

A MULTI-DIMENSIONAL PARTICLE TRACKING COMPUTER PROGRAM FOR ENVIRONMENTAL RESEARCH AND STUDY

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We summarize the initial efforts undertaken in developing an accurate and efficient multi-dimensional particle tracking computer program: PT123. PT123 was developed as part of the advancement of modeling capability for solving transport-related environmental problems. The particle tracking technique has a wide range of application in environmental sciences and engineering. It can be used to provide quick estimates of the migration of chemicals in complex surface water and groundwater systems, to understand, visualize, and analyze flow fields, and to study sediment transport, oil spill, and natural or man-induced retardation mechanisms that may be used for the remediation or prevention of environmental pollution. It can also be employed to understand and predict animal behavior for investigations concerning food supply and ecosystem restoration and preservation. It is an essential and crucial component in the Eulerian-Lagrangian (EL) approximation for numerically solving transport equations numerically. The quality of particle tracking dictates much of the accuracy of the whole EL approximation as well as efficiency on serial and parallel platforms. The purposes of developing PT123 are two-fold. One is to construct accurate and efficient PT computer routines that can be used for solving multi-dimensional transport problem using the EL-based numerical method. The other is to develop a modularized computer program that can be easily incorporated into or linked to ERDC's existing flow or transport models to enhance modeling capability for various applications.

Given velocities, PT123 can track particles in 1-, 2-, and 3-D unstructured meshes. The elements used to construct unstructured meshes are line elements in 1-D, triangular and/or quadrilateral elements in 2-D, and tetrahedral, triangular prism, and/or hexahedral elements in 3-D. Various Runge-Kutta methods are included in PT123 to solve the ordinary differential equations describing the motion of particles. Adaptive time integration can be used to meet a user-specified accuracy requirement. Both element-by-element (EBE) and non-element-by-element (NEBE) tracking approaches are incorporated into PT123. Both node- and element-based velocity can be used for particle tracking. PT123 tracks particles along the closed boundary and stops tracking when a particle encounters the open boundary. It can execute forward and backward tracking and output tracking history at specified time intervals. In the presentation, the details of the aforementioned numerical techniques and capabilities will be briefly described. Also, several test examples in multiple dimensions will be used for verification and demonstration.