Grid Refinement in Cartesian Coordinates for Groundwater Flow Models Using the
 Divergence Theorem and Taylor's series.

3

4 Mansour M.M. and Spink A.E.F.

5

6 Abstract

7

8 Grid refinement is introduced in a numerical groundwater model to increase the accuracy of 9 the solution over local areas without compromising the run time of the model. Numerical methods developed for grid refinement suffered certain drawbacks, for example deficiencies in 10 the implemented interpolation technique; the non-reciprocity in head calculations or flow 11 calculations; lack of accuracy resulting from high truncation errors, and numerical problems 12 resulting from the construction of elongated meshes. A refinement scheme based on the 13 14 divergence theorem and Taylor's expansions is presented here. This scheme is based on the work of De Marsily (1986) but includes more terms of the Taylor's series to improve the 15 numerical solution. In this scheme flow reciprocity is maintained and high order of refinement 16 was achievable. The new numerical method, investigated by modelling flows in homogeneous 17 confined aguifers, produced results with acceptable degrees of accuracy. It converges and 18 reproduces the desired solution in heterogeneous aquifers. This method also shows the 19 20 potential for application to solving groundwater heads over nested meshes with irregular shapes. 21

22

23 Introduction

The finite difference technique is a numerical method that is used to solve the differential 25 equation representing the spatial and temporal variations of the groundwater heads of 26 groundwater systems. Like other numerical techniques, for example, the subsurface flow finite 27 28 element models FEHM (Zyvoloski et al., 1997) and FEFLOW (Diersch, 2005), the continuous aquifer domain is discretised into a set of sub-domains or nodes, where groundwater heads are 29 calculated. The increased number of nodes both improves the accuracy of the numerical 30 solution and improves the processing time required to produce the solution. In the early days 31 of finite difference applications, computational resources were limited in terms of both storage 32 33 capacity and computational speed. This made the efficiency of a numerical method an important feature and most often the resolution of the numerical grids holding nodes was 34 compromised to benefit run time. Today, storage capacity imposes few restrictions and 35 computer speed is ever-increasing allowing more complicated and accurate numerical methods 36 to be applied. However, the complexity of groundwater applications is increasing in parallel 37 with the development of computer abilities and this has led researchers, for example Szekely 38 (1998), Hayes(1999), Jackson (2000), Mehl and Hill (2004), Mehl et al. (2006), Dickinson et al. 39 (2007), Szekely (2008) to continue to work on the development of numerical applications that 40 41 satisfy both speed and accuracy.

42

The speed of solving a groundwater problem is mainly controlled by the power of the processor and by the number of nodes included in the numerical model. The accuracy of the solution, on the other hand, depends on many factors. A major factor is the spacing between adjacent nodes of the numerical grid. This affects the truncation error introduced into the numerical approximations and the accuracy of the representation of the rate of change of groundwater head over distance. A smooth change in the hydraulic gradient, as is the case in regional aquifers, for example, allows the use of a large interval without affecting the accuracy

of the solution. In radial flow modelling, for example Rushton and Redshaw (1979) or Mansour 50 et al. (2011), the use of a logarithmic radial mesh increases the node density in the region 51 around the well where steep hydraulic gradients occur and reduces the node density in the 52 53 more distant parts of the aquifer. However, steep hydraulic gradients may occur in a regional aquifer due to the existence of special features, such as rivers, wells, faults, and changes in the 54 aquifer properties. This requires the use of a small space interval over these limited areas. 55 Mesh refinement is a useful technique that increases the accuracy of the model without 56 limiting its run-time efficiency or increasing computer memory. 57

58

Mesh refinement techniques were investigated as early as 1946 (Southwell, 1946) and 59 different mesh refinement schemes have been developed over the years. For example 60 telescopic refinement schemes with multiple scale models are used by Ward et al. (1987), 61 Bravo et al. (1996) and Miller and Voss (1987), adaptive mesh refinement schemes are used by 62 Berger and Oliger (1984), Arney and Flaherty (1989) and De Lange and De Goey (1994) and 63 local grid refinement schemes are used by Szekeley (1998), Bennet and Smooke (1999), Hayes 64 (1999), Jackson (2000) and Mehl et al. (2006). These methods successfully served the needs of 65 their users giving acceptable accuracy for the type of problem investigated. However, each of 66 these methods suffers from certain drawbacks, for example deficiencies in the implemented 67 interpolation technique, lack of accuracy resulting from high truncation errors, and numerical 68 problems resulting from the construction of elongated meshes. Other methods do not 69 maintain grid reciprocity, which specifies that if point A is included in the finite difference 70 approximation at point B, then point B must be included in the approximation at point A. If 71 72 reciprocity exists then the approximation of flux leaving A and entering B can be formulated in exactly the same way as the approximation of the flux leaving B and entering A (Jackson, 2000; 73 Mehl et al., 2006). De Marsily et al. (1978) present a refinement scheme based on integrated 74

finite differences that has certain attractions. This scheme uses the Green Theorem to calculate the groundwater flows at the sides of the nodes located at the coarse-fine grid interfaces. It fits, therefore, neatly within the conventional finite differences and maintains a flow balance. However, the one drawback of the method as presented by De Marsily (1986) is its limited accuracy.

80

Jackson (2000) developed equations that are more accurate than De Marsily et al. (1978) and De Marsily (1986) although they do not maintain flow reciprocity. The lack of accuracy in the scheme developed by De Marsily (1986) originates from limiting the number of terms in the Taylor's series used to develop the numerical equations to just three, i.e. the heads and first gradients of heads.

86

This paper presents a refinement scheme based on the refinement scheme developed by De 87 Marsily (1986) but improved by including more terms of the Taylor's series to derive the 88 necessary numerical equations. The challenges of this are first to produce numerical equations 89 that have the desired groundwater equation forms as the product of head differences 90 91 multiplied by conductance parameters and second that the developed numerical technique is stable and converges to the required solution with an acceptable degree of accuracy. This 92 paper discusses the steps required to derive the numerical equations and presents the grid 93 94 discretisation scheme that reduces the effort required to derive these equations. The convergence of the numerical scheme is demonstrated by simulating groundwater flows in one 95 and two dimensional homogeneous aquifers under steady state conditions. The convergence 96 97 of the numerical scheme in transient problems is demonstrated by comparing the numerical results to the Theis solution. Finally the limitations of the method and recommendation for 98 future development are discussed. 99

Description of the Methods

102 Integrated Finite Differences.

103 The basic flow equation in an anisotropic and heterogeneous aquifer is given by:

104
$$\frac{\partial}{\partial x} \left(T_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(T_y \frac{\partial h}{\partial y} \right) = S \frac{\partial h}{\partial t} - q$$
 Equation 1
105 De Marsily et al. (1978) introduced the integrated finite difference technique based on the

Divergence Theorem, or Green's Theorem. In two dimensions, the Divergence Theorem states that for any continuous vector function **V** with continuous first partial derivatives, the double integral of the divergence of this function over a closed area A can be transformed into a contour integral of the scalar product of the vector function with the unit outward normal evaluated along the perimeter C of the area A. This is expressed by, for example Boas (1983), De Marsily et al. (1978):

112
$$\iint_{A} div(\mathbf{V}) dA = \oint_{C} \mathbf{V} \cdot \mathbf{n} ds$$
 Equation 2
113

To generalise the method, De Marsily (1986) considered an anisotropic aquifer and constructed a mesh where the grid elements have a polygonal shape with nodes located within them. In a conventional finite difference approximation, Equation 1 would be written at each of the nodes. In integrated finite differences, the integral of the flow equation over the area A_i surrounding each node is formed. This leads to:

119
$$\iint_{A} \left[\frac{\partial}{\partial x} \left(T_{x} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(T_{y} \frac{\partial h}{\partial y} \right) \right] da = \iint_{A} \left(S \frac{dh}{dt} - q \right) da$$
 Equation 3

and by recognising that the left hand side is a divergence term Equation 3 can be written as:

121
$$\iint_{A} div (T \text{ grad } h) da = \iint_{A} \left(S \frac{dh}{dt} - q \right) da$$
 Equation 4

122 Finally the divergence theorem allows the left-hand side to be replaced by a line integral:

123
$$\oint_{\tau_i} \left(T_x \frac{\partial h}{\partial x} n_x + T_y \frac{\partial h}{\partial y} n_y \right) ds = \iint_A \left(S \frac{dh}{dt} - q \right) da$$
Equation 5

Where n_x and n_y are the direction cosines of the unit vector **n** perpendicular to the boundary, and ds is an element of τ_I , the boundary of the element surrounding the node. As a result of this transformation, numerical approximations to $\frac{\partial h}{\partial x}$ and $\frac{\partial h}{\partial x}$ are required rather than to $\frac{\partial^2 h}{\partial x^2}$ and $\frac{\partial^2 h}{\partial x^2}$.

128

To evaluate the hydraulic gradients
$$\frac{\partial h}{\partial x}$$
 and $\frac{\partial h}{\partial x}$ at an arbitrary point (m) moving along line AB
(Figure 1), De Marsily (1986) wrote three Taylor's series expansions for the head values at I, J
and K. Only three terms of the Taylor's series are retained, as shown in Equation 6, allowing the
gradients $\frac{\partial h}{\partial x}\Big|_m$ and $\frac{\partial h}{\partial y}\Big|_m$ at the point m to be calculated in terms of the heads at the

133 surrounding nodes and their positions.

134
$$h_I = h_m + (x_I - x_m) \frac{\partial h}{\partial x}\Big|_m + (y_I - x_m) \frac{\partial h}{\partial y}\Big|_m$$
 Equation 6

De Marsily (1986) showed that the gradients are independent of the location of point m and that they are constant along AB. This allows the rearrangement of the left-hand side of Equation 5 by writing the head gradients outside the integrals. This greatly reduces the mathematical procedure required to carry out the integration and yields a relatively simple form as given in Equation 7.

140
$$\int_{AB} \left(T_x \frac{\partial h}{\partial x} n_x + T_y \frac{\partial h}{\partial y} n_y \right) ds = C_{IJ} \left(H_J - H_I \right) + C_{IK} \left(H_K - H_I \right)$$
Equation 7

141 C_{IJ} and C_{IK} are constants that depend on the aquifer characteristics, specifically the 142 transmissivity and the dimensions of the mesh. Equation 7 shows that integrated finite differences lead to an expression for flow in the form of head differences multiplied by constants. This is similar to the structure in conventional finite difference formulae. In addition, the method maintains both a flow balance and the reciprocity requirement. However, it also generates a high truncation error.

147

In conventional finite differences, the truncation error resulting from the calculation of $\frac{\partial h}{\partial r}$ 148 or $\frac{\partial^2 h}{\partial r^2}$, using the central difference scheme, is in the order of O(Δx^2). The approach used by 149 De Marsily results in an error in the order of O(Δx) for the calculation of $\frac{\partial h}{\partial x}$ or $\frac{\partial h}{\partial y}$. De Marsily 150 et al. (1978) recognised that a model based on this approach does not represent the system 151 152 accurately and De Marsily (1986) restricted the refinement by halving the mesh interval to maintain accuracy. This makes other refinement approaches such as the one developed by 153 Jackson (2000) more desirable, even without maintaining reciprocity, since they produce better 154 quality results. 155

156

157 **The New Formulation**

158

De Marsily et al. (1978) described their work as having a "logical synthesis" and as being "hydrogeologically plausible". Indeed, integrated finite differences fit neatly with conventional finite differences and keep important features such as providing clear discretised aquifer units, maintaining a flow balance, and dealing with heterogeneous aquifers. However, the major problem with the method, as represented by De Marsily et al (1978) and De Marsily (1986), is the limited accuracy. To overcome this difficulty, a new formulation for the head gradients $\frac{\partial h}{\partial x}$ and $\frac{\partial h}{\partial y}$ is developed. Like De Marsily et al. (1978) it is based on using Taylor's series at



167

There are three main challenges to this approach. The first is that the approximations become large and a tidy outcome where the fluxes consist of expressions composed of head differences multiplied by constants is not guaranteed. Second, the head gradients depend on the position of the point m as it moves along the interface and this complicates the integration to determine the flow. Finally, the equations must produce an accurate solution.

173

To increase the accuracy of the head gradient approximation to the order of $O(\Delta x^2)$ three extra 174 terms of Taylor's series involving the terms $\frac{\partial^2 h}{\partial x^2}$, $\frac{\partial^2 h}{\partial y^2}$ and $\frac{\partial^2 h}{\partial x \partial y}$ are included in the head 175 176 equation at a given node in addition to the three used by De Marsily et al. (1978) and shown in The calculation of the values of these six terms necessitates the application of 177 Equation 6. Taylor's series at six nodes. However, the locations of these nodes define the structure of the 178 equations. It is, therefore, preferable to arrange the nodes carefully in a definite geometrical 179 layout so the mathematical manipulation is reduced. Two possible grid layouts for the 180 refinement scheme are presented here. The first is similar to the one implemented by Jackson 181 182 (2000) and is illustrated in Figure 2. This layout consists of a coarse grid with a refined region giving elongated rectangular flow interaction areas at the mesh interface. 183

184

For a typical node, I, on the fine-coarse interface, there are three sides of the flow interaction area , AB, BC and AD that require a new formulation of the head gradient, $\frac{\partial h}{\partial x}$ or $\frac{\partial h}{\partial y}$, while on the fourth side, CD, the conventional finite difference expression can be applied. Many

problems arise in this case, especially along the sides BC and AD. Along segment BC for 188 example, the determination of the hydraulic gradient $\frac{\partial h}{\partial v}$ requires two different evaluations, 189 one along BE and the other along EC. The same is true for the determination of $\frac{\partial h}{\partial y}$ along AD. 190 A second more serious problem concerns the water balance. Line AF, for example, represents 191 a common boundary between nodes K and I. For the flow balance at node K, the expression 192 for $\frac{\partial h}{\partial v}$ is based on head values at points L, I, K, R and J. When considering node I, the gradient 193 is based on head values at points L, N, I, K, and J. In theory the two expressions should 194 produce the same results, but because of the truncation errors this is not guaranteed. In 195 196 general, the use of different combinations of head values will lead to inconsistent estimates of 197 flow across a common boundary.

198

The second layout divides the coarse grid into a number of discrete areas for which flow balances are calculated. In this case, the areas can extend beyond the original coarse grid lines, as shown in Figure 3. This eliminates the elongated areas and ensures that all nodes in all meshes have a square or a rectangular shape with an aspect ratio similar to that of the coarse grid. The advantage of this arrangement is that for all the nodes located on the interface, there is only a need to derive one expression for one head gradient, either $\frac{\partial h}{\partial x}$ or $\frac{\partial h}{\partial y}$ depending on

the direction of the node face.

206

In the new scheme groundwater heads at the six points I, K, J, L, N and P, shown in Figure 3, are expressed by Taylor's expansions based on a point m that is moving along the line AB. Equation 8 shows the expression for Node I; the heads at the other nodes take the same form.

211

212

$$h_{I} = h_{m} + (x_{I} - x_{m})\frac{\partial h}{\partial x}\Big|_{m} + (y_{I} - y_{m})\frac{\partial h}{\partial y}\Big|_{m} + \frac{(x_{I} - x_{m})^{2}}{2!}\frac{\partial^{2}h}{\partial x^{2}}\Big|_{m} + \frac{2}{2!}(x_{I} - x_{m})(y_{I} - y_{m})\frac{\partial^{2}h}{\partial x\partial y}\Big|_{m} + \frac{(y_{I} - y_{m})^{2}}{2!}\frac{\partial^{2}h}{\partial y^{2}}\Big|_{m}$$
Equation 8

214

213

This equation was used by Quandalle and Franlab (1985) who built a numerical model with composite grids. However, they considered refinement in one direction only and estimated the hydraulic gradient at a single node at the mid-point of line AB. They did not derive a general expression for the hydraulic gradient and integrate it along the interface.

219

220 The next stage consists of solving the six equations containing values of six unknown head and

head gradients to evaluate the hydraulic gradient $\frac{\partial h}{\partial x}$. This yield Equation 9:

222
$$M\frac{\partial h}{\partial x} = C_1(h_L - h_I) + C_1(h_J - h_I) + (C_2 + C_{10}C_7 + y_mC_{10}C_6)(h_L - h_J) + C_4(h_P - h_I) + (C_3 + C_5 + C_9C_7 + y_mC_9C_6)(h_K - h_I) + C_5(h_N - h_I) + (C_5 + C_8 + y_mC_8C_6)(h_N - h_I)$$
223 Equation 9

Where:

225
$$M = \frac{-3\Delta x - \Delta X}{4\Delta x}$$

226
$$C_1 = \frac{-1}{\Delta x + \Delta X}$$
, $C_2 = \frac{-(2y_I - y_L - y_J)}{2\Delta Y(\Delta x + \Delta Y)}$, $C_3 = \frac{-(2y_I - y_L - y_J)}{2\Delta y(\Delta x + \Delta X)}$

227
$$C_4 = \frac{-(\Delta x - \Delta X)}{4\Delta x^2}, \quad C_5 = \frac{\left[(2y_I - y_L - y_J)\Delta y - \Delta Y^2\right]}{4\Delta y^2(\Delta x + \Delta X)}$$

228
$$C_{6} = \frac{-(3\Delta x^{2} + \Delta X^{2} + 4\Delta x\Delta X)}{4\Delta x(\Delta x + \Delta X)}, \qquad C_{7} = \frac{[(\Delta x + \Delta X)(y_{I}(\Delta x + \Delta X) + (y_{I} + y_{L})\Delta x)]}{4\Delta x(\Delta x + \Delta X)}$$

229
$$C_8 = \frac{\left(y_I + y_N - y_L - y_J - 2\Delta y\right)}{\Delta y^2 \left(\Delta x + \Delta X\right)}, \qquad C_9 = \frac{\left(y_I + y_N - y_L - y_J\right)}{\Delta y^2 \left(\Delta x + \Delta X\right)}, \qquad C_{10} = \frac{2}{\Delta Y \left(\Delta x + \Delta X\right)}$$

230

Where Δx and Δy are the grid intervals on the fine grid and ΔX and ΔY are the corresponding values on the coarse grid as shown in Figure 3. Integrating Equation 9 over the interval AB and multiplying by the transmissivity in the x direction, gives the flow across AB. In the case of node I shown in Figure 3, the integration is carried out in the y direction. This only affects the variable y_m in Equation 9, since all other terms are independent of the position of m. The integration results in multiplying all terms that do not include y_m by Δy and in replacing y_m , by $\frac{1}{2}(y_B^2 - y_A^2) = y_I \Delta y$. The flow equation becomes:

239

240
$$Q_{AB} = \frac{T\Delta y}{M} \begin{bmatrix} C_1(h_L - h_I) + C_1(h_J - h_I) + (C_2 + C_{10}C_7 + P \cdot C_{10}C_6)(h_L - h_J) + C_4(h_P - h_I) \\ + (C_3 + C_5 + C_9C_7 + P \cdot C_9C_6)(h_K - h_I) + C_5(h_N - h_I) + (C_5 + C_8 + P \cdot C_8C_6)(h_N - h_I) \end{bmatrix}$$
241 Equation 10

242

243 The symbol P in Equation 10 is used to indicate a term which changes for certain nodes. In general P is equal to y_I. The value changes when nodes fall along the line of the original coarse 244 245 grid. Node N in Figure 3 represents one such node where the integration of Equation 9 over the interval BF is achieved in two steps. The first integral occurs over BE using head values 246 located below the line LN while the second occurs over EF and uses head values located above 247 LN. In both cases the equations are based on the hydraulic characteristics of node N and are 248249 similar to Equation 10. However, for the flow moving across segment BE, the value of P is adjusted to: $\left(y_N - \frac{\Delta y}{4}\right)$ and across EF the value of P is: $\left(y_N + \frac{\Delta y}{4}\right)$. With these modifications, 250 Equation 10 is a general equation that takes a desirable numerical form of head differences 251

252 multiplied by constants and it can be applied at all nodes along the grid interface.

The corresponding equations for interfaces oriented in decreasing x, and increasing and decreasing y directions can be obtained by careful re-arrangement of Equation 10. An example of this treatment can be found in Jackson (2000).

257

One slight problem arises at the extremities of the expanded mesh. The procedure does not allow the determination of groundwater head at nodes located at the corners of a child grid. This arises from the need for six points to calculate the flow balance as demonstrated for node I in Figure 4. For a point such as C in Figure 4, which is located at the corner of the child grid, the sixth node required for the calculation of the flow across DE is missing. To overcome this difficulty a virtual node is introduced beyond the extreme corner of a fine mesh. The head value at this extra node has to be estimated by interpolation.

265

Convergence of the Numerical Scheme

267 **Convergence to steady state conditions**

A first check on the new refinement scheme is to examine a simple steady state problem. This consists of a 2.5 km square aquifer, refined as shown in Figure 5a. The parent and the child grids are composed of 500 m and 100 m square cells respectively. The child grid lies at the middle of the coarse grid and both have the same transmissivity values of 100 m² day⁻¹.

272

Successive Over Relaxation (SOR) is used to solve the numerical system. SOR is a point iterative approach based on the Jacobi and the Gauss-Seidel iteration methods to solve a system of linear equations. The allowable error, representing the maximum flow imbalance at each node and at which the SOR procedure terminates, is set to a very small value of 1×10^{-8} m³ day⁻¹. The head values generated by the model fit the analytical solution with maximum differences between the results of the analytical and numerical solutions not exceeding 0.15%. In this special case the interpolation technique calculates the groundwater heads at the missing nodes and the groundwater heads at the extreme ends of the child grid. The flows calculated by the model confirm that no flow is generated in the y direction and that the flow in the x direction is equal to that calculated using the analytical solution. This is an important check of the coding of the model because it confirms the correct implementation of the various forms of the refined area equations as well as the proper linkage between the different types of node.

285

The boundary conditions are specified as fixed head values on all sides and zero groundwater heads are specified everywhere as initial condition. A curved surface is created by introducing an abstraction well approximately in the centre of the child grid at the location labelled Node C in Figure 5a.

290

The numerical solution resulting from the proposed refined grid is compared to that produced 291 292 using a regular fine mesh grid having 100 m square cells over the whole aquifer. After a certain period of continuous abstraction at a rate of 1000 m³ day⁻¹, a steady state condition is reached. 293 Figure 5b shows the contour lines resulting from both grids. The results are in close agreement 294 and the contour lines of both solutions almost coincide. However, a closer examination reveals 295 that some differences in head exist, reaching at certain locations an absolute value of 1.4%. 296 This behaviour becomes clearer when the difference between the two solutions at the child 297 grid boundary is examined. Since a line of symmetry crosses the aquifer diagonally, as shown 298 in Figure 5a, only the upper and the lower faces of the child grid need be considered. Figure 6 299 shows the absolute head difference along these two boundary lines. The head difference 300 301 varies from a minimum of 0.1% to a maximum value of 1.4% with the maximum difference located at the node opposite the abstraction point. The flow crossing the coarse-fine interface 302 at the nodes common to both models is also compared in Figure 6. The absolute percentage 303

difference in flow ranges from a minimum of zero to a maximum of 5.0%. It is clear that a 304 small error in the computed head leads to a larger error in the flow. Reciprocally, a relatively 305 large error in the flow may lead to insignificant differences in the corresponding head values. 306 307 This is the main reason for basing the convergence criterion on an accurate determination of flow, i.e. minimising the flow imbalance, which certainly leads to an accurate head 308 determination. This is also an advantage of the integrated finite difference refinement method 309 which relies on the calculation of flow as a means of to determining head at the coarse-fine 310 interface and not vice versa. 311

312 Reproducing time variant groundwater heads

Theis' (1935) analytical solution is used to investigate the capability of the new refinement 313 scheme to produce the groundwater flow solution under time variant conditions. 314 Groundwater flows are simulated in a large 10 km square aquifer with fixed heads at its outer 315 boundaries. Large dimensions of the aquifer are necessary to reduce the interference of the 316 outer boundaries with the numerical results, especially at the later times of the simulation. the 317 transmissivity of the aquifer is set to a value of 100 m² day⁻¹ and the storage coefficient is set to 318 319 a value of 0.0001. To satisfy the Theis assumptions, no recharge is applied, the initial head values are set to zero, i.e. no drawdown occurs at time zero, and the abstraction increases 320 instantaneously to the rate of 1000 m³ day⁻¹. Finally, to allow a small nodal area at the 321 abstraction borehole so that it resembles an infinitely small well, the aquifer is refined in three 322 stages; at the coarsest level, a grid with 500 m square cells is used, followed by a grid with 100 323 m square cells as an intermediate stage and finally a grid with 20 m square cells is used for the 324 325 finest mesh. These settings are shown in Figure 7.

326

Time drawdown curves generated by the model are compared to the Theis solution at three observation wells. The locations of the observation (Figure 7) wells are selected to show

groundwater head values calculated at nodes located on the three grids. The distances 329 between the observation boreholes and the abstraction borehole are 141 m, 500 m and 1500 330 m. Figure 8 shows the simulated time drawdown curves and those produced using the Theis 331 solution. It is clear that there is good agreement between these curves except at the early 332 times of pumping. The disparity between the results is attributed to the difference in the 333 representation of the sink in the numerical model and it representation as a line source in the 334 Theis analytical solution. After day 7 the outer boundary effects start to appear in the 335 simulated results. This is reflected by the reduction of the gradient of the time drawdown 336 curves indicating that some water is being supplied by the outer fixed head nodes to the 337 pumped borehole. 338

339 Simulation of groundwater heads in heterogeneous aquifers

The presented numerical scheme can be readily used to simulate groundwater heads in heterogeneous aquifers on condition that the transmissivity value specified at one coarse grid node is the same as the transmissivity values of the child nodes in contact with it. Reproducing the groundwater heads in heterogeneous aquifers is tested in this section.

An aquifer that is 5 km long and 2.5 km wide with a global transmissivity value of 100 m2 day-1 344 and a storage coefficient value of 0.0001 is discretised using a grid with 500 m square cells, 345 which is refined at its centre as illustrated in Figure 9a. The refining grid has 100 m square cells. 346 347 The aquifer has zones with transmissivity values of 50 and 200 m2 day-1 as shown in Figure 9a. The aquifer has fixed head boundaries along its sides, has no recharge and is pumped at a rate 348 of 1000 m3 day-1 at its centre. Figure 9b shows the groundwater head contour lines produced 349 from this model and those produced from a model using a fine with 100 m square cells after a 350 simulation time of 10 days. These contours are in close agreement with the observed 351 352 discrepancy related to contouring artefact. A closer comparison between the simulated results shows that the overall discrepancy is ranging between 3 and 5% but with few cells showing 353

high error values of up to 13%. While the latter error figure recommends further investigations into its source, the cells associated with it are located next to the fixed head boundaries. The groundwater heads calculated at these cells are in the order of 10 cm while the highest drawdown values calculated at the centre is 1%.

358

Discussion and Conclusion

360

The refinement scheme is based on the integrated finite differences approach. It is similar to 361 that used by De Marsily et al. (1986) as it relies on the divergence theorem and Taylor's 362 expansions. The divergence theorem is used to transform a double integral of the basic flow 363 equation over the area associated with a node into a contour integral around the perimeter of 364 this same area. Taylor's expansions are used to determine the hydraulic gradient along the 365 366 perimeter. The accuracy of the developed numerical equations is improved by including terms 367 up to the second order from the Taylor's expansions. This is the main difference from the work presented by De Marsily et al. (1986); however, the inclusion of these additional terms requires 368 extra mathematical computation to derive the numerical equations that describe the flow 369 across the fine-coarse mesh interface. Significantly, the new flow equations maintain the 370 desired form, which calculates the flow as the product of head differences multiplied by a 371 372 constant as in the conventional finite difference formulae.

373

The numerical grid layout used to refine the grid affects the difficulties associated with producing the numerical equations. It has been found that dividing the nodes rather than the mesh increases the number of sides over which the conventional finite difference equations are applied, and increases the accuracy of the model. The derived numerical equations converged to the required solution without difficulty, although in some cases the over

379 relaxation factor had to be limited to values less than 1.4 to ensure the convergence of the380 solution.

381

The new refinement scheme is tested for its ability to represent the groundwater heads in 382 homogeneous and heterogeneous aquifers under steady state and time variant conditions. 383 The developed numerical technique relies on the principle of using the Taylor's series to 384 calculate the groundwater head gradients at a point moving along a node face. This requires 385 that the groundwater surface is continuous and differentiable between all the nodes in order 386 387 to calculate the gradient at that point. For a heterogeneous aquifer, the refining grid must be selected such that the aquifer does not change in its properties between the nodes 388 surrounding the point where the hydraulic gradients are calculated 389

390

Accurate results were generated for a drawdown surface that curves in one direction only. 391 392 However, the technique generated undesirable but small errors in the representation of a drawdown surface that curves in two directions. 393 These errors arise because of the interpolation necessary to calculate head values at the imaginary nodes at the corners, which 394 395 are required to comply with the new formulae. However, the differences between the numerical results and the analytical results fall within an acceptable range. The flow errors are 396 found to be higher than the head errors; this is expected since a very small change in the head 397 values can lead to relatively high changes in water flows. It is therefore much better to stop 398 the iteration process in the numerical model when it attains an acceptable water balance 399 rather than when the heads stop changing significantly. This is where the integrated finite 400 401 difference approach, where the calculation of flows at all node faces is possible, prevails over other refinement schemes. 402

This refinement scheme shows the potential of having more advantages than other refining techniques so far reported in the literature. For example, the order of refinement can be increased to order of refinement higher than 5, the limit imposed by Jackson (2000) on his refinement technique. This refinement approach together with the layout of the grid described in this paper also offers the possibility of setting a concave refinement configuration, i.e. when the part of the child grid takes an L shape. In addition, the integrated finite difference application presented here can be applied to non-linear grid interface. This opens the possibility of deriving groundwater flow equations to nodes located at the edges of a cylindrical grid model and consequently embedding the cylindrical grid model in a Cartesian model. This investigation is ongoing.

429 References

- Arney, D.C., and Flaherty J.E. 1989. An adaptive local mesh refinement method for time-dependent
 partial differential equations. *Applied Numerical Mathematics*, 5, 257-274.
- 432 Bennett B.A.V., and Smooke M.D. 1999. Local rectangular refinement with application to nonreacting
- 433 and reacting fluid flow problems. *Journal of Computational Physics*, 151, 684-727.
- 434 Berger M.J., and Oliger J. 1984. Adaptive mesh refinement for hyperbolic partial differential equations.
- 435 *Journal of Computational Physics*, **53**, 484-512.
- 436 Boas M.L. 1983. *Mathematical methods in the physical sciences*. New York: John Wiley and Sons.
- 437 Bravo R., Rogers J.R., and Cleveland T.G. 1996. Modelling groundwater flow using flux boundary
- 438 conditions. *Water Resources Bulletin*, 32, 1, 39-46.
- 439 De Lange H.C., and De Goey L.P.H. 1994. Numerical flow modelling in a locally refined grid.
- 440 International Journal for Numerical Methods in Engineering, 37, 487-515.
- De Marsily G., Ledoux E., Levassor A., Poitrinal D., and Salem A. 1978. Modelling of large multilayered
 aquifer systems: Theory and applications. *Journal of Hydrology*, 36, 1-34.
- 443 De Marsily G. 1986. *Quantitative Hydrogeology*. San Diego: Academic Press.
- 444 Dickinson E.J., James S.C., Mehl S., Hill M.C., Leake S.A., Zyvoloski G.A., Faunt C.C., and Eddebbarh A.
- 445 2007. A new ghost-nod method for linking different models and initial investigations of heterogeneity
- and nonmatching grids. *Advances in Water Resources*, 30, 1722-1736.
- 447 Diersch H.j.G. 2005. FEFLOW finite element subsurface flow and transport simulation system reference
- 448 manual. WASY GmbH Institute for Water Resources planning and Systems Research. Berlin
- 449 Hayes P.J. 1999. An r-theta co-ordinate numerical model, incorporating mesh refinement, for the
- 450 investigation of pumping tests in heterogeneous aquifers. Ph.D. Thesis, The University of Birmingham,
- 451 Birmingham, U.K.
- 452 Jackson J.R. 2000. A novel grid refinement method for regional groundwater flow using Object Oriented
- 453 technology. Ph.D. Thesis, The University of Birmingham, Birmingham, U.K.

- Mansour M.M., Hughes A.G., Spink A.E.F., Riches J. 2011. Pumping Test Analysis Using a Layered
 Cylindrical Grid Numerical Model in a Complex, Heterogeneous Chalk Aquifer. *Journal of Hydrology*, 1-2,
 14 21.
- 457 Mehl S., and Hill M.C. 2004. Three-dimensional local grid refinement for block-centered finite-458 difference groundwater models using iteratively coupled shared nodes: a new method for interpolation 459 and analysis of errors. *Advancs in Water Resources*, 27, 899 – 912.
- Mehl S., Hill M.C., and Leake A.A. 2006. Comparison of local grid refinement methods for MODFLOW. *Ground Water*, 44, 6, 792 796.
- 462 Miller R.T. and Voss C.I. (1987). Finite-difference grid for a doublet well in an anisotropic aquifer.
- 463 Ground Water, 24, 4, 490-496
- 464 Quandalle P. and Franlab P.B. 1985. Reduction of grid effects due to local sub-gridding in simulations
 465 using a composite grid.
- 466 Rushton K. R. And Redshaw S.C. 1979. *Seepage and groundwater flow*. Chichester : Wiley.
- 467 Southwell R.V. 1946. *Relaxation methods in theoretical physics*. Oxford : Clarendon Press.
- Szekely F. 1998. Windowed spatial zooming in finite-difference ground water flow models. *Ground Water*, 36, 5, 718-721.
- Szekely F. 2008. Three-dimensional mesh resolution control in finite difference groundwater flow
 models through boxed spatial zooming. *Journal of Hydrology*, 351, 261-267.
- 472 Theis C.V. 1935. The relation between the lowering of the piezometric surface and the rate and
- 473 duration of discharge of a well using ground-water storage. *Transactions of the American Geophysical*
- 474 Union, 16th annual meeting, 519-524.
- 475 Ward D.S., Buss D.R., Mercer J.W., and Hughes S.S. 1987. Evaluation of groundwater corrective action
- 476 at the Chem-Dyne hazardous waste site using a telescopic mesh refinement modeling approach. *Water*
- 477 *Resources Research*, 23, 4, 603-617.
- 478 Zzvoloski G.A., Robinson B.A., Dash Z.V., and Trease L.L. 1997. Summary of the models and methods for
- the FEHM application: A finite-element heat- and mass-transfer code. Los Alamos National Laboratory
- 480 Report LA-13306-MS.





Figure 4: An imaginary node replaces the missing node adjacent to the corner node.









546 Figure 10: Comparison between simulated time drawdown curves and the Theis solution at