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**Modeling spatially and temporally distributed phenomena: new methods
and tools for GRASS GIS**

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Abstract. The concept of GRASS (Geographic Resources Analysis Support System) as an open system has created a favorable environment for integration of process based modeling and GIS. To support this integration a new generation of tools is being developed in the following areas: a) interpolation from multidimensional scattered point data, b) analysis of surfaces and hypersurfaces, c) modeling of spatial processes, d) 3D dynamic visualization. Examples of two applications are given - spatial and temporal

modeling of erosion and deposition, and multivariate interpolation and visualization of nitrogen concentrations in the Chesapeake Bay.

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1. Introduction

In environmental sciences, various phenomena can be modeled at a certain level of approximation by smooth functions: terrain, climatic phenomena, surface water depth, concentrations of chemicals, *etc.* (e.g., Mitasova 1992, 1993, 1994). Multivariate smooth functions are also important for modeling processes described by scalar fields and their associated vector fields representing fluxes (Moore *et al.* 1993, Maidment 1994). Current GIS systems support modeling with 2D fields and some geoscientific systems also support 3D fields and temporal data sets (What is a Scientific GIS 1991). We anticipate that with environmental models incorporating the study of interacting systems, and with the increasing need of analysis of multiparametric models, higher dimensional tools become necessary (Compton and Miller 1994). The concept of GRASS (Geographic Resources Analysis Support System) as an open, public domain system with documented source code organized as libraries of functions and open data structures, provides the environment not only for the development of GIS applications but also for programming and implementation of new GIS methods and tools such as the modeling and visualization with multidimensional continuous fields.

In this paper, we at first present an interpolation method which allows computation of grid representations of continuous fields from scattered point data, then we briefly describe the analysis of geometry of these fields and give an overview of multidimensional visualization capabilities. Presented methods are then illustrated on two environmental modeling applications. In conclusion, we provide the information on programs integrated with GRASS.

2. Multivariate spline interpolation

One of the basic tools needed for multidimensional modeling in environmental sciences is interpolation and approximation from d -dimensional scattered point data to

d -dimensional grids. Although numerous interpolation methods, especially for bivariate case, are available, significant progress was achieved recently using methods obtained as solutions to variational problems, commonly known as splines (Franke 1987, Hutchinson 1989, 1991, 1994, Wahba 1990, Mitas and Mitasova 1988, Mitasova and Mitas 1993). We recall some of the basic principles of this approach and present a general expression for d -variate smoothing spline with tension and its special cases implemented in GIS.

Spline methods are based on the assumption that the approximation function should pass as closely as possible to the data points and should be at the same time as smooth as possible. These two requirements can be combined into a single condition of minimizing the sum of the deviations from the measured points and the smoothness seminorm of the function, which is formulated as follows:

Given N values of the studied phenomenon $z^{[j]}$, $j = 1, \dots, N$ measured at discrete points $\mathbf{x}^{[j]} = (x_1^{[j]}, x_2^{[j]}, \dots, x_d^{[j]})$, $j = 1, \dots, N$ within a certain region of a d -dimensional space, find a function $S(\mathbf{x})$ which fulfils the condition

$$\sum_{j=1}^N |z^{[j]} - S(\mathbf{x}^{[j]})|^2 w_j + w_0 I(S) = \text{minimum} \quad (1)$$

where w_j, w_0 are positive weighting factors and $I(S)$ is the smooth seminorm. The solution of this problem can be expressed as a sum of two components (Talmi and Gilat 1977)

$$S(\mathbf{x}) = T(\mathbf{x}) + \sum_{j=1}^N \lambda_j R(\mathbf{x}, \mathbf{x}^{[j]}) \quad (2)$$

where $T(\mathbf{x})$ is a 'trend' function and $R(\mathbf{x}, \mathbf{x}^{[j]})$ is a radial basis function with an explicit form which depends on the choice of $I(S)$. For our choice of the smooth seminorm (Mitasova and Mitas 1993) the 'trend' function $T(\mathbf{x})$ is a constant

$$T(\mathbf{x}) = a_1 \quad \text{for an arbitrary } d \quad (3)$$

and the general form of radial basis function for d -variate case (Mitas and Mitasova 1994) is given by

$$R_d(\mathbf{x}, \mathbf{x}^{[j]}) = R_d(|\mathbf{x} - \mathbf{x}^{[j]}|) = R_d(r) = \varrho^{-\delta} \gamma(\delta, \varrho) - \frac{1}{\delta} \quad (4)$$

where $\delta = (d - 2)/2$, and $\varrho = (\varphi r/2)^2$. Further, φ is a generalized tension parameter, $r^2 = \sum_{i=1}^d (x_i - x_i^{[j]})^2$, and finally, $\gamma(\delta, \varrho)$ is the incomplete gamma function (Abramowitz and Stegun 1964). For the the special cases $d = 2, 3, 4$ the equation (4) can be rewritten as

$$R_2(r) = \lim_{\delta \rightarrow 0} \left[\varrho^{-\delta} \gamma(\delta, \varrho) - \frac{1}{\delta} \right] = -[E_1(\varrho) + \ln \varrho + C_E] \quad (5)$$

$$R_3(r) = \sqrt{\frac{\pi}{\varrho}} \operatorname{erf}(\sqrt{\varrho}) - 2 \quad (6)$$

$$R_4(r) = \frac{1 - e^{-\varrho}}{\varrho} - 1 \quad (7)$$

where $C_E = 0.577215\dots$ is the Euler constant, $E_1(\cdot)$ is the exponential integral function and $\operatorname{erf}(\cdot)$ is the error function (Abramowitz and Stegun 1964). The limit for $d = 2$ case can be verified by using the properties of the generalized gamma function (Abramowitz and Stegun 1964, Mitas and Mitasova 1994). The coefficients $a_1, \{\lambda_j\}$ are obtained by solving the following system of linear equations

$$a_1 + \sum_{j=1}^N \lambda_j \left[R(\mathbf{x}^{[i]}, \mathbf{x}^{[j]}) + \delta_{ji} w_0 / w_j \right] = z^{[i]}, \quad i = 1, \dots, N \quad (8)$$

$$\sum_{j=1}^N \lambda_j = 0. \quad (9)$$

Besides the high accuracy on smooth test data (Mitasova and Mitas 1993), the derived functions have several useful properties. They have regular derivatives of all orders which make them suitable for direct analysis of surface and hypersurface geometry. The generalized tension φ controls the distance over which the given point influences the resulting surface or hypersurface. For the bivariate case tuning the tension can be interpreted as tuning the character of the resulting surface between membrane and thin plate. The proper choice of smoothing and tension parameters is important for successful interpolation or approximation. One possibility for finding the optimal smoothing parameter is to use ordinary or general cross-validation scheme (Wahba 1990, Hutchinson and Gessler 1993). We have an ordinary cross-validation to find both optimal tension and smoothing. If we assume that $\{w_j\}$ are the same for all data points then the smoothing parameter is $w = w_j/w_0$. Let $S_{N,\varphi,w}^{[k]}$ be the smoothing spline with tension using all the data points except the k -th. We can take the ability of $S_{N,\varphi,w}^{[k]}$ to predict the missing data point z_k as a measure of predictive capability of the spline with the given tension φ and smoothing w , which can be represented by a mean error V_0

$$V_0(\varphi, w) = \frac{1}{N} \sum_{k=1}^N |S_{N,\varphi,w}^{[k]}(\mathbf{x}^{[k]}) - z^{[k]}|. \quad (10)$$

Then the optimal values of tension φ_O and smoothing w_O are found by minimizing $V_0(\varphi, w)$. The example for Chesapeake Bay nitrogen concentration data (figure 1) shows that for smoothing $w = 0$ the predictive error sharply increases for tension $\varphi < \varphi_O$. A small value of smoothing can significantly reduce the predictive error for the low values of tension. Although it is possible that $V_0(\varphi, w)$ has multiple minima (Dietrich and Osborne 1991), this approach is useful for finding at least an interval of values of the parameters where the cross-validation error does not exceed acceptable values.

The cross-validation error computed for each point can also be used for the analysis of spatial distribution of predictive error and location of areas where this error is high and denser sampling is needed.

Due to the solution of system of linear equations (8, 9) the computational demands for the presented method are proportional to N^3 and its application to large data sets becomes problematic. To overcome this limitation, an algorithm for segmented processing has been proposed (Mitasova and Mitas 1993) and then further developed using quad-trees (Kosinovsky *et al.* 1994). Segmentation is based on the division of the given region into (hyper)rectangular segments. The size of each segment is adjusted to the density of points in the given subregion using 2^d -trees (quad-trees for 2D, oct-trees for 3D, *etc.*). Then, the interpolation function is computed for each segment using the points from this segment and from its neighborhood, located in the window which adjusts its size to the density of points in the neighborhood of each segment (figure 2). Sufficiently large overlapping neighborhood ensures the smooth connection of segments. This segmentation is dimension independent, applicable to data with heterogeneous spatial distribution and the resulting algorithm has favorable scaling as the computation time is proportional to N .

Multidimensional interpolation is also a valuable tool for incorporating the influence of an additional variable into interpolation, e.g. for interpolation of precipitation with the influence of topography or concentration of chemicals with the influence of the environment where it is distributed. We have implemented the approach proposed by Hutchinson and Bischof (1983) to support this type of modeling. To model the spatial distribution of a d -dimensional phenomenon $u = F(x_1, \dots, x_d)$ from the given point data $(x_1^{[i]}, \dots, x_d^{[i]}, u^{[i]}) = (\mathbf{x}^{[i]}, u^{[i]})$, $i = 1, \dots, N$ influenced by another d -dimensional phenomenon $z = G(x_1, \dots, x_d)$, we can take the values of the 'influencing' phenomenon

as a $d + 1$ coordinate $x_{d+1}^{[i]} = cG(\mathbf{x}^{[i]})$ where c is a rescaling factor, so that we get the points $(x_1^{[i]}, \dots, x_{d+1}^{[i]}, u^{[i]}) = (\mathbf{x}^{*[i]}, u^{[i]})$. The values of $x_{d+1}^{[i]}$ can be either given with data or can be interpolated from the function $z = G(\mathbf{x})$. Now we can interpolate from these points using the $(d + 1)$ -variate function $S^*(\mathbf{x}^*)$ and compute the resulting $S(\mathbf{x})$ as $S(\mathbf{x}) = S^*(\mathbf{x}, cG(\mathbf{x}))$. The $(d + 1)$ th variable can be either a real surface like terrain or geological layer, its modification, or an abstract surface. Figures 3, 4 illustrate the difference between the bivariate spline interpolation of annual precipitation in the tropical South America, and the interpolation with the influence of topography. The importance of incorporating the terrain data is especially visible in the mountainous areas, where the barrier effect of the Andes is very well represented in the results of trivariate interpolation (figure 4).

3. Surface geometry analysis

For process based modeling it is often necessary to compute the geometrical parameters of surfaces and hypersurfaces directly related to the fluxes in landscape. We have used d -dimensional differential geometry (Thorpe 1979) to formulate the algorithms for d -dimensional topographic analysis. Assume, that the studied phenomenon is modeled by a d -dimensional surface (d -surface) in a $d + 1$ -dimensional space represented by a smooth d -variate function $z = g(x_1, \dots, x_d)$. If we set $z = x_{d+1}$ we can represent this function in an implicit form as $f(x_1, \dots, x_{d+1}) = x_{d+1} - g(x_1, \dots, x_d) = 0$ and then use the general expressions for d -surface analysis, applicable also to d -surfaces which are not functions (e.g. isosurfaces). Associated with each function $f(\mathbf{x})$ is a smooth vector field called the gradient ∇f , defined by

$$\nabla f = \left(\frac{\partial f}{\partial x_1}, \dots, \frac{\partial f}{\partial x_{d+1}} \right) = \left(-\frac{\partial g}{\partial x_1}, \dots, -\frac{\partial g}{\partial x_d}, 1 \right). \quad (11)$$

Such vector fields often arise in geosciences as velocity fields or fluid flows. Scalar fields

associated with gradient are gradient magnitude $\|\nabla f\|$ and gradient direction $(\alpha_1, \dots, \alpha_d)$

$$\|\nabla f\|^2 = \sum_{i=1}^{d+1} \left(\frac{\partial f}{\partial x_i} \right)^2, \quad \cos \alpha_i = \frac{1}{\|\nabla f\|} \frac{\partial f}{\partial x_i} \quad i = 1, \dots, d. \quad (12a, b)$$

For the bivariate case, in most applications a horizontal projection of ∇f : $\nabla f' = (\partial f/\partial x_1, \partial f/\partial x_2, 0) = (-\partial g/\partial x_1, -\partial g/\partial x_2, 0)$ is being used and gradient magnitude is measured by the slope angle β , $\tan \beta = \|\nabla f'\|$ or $\cos \beta = (\partial f/\partial x_1)/\|\nabla f\|$. The direction of $\nabla f'$ is used as aspect. Besides these scalar fields, associated with a gradient field is a family of curves called flow lines. To generate the flow lines and their related parameters we have developed an improved flow tracing algorithm based on a vector-grid approach (Mitasova and Hofierka 1993, Mitasova *et al.* 1994b). The points defining the flow line are computed as the points of intersection of a line constructed in the $\nabla f'$ direction and a grid cell edge. Flow lines can be generated in the direction of $\nabla f'$ (downhill) for the computation of upslope contributing areas (Moore and Wilson 1992) and extraction of streams because downhill flow lines merge in valleys (figure 5). Flow lines generated in the direction of $-\nabla f'$ (uphill) are useful for computation of flow path length and extraction of ridge lines as these flow lines merge on ridges (figure 6). A modified version of this algorithm has been developed for tracing the flow lines in 3D by Zlocha and Hofierka (1992).

To study the rate of change in the velocity of flow due to the shape of d -surface, the Weingarten map or *shape operator* $L_p(\mathbf{v})$ (Thorpe 1979) is defined as

$$L_p(\mathbf{v}) = -\nabla_{\mathbf{v}} \mathbf{N} = -\frac{1}{\|\nabla f\|} \left(\sum_{i=1}^{d+1} \frac{\partial^2 f}{\partial x_i \partial x_1} v_i, \dots, \sum_{i=1}^{d+1} \frac{\partial^2 f}{\partial x_i \partial x_{d+1}} v_i \right) \quad (13)$$

where $\nabla_{\mathbf{v}}$ denotes the directional derivative in the direction given by a vector $\mathbf{v} = (v_1, \dots, v_{d+1})$ where \mathbf{v} belongs to the tangent space of the modeled d -surface. The shape operator $L_p(\mathbf{v})$ measures the turning of the normal $\mathbf{N} = \nabla f/\|\nabla f\|$ in the point moving

on a d -surface. Normal component of acceleration at this point in the direction \mathbf{v} is measured by a normal curvature $k(\mathbf{v})$ computed directly for the $\|\mathbf{v}\| = 1$ from the Weingarten map as

$$k(\mathbf{v}) = L_p(\mathbf{v}) \cdot \mathbf{v} = -\frac{1}{\|\nabla f\|} \sum_{i,j=1}^{d+1} \frac{\partial^2 f}{\partial x_i \partial x_j} v_i v_j \quad (14)$$

For the bivariate case, when we consider flow over a 2-surface in a 3D space, we get the profile curvature related to the flow acceleration for the vector \mathbf{v} representing the tangent to the surface in the direction of flow. If \mathbf{v} represents the tangent to the surface in the direction of a tangent to the contour we get the tangential curvature related to the flow convergence/divergence (Mitasova and Hofierka 1993). Figures 7, 8 show the importance of using an appropriate method for the estimation of first and second order derivatives. While local polynomial interpolation applied to the noisy data with insufficient resolution produced unacceptable results (figure 7), tangential curvature computed from smoothing spline (figure 8) reflects the basic structure of ridges and valleys.

Various other measures related to acceleration and shape of the d -surface can be derived from Weingarten map (e.g. mean, Gauss-Kronecker and principal curvatures), and used not only in process based models but for enhancing the visualization as well (e.g., Nielson *et al.* 1991).

4. Multidimensional dynamic visualization

For the implementation and applications of the presented approach within GIS a highly interactive and efficient tool for visualization of data and the resulting surfaces was important (Mitasova *et al.* 1994a). It was needed both for the visual evaluation of the functionality of methods, algorithms and programs as well as for the communication of the results of applications. To support the use of visualization as both an analytical

and communication tool a program *SG3d* was developed and fully integrated with the data structure of GRASS. The program enables users to view all types of currently supported geographic data (raster, point, vector) in the same 3D space and allows scripting for producing dynamic visualizations via animation. The support for the volumetric visualization of 3D data sets (3D raster, 3D point and 3D vector) not currently supported by the GIS, is being integrated with *SG3d*.

SG3d has the following capabilities (Brown and Gerdes 1992):

- a) visualization of 2D raster data as 2-surfaces in 3D space, using one data set for surface topography and a second one for surface color (e.g. figures 7, 8, 9);
- b) interactive, easy positioning, zooming, and z-scaling, important for the efficient use in analysis of the results of models;
- c) interactive lighting with adjustable light position, color, intensity and surface reflectivity, useful for detecting noise or small errors in data or models, and enhancing the 3D perception of surface topography;
- d) draping vector (figure 5, 6) and point data, with the "glyphs" option for point data to facilitate the visualization of data with uncertainty (figure 9);
- e) animation capabilities with two options: i) scripting for automatically generating animations from temporal data, ii) key-frame animation to establish a path for moving the viewpoint through the data and automatically rendering and saving a user-defined number of frames;
- f) displaying and animation of multiple related surfaces, e.g., for hydrologic modeling: rainfall intensity surface, terrain with water surface depth draped as a color, and infiltration depth surface, all displayed and animated in one 3D space (Saghafian 1994);
- f) fast querying of raster data displayed as a surface topography and a surface color;

g) display in spherical coordinate system for rendering the surfaces draped over the whole globe or a portion of it;

A new version of the visualization program which integrates the capabilities of *SG3d* with programs for volumetric visualization of *3D* data sets has been developed. This program combines the standard 2-surfaces, vectors and points with isosurfaces, solids, slices, and points representing *3D* phenomena (figure 11), in the same *3D* space, while preserving the flexibility and efficiency of *SG3d*.

5. Examples of application

5.1 Spatial and temporal distribution of soil erosion/deposition

By analyzing several erosion models and sediment flux equations, Moore and Wilson (1992) have derived a dimensionless index of sediment transport capacity T representing the influence of terrain on soil erosion:

$$T = \left(\frac{A}{22.13} \right)^m \left(\frac{\sin \beta}{0.0896} \right)^n \quad (15)$$

which is the unit stream power based length-slope (LS) factor proposed by Moore and Burch (1986). In this equation, A is the upslope contributing area per unit contour width [$m^2 m^{-1}$], β is the steepest slope angle [deg], and m , n are constants. The index becomes unity for the case when the upslope area $A = 22.13 m^2 m^{-1}$, and the slope is $5.14 deg$ (9%), because these conditions refer to the reference slope used in the original derivation of the Universal Soil Loss Equation (USLE). It has been shown that the values of $m = 0.6$, $n = 1.3$ give results consistent with the revised USLE (RUSLE) LS factor for the slope lengths $\lambda < 100m$ and the slope angles $\beta < 14 deg$ (Moore and Wilson 1992).

By considering the sediment transport limiting case, the topographic potential of landscape for erosion or deposition E can be computed as a change in the sediment

transport capacity in the direction of flow (figure 9). As an alternative to the finite difference approach proposed by Moore and Wilson (1992), E can be computed as a directional derivative of the surface $T = g(x_1, x_2)$ representing the sediment transport capacity, (Mitasova *et al.* 1994b.)

$$E = \frac{\partial g}{\partial s} = \frac{\partial g}{\partial x_1} \cos \alpha + \frac{\partial g}{\partial x_2} \sin \alpha \quad (16)$$

where (x_1, x_2) are the georeferenced coordinates, and α is the aspect angle [*deg*] representing the direction of flow and computed from the elevation surface $z = f(x_1, x_2)$. The smoothing spline with tension is used for the estimation of partial derivatives in the equation (16). The equation (16) incorporates the influence of slope angle, shape of terrain in flow direction (through the derivative in the direction of flow) as well as water flow convergence/divergence (through the upslope area). To compare the erosion/deposition potential for various land covers, rainfall intensities and soil properties, it is possible to combine the unit stream power based LS factor T with the RUSLE C, R, and K factors respectively.

We have used this approach to model the spatial and temporal distribution of erosion and deposition potential at a military installation undergoing significant changes in land use during the year. The high resolution (5m) DEM with slope and aspect was created from digitized contours using the smoothing spline with tension. Upslope contributing area for each grid cell was computed by the vector-grid based flow tracing algorithm. Unit stream power based LS-factor T and erosion/deposition potential E were computed using the raster map calculator *r.mapcalc* (Shapiro and Westervelt 1992). The series of raster maps representing the spatial and temporal distribution of potential soil loss index L during the year was then computed as

$$L(x_1, x_2, t_i) = R(t_i).C(x_1, x_2, t_i).K(x_1, x_2).T(x_1, x_2), \quad i = 1, \dots, 12 \quad (17)$$

where R is the rainfall factor uniform over the area, but significantly changing during the year, C is the cover factor, which varies in space and time, and K is the soil factor. The study has shown that both spatial and temporal distribution of erosion are important for land use management to minimize the soil loss. Spatial analysis allowed us to propose to locate the intensively used areas in regions least susceptible to erosion and to create protective buffers with natural vegetation along the streams in areas of high erosion and deposition. Temporal analysis showed that rescheduling the timing of intensive use so that it does not coincide with the highest rainfall intensity can further reduce the soil erosion risk.

5.2 Multivariate interpolation of nitrogen concentrations

The presented methods have been applied to interpolation, analysis and visualization of the concentrations of dissolved inorganic nitrogen (DIN) in the Chesapeake Bay. DIN is measured at 43 stations at 2 or 4 depths at each station approximately twice per month and it takes about 3 days to collect the data from all stations (Trends in Nitrogen in the Chesapeake Bay 1992). If we consider time to be an independent variable, then the data represent scattered points in $4D$ space and the distribution of DIN in space and time can be modeled by a function $u = S(x_1, x_2, x_3, x_4)$ where the fourth variable x_4 is proportional to time. To compare the differences between interpolation at various dimensions we have applied bivariate interpolation to model the spatial distribution of DIN at the surface layer and trivariate interpolation to model the concentrations of DIN in the volume of water. The 4-variate function was used to model both spatial and temporal distribution of DIN concentrations during the one year cycle with 7 days time step.

SG3d was used to visualize the dynamics of spatial distribution of DIN concentrations at the surface layer of the bay during the year, with surface and color rep-

representing concentrations of DIN, and glyphs, representing sampling sites, colored and sized according to the cross-validation error (figure 10). The integrated *SG3d* and volume visualization tool was used to create animations from the results of trivariate and 4-variate interpolation. Although trivariate interpolation and volume visualization provided good representation of spatial distribution of DIN in the volume of water (figure 11), the animations created from a series of 3D grids interpolated by trivariate interpolation failed to capture the dynamic character of DIN movement. However, application of 4-variate interpolation and computation of 3D grids with 7-day steps resulted in an excellent animation (see *Mosaic*, <http://www.cecer.army.mil/grass/viz/ches.html>) and proved the importance of using time as a 4th independent variable when processing the time series of data measured in 3D space.

6. Integration with GIS

We have used GRASS as an environment for implementing the presented system for multidimensional modeling, analysis and visualization for environmental applications. We were able to fully integrate the tools for the bivariate case with GRASS as commands *s.surf.tps/v.surf.tps* for interpolation and topographic analysis from scattered point data or vector data (e.g. digitized isolines), *r.resample.tps* for smoothing, resampling and topographic analysis of noisy raster data, *r.flow* (contributed by J. Hofierka and M. Zlocha) for the construction of flow lines, computation of flow path lengths and upslope contributing areas, as well as the interactive visualization tool *SG3d* (GRASS4.1 Reference Manual). We were able to handle time series quite efficiently using shell scripts with GRASS commands, however a more appropriate data structure is desirable. The programs supporting the higher dimensional interpolation and visualization (*s.surf.3d*, *s.surf.4d*, *sg4d*) are consistent with GRASS and linked to it through the geographic region. Because the standard GRASS GIS does not support 3D and 4D data we have

used our own data structure which may be potentially incorporated into GRASS.

The presented approach to the integration of multidimensional modeling and GIS based on the open, public domain GIS system such as GRASS, creates the basis for the development of a new generation of GIS technology which supports the study of complex interacting systems needed for environmental modeling. More information about the presented tools and applications, including the images and animations, can be found via Internet using the *Mosaic* browser at <http://www.cecer.army.mil/grass/viz/VIZ.html>. The latest releases of programs are available from the anonymous ftp site [moon.cecer.army.mil](ftp://moon.cecer.army.mil).

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short title for a running headline:

Modeling spatially and temporally distributed phenomena.