beta-LTRANS-ADCIRC

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Model Description

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Preface

Much of this text appears in the LTRANS v2b User's Guide (Schlag and North 2012), was originally written by E. North, and has been updated for this description of beta-LTRANS-ADCIRC by E. North. The objective of this Model Description is to provide basic information for developers who are interested in adapting beta-LTRANS-ADCIRC to their ADCIRC model domain. Section II of the LTRANS v2b User's Guide (Schlag and North 2012) provides information on how to set up and run LTRANS.

Introduction

beta-LTRANS-ADCIRC is a particle-tracking model that runs with stored predictions from the 3D ADCIRC hydrodynamic model (http://adcirc.org/). The code is based on the **L**agrangian **TRANS**port model (LTRANS v2b, http://northweb.hpl.umces.edu/LTRANS.htm) which is an off-line particle-tracking model that runs with the stored predictions the Regional Ocean Modeling System (ROMS). beta-LTRANS-ADCIRC is intended to simulate passive particles, particles with sinking or floating behavior like sediment or oil droplets and planktonic organisms like oyster larvae. beta-LTRANS-ADCIRC is written in Fortran 90 and is designed to track the trajectories of particles in three dimensions. It includes a 4th order Runge-Kutta scheme for particle advection and a random displacement model for vertical turbulent particle motion. Reflective boundary conditions, particle behavior, and settlement routines are also included.

LTRANS v.1 was built by Elizabeth North and Zachary Schlag of University of Maryland Center for Environmental Science Horn Point Laboratory. Modifications for LTRANS v.2 were undertaken by Zachary Schlag and updates for LTRANS v.2b were conducted by Ian Mitchell. Funding for LTRANS development was provided by the National Science Foundation Biological Oceanography and Physical Oceanography Programs, Maryland Department of Natural Resources, NOAA Chesapeake Bay Office, and the NOAA-funded UMCP Advanced Study Institute for the Environment. Components of LTRANS have been in development since 2002 and are described in the following publications: North et al. (2005, 2006a, 2006b, 2008, 2011, 2015), Schlag and North (2012), and Mitchell (2013).

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Model structure

beta-LTRANS-ADCIRC is designed to predict the movement of particles based on advection, turbulence and behavior. It has an external and internal time step (Fig. 1) and boundary condition algorithms that keep particles from leaving the model domain. The external time step is the time step of hydrodynamic model output (e.g., 10 min). The internal time step is the time interval during which particle movement is calculated (e.g., 120 s). The internal time step is smaller than the external time step so that particles do not move in large jumps that could cause inconsistencies between predictions of the hydrodynamic model and the particle tracking model. At each internal time step of beta-LTRANS-ADCIRC, particle motion is calculated as the sum of movement due to advection, turbulence and behavior. The model contains sub-models for each of these components. The turbulence and behavior routines can be turned off so that particle movement is based solely on advection. beta-LTRANS-ADCIRC also includes sub-models for boundary conditions, particle settlement (i.e., target areas, habitats) and handing wetting-and-drying which occurs in ADCIRC (i.e., 'beaching' of particles in 'dry' elements).

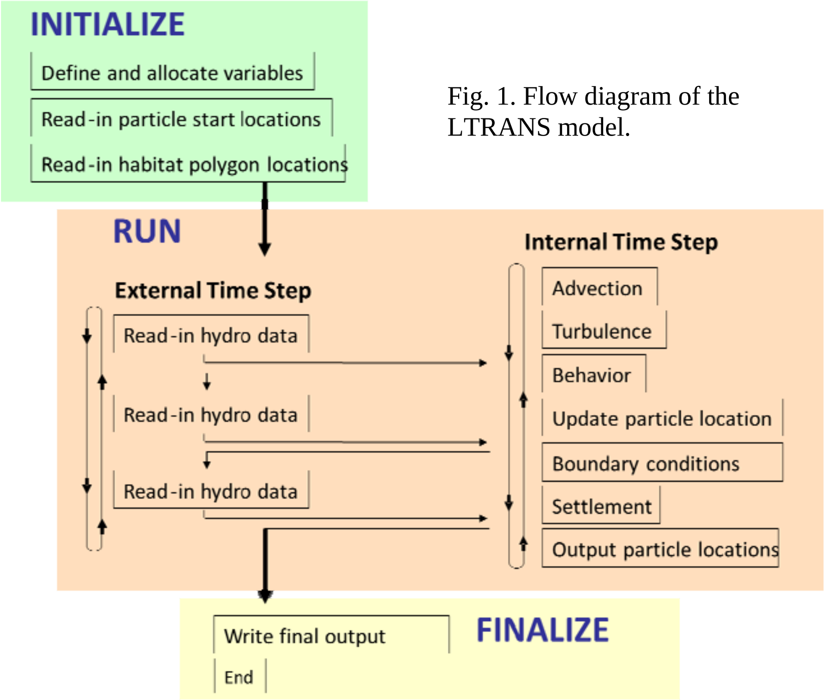

Fig. 1. Flow diagram of the LTRANS model.

Interpolation scheme

Hydrodynamic model predictions (stored in NetCDF format) are read in and interpolated in space and time to the particle location. The first step in the process of interpolating the water properties (e.g., current velocities, salinity, temperature, sea surface height, and vertical and horizontal diffusivities) to the particle location is to determine the grid element in which the particle is located. For this, we use the 'crossings' point-in-polygon approach. Once the particle is located in an element, water properties are interpolated in space to the particle location. All water properties are interpolated from the native ADCIRC nodes. For two-dimensional water properties (e.g., sea surface height, water depth) bilinear interpolation is used. For three-dimensional water properties (e.g., current velocities, diffusivities, salinity), a water-column profile scheme is applied (North et al. 2006a). In this scheme, values are interpolated along each s-level to create a vertical profile of values at the x-y particle location (see Fig. 3 in Schlag and North (2012). A tension spline curve is then fit to the vertical profile and used to estimate the water property at the particle location. The interpolation scheme was adapted from North et al. (2006a), streamlined to increase computational speed, and enhanced to handle model domains with irregular bottoms and non-rectangular grid geometries. More discussion of the tension spline interpolation scheme can be found in Schlag and North (2012).

The tension spline interpolation scheme in beta-LTRANS-ADCIRC is based on the Tension Spline Curve Fitting Package (TSPACK). TSPACK (TOMS/716) was created by Robert J. Renka (renka@cs.unt.edu, Department of Computer Science and Engineering, University of North Texas) and is available for download from http://www. netlib.org and http://portal.acm.org/citation.cfm?id=151277. TSPACK fits tension splines to data that preserve the concavity and monotonicity of the data. TSPACK is copyrighted by the Association for Computing Machinery (ACM). With the permission of Dr. Renka and ACM, TSPACK was modified for use in LTRANS by removing unused code and call variables and updating it to Fortran 90. The modified version of TSPACK is included in the LTRANS source code in the Tension Spline Module (tension_module.f90). If you would like to use LTRANS with the modified TSPACK software, please read and respect the ACM Software Copyright and License Agreement (http://www.acm.org/publications/policies/softwarecrnotice). For noncommercial use, ACM grants "a royalty-free, nonexclusive right to execute, copy, modify and distribute both the binary and source code solely for academic, research and other similar noncommercial uses" subject to the conditions noted in the license agreement. Note that if you plan commercial use of LTRANS with the modified TSPACK software, you must contact ACM at permissions@acm.org to arrange an appropriate license. It may require payment of a license fee for commercial use.

For particle tracking, it is necessary to interpolate in time as well as space because the duration between successive outputs of the hydrodynamic models (i.e., the external time step) is longer than the time step of particle motion (i.e., the internal time step). To do this, water properties are estimated at the particle location (as above) at three time points that correspond to the hydrodynamic model output (i.e., at the 10-min intervals of the external time step). Then a polynomial curve is fit to the water properties at three time points and used to calculate the water properties at the time of particle motion (i.e. for the internal time step). The advection, turbulence and behavior sub-models incorporate these spatial and temporal interpolation techniques; specifics associated with each sub-model are discussed below.

Advection sub-model. A 4th order Runge-Kutta scheme in space and time is used to calculate particle movement due to advection. This scheme solves for the *u*-, *v*-, and *w*- current velocities (representing the x-, y-, and z-directions) at the particle location using an iterative process that incorporates velocities at previous and future times to estimate the trajectory of particle motion. Current velocities (m s^{-1}) provided by the Runge-Kutta scheme are multiplied by the duration of the internal time step (δt) to calculate the displacement of the particle in each component direction. Displacements (m) are then added to the original location of the particle (x_n, y_n, z_n) in order to calculate the new location of the particle ($x_{n+1}, y_{n+1}, z_{n+1}$):

(1) $$x_{n+1} = x_n + u\delta t$$

(2) $$y_{n+1} = y_n + v\delta t$$

(3) $$z_{n+1} = z_n + w\delta t$$

Law-of-the-wall (a log layer calculation) is applied to the current velocities within one s-level of bottom to simulate reduction in current velocities near bottom.

Turbulence sub-model

Hydrodynamic models do not simulate turbulent motion at scales smaller than the grid resolution of the model. In particle-tracking models, particles can be moved in millimeter to centimeter steps -- much less than the hydrodynamic model grid scale. A random component must be added to particle motion in order to reproduce turbulent diffusion that occurs at the scale of particle motion (Hunter et al. 1993, Visser 1997, Brickman and Smith 2002). A random displacement model (Visser 1997) is implemented within the LTRANS to simulate sub-grid scale turbulent particle motion in the vertical (z) direction:

$$z_{n+1} = z_n + K_v' \delta t + R\left[2r^{-1} K_v \delta t\right]^{1/2} \tag{4}$$

where z_n = initial particle location, K_v = vertical diffusivity evaluated at ($z_n + 0.5 K_v' \delta t$), δt = time step of the random displacement model, $K_v' = \partial K_v / \partial z$ evaluated at z_n, and R is a random number generator with mean = 0 and standard deviation $r = 1$. Unlike random walk models, random displacement models do not result in numerical artifacts if the vertical resolution is adequate to resolve sharp variations in vertical diffusivity (Visser 1997; Brickman and Smith 2002). In LTRANS, the turbulent particle motion sub-model uses the same approach for determining K_v and K_v' at the particle location as that used in the advection model, except that 1) a smoothing algorithm is applied to the water column profile of K_v to prevent artificial aggregation of particles in regions of sharp gradients in diffusivity (North et al. 2006a), and 2) a 4th order Runge-Kutta was applied in time but not in space due to computational constraints.

A random walk model is used to simulate turbulent particle motion in the horizontal direction (x- or y- directions). When K_h is constant, the random displacement model defaults to a random walk model (Visser 1997):

$$x_{n+1} = x_n + R\left[2r^{-1} K_h \delta t\right]^{1/2} \tag{5}$$

where K_h = horizontal diffusivity evaluated at (x_n). This was suitable for the ROMS model for which LTRANS was developed (Li et al. 2005, 2006, Zhong and Li 2006) because it was implemented with a constant value for K_h (1 m^2 s^{-1}). The model output was interpolated to the particle location using the same approach as was used for advection (described above), except that a 4th order Runge-Kutta was applied in time only (not space) due to the computational constraints. Note that a random displacement model might be needed if horizontal diffusivity is not constant in the hydrodynamic model to maintain fidelity with hydrodynamic model predictions.

Behavior sub-model

The behavior sub-model assigns vertical sinking, floating, or swimming velocities to particles. This velocity includes a speed component and an orientation (up or down) component that can depend upon particle characteristics such as species and developmental stage. The speed component controls the speed of particle motion due to sinking, floating or swimming. The speed can be set as constant or as a function of particle age. The orientation component regulates the direction of particle movement (i.e., sink, float, swim down in the presence of light, etc.). To simulate random variation in the movements of individual larvae, the direction of particle motion is assigned a random component that can be weighted so that particles have a tendency to move up or down depending on species and/or age of particle.

Settlement sub-model

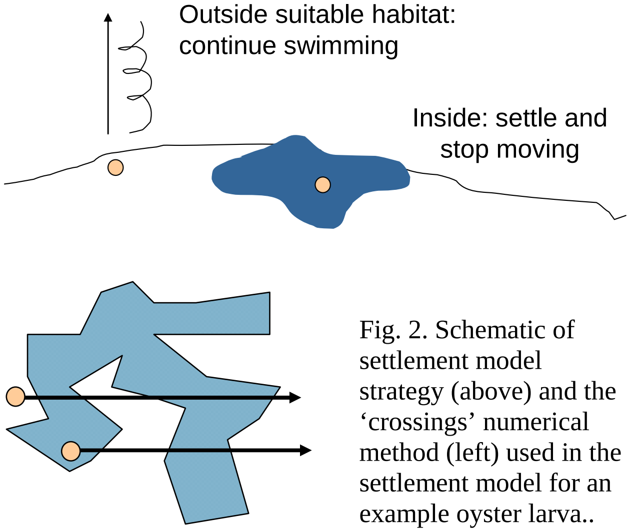

Fig. 2. Schematic of settlement model strategy (above) and the ‘crossings’ numerical method (left) used in the settlement model for an example oyster larva..

The purpose of the settlement sub-model is to determine if a particle is inside or outside an irregularly shaped polygon such as suitable habitat (e.g., marine reserve, seagrass bed, oyster reef). Once a particle reaches a specified age, the Settlement Module tests the location of settlement-stage particles at each internal time step (e.g., every 2 min) to determine if they are within the boundaries of a habitat polygon. If so, they stop moving (Fig. 2). To determine if the particle is inside or outside an irregularly shaped polygon, the ‘crossings method’, a ‘point-in-polygon’ technique, is applied. A ray, parallel to the x-coordinate axis, is shot from the particle (a point) to the east. The number of times the ray intersects with the line segments of each polygon is calculated. If the number of intersections is odd, then the particle is within the polygon. If the number is even, then the particle is outside the polygon boundaries. A search restriction algorithm ensures that the locations of particles are tested only for nearby polygons to reduce computation time.

Boundary conditions

Before particles settle or die (i.e., between the time they are released and the time they stop moving), the location of each particle is tested every internal time step to ensure that it remains within the model boundaries. If the motion of the particle causes it to exceed the boundaries, the particle is placed within the model domain as specified below.

Vertical boundaries (surface and bottom) are specified for each particle by interpolating sea surface height and bottom depth to the x-y location of the particle. If a particle passes through the surface or bottom boundary due to turbulence or vertical advection, the particle is placed back in the model domain at a distance that is equal to the distance that the particle exceeds the boundary (i.e., it is reflected vertically). If a particles passes through the surface or bottom due to particle behavior, the particle is placed just below the surface or above the bottom (i.e., it stops near the boundary).

Reflective horizontal boundary condition routines keep particles within the model domain. beta-LTRANS-ADCIRC uses the boundaries defined by the ADCIRC model. If there are islands inside the ADCIRC model domain, beta-LTRANS-ADCIRC does not yet have the capability of handling then (or at least it has not been tested). The ‘crossings’ point-in-polygon approach is used to determine if a particle is inside or outside the model boundaries. If the particle is on land (outside the model boundaries), the particle is reflected off the boundary with an angle of reflection that equals the angle of approach to the boundary. The distance that the particle is reflected is equal to the distance that the particle exceeded the boundary. The horizontal boundary condition routine allows multiple reflections within one time step. At open ocean boundaries, the user may specify either reflection or ‘sticking’. For ‘sticking’, if the particle intersects the open ocean boundary, it would stop moving at the boundary and remain there until the end of the simulation. (Note: changes in particle behavior at open ocean boundaries has not been tested in beta-LTRANS-ADCIRC).

Particle status

The status of a particle is updated every internal time step and is written to the para*.csv output files. The status of the particle provides information about the behavior of the particle (0 = passive, 1 = near-surface orientation, 2 = near-bottom orientation, 3 = diel vertical migration, 4 = *Crassostrea virginica* oyster larvae, 5 = *Crassostrea ariakensis* oyster larvae, 6 = constant sinking or floating). Depending upon the user-defined preferences (in LTRANS.data), an individual particle’s status can change over the course of the model run (-1 = dead, -2 = settled in a habitat polygon, -3 = out of model boundaries, -4 = beached, or has been beached, in a dry element within model boundaries).

Concluding thoughts

The beta-LTRANS-ADCIRC model is designed to maintain fidelity with ADCIRC hydrodynamic model predictions. The original LTRANS model was developed to simulate oyster larvae in Chesapeake Bay, a region with complex bathymetry and horizontal and vertical current shears. It is not known whether the LTRANS interpolation schemes would be appropriate in other systems, and, if so, in what conditions they should be used. We invite the particle tracking community to participate in cross-system comparisons to help develop standardized methods for interpolation, turbulence and time stepping for different systems.

Open Source License

beta-LTRANS-ADCIRC is an open-source model and licensed under the MIT/X License. This license is similar to the LTRANS v2b model license. Here is a copy of the beta-LTRANS-ADCIRC model license file:

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Literature Cited

Brickman, D., and P. C. Smith, 2002. Lagrangian stochastic modeling in coastal oceanography. Journal of Atmospheric and Ocean Technology 19: 83–99.

Hunter, J., P. Craig, and H. Phillips. 1993. On the use of random-walk models with spatially-variable diffusivity. Journal of Computational Physics 106:366-376.

Li, M., L. Zhong, and W. C. Boicourt. 2005. Simulations of Chesapeake Bay estuary: Sensitivity to turbulence mixing parameterizations and comparison with observations, Journal of Geophysical Research, 110, C12004, doi:10.1029/2004JC002585.

Li, M., L. Zhong, W. C. Boicourt, S. Zhang and D.-L. Zhang. 2006. Hurricane-induced stormsurges, currents and destratification in a semi-enclosed bay. Geophysical Research Letters 33: L02604, doi:10.1029/2005GL024992.

Mitchell, I. 2013. Updates in LTRANS v.2b. University of Maryland Center for Environmental Science, Horn Point Laboratory. Cambridge, MD. 2 pp. Available at http://northweb.hpl.umces.edu/LTRANS.htm

North, E. W., R. R. Hood, S.-Y. Chao, and L. P. Sanford. 2005. The influence of episodic events on transport of striped bass eggs to an estuarine nursery area. Estuaries 28(1): 106-121.

North, E. W., R. R. Hood, S.-Y. Chao, and L. P. Sanford. 2006a. Using a random displacement model to simulate turbulent particle motion in a baroclinic frontal zone: a new implementation scheme and model performance tests. Journal of Marine Systems 60: 365-380.

North, E. W., Z. Schlag, R. R. Hood, L. Zhong, M. Li, and T. Gross. 2006b. Modeling dispersal of Crassostrea ariakensis oyster larvae in Chesapeake Bay. Final Report to Maryland Department of Natural Resources, July 31, 2006. 55 p.

North, E. W., Z. Schlag, R. R. Hood, M. Li, L. Zhong, T. Gross, and V. S. Kennedy. 2008. Vertical swimming behavior influences the dispersal of simulated oyster larvae in a coupled particle-tracking and hydrodynamic model of Chesapeake Bay. Marine Ecology Progress Series 359: 99-115.

North, E. W., E. E. Adams, S. Schlag, C. R. Sherwood, R. He, S. Socolofsky. 2011. Simulating oil droplet dispersal from the Deepwater Horizon spill with a Lagrangian approach. AGU Book Series: Monitoring and Modeling the Deepwater Horizon Oil Spill: A Record Breaking Enterprise 195: 217-226

North, E. W., E. E. Adams, A. E. Thessen, Z. Schlag, R. He, S. Socolofsky, S. M. Masutani, and S. D. Peckham. 2015. The influence of droplet size and biodegradation on the transport of subsurface oil droplets during the Deepwater Horizon spill: a model sensitivity study. Environmental Research Letters 10: 024016 (doi:10.1088/1748-9326/10/2/024016).

Schlag, Z. R., and E. W. North. 2012. Lagrangian TRANSport model (LTRANS v.2) User's Guide. University of Maryland Center for Environmental Science, Horn Point Laboratory. Cambridge, MD. 183 pp. Available at http://northweb.hpl.umces.edu/LTRANS.htm

Visser, A.W., 1997. Using random walk models to simulate the vertical distribution of particles in a turbulent water column. Marine Ecology Progress Series 158: 275–281.

Zhong, L. and M. Li. 2006. Tidal energy fluxes and dissipation in the Chesapeake Bay. Continental Shelf Research 26: 752-770.