A hardware-accelerated particle filter for the geolocation of

demersal fishes

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${f Abstract}$

Geolocation is increasingly employed to reconstruct the movements of demersal fishes using data retrieved from electronic archival tags. However, geolocation methods commonly suffer from limitations such as low horizontal resolution of locations, flawed land boundary treatment, and extensive computation time. We addressed these issues using a state-space approach based on the particle filter (PF), and developed a geolocation package with graphics processing unit (GPU) acceleration. Our method focused on application to demersal fish and utilizes comparison of the tag-recorded depth and temperature to the same variables from an unstructured grid regional oceanographic model. A rigorous boundary treatment scheme was implemented to handle regions with complex coastline geometry. Validation exercises using stationary mooring tags and double-electronic-tagged (archival and acoustic tags) Atlantic cod in the Gulf of Maine resulted in <10 km median errors of the estimated tracks. Sensitivity analyses suggest that using 200,000 particles was adequate to stabilize the location track estimation. Acceleration of the particle filter using GPUs resulted in faster processing than the single threaded CPU (central processing unit) implementation, enabling rapid geolocations using consumer grade computer hardware. The geolocation output of each tagged fish includes the most probable track and the associated spatial probability distribution. The resulting PF geolocation package enables high resolution and accelerated geolocation analyses to be performed on affordable consumergrade computer hardware, resolving the time intensiveness problem of the PF that may have prevented its adoptions in marine animal geolocation. Expanded application of geolocation will yield more reliable migration information to support management. Geolocation results from archival tagging will contribute to our understanding of the spatial ecology of marine species.

$_{\scriptscriptstyle 40}$ 1 Introduction

Electronic tagging has offered improved fishery-independent insights into behavior and population structure of marine species (Galuardi and Lam, 2014; Hussey et al., 2015). Two commonly employed variants of electronic archival tags are data storage tags (DSTs) and pop-up satellite archival tags (PSATs). These are relatively compact devices that can be attached to a fish and are capable of recording key environmental data such as pressure (i.e., depth), light level, and temperature at precise time intervals, typically seconds to minutes. These data may be used to estimate locations and possible migration paths of the tagged individual through geolocation. The majority of geolocation methods for tracking individual aquatic animals use GPS and light level (Galuardi and Lam, 2014). However, due to attenuation in the water column, these signals are not suitable for geolocation of demersal species that reside at depth on or near the bottom of the water column. For demersal fish, geolocation using tag-recorded depth and temperature data is a more appropriate approach and has been incorporated into several methods, including Metcalfe and Arnold (1997); Hunter et al. (2003); Andersen et al. (2007); Righton and Mills (2008); Pedersen et al. (2008). Many of these prior approaches are based on state-space models that account for uncertainties related to the observations and the estimated quantities (Pedersen et al., 2008; Thygesen et al., 2009; Patterson et al., 2008; Jonsen et al., 2013). The particle filter (PF), also known as sequential importance resampling or sequential Monte Carlo, is a statistical method that is commonly applied to tracking applications in fields such as robotics and image processing (Gustafsson et al., 2002). The PF has also been employed for fish geolocation using archival tagging data (Nielsen, 2004; Royer et al., 2005; Andersen et al., 2007; Brickman and Thorsteinsson, 2008; Coleman, 2015), where the possible geographic location of the fish is modeled by an ensemble of samples, or particles, filtered by the likelihood distributions in an iterative manner. An approach that has been more widely applied to the archival tagging geolocation problem is the hidden Markov model (HMM). HMMs typically require a known, finite number of states, thus the HMM-based geologation methods operate on a horizontal regular rectangular grid. HMM-based geolocation software packages have been developed and made available by several research groups (e.g., Pedersen et al. 2008, 2011a; Liu et al. 2017; Braun et al. 2018). In comparing these two methods, the PF has two key advantages over the HMM-based methods for state-space modeling in the context of the geolocation problem. The first is that the PF is better suited for filtering both nonlinear and non-Gaussian probability density distributions for the horizontal locations. This is particularly advantageous for handling simulations when the fish is in coastal waters near land (Andersen et al., 2007) where Gaussian distributions are not suitable. In the PF, confinement to the domain can be implemented in a straightforward and robust manner. The second advantage of the PF over HMM-based geolocation is that the PF assumes a continuous state space for particle locations, i.e., modeled particle locations are not constrained to a finite set of discrete grid points of an underlying horizontal grid. This avoids the need for any interpolation or discretization of the 2-D spatial distributions onto fixed grids as required by the HMM approach, which may lead to information loss and render geolocation results dependent on the horizontal resolution.

Previous studies identified that a major drawback of the PF is that it can be computationally intensive 77 due to the large number of particles needed for a given simulation (Pedersen et al., 2008; Thygesen et al., 2009; Woillez et al., 2016). This is likely the reason why the PF has been infrequently employed in geolocation studies despite the clear benefits of the approach. Fortunately, the nature of the PF algorithm enables the employment of modern computer hardware acceleration approaches to significantly reduce the computation time. The parallelization of the PF algorithm using multiple CPU cores or graphics processing units (GPU) to reduce runtime has been studied in the context of other applications (Hendeby et al., 2010; Goodrum et al., 2011). A GPU is a computer hardware device that was traditionally used to create images to be rendered on a display. Over the last two decades, software tools and algorithms have been developed to enable GPUs to be used to accelerate general purpose scientific computation (Vuduc and Choi, 2013). GPUs typically contain 100s to 1,000s of processing elements (cores) that can perform simple computations in parallel. Parallelization of the particle filtering problem can be implemented straightforwardly by taking advantage of the independence of the particles. The lack of interaction between particles allows processing elements to handle particles or groups of particles without incurring overhead costs related to exchanging information among particles. In contrast, the HMM geolocation approach is less amenable to straightforward parallelization and is thus less likely to benefit from modern hardware acceleration approaches.

The primary objective of this work was to develop an efficient geolocation method based on the PF for demersal fishes using archival tagging data. The approach builds from previous work on an HMM-based model (HMM Geolocation Toolbox, Liu et al. (2017)) and PF models (Royer et al., 2005; Andersen et al., 2007), and improves on some of the algorithmic deficiencies from these prior efforts. The computational approach is accelerated using GPUs, enabling significant speedup of the geolocation and rapid execution of the model with affordable desktop computing components. The PF geolocation package was developed in Python

with CUDA for the accelerated sections and is available at https://github.com/cliu3/pf_geolocation.

To the best of our knowledge, this work is the first to apply GPU-based parallelization to individual animal tracking applications and to introduce an open-source geolocation code for archival tagging based on the PF.

In the following sections, we describe the specifics of the PF geolocation method and the implementation of hardware acceleration. We then present a skill assessment of the method using fixed location mooring tags and double-electronically-tagged Atlantic cod from the western Gulf of Maine. Finally we demonstrate an application of the approach by presenting geolocations of two cod.

2 Methods

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2.1 The particle filter algorithm

Demersal fish geolocation can be described as a nonlinear filtering problem using the following state-space system (Royer et al., 2005):

$$\mathbf{x}^{(k)} = f(\mathbf{x}^{(k-1)}),$$

$$\mathbf{y}^{(k)} = g(\mathbf{x}^{(k)}) + \mathbf{e}_t.$$
(1)

Here, $\boldsymbol{x}^{(k)}$ is the state variable (geographic horizontal location of the fish) at time $t = k\Delta t$ where Δt is the observation time step; $\boldsymbol{y}^{(k)}$ is the observation (temperature and depth recorded by the archival tag) at the concurrent time; f is a function describing the fish's horizontal movement; g is the observation function; and \boldsymbol{e}_t is the observation error (tag sensor errors). The goal is to estimate the daily location distribution of the tagged fish, i.e., the unknown state series \boldsymbol{x} , which requires estimating a probability distribution series $p(\boldsymbol{x}^{(k)}|\boldsymbol{y}^{(0:k)})$, given the tag-recorded full observation series $\boldsymbol{y}^{(0:k)} = \{\boldsymbol{y}^{(0)}, \boldsymbol{y}^{(1)}, ..., \boldsymbol{y}^{(k)}\}$. This is achieved using Bayesian inference:

$$p(\boldsymbol{x}^{(k)}|\boldsymbol{y}^{(0:k-1)}) = \int p(\boldsymbol{x}^{(k)}|\boldsymbol{x}^{(k-1)})p(\boldsymbol{x}^{(k-1)}|y^{(0:k-1)})d\boldsymbol{x}^{(k-1)},$$

$$p(\boldsymbol{x}^{(k)}|\boldsymbol{y}^{(0:k)}) = \frac{p(\boldsymbol{y}^{(k)}|\boldsymbol{x}^{(k)})p(\boldsymbol{x}^{(k)}|\boldsymbol{y}^{(0:k-1)})}{p(\boldsymbol{y}^{(k)}|\boldsymbol{y}^{(0:k-1)})},$$
(2)

where the initial distribution $p(\mathbf{x}^{(0)}|\mathbf{y}^{(0)})$ is a Gaussian distribution centered at the release location of the tagged fish, with a small standard deviation of <50 m. A PF is an algorithm for estimating a state-space

model in which a set of discrete samples in state space (referred to as particles) and weights indicating the relative importance of the particles are used to approximate the predicted distribution. With respect to the geolocation problem, each particle $x_i^{(k)}$ where i is the particle index represents the possibility of the fish's horizontal location at discrete time k. Each particle has a corresponding weight $(w_i^{(k)})$ which quantifies that possibility. Given sufficiently large particle count, N, the particles collectively approximate the continuous probability distribution of the fish's location.

A likelihood function connects the observations and the corresponding hidden states at each discrete time 127 k. Constructing the likelihood function requires a comparison between the environmental data from archival tagging and a regional environmental database. We used bottom water temperature, bathymetry, and tidal elevation output from the Northeast Coastal Ocean Forecasting System (NECOFS) (Beardsley et al., 2013; NECOFS, 2013), which was developed using the Finite-Volume Community Ocean Model (FVCOM) (Chen et al., 2006; Cowles et al., 2008). FVCOM utilizes unstructured triangular grids which enable variation in the horizontal resolution. In the NECOFS database, the horizontal resolution ranges from 5 km near the open boundary to 500 m along the coast and in the vicinity of persistent tidal mixing fronts. Values of bathymetry 134 and bottom temperature are located at the vertices of the triangles. Previous skill assessment studies 135 compared the NECOFS-estimated bottom temperature with in situ bottom temperature measurements and 136 reported strong agreement (Li et al., 2017; Liu et al., 2017). The likelihood function L(x,t) is derived from 137 a statistical comparison of environmental data from the tag and from the FVCOM database over a tolerance 138 interval following Le Bris et al. (2013); Liu et al. (2017); Zemeckis et al. (2017):

$$L_{dt}(\boldsymbol{x}) = \int_{z-\Delta z}^{z+\Delta z} N\left(z; \mu_z(\boldsymbol{x}), \sigma_z(\boldsymbol{x})\right) dz \times \int_{T-\Delta T}^{T+\Delta T} N\left(T; \mu_T(\boldsymbol{x}), \sigma_T(\boldsymbol{x})\right) dT,$$
(3)

where Δz and ΔT are the tag measurement error for depth and temperature, respectively; z and T are daily bottom depth and the associated temperature determined from the tag data; $N(\mu, \sigma^2)$ is a normal distribution function of mean μ and standard deviation σ , and μ_z and μ_T are NECOFS depth and temperature. The standard deviations of bathymetry $\sigma_z(\boldsymbol{x})$ and temperature $\sigma_T(\boldsymbol{x})$ were determined using the NECOFS depth and temperature values from the neighboring vertices of \boldsymbol{x} on the unstructured grid. Subsequently, likelihood values are assigned a value of zero at locations where the possible tidal range interval estimated from NECOFS does not include the range of tidal signal detected from the tag data (see Liu et al. (2017) for details). The known recapture location was also incorporated in the likelihood function to influence movement towards this location over the last several time steps, by confining the likelihood distribution within a circle of decreasing radius R_t around the reported recapture location, and the radius is informed by the remaining time until recapture, and the typical swimming speed of the species v_m , until the radius equals the reported uncertainty radius r_u associated with the recapture location:

$$R_t = \max(r_u, 0.5v_m(T-t)). \tag{4}$$

The likelihood approach is described in detail in Liu et al. (2017) and was implemented in MATLAB in the
HMM Geolocation toolbox. For the present work, the routines that construct the daily likelihood function
were converted to Python and are incorporated in the PF geolocation package.

There are four main steps in the PF geolocation scheme: release, prediction, update, and resampling (Fig. 1). In the first step, the particles are initiated at the release location of the fish (Fig. 1a). This occurs only at the beginning of the simulation. The remaining three steps are repeated each day of the geolocation and are implemented in this study following the basic PF approach of Royer et al. (2005) and Andersen et al. (2007) and are described in detail below.

The prediction step models the horizontal movement of the fish and represents behavior (see Fig. 1b).

This movement is approximated here by a random walk and was modeled directly for each particle using:

$$\widetilde{\boldsymbol{x}}_{i}^{(k)} = \boldsymbol{x}_{i}^{(k-1)} + \frac{\Delta t}{\delta t} \boldsymbol{R} \sqrt{2D_{m}\delta t}, \tag{5}$$

where i is the particle index, $\Delta t = 24$ h is the time interval between observations, δt is the prediction sub-step, R is drawn from the standard normal distribution (mean = 0; s.d. = 1) representing the process error, and D_m is a diffusion coefficient corresponding to the behavior state m. Approximating fish movement behavior via random walk is common and estimated movement can encompass a range of possible mechanisms and behaviors, both in geolocation applications (e.g., Sibert et al., 2003; Andersen et al., 2007; Nielsen and Sibert, 2007; Pedersen et al., 2008, 2011a; Galuardi and Lam, 2014; Braun et al., 2018) and estimating fish

movements in the context of spatial stock structure (e.g., Sibert et al., 1999; Goethel et al., 2011; Schwarz, 171 2014). We selected a prediction sub-step of $\delta t = 1$ h which prevented particle displacements from exceeding 172 the FVCOM mesh resolution along the coast. The values used for the diffusivity coefficients D_m , are species-173 specific and are tied to discrete behavior states. The behavior state is established based on the detection 174 and duration of a tidal signal in the tag data on a given day following the approach used in our HMM 175 geolocation package (Liu et al., 2017; Zemeckis et al., 2017) based on the premise that a tidal signal is more 176 discernible in low activity fish when they are sedentary on the bottom, and the diffusivity coefficient values 177 were determined considering the typical swimming speed of the species (e.g., Fernö et al., 2011). For Atlantic cod, we allowed the behavior state m to be sedentary (low activity, 13 h tidal signal, $D_m = 1 \text{ km}^2 \text{ day}^{-1}$), intermediate (moderate activity, 5 h tidal signal, $D_m = 5 \text{ km}^2 \text{day}^{-1}$), or migratory (high activity, no tidal signal, $D_m = 10 \text{ km}^2 \text{ day}^{-1}$).

A rigorous boundary treatment was implemented to conserve the number of particles in the simulation by 182 preventing particles from crossing onto land. To determine if a particle moved onto land during a prediction 183 sub-step (δt) , a nearest-neighbor search was performed to find the two FVCOM mesh vertices nearest the 184 new particle location. A particle that is not contained within any of the triangular cells that are connected 185 to these two vertices was considered to have exited the domain and is subsequently reset to its prior position 186 within the domain at the previous prediction sub-step (Fig. 2a). Conversely, a particle that is inside any 187 of the triangular cells that are connected to the two vertices nearest the particle was considered to be in 188 the domain and the new particle location is retained (Fig. 2b). This boundary treatment approximates a 189 reflecting boundary condition, which is appropriate for modeling fish movements (Sibert et al., 1999). In 190 the serial CPU version of the code, the nearest neighbor search is performed using a k-d tree algorithm 191 (Maneewongvatana and Mount, 1999) from the SciPy Python package (Jones et al., 2001). The k-d tree is 192 an efficient search algorithm that is optimized for the CPU. For the present work it is considerably faster 193 than a brute-force nearest neighbor search, providing a factor of 35 speedup in benchmark testing. 194

In the update step, particle weights are first drawn from the likelihood function L(x,t) evaluated at

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particle locations $oldsymbol{x}_i^{(k)}$ and time $t=k\Delta t$:

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$$\widetilde{w}_i^{(k)} = L(\boldsymbol{x}_i^{(k)}, t), \tag{6}$$

The particle likelihood values are computed using data that is stored discretely on the horizontal unstructured grid of the NECOFS database. Execution of eq. (6) requires interpolating $L(\boldsymbol{x},t)$ onto each particle location. For this work we use a routine for bilinear interpolation on triangular grids provided in the Python package Matplotlib (Hunter, 2007). The particle weights are then normalized into the range $0 \le w_i^{(k)} \le 1$

$$w_i^{(k)} = \widetilde{w}_i^{(k)} / \sum_i \widetilde{w}_{(k)}^{(k)}, \tag{7}$$

to give the resulting posterior probability distribution at time t (Fig. 1c).

In the last step of the daily iteration, particles are resampled according to the particle weights $(w_i^{(k)})$, 204 such that particles with low weights are removed and replaced by those with higher weights and particle 205 numbers are reordered in the new set of particles so that they are proportional to their weights (Fig. 1d). 206 The resampling is implemented following the approach of Labbe (2016) and is demonstrated in Fig. 3 for a 207 simple simulation with N = 10 particles. In the first step, a cumulative density function (cdf; blue line) is 208 constructed using the normalized weights $(w_i^{(k)})$. The cdf is then divided into N equal divisions where N is 209 the number of particles and a random offset is used to displace these divisions (Fig. 3, green arrows). The 210 N particles identified by the green arrows in the cdf curve are then selected for resampling. Note that the 211 particle multiplicity may be greater than one. For the cdf and divisions shown in Fig. 3, the selected set 212 of particles is $I = \{0, 0, 1, 3, 4, 4, 6, 8, 8, 9\}$. The particles with multiplicity greater than unity $\{0, 4, 8\}$ are 213 particles with greater weight. The particles with lower weights {2,5,7} will be re-initialized at the locations 214 of particles $\{0,4,8\}$, respectively. The particle position histories are transferred using the indexing array I 215 so that particles initialized to a new location carry the location time series of the particle in that location at time t:

$$\boldsymbol{x}_{i}^{(j)} = \widetilde{\boldsymbol{x}}_{\boldsymbol{I}_{i}}^{(j)} \qquad j = 0...k. \tag{8}$$

To conduct this step we used the systematic resampling function from the package FilterPy (Labbe, 2016) to generate an index array I to the particles that have been chosen for resampling such that the numbers of the indices to the particles before resampling equals these particles' weights:

$$P(I_i = j) = w_j. (9)$$

After the model has been integrated from release to recapture, the estimated most probable track (MPT) is determined. The MPT represents the track of the particle with the highest overall importance score, defined as the product of the weight at the last time step and the sum of the weights from the first to the second to last time steps. The index of the particle associated with the MPT is given by

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$$I_{MPT} = \arg\max_{i} \left(w_i^{(T)} \sum_{k=0}^{T-1} w_i^{(k)} \right)$$
 (10)

where T is the last time step of the filter. In addition to the MPT, daily posterior probability distributions of the fish are reconstructed from the horizontal distribution of particles using non-parametric kernel density estimation. These may also be interpreted as the uncertainty distribution around the most probable track and may be useful in interpreting the results.

A summary of the work flow in the present PF geolocation algorithm is provided in the table below.

- 1. Initialize the particles by placing them at the release location of the tagged fish (Fig. 1a).
- 2. FOR each day the fish is at large, do steps (a)-(c):
 - (a) Predict: move the particles horizontally using a random walk and ensure that particles do not exit the domain (Fig. 1b).
 - (b) Update: weight the particles by interpolating the observation likelihood function to the particles, and normalize the weights (Fig. 1c).
 - (c) Resample: remove particles with lower weight and replace them by those with higher weight (Fig. 1d).
- 3. Construct the overall probability distribution.
- 4. Determine the most probable track (MPT)

$_{34}$ 2.2 GPU parallelization

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The PF geolocation algorithm was first implemented as serial CPU code. To achieve acceleration of the ge-235 olocation computation, the serial CPU code was parallelized by taking advantage of the significant computing 236 capabilities of modern GPUs, specifically those manufactured by NVIDIA. For this we used the PyCUDA 237 package (Klöckner et al., 2012), a Python library that provides access to the NVIDIA CUDA parallel com-238 putation platform (Nickolls et al., 2008). In the CUDA platform, memory spaces on the host (CPU) and 239 the device (GPU) are handled separately, and data must be available in the device memory for the GPU to 240 perform computations. Transfers of data between the host and the device are explicitly programmed and 241 must be carefully planned because they can incur a significant overhead. Functions that are submitted to 242 the GPU for parallel execution are referred to as kernels and are written in CUDA C, a variant of the C programming language. Here we describe the details of the GPU-accelerated version of the PF geolocation, hereby referred to as the GPU code. We refer explicitly to the three primary steps of the PF algorithm: prediction, update,

and resample (Fig. 4). During the initial benchmarking and profiling of the serial CPU code, the nearest

neighbor search was identified to be the most computationally intensive component. Therefore, the GPU implementation focuses primarily on the parallelization of the prediction step. In the GPU code, the x and 249 y arrays representing the horizontal coordinates of the particles are first initiated on the host at the reported 250 release location of the fish. These arrays are then transferred to the global memory on the device. In the 251 prediction step, random numbers required for the random walk are generated on the device using an intrinsic 252 function provided by PyCUDA and the particle positions are updated on the device. To apply the boundary 253 conditions, a brute force nearest neighbor search is used. This required two separate kernels, one to determine 254 the mesh elements surrounding the two mesh vertices nearest to each particle and a second to determine if the particle resides within any of these elements. In the update step, the x and y arrays are transferred from the host to the device. The likelihood distribution L is then interpolated onto the particle positions (x, y) on the host to compute particle weights. These interpolated weights are subsequently transferred to the device. In the resampling step, the index array I is generated on the host. A kernel was written to re-arrange the x and y arrays according to I on the GPU. Arrays x and y are subsequently transferred from the device to the host and stored in an array that is archived to an external data file.

²⁶² 3 Validation and Performance Results

263 3.1 Tag Data and Skill Metrics

Following Liu et al. (2017), two types of tag data were used for assessing the skill of the PF geolocation 264 method. First, bottom-mooring tags which challenge the model to maintain a fixed position over time. A 265 total of 14 Star-ODDI DSTs were moored on the bottom of different known fixed locations in Massachusetts 266 Bay, Ipswich Bay, and Jeffreys Ledge between 2010 and 2015 (Fig. 5). The second set of tag data is derived 267 from double-tagged Atlantic cod. During a study conducted from 2010 to 2012, individual Atlantic cod were 268 tagged with both Star-ODDI milli-L DSTs and Vemco V16P-6H acoustic transmitters in the Spring Cod 269 Conservation Zone (SCCZ; Fig. 5), located in northern Massachusetts Bay in the western Gulf of Maine, USA (See Dean et al. (2014); Zemeckis et al. (2014, 2017) for full tagging methods). Importantly, ten double-271 tagged fish were recaptured and the acoustic transmitters carried by these fish provide an independent set of 272

location estimates accurate to <10 m in the SCCZ and <1 km otherwise, when the tagged fish were detected within the receiving range of acoustic receiver arrays. Since the position of the animal is accurately known at these discrete locations while at-liberty, these data can be directly incorporated in the skill assessment of the geolocation method. Three error metrics were used to evaluate the model skill. The first metric (E1) is the distance between known locations and the location of the nearest modeled particle on the day of detection. The second metric (E2) is the distance between known locations and the position of the fish along the MPT on the day of detection. The third metric (E3) is whether the known location falls within the 95% credible area of the same-day probability distribution, reconstructed from all particles. The 95% credible area is defined such that the sum of the probability within the area is 95% of the total probability.

282 3.2 Sensitivity to the number of particles

A study was carried out to examine the influence of the particle count N on the geologation. Seven sets of 283 geolocation tests were conducted using particle numbers N ranging from 2×10^3 to 400×10^3 . For each N, 284 an ensemble of 30 runs were made with identical parameters. Both the E1 and E2 metrics were computed 285 for each model run and used to evaluate convergence of the solution with N. The mean value of E1 over 286 the ensemble decreases rapidly with increasing particle count to around 200×10^3 particles and then begins 287 to asymptote towards a fixed value with further increases in particle count (Fig. 6a). Statistics for the root 288 mean square (RMS) of the E2 metric were also evaluated. The median value of the RMS of the E2 does not 289 depend on particle count (Fig. 6b). However, the variation of the RMS of the E2 decreases with particle 290 count up to around $N = 200 \times 10^3$ particles and remains fairly static for $N \ge 200 \times 10^3$. This indicates that 291 the geolocation reaches a particle-converged solution at $N \sim 200 \times 10^3$ particles. Results from both the E1 292 and E2 metrics indicate that using $N = 200 \times 10^3$ particles is an optimal choice for both accuracy in particle filtering and computational load. This particle number was thus used in all experiments.

5 3.3 Skill Assessment

A skill assessment based on the E2 metric (error in the MPT) and E3 (whether known locations fall within 95% credible areas) was conducted using tags from 14 mooring and 10 double-tagged cod representing 984

d of data. The MPT estimations of the PF geolocation method for the mooring DST locations had an RMS error of 14.95 km, and the error range was 0.01–27.53 km. The median MPT error for all mooring tags was 9.71 km (Table 1), and 61.9% of the known locations fell within the 95% credible areas of the same-day posterior probability distributions. For the 10 double-tagged cod with high-resolution positions determined by acoustic telemetry detections, the RMS error of the same-day MPT estimation was 18.19 km and the median error was 6.0 km. The error range was 0.29–46.77 km (Table 1). All known locations fell within the 95% credible areas of the same-day posterior probability distributions. These results indicate that the MPT determined using PF geolocation method was able to provide accurate location estimates typically on the horizontal scale of <18 km.

307 3.4 Benchmarking and profiling

Wall clock time for the PF geolocation code executed on serial CPU and GPU was evaluated on a high-308 performance computing cluster. Each node in the cluster was equipped with an Intel Core i7-950 CPU 309 and an NVIDIA GeForce GTX 560 Ti GPU. A range of problem sizes from 12,500 to 200,000 particles 310 was tested on data from a tagged cod with 56 d at liberty. Using the Python profiling module "cProfile". 311 the total runtime was decomposed into fractions spent in the prediction, update, and resampling steps. 312 Profiling demonstrated that the majority of the computational time (>97\% for all serial CPU cases, >52\% 313 for all GPU cases) was spent in the prediction step (Fig. 7a). The relationship between runtime and particle 314 number is approximately linear for both the serial CPU and GPU implementations, and the speedup that 315 the GPU implementation provides over the serial CPU approach increases with increasing particle count 316 N, ranging from a factor of 19.0 to 48.9 (Fig. 7b). Furthermore, in both CPU and GPU implementations, 317 time spent in prediction and resampling steps increases as N increases, whereas the time spent in other 318 parts is nearly constant regardless of particle counts, resulting in decreasing portion of total time (Fig. 7a). Thus, accelerating the prediction step through GPU parallelization effectively reduced overall runtime of PF geolocation.

A performance study of the PF geolocation method was also conducted on a wide range of NVIDIA GPUs.

The set included products from four generations of hardware microarchitectures (Fermi, Kepler, Maxwell,

and Pascal) and both consumer (GeForce) and high-performance computing (Tesla) lines (Table 2) and 324 represents a factor of 10 in the range of theoretical single-precision performance. These tests were conducted 325 using 200,000 particles and tag data from the same Atlantic cod used in the CPU-GPU comparison study. 326 CUDA Toolkit version 9.1 was used to compile kernels for all tests with the exception of those run on the 327 legacy Fermi generation GPUs which are not supported beyond CUDA 8.0. CUDA 9.1 contains optimizations 328 in routines used by the PF package which enable a 10% increase in performance over CUDA 8.0. Throughput, 329 measured as the number of days at liberty that can be geolocated in an hour of compute time using 200,000 330 particles, was used as the performance metric. The throughput on the serial CPU code was 6.4 d/h. The 331 results suggest that performance of the model generally correlates with the theoretical performance of the hardware (GFLOPS) and that throughput is enhanced on the newer architectures with greater memory bandwidth. The greatest performance was achieved on the NVIDIA Volta V100, a powerful GPU aimed at deep learning applications with an approximate price of \$10,000 USD. Such high end hardware, however, is not necessary. The GeForce GTX 1050 is capable of geolocating 483 d of fish movement in under an hour of wall clock time. The 1050 is commonly specified in laptops and entry-level desktops and sells for \sim \$100 337 USD, considerably less than the cost of an archival storage tag. In summary, this study indicates that the GPU enables routine PF geolocations to be performed on affordable consumer-grade computers.

3.5 Geolocation of Atlantic cod in western Gulf of Maine

To demonstrate the capabilities of the PF geolocation package, we applied it to the geolocation of two
Atlantic cod. For each fish, the estimated MPT and daily posterior probability distributions for each day
the fish was at liberty are shown in Figs. 8 and 9. The reconstructed depth and temperature time series
from the MPT are generally in good agreement with the raw tag data (Fig. 10).

Cod #13 was released on 11 May 2010 and recaptured on 21 Nov. 2010. During its 194 d at large, the tidal fitting algorithm identified 151 d as low activity, 32 d as moderate activity, and 11 d as high activity.

The cod migrated southward from the tagging location and remained in the region between Stellwagen Bank and Cape Cod Bay for a prolonged period of time (approximately from day 20 to 120) before heading north to the location of its recapture (Fig. 8). The prolonged period of sedentary behavior was also evident in

the depth time series data recorded by the DST (Fig. 10a). The considerable time spent on Stellwagen
Bank, away from the release and recapture locations represents information that would not be possible to
determine from conventional tagging which can only inform release and recapture locations.

Cod #17 was released on 18 June 2010 and recaptured on 29 Aug. 2010 (72 d at large); 26, 33, and 13 days
were classified as low, moderate, and high activity days, respectively. As the fish migrated northward after
day 30 towards the recapture location, the posterior probability distribution exhibited a bimodal pattern,
suggesting two plausible trajectories: one that extended directly northward and the other that took a more
circuitous route to the east around the southern portion of Jeffreys Ledge (Fig. 9). In an ensemble of model
runs, MPTs along both of these trajectories were observed, although the circuitous route was the dominant
solution. The MPT from the particular model run shown in Fig. 9 follows this circuitous second trajectory.

$_{ ext{\tiny 360}}$ 4 Discussion

The open source PF geolocation package presented in this work was developed with the goal of making geolocation analyses more accessible to fisheries researchers who conduct archival tagging studies on demersal fishes. The kernel of the solver represents an implementation of the basic filter outlined in Andersen et al. (2007) combined with the likelihood function approach developed in our prior geolocation work (Liu et al., 2017). The implementation of a rigorous boundary treatment scheme and GPU parallelization enables this software package to estimate movement in regions with complex coastline geometry and provides rapid solutions using consumer grade computer hardware readily available to researchers.

Results of MPT errors from PF geolocation of both mooring and double-tagging validation tests were similar to those obtained using the HMM geolocation toolbox (Liu et al., 2017): RMS error for mooring tags were 14.95 km with PF and 11.07 km with HMM, while for double-tagged cod errors were 18.19 km with PF and 21.87 km with HMM. The PF geolocation exhibited slightly better overall skill in the geolocations of double-tagged fish, but with shorter runtime. For six out of ten double-tagged fish, the PF geolocation code outperformed the HMM geolocation toolbox in median geolocation error by 0.45–34.8 km. These errors were not found to decrease substantially with further increases in the number of particles in the PF or refinement of the mesh in HMM. This indicates that for this specific combination of species, tag type, and the given

environmental database, we may be at the limit of estimation accuracy that can be provided by state-space methods. The PF geolocation performances are similar to or better than other geolocation efforts. For example, Hunter et al. (2003) and Thorsteinsson et al. (2012) used mooring tags fixed at known locations to validate their tidal-based method and reported average error of 15.7 ± 3.5 km and 18.91 km, respectively. Double-tagging studies of sharks (Teo et al., 2004; Winship et al., 2012) found errors >0.5°(approximately 55 km). A recent HMM-based geolocation study of shark species reported median errors of 66–150 km compared to known locations with accuracy of <10 km (Braun et al., 2018). Precision obtained with this methods is the among highest documented in tracking marine animals.

The GPU implementation of the PF geolocation package achieves up to $75\times$ the speed of the serial CPU implementation on the affordable, consumer-grade NVIDIA GTX 1050, and up to 266× on a highend Tesla V100 GPU. The runtime of PF geolocation of a 210 d track is well under an hour running on a typical consumer grade NVIDIA GPU with minimal specifications. This acceleration factor may be even higher if the suboptimal brute force nearest neighbor search were used in the CPU implementation rather than the optimized k-d tree algorithm. The significant acceleration achieved through GPU parallelization eliminates the requirements for costly specialized hardware. For comparison with the computation time of other geolocation applications on consumer-grade hardware, Pedersen et al. (2011b) reported that the 391 finite-element geolocation method they developed takes on the order of days to estimate a 294 d track on a 392 1.4 GHz laptop and the recently published HMM-based geolocation package HMMoce (Braun et al., 2018) 393 written in R takes nearly a full day to run a 134 d track on a quad-core personal computer. Parts of 394 the current PF geolocation package may be further parallelized, but doing so is not likely to result in any 395 significant improvement in performance. For example, in the current method, the prediction step is the 396 most computationally intensive. Brute-force nearest neighbor search represents an embarrassingly parallel 397 algorithm and the GPU implementation is much faster than the optimized k-d tree on serial CPU. The k-d tree is an optimized algorithm for serial execution that may provide $35 \times$ speedup over serial brute-force, but it is not suitable for parallel execution (Hering, 2013). Implementing this k-d tree on GPU would require a considerable undertaking with no guarantee of performance gain over the brute-force algorithm. As another example, the PF resampling in the current method is not parallelized. While parallelized PF resampling algorithms have been proposed (McAlinn et al., 2016), the benefit to the overall performance would be nominal, because resampling accounts for only <1.2% of the total runtime, and Amdahl's Law (Amdahl, 1967) predicts a maximum speedup of only $S = 1/\left(1 - \frac{1.2}{100}\right) \approx 1.2\%$.

Most approaches to marine animal geolocation do not place emphasis on the boundary treatment. Sim-406 ple boundary schemes, such as masking out values on grid points representing land, may be sufficient for 407 estimating large-scale movements of pelagic animals in which case the influence of land boundaries may 408 be negligible, but these simple schemes cannot adequately handle the estimations of movements of coastal 409 species in regions with complex land boundaries. In the present work, we use the unstructured triangular 410 mesh of NECOFS database which provides significantly better resolution of the coastline compared with structured grid approaches (Chen et al., 2006). This enables us to implement a robust reflection boundary scheme in the PF geolocation package that effectively prevents particles from moving onto or crossing over land and models the fish movements more realistically. As an alternative boundary treatment, particles that move out of the domain can be eliminated. This is equivalent to an absorbing boundary condition 415 which is not appropriate for the land-ocean boundary in modeling marine animal movements (Sibert et al., 416 1999). The PF geolocation package can potentially be adapted to work with other oceanographic databases 417 that provide bathymetry and bottom temperature data for other regions. Since the boundary treatment in 418 the PF geolocation package is dependent on the grid of the FVCOM bottom temperature data, using data 419 from other databases requires re-implementation of the boundary treatment scheme. Bottom temperature 420 data from many of the oceanographic databases are based on popular ocean models such as ROMS or HY-421 COM that use curvilinear grids, which would make the particle-based boundary treatment scheme easier to 422 implement than the triangular grid of FVCOM (e.g., Sumner et al., 2009). 423

The PF geolocation results include the daily posterior probability distributions and the MPT. Due to the stochastic nature of the simulation, two runs with identical parameters will not produce identical results. The particle number sensitivity experiments indicate that using larger particle numbers will decrease the variability of the outcome (MPT), but there is a limit beyond which further increase in the particle count will not provide further convergence of the MPT over an ensemble of runs. As an alternative point estimate metric, maximum a posteriori (MAP) (Saha et al., 2009) may provide less stochastic location track estimates,

but the high computational complexity is likely prohibitive, especially when the particle number is large. In
addition, being a single sample of all the particles, the MPT ensures that the movement model is strictly
followed, making MPT a more plausible track than one estimated by the MAP. It should be noted that, as
the daily posterior distributions are largely consistent across an ensemble of runs using a fixed model setup,
any point estimate metric including the MPT should not be the sole information to be considered when
interpreting and understanding the movements of the tagged individual.

The PF geolocation method uses the random walk to model individual movements, because the random 436 walk and the equivalent Fokker-Planck diffusion model are widely accepted as appropriate for the spatial 437 and temporal scales corresponding to tagging studies of fishes (e.g., Sibert et al., 1999; Andersen et al., 2007; Pedersen et al., 2008; Goethel et al., 2011), and for animal movement modeling using the particle filter (e.g., Andersen et al., 2007; Tremblay et al., 2009; Dowd and Joy, 2011; Rakhimberdiev et al., 2015). The random walk was also the choice of the movement model in many popular geolocation software packages for marine animals (e.g., hmmgeolocation: Pedersen et al. 2008; Wildlife Computers GPE3: based on Pedersen et al. 2011a; TrackIt: Lam et al. 2010; HMMoce: Braun et al. 2018). Alternative movement models, such as Lévy flight, have been shown to have a negligible effect in geolocation applications compared to the random walk (Thygesen and Nielsen, 2009). Furthermore, the random walk model is effectively 445 being used as a prior on possible moves and the estimated movement is being updated by the data very 446 frequently, therefore the performance may be less sensitive to the choice of the movement model. Given the 447 reasonably good performance indicated by the validation results, implementing a different movement model 448 may unnecessarily increase the complexity of the geolocation method. In geolocating the double-tagged cod, 449 the diffusion coefficient was estimated from the measured modal swimming speed of Atlantic cod (0.1–0.4 450 body lengths per second, Fernö et al. 2011). Given that the lengths of the double-tagged cod are in the 451 range of 70–110 cm, the appropriate diffusion coefficient was estimated to be $1 \text{ km}^2 \text{ day}^{-1}$ for the low activity 452 level, considering a small, slow fish (70 cm, 0.05 body lengths per second) and 10 km² day⁻¹ for the high 453 activity level, considering a larger, faster fish (110 cm, 0.1 body lengths per second), using the equation $D = \rho v^2/2$, where v is the swimming speed and $\rho = 6$ h is an assumed decorrelation time (Pedersen, 2007). The PF geolocation results were found to be sensitive to values selected for the diffusion coefficients. We performed the double-tagged cod validation with the increased diffusion coefficient values for low, moderate,
and high activity levels of 5, 25, and 50 km² day⁻¹, and the overall median error increased 23 km. The
PF geolocation method may be further improved to be capable of estimating unknown parameters, such
as the diffusion coefficient, based on a maximum likelihood approach. For example, Andersen et al. (2007)
proposed using Random Walk Metropolis-Hastings combined with the PF to approximate the probability
distributions of the unknown parameters. Parameter estimation for the PF is an active field of research (see
e.g., Kantas et al., 2015), and developing the GPU implementation of the optimal approach is a promising
future direction.

The main contribution of this work is the successful development of a GPU-accelerated open-source geolocation package using archival tagging data that can be executed on affordable computers. The source code
is available on a GitHub repository at https://github.com/cliu3/pf_geolocation, where instructions for
users and an example case that can be executed are also available. Researchers can further adapt the source
code for applications to other species and regions.

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478 Author Contributions

CL designed methodology, developed the PF geolocation package, and performed analyses; DZ collected the cod DST and acoustic telemetry data; CL and GC led the writing of the manuscript. All authors contributed

critically to the drafts and gave final approval for publication.

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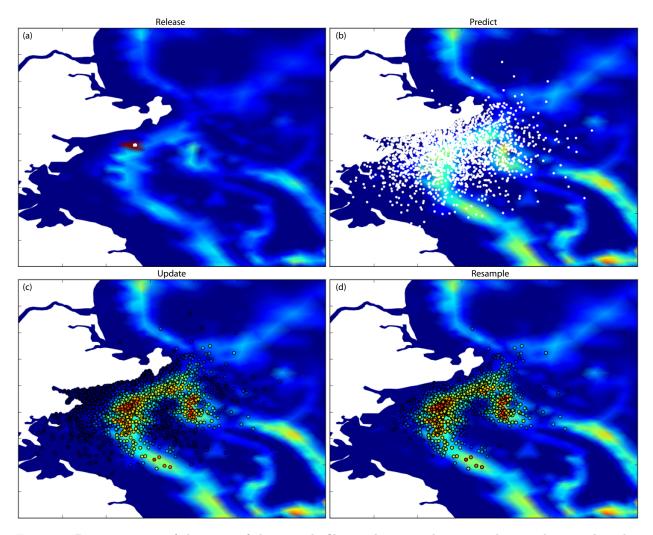


Figure 1: Demonstration of the steps of the particle filter: release, prediction, update, and resample. This is an example of cod in the Gulf of Maine. Color indicates values of the daily likelihood distribution L_{dt} .

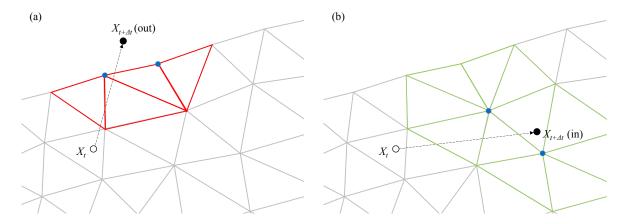


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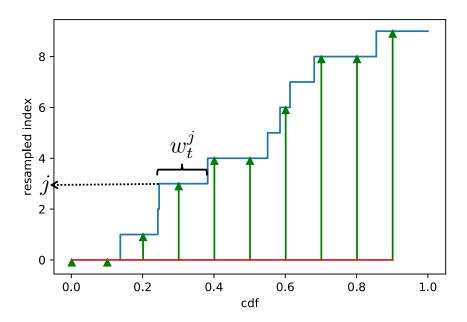


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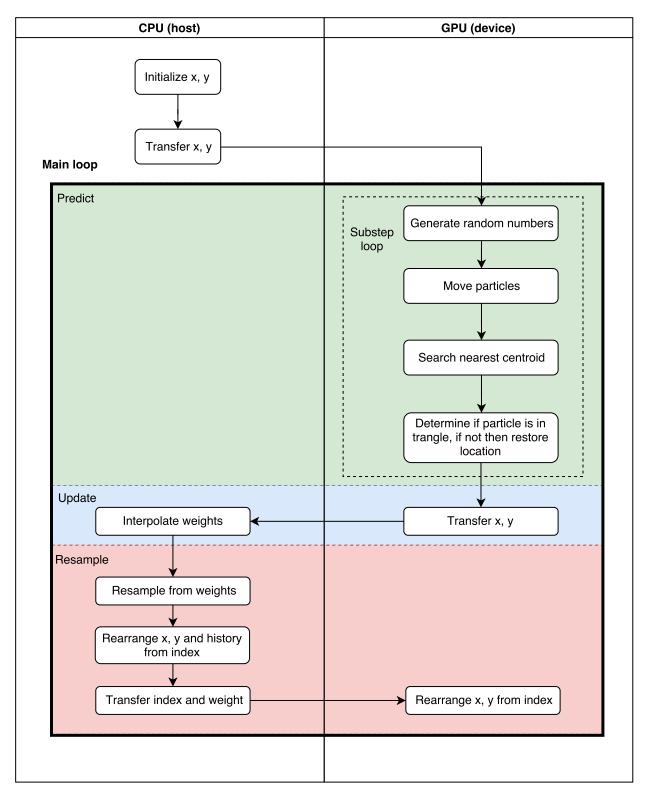


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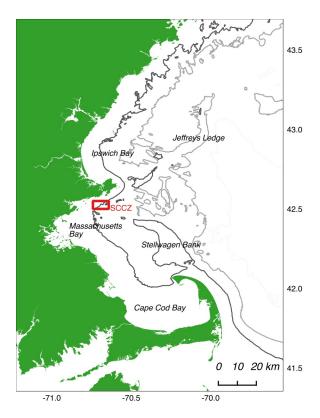


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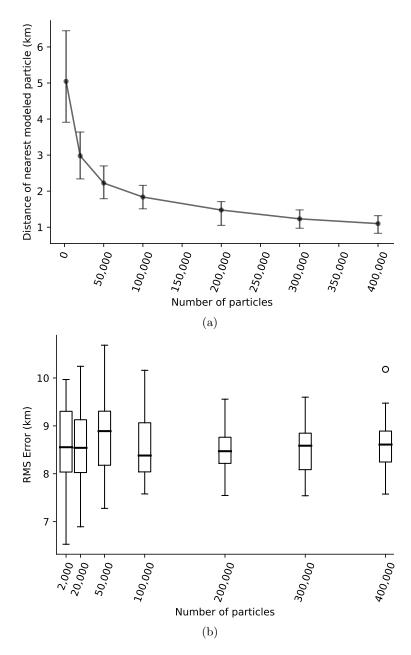


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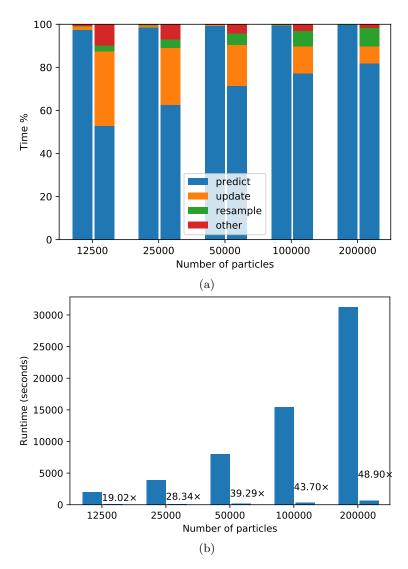


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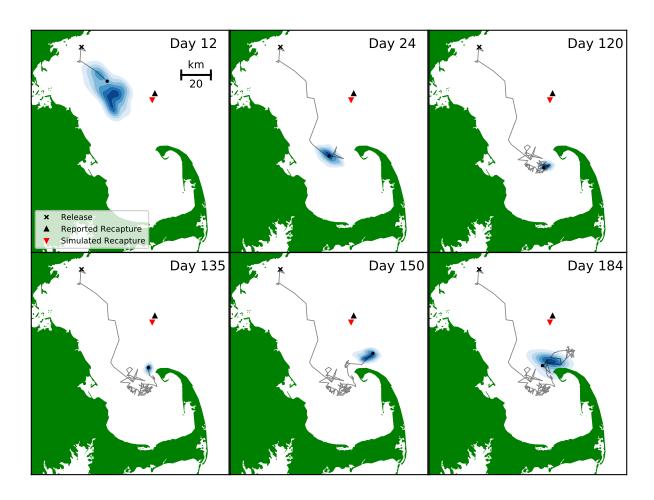


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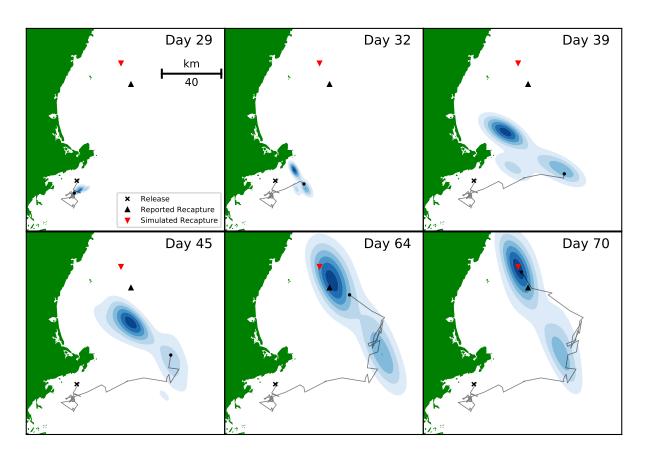


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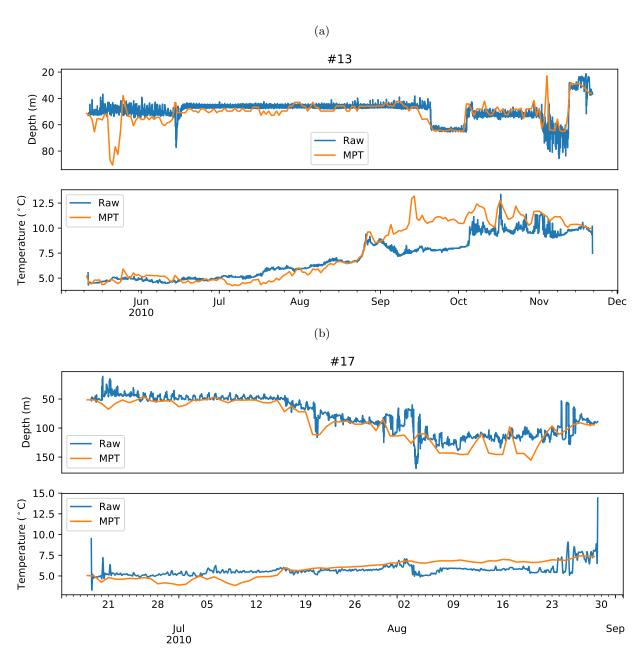


Figure 10: Comparison of the raw depth and temperature time series data recorded by the data storage tags (DSTs; blue line) and the daily depth and temperature data reconstructed from environmental database along the most probable track (MPT; orange line) for (a) cod #13 and (b) #17.

Table 1: Skills of the most probable track (MPT) of the PF geolocation method for mooring and double-tagging

Data Source	Mooring	Double-tagged fish
# tag deployments	14	10
# geolocation days with known locations	762	222
E2 Error range (km)	0.01 - 27.53	0.29 – 46.77
E2 RMS (km)	14.95	18.19
E2 Median (km)	9.71	6.0
$E2 Mean \pm S.D. (km)$	12.03 ± 8.87	$12.47{\pm}13.28$
E3 %days within $95%$ credible area	61.9	100

Table 2: Hardware specifications and PF-Throughput in geolocation-days per wall clock hour (d/h) on ten GPUs.

NVIDIA GPU Model	Architecture Generation	Compute Cores	Base Clock (MHz)	Memory Band- width (GB/s)	Single Precision GFLOPS	PF-Throughput (d/h)
Tesla V100	Volta	5120	1455	900.0	14899.0	1705
Titan X	Pascal	3584	1417	480.0	10157.0	1090
Tesla M60	Maxwell	4096	899	320.0	7365.0	877
Tesla K80	Kepler	4992	560	480.0	5591.0	657
GeForce GTX 1050 Ti	Pascal	768	1290	112.1	1981.4	638
GeForce GTX 1050	Pascal	640	1354	112.0	1733.1	483
Tesla K40c	Kepler	2880	745	288.0	4291.0	413
GeForce GTX 750 Ti	Maxwell	640	1020	86.4	1305.6	391
GeForce GTX 560 Ti	Fermi	384	1645	128.0	1263.4	315
Tesla C2050	Fermi	448	1150	144.0	1030.4	228