An Unstructured Version of PATH3D, PATH3DU

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ABSTRACT

Common particle tracking techniques, such as the method embodied in MODPATH (Pollock, 1994) and the Runge-Kutta scheme embodied in Path3D (SSP&A, 2003), were principally developed for use in regular rectangular finite-difference grids as used by MODFLOW. Since they use linear interpolation to estimate velocities from the node-based flow solution, these methods do not readily lend themselves to use for unstructured and/or non-rectangular grids, or in the vicinity of strongly curvilinear flow fields. Furthermore, the results of particle tracking analyses can be severely grid-dependent (Zheng, 1994). This presentation describes improvements to the PATH3D code (referred to here as PATH3DU), enabling generalized particle tracking for unstructured and/or non-rectangular grids. In PATH3DU, linear interpolation from the node-based flow solution is replaced with a universal kriging technique. This has the advantages that it can (a) compute velocity components for an arbitrary node pattern, and (b) incorporate hydrologic drift (trend) terms in the velocity interpolation that effectively lead to 'grid-independent' resolution in the vicinity of pumped wells for calculating capture zones using coarsely discretized models.

INTRODUCTION

Particle tracking is an important component of groundwater modeling. An example of its use is the delineation of source areas for different features of a model, such as the capture zone of an extraction well. This paper discusses updates to the particle tracking program PATH3D for use with unstructured grids, in particular the version of MODFLOW discussed by Panday (2011: see presentation this conference).

Cells in an unstructured grid can theoretically be any shape or size. The tracking (Pollock) method employed by MODPATH and the (bilinear) interpolation routine originally employed by PATH3D are currently dependent upon a rectangular grid of flows and hydraulic-heads calculated by MODFLOW. The interpolation routine in PATH3DU is replaced with a universal kriging one that can be used to calculate velocity components for an arbitrary node pattern. With appropriate hydrologic drift terms this technique has the added advantage of being able to resolve velocities in a 'grid-independent' manner.

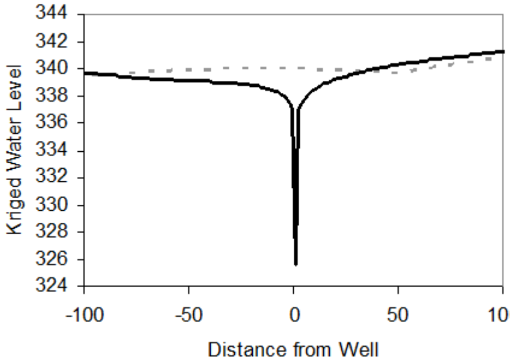


Figure 1 Kriged water levels in the vicinity of a pumped well using ordinary kriging (dashed line) and universal kriging (solid line).

The applicability of this approach is first demonstrated using an unstructured MODFLOW model. The benefits of the universal kriging velocity interpolation scheme in the vicinity of pumped wells are then demonstrated using a model for which pumping is assigned using the Area-based Redistribution (ABRD) method (Pinales et al., 2003; 2005) that mimics off-node-center pumping by distributing pumping to the neighboring cells.

UNIVERSAL KRIGING

Kriging is often used to interpolate irregularly spaced measurement data to unsampled locations (typically a grid of points suitable for contouring). 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*. In ordinary kriging, the mean is assumed to be unknown *a-priori*, but is estimable using some function of the measured data. However, 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. Essentially, 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 as shown in Figure 1. It is important to note that kriging is an exact interpolator in the absence of measurement error or co-located data. In the context of particle tracking, 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.

PARTICLE TRACKING ON AN UNSTRUCTURED GRID

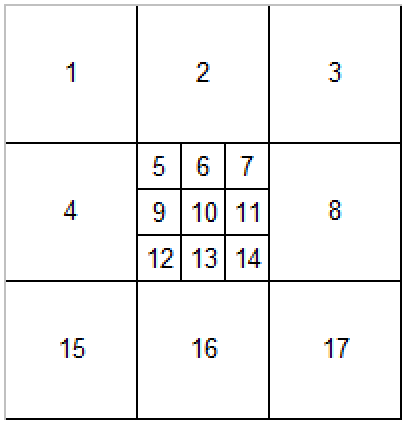


Figure 2 The unstructured grid used to test PATH3D. The numbers identify each model cell.

To demonstrate the applicability of the new kriging interpolator in PATH3DU - especially the utility of drift terms - a simple, isotropic and homogeneous single layer unstructured model was developed for the unstructured version of MODFLOW. The model consists of a central 3x3 regularly spaced grid, with each of the resulting 9 cells being 10 x 10m in size. This central grid was then surrounded by (8) 30 x 30m cells as in Figure 2. Constant head boundary conditions were specified on opposite sides of the domain (at 90m and 85m respectively). This test case was chosen for its simplicity as the “true” path of a particle is a straight line from left to right across the domain. In addition, particle paths using the Pollock method can still be calculated and compared to the PATH3DU paths.

Because the model uses an unstructured grid, there is a component to flow in the y-direction between cell 2 and cells 5, 6, and 7 (and between cell 16 and cells 12, 13, and 14) (Figure 3). The head calculated for cell 2 represents the bulk average head for the cell. As such, resolution is lost compared to the refinement provided by cells 5, 6, and 7 which results in artificial flow between these cells (Figure 3) as shown by the particle paths calculated with the Pollock method (Figure 4). However, by incorporating a linear-drift with the universal kriging approach, the effects of this artificial flow component can be mitigated resulting in more linear particle paths as shown in Figure 4.

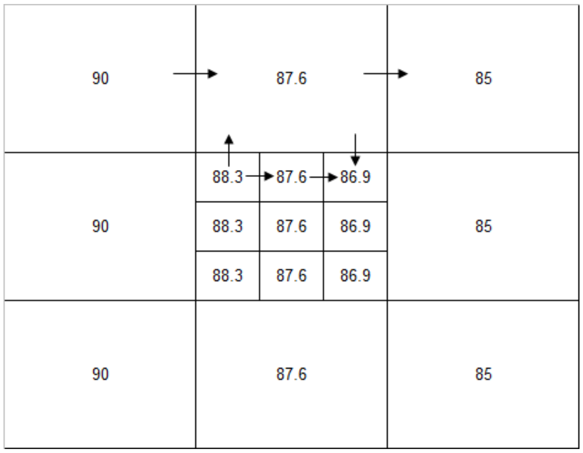


Figure 3 Model calculated heads for the unstructured test model. The arrows show the direction of flow between model cells.

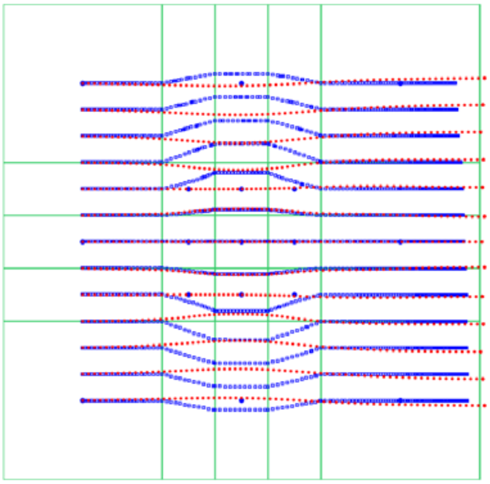


Figure 4 Particle paths calculated with the Pollock method (blue-square) and the kriging approach available to PATH3DU (red-x).

GRID INDEPENDENT RESOLUTION IN THE VICINITY OF PUMPED WELLS

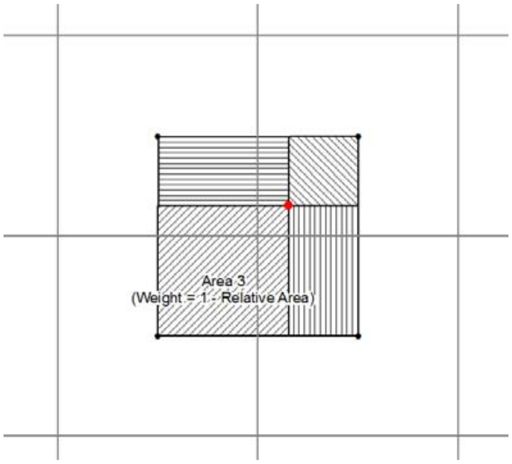
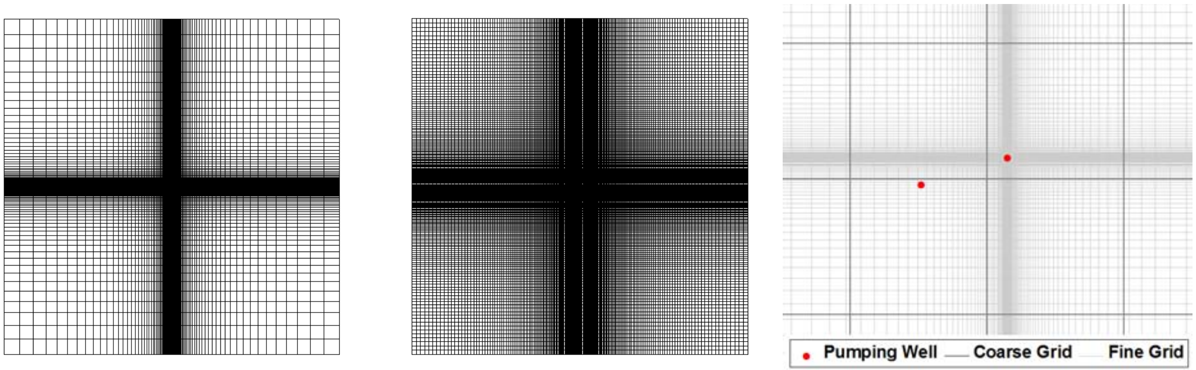


Figure 5 Area-based bilinear interpolation weights used with the ABRD approach of Pinales et al. 2003.

Traditionally, model domains are refined in the area of pumping wells to improve accuracy as MODFLOW requires a well be specified at the center of a model cell. However, such an approach results in longer simulation times owing to the additional model cells. Pinales et al. (2003;2005) demonstrate that the effects of off-center pumping wells can be incorporated into MODFLOW by distributing the total pumping of a well to the 4 model cells surrounding it (referred to as the Area Based Redistribution, or ABRD, approach). The pumping is distributed using a bilinear area-based approach as in Figure 5. With the ABRD approach, refinement in the area of pumping wells is no longer necessary for a wide variety of simulation objectives, thereby reducing model run times.

However, the effect of employing the ABRD approach on the capture zones of wells modeled in this manner has not previously been demonstrated in detail. Pinales et al. (2003;2005) show that the drawdown calculated at the 4 nodes to which pumping was distributed are equivalent to the expected drawdown given their relative cell-center distance from the actual well location. This result suggests that, in the presence of a single pumped well, the correct capture zone would be delineated by the Pollock method or the bilinear Runge-Kutta scheme of PATH3D.

To demonstrate the utility of the universal kriging approach available with PATH3DU, regular MODFLOW models were created. First, a fine grid model (center cell of 1 x 1m – coarsening outwards with cell widths 1.5 times the preceeding width until the domain was approximately 50,000 x 50,000m as in Figure 6a) was developed with two wells, the first (260 gpm) in the center of the domain and the second about 65m to the southwest pumping 180gpm. This model constitutes the “true” solution. A second, coarse version of the same model was created in which the central 5000 x 5000m area of the domain is discretized using 100 x 100m cells (Figure 6b). Cell widths coarsen outward from this refined area by a factor that ensures the total width of both domains is the same. In each model, two wells were modeled using the ABRD approach. The location of these wells within both model domains is shown in Figure 6c. The predominant groundwater flow direction is from north to south due to constant heads defined at these boundaries.

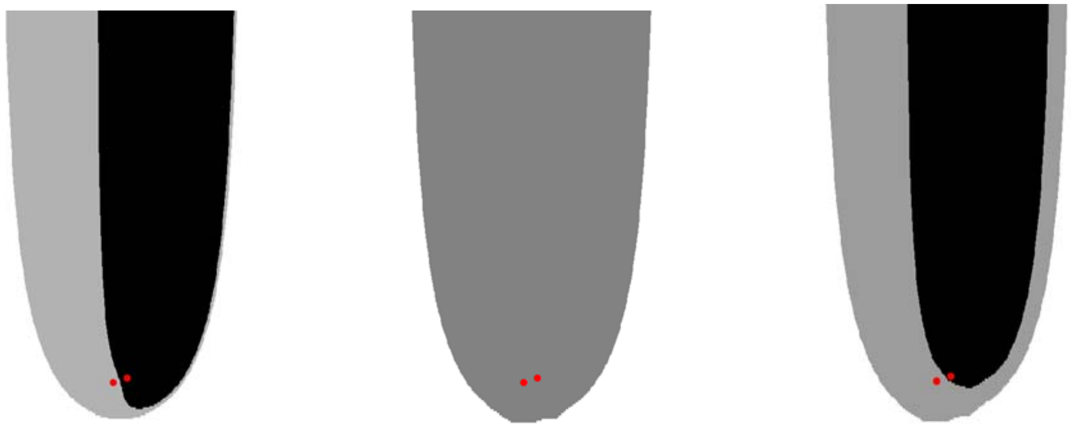


a) b) c)

Figure 6

- **a) Fine grid of model used to determine "true" capture zones (using the Pollock method) of two pumped wells near center of domain.**
- **b) Coarse grid of model upon which universal kriging with a well “drift” is used to calculate capture zones for the same two wells as (a).**
- **c) The locations of the two pumping wells relative to each of the model grids**

Figure 7 shows the capture zone(s) calculated using (a) MODPATH on the fine-grid, (b) MODPATH on the coarse-grid, and (c) universal kriging with a point sink in PATH3DU on the coarse grid. The capture zones calculated by MODPATH on the fine grid represent the “true” zones. It is clear that the universal kriging interpolator in PATH3DU delineates capture zones that are very similar to the “true” solution. The differences are likely due to the fact that a much coarser grid (exhibiting a length ratio to the true grid of 100:1) in the vicinity of the pumping wells was used: this represents an extreme case for most modeling applications. As expected, MODPATH correctly delineated the *combined* capture for both wells on the coarse grid, but could not differentiate their respective zones.



a) b) c)

Figure 7

a) Capture zones calculated using the Pollock method (MODPATH) on the fine model grid
b) Composite capture zone calculated using the Pollock method on the coarse model grid
c) Capture zones calculated using the universal kriging approach (PATH3D) on the coarse model grid

CONCLUSIONS

Replacement of the bilinear interpolation routine in PATH3D with a universal kriging one makes PATH3DU a general particle tracking program applicable to a wide range of grids, discretization techniques, and levels of refinement.

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