Corrections to flow equations involving structural strike and dip

John R. Hoaglund, III and David Pollard

Abstract

Darcy flow equations relating vertical and bedding-parallel flow to vertical and bedding-parallel gradient components are derived, correcting for structural dip given the principal permeabilities in bedding-parallel and bedding-orthogonal directions. Incorrect-minus-correct error results are presented for ranges of structural dip ($0 \le \theta \le 90$) and gradient directions ($0 \le \varphi \le 360$). The equations can be coded into ground-water models (e.g. MODFLOW) that can use a skewed Cartesian coordinate system in structural terrane.

Structure, Scaling, and Anisotropy

Regional ground water modelling over structural terranes requires the rescaling of intra-aquifer distances along dip, as well as the rotation of transverse anisotropy with dip. In structural terranes at the scale of a groundwater or reservoir model, the intra-aquifer distances and directional components of an arbitrary flow direction become functions of the angle of dip, rotated into the plane of the regional and/or local fold-controlled bedding.

We present corrections to the Darcy flow equations relative to a skewed Cartesian coordinate system (Butkov, 1968) that is commonly used in standard MODFLOW (McDonald and Harbaugh, 1988) models, plotting incorrect-minus-correct flow error for different conditions of gradient, structural dip, and degree of anisotropy.

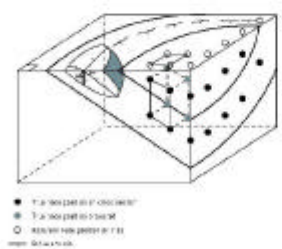

Figure 1 Block diagram showing relationships between true and apparent nodes, strike and dip of bedding, principal conductivity directions (a and b), and vertical direction (V) between nodes.

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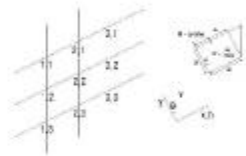

Figure 2 and 3. Skewed cartesian coordinate system (Butkov, 1968) used in MODFLOW. The vertical plane, oriented in an inter-nodal direction, shows "h" and "v" independent axes, corresponding to the bedding-parallel and vertical directions respectively, and "x" and "y" independent axes, corresponding to the bedding-parallel and bedding-orthogonal principal permeabilities. The "h" and "x" directions are shared while the "v" direction is offset from the "y" direction by the apparent dip angle, theta (θ) The non-orthogonal, stratally centered nodes are similar to those of Weiss (1985), but we neglect the effects related to thickness changes and curvature.

The "h" and "v" components of flow in terms of "h" and "v" components of gradient are given by:

$$\begin{Bmatrix} q_h \\ q_v \end{Bmatrix} = \begin{bmatrix} K_x\cos^2\theta + K_y\sin^2\theta & -K_y\tan\theta \\ -K_y\tan\theta & \dfrac{K_y}{\cos^2\theta} \end{bmatrix} \begin{Bmatrix} \dfrac{\partial H}{\partial h} \\ \dfrac{\partial H}{\partial v} \end{Bmatrix}$$

This correction for structural dip cannot be accommodated in most ground water flow models by input modification alone due to off-diagonal terms. To evaluate the error, we subtract these correct flows from incorrect flows derived by setting $\theta = 0$. We transform both sets of flow equations to an orthogonal coordinate system and specify the direction of a unit gradient with an angle phi (φ) where bedding parallel gradients are given by $\varphi = 0°$ and $\varphi = 180°$ and bedding orthogonal gradients are given by $\varphi = 90°$ and $\varphi = 270°$.

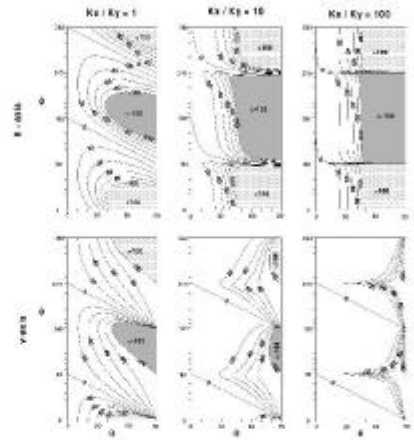

Figure 4. [illegible]

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Constraining fold-shape models with simultaneous non-linear regression to characterize fold related fractures

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Abstract

edding-plane partings and axial-plane spaced cleavage are examples of ractures in sedimentary rocks that can be related to field scale fold ructures. These fracture systems can be modelled regionally if the fold ructure can be approximated mathematically through the use of fold hape models. The theory of a new technique to estimate parameters of old shape models using geologic horizon elevation and bedding plane ata is presented. Observations of the elevation of a geologic horizon are sed to regress the parameters of a model of the horizon in a fold, while bservations of bedding planes are used to regress the same parameters in he gradient of an isotimic surface function that reduces to the horizon odel when the isotimic constant is zero. The gradient thus corresponds o the normal to the tangent (bedding) plane to the horizon, i.e. the pole to edding. Therefore the normalized components of the gradient correspond o the direction cosines of the pole to bedding, and comprise three models n the same parameters as the horizon model. A simultaneous regression an be constructed using both the horizon elevation and bedding plane bservations. The sensitivities of both the horizon model and gradient odels depend upon the values of the parameters, and thus the regression non-linear. The theory is developed and an example using a sum-of-nes function is presented for upright, symmetric folds in the Mahantango reek watershed of Pennsylvania.

A simplified model of a fold horizon

A sum-of-sines function is presented as a parsimonious model of a fold orizon in a regional doubly plunging fold system, e.g., the Valley and idge structural terrain of Pennsylvania, as an example to illustrate the heory of the technique:

$$z(x,y) = A\sin(k_1[y-y_0]) + B\sin(k_2[x-x_0]) + z_0$$

vith

$$k_1 = \frac{2\pi}{\lambda_1} \quad \text{and} \quad k_2 = \frac{2\pi}{\lambda_2}$$

where λ_1 and A, and λ_2 and B are the wavelength and amplitude of the olding and the plunging respectively, and x_0, y_0, and z_0 are offsets for the rigin. Figure 1 shows the surface generated by the function.

Non-linear regression of the models, η, to data, Y

Non-linear regression follows Cooley and Naff, 1990:

$$b^{k+1} = b^k + \rho[(C^T X^T W X C + \mu I)C^{-1}]^{-1} C^T X^T W (Y - \eta)$$

where b is the parameter vector, ρ is the damping parameter, C is the Forsythe and Strauss (1955) scaling matrix, W is a weight matrix, μ is the Marquardt (1963) parameter, I is the identity matrix, and X is the sensitivity matrix given by:

$$X_{\substack{i=1,ND \\ j=1,NP}} = \frac{\partial \eta}{\partial \beta}$$

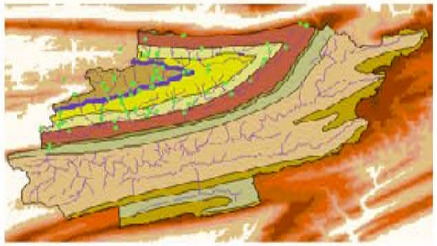

Figure 2. Mahantango Creek watershed, PA, showing locations of bedding measurements (green) and contact points (purple) where DEM elevations were used as horizon elevation data.

References

Cooley, R.L. and R.L. Naff, 1990. Regression modeling of ground-water flow. Techniques of Water Resources Investigations of the U.S. Geological Survey, Book 3, Chapter B4, Applications of Hydraulics.

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3 Gradient Component Models

Direct observations of bedding planes (strike and dip of bedding) amount to direct observations of tangent planes to the surface z(x,y) and can be used to further constrain the parameters in a simultaneous regression. Poles to bedding are normal to the surface z(x,y). If we define an isotimic surface, w(x,y,z), equal to a constant (zero):

$$w(x,y,z) = A\sin(k_1[y-y_0]) + B\sin(k_2[x-x_0]) + z_0 - z = 0$$

then ∇w is normal to the surface z(x,y), parallel to the pole to bedding. The normalized components of ∇w are:

$$\frac{f_x}{\sqrt{f_x^2+f_y^2+f_z^2}} = \frac{Bk_2\cos(k_2[x-x_0])}{\sqrt{B^2k_2^2\cos^2(k_2[x-x_0]) + A^2k_1^2\cos^2(k_1[y-y_0]) + 1}}$$

$$\frac{f_y}{\sqrt{f_x^2+f_y^2+f_z^2}} = \frac{Ak_1\cos(k_1[y-y_0])}{\sqrt{B^2k_2^2\cos^2(k_2[x-x_0]) + A^2k_1^2\cos^2(k_1[y-y_0]) + 1}}$$

$$\frac{f_z}{\sqrt{f_x^2+f_y^2+f_z^2}} = \frac{-1}{\sqrt{B^2k_2^2\cos^2(k_2[x-x_0]) + A^2k_1^2\cos^2(k_1[y-y_0]) + 1}}$$

comprising three models in the same parameters as in the model for z(x,y). The models correspond to the x, y, and z direction cosines respectively of the pole to the bedding observations, calculated using an East, North, Up (ENU) convention from:

East (for f_x): $\cos(\alpha) = \cos(\psi)\cos(\theta)$

North (for f_y): $\cos(\beta) = \cos(\psi)\sin(\theta)$

Up (for f_z): $\cos(\gamma) = \sin(\psi)$

where ψ is the plunge and θ is the azimuth (bearing) of the pole to bedding [the rotation-flip of the North, East, Down (NED) convention of Watson (1965) used for southern hemispheric statistical analysis of poles to bedding]. Each strike and dip measurement can thus be used to regress the parameters in three separate models, one for each component of the gradient. Simultaneously the direct observations of the geologic horizon can be regressed to its model z(x,y).

Improving ground water models by adjusting transverse anisotropy regressed from a structural model.

2003-35102-13587

John R. Hoaglund, III

Currently at Bloomsburg University of PA

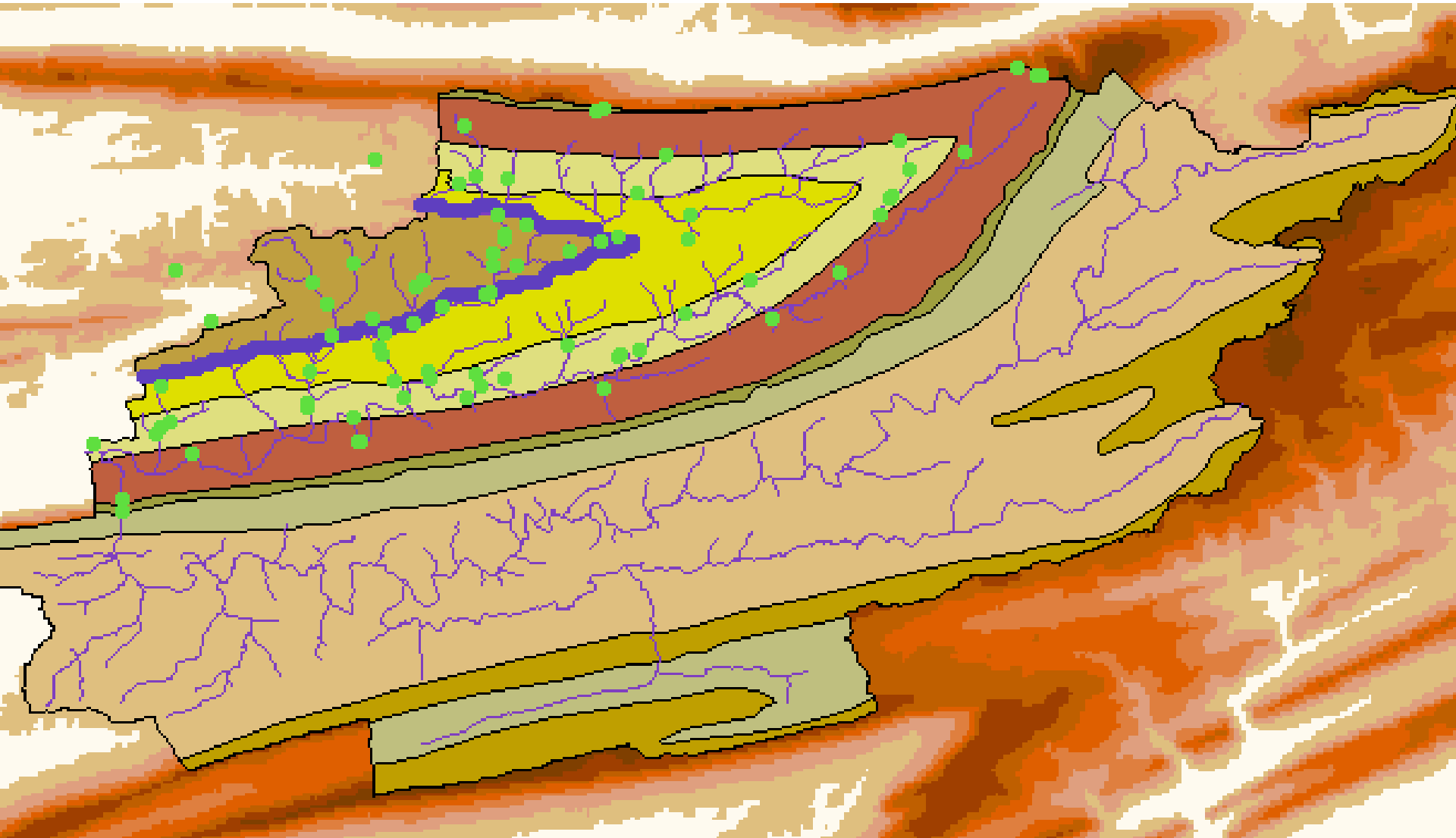
Project is Penn State University sponsored research.

- Part I: Ground water flow model corrections needed for transverse anisotropy
- Part II: Structural model regression from bedding horizon and gradient data.
- Part III: Viewxsxn for structurally consistent solid model generation.

ext slide

Mahantango Watershed, Pennsylvania

Geologic map on shaded relief showing strike-and-dip data points



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Sum of sines model for doubly-plunging folds

$$z(x, y) = A\sin(k_1[y - y_0]) + B\sin(k_2[x - x_0]) + z_0$$

$$k_1 = \frac{2p}{l_1} \qquad k_2 = \frac{2p}{l_2}$$

A is amplitude and ?$_1$ is wavelength for folding

B is amplitude and ?$_2$ is wavelength for plunging

x_0 , y_0 , and z_0 are offsets

3 gradient component models

$$w(x,y,z) = A\sin(k_1[y-y_0]) + B\sin(k_2[x-x_0]) + z_0 - z = 0$$

$$\frac{f_x}{\sqrt{f_x^2 + f_y^2 + f_z^2}} = \frac{Bk_2\cos(k_2[x-x_0])}{\sqrt{B^2k_2^2\cos^2(k_2[x-x_0]) + A^2k_1^2\cos^2(k_1[y-y_0]) + 1}}$$

$$\frac{f_y}{\sqrt{f_x^2 + f_y^2 + f_z^2}} = \frac{Ak_1\cos(k_1[y-y_0])}{\sqrt{B^2k_2^2\cos^2(k_2[x-x_0]) + A^2k_1^2\cos^2(k_1[y-y_0]) + 1}}$$

$$\frac{f_z}{\sqrt{f_x^2 + f_y^2 + f_z^2}} = \frac{-1}{\sqrt{B^2k_2^2\cos^2(k_2[x-x_0]) + A^2k_1^2\cos^2(k_1[y-y_0]) + 1}}$$

gradient component data

East for f_x $\cos(a) = \cos y \ \cos q$

North for f_y $\cos(b) = \cos y \ \sin q$

Up for f_z $\cos(g) = \sin y$

a, ß, ? Direction cosines

? Plunge of pole to bedding

? Azimuth of pole to bedding

Mahantango Watershed, Pennsylvania

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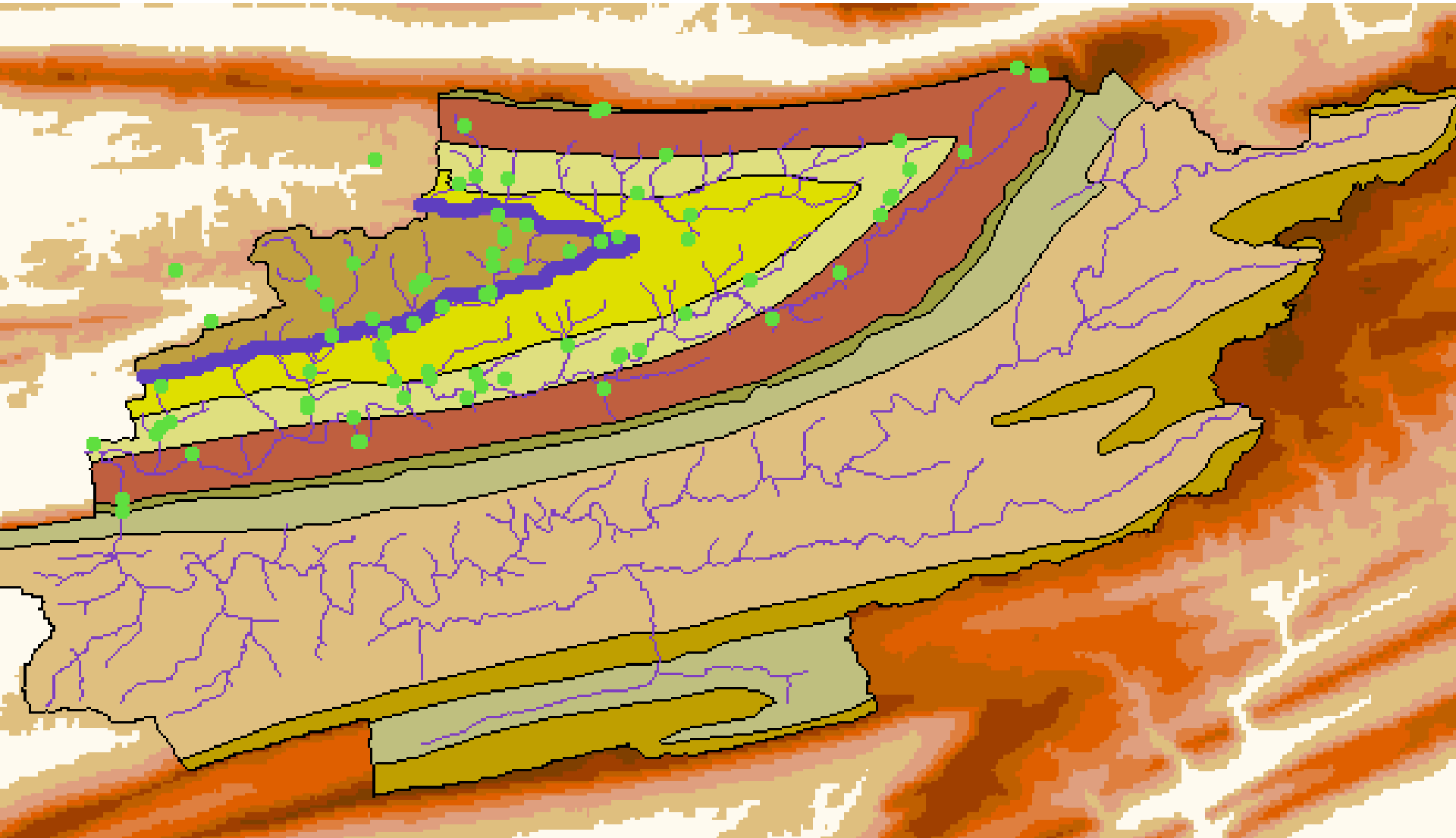

Structural Model Regression

- Non-linear regression coded in Matlab
- z model dampens amplitude
- Gradient component model increases amplitude
- Need better z data definition; re-run regressions
- The need to visualize fold parameter sets initiated development of Viewxsxn
- Viewxsxn is a solid model builder and solid model cross section viewer

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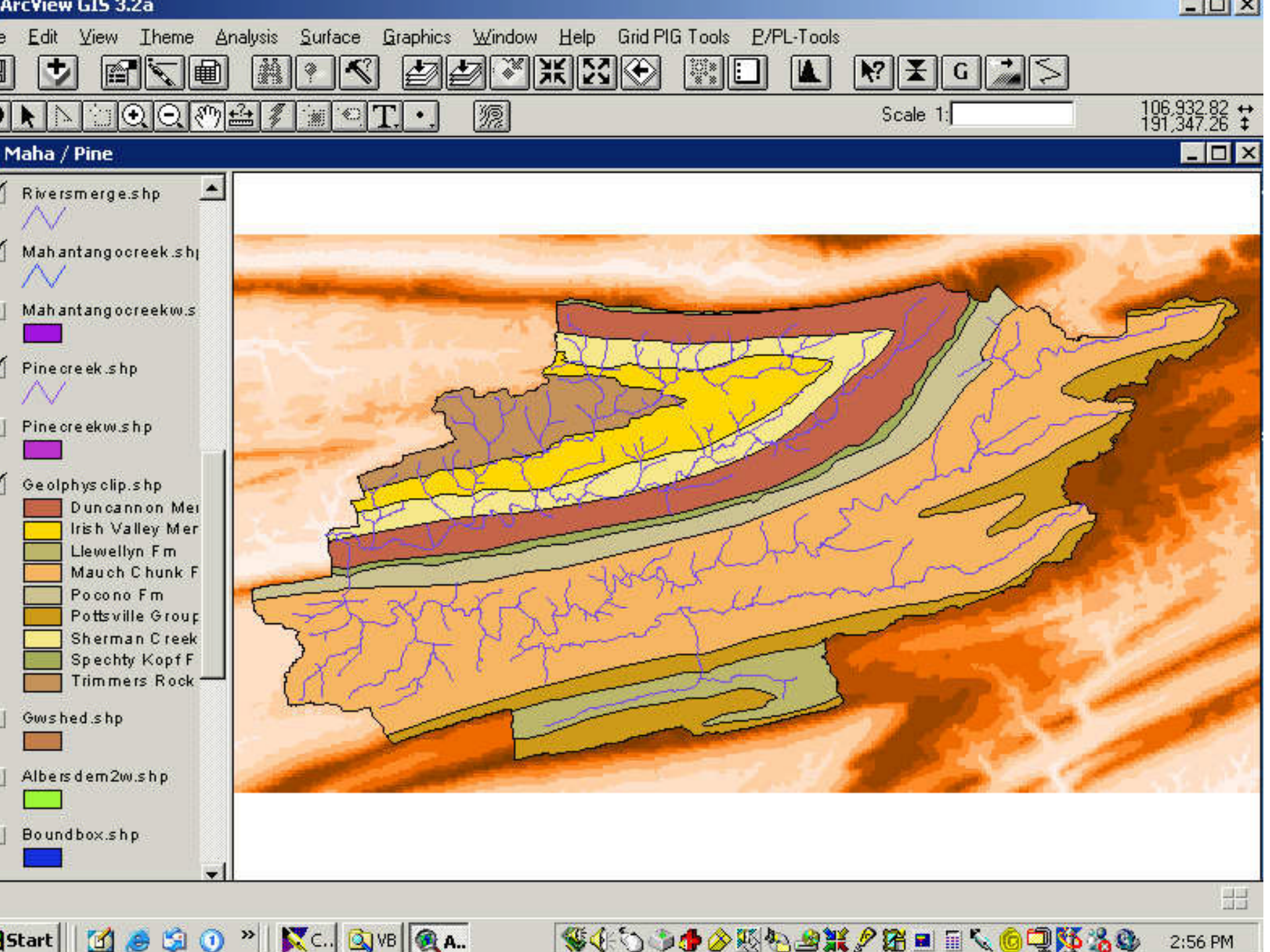
Viewxsxn

- User inputs geologic map raster and coincident DEM, both from ArcView
- Geologic map clipped to TauDEM defined watershed
- User specifies stratigraphic sequence of geologic map units, and number of tops to construct for the solid model
- Viewxsxn interprets geologic map for stratigraphic younging direction for either a fold or homoclinal reconstruction.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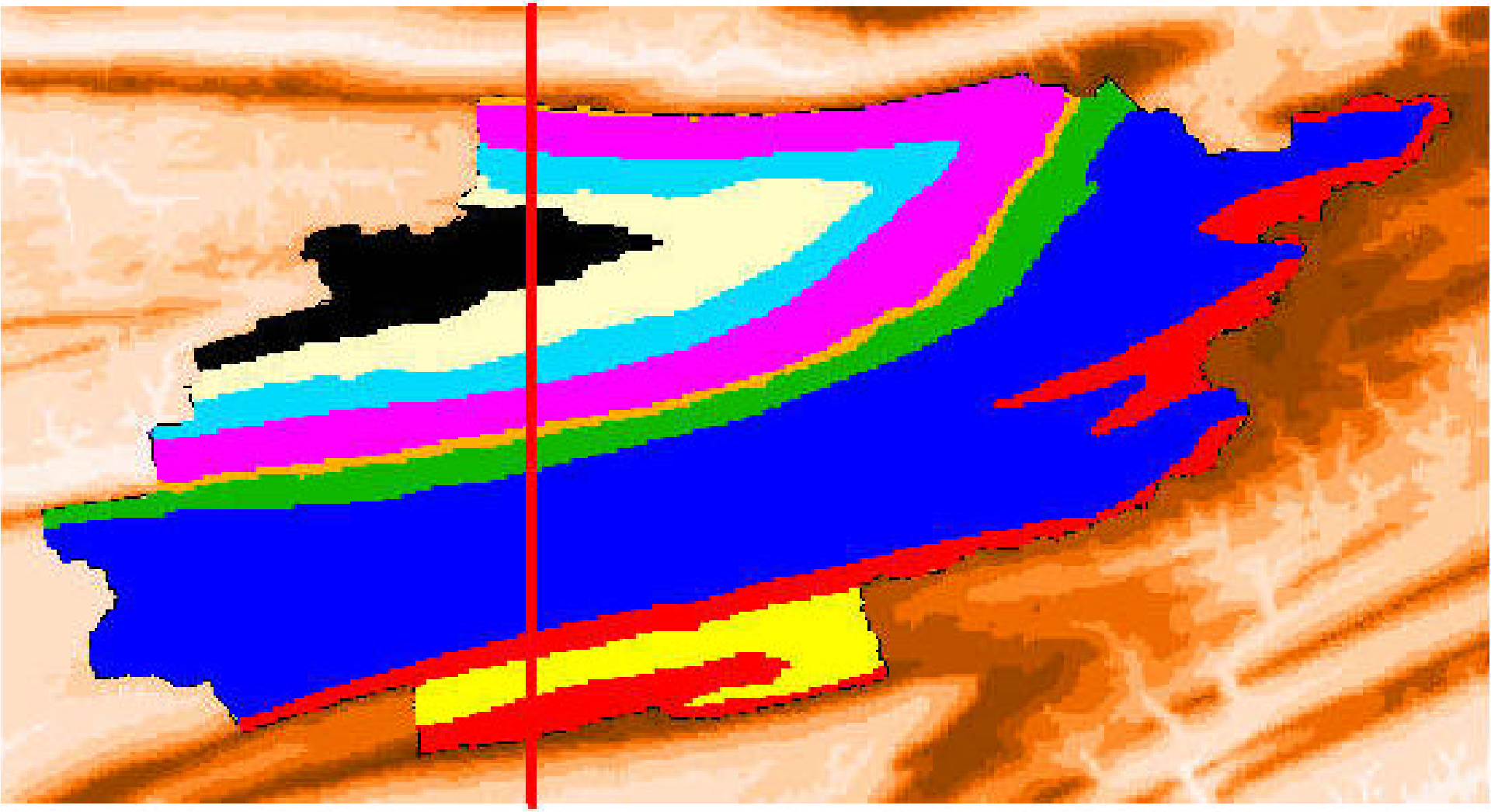

Next Slide

Viewxsxn

- Takes solid model defined as tops and generates Modflow-compliant layers, coincident with structural tops AND accommodating the pinchout problem.
- Builds LARGE (Arc-grid coincident) Modflow models using a river raster from ArcView, watershed boundary from the geologic map clip, and user specified heads.
- Models are importable into Argus, using Modflow96 import procedures and new DLL’s to handle variable-sized grids, for conversion to Sutra.
- Tensor orientation file generated from structurally coincident tops.

Current Progress

1) Regional and field-scale Modflow models have been generated for Mahantango Creek (siliciclastic) and Nittany Valley (carbonate).

2) Modflow models have been imported into Argus where equivalent Sutra models are under construction

3) Comparing simulations of uncorrected Modflow/Modpath models to uncorrected and corrected Sutra models.

Measure of Improvement?

Mahantango Creek regional modeling being onducted by John Hoaglund, with field-scale ransport compared to USDA pasture site, and ransport result, of Burton et al., 2002.

Nittany Valley regional modeling being onducted by Christopher Casler, Penn State lissertator, with field-scale transport compared to ontaminant plume in State College.

Research Ideas

Go straight from Viewxsxn to Sutra (Argus is expensive).

Visualization is key. Move Viewxsxn graphics to the 3D GeoWall

Incorporate Viewxsxn into David Maidment's (UT Austin) ArcHydro

Design a river package (Cauchy boundary) for Sutra

Re-visit Weiss for new solver techniques. Incorporate result into Modflow**.

Research toward incorporating generalized anisotropy into Modflow is ongoing at USGS. Ken Kipp and Mary Hill have implemented generalized anisotropy for radial jointing trends in the Death Valley model in **MAP view.

The Wedding Cake Analogy

- Wedding cakes are not allowed
- Upside down wedding cakes are allowed