

On the performance of four methods for the numerical solution of ecologically realistic size-structured population models

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Abstract

- Size-structured population models (SSPMs) are widely used in ecology to account for intraspecific variation in body size. Three characteristic features of size-structured populations are the dependence of life histories on the entire size distribution, intrinsic population renewal through the birth of new individuals, and the potential accumulation of individuals with similar body sizes due to determinate or stunted growth. Because of these three features, numerical methods that work well for structurally similar transport equations may fail for SSPMs and other transport-dominated models with high ecological realism, and thus their computational performance needs to be critically evaluated.
- Here, we compare the performance of four numerical solution schemes, the fixed-mesh upwind (FMU) method, the moving-mesh upwind (MMU) method, the characteristic method (CM), and the Escalator Boxcar Train (EBT) method, in numerically solving three reference problems that are representative of ecological systems in the animal and plant kingdoms. The MMU method is here applied for the first time to SSPMs, whereas the three other methods have been employed by other authors.
- Our results show that the EBT method performs best, except for one of the three reference problems, in which size-asymmetric competition affects individual growth rates. For that reference problem, the FMU method performs best, closely followed by the MMU method. Surprisingly, the CM method does not perform well for any of the three reference problems.
- We conclude that life-history features should be considered when choosing numerical method.

Keywords: Size-structured population, Escalator Boxcar Train, life history, asymmetric competition, upwind scheme, moving mesh, characteristic curve

1. Introduction

Intraspecific variation in individual physiological states such as body size is a ubiquitous feature of ecological communities. This variation typically arises from individual ontogenetic growth, although it can also arise from other processes such as genetic variation, phenotypic plasticity, or morphological sex differences. As body size changes during individual life cycles, many size-dependent life-history processes such as consumption, growth, reproduction, and mortality, vary accordingly. These in turn affect the environment that the species experience, for example, by depressing resource abundances or aggravating size-dependent mortality. This interplay between individual variation and the experienced environment is often important for the population dynamics and can give rise to emergent phenomena such as alternative stable states and population cycles (de Roos et al., 2003; Persson and de Roos, 2013).

Size-structured population models (SSPMs) account for intraspecific variation by assigning body sizes to individuals and tracking how the number of individuals with a given body size change over time as a consequence of growth, mortality, and reproduction. While it can sometimes suffice to classify individuals into two or more body-size classes (de Roos et al., 2008; Bodin et al., 2012; Meng et al., 2013), these models generally account for continuous changes in individual size and associated vital rates. Although the lack of widely available standardized tools complicates numerical investigations of SSPMs, three principal types of numerical methods are used for this purpose: the upwind finite-difference method, the characteristic method, and the Escalator Boxcar Train (EBT) method. These are either adapted from, or closely related to, numerical methods for partial differential equations, but they differ in incorporating feedback from the population to individual vital rates and to the inflow of newborn individuals.

First, the upwind finite difference method (e.g., Sulsky, 1994; Ackleh and Ito, 1997; Ackleh et al., 2002; Fischer et al., 2006; Krzyzanowski et al., 2006) works by discretizing the distribution of individuals in the state variable, body size, and in time. For each of the resulting mesh points (i.e., the discretized state variables), the finite difference method approximates the density of individuals with the corresponding body size at that particular time. The change in the density from the mesh point at a given time to the mesh point at the next time is determined by approximating the rates of change as finite-difference quotients. These quotients include more mesh points in the direction of individual growth, referred to as the “upwind” direction. We use the name fixed-mesh upwind (FMU) for the most common case of a fixed, unchanging mesh. The FMU method is often very fast, but it can fail at correctly resolving the population dynamics of populations for which the population density vary rapidly with body size. One way to deal with this problem, which has proven successful in computational fluid dynamics, is to redistribute the mesh dynamically according to the gradient of the solution (Huang et al., 1994; Li and Petzold, 1997; Stockie et al., 2001). We adapt this technique for SSPMs and evaluate the performance of the resulting moving-mesh upwind (MMU) method.

Second, the characteristic method, by contrast, tracks the population density along growth trajectories of individuals. Along these trajectories, known in the literature as characteristic curves, the change in the population density can be determined directly from individual growth and mortality rates. A SSPM can thus be approximated by a system of coupled ordinary differential equations, in which the coupling reflects the feedback from the environment (Ito et al., 1991; Sulsky, 1994; Angulo and Lopez-Marcos, 2002; Kostova, 2003; Angulo and López-Marcos, 2004; Angulo et al., 2005a; Angulo and López-Marcos, 2005b, Angulo et al., 2014, 2016, Falster et al., 2016). A key advantage of these methods is that they avoid numerical diffusion, i.e., the artificial difference in the behavior between the simulated system and

the intended system (an illustration of this effect is given in Supplementary Fig. S1, Appendix S1).

Third, the Escalator Boxcar Train (EBT) (de Roos, 1988; de Roos et al., 1992; Brännström et al., 2013), which among the investigated numerical methods is probably the one most commonly used among theoretical biologists, is analogous to particle methods in computational physics (Brännström et al., 2013; Carrillo et al., 2014). The EBT method partitions the population into a number of cohorts (individuals of similar age and size) and tracks the total abundance as well as the mean body size of the individuals contained in each cohort. It thus differs from the characteristic method which tracks the population density of individuals with a given size. The fact that the EBT method allows a natural biological interpretation as the number of individuals in cohorts, along with the desirable property that it avoids numerical diffusion, has most likely contributed to its adoption by theoretical biologists.

In this paper, we evaluate the performance of representative numerical methods of the three aforementioned types as measured by their numerical accuracy and computational efficiency. Specifically, we compare the FMU method, the MMU method, the characteristic method, and the EBT method in order to distinguish their strengths and weaknesses in solving SSPMs. To maximize the chances that our conclusions reflect the needs of practitioners, we use three representative SSPMs as our reference problems and compare the accuracy of the four numerical methods using two geometric measures and four ecological statistics. Although we specifically consider SSPMs, most of the insights from our study should be relevant also for theoretical ecologists who work with transport-dominated ecological models.

Our paper is structured as follows. In Sect. 2, we specify the four numerical methods and introduce the three reference problems that we use for benchmarking. In Sect. 3, we compare the performance of the four numerical methods. Finally, in Sect. 4, we summarize our conclusions and discuss the strengths and weaknesses of the investigated numerical methods.

2. Methods

We start by describing how size-structured population models (SSPMs) are represented in the framework of partial differential equations. We continue with a brief overview of the four numerical methods. A detailed description can be found in Appendix S2-S5. The three reference problems and their associated measures of performance are presented next, with the life-history functions of the three reference problems given in Appendix S6-S8.

2.1 Representation of size-structured population models

Size-structured population models are often formulated with the McKendrick-von Foerster equation (McKendrick, 1926; von Foerster, 1959),

$$\frac{\partial}{\partial t} u(x, t) + \frac{\partial}{\partial x} (g(x, E_t) u(x, t)) = -\mu(x, E_t) u(x, t), \quad (1a)$$

$$u(x_b, t) = \frac{1}{g(x_b, E_t)} \int_{x_b}^{x_m} \beta(x, E_t) u(x, t) dx, \quad (1b)$$

$$u(x, 0) = u_0(x), \quad (1c)$$

in which the size of an individual, x , increases from its size at birth, x_b , to a maximum value, x_m . The individual size x can, for example, represent the body mass or length of animals (e.g., de Roos, 1988; Hartvig et al., 2011), or the height or leaf mass of plants (Falster et al., 2010). The size distribution of individual abundance is denoted by $u(x, t)$; it changes over time depending on the rates of individual growth, $g(x, E_t)$, mortality, $\mu(x, E_t)$, and fecundity, $\beta(x, E_t)$. These size-dependent vital rates determine an individual's life history. $u_0(x)$ is the initial size distribution. Finally, E_t represents the dependence on relevant aspects of the envi-

ronment, such as resource abundance, or light availability and might be represented by a single number, a vector, or a function of size, depending on the environmental dimensionality. Based on these ingredients, Eq. (1) deterministically describes the population dynamics.

In this equation, individuals interact through the environment E_t . The environment affects the vital rates of individuals which, in turn, often depend directly or indirectly on the size distribution $u(x, t)$. In our reference problems, the environment either follows an ordinary differential equation (ODE) (the Daphnia model) or a weighted integral (the fish and vegetation model), and changes dynamically (therefore denoted E_t).

2.2 Numerical methods

Figure 1 gives a schematic overview of the four numerical methods which we use to numerically approximate the solution to Eq. (1). We have implemented the methods in Matlab R2014b and use the Matlab function ODE45 (Runge-Kutta method at 4th and 5th order; Dormand and Prince, 1980) with default error tolerance for the integration of ODEs. We now briefly describe each of the four implemented methods in turn and refer the reader to Appendix S2-S5 for details.

The fixed-mesh upwind (FMU) method and the moving-mesh upwind (MMU) methods both partition the size range (i.e., the interval from x_b to x_m) into a number of non-overlapping size classes. A finite difference scheme is used to update the density of individuals in a size class at the next time step. This finite difference in the state variable is biased in the direction of growth so that only information about abundances in the focal and smaller size class is used. This ensures that a small disturbance to the solution can only propagate in the direction of growth. The term “upwind” stands for the direction from which individuals are growing

into the focal size class. Higher-order versions of the differencing scheme exist which predominantly, but not exclusively, use size classes in the upwind direction. For this paper, we study the most common first-order scheme. The FMU and MMU methods differ in that the former employs a static mesh which we take to be equally spaced (arrows in Fig. 1A) while the latter employs a dynamic mesh which continuously resizes to maintain relatively high resolution in the size distribution with steep changes (arrows in Fig. 1B). In general, any measure of mesh “badness” can be used in the moving-mesh method which then aims to place the mesh points so that each size class has the “same amount” of badness (see Huang and Russel, 2011, and Appendix S3).

We have adapted the characteristic method (CM) from Angulo and López-Marcos (2004). As their constraints on the smoothness of the life-history functions are generally not satisfied by our reference problems, the convergence of the method is not guaranteed. The characteristic method solves Eq. (1a) along characteristic curves (arrows in Fig. 1C) on which the underlying partial differential equation reduces to an ordinary differential equation (ODE). Each characteristic curve, which corresponds to a growth trajectory of an individual, has two associated ODEs that track the characteristic curve (red curves with arrowheads in Fig.1C) and the population density (solid circles in Fig.1C). The ODEs are coupled through the environmental variable (E_t) and the system is integrated for a time interval Δt , at the end of which a new characteristic curve (orange circle in Fig.1C) is introduced to accommodate newborn individuals of size at birth. The initial population density of the new characteristic curve is determined by the boundary condition (1b). As new characteristic curves are introduced at fixed time intervals, the number of characteristic curves increases linearly over time. We maintain a constant number of characteristic curves by removing the interior characteristic curve with the least distance to the closest to its two neighbors (Appendix S4).

The Escalator Boxcar Train (EBT) method was designed by de Roos (1988) for solving physiologically structured population models and it is widely used in theoretical biology, possibly since the numerical scheme admits a simple biological interpretation. In contrast to the CM method, the EBT method divides the population into a number of cohorts and tracks the average size of individuals in the cohorts (red curves with arrowheads in Fig. 1D) and their abundance (boxes in Fig. 1D) through a system of ODEs. Since the EBT method tracks the number of individuals in a cohort rather than the density of individuals with a certain size, it can work well when individual growth ceases at a certain size, which usually causes sharp peaks in the size distribution when a large fraction of all individuals in the population have very similar size. A boundary cohort (orange boxes in Fig. 1D) with slightly different dynamics accounts for offspring of mature individuals (Appendix S5). The boundary cohort is internalized at regular time intervals and, if the internal cohorts exceed the maximal number allowed, the cohort with the lowest abundance is deleted.

Since the EBT method does not approximate the density distribution *per se*, we track the boundaries of each cohort through an additional system of ODEs so that the size distribution can be obtained and compared to other methods, but we exclude the computational time for calculating the cohort boundaries when we compare the EBT method to other methods in terms of the measures given in Subsection 2.4, Eq. (2).

The environment E_t in Eq. (1) has to be approximated in order to evaluate individual vital rates of growth, mortality, and reproduction. For two of our reference problems (fish and vegetation models), this requires integrating the size distribution weighted with a size-dependent factor that scales the influence of individuals with this size. These integrals appear in the life-history functions as specified in Table S4 and S5 in Appendix S7 and S8, and are calculated

from the computed size distribution (green curves in Fig. 1) in the FMU, MMU, and CM method. In the EBT method, they are instead calculated as a sum over cohorts (de Roos et al., 1992).

2.3 Reference problems

We investigate how well the four numerical methods approximate the solution to three representative SSPMs covering both the animal and plant kingdoms:

- A *Daphnia* model of a size-structured consumer feeding on unstructured dynamic resource algae (de Roos, 1990). Individuals cease to grow at a certain size due to competition for food, resulting in a singularity in the size distribution of individual abundance. The life-history functions are given in Appendix S6.
- A fish-population model in which all life-history functions are density-dependent. This model is adapted from the size-structured food-web framework of Hartvig et al. (2011). Predation is size dependent, with larger individuals preying upon smaller. We consider a single size-structured fish population feeding on a dynamic resource. Individuals slow down their growth as they mature, resulting in an accumulation of individuals near the size at maturation. The life-history functions are given in Appendix S7.
- A simplified single-patch version of the Falster et al. (2010) vegetation model. As a consequence of strong asymmetric competition for light among trees of different heights, the growth trajectories of trees (hence also the characteristic curves) can diverge substantially over time even if they start growing at almost the same time. The equilibrium size distribution has two peaks, corresponding to understory and canopy vegetation. The life-history functions are given in Appendix S8.

For the Daphnia model, the analytical equilibrium solution to Eq. (1) can be determined (Appendix S9). As reference equilibrium solutions for the other two reference problems we use a finely resolved numerical approximation with 4000 size classes obtained with the FMU method. It is worth pointing out that setting the time derivative to zero in equation (1) to solve equilibrium solution generally fails for SSPMs (e.g., the fish and vegetation models) as the vital rates often depend on the entire size distribution.

2.4 Performance measures

We compare the performance of the four numerical methods in terms of their computational efficiency, as measured both by computational load (CPU time in seconds), and in terms of their numerical accuracy as quantified by the error of the computed numerical solution relative to the reference solution. We quantify this error once the solution reaches dynamical equilibrium using two geometric measures of the error in the size distribution and four ecological measures that reflect difference in salient population statistics¹.

We define the two geometric measures as follows,

$$R_\infty = \frac{\max_{x_b \leq x \leq x_m} |u_c(x) - u_e(x)|}{\max_{x_b \leq x \leq x_m} u_e(x)} \quad \text{and} \quad R_1 = \frac{\int_{x_b}^{x_m} |u_c(x) - u_e(x)| dx}{\int_{x_b}^{x_m} u_e(x) dx}. \quad (2a)$$

These two quantities measure the relative difference between the computed equilibrium solution u_c and the reference equilibrium solution u_e . The first measure, R_∞ , is the maximal relative difference between the computed and reference size distribution at any one value of individual size, whereas R_1 is the sum of the relative difference across the size distribution. The

¹As the density at the maximum realized size is infinite in the reference solution of the Daphnia model (Appendix S9), the two geometric measures will be inappropriate. To enable a meaningful comparison, we only compare the part of the solution between the offspring size and 95% of the maximum size at equilibrium.

four ecological measures are the relative errors in total abundance, R_n , total biomass, R_b , average body size, R_s , and total fertility, R_f . Specifically, we let

$$R_n = |N_c - N_e|/N_e, R_b = |B_c - B_e|/B_e, R_s = |\bar{x}_c - \bar{x}_e|/\bar{x}_e, R_f = |F_c - F_e|/F_e. \quad (2b)$$

Here, $N = \int_{x_b}^{x_m} u(x)dx$ is the population abundance, $B = \int_{x_b}^{x_m} xu(x)dx$ is the population biomass, $\bar{x} = B/N$ is the average individual body size, and $F = \int_{x_b}^{x_m} \beta(x)u(x)dx$ is the population's fecundity rate. As before, the subscript indicates whether the quantity is calculated from the computed numerical solution or from the reference equilibrium solution.

When we determine numerical solutions for comparative purposes, using either of the four numerical methods we investigate, the integration times for the respective reference problems are 150 for the Daphnia model, 10 for the fish model, and 400 for the vegetation model, by which the considered models have reached equilibrium size distribution. The frequency (i.e., $1/\Delta t$) of introducing a new characteristic curve or cohort is also different for each reference problem. Specifically, we double the frequency while doubling the number of characteristic curves and cohorts. The time interval Δt for 50 mesh points (characteristic curves and cohorts) is 0.2 for the Daphnia model, 0.01 for the fish model and 0.1 for the vegetation model.

3. Results

To start with, we find that the characteristic method (CM) does not perform well for any of the three reference problems. Specifically, the CM method fails for the Daphnia model as the density of individuals at size of maturation in the equilibrium size distribution is infinite (Appendix S6). This sharp peak causes large numerical errors when approximating growth rates. The CM method can work for the fish model but only with poor resolution (Appendix S10). The poor resolution results from the steep changes in the size distribution (solid lines in Fig. 2) that leads to poor approximation of the growth rate. The CM method also fails for the vegeta-

tion model due to the sharp changes in the size distribution (solid lines in Fig. 2) and the significant divergence of the individual growth trajectories as a consequence of size-asymmetric competition for light. This divergence detrimentally leads to uneven resolution of the size distribution, and numerical aggregation of individuals at both small and large body size. For SSPMs with neither sharp changes in the size distribution nor diverging characteristic curves, such as the model presented by Angulo and López-Marcos (2004), we show in Appendix S11 that the CM method performs satisfactory. The problem of diverging characteristic curves can be overcome with an adaptive time schedule for the introduction of characteristic curves (Falster et al., 2016), but this recently developed improvement to the CM method is out of the scope of the present work. To focus on the performance of the other three numerical methods, we will not consider the CM method further in this section.

Figure 2 shows the numerically computed size distributions obtained using the fixed-mesh upwind method (FMU), the moving-mesh upwind method (MMU), and the Escalator Boxcar Train (EBT) method. The FMU method is accurate for solutions with small to intermediate gradients but is otherwise inaccurate (Fig. 2A-C). This is expected since the FMU method employs (logarithmically) equally spaced mesh points, which do not account for the solution structure. Consequently, excessive mesh points may be used to resolve regions of the solution that only require a few mesh points for high accuracy, while too few mesh points are in the regions that require a finer mesh for high accuracy. In contrast, the MMU method redistributes mesh points dynamically to ensure more mesh points in places with sharp changes, thus overcoming the shortcomings of the FMU method (Fig. 2D-F) at the expense of higher computational demands.

The EBT method approximates solutions fairly accurately and captures the steep gradients in the Daphnia and fish models (Fig. 2G, H). While the EBT method successfully resolves steep gradients, it uses relatively few cohorts for small individuals as a consequence of infrequent internalization of the boundary cohort (i.e., large Δt in Eq. S8 in Appendix S5). Increasing the frequency of internalizations decreases the cohort width, but since we keep the number of cohorts fixed for comparative purposes, more frequent internalization (smaller Δt) causes larger numerical errors since cohorts that still exert significant effects on the population dynamics will then be removed or merged. The accuracy of the EBT method is unsatisfactory for the vegetation model (Fig. 2I), for the same reason that the CM method fails to accurately resolve the size distribution. Size-asymmetric competition causes divergence in growth trajectories and hence cohorts, which increases the maximum width between approximating cohorts and undermines the numerical approximation.

Figure 3 shows how the performance of the numerical methods compare in terms of numerical accuracy and computational efficiency, as measured by the geometric measure (R_1), the ecological measure of population biomass (R_b), and the computational time required. Results for other measures are similar and presented in Appendix S12. The EBT method is the most accurate method for the Daphnia and fish models, but not for the vegetation model. The MMU method is with few exceptions more accurate than the FMU method for the same number of mesh points (computational time is not considered here), in particular in determining the population biomass in the Daphnia model and vegetation model. The EBT and FMU method are computationally more efficient than the MMU method, except in the vegetation model for which the FMU method is computationally more efficient than both the EBT and MMU method

In summary, Fig. 3 shows that the EBT method has the best performance for the Daphnia and the fish model. For the vegetation model, either the MMU or the FMU method performs best depending on whether one values numerical accuracy or computational efficiency highest. Moreover, our results are robust also when considering transient dynamics (Appendix S13).

4. Discussion

In this paper we have evaluated the performance of four numerical methods for size-structured population models (SSPMs) in solving three ecologically relevant reference problems. Our conclusions can be stated as follows.

(i) The fixed-mesh upwind (FMU) method is computationally the most efficient (has the fastest execution time for the same number of mesh points) for all three reference problems. The static mesh used in the FMU method makes it possible to repeatedly use size-dependent interaction kernels such as the predation kernel in the fish model (Appendix S7) or the shading kernel and the assimilation kernel in the vegetation model (Appendix S8), while the other three numerical methods require evaluating size-dependent interaction kernels at each iteration. This numerical method therefore has good performance across the board when the size distribution does not have very steep gradients, but when very steep gradients are present, such as the sharp peak in the Daphnia model, the method may fail to accurately resolve the size distribution. Since the FMU method is easy to implement and generally performs well, we recommend it as the first choice for numerically solving SSPMs, especially when there is no a priori reason to expect very steep gradients in the size distribution.

(ii) The moving-mesh upwind (MMU) method is suited for SSPMs in which asymmetric competition significantly affects growth rates, in particular when the number of mesh points is

low. By dynamically adjusting the mesh according to the gradient of the size distribution, this method efficiently captures rapid changes in the size distribution and hence enhances the numerical accuracy. The moving-mesh technique has been widely used in computational fluid dynamics (Huang and Russell, 2011) and numerical experiments have shown that, for certain partial differential equations, the moving-mesh technique with the equidistribution principle (equal arc-length between mesh points; de Boor, 1973) decisively improves computational performance (e.g., Huang et al., 1994; Stockie et al., 2001; Beckett et al., 2001; Huang and Russell, 2011). In contrast to this finding in computational fluid dynamics, our numerical investigations indicate that the moving-mesh technique is not of fundamental importance for enhancing computational performance in investigations of ecological SSPMs. The primary reason for our contrasting conclusion is the need to repeatedly evaluate the nonlinear size-dependent life-history functions. This repetitive calculation of the size-dependent interaction kernels reduces the computational efficiency and overall performance of the method. In fact, the time required to evaluate the interaction kernels is roughly half of the total computational time (around 40% in the fish model and 60% in the vegetation model), whereas the calculation of mesh equation (Eq. S3 in Appendix S3) consumes only around 10% of the total computational time. Thus, we conclude that the drawback of having to repeatedly evaluate the vital rates either offsets (vegetation model) or exceeds (fish model) the advantage of enhanced numerical accuracy. One more disadvantage of the MMU method is that some trial-and-error is needed to choose a good monitor function, and inappropriate choice can undermine the performance.

(iii) The characteristic method (CM) appears generally unsuited for SSPMs in which steep gradients are present in the size distribution. Since the environment E_t will generally depend directly or indirectly on the entire individual size distribution, the appearance of steep gradi-

ents in the size distribution (e.g., Fig. 2) results in large approximation errors for the vital rates for individual life histories. These approximation errors can be reduced by allowing for more characteristic curves, but this further increases computational time. For SSPMs in which size-asymmetric competition significantly impedes growth rates (e.g., the vegetation model), growth of small individuals can be stunted and the characteristic method can effectively fail. A similar conclusion applies to the Escalator Boxcar Train (EBT) method, and we will discuss the reason below.

(iv) The EBT method has high overall performance except for SSPMs in which asymmetric competition significantly impedes growth rate (Fig. 2I, Table S10 in Appendix S12). As no mesh is required, the EBT method is free of numerical diffusion. Moreover, the representation of the solution as a set of cohorts means that integrals over the size distribution, such as those which typically appear in the environmental variable, can be conveniently evaluated as a summation of the contribution from the different cohorts. The convergence of the EBT method has recently been proved in a modern framework of measure-valued solutions (Brännström et al., 2013). A recent study by Carrillo et al. (2013) which introduced a new numerical method for SSPMs based on operator splitting has further shown that the convergence of the EBT method is of first order in a specific but natural metric for measure-valued solutions. Importantly, this study also found that insufficiently frequent internalizations may cause a failure in the ordinary differential equations describing the boundary cohort (also see Gwiazda et al., 2014).

The numerical accuracy of the EBT method and the CM method is impeded if the distances between two successive cohorts (or characteristic curves) become large. This problem is particularly severe when individual growth rates are affected by asymmetric competition such as in the vegetation model. Plants in the understory can grow at ever lower speed, or even stop

growing entirely due to heavy shading by taller plants, while canopy plants keep growing fast (Fig. 4). Consequently, cohorts diverge and the maximum difference between two successive cohorts increases, leading to the loss of accuracy. It is worth mentioning that the loss of accuracy is because of the divergence of growth trajectories rather than the way we keep the number of cohorts constant (see Falster et al., 2017). However, a recent numerical implementation of a closely related vegetation model (Falster et al., 2016) shows that an adaptive time schedule for the introduction of characteristic curves can resolve the problem of divergence in the CM method. A similar implementation of the EBT method can also overcome the problem of cohort divergence (Falster et al. 2017). Considering that the EBT method had the best performance for all reference problems but the vegetation model, we believe that an EBT implementation with adaptive spacing of cohort introduction times, similar to Falster et al. (2017), offers the best overall performance for SSPMs.

We have discussed the strengths and weaknesses of the four numerical methods in solving physiologically structured population models with one structuring variable. In real ecological systems, populations may need to be described by additional state variables, which could take the form of individual age in the *Daphnia* and fish model, or root size in the vegetation model. The FMU method can theoretically be extended to higher-dimensional structured population models, but it may in practice perform poorly as the population will in many cases cover only a part of the entire state space, typically a one-dimensional curve. This means that most of the mesh points will be in areas where there are few to no individuals, resulting in low accuracy. This problem may be alleviated through the MMU method, but we believe that large problems with numerical diffusion would still remain. In stark contrast, the EBT method would by construction ensure that the cohorts are located in the part of the state space where the population resides while also not having the problem of numerical diffusion. Thus, we

believe that the advantage of the EBT method will be even greater for PSPMs with two or more individual states.

In summary, the dependence of life-history functions on the entire size distribution and the potential for individuals to aggregate at certain body sizes makes numerical investigation of SSPMs challenging. The EBT method is generally most accurate, but it can fail for SSPMs in which individual growth rates are significantly affected by asymmetric competition. The FMU method has generally good performance for SSPMs, except when very steep gradients are present in the size distribution. The CM and MMU method did not perform well or did not offer sufficient added value over the other two methods. These conclusions should apply also to other transport-dominated ecological models with non-linear environmental feedback from population to population dynamics. Taken together, our findings demonstrate important differences between numerical solution of SSPMs and PDEs and show that the nonlinear environmental dependence is of key importance when selecting suitable numerical methods to solve SSPMs.

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Author contributions

LZ and ÅB designed the study. LZ performed numerical analysis, and wrote the manuscript draft with input from ÅB. All authors contributed to the discussion of results and the final text.

Data accessibility

No data were used in this paper.

Supporting Information

Additional supporting information can be found in the online version of this article:

Appendix S1: Illustration of numerical diffusion in transport-dominated PDEs.

Appendix S2: Description of the fixed-mesh upwind method.

Appendix S3: Description of the moving-mesh upwind method.

Appendix S4: Description of the characteristic method.

Appendix S5: Description of the Escalator Boxcar Train method.

Appendix S6: Specification of the Daphnia model.

Appendix S7: Specification of the fish model.

Appendix S8: Specification of the single-patch vegetation model.

Appendix S9: Analytical equilibrium of the size-structured Daphnia model.

Appendix S10: Numerical performance of the characteristic method for the fish model.

Appendix S11: An analytically tractable test model without ecological interpretation.

Appendix S12: Computational performance of the numerical methods.

Appendix S13: Robustness for transient dynamics.

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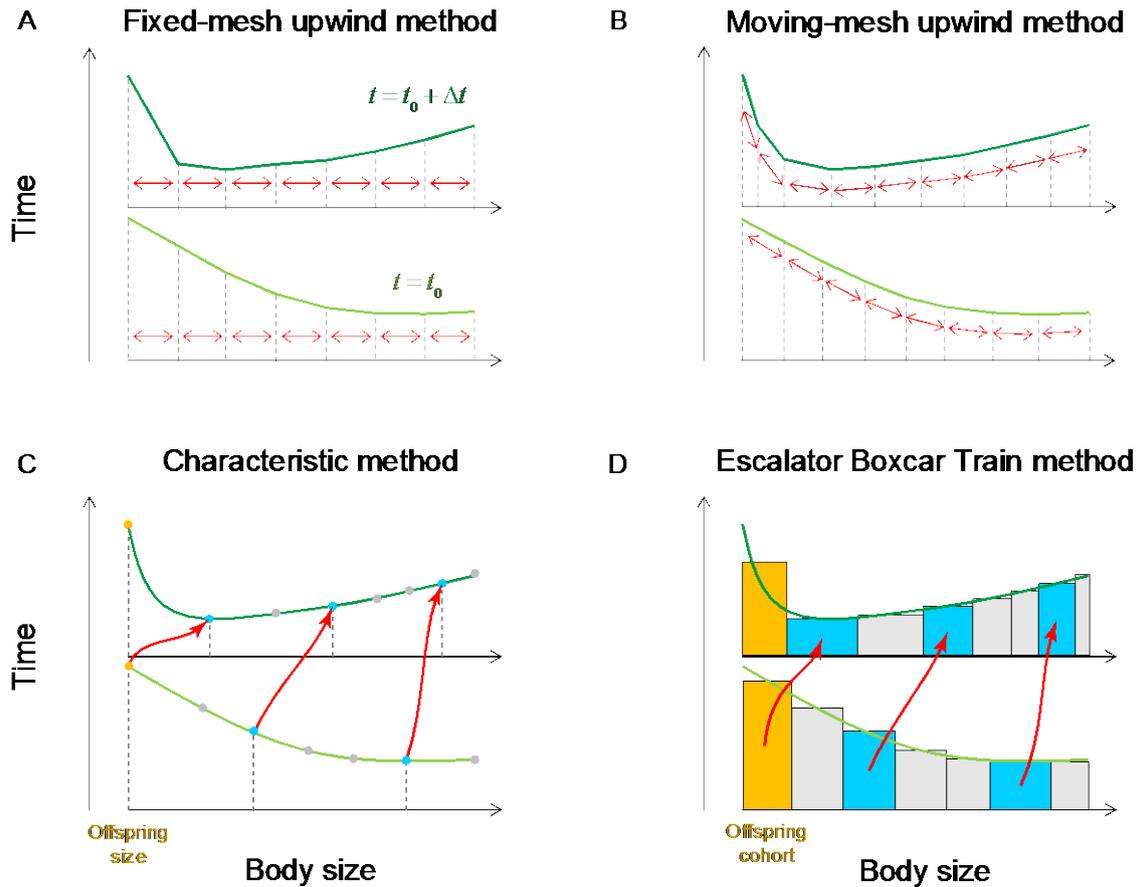
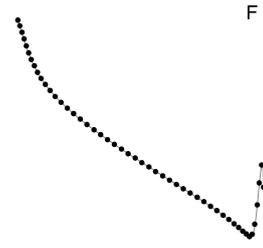
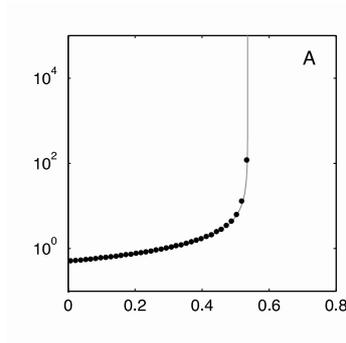


Fig. 1: Schematic overview of the investigated methods. A) The fixed-mesh upwind (FMU) method uses a static mesh and finite differences of size classes in the direction of growth to approximate the solution. B) The moving-mesh upwind (MMU) method, by contrast, uses a dynamic mesh, which resizes to maintain approximately equal arc lengths of the size distribution. C) The characteristic method tracks the size distribution along growth trajectories. D) The Escalator Boxcar Train (EBT) method tracks average individual size and numbers of individuals in discrete “cohorts”. Further explanations are given in Section 2.2 and full details are provided in Appendix S2-S5.



Body size

Body size (gram)

Body size (kg)

Fig. 2: Computed size distributions at equilibrium (shown as points) for the three reference problems using the fixed-mesh upwind method (FMU; top panels), the moving-mesh upwind method (MMU; middle panels), and the Escalator Boxcar Train method (EBT; bottom panels) with the corresponding reference solutions (continuous curves). While both the MMU and the EBT methods resolve sharp changes well, the EBT method is inaccurate for the vegetation model. The numerical solutions were computed using 50 mesh points (FMU and MMU method) or 50 cohorts (EBT method).

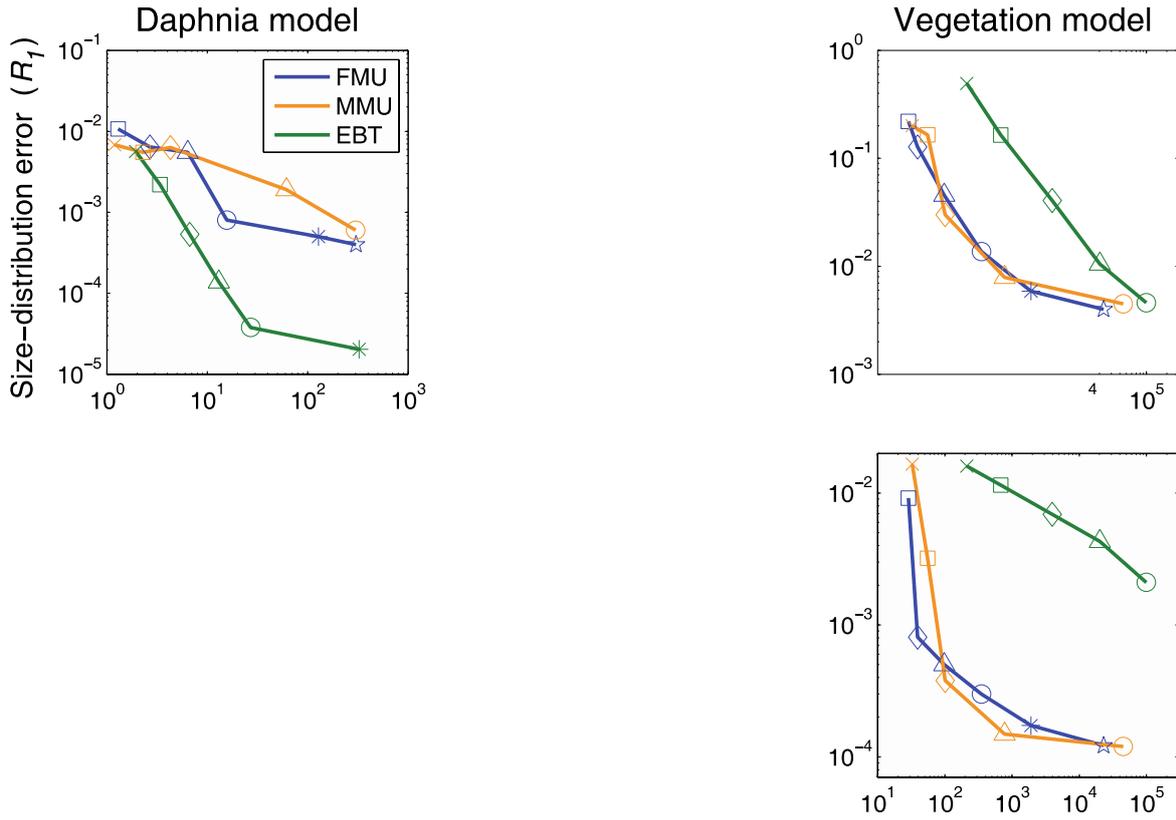


Fig. 3: Performance for the three reference problems as measured by numerical accuracy and computational requirements. Total relative error in the size distribution (R_1 ; top panels) and relative error in the population biomass (R_b ; bottom panels) are plotted against the used CPU time for the fixed-mesh upwind method (FMU), the moving-mesh upwind method (MMU), and the Escalator Boxcar Train (EBT) method. The EBT method is the most efficient method for the Daphnia and fish models, but it is numerically inaccurate when growth rates are impaired by size-asymmetric competition. The MMU method is, with few exceptions, more accurate than the FMU method for the same number of mesh points, but requires more CPU time. The CPU time required for tracking the cohort boundaries in the EBT method is excluded from the shown CPU times. Markers indicate the number of mesh points/cohorts: 13 (cross), 25 (square), 50 (diamond), 100 (triangle), 200 (circle), 400 (star), and 800 (pentagram).

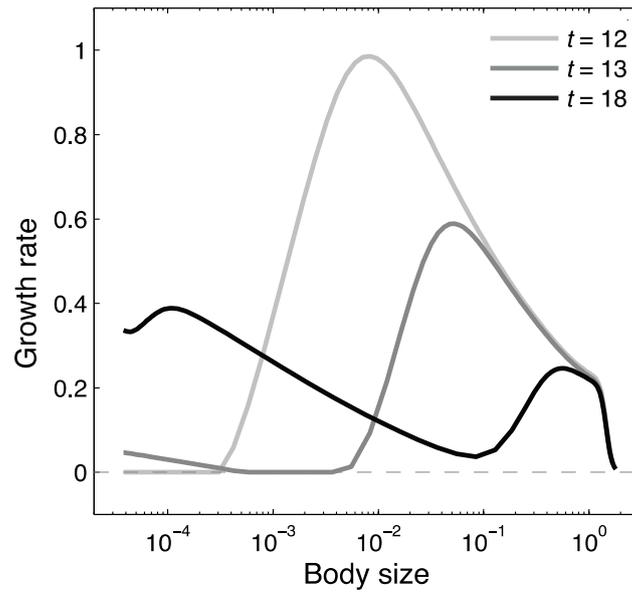


Fig. 4: Individual growth rates at three different times for the vegetation model. Understory individuals with small size can stop growing due to heavy shading from canopy individuals with large size. Thus, aggregation occurs in both the understory and the canopy.