

**PRO-GRADE User's Guide**

***Pattern Recognition Organizer  
and  
Groundwater Recharge and Discharge Estimator  
for  
Geographic Information Systems***

By

Yu-Feng Lin  
Center for Groundwater Science  
Illinois State Water Survey / University of Illinois at Urbana-Champaign

Jihua Wang  
Department of Civil and Environmental Engineering  
University of Illinois at Urbana-Champaign

Albert J. Valocchi  
Department of Civil and Environmental Engineering  
University of Illinois at Urbana-Champaign

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## Chapter 1: Introduction

PRO-GRADE is a Geographic Information System (GIS) plug-in tool package for recognizing patterns from raster data, such as groundwater recharge and discharge patterns, in ArcGIS 9.2-SP2 or 9.3X. The package consists of two separate programs: (1) the Pattern Recognition Organizer for GIS (PRO-GIS), and (2) the Groundwater Recharge and Discharge Estimator for GIS (GRADE-GIS). PRO-GIS is a general utility that organizes several image processing algorithms into one user interface to offer the flexibility to extract spatial patterns according to the user's needs. It provides generic pattern recognition functions that support virtually any Spatial Decision Support Systems (SDSS) used to assist in management applications such as water resources, land use and agricultural development. GRADE-GIS is a groundwater recharge and discharge estimation interface that requires only hydraulic conductivity, water table and bedrock elevation data for two-dimensional steady state aquifers based on mass balance approaches (Stoertz and Bradbury, 1989; Lin and Anderson, 2003).

PRO-GRADE adheres to the default raster file format developed by the Environmental Systems Research Institute, Inc. (ESRI) as the standard for storing spatial information. The computations are performed in double-precision floating point although the raster files store the data in single-precision floating point using scientific notation. Several ArcObjects developed by ESRI were also utilized for spatial data access and mapping. The package was coded using Microsoft Visual Basic in Microsoft Visual Studio 2005.

## Chapter 2: Installation instructions

The software environment configuration, preinstallation requirements and installation steps are described in this chapter. The current version of PRO-GRADE has been tested on personal computers using Microsoft Windows XP and Vista operating systems.

### 2.1 Important notes before installation

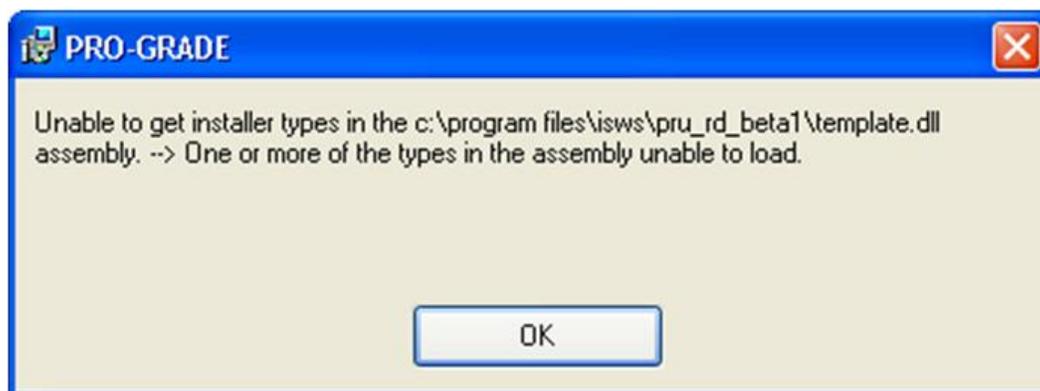
If the previous version of PRO-GRADE (called “PRU” in the beta version) is installed, it must be uninstalled by using Add or Remove Programs in the Control Panel prior to installing the current version of PRO-GRADE. If the user needs to upgrade from ArcGIS 9.1 to ArcGIS 9.2, the previous version of PRO-GRADE must be uninstalled **before** uninstalling ArcGIS 9.1. Otherwise, the previous version of PRO-GRADE cannot be uninstalled because the ArcGIS 9.1 environment will not be available.

### 2.2 Software requirements and configuration for PRO-GRADE

#### PRO-GRADE requires the following preinstalled software:

1. Operating System: Windows XP – SP2 or Windows Vista
2. ArcGIS Release: 9.2-SP2 and 9.3X
3. ArcMap Spatial Analyst Extension
4. ArcGIS.NET support
5. Minimum .NET Release: .NET Framework 2.0

Several error messages may appear during the PRO-GRADE installation process if the required software packages are not completely installed prior to the PRO-GRADE installation. Figure 1 shows an example of an error message that can occur during the PRO-GRADE installation process.

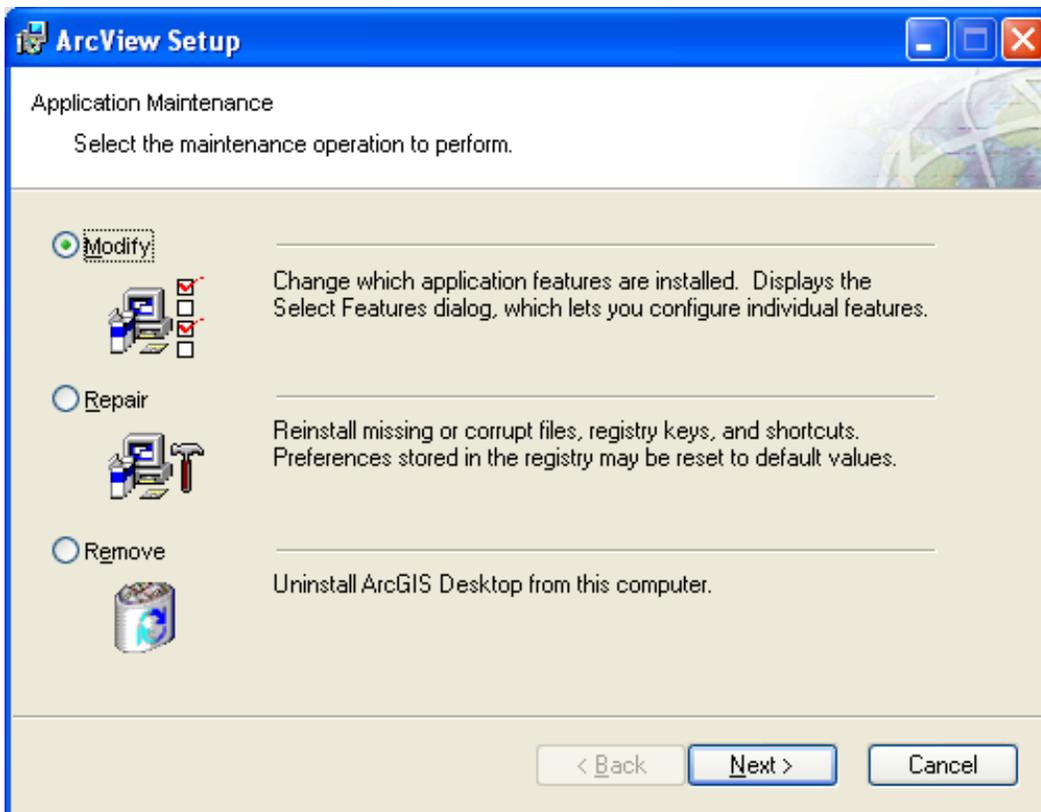


**Figure 1. Example error message during installation process caused by insufficient software requirements in ArcGIS**

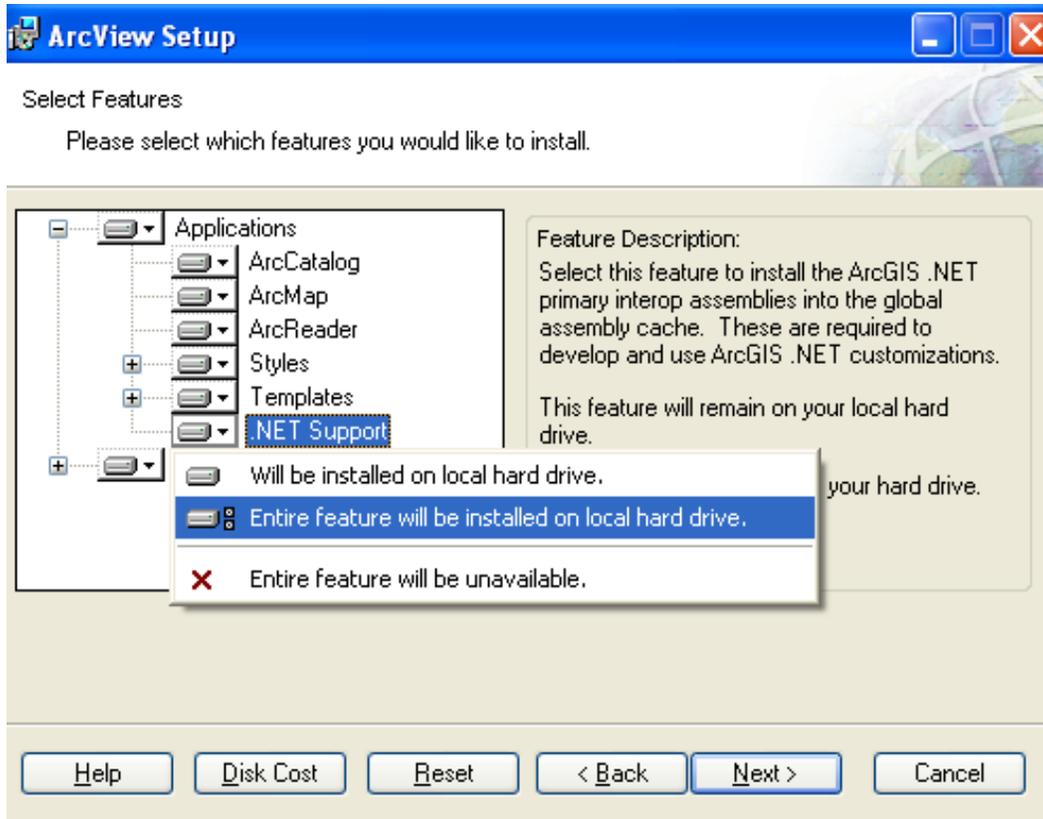
## 2.3 Installation processes

### Step 1: Install full ArcGIS.NET support.

Full ArcGIS.NET support must be installed before installing the PRO-GRADE package. ArcGIS.NET support can be verified in Windows by clicking Start | Control Panel | Add or Remove Programs | ArcGIS | change-modify. Then select Modify in ArcView Setup (Figure 2) and enable the entire .NET support feature (Figure 3).



**Figure 2. ArcView Setup**



**Figure 3. Selecting and installing ArcGIS.NET**

## Step 2: Install ArcGIS9.2 Updates

Service packs (SP2 or later) for ArcGIS 9.2 must be installed prior to installing PRO-GRADE. An error message similar to the error message shown in Figure 2 may appear during the PRO-GRADE installation if SP2 or later is not preinstalled. Be sure to contact your GIS manager for proper SP2 installation since every organization has different GIS server configurations.

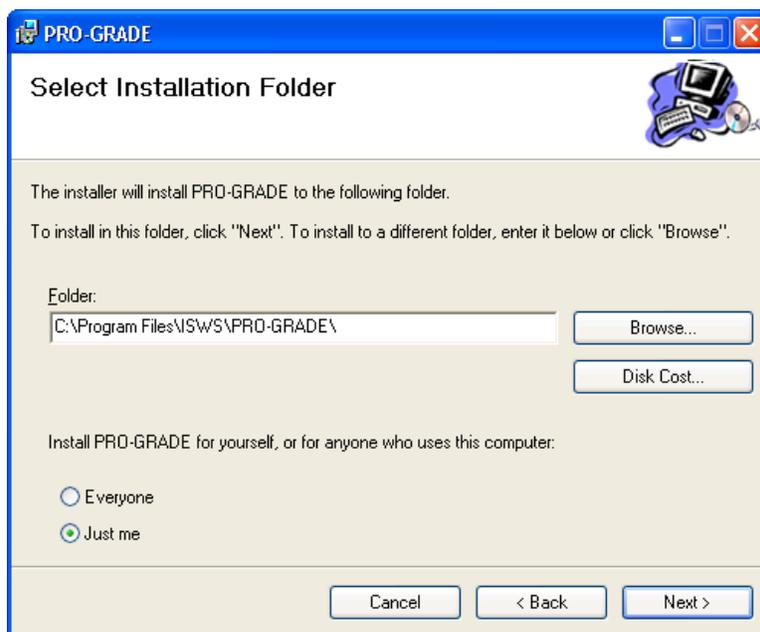
## Step 3: Install the .NET framework

Microsoft.NET framework 2.0 (or later) must be installed prior to installing PRO-GRADE,. At the time of the writing of this guide, Microsoft .NET Framework Version 2.0 was available for free download at:

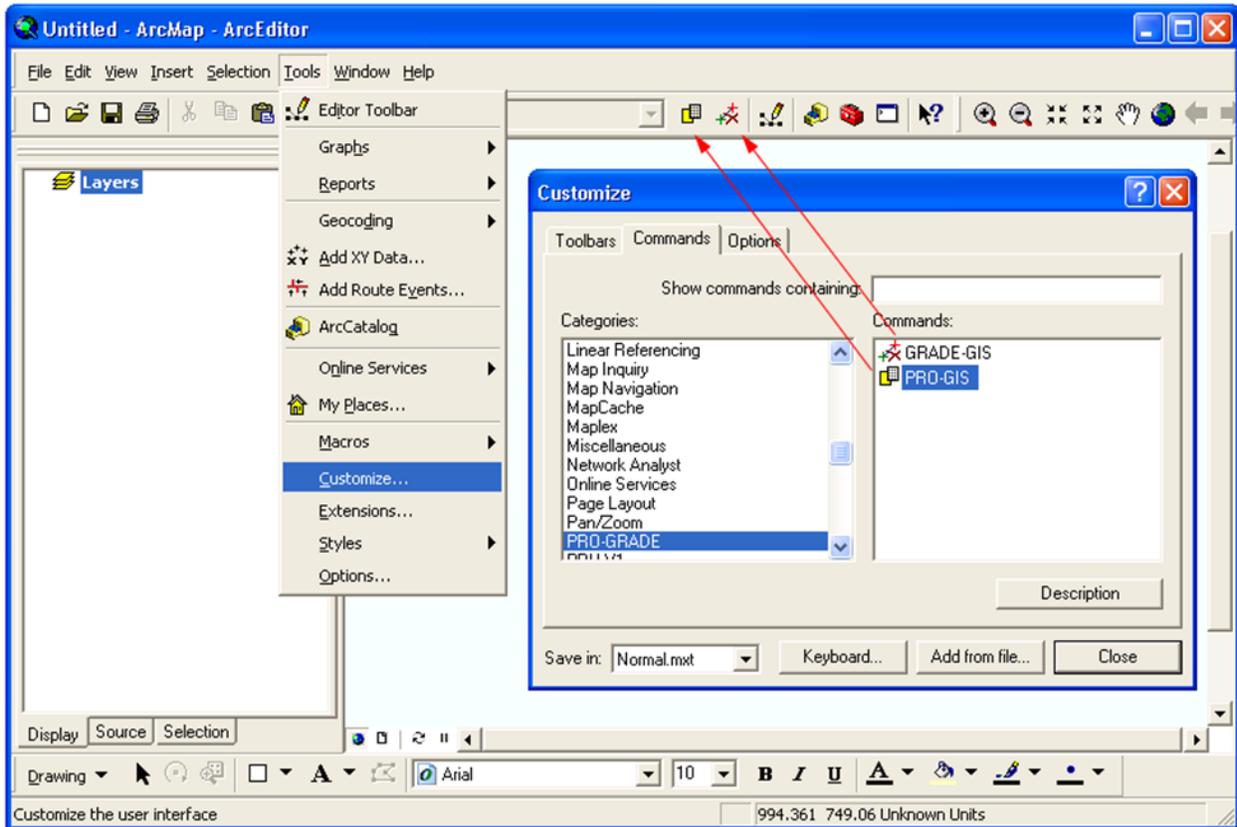
<http://www.microsoft.com/downloads/details.aspx?familyid=0856eacb-4362-4b0d-8edd-aab15c5e04f5&displaylang=en>

## Step 4: Install PRO-GRADE.

Download and unzip the PRO-GRADE zip file to a temporary folder. From the unzipped package, select the PRO-GRADE folder and click setup.exe; PRO-GRADE installation will start. The program directory can be specified during installation as shown in Figure 4. After installation is complete, start ArcMap, then click Tools | Customize as shown in Figure 5. Clicking on PRO-GRADE in the Categories window will display two icons in the Commands window. Drag the icon  for PRO-GIS and the icon  for GRADE-GIS from Commands to the ArcMap toolbar as the red arrows show in Figure 5. Complete the step by clicking Close in the Customize dialog box.



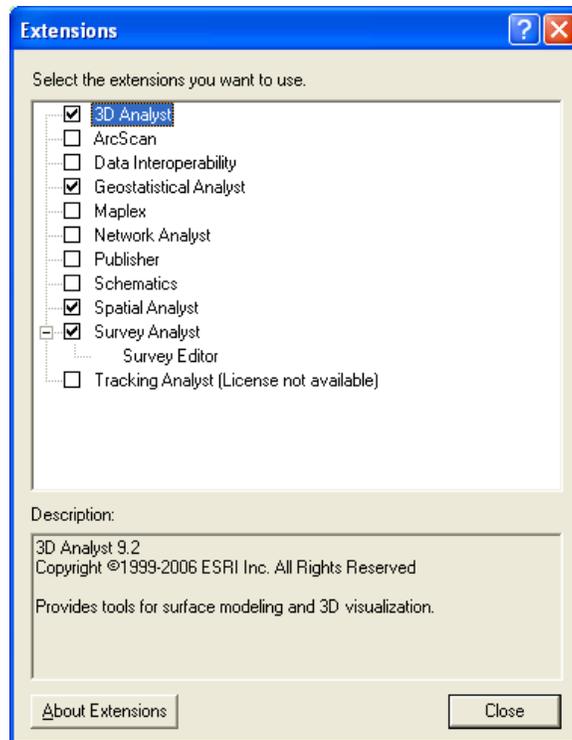
**Figure 4. Installing PRO-GRADE in a user-specified directory**



**Figure 5. Installing PRO-GIS and GRADE-GIS icons in the ArcMap toolbar**

### **Step 5: Enable Spatial Analyst.**

The spatial analyst extension must be activated in ArcMap in order to fully utilize PRO-GIS. This extension can be accessed from the ArcMap main menu bar by clicking on Tools | Extensions (Figure 5). Check Spatial Analyst in the Extensions window and then click on Close as shown in Figure 6. If the spatial analyst extension is not activated, an error message (“Check spatial analyst license: the parameter is incorrect”) will appear when the 2D Moving Average is executed in PRO-GIS.



**Figure 6. Enabling the Spatial Analyst extension**

## Chapter 3: Pattern Recognition Organizer for GIS (PRO-GIS)

PRO-GIS demonstrates the benefit of organizing multiple image processing algorithms into one graphical user interface (GUI). This organization provides an efficient and systematic approach for scientists to analyze and compare data and unquantifiable information. Numerous image processing algorithms can be added to the GUI through the use of Microsoft Visual Basic. PRO-GIS can work with three methods of image processing: (1) existing program objects, (2) existing codes for traditional algorithms, and (3) code written within PRO-GIS for new algorithms. Future developers will be able to use these three methods to expand the capabilities of PRO-GIS and tailor the application to the needs of each individual project.

### Launching PRO-GIS

Before using PRO-GIS, the user must import at least one raster file into ArcMap. If the user has only feature layers instead of raster files, the feature layers can be converted

to raster files using ArcToolbox  by clicking Conversion Tool | To Raster | Feature to Raster.

Clicking the PRO-GIS icon  on the ArcMap tool bar launches the GUI, as shown in Figure 7. The input raster layer for the pattern recognition process can be selected from the dropdown list or by clicking “Browse”  to select a raster in the “Input/Output” area.

There are three image processing methods available in the present version of PRO-GIS: 2D Moving Average, Normalization and TVL1 Low Pass Filter.

After PRO-GIS processes the data, the output files can be saved to the default output directory (C:\) or to a user-specified directory. The user-specified directory must be present before trying to save the result raster file. PRO-GIS is not currently capable of generating new folders. If the user-specified directory does not exist, an error message (“Could not find a part of the path ...\\treatpru.txt”) may appear. PRO-GIS closes after the output raster file is successfully saved to the specified directory. PRO-GIS will not overwrite the existing file. Therefore, the user must create a new output raster name in the specified directory in order to prevent the error message “Raster: SaveAs File already exists”. The default symbology for the result raster file is “stretched”, but can easily be modified using the properties dialog for the raster layer.

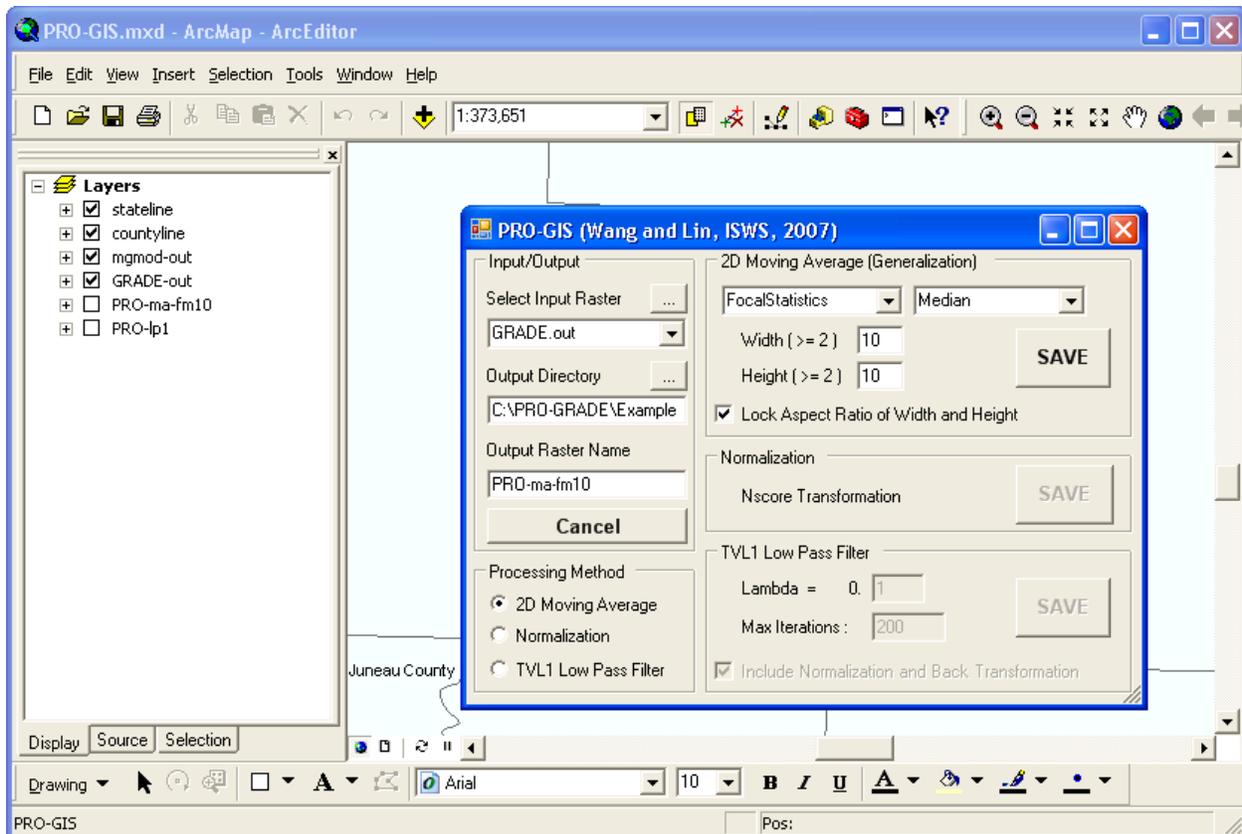


Figure 7. The PRO-GIS GUI

### 3.1 2D Moving Average (Generalization)

The Spatial Analyst Extension must be enabled (Section 2.1, Step 5, Figure 6) before trying to calculate the 2D moving average, because the average is calculated using the Generalization ArcObject in Spatial Analyst. This function set will demonstrate the flexibility of PRO-GIS in using existing program objects as mentioned above.

There are two main methods to calculate a 2D moving average: focal statistics and block statistics, which use the FocalStatistics and BlockStatistics ArcObjects, respectively. For each method, several statistical calculations are available, including majority, maximum, median, minimum, minority, range, standard deviation (STD) and variety. The default method is focal statistics - median.

As shown in Figure 7, the width and height of the moving window for averaging computations can be specified in the corresponding textboxes. The default width and height must be equal to or greater than 2 in order to generate sufficient results. If the “Lock Aspect Ratio of Width and Height” checkbox is activated, the width and height will be modified simultaneously. A larger sized moving window usually requires more computation time.

Since the functions for 2D Moving Average are directly inherited from Generalization ArcObjects, the following subsections are summaries taken from the ESRI Developer Network website and ArcGIS 9.2 Desktop Help (ESRI, 2005) for users' convenience. More detailed information regarding Generalization in the Spatial Analyst Extension is available at the ESRI Developer Network website.

### 3.1.1 Focal Statistics (FocalStatistics) and Block Statistics (BlockStatistics)

The Focal Statistics and Block Statistics options calculate a statistic on a raster over a specified neighborhood (ESRI, 2005) based on different neighborhood configurations. Although the original Generalization ArcObjects offers more options, the default neighborhood shape (or moving window) of the area around each cell used to calculate the statistic in PRO-GIS is a rectangle.

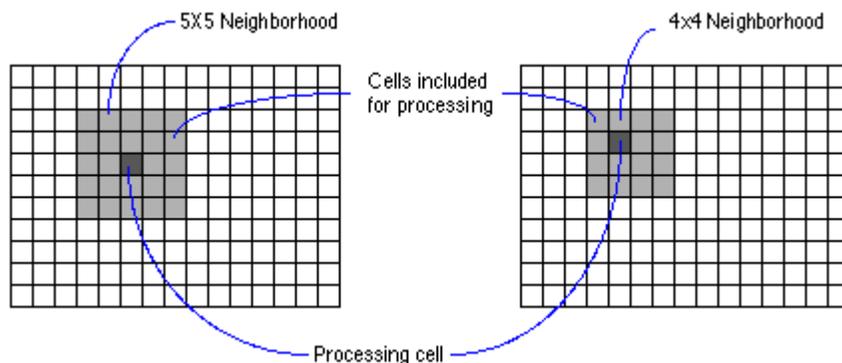
#### 3.1.1.1 Neighborhood Settings for Focal Statistics

The Focal Statistics function calculates a statistic on a raster over a specified neighborhood. The rectangle is the default shape of the area around each cell used to calculate the statistic. The x, y position for the processing cell within the neighborhood, with respect to the upper-left corner of the neighborhood, is determined by the following equations:

$$x = (\text{width of the neighborhood} + 1) / 2$$

$$y = (\text{height of the neighborhood} + 1) / 2$$

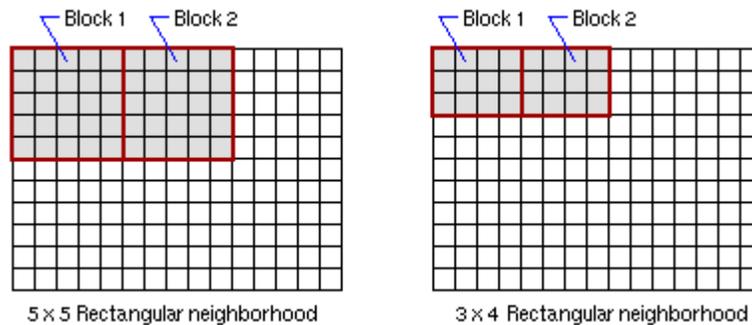
If the input number of cells is even, the x, y coordinates are computed using truncation. For example, in a 5 x 5 cell neighborhood the x- and y-values are 3, 3. In a 4 x 4 neighborhood the x- and y-values are 2, 2.



**Figure 8. Neighborhood Settings for Focal Statistics (from ArcGIS 9.2 Desktop Help)**

### 3.1.1.2 Neighborhood Settings for Block Statistics

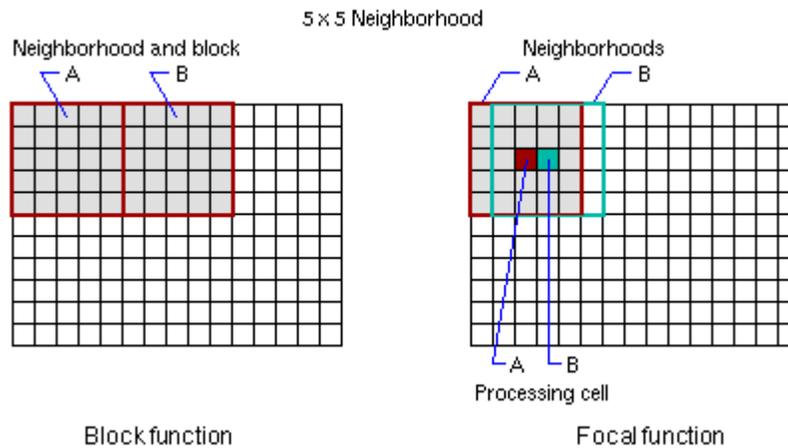
With the Block Statistics function, values are calculated for a fixed set of non-overlapping windows or neighborhoods. The resultant value for an individual neighborhood is assigned to all cell locations contained in the rectangle of the specified neighborhood. The block function partitions the remaining area of the raster into defined blocks (no blocks can overlap). It calculates the output value for each neighborhood of each block. The resultant values are assigned to every cell location in the corresponding output block.



**Figure 9. Neighborhood Settings for Block Statistics  
(from ArcGIS 9.2 Desktop Help)**

### 3.1.1.3 Differences between Focal Statistics and Block Statistics

The neighborhoods in the block statistics function do not overlap, while the neighborhoods in the focal statistics function are based around a processing cell and always overlap. In a block function, a block of cells corresponding to the minimum bounding rectangle of a neighborhood receives the resultant value, while in a focal function only the processing cell receives the resultant value.



**Figure 10. Differences between the block function and the focal function (from ArcGIS 9.2 Desktop Help)**

### 3.1.2 Functions and formats for statistical calculations

The choices of statistical calculations for both Focal Statistics and Block Statistics include the following: Majority, Maximum, Median, Minimum, Minority, Range, STD and Variety.

#### Majority

- Majority calculates the majority value (the value that occurs most often) of the cells in the neighborhood
- If the input raster contains integers, the values on the output raster will be integers. If the values on the input are floating point, the values on the output will be floating point.
- When there is more than one majority value within a neighborhood, the processing cell location will result “No Data” on the output.

#### Maximum

- Maximum calculates the maximum value (the largest value) of the cells in the neighborhood.
- If the input raster contains integers, then the values on the output raster will be integers. If the values on the input are floating point, the values on the output will be floating point.

## Median

- Median calculates the median value of the cells in the neighborhood.
- If the input raster contains integers, the values on the output raster will be integers. If the values on the input are floating point, the values on the output will be floating point.
- When the number of the valid cell values in the neighborhood is odd, the median value is calculated by ranking the values and then selecting the middle value. If the number of values in a neighborhood is even, the values will be ranked and the middle two values will be averaged.

## Minimum

- Minimum calculates the minimum value (the smallest value) of the cells in the neighborhood.
- If the input raster contains integers, the values on the output raster will be integers. If the values on the input are floating point, the values on the output will be floating point.

## Minority

- Minority calculates the minority value (the value that occurs least often) of the cells in the neighborhood.
- If the input raster contains integers, the values on the output raster will be integers. If the values on the input are floating point, the values on the output will be floating point.
- When there is more than one minority value within a neighborhood, the processing cell location will result “No Data” on the output.

## Range

- Range calculates the range (the difference between the largest and the smallest values) of the cells in the neighborhood
- If the input raster contains integers, the values on the output raster will be integers. If the values on the input are floating point, the values on the output will be floating point.
- The values for each cell location on the output grid are determined on a cell-by-cell basis by applying the simple formula:

$$\text{Focal Range} = \text{Focal Maximum} - \text{Focal Minimum}$$

## Standard Deviation (STD)

- STD calculates the standard deviation of the cells in the neighborhood.
- The output raster will always be in the form of floating points.

### Variety

- Variety calculates the variety (the number of unique values) of the cells in the neighborhood.
- The output raster will always be in integer form.

## 3.2 Normalization

Normal score transformation is provided in PRO-GIS as an option for transforming input data with significantly asymmetric distribution to a normal distribution. The normal score transformation is helpful in reducing the skewness and may provide a clearer result. The following explanation is summarized from Deutsch and Journel (1998) for convenience. For more complete information, please read this reference directly. The Normalization function will demonstrate the capability of PRO-GIS to utilize existing codes for traditional algorithms as mentioned at the beginning of Chapter 3.

According to Deutsch and Journel (1998), the original z-data are first transformed into y-values with a standard normal histogram. The transform  $y = \phi(z)$  identifies the cumulative probability corresponding to the Z and Y p-quantiles:

$$F_Y(y_p) = F_Z(z_p) = p, \forall p \in [0,1] \quad \text{hence}$$

$$y = F_Y^{-1}(F_Z(z))$$

*with  $F_Y^{-1}(\cdot)$  being the inverse cumulative distribution function (CDF) or quantile function.*

If Y is standard normal with CDF  $F_Y(y) = G(y)$ , the transform  $G^{-1}(F_Z(\cdot))$  is the normal score transform.

In practice, the n z-sample data are ordered in increasing value:  $z^{(1)} \leq z^{(2)} \leq \dots \leq z^{(n)}$ . The cumulative frequency corresponding to the  $k_{\text{th}}$  largest z datum is  $F_Z(z^{(k)}) = k/n$ .

Then the normal score transform of  $z^{(k)}$  is the  $k/n$  quantile of the standard normal CDF, i.e.,

$$y^{(k)} = G^{-1}(k/n)$$

Generally the above solution may be sensitive to the sample size and is not flexible to model the distribution tails. To avoid the problem of sensitivity to sample size, the cumulative probability of each data is reset to the average between its cumulative probability and that of the next lowest datum.

For example, if  $c_i$  is the cumulative probability with the  $i_{th}$  largest data value

$z_i(c_i = \sum_{j=1}^i p_j)$ , the normal score transform  $y_i$  with  $z_i$  is calculated as

$$y_i = G^{-1}\left(\frac{c_i + c_{i-1}}{2}\right)$$

with  $G(y)$  being the standard normal CDF and  $c_0 = 0$ .

The normalization function in PRO-GIS was implanted based on the FORTRAN code `nscore.f`, in GSLIB (Deutsch and Journal, 1998). The default parameters for numerical computation suggested by Deutsch and Journal (1998) were used and no weight for declustering was applied for  $Fz$  computation.

### 3.3 TV+L<sup>1</sup> Low Pass Filter (TVL1)

An advanced image-processing algorithm, TV+L<sup>1</sup> which stands for Total Variation Regularized L<sup>1</sup> Function Approximation (Chan and Esedoglu, 2005), is incorporated in PRO-GIS. TV+L<sup>1</sup> minimizes the total variation of the image subject to an L<sup>1</sup>-norm fidelity term. The main advantages of this algorithm include the well known edge-preserving capacity, simplicity of parameter selection, minimal signal distortion and the flexibility to extract variable degrees of spatial details (Chen et al, 2006). This recently developed image-processing algorithm has been applied in several advanced pattern-recognition applications (Chen et al, 2006; Yin et al., 2005), including a current study for identifying human brain anomalies in MRI (Magnetic Resonance Imaging) scans. TV+L<sup>1</sup> includes a high-pass filter for extracting detail features and a low-pass filter for removing noise and identifying the overall pattern. Only the low-pass filter TV+L<sup>1</sup> was implanted in PRO-GIS. Use of this algorithm illustrates the ability to incorporate other algorithms in PRO-GIS as mentioned at the beginning of Chapter 3.

The TV+L<sup>1</sup> Low Pass Filter (TVL1) requires two parameters: Lambda and Max Iterations.

- Lambda ( $\lambda$ ) is the Lagrange multiplier. The determination of lambda is based on the radius of the pattern desired. For a2D image,  $\lambda=2/r$ .

- Max Iterations is the stop condition of maximum iteration in computation.

In the TV-based framework, an image  $f$  is modeled as the sum of image pattern  $u$  (low-pass signal) and texture  $v$  (high pass signal), where  $f$ ,  $u$  and  $v$  are defined as functions in appropriate spaces. Pattern  $u$  contains background hues and significant boundaries, specifically the large-scale spatial patterns identified in PRO-GIS. The rest of the image  $v$ , which is texture characterized by small-scale oscillation patterns, is not utilized in PRO-GIS since noise and small artifacts are included.

Since pattern  $u$  is more regular than texture  $v$ , we can obtain  $u$  by minimizing the irregularity measure while being close to  $f$  with respect to a fidelity (distance) measure (Yin et al., 2005). The TV+L<sup>1</sup> model was formulated by Chan and Esedoglu (2005) as

$$\min \int_{\Omega} |\nabla u(x)| dx \quad s.t. \quad \|f(x) - u(x)\|_{L^1} \leq \sigma$$

where  $\Omega$  is the image domain, and functions  $f$  and  $u$  are defined on  $\Omega$ .

$\|\bullet\|_*$  denotes the dual norm of total variation

Since the formula above is a convex optimization problem, it can be formulated as

$$\min \int_{\Omega} [|\nabla u(x)| + \lambda |f(x) - u(x)|] dx$$

where  $\lambda$  is the Lagrange multiplier.

The first integral is the regularization term, which disfavors oscillations and is responsible for the elimination of noise in noisy images. The second integral is the L<sup>1</sup>-norm fidelity term, which encourages the solution  $u(x)$  being sought close to  $f(x)$ .

The TV+L1 model keeps the sharp object edges in  $u$  because minimizing the TV regularization term penalizes all intensity variations in a uniform way. Thus the decomposition is dependent only on the scale of the pattern (the geometric features) but is independent of the intensity of the pattern (the contrast of image features) (Chan and Esedoglu, 2005).

The value of Lambda can be modified with a positive number less than 1.0. Usually, the smaller value of Lambda will produce a smoother image. The Max Iterations is generally 200 or greater for a larger map. The PRO-GIS default values of Lambda and Max Iterations are 0.1 and 200, respectively. If the data structure is distributed asymmetrically with a few extreme values, the result of TVL1 may look unreasonable. This problem might be compensated by activating the checkbox of "Including Normalization and Back Transformation" (see the "Normalization and Back Transformation" section below for more information) prior to saving the TVL1 result.

The value selection of Lambda is based on the user's need. In most cases, the higher lambda will enable TVL1 to catch more detailed signals (and noise) from the input image. Therefore, the output of TVL1 should be similar to the input image if lambda is 0.99. Higher values of Max Iterations will require more computation time and generally

will generate a more accurate result. If two different iteration numbers with the same lambda generate the same image, it is an indication that the smaller iteration number should be sufficient.

## Normalization and Back Transformation Option

If the checkbox for “Include Normalization and Back Transformation” is activated in the TVL1 option, the original data will be transformed into normal score (section 3.2) and then processed by the TV+L<sup>1</sup> low-pass filter and then back-transformed to the original range. Therefore, the resultant data range will be the same scale as the original data range.

Deutsch and Journel (1998) showed the back transformation  $z_i$  of the standard normal deviate  $y_i$  is given by

$$z_i = F^{-1}(G(y_i))$$

where  $F(z)$  is the CDF of the original data (section 3.2)

Usually, the value  $G(y_i)$  will not correspond exactly to an original sample CDF value  $F$ ; therefore, some linear interpolation between the original sample values or extrapolation beyond the smallest and largest z-value may be required if the scaling issue is significant.

The normalization and back transformation functions in PRO-GIS are based on the FORTRAN codes `nscore.f` and `backtran.f` in GSLIB (Deutsch and Journel, 1998), and the default parameters are used for numerical computation. These functions in PRO-GIS exclude weights for declustering, which means equal weight is used for calculating  $Fz$  (same as section 3.2).

## Chapter 4 Groundwater Recharge And Discharge Estimator for GIS (GRADE-GIS)

PRO-GIS provides generic pattern recognition functions that can be used for a wide variety of purposes, including but not limited to groundwater recharge and discharge pattern recognition. GRADE-GIS is a user-friendly interface for estimating groundwater recharge and discharge based on the mass balance concept of Stoertz and Bradbury (1989). Lin and Anderson (2003) discussed the concept of coupling the mass balance method and the image processing approach for more advanced groundwater recharge and discharge estimation. PRO-GIS and GRADE-GIS are individual programs and can be used independently. To facilitate compatibility, output from GRADE-GIS is formatted correctly for use in PRO-GIS as shown in the example case (see Appendix).

### 4.1 Graphical User Interface

The GRADE-GIS GUI (Figure 11) is activated by clicking the button  from the ArcMap tool bar, which is installed as shown in Step 4 of section 2.1. Three input raster files of hydraulic conductivity, water table and bedrock elevation must be selected from the dropdown list, or the user can click on “Browse”  to select the raster files from file directories. The coordinate projections, grid size and grid number of the three input raster files must be synchronized prior to processing in GRADE-GIS. The result raster will appear after the “Save” button is clicked. If the “Cancel” button is clicked, the GRADE-GIS GUI will be terminated without performing any calculations.

After GRADE-GIS processes, the result files can be saved to the default output directory (C:\) or to a user-specified directory. The user-specified directory must exist before saving the result raster file because PRO-GRADE is not capable of generating new folders. The GRADE-GIS GUI is designed terminate after the result raster file is saved to the specified directory successfully. The GRADE-GIS interface will not overwrite the existing file; therefore, the user needs to create a new output raster name in the specified directory in order to prevent an error message (“output file already exists”).

In GRADE-GIS, the user can specify the minimum saturated thickness as equal to or greater than 0.0. For more discussion of the minimum saturated thickness, please see assumption 3 in the section 4.2.

### 4.2 Methodology

GRADE-GIS provides groundwater recharge and discharge estimations in steady state and two-dimensional aquifers based on the mass balance approach of Stoertz and Bradbury (1989).

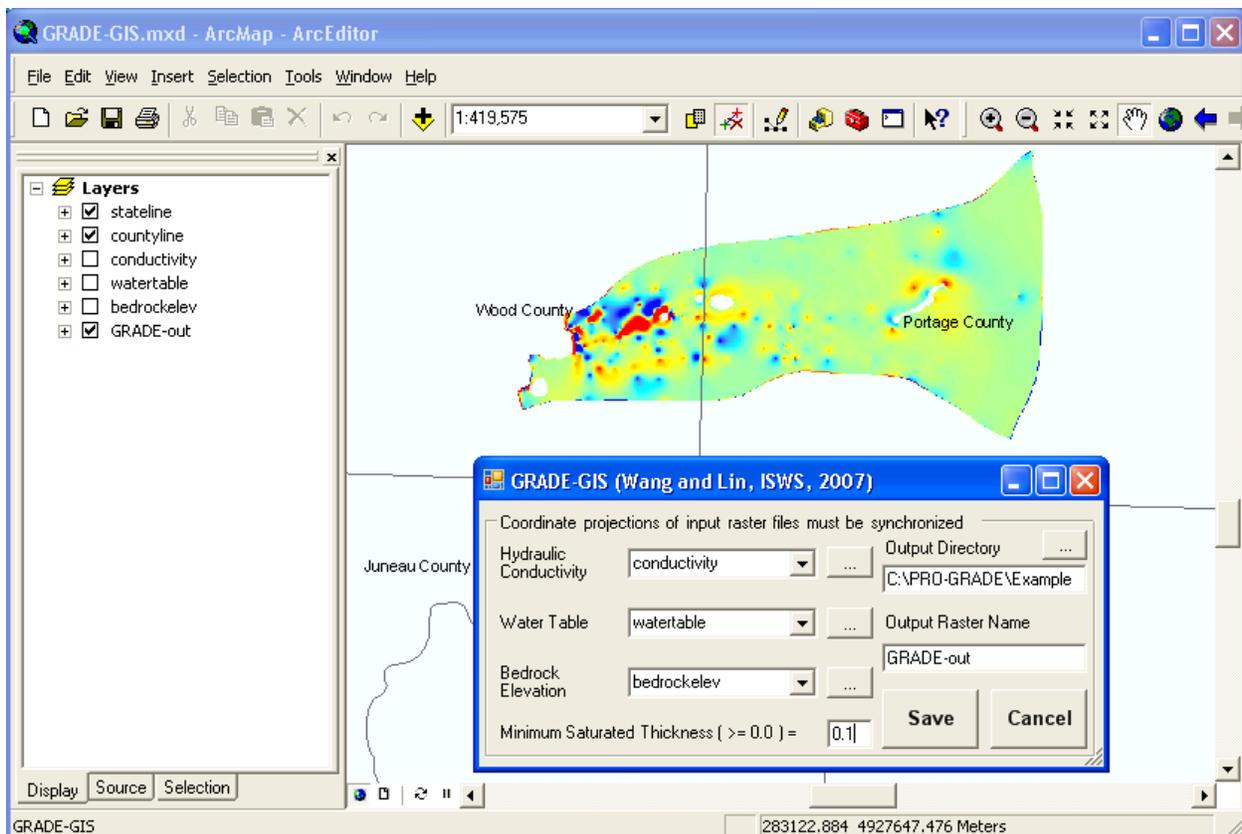
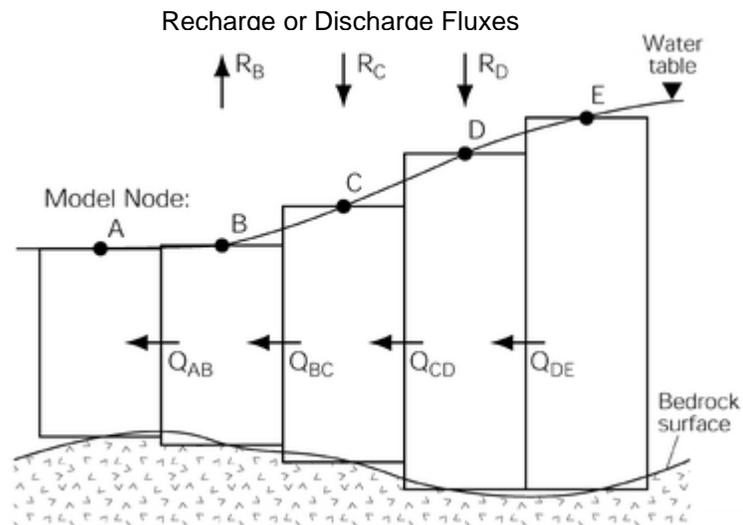


Figure 11. The GRADE-GIS interface

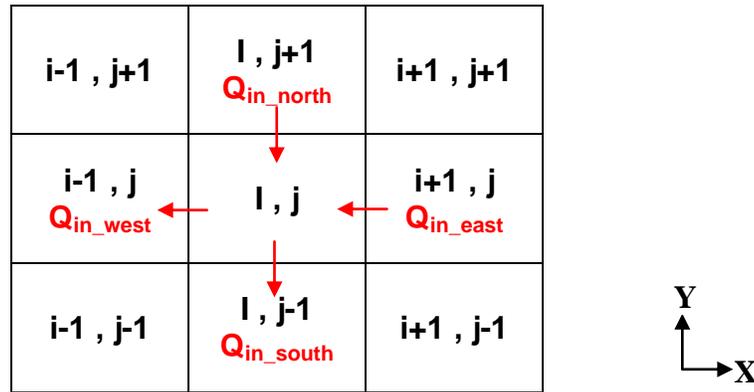
Figure 12. Stoertz and Bradbury (1989) developed a 2D steady state groundwater recharge and discharge mapping method which modifies MODFLOW-88 to compute a water balance whereby lateral flow in and out of a cell is balanced by water that enters or leaves via groundwater recharge or discharge. (from Stoertz and Bradbury, 1989)



There are three assumptions in the GRADE-GIS computation:

1. The groundwater system has horizontal two-dimensional flow under steady-state conditions in the aquifer with isotropic hydraulic conductivities.

2. There are no source and sink terms except recharge and discharge (i.e., recharge and discharge are the lump sums for all source and sink terms).
3. The water table is always higher than the bottom elevation. If the water table is less than or equal to the sum of the bottom elevation and the minimum saturated thickness, the cell is considered an inactive cell (NoData value in ArcGIS) and will be excluded from computation.
4. The resultant recharge and discharge raster cells will have NoData values for the cells that have NoData values in any of the input raster files.



**Figure 13. Grid orientation and notation for numerical computation**

As shown in Figure 13, if all the grids have the same size (which is required for the raster file), for every grid( $i,j$ )

$$Q_{in} = -R_{i,j} \cdot \Delta x_{i,j} \cdot \Delta y_{i,j}$$

$$Q_{in} = \frac{dh}{dt} \cdot K \cdot A = Q_{in\_west} + Q_{in\_east} + Q_{in\_north} + Q_{in\_south}$$

$$Q_{in\_west} = \frac{h_{i-1,j} - h_{i,j}}{\Delta x_{i-1/2,j}} \cdot K_{i-1/2,j} \cdot b_{i-1/2,j} \cdot \Delta y_{i,j} = \frac{h_{i-1,j} - h_{i,j}}{\Delta x_{i-1/2,j}} \cdot T_{i-1/2,j} \cdot \Delta y_{i,j}$$

$$Q_{in\_east} = \frac{h_{i+1,j} - h_{i,j}}{\Delta x_{i+1/2,j}} \cdot K_{i+1/2,j} \cdot b_{i+1/2,j} \cdot \Delta y_{i,j} = \frac{h_{i+1,j} - h_{i,j}}{\Delta x_{i+1/2,j}} \cdot T_{i+1/2,j} \cdot \Delta y_{i,j}$$

$$Q_{in\_north} = \frac{h_{i,j+1} - h_{i,j}}{\Delta y_{i,j+1/2}} \cdot K_{i,j+1/2} \cdot b_{i,j+1/2} \cdot \Delta x_{i,j} = \frac{h_{i,j+1} - h_{i,j}}{\Delta y_{i,j+1/2}} \cdot T_{i,j+1/2} \cdot \Delta x_{i,j}$$

$$Q_{in\_south} = \frac{h_{i,j-1} - h_{i,j}}{\Delta y_{i,j-1/2}} \cdot K_{i,j-1/2} \cdot b_{i,j-1/2} \cdot \Delta x_{i,j} = \frac{h_{i,j-1} - h_{i,j}}{\Delta y_{i,j-1/2}} \cdot T_{i,j-1/2} \cdot \Delta x_{i,j}$$

where

$\Delta x_{i,j}$  and  $\Delta y_{i,j}$  are horizontal cell dimensions [l];

$\Delta x_{i,j}$  and  $\Delta y_{i,j}$  with  $\pm 1/2$  in i and j notations are the lengths between centers of cell (i,j) and its four adjacent cells [l];

$R_{i,j}$  is recharge / discharge rate of grid(i,j) [l/t];

$h_{i,j}$  is the hydraulic head of grid(i,j) [l];

$K_{i,j}$  is hydraulic conductivity of grid(i,j) [l/t];

$b_{i,j}$  is saturated thickness and equal to hydraulic head minus bottom elevation [l];

$T_{i,j}$  is the transmissivity of grid(i,j),  $T_{i,j} = K_{i,j} \bullet b_{i,j}$  for unconfined aquifer [l<sup>2</sup>/t];

$T_{i+1/2,j}$  is the harmonic mean of transmissivity between grid(i+1,j) and grid(i,j) [l<sup>2</sup>/t],

$$\frac{1}{T_{i+1/2,j}} = \frac{\frac{1}{T_{i+1,j}} + \frac{1}{T_{i,j}}}{2} \text{ which means } T_{i+1/2,j} = \frac{2}{\frac{1}{K_{i+1,j} \bullet b_{i+1,j}} + \frac{1}{K_{i,j} \bullet b_{i,j}}};$$

If grid(i,j) is on the boundary, the flow rate from the neighboring inactive grid is equal to zero. For example, if the grid is located on the west boundary with  $i-1 = 0$ ,  $Q_{in\_west} = 0$

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## **Appendix: Example Case**

During the installation of PRO-GRADE, an example folder is copied to the directory ..\PRO-GRADE\Example. In the example folder, there are two additional folders, PRO-GIS and GRADE-GIS, that contain example files from the Buena Vista Groundwater Basin in Wisconsin. That basin has been intensively studied in several research projects (Stoertz and Bradbury, 1989; Lin and Anderson, 2003). In the PRO-GIS folder, PRO-GIS.mxd is an ArcMap file with test input files (i.e., raster layers) that can be used with the PRO-GIS application. In the GRADE-GIS folder, GRADE-GIS.mxd is an ArcMap file with test input files (i.e., raster layers) that can be used with the GRADE-GIS application. Both of the ArcMap files have example output and can be used to experiment with the functions of the PRO-GRADE package.