# User's Guide for mod-PATH3DU

## A groundwater path and travel-time simulator

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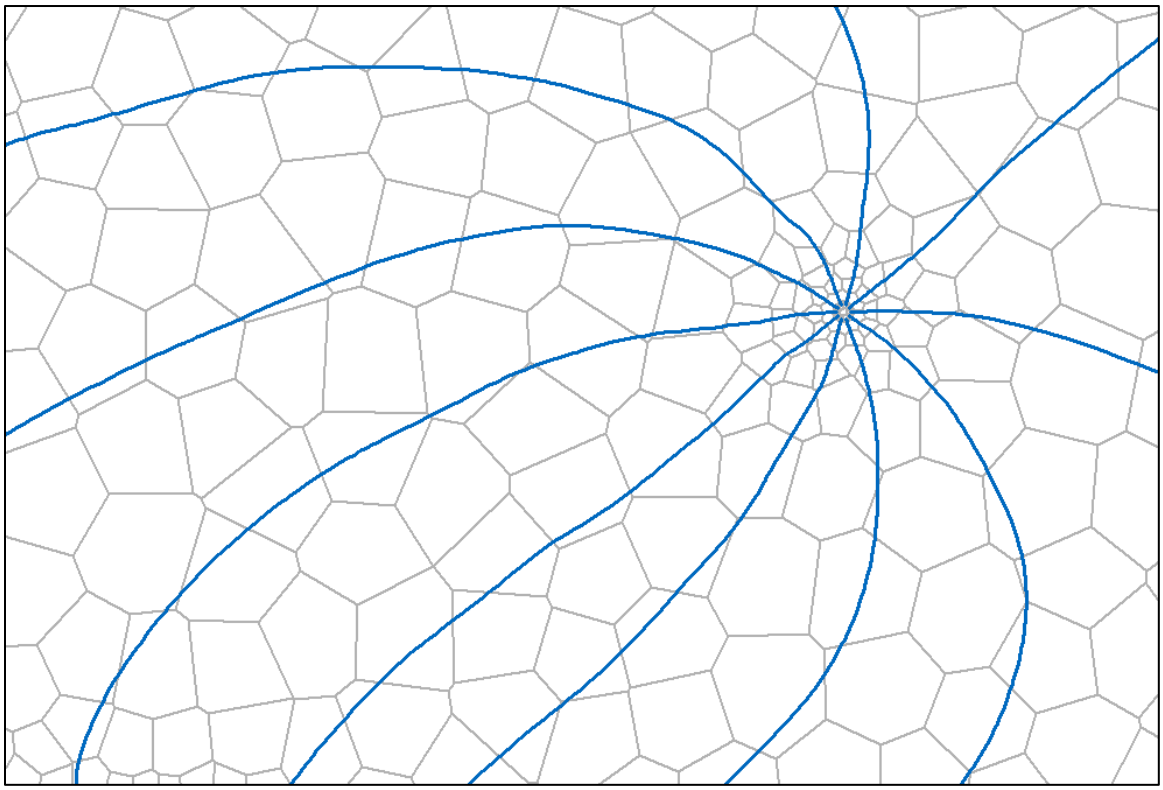

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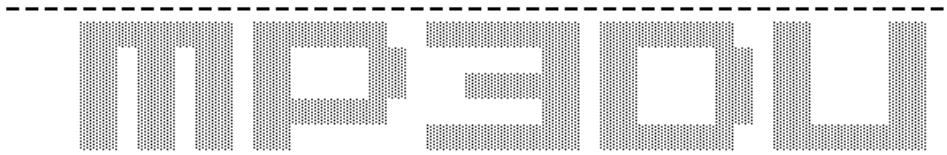

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S.S. Papadopulos & Assoc. Inc.

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# Preface

This report describes a particle tracking program, called mod-PATH3DU, which supports the latest MODFLOW release by the U.S. Geological Survey, MODFLOW-USG (Panday et al. 2013). mod-PATH3DU currently implements the Pollock method (Pollock, 1994), together with a novel technique, referred to herein as the SSP&A method, for calculating groundwater path and travel-time for unstructured grids. The focus of mod-PATH3DU development to date has been on the logic to map shared faces between cells, and validating the SSP&A tracking algorithm for a variety of simple systems. Future applications of mod-PATH3DU may reveal errors that were not detected during testing. In the event a bug is found please contact the corresponding author listed below; every effort will be made to correct any identified bugs.

S.S. Papadopulos & Associates Inc. developed mod-PATH3DU to support specific project applications, but is distributing it free-of-charge as a service to our industry. As such, only limited technical support can be provided by S.S. Papadopulos & Associates Inc. through the corresponding author.

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## Quick Start Guide

1. Read this manual in its entirety.
2. Download the mod-PATH3DU executable, mod-PATH3DU.exe, from SSP&A's website at www.sspa.com/software.
3. Create the (4) required input files (MPSIM, MPBAS, MPNAM, particle starting location) following the instructions in the Input Instructions section of this manual. Create the optional MP3DU file if desired.
4. Put these 4 (or 5) files in the same folder as the MODFLOW-USG model files
5. At a command prompt enter the name of the mod-PATH3DU executable, followed by the name of the MPSIM file. For example : *mod-PATH3DU.exe NAME.MPSIM*
6. Review the log and listing files created, in particular mp3du.log and the MPLST file to ensure the program executed as expected.

To support mod-PATH3DU, SSP&A has, through the mod-PATH3DU webpage, created a simple interface that can be used to generate an initial set of the required (and optional) input files (Step 3). On the webpage users can enter some basic information about their problem (i.e. number of model layers, tracking direction, etc.) and download the corresponding input files. These files can then be modified as needed by the user following the Input Instructions section of this manual.

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# Abstract

mod-PATH3DU is a particle tracking code for calculating the three-dimensional flow pathlines of purely advective solute particles. This program is fully compatible with the groundwater simulation model MODFLOW, including MODFLOW-USG, an unstructured-grid version based on an underlying control volume finite difference (CVFD) formulation (Panday et. al, 2013).

mod-PATH3DU contains two different particle tracking schemes: the Pollock method (Pollock, 1989), and the SSP&A method. The Pollock method is implemented in the different versions of the U.S. Geological Survey (USGS) particle tracking code MODPATH (Pollock, 2012) and is applicable to rectilinear, structured cells. The SSP&A method is grid independent. It uses universal kriging of a MODFLOW hydraulic-head solution and Darcy's law to calculate the velocity vectors necessary to advect a particle. The pathlines are generated using a higher-order Runge-Kutta scheme or a simple Euler approach. Currently, the SSP&A method uses the Pollock method to track particles in the *z*-direction. Because the SSP&A method is grid independent it can be used to track particles on structured and unstructured grids. Users can specify which tracking method to use on a per-cell basis as each has their strengths and weaknesses and may be more appropriate in some areas of a model domain. A third tracking scheme is being developed by Dr. James Craig at the University of Waterloo with his student Muhammad Ramadhan and will be a second option for tracking on unstructured grids when it becomes available.

The program uses the input file structure of MODPATH6 with some changes detailed in the Input Instructions section. Depending on the type of simulation specified, the program writes different output files, but a summary of the input and simulation results is always generated.

The executable file of mod-PATH3DU is available for download at www.sspa.com/software.

# Introduction

The U.S. Geological Survey (USGS) has recently developed a new version of the groundwater flow model MODFLOW, called MODFLOW-USG, to support a wide variety of structured and unstructured grid types. However, there is not any particle tracking code adapted to it. The USGS particle tracking model MODPATH6 and its previous versions can only support groundwater flow simulations for structured grids based on MODFLOW. Therefore, a particle tracking code accommodating the newly developed flow model MODFLOW-USG is required, and mod-PATH3DU has been developed for this purpose.

The main difference between mod-PATH3DU and MODPATH lies in the particle tracking scheme. Currently, two different tracking schemes are implemented in mod-PATH3DU, the Pollock and SSP&A methods. The semi-analytical particle tracking scheme, the Pollock method, implemented in MODPATH, evaluates the velocity field using linear interpolation of the groundwater velocities within each finite-difference grid (Pollock, 1989). A particle's path is then computed by moving the particle from one cell to another until it reaches a boundary or meets another termination criterion. For unstructured grids that provide greater flexibility in spatial discretization, the linear velocity interpolation used in the Pollock method is not applicable. The Pollock method is incorporated in mod-PATH3DU for situations in which the grid (or a subset of the grid) is structured. The SSP&A method computes the velocity field based on the hydraulic head distribution generated by MODFLOW-USG using kriging. It uses a higher order numerical Runge-Kutta scheme (Zheng, 1992) or a simple Euler approach to track a particle within an unstructured cell.

This document describes the particle tracking program mod-PATH3DU and provides instructions for using the program. Some of the required input files are created outside of MODFLOW-USG and it is important to read the instructions to make sure that all of the required input is specified. mod-PATH3DU does not include either a graphical user interface or tools for visualizing the results, although it is expected that the program will be supported by popular modeling interfaces[1]. Users will need to devote care to preparing the input and analyzing the output. All of the files for the test cases detailed in the Examples section are available for download. These files illustrate the structure of the input and the procedures required to execute mod-PATH3DU. mod-PATH3DU is intended to be compatible with MODPATH6 and MODFLOW-USG in terms of input and output formats. The variable names and the corresponding definitions are consistent with the two programs as well. More detailed descriptions of the input parameters are presented in Harbaugh (2005), Panday et al. (2013) and Pollock (2012).

This document is organized into five major sections:

[1] SSP&A has developed 3D visualization software for MODFLOW-USG that fully supports mod-PATH3DU. It is available at www.groundwaterdesktop.com

- Background,
- Overview,
- Input Instructions,
- Output File Formats, and
- Examples.

## Compatibility with MODFLOW

mod-PATH3DU uses information in both the cell-by-cell flow (CBB)[2] and head-save (HDS) files written by MODFLOW to calculate velocity. These files list the components of flow and hydraulic head for each cell. The Pollock method relies exclusively on the CBB file, while the SSP&A method requires both. In structured grid mode, MODFLOW-USG writes these two files in a format identical to previous releases. As such, mod-PATH3DU is compatible with previous versions of MODFLOW, specifically MODFLOW-2000 and MODFLOW-2005. It does not support earlier releases.

MODFLOW-USG is built upon the MODFLOW-2005 framework and uses modified versions of its predecessor's subroutines to read input files. These modified routines are incorporated into mod-PATH3DU. As such, mod-PATH3DU does not support the global (GLO) package available with MODFLOW-2000. Further, the connected-linear network (CLN) package available with MODFLOW-USG supersedes the multi-node well (MNW) package in previous releases of MODFLOW. mod-PATH3DU relies on the CBB file for boundary and source/sink flow information and not the input packages for these routines explicitly, as such, it supports both the MNW and CLN packages. Currently, it does not track particles within a CLN network.

MODFLOW-USG does not require information about cell shapes or how cells are positioned in space (Panday et al. 2013). Spatial information about cells, however, is critical to a particle tracking model. Fortunately, a grid specification file (GSF) was decided upon that provides x, y and z coordinates for the vertices of a cell. mod-PATH3DU requires this file for unstructured grid models. If a structured grid is used and a GSF file is not provided, mod-PATH3DU uses the information in the DELR, DELC and BOTM arrays of the DIS file for the necessary spatial information. The format for the GSF file is provided in the Input Instructions section. This GSF file is supported by Groundwater Desktop and many of the popular MODFLOW-USG interfaces.

[2] mod-PATH3DU requires the CBB file be written using the COMPACT BUDGET option in the MODFLOW output control (OC) file.

# Background

## Structured Grids

The type of grid available to the original MODFLOW formulation is a structured grid. A structured grid is characterized by regular connectivity. In the case of a structured MODFLOW grid this connectivity is seven-point: each cell in the grid is connected to the two adjacent cells along each coordinate direction. Each cell in a structured grid can be addressed by index (*i*,*j*) in two-dimensions (2D) or (*i*,*j*,*k*) in three-dimensions (3D), where *i*, *j*, *k* refer to row, column and layer number, respectively. An example of a 2D projection of a 3D structured grid is shown in Figure 1. The grid spacing between each cell in the *x*-, *y*- or *z*- direction is *dx*, *dy* or *dz*. Structured grids may be used in different numerical approximation algorithms of differential equations, for example, the finite element method, the finite volume method, as well as, the finite difference method.

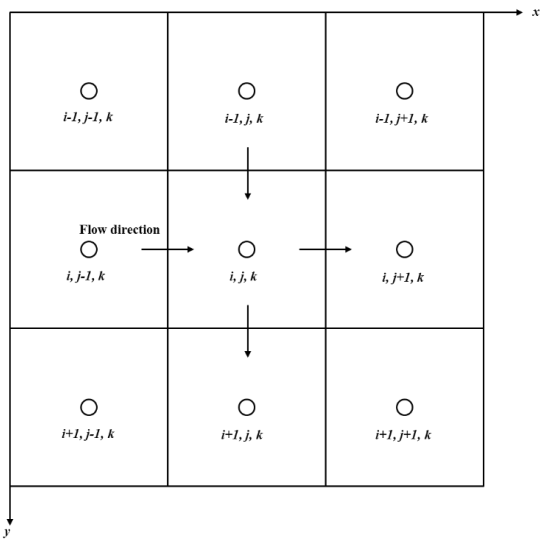



Figure 1 - Example of a 2D structured grid

## Unstructured Grids

An unstructured grid is characterized by irregular connectivity, that is, the number of adjacent cells is variable for each cell. The commonly used elements for this grid type are triangles and quadrilaterals in 2D or tetrahedra and hexahedra in 3D, in irregular patterns. Compared with structured grids, unstructured grids provide better representation of complex boundaries and can facilitate refinement of the spatial discretization of a model in areas of abrupt changes in groundwater velocities, for example in the vicinity of sources and sinks. The tradeoff is that increased computer memory is required to explicitly store neighboring connectivity. Grids of this type may be used with the finite volume or finite element methods. MODFLOW-USG supports a variety of unstructured grid types. Examples of unstructured grid types are shown in Figure 2.

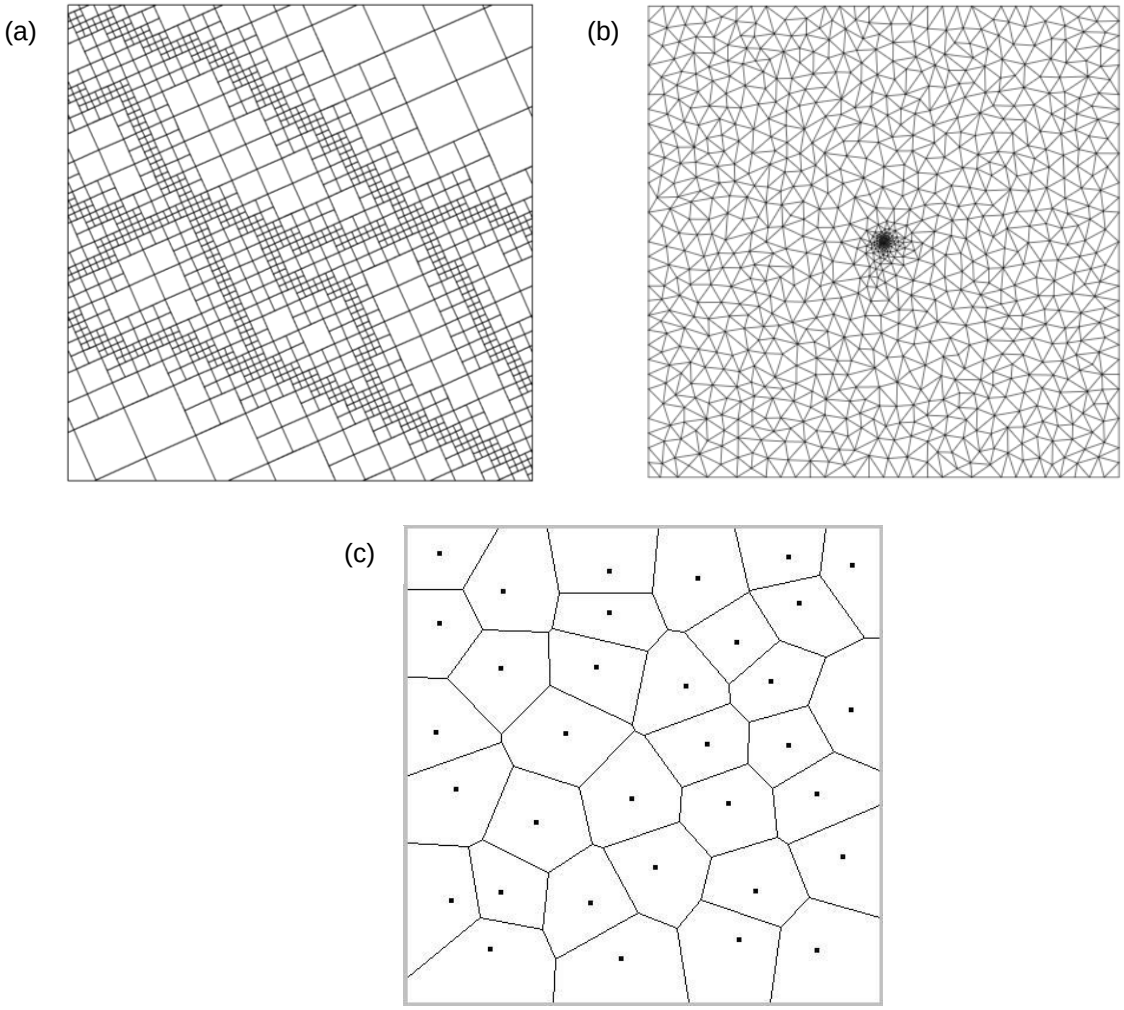



Figure 2 - Examples of unstructured grids: (a) rectangular quadtree, (b) triangular, and c) Voronoi

A stable type of unstructured grid, Voronoi cells, is used widely in the fields of science and technology. In this type of grid, each of the finite difference cells is a Voronoi tessellation of a Delaunay triangulation. An example Voronoi grid is shown in Figure 2.

## Particle Tracking Algorithms

### The Pollock Method

The Pollock (1989) method is a semi-analytical particle tracking method implemented for structured grids in MODPATH (Pollock, 2012). The principle components of the velocity vector of

a particle within an individual cell are computed using linear interpolation based on the velocity components on the cell faces.

$$v_x = A_x(x - x_1) + v_{x_1} \quad \text{(2-1a)}$$
$$v_y = A_y(y - y_1) + v_{y_1} \quad \text{(2-2a)}$$
$$v_z = A_z(z - z_1) + v_{z_1} \quad \text{(2-3a)}$$

where

$$A_x = \frac{v_{x_2} - v_{x_1}}{\Delta x} \quad \text{(2-2a)}$$
$$A_y = \frac{v_{y_2} - v_{y_1}}{\Delta y} \quad \text{(2-2b)}$$
$$A_z = \frac{v_{z_2} - v_{z_1}}{\Delta z} \quad \text{(2-2c)}$$

The components of the velocity of a particle, p, are defined as:

$$v_{xp} = \frac{dx}{dt}; \qquad v_{yp} = \frac{dy}{dt}; \ldots \qquad v_{zp} = \frac{dz}{dy}$$

Therefore:

$$\left(\frac{dx}{v_x}\right)_p = dt \quad \text{(2-3a)}$$
$$\left(\frac{dy}{v_y}\right)_p = dt \quad \text{(2-3b)}$$
$$\left(\frac{dz}{v_z}\right)_p = dt \quad \text{(2-3c)}$$

Substituting Equations (2-1) into Equations (2-3) and integrating Equations (2-3) over $[t_1, t_2]$:

$$\int_{x_p(t_1)}^{x_p(t_2)} \frac{dx_p}{A_x(x_p - x_1) + v_{x_1}} = \int_{t_1}^{t_2} dt \quad \text{(2-4a)}$$
$$\int_{y_p(t_1)}^{y_p(t_2)} \frac{dy_p}{A_y(y_p - y_1) + v_{y_1}} = \int_{t_1}^{t_2} dt \quad \text{(2-4b)}$$
$$\int_{z_p(t_1)}^{z_p(t_2)} \frac{dz_p}{A_z(z_p - z_1) + v_{z_1}} = \int_{t_1}^{t_2} dt \quad \text{(2-4c)}$$

Since, $A_x$, $A_y$, and $A_z$ are constant within a given finite-difference cell, Equation (2-4a) can be integrated to yield a closed form expression:

$$\ln\frac{A_x[x_p(t_2)-x_1]+v_{x_1}}{A_x[x_p(t_1)-x_1]+v_{x_1}}=A_x\Delta t \tag{2-5}$$

Rearranging Equation (2-5) by substituting $A_x[x_p(t_1)-x_1]+v_{x_1}$ for $v_{x_p}(t_1)$:

$$x_p(t_2)=x_1+\frac{1}{A_x}[v_{x_p}(t_1)\exp(A_x\Delta t)-v_{x_1}] \tag{2-6a}$$

Similarly, Equations (2-4) in the *y*- and *z*- directions can be rewritten as:

$$y_p(t_2)=y_1+\frac{1}{A_y}[v_{y_p}(t_1)\exp(A_y\Delta t)-v_{y_1}] \tag{2-6b}$$

$$z_p(t_2)=z_1+\frac{1}{A_z}[v_{z_p}(t_1)\exp(A_z\Delta t)-v_z] \tag{2-6c}$$

The Pollock particle tracking algorithm can be illustrated using a two-dimensional example in the *x*-*y* plane shown in Figure 3. As shown in the figure, the particle trajectory starts at point $(x_p, y_p)$ at time $t_p$ and ends at the particle exiting point $(x_e, y_e)$ at time $t_e$. This example assumes that the velocity components in the *x*- and *y*- directions at each face, $v_{x_1}$, $v_{x_2}$, $v_{y_1}$, and $v_{y_2}$, are all greater than zero. The particle is expected to exit the cell across either face $x_2$ or face $y_2$ depending on the time required for the particle to reach the two downstream faces. The time required to reach face $x_2$ can be computed using Equation (2-5):

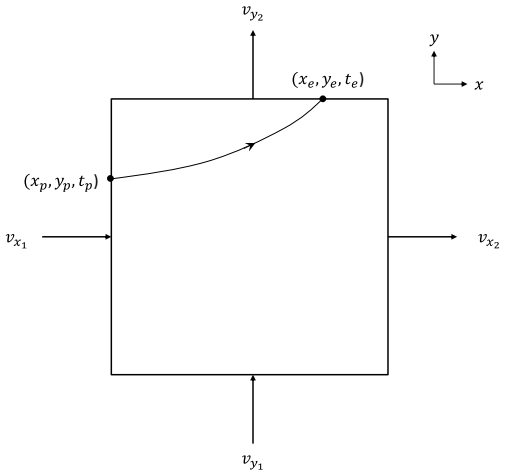



Figure 3 - Example of computing pathlines using the Pollock method

$$\ln\frac{v_{x_2}}{v_{x_p}}=A_x\Delta t_x \tag{2-7}$$

where $A_x[x_p(t_2)-x_1]+v_{x_1}=A_x[x_2-x_1]+v_{x_1}=v_{x_2}$
and $A_x[x_p(t_1)-x_1]+v_{x_1}=v_{x_p}(t_p)=v_{x_p}$

Rearranging Equation (2-7) for $\Delta t_x$ yields:

$$\Delta t_x = \frac{1}{A_x} \ln \frac{v_{x_2}}{v_{x_p}} \tag{2-8}$$

Similarly, the time required to reach face $y_2$ is expressed as:

$$\Delta t_y = \frac{1}{A_y} \ln \frac{v_{y_2}}{v_{y_p}} \tag{2-9}$$

The time required for the particle to move from the initial position to the exit point, $\Delta t_e$, is the smaller of $\Delta t_x$ and $\Delta t_y$. If $\Delta t_x$ is smaller than $\Delta t_y$, the particle will leave the cell from face $x_2$; If $\Delta t_y$ is smaller than $\Delta t_x$, the particle will leave the cell from face $y_2$. The corresponding exit coordinates $(x_e, y_e)$ are:

$$x_e = x_1 + \frac{1}{A_x}[v_{x_p} \exp(A_x \Delta t_e) - v_{x_1}] \tag{2-10a}$$

$$y_e = y_1 + \frac{1}{A_y}[v_{y_p} \exp(A_y \Delta t_e) - v_{y_1}] \tag{2-10b}$$

The total elapsed time at which the particle leaves the cell is given by $t_e = t_p + \Delta t_e$. The same procedure is then repeated to move the particle through the next cell until it reaches a discharge point or one of the termination criteria is met (for example, the particle enters a hydraulic sink).

The Pollock method assumes that the velocity field varies linearly across a cell and a constant velocity vector at each cell face is used to represent the local velocity field within a cell. The velocity components of a particle in the *x*-, *y*- or *z*- directions depend only on the local coordinate of the particle's position in that direction. The particle path and travel time within a cell are computed by integration for the finite difference method with structured grids. This method cannot be used for finite-element or integrated finite-difference schemes that have unstructured grids with more complex cell and node connections.

**The SSP&A Method**

The SSP&A method was originally developed by Tonkin and Larson (2002) to track particles and estimate hydraulic capture on a mapping of ground water level data under the influence of pumping. Later it was used by Karanovic et al. (2009) to calculate capture frequency maps. It is a grid independent approach and therefore, sufficiently flexible to be used with either structured or unstructured grids (e.g., triangular, quadtree, Voronoi). Unlike the Pollock method, which uses linear velocity interpolation based on the flow rates at cell faces calculated by MODFLOW, the SSP&A method evaluates the velocity components of a particle in *x*- and *y*- directions using the interpolated head based on the distribution solved for by MODFLOW. The head interpolation is implemented in the vicinity (blue points) of a particle (black point) using universal kriging, from

which the velocity components in the *x*- and *y*- directions (red lines) are calculated according to Darcy's law (Figure 4). The fourth-order Runge-Kutta scheme used in PATH3D (Zheng, 1989; Zheng, 1992) or a simple Euler approach can be employed in this method for the particle tracking calculations. Currently, in the vertical (*z*) direction the SSP&A method implements the Pollock method.

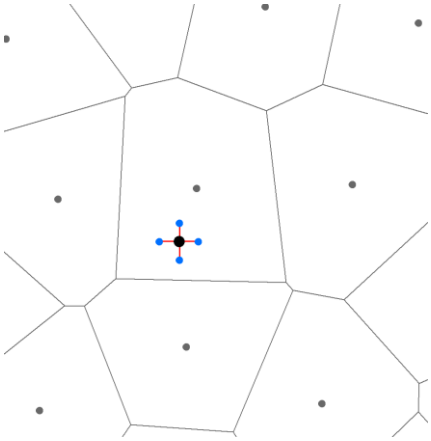


Figure 4 - Schematic of SSP&A method velocity calculation

***Kriging***

Kriging is often used to interpolate irregularly spaced measurement data to unsampled locations (typically a grid of points suitable for contouring). The values at unknown locations are then estimated by minimizing the error variance of predicted values based on their spatial distribution. In the context of mod-PATH3DU, the heads calculated by MODFLOW that are used to determine velocity constitute the "measured" data, while the position of a particle is the "unsampled" location. Kriging is an exact interpolator in the absence of measurement error or co-located data. Two popular forms of kriging are simple and ordinary. In simple kriging, the mean of the data is assumed to be constant everywhere and its value known *a-priori*. With ordinary kriging, the mean is assumed to be unknown, but is estimable using some function of the measured data. In addition, ordinary kriging can support a spatially varying mean that is not only a function of the data, but includes some trend or "drift". This form of ordinary kriging is called universal kriging. Universal kriging is a means of incorporating the shape associated with different hydrologic features into the estimate at an unsampled location. For example, in the vicinity of a pumping well, a point sink/source of known strength, derived from the Thiem equation, can be used to incorporate the logarithmic drawdown shape (Tonkin and Larson, 2002). The mathematical details on kriging have been well documented by Journel and Huijbregts (1992), Cressie (1993) and Deutsch and Journel (1998). The kriging algorithm used in the SSP&A method is adapted from the public domain software Geostatistical Software Library (GSLIB) (Deutsch and Journel, 1998) and Skrivan and Karlinger (1980). Use of drift terms with the SSP&A method is invoked

using the IFACE variable discussed in the Boundary Packages and Internal Sinks/Sources section.

## Runge-Kutta Numerical Scheme

To increase the accuracy of the particle tracking calculations relative to a first-order Euler tracking scheme, a higher order of numerical scheme is desired. The SSP&A tracking algorithm uses a fourth-order Runge-Kutta method. The basic principle of this method for solving the particle tracking equation is to advance a particle from the initial position $(x_n, y_n, z_n)$ over a time interval $\Delta t$ by combining the information from several trial steps, and then using the information to match a fourth-order Taylor series expansion. The velocity is evaluated four times for each particle tracking step: once at the initial point ($p_1$), twice at trial midpoints of the step ($p_2$ and $p_3$) and once at a trial endpoint ($p_4$), as shown in Figure 5. Based on the velocities evaluated at the four points, the position of the particle at the beginning of the next step $(x_{n+1}, y_{n+1}, z_{n+1})$ is calculated as:

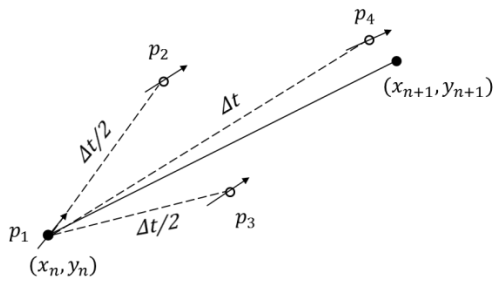



Figure 5 - Illustration of the fourth-order Runge Kutta method

$$x_{n+1} = x_n + \frac{(k_1 + 2k_2 + 2k_3 + k_4)}{6} \quad (2\text{-}11a)$$

$$y_{n+1} = y_n + \frac{(l_1 + 2l_2 + 2l_3 + l_4)}{6} \quad (2\text{-}11b)$$

$$z_{n+1} = z_n + \frac{(m_1 + 2m_2 + 2m_3 + m_4)}{6} \quad (2\text{-}11c)$$

where

$$\begin{aligned} k_1 &= \Delta t v_x(x_n, y_n, z_n, t_n) \\ k_2 &= \Delta t v_x(x_n + \frac{k_1}{2}, y_n + \frac{l_1}{2}, z_n + \frac{m_1}{2}, t_n + \frac{\Delta t}{2}) \\ k_3 &= \Delta t v_x(x_n + \frac{k_2}{2}, y_n + \frac{l_2}{2}, z_n + \frac{m_2}{2}, t_n + \frac{\Delta t}{2}) \\ k_4 &= \Delta t v_x(x_n + k_3, y_n + l_3, z_n + m_3, t_n + \Delta t) \end{aligned} \quad (2\text{-}12)$$

$$\begin{aligned} l_1 &= \Delta t v_y(x_n, y_n, z_n, t_n) \\ l_2 &= \Delta t v_y(x_n + \frac{k_1}{2}, y_n + \frac{l_1}{2}, z_n + \frac{m_1}{2}, t_n + \frac{\Delta t}{2}) \end{aligned} \quad (2\text{-}13)$$

$$
\begin{aligned}
l_3 &= \Delta t v_y(x_n + \frac{k_2}{2},\ y_n + \frac{l_2}{2},\ z_n + \frac{m_2}{2},\ t_n + \frac{\Delta t}{2}) \\
l_4 &= \Delta t v_y(x_n + k_3,\ y_n + l_3,\ z_n + m_3,\ t_n + \Delta t)
\end{aligned}
$$

$$
\begin{aligned}
m_1 &= \Delta t v_z(x_n,\ y_n,\ z_n,\ t_n) \\
m_2 &= \Delta t v_z(x_n + \frac{k_1}{2},\ y_n + \frac{l_1}{2},\ z_n + \frac{m_1}{2},\ t_n + \frac{\Delta t}{2}) \\
m_3 &= \Delta t v_z(x_n + \frac{k_2}{2},\ y_n + \frac{l_2}{2},\ z_n + \frac{m_2}{2},\ t_n + \frac{\Delta t}{2}) \\
m_4 &= \Delta t v_z(x_n + k_3,\ y_n + l_3,\ z_n + m_3,\ t_n + \Delta t)
\end{aligned}
\qquad (2\text{-}14)
$$

The velocity components at points $p_1$, $p_2$, $p_3$ and $p_4$ are calculated using Darcy's law from the heads in the vicinity of a particle by interpolation using kriging. The series of calculations is repeated to move a particle step by step until the particle reaches a discharge point or until a termination criterion is met.

Compared with the Pollock (1994) semi-analytical method, the fourth-order Runge-Kutta method is generally more computationally intensive and may introduce numerical truncation errors. However, the Runge-Kutta method is more general, in that it is not limited to linear interpolation, but applicable to any velocity interpolation scheme.

The accuracy of the Runge-Kutta method depends on the tracking step size $\Delta t$. If $\Delta t$ is too large, the calculation of the velocity components may be inaccurate and the particle tracking pathline may divert from the actual flow path. If $\Delta t$ is too small, significant computational effort may be required to move a particle over a given distance. Thus, it is important to determine an appropriate step size $\Delta t$ for the particle tracking process. The adaptive step size control procedure used in the PATH3D code (Zheng, 1989; Zheng, 1992), "step doubling", is also implemented in mod-PATH3DU. The tracking step $\Delta t$ is taken twice: once as a full step and once as two half steps, illustrated in Figure 6. If $\Delta t$ is sufficiently brief for accurate tracking, the difference between the particle endpoint locations calculated with a full step and by taking two half steps, denoted as $\Delta S$, will be small. Because the Runge-Kutta is a fourth-order accurate method, $\Delta S$ can be scaled as $(\Delta t)^5$:

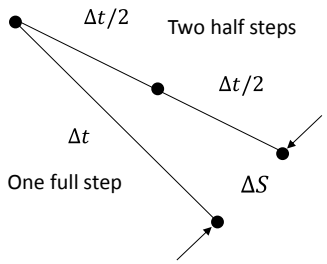



Figure 6 - Illustration of the adaptive step size control procedure

$$
(\frac{\Delta t_0}{\Delta t})^5 = \frac{\Delta S_0}{S} \qquad (2\text{-}15)
$$

where $\Delta S_0$ and $\Delta S$ are the differences in particle locations with respect to time steps $\Delta t_0$ and $\Delta t$. To estimate the step size $\Delta t_0$, a "safety factor", $f_s$, is assigned in Equation (2-15) and rearranging the equation to yield,

$$\Delta t_0 = f_s \Delta t \left(\frac{\Delta S_0}{S}\right)^{0.2} \quad (2\text{-}16)$$

The safety factor has a value slightly smaller than unity (e.g., 0.9). Equation (2-16) is implemented in every tracking step to estimate the required step size adjustment. If the value of $\Delta S$ calculated with respect to the step size $\Delta t$ is larger than the required accuracy specified by $\Delta S_0$, the step size is then reduced to $\Delta t_0$ and the tracking calculation is repeated for that step. If $\Delta S$ is smaller than $\Delta S_0$, the tracking calculation based on the step size $\Delta t$ is acceptable, and the initial step size for the next step is taken as $\Delta t_0$. The difference in particle locations $\Delta S$ is treated as an indicator for the step size adjustment and is a vector in *x*-, *y*- and *z*- directions which can be expressed in terms of a single error criterion, ***ε***, as,

$$\begin{aligned} \Delta X_0 &= \varepsilon \times XMAX \\ \Delta Y_0 &= \varepsilon \times YMAX \\ \Delta Z_0 &= \varepsilon \times ZMAX \end{aligned} \quad (2\text{-}17)$$

where $XMAX$, $YMAX$ and $ZMAX$ are scaling factors in the three directions and are the maximum lengths of the flow domain in *x*-, *y*- and *z*- directions. Given an error criterion, ***ε***, as specified by the user, the maximum allowed error in all directions can be calculated according to Equation (2-17).

## Boundary Packages and Internal Sinks/Sources

### IFACE

MODPATH computes the velocity vector based on the flow components of the cell faces. It is important that the flux across each cell face include boundary condition flows when appropriate. The auxiliary variable IFACE is the mechanism by which boundary flows are assigned to a particular cell face. For example, consider recharge, its flux is vertical and enters a cell through the top face. If the recharge flux is not assigned to the top face the velocity in the *z*-direction calculated by MODPATH would be incorrect for the upper layer and a particle could only be reliably tracked within layers below. In MODPATH, IFACE ranges from 0 to 6, where 1 through 4 represent the different side faces of a cell (Figure 7), 5 and 6, denote the bottom and top faces, respectively, and 0 is used to specify an internal sink/source (i.e. flow is not assigned to a face). The default IFACE for cells not explicitly specified is 0.

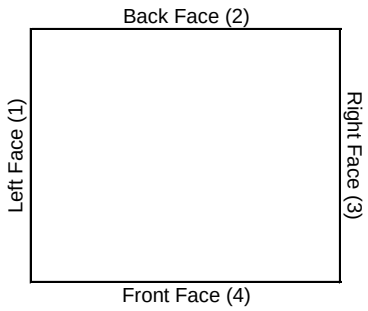



Figure 7 - MODPATH IFACE designation for side faces

IFACE can be specified in two ways: 1) using the auxiliary IFACE variable available to MODFLOW, or 2) using the default IFACE specification of MODPATH. By specifying IFACE through MODFLOW, it can be assigned on a per-cell basis, whereas, the default IFACE option of MODPATH specifies IFACE for all cells belonging to a particular boundary package. For example, if the WEL package of MODFLOW is being used to represent both recharge and pumping wells, specifying IFACE through MODFLOW would allow IFACE to be set to 6 for the recharge "wells", and 0 for the pumping wells. The default IFACE specification in MODPATH would set all cells listed in the WEL package to the desired IFACE value (0 or 6, for example).

### Internal Strong/Weak Sinks/Sources (and UK drift terms)

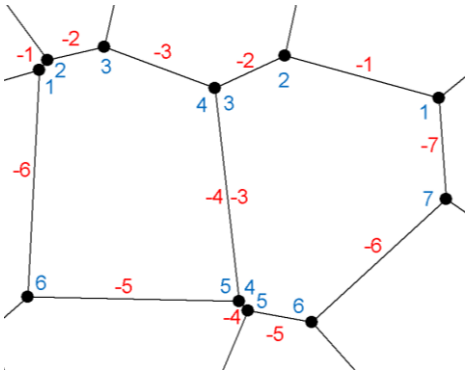



Figure 8 - mod-PATH3DU IFACE designation for side faces

In mod-PATH3DU use of IFACE is maintained to support the Pollock method and is the mechanism by which drift terms are invoked in the SSP&A method. With mod-PATH3DU, the side face designation is different because the number of faces can vary from cell-to-cell in an unstructured grid. Figure 8 illustrates how side faces (red) are numbered. It is dependent on the order in which the vertices (blue) of a cell are listed in the grid specification file (GSF). The face between the first and second node is assigned -1, between the second and third -2, and so on. Bottom and top faces are denoted in the same way as MODPATH, with 5 and 6, respectively. Specification of an internal sink/source is different. In the vicinity of a pumping well, the SSP&A method uses a local analytic solution to augment its calculation of velocity. IFACE is the mechanism by which this functionality is activated. If IFACE is set to 0 for a boundary cell, it is assumed that boundary is a pumping well and is used in the local analytic approximation. IFACE of 7 is used to indicate an internal sink/source for which the local analytic solution does not apply, for example constant-head. As development of the SSP&A tracking method continues, IFACE will be used to indicate different universal kriging drift terms for other boundary packages.

## Special Cases

### Quasi Three-dimensional Representation of Confining Layers

Implicit confining layers are not supported at this time. The program is setup to handle these layers, but at the time of this writing the option was not tested. If there is interest in this option please contact the corresponding author.

### Distorted Vertical Discretization and the Water Table

The manner in which distorted vertical discretization is handled in mod-PATH3DU is identical to MODPATH. In each cell, elevation, $z$, is transformed to a local coordinate system, $z_L$, that ranges from 0 at the bottom of a cell to 1 at the top or water table elevation. By scaling the velocity in the vertical direction by the saturated thickness of the cell, a particle can be tracked in this transformed space provided that $z_L$ is updated when a particle changes layers. The "Non-Rectangular Vertical Discretization" and "Water Table Layers" sections of the MODPATH manual (Version 4) provide excellent discussions of tracking in this transformed space.

### Cross Section Models

To track on a cross section model using the SSP&A method the XSECTION option must be specified in the basic package (BAS) of MODFLOW-USG. This requirement is necessary because the SSP&A method is head based and velocity in the y-direction cannot be accurately calculated for cross section models. When the XSECTION option is used velocity in the y-direction is set to 0.

### Weak/Strong Sinks/Sources

mod-PATH3DU does not currently support the weak sink/source options that are incorporated within either MODPATH (Pollock, 1994) or Path3D (Zheng, 1992). Testing indicates the SSP&A method provides more meaningful results in the vicinity of pumped wells regardless of grid geometry. Since calculation of the approximate stagnation zone is incorporated within the SSP&A method based on a local regression, particles should track quite accurately within a cell unless the sink is very weak and its signal is overwhelmed by other local factors.

### Connected Linear Networks (CLN)

Currently, mod-PATH3DU only supports the CLN package if it is used to simulate a well. It does not track particles within networks, however, it is hoped a future release will. To track particles in the vicinity of a CLN well a default IFACE of 0 must be assigned to the CBB file property "GWF TO CLN" in the MPBAS file (see Input Instructions). Currently, it is assumed all networks in the CLN package represent a pumping well. This assumption will be rectified in a future release when support for additional boundary packages, such as the river (RIV) and drain (DRN), are supported.

# mod-PATH3DU Overview

## Time Concepts

To understand the particle tracking process in mod-PATH3DU, it is necessary to be familiar with the time concepts defined in the program, illustrated in
Figure 9. The time concepts are defined below.

- MODFLOW-USG simulation time: the time generated from the MODFLOW-USG simulation. It starts from zero and increases through to the end of the simulation.
- Reference time: the starting time for the particle-tracking with respect to the start of the MODFLOW-USG simulation.
- mod-PATH3DU simulation time (or tracking time): the mod-PATH3DU simulation time which for forward tracking is defined as the difference between the MODFLOW-USG simulation time and the reference time, and for backward tracking is defined as the difference between the reference time and the MODFLOW-USG simulation time. The tracking time is always a positive value.
- Release time: is the value of time when a particle is released with respect to the mod-PATH3DU simulation time.
- Stop time: the time at which to stop the tracking. For forward tracking, any timesteps after the timestep within which the stop time is will be erased; for backing tracking, any timesteps after the stop time will be completely erased.
- If the *StopOption* equals to 3, mod-PATH3DU will allow specifying a value at which to stop the particle tracking. This time value is not the absolute MODFLOW simulation time, but a relative value with respect to the reference time:
  *The absolute stop time = reference time + stop time (forward tracking);*
  *The absolute stop time = reference time – stop time (backward tracking).*

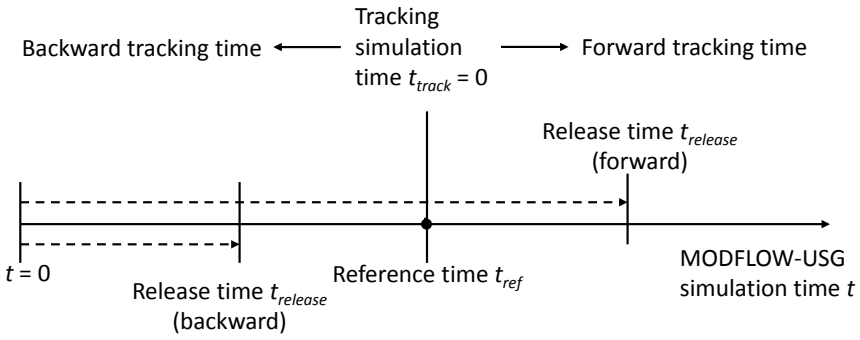
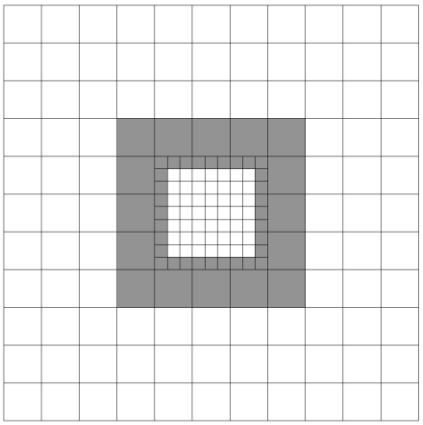



Figure 9 - Illustration of time concepts in mod-PATH3DU

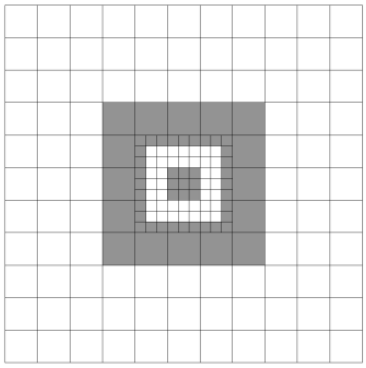
## Tracking Scheme Selection

Currently, mod-PATH3DU provides two schemes for tracking particles: the Pollock method, and the SSP&A method. This section provides guidance on which scheme to use for a particular application. mod-PATH3DU is quite flexible in that it allows users to choose which tracking method to use on a per-cell basis. As such, one method is not required for an entire application, rather, the choice of method is dictated by the computational efficiency of each method and grid and flow characteristics in different parts of the groundwater model domain.



Certainly, for grids that use non-rectangular cells, i.e. Voronoi, the SSP&A method must be used throughout the domain. However, for grids based on rectilinear cells, i.e. quadpatch and quadtree, the choice of tracking method is more nuanced. Consider the quadpatch grid shown in the figure to the left. Each cell is rectilinear, and only those cells shaded gray have more than the seven-point connectivity required by the Pollock method. As such, with mod-PATH3DU, the Pollock method can be used to track on the unshaded cells because it is computationally faster and the SSP&A method used on the shaded cells as they are “unstructured”.

Consider further a pumping well in the center of the same quadpatch grid shown above. To get the smooth particle paths in the vicinity of this well possible with the SSP&A method, the user can specify its use for surrounding cells as in the figure to the right.



Generally speaking, use of the Pollock method is advantageous for rectilinear cells with structured connectivity not near any important boundaries (hydrologic features) or sinks/sources because it is computationally faster. The SSP&A method is required for unstructured cells and is more robust in the vicinity of hydrologic features (although these are not supported at this time) and point sinks/sources. Further, both methods have limitations and understanding these is critical to choosing the appropriate algorithm for a problem. See the Limitations section for a discussion of these constraints.

## Limitations

### Pollock Method

For a detailed discussion of the limitations of the Pollock method – please refer to the MODPATH manual.

### SSP&A Method

The applicability of the SSP&A method to tracking problems is limited by 1) the assumptions in the underlying tracking scheme, 2) the interpolation method it employs, and 3) limitations in the groundwater flow model, including discretization and boundary effects.

The accuracy of the Runge-Kutta scheme depends on the tracking step size $\Delta t$. If $\Delta t$ is too large, the calculation of the velocity components may be inaccurate and the particle tracking pathline may divert from the actual flow path. However, mod-PATH3DU mitigates this error by implementing the adaptive step size control procedure used in PATH3D called "step doubling". For more information on the Runge-Kutta scheme please see Zheng (1989;1992;1994) and Zheng and Bennett (2002).

The accuracy of the universal kriging interpolation is dictated by (a) grid discretization, (b) severe heterogeneities, and (c) proximity to certain boundaries. The refinement obtained by adding more cells spaced closer together will provide the approach with better information to calculate velocity. Nevertheless, the use of universal kriging can overcome many discretization and boundary effects provided an appropriate drift term is used. However, because the coefficients of these drift terms are determined through a regression, they can be made zero or their sign reversed (although this is unlikely). For example, when pumping in the presence of a strong regional gradient, the pumping well signal (its contribution to the hydraulic-head in a cell) may be overwhelmed by the signal from the regional gradient and thus made zero in the regression. Drift terms to overcome hydraulic conductivity dichotomies between two cells and to account for additional boundaries, including no-flow and streams/rivers, are possible, but are not yet available in this version of mod-PATH3DU.

Because the Pollock method is used to calculate velocity in the *z*-direction vertical sub-discretization is not supported at this time. Further, the cell structure in each layer must be identical.

# Input Instructions

## Input Data Format

mod-PATH3DU supports the input and output file formats of MODPATH6 detailed by Pollock, 2012. These files include the simulation, name, basic, and pathline files. However, with MODPATH6, some of the required information is already listed in MODFLOW-USG input files. All references to duplicate information are removed from the input files in mod-PATH3DU. Detailed input directions for each file are provided in this section.

Input data are read free format: the spacing of values for each record is not fixed and between two records a SPACE or COMMA can be used for separation. It is important to specify all input data items explicitly. Apostrophes are not required for character data items if the character data item is the only record on a line; otherwise, if multiple records on a line and a character data item contains a space, apostrophes must be used for data specification. For reading array input, mod-PATH3DU uses the same array reader subroutines (U2DREL, U2DINT, and U1DREL) used by MODFLOW (Harbaugh, 2005); detailed information can be found in Harbaugh (2005).

## Tracking Simulation File (MPSIM)

The mod-PATH3DU simulation file contains information for defining a particle tracking problem and specifying the tracking method. The name of the simulation file can be specified on the mod-PATH3DU command line.

```
(1)  Example.mpnam
(2)  Example.mplist
(3)      2       1       1       1       2       3       2       1       2       2       1       1
(4)  Example.ept
(5)  Example.ptl
(6)          1           1      1.000
(7)      365.0
(8)  Example.ptr
(9)          0
```

Figure 10 - Example MPSIM file

Table 1 - MPSIM input instructions

| Item | Variable[1] | Type[2] | Options / Values | Description |
|---|---|---|---|---|
| 0 | [HEADER] | C | #TEXT | Header. |
| 1 | MPNAMFile | C | - | Name of the MPNAM file. |
| 2 | MPLSTFile | C | - | Name of the mP3DU listing file. |
| 3 | SimulationType | I | 2 - Pathline simulation | A flag indicating the type of particle-tracking simulation. |
| | TrackingDirection | I | 1 - Forward tracking<br>2 - Backward tracking | A flag indicating the direction of the particle tracking computation. |
| | WeakSinkOption | I | 1 - Allow particles to pass through weak sinks | Flag indicating how weak sinks are to be treated. Only used with Pollock method. |
| | WeakSourceOption | I | 1 - Allow particles to pass through weak sources | Flag indicating how weak sources are to be treated. Only used with Pollock method. |
| | ReferenceTimeOption | I | 1 - Specify a value for reference time<br>2 - Specify stress period, time step and relative time position within the time step to use to compute the reference time | A flag indicating how reference time will be specified. |
| | StopOption | I | 1 - Stop at the end (forward tracking) or | A flag indicating how the particle |

| | | | | |
|---|---|---|---|---|
| | | | beginning (backward tracking) of the MODFLOW-USG simulation<br>2 - Track until all particles reach their termination points<br>3 - Specify a value of tracking time at which to stop | tracking simulation should be terminated. |
| | ParticleGenerationOption | I | 2 - Read particle locations from an external file | A flag indicating how particle starting locations are generated. |
| | TimePointOption | I | 1 - Time points are not specified | Ignored. |
| | BudgetOutputOption | I | 1 - No budget checking | Ignored. |
| | ZoneArrayOption | I | 1 - Zone data are not supplied | Ignored. |
| | RetardationOption | I | 1 - Retardation factors are not read or used in the velocity calculations | Ignored. |
| | AdvectiveObservationOption | I | 1 - Advective observations are not computed or saved | A flag indicating if advective observations are computed and saved as output. |
| 4 | EndpointFile | C | - | File name for the endpoint file (ignored). |
| 5 | PathlineFile | C | - | File name for the pathline file. |
| 6 | [ReferenceTime] | R | Reference time | If ReferenceTimeOption = 1 |
| | | I | Stress period | If ReferenceTimeOption = 2 |
| | | I | Time step | If ReferenceTimeOption = 2 |
| | | R | Relative time (between 0 and 1) | If ReferenceTimeOption = 2 |
| 7 | [StopTime] | R | Stop time | If StopOption = 3 |
| 8 | StartingLocationsFile | C | - | File name of the particle starting locations file. |
| 9 | StopZone | I | 0 - Particles should not be stopped at a user specified zone | Ignored. |

1 Square brackets indicate optional or dependent variables
2 C Character
I Integer
R Real

## Tracking Name File (MPNAM)

The name file contains the names of input files that are used by mod-PATH3DU. Currently, the files required by mod-PATH3DU are (1) the MODFLOW-USG name file, (2) mod-PATH3DU basic file, and (3) the grid specification file if MODFLOW-USG was executed in "unstructured" mode.

```
(1)    MFNAM                11    Example.nam
(1)    GSF                  12    Example.gsf
(1)    MPBAS                13    Example.mpbas
(1)    MP3DU                14    Example.mp3du
```

Figure 11 - Example MPNAM file

Table 2 - MPNAM input instructions

| Item | Variable[1] | Type[2] | Options / Values | Description |
|---|---|---|---|---|
| 0 | [HEADER] | C | #TEXT | Header. |
| 1[3] | FileType | C | MFNAM - MODFLOW-USG NAM file<br>GSF - Grid specification file<br>MPBAS - mod-PATH3DU basic data file<br>MP3DU – mod-PATH3DU settings file | Type of the file. |
| | FileUnit | I | Greater than 10 | Unique unit number to be assigned to the file. |
| | FileName | C | - | Name of the file. |

1 Square brackets indicate optional or dependent variables
2 C Character
I Integer
R Real
3 Repeat for each file to be listed

## Tracking Basic Package (MPBAS)

The mod-PATH3DU basic file contains additional data that is dependent on the MODFLOW-USG grid and boundary conditions. The name of the MPBAS file is specified in the MPNAM file.

```
(1)                  1
(2)    RECHARGE
(3)    6
(4)    CONSTANT                    0.200   Porosity Layer 1
(4)    CONSTANT                    0.200   Porosity Layer 2
(5)    CONSTANT                        2   MTH Layer 1
(5)    CONSTANT                        2   MTH Layer 2
```

Figure 12 - Example MPBAS file

Table 3 - MPBAS input instructions

| Item | Variable[1] | Type[2] | Options / Values | Description |
|---|---|---|---|---|
| 0 | [HEADER] | C | #TEXT | Header. |
| 1 | DefaultIFACECount | I | Greater than or equal to 0 | The number of budget items for which a default IFACE is specified. |
| | | | Repeat items 2 and 3 DefaultIFACECount times | |
| 2 | BudgetLabel | C | CONSTANT HEAD<br>WELLS<br>RECHARGE<br>etc. | Text label used in the MODFLOW-USG budget file. The mod-PATH3DU log reports these for each stress period if in doubt. |
| 3 | DefaultIFACE | I | less than 0 - Flow is assigned to the corresponding cell face (see IFACE section)<br>0 - Flow is treated as an internal sink or source, point-logarithmic drift activated for this cell<br>5 - Flow is assigned to the bottom face of the cell<br>6 - Flow is assigned to the top face of the cell<br>7 – Flow is treated as an internal sink or source | The value of IFACE to be assigned to this BudgetLabel |
| 4[3] | Porosity | R | Between 0.0 and 1.0 | Porosity. Read using U2DREL. |
| 5[3] | MTH | I | 1 - Pollock Method<br>2 - SSP&A Method | The particle tracking algorithm to use. Read using U2DINT. |

1 Square brackets indicate optional or dependent variables
2 C Character
I Integer
R Real
3 Repeat NLAY times

## mod-PATH3DU Tracking Options Package (MP3DU)

The MP3DU package is an optional input file that can be used to control tracking options, specifically related to the SSP&A method. It uses a keyword input style as detailed below. The keywords are optional and can be listed in any order. If a keyword is not present the default value is used for that option.

```
(1)    TRACK_TYPE                RK4
(2)    STEP_ERROR              1.00E-06
(3)    DT_INIT                 1.00E+01
(4)    DT_MAX                  1.00E+06
(5)    WELL_CAPTURE_RADIUS     1.00E+01
```

Figure 13 - Example MP3DU file

Table 4 – MP3DU file input instructions

| Item | Variable[1] | Type[2] | Options / Values | Description |
|---|---|---|---|---|
| 1 | [TRACK_TYPE] | C | "RK4" (Default)<br>"EULER" | Tracking method. Default is "RK4". |
| 2 | [STEP_ERROR] | R | - | Adaptive stepsize error term, $\varepsilon$, in equation 2-17. Default is 1.00E-06. Larger values will result in a faster runtime with, potentially, less accurate paths. To turn-off the adaptive step size option make STEPERROR large (1.00E+06). |
| 3 | [DT_INIT] | R | - | Initial step size. Default is 10. |
| 4 | [DT_MAX] | R | - | Maximum step size. Default is 1.00E+06. |
| 5 | [WELL_CAPTURE_RADIUS] | R | - | When FORWARD tracking using the adaptive time step option (STEP_ERROR < 1), WELL_CAPTURE_RADIUS is the radial distance from the well, within which, a particle is considered captured. |

1 Square brackets indicate optional or dependent variables
2 C Character
I Integer
R Real

If a simple Euler scheme is desired make STEP_ERROR large (1.00E+06) and set an appropriate maximum time step size.

## Particle Starting Locations File

The mod-PATH3DU particle starting locations file contains information on the time and locations of starting particles. The format for this file has not been finalized and may change in future releases. A particle starting location has two facets: 1) temporal options, and 2) spatial options. As mod-PATH3DU continues to develop, the plan is to evolve the format of this file (and corresponding output files) in such a way as to make typical tracking exercises more automated and therefore, user friendly. For example, a future release will have a "capture zone" starting option. The user will simply indicate wells or stream segments and mod-PATH3DU will execute and write a polygon-shapefile of the capture zone for each of the listed elements.

```
(1)    GRID2D
(2)                 1              0.0
(5)                 1              0.5
(6)            1000.0           1000.0            100.0
(7)            1000.0           1000.0            100.0
(1)    WELL2D
(2)                 1              0.0
(5)                 6              0.1
(8)             100.0            100.0               10              20.0
(1)    OTHER
(2)                 1              0.0
(9)              10.0             10.0                1              0.5
(9)              20.0             20.0                1              0.5
(9)              30.0             30.0                1              0.5
```

Figure 14 - Example particle starting locations file

Table 5 - Particle starting locations input instructions

| Item | Variable[1] | Type[2] | Options / Values | Description |
|---|---|---|---|---|
| | | | Repeat as needed (unless SpatialOption = OTHER, see note 3) | |
| 1 | SpatialOption | C | "GRID2D" - Release particles in a regular grid pattern for a specified layer<br>"WELL2D" - Release particles at some radius around a well for a specified layer<br>"OTHER"[3] - Release particles at listed global X, Y coordinates | Release option. |
| 2 | TemporalOption | I | 1 - A single ReleaseTime will be used for all particles<br>2 - Particles will be released | A flag indicating whether a single or multiple release events will be used for particles. |

| | | | | |
|---|---|---|---|---|
| | | | 3 - ReleaseEventCount times every ReleasePeriodLength<br>Particles will be released ReleaseEventCount times at the specified ReleaseTimes | |
| | ReleaseTime | R | Greater than 0.0 | Release time of particles relative to mod-PATH3DU tracking time. |
| 3 | [ReleaseEventCount] | I | Greater than 0 | If TemporalOption = 2 or 3<br>The number of release events. |
| | [ReleasePeriodLength] | R | Greater than 0.0 | If TemporalOption = 2<br>The time interval between particle release events. |
| 4 | [ReleaseTimes] | R | Greater than 0.0 | If TemporalOption = 3<br>ReleaseEventCount release times relative to mod-PATH3DU tracking time. |
| 5 | [ReleaseLayer] | I | 1 - NLAY | Layer number. If SpatialOption is not OTHER |
| | [RelZ] | R | 0.0 - 1.0 (bottom - top or WT) | Local Z coords. |
| 6 | [XMIN] | R | - | If SpatialOption = GRID2D |
| | [XMAX] | R | - | |
| | [DX] | R | - | |
| 7 | [YMIN] | R | - | If SpatialOption = GRID2D |
| | [YMAX] | R | - | |
| | [DY] | R | - | |
| 8 | [X] | R | - | If SpatialOption = WELL2D |
| | [Y] | R | - | |
| | [NumberOfParticles] | I | - | |
| | [Radius] | R | - | |
| 9 | [X] | R | - | If SpatialOption = OTHER |
| | [Y] | R | - | |
| | [Layer] | I | - | |
| | [Relz] | R | - | |

1 Square brackets indicate optional or dependent variables
2 C Character
I Integer
R Real
3 If SpatialOption = OTHER it is assumed that, following entry of item 2, all remaining lines in the file are item 9

## Grid Specification File (GSF)

The grid specification file provides *x*, *y*, and *z*- coordinates for the cells in a MODFLOW-USG grid. If MODFLOW-USG is being executed in "structured" mode, that is DELR and DELC are specified, this file is not required – mod-PATH3DU will track in local model coordinates using the DELR, DELC and BOTM arrays in the MODFLOW-USG DIS file. At this time, mod-PATH3DU does not recognize the "STRUCTURED" option in the GSF file.

It is expected that many of the popular MODFLOW interfaces will support this file and write it as part of their programs. However, in the event this file is not available, the following input instructions can be used to create the file as needed.

```
(1)  UNSTRUCTURED
(2)                    73775            8          1            1
(3)                   156956
(4)                   2226.0      10230.0   393.037
(4)                   2226.0      10230.0   391.769
(4)                        …
(4)                   2234.0       9910.0   336.513
(5)        1  2228.0  10170.0  416.9   1   8   29   30   39   38   7857   7858   7857   7856
(5)        2  2229.0  10170.0  439.7   1   8   30   47   55   39   7858   7855   7853   7857
(5)        …
(5)    73775  2238.7   9703.2  194.1   8   8 7848 7842 3036 7844  15696  15690  10884  15692
```

Figure 15 - Example GSF file

Table 6 - GSF input instructions

| Item | Variable[1] | Type[2] | Options / Values | Description |
|---|---|---|---|---|
| 1 | GridType | C | "UNSTRUCTURED" | Grid type |
| 2 | NCELL | I | - | Number of cells in model domain (all layers). Equivalent to MODFLOW-USG DIS parameter NCELL. |
| | NLAY | I | NLAY | Number of layers |
| | IZ | I | 0 - Elevations of node and mesh element vertices are not supplied<br>1 - Elevations of node and mesh element vertices are supplied | mod-PATH3DU only supports IZ = 1 |
| | IC | I | 0 - Cell definitions are not provided | mod-PATH3DU only supports IC |

| | | | | | |
|---|---|---|---|---|---|
| | | | 1 - Cell definition of each node is supplied | | = 1 |
| 3 | NVERT | I | | - | Total number of vertices. Vertices are required for both cell top and bottom. |
| | | | Repeat Item 4 NVERT times | | |
| 4 | XVertex | R | | - | X-coordinate of vertex |
| | YVertex | R | | - | Y-coordinate of vertex |
| | ZVertex | R | | - | Z-coordinate of vertex |
| | | | Repeat Item 5 NCELL times | | |
| 5 | CellID | I | | - | Id of cell. |
| | XCellCenter | R | | - | X-coordinate of cell center. |
| | YCellCenter | R | | - | Y-coordinate of cell center. |
| | ZCellCenter | R | | - | Z-coordinate of cell center. |
| | Layer | I | 1 - NLAY | | Layer cell is in. |
| | NumberOfVertices | I | | - | The number of vertices that define this cell. This number includes top and bottom definitions. For example, for a square cell, the number of vertices is 8. |
| | Repeat the following item NumberofVertices times. The vertices must be listed in order (clockwise or counter-clockwise) and list all top or bottom vertices first, and then the other set. | | | | |
| | VertexID | I | | - | The id of the vertex – corresponds to the order in which they are listed as Item 4. |

1 Square brackets indicate optional or dependent variables

2 C Character
I Integer
R Real

# Output File Formats

mod-PATH3DU writes a variety of output files. Primarily these files are listing or log files that report particle tracking options, MODFLOW-USG input, and progress. The endpoint file is not supported at this time. Particle paths are only reported in the pathline file. The format of this file is similar to MODPATH6 and is detailed in the Output File Formats section.

## Pathline File

The pathline file provides temporal and spatial information for each particle as it moves through the flow field calculated by MODFLOW-USG. It lists the time and *x*, *y*, and *z*-coordinates of every step a particle takes.

Table 7 - Pathline file format

| Item | Variable[1] | Type[2] | Options / Values | Description |
|---|---|---|---|---|
| 1 | Label | C | - | mod-PATH3DU does not support these header entries. It writes defaults to the file every time. |
| | Version | I | - | |
| | Revision | I | - | |
| 2 | TrackingDirection | I | - | Echo tracking direction. |
| | ReferenceTime | R | - | Echo reference time. |
| 3 | EndHeader | C | "END HEADER" | End-of-header flag. |
| | Item 4 is repeated for every step every particle takes | | | |
| 4 | ParticleID | I | - | Particle identification number. |
| | ParticleGroupNumber | I | - | Particle group number. |
| | UnusedFlag | I | - | - |
| | Ktime | I | - | Cumulative time step, from 1 to the last time step of the MODFLOW-USG simulation. |
| | Time | R | - | mod-PATH3DU tracking time. |
| | X | R | - | Global *x*-coordinate. |
| | Y | R | - | Global y-coordinate. |
| | Z | R | - | Global z-coordinate. |
| | CellID | I | - | Cell ID particle is within. Cell ID |

| | | | | |
|---|---|---|---|---|
| | | | | corresponds to the MODFLOW-USG cell number. |
| | UnusedFlag | I | - | - |
| | Layer | I | - | Layer number. |
| | UnusedFlag | I | - | - |
| | UnusedFlag | R | - | - |
| | UnusedFlag | R | - | - |
| | UnusedFlag | R | - | - |
| | Zloc | R | - | Local *z*-coordinate. |

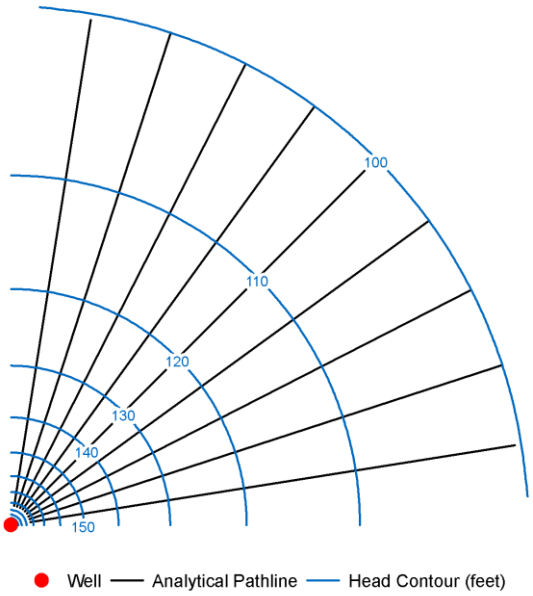
1 Square brackets indicate optional or dependent variables
2 C Character
I Integer
R Real

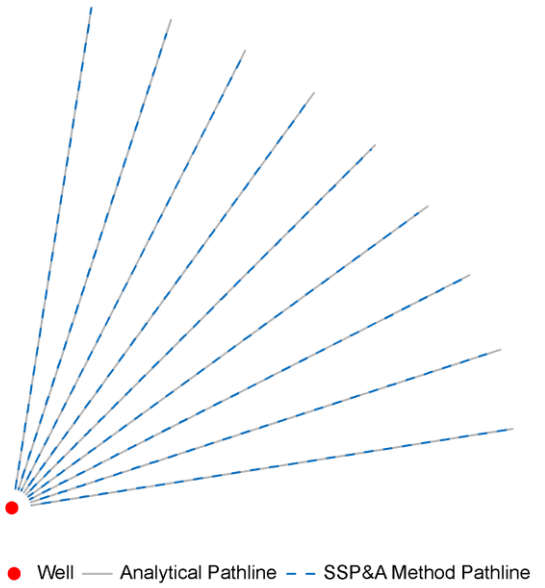
# Examples

## Example 1

### Radial Flow

This example is taken from Pollock (1988). It is a simple radial flow problem - water is injected at a constant rate of 160,000 feet$^3$/day into a 100 foot thick confined aquifer with a hydraulic conductivity of 10 feet/day and porosity of 0.3. At a radial distance of 4000 feet from the well, hydraulic-head is constant at 100 feet. Pollock (1988) presented results and focused his discussion on the basis of a numerical approximation of this problem. The analysis presented here, however, focuses on the analytic solution to illustrate the benefit of the well drift term employed by the SSP&A method in the vicinity of a pumping well. The analytic head solution and particle paths are shown on the figure to the right.




In order to track particles on the analytic solution to this problem using mod-PATH3DU, a numerical model was constructed of the problem, similar to the one described by Pollock (1998), to get the MODFLOW input files (DIS, LPF etc.) required by mod-PATH3DU. The grid is uniform and each cell has dimensions of 100 feet by 100 feet. The head at each cell center is calculated analytically and written to a MODFLOW head-save file. The particle paths calculated by mod-PATH3DU are shown in the figure to the left. The SSP&A method paths are perfect because the universal kriging algorithm it employs interpolates a value of head anywhere in the model domain that is equivalent to the analytic solution at that point.

# Example 2a

### Tracking in the Vicinity of a Pumping Well (Structured Grid)

The purpose of this example is to highlight the strength of the SSP&A method in tracking near a pumping well. The groundwater system is confined (50 feet thick), steady-state and two-dimensional, in plan-view. The ambient groundwater flow field is uniform throughout the whole domain and flow is from left to right. The fully penetrating well is pumped at a constant rate of 50 feet$^3$/d. Hydraulic conductivity is 10 feet/d and porosity is 0.3. The numerical domain consists of 21 rows, each 5 feet wide, and 87 columns with varying widths ranging from 5 to 20 feet, for a total model width of 500 feet. The conceptual model is shown in Figure 16. The flow balance is presented in Table 8.

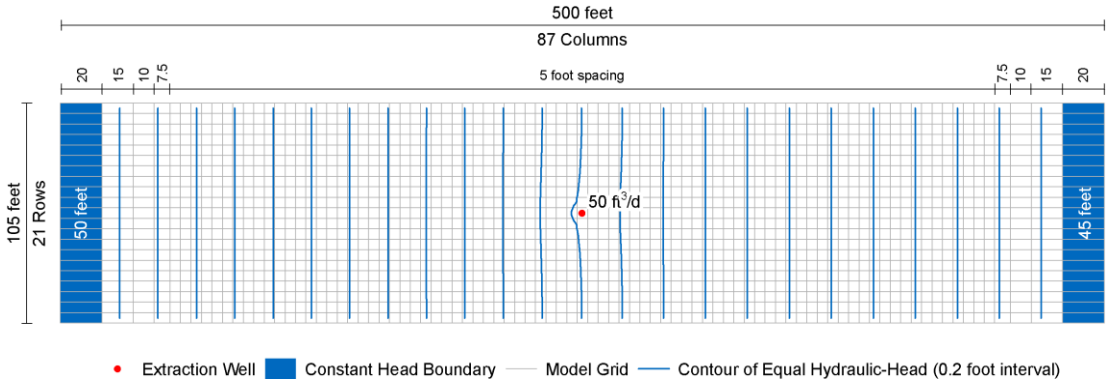



Figure 16 - Conceptual Model - Example 2a

Table 8 - Flow Balance - Example 2a

| Item | In (ft$^3$/d) | Out (ft$^3$/d) | Net |
|---|---|---|---|
| Constant Head | 571.9 | 521.9 | 50.0 |
| Well (MNW2) | 0.0 | 50.0 | -50.0 |
| Total | 571.9 | 571.9 | 0.0 |

Particle paths, in the vicinity of the pumping well, calculated by MODPATH6 and the SSP&A method of mod-PATH3DU are shown in Figure 17. The SSP&A method provides smooth pathlines as particles approach the well, in addition, the particles can be tracked in the cell containing the well. The head contours presented are an expression of what mod-PATH3DU tracks on in the vicinity of a well. They were calculated by interpolating from the MODFLOW heads to a very fine grid using the universal kriging algorithm available with mod-PATH3DU. The shape visible around the well is determined by the linear-log drift term applied in this case.

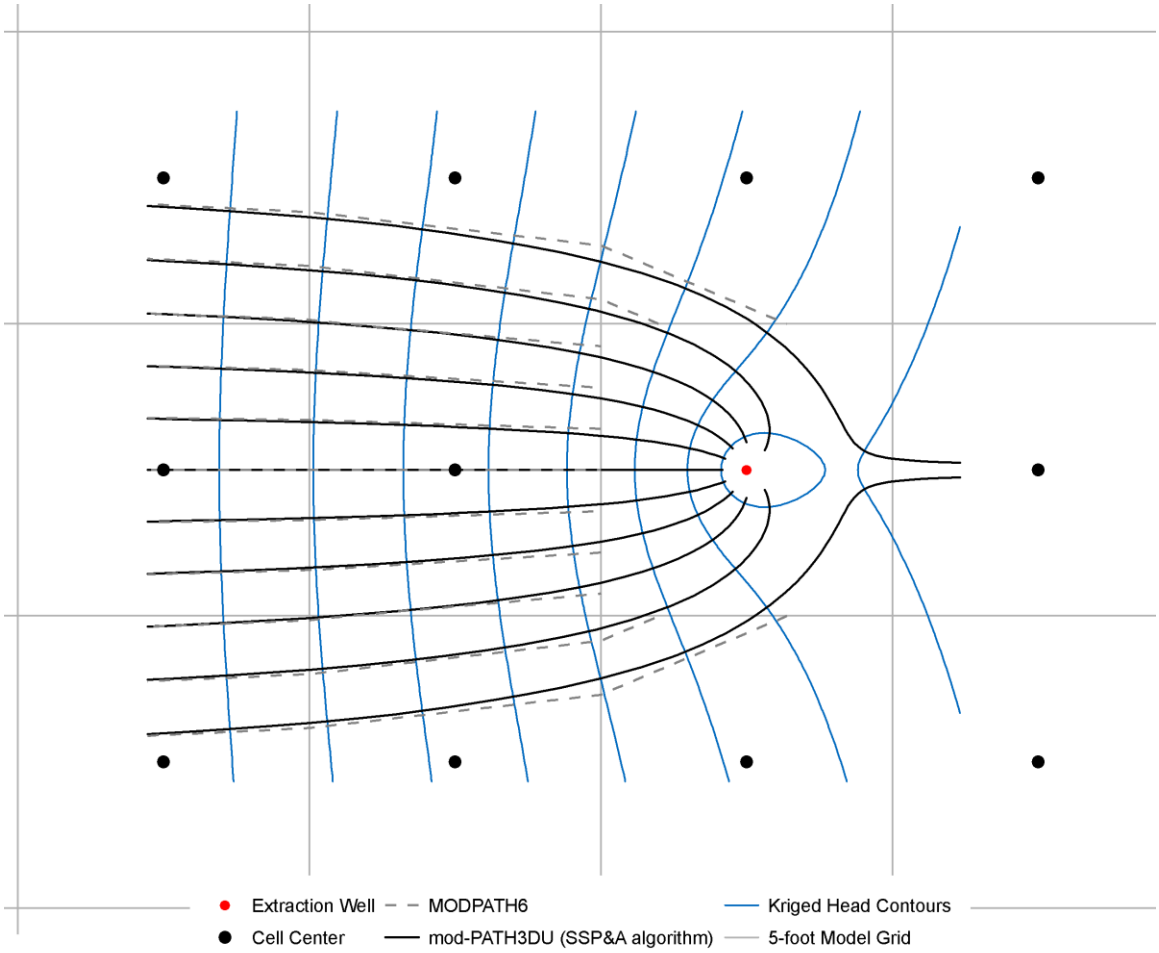



Figure 17 – Particle paths calculated using MODPATH6 and mod-PATH3DU - Example 2a

Because the SSP&A method imposes an analytic solution when tracking near a well, it can mitigate some coarse grid discretization issues. A second version of this same model was constructed with 20-foot grid spacing in the *x* and *y* directions (5 rows and 25 columns). This coarser grid was offset in the *y*-direction 2.5 feet to ensure the central cell aligned with the well location of the original, finer, grid. All other properties and boundaries remained the same between the two models. Figure 18 shows the capture zones calculated by mod-PATH3DU for the coarser grid model and the finer grid model and an analytical solution computed using Jacob, 1949; p.344. Note, the extent of Figure 18 is less than 20 feet in both the *x*- and *y*- directions; thus it is encapsulated by a single coarse grid cell. The capture zones delineated using mod-PATH3DU for the numerical models agree very well with the analytical solution. The difference between them is caused primarily by the upgradient coarse boundary cell size (20 feet) in both the fine and coarse models. An example of how mod-PATH3DU can be used to calculate capture

zones for off-center pumping wells using the Area Based Redistribution (ABRD) approach of Pinales et al. (2003;2005) is presented in Muffels et al. 2011.

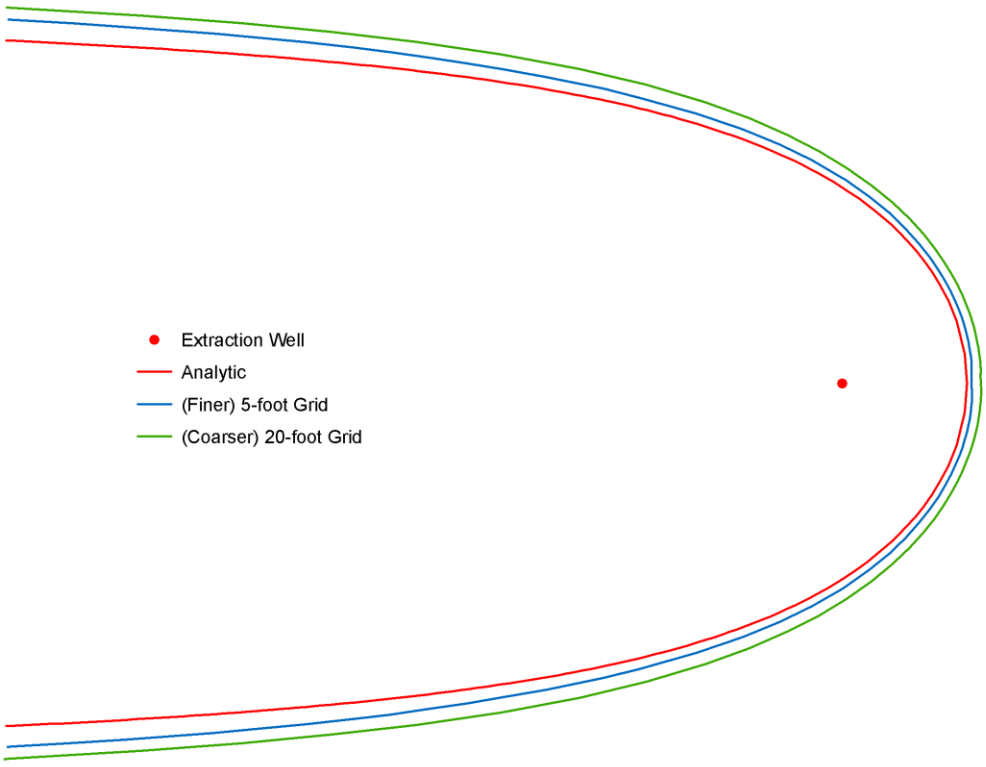



Figure 18 – Comparison of capture zones calculated by mod-PATH3DU (fine and coarse structured grids) with an analytical solution – Example 2a

## Example 2b

### Tracking in the Vicinity of a Pumping Well (Unstructured Grid)

The modeling exercise in Example 1a is repeated using an unstructured grid defined by Voronoi cells, Figure 19. The resulting flow balance is presented in Table 9. The difference in the flow entering the system between this model and the five-foot structured model is due to the smaller cell size along the boundaries.

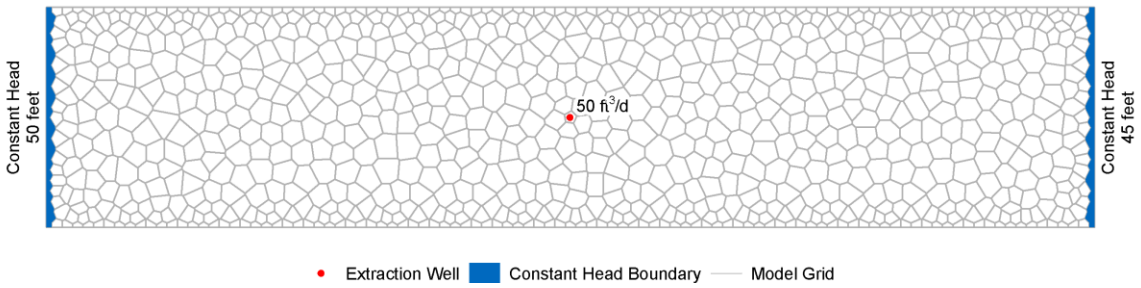



Figure 19 - Conceptual Model - Example 2b

Table 9 - Flow Balance - Example 2b

| Item | In ($ft^3/d$) | Out ($ft^3/d$) | Net |
|---|---|---|---|
| Constant Head | 524.3 | 474.0 | 50.3 |
| Well (MNW2) | 0.0 | 50.0 | -50.0 |
| Total | 524.3 | 524.0 | 0.3 |

The mod-PATH3DU calculated particle paths for this model are shown in Figure 20, and the computed capture zone is compared to the analytic solution in Figure 21.

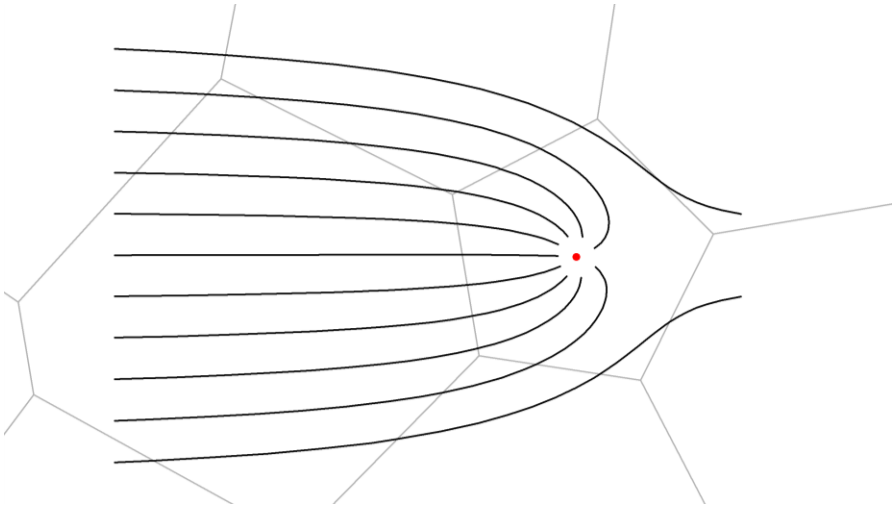


Figure 20 - Particle paths calculated by mod-PATH3DU in the vicinity of a pumping well for a MODFLOW-USG model with Voronoi cells - Example 2b

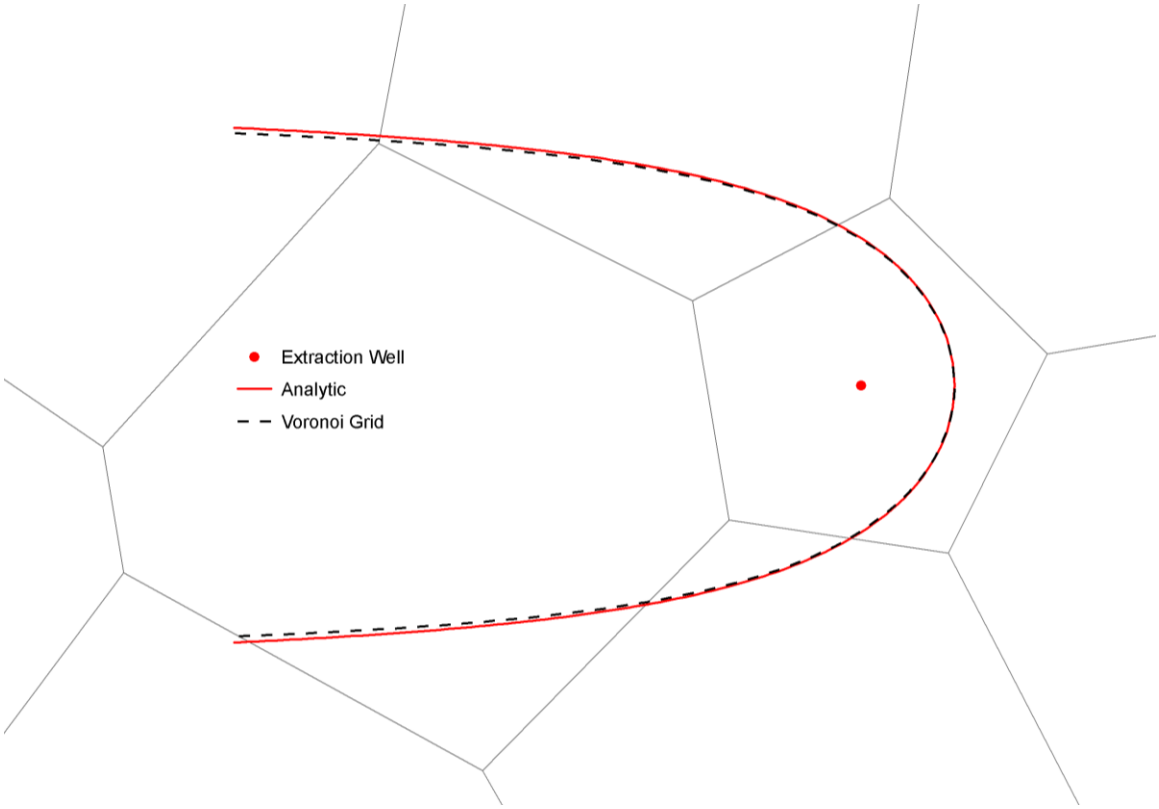



Figure 21 – Comparison of capture zone calculated with mod-PATH3DU (unstructured Voronoi grid) with an analytical solution - Example 2b

# Example 3

### Flow Path in Heterogeneous Cross-section

This example is adapted from the documentation of PATH3D ver. 4.6. The example was developed to test the calculation of groundwater pathlines in a heterogeneous cross-section. The groundwater model comprises three strata; the hydraulic conductivity of each stratum is shown in Figure 22. The model is discretized into 20 layers. The cross-section is bordered by no-flow boundaries along the left, right and bottom edges. The top boundary is assigned specified-heads to represent a linear water table declining from 41 feet at $x$ = 100 feet to 40 feet at $x$ = 0 feet. Porosity is 0.2. The resulting flow balance in presented in Table 10.

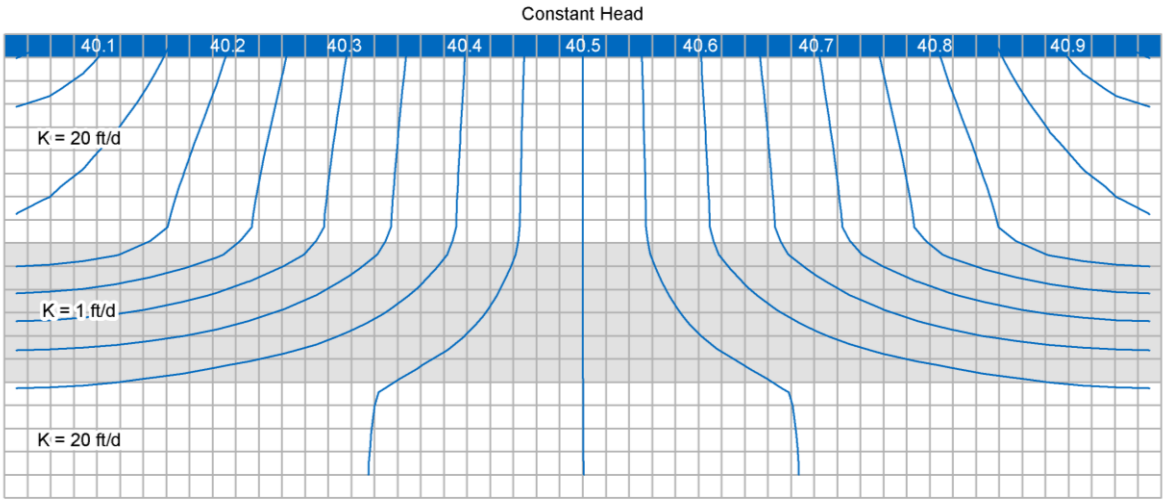



Figure 22 - Conceptual Model - Example 3

Table 10 - Flow Balance - Example 3

| Item | In ($ft^3/d$) | Out ($ft^3/d$) | Net |
|---|---|---|---|
| Constant Head | 3.7 | 3.7 | 0.0 |
| Total | 3.7 | 3.7 | 0.0 |

A particle is tracked backwards from $x$ = 1 foot. The particle paths calculated using PATH3D v.4.6 and both the Pollock and SSP&A methods in mod-PATH3DU for this particle are shown in Figure 23. The total travel time calculated by each approach are nearly identical; PATH3D calculated 636 days, while mod-PATH3DU calculated 637 and 635 days using the SSP&A and Pollock methods, respectively. This example primarily serves to demonstrate the implementation of the Pollock method, especially in the $z$-direction when used in conjunction with the SSP&A method, is

correct and that the method can be applied to cross-section models. This example, in and of itself, is not particularly challenging for the Pollock method.

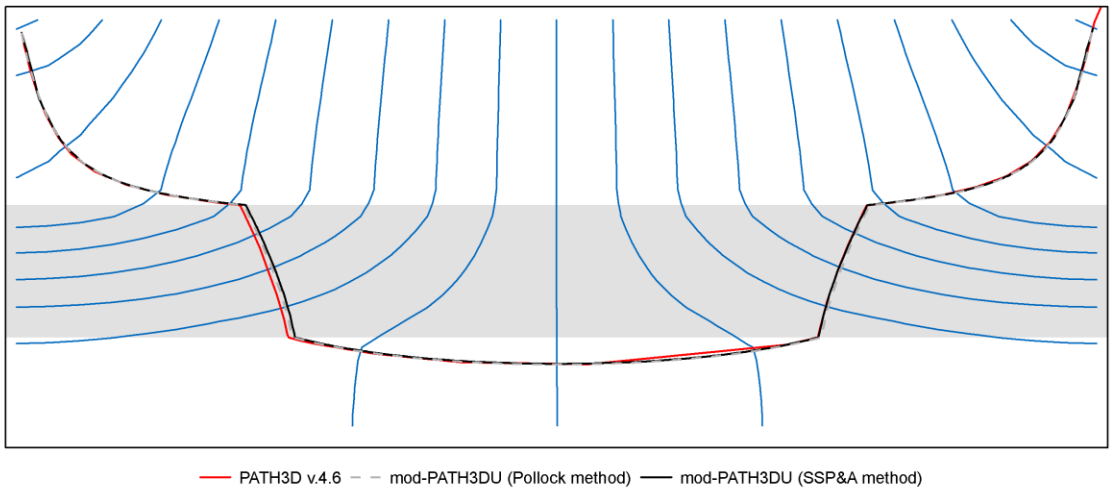



Figure 23 - Comparison of pathlines computed using mod-PATH3DU and PATH3D v4.6 - Example 3

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