Linked Lists for Transport Simulations Using Lagrangian Parcels

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Abstract: The linked-list method is explained using transport simulations involving Lagrangian discrete parcels. Parcel insertion and removal as well as storing of variables in a multispecies problem are explained through examples. The advantages of the linked-list method over the sequential-list method are discussed. Both single-species and multispecies applications are addressed. It is shown that for maintaining parcel lists, insertions, and removals, use of the linked-list approach optimizes the use of memory and is significantly more efficient than using sequential lists.

INTRODUCTION

The linked-list method provides a way to manage and manipulate efficiently a list or lists of variables during various computations in a program. In numerical simulations involving fluid flows, particularly ones that use Lagrangian parcels, the advantages of the linked-list method are great.

The linked list method has been in use for at least 20 years. Early explanations of this method can be found in the classic book by Knuth (1973) on computing algorithms. The linked-list method is regularly studied in computer science courses on data structures and is used widely in commercial software development (e.g., database programs). The use of the linked-list method has not been widely exploited in the modeling of fluid flows in environmental and hydraulic engineering. One reason for this lack of usage is that these numerical models are usually coded in FORTRAN computer language. Linked lists and data structures are not well-known to FORTRAN programmers, and are rarely described in FORTRAN books. It must be pointed out that the use and merits of the linked-list method are not limited to any particular programming language or languages, and that FORTRAN can be used easily for this purpose. A second reason for the lack of usage is that in numerical modeling of fluid flows using Eulerian systems, the advantages of using linked lists are not as clear as when using the Lagrangian parcels method. However, the use of linked lists can benefit Eulerian models as well.

The recent emergence of the Lagrangian parcel method in successfully modeling transport processes in fluid flows such as oil-spill fate and transport (Yapa et al. 1994) and ice transport and dynamics (Shen et al. 1993) provides examples in which the linked-list method could be used to gain enormous modeling advantages. These advantages will be more apparent in multispecies problems such as an oil- or chemical-spill transport model or a model to simulate the behavior and movement of fish. For example, in an oil-spill fate and transport model, the multiple species are parent oil, weathered (emulsified) oil, surface oil, oil present as globules in the water column, oil attached to sediment particles but moving in the water column, and oil that has sunk to the bed. In a model simulating the behavior and movement of fish, multiple species are different types of fish (e.g., salmon, trout). With each fish type, different variables have to be linked up to describe their movement patterns, spawning behavior, growth rate, etc.

The purposes of this technical note are (1) to explain the concept of the linked-list method to programmers with no background in data structures; (2) to show the advantages of using the linked-list method when using Lagrangian parcels techniques; and (3) to show the suitability and advantages of using the linked-list method for multispecies modeling problems.

EXPLANATION OF METHOD

A linked list consists of a series of items in which each item contains a link (or pointer) to the next item in the list. The link (or pointer) is the value of the subscript of the variable used for storing information corresponding to a particle. Fig. 1 shows a linked list of five items sorted and maintained as a list, with links shown in column 3 stored in a separate array. An item (as shown in Fig. 1) is a logical identification for a series of properties associated with the item. The beginning point of the list is maintained in a separate variable (let's say B) and the end of the list is indicated by storing a flag value of −1 in the list. In the example discussed, $B = 3$. Once the value of B is known, the rest of the sequence is found through links in the list. At this point, the advantages of the linked-list method are not obvious. The advantages and more details of the linked-list method are explained in the next section when the insertion and deletion of items are discussed.

In a typical modeling problem, a list contains several variables. Let's consider the case of a three-dimensional oil-spill trajectory model that uses Lagrangian parcels (the Lagrangian parcel method has been described in detail in other papers, e.g., Shen and Yapa (1988) and Monaghan (1985)]. In this case, at least four variables are needed to define each parcel, i.e., spatial coordinates (x, y, z), and the volume (v). It should be noted that the size of array necessary for maintaining the links is independent of the number of variables associated with the list (see Fig. 2).

One of the advantages of the linked-list method is the ease

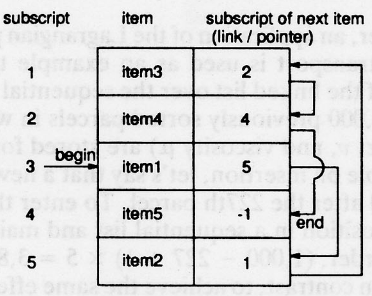

FIG. 1. Basic Item List and Links

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