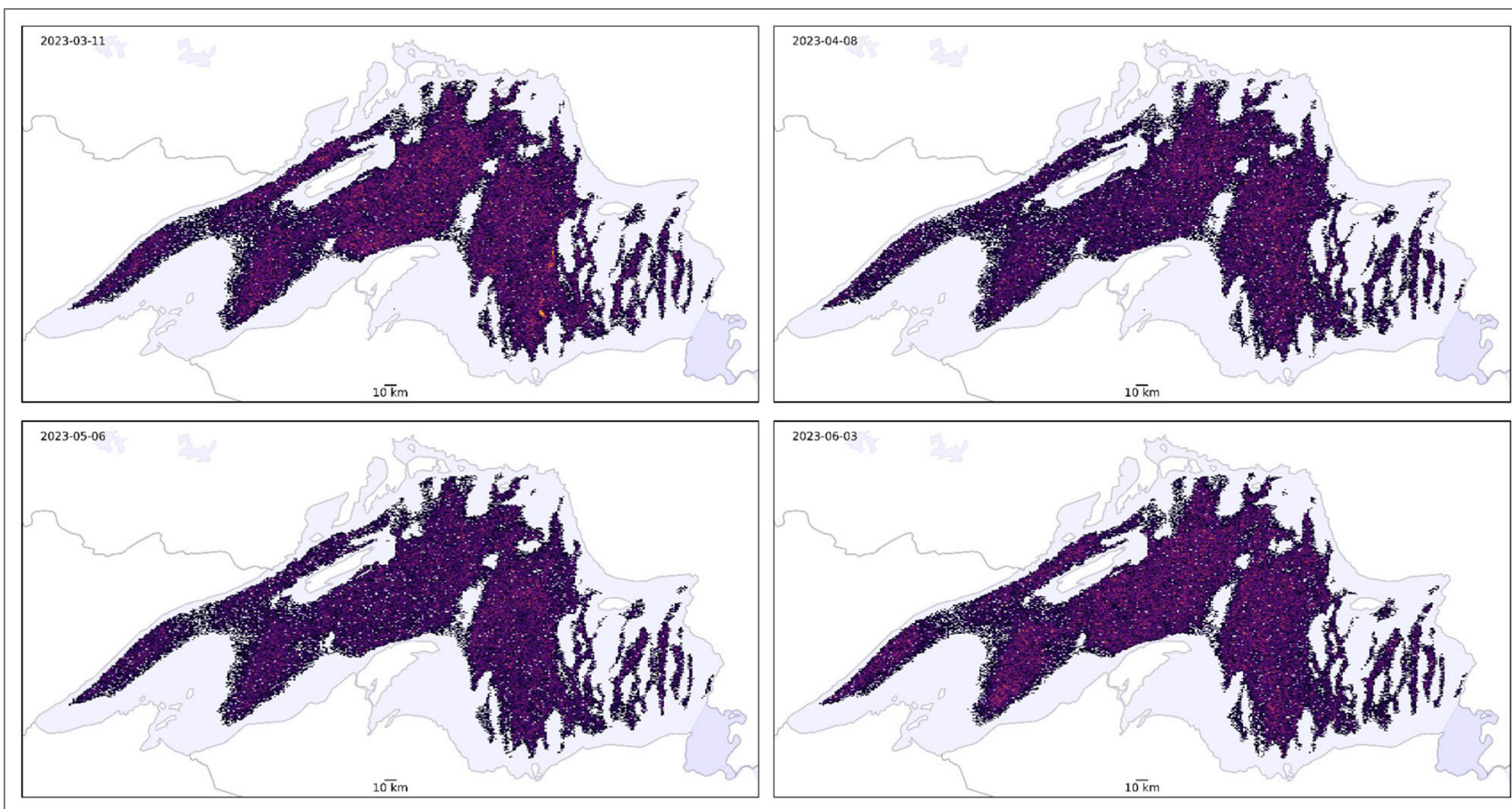


Figure 18. Array of monthly snapshots of particle concentrations integrated over the 150- to 200-m depth section on the indicated dates in March to June 2023.

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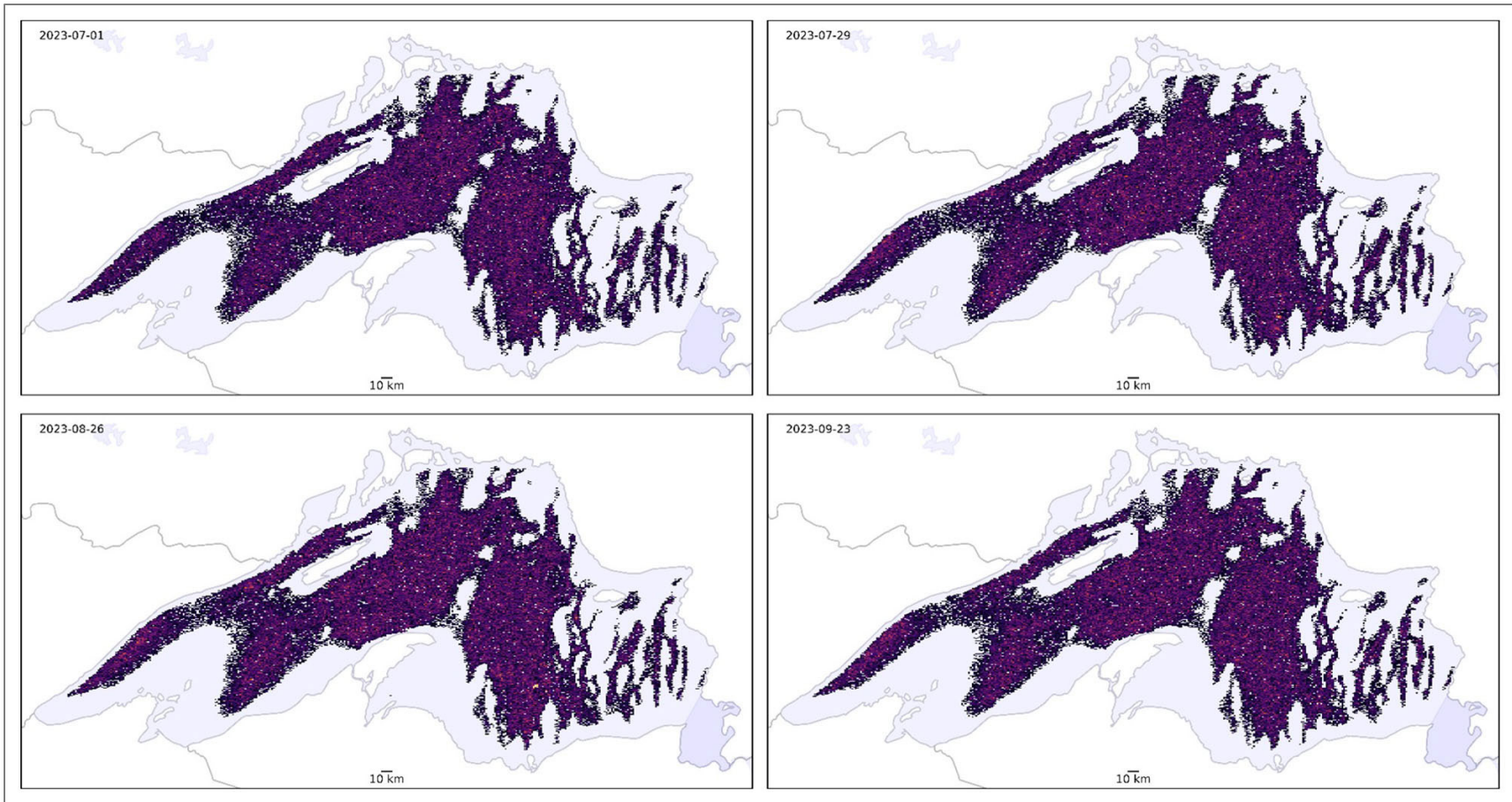


Figure 19. Array of monthly snapshots of particle concentrations integrated over the 150- to 200-m depth section on the indicated dates in July to September 2023.

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These simulations demonstrate a method to identify particle accumulation hotspots and are useful to aid inference of the physical drivers of accumulation. It is important to note that the hotspot locations identified in this analysis may not correspond with actual locations of particle accumulation in Lake Superior, as further ground-truthing of this model is needed to connect model output with observation, especially with respect to vertical particle transport. Transforming this model into a tool for limnological study, management, and regulatory work should be a focus of further research, which might seek to expand the community of practice for particle tracking in the aquatic science community, explore the effect of user-defined particle properties on model outcomes, establish standard procedures for simulations, and compare this model with tools such as the General NOAA Operational Modeling Environment (Song et al. 2024).

Experiment 3: Backtracking Harmful Algal Blooms

Summary

OceanTracker facilitates particle tracking forward through time or in reverse. Particle movement is modeled as the sum of current-driven Lagrangian motion and a three-dimensional random walk representing processes below the hydrodynamic field resolution (e.g., turbulence). This two-part motion makes it difficult to “backtrack” motion of a particle by running the model in reverse, for while Lagrangian advective motion can be solved with time in reverse, random walks cannot. To the extent that the net Lagrangian transport is larger than random diffusive transport, backtracking simulations can still indicate potential particle source locations, or at least general transport patterns.

This particle tracking strategy was applied to explore the drivers of harmful algal bloom (HAB) formation in Lake Superior. The key questions in this experiment were:

1. What hydrodynamic conditions precede HAB reports?
2. What are the sources of water masses that develop HABs?

To explore these questions, we backtracked particles released in bloom and non-bloom conditions at two sites on the south shore of Lake Superior. The morphology of the backtracked particle distribution was used to infer water mass source with mixed results. Advection-dominated transport of a water mass from tributaries with relatively little mixing may be connected with bloom-forming conditions for some sites, but more detailed study of more blooms is necessary to test this connection.

Setup

HABs were observed at two sites along the Wisconsin Lake Superior shoreline: on 7 August 2023 near Mawikwe Bay (N 46.89°, W 91.06°) and on 3 September and 21 September 2023 near Quarry Point (N 46.80°, W 91.41°). These locations were used as destination points where simulated particles were released and backtracked for three weeks. This period was determined by iterative comparison of particle plumes over periods up to one month. Particle plumes backtracked from the south shore of Lake Superior lost cohesion over longer periods due to dispersive transport overwhelming advective transport on the scale of three to four weeks, resulting in diffuse particle sources spread across the western arm of Lake Superior and an implied upper limit for backtracking simulations in this system during the simulated period. A nebulous backtracked result may obscure HAB source water formation mechanisms, which is a limitation of this method that might be addressed by forward modeling. This three-week period also falls within the range of observed lags between tributary input and cyanobacterial blooms observed in previous work (Stern et al. 2020).

Particles were released daily for the period 1 August 2023–30 September 2023 in 61 pulses of 1,024 particles. Their movements were tracked every 1,024 seconds (ca. 17 minutes) before they were removed from the simulation after 21 days. Particles were confined to the upper three meters of the water column (by applying an overriding upward velocity) in the expectation that strongly stratified

summer waters would restrict vertical movement, which is less-well constrained in this model than horizontal movement.

Results

Pulses of identical neutrally buoyant particles deposited at the same location and time experienced a broad array of backtracked sources in Lake Superior. This was likely driven by the competition between advection and turbulent dispersion, which in calmer waters without large currents was expected to favor dispersion.

Sequential heatmaps were created depicting the spatial distribution of source locations for each particle pulse (Figures 20, 21). Particles backtracked from HAB conditions at Quarry Point appeared to exhibit relatively rapid transport from the far western arm of Lake Superior near the St. Louis River estuary, with relatively cohesive particle groups backtracked to that region approximately nine days before HAB events. Non-HAB event simulations generally exhibited dispersed particle pulses, with slow or no arrival of particle pulses near the St. Louis River estuary within the modeled period.

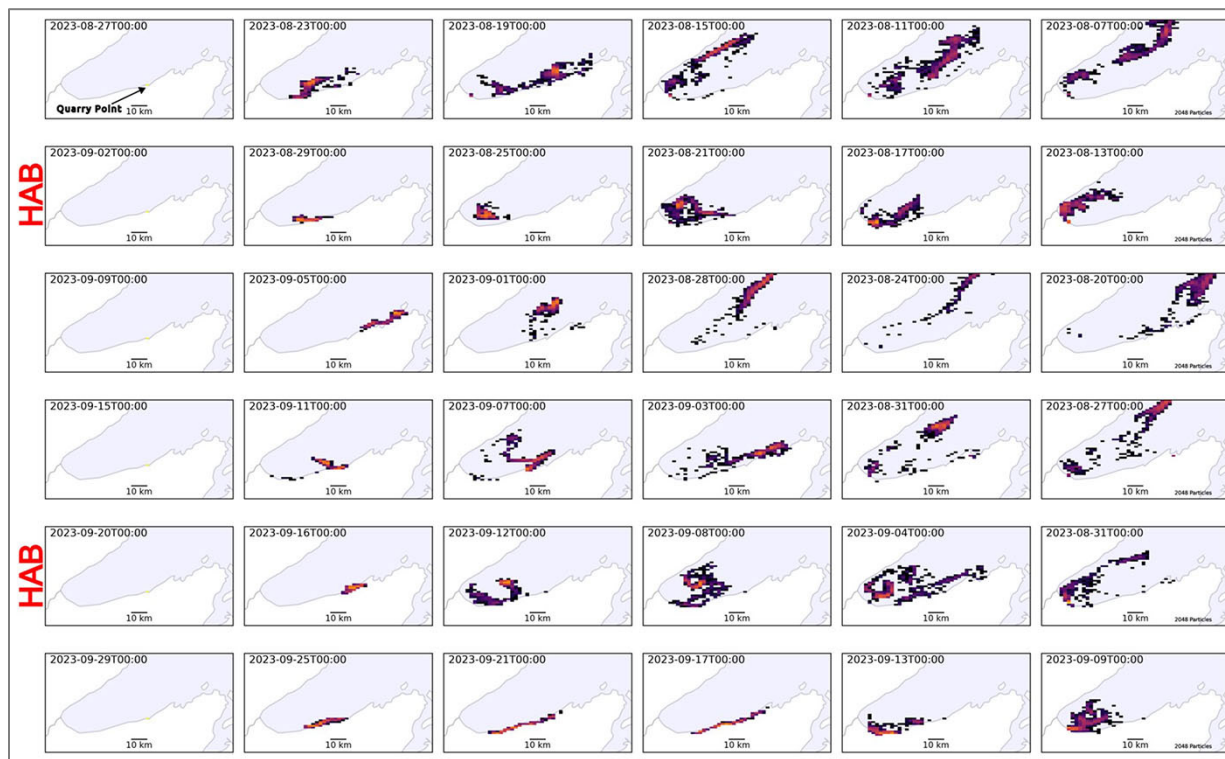


Figure 20. Particles released from Quarry Point, Wisconsin, in September 2023 (release dates shown at top of each map). HABs were observed on 3 September and 21 September 2023 near Quarry Point. A series of heatmaps starting 24 hours after release (left-most column) and continuing every 96 hours from left to right illustrates the paths of particles backtracked for up to 21 days. Particle colors indicate relative particle concentrations on a logarithmic scale. Labels at left indicate HAB status at the release time and location.

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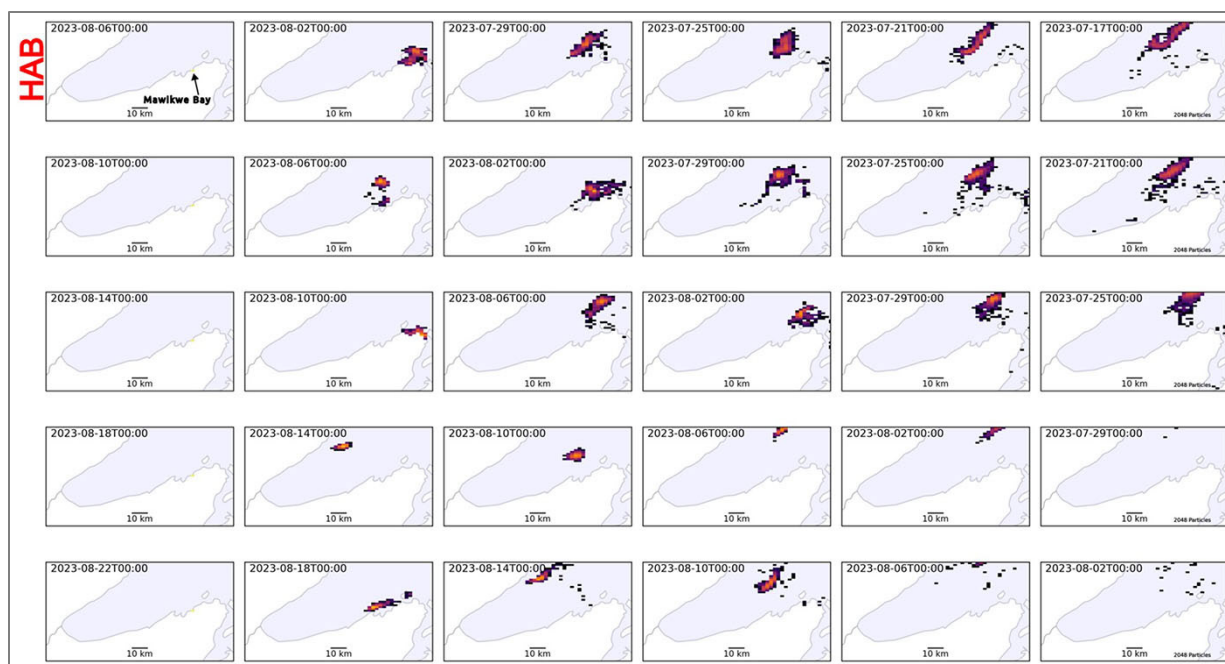


Figure 21. Particles released from Mawikwe Bay, Wisconsin, in August 2023 (release dates shown at top of each map). HABs were observed on 7 August 2023 near Mawikwe Bay. A series of heatmaps starting 24 hours after release (left-most column) and continuing every 96 hours from left to right illustrates the paths of particles backtracked for up to 21 days. Particle colors indicate relative particle concentrations on a logarithmic scale. Labels at left indicate HAB status at the release time and location.

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The results of these backtracking experiments indicated some association between physical transport mechanisms in the open waters of Lake Superior and formation of HABs. Although only a handful of releases in late summer 2023 were simulated, it was clear that particles released at observed HAB sites and times experienced more advective, non-dispersive transport relative to non-HAB conditions. This may imply transport of nutrient-rich water from tributaries such as the St. Louis River to Quarry Point via longshore currents with little mixing, or offshore bloom development followed by concentration at places like Mawikwe Bay. The Quarry Point results are consistent with literature describing the role of tributaries to “seed” HABs (Reinl et al. 2020). The simulations carried out in this research provide a demonstration of a research tool, rather than proof of HAB causal factors. Careful consideration of these and other limitations of this experiment may inform future improvements.

This experiment was limited by relatively few HAB observations with which to compare to non-bloom conditions, as well as by the qualitative nature of this brief illustration. Additionally, lack of a report of a HAB is not proof of absence of a HAB, so some blooms may mistakenly be included in non-bloom simulations. This simulation is also blind to temperature and nutrient conditions, both thought to play major roles in HAB formation (Reinl et al. 2020). Future work should seek to produce quantitative descriptions of particle transport, compare a larger set of locations and HAB

occurrences, and incorporate temperature and nutrient information (e.g., via a coupled hydrodynamic-biogeochemical model).

Discussion and Next Steps

These experiments serve as applied demonstrations of the potential for particle tracking models to aid scientific study of physical and ecological processes in Lake Superior as well as the other Laurentian Great Lakes. Experiment 1 highlighted rapid transport of particles (representing AIS vectors) from tributaries to destinations of interest around Lake Superior, as well as high variability in transport efficiency and speed. Experiment 2 depicted regions of relatively high particle accumulation (termed “hotspots”) in space and time, which were generally clustered on Lake Superior’s south and east shores and within embayments. Experiment 3 illustrated potential water circulation drivers of HAB events by backtracking particles (representing HAB-forming water masses) from the event to an array of sources. These experiments serve as demonstrations of scientific methods, and as starting points for future research.

Future studies can use this particle tracking framework to answer scientific questions, but several concerns must be addressed. First, it remains unclear how well this particle tracking model represents actual particle transport. The hydrologic model output and particle tracking routines driving the model presented here are state-of-the-art and based on the best available knowledge of lake and Lagrangian particle physics; still, ground-truthing should be attempted to qualify the results of future work. This could be accomplished by comparison of particle tracking model output with *in situ* measurements of intentionally-released dyes (Minor et al. 2016) or Lagrangian floats (Manley et al. 2012). This process would aid further model tuning of parameters such as resuspension and buoyancy to support realistic particle tracking. Similarly, efforts should be made to better couple particle tracking software with more modeled diffusivities, ice cover, and buoyancy forcing. These additional drivers introduce further complexity and opportunities for model error or artifacts (cf. Rowe et al. 2016), but are important to consider for scientific and management studies seeking to understand real lacustrine systems.

Second, extension of this model to other Laurentian Great Lakes should be completed to broaden the scope and impacts of this work. The flexible nature of OceanTracker and the readily available FVCOM model output from the Great Lakes Observational Forecast System makes this step trivial in theory but may require terabytes of data storage, access to high-performance computational resources, and refinement of the code produced for this work to ensure robustness. The resources of the Minnesota Supercomputing Institute proved very helpful in these respects. Future research may benefit from partnerships leveraging the computational expertise and resources of similar high-performance computing facilities, which can provide on-demand storage and processing of simulations.

Third, connections between particle tracking model experiments and questions of scientific/regulatory/management importance should be refined. AIS transport was addressed in this work because *Dreissena veligers* can be considered Lagrangian particles, even though several aspects of veliger physics (e.g., buoyancy, settling) are not constrained in this model. A temptation is to treat particle tracking as a tool in search of a problem, but the relationship should be reversed (or at least treated with caution) when considering applications of particle tracking to limnological problems

including AIS vectors, HAB formation, microplastic transport, pollutant plumes, and others. Again, observational and theoretical ground-truthing will be required.

Despite these concerns, we believe particle tracking holds great potential to shed light on the limnology of the Laurentian Great Lakes, with ready application to important questions of ecology and management. Parallel advances in marine and estuarine particle tracking science have proven to be fruitful areas of study, and the comparatively recent availability of this technique in the Laurentian Great Lakes holds similar potential. Notably, multiple management questions at Sleeping Bear Dunes National Lakeshore in Lake Michigan would benefit from particle-tracking applications, including understanding pollutant time of travel from a potential Line 5 (crude oil pipeline) rupture in the Straits of Mackinac (Song et al. 2024), backcasting origins of botulism-affected birds (adding new detail to Kenow et al. 2016), or for predicting transport of sloughed algae (Shen et al. 2022) or fish eggs to areas of management interest.

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