GRASS and modeling landscape processes using duality between particles and fields

Jaroslav Hofierka*,**, Helena Mitasova*, Lubos Mitas***

* Department of Marine, Earth and Atmospheric Sciences, North Carolina State University, Raleigh, NC, USA, hmitaso@unity.ncsu.edu.
** Department of Geography and Geoecology, Faculty of Humanities and Natural Science, University of Prešov, 17. novembra 1, 081 16 Prešov, Slovak Republic, e-mail hofierka@geomodel.sk
***Department of Physics, North Carolina State University, Raleigh, USA.

1 Introduction

Emergence of new mapping and automated monitoring technologies created new opportunities to predict consequences of anthropogenic activities and use such predictions to find sustainable solutions for development. Modeling of landscape processes plays an important role in this effort by allowing us to simulate the impact of proposed changes before irreversible damage is done and by providing tools to explore a wide range of alternatives. Traditional, spatially averaged models, such as BASIN and to some extent SWAT [3], [11], have limited capabilities to identify locations of problems (e.g. pollution sources) and the pattern of their propagation through landscapes. Also the possibilities to explore various alternatives of land use pattern and to find optimal organization of landscape are restricted. Spatially distributed models based on continuous fields provide such insight, however, they are much more complicated in terms of their implementation and data requirements. As the availability of high resolution data improves and the GIS capabilities are enhanced, such models are becoming more feasible for practical applications.

Coupling with GIS makes running the distributed models more efficient, especially when larger, complex areas are involved and a number of alternatives needs to be evaluated. Direct access to GIS database is useful for adjusting and optimizing model parameters, which can have high level of uncertainty. The parameter and land use optimization techniques can be integrated within GIS as well. GIS also provides powerful tools for comprehensive analysis of the results.

In early nineties, GRASS as a public domain GIS provided an environment for pioniering work in integrating GIS and landscape process modelling, for example [11], [10], [14]. While most of these models are now linked to proprietary GIS, the release of GRASS5.0 within the open source computational infrastructure creates opportunities for development and GIS integration of a new generation of simulation tools. Fully disclosed GRASS source code provides specialized libraries which make software implementation of the model simpler, faster and more effective.

In this paper we describe a full GIS integration of path sampling method for modeling fluxes represented by continuity equation with advection and diffusion term (e.g. overland water flow) and with added rate term describing the local rate of proliferation or decay (deposition) of modeled substance. The method incorporates both deterministic and stochastic influences.

2 Method

Because of the complexity of the Earth systems, process-based modeling of geospatial phenomena relies in practice on the best possible combination of physical models, empirical evidence, intuition and available measured data. To build a physical model of a natural process we need to define:

1. *Configuration space* for fields and/or particles and a corresponding range of its physical validity. This includes specification of relevant initial, external or boundary conditions, as well as physical conditions and parameters. The definition of configuration space relies on observed data and GIS plays an important role in their processing including transformations into digital representations suitable for the particular model.

2. *Interactions* between the constituents such as impact of one field on another or interaction between particles and fields. While it is not practical to take into account every interaction influencing the studied process, it is crucial to identify and incorporate those interactions which control the modeled process at the given scale.

3. *Governing equations* derived from natural laws which describe the behavior of the system in space, and time. The typical examples are continuity, mass and momentum conservation, diffusion-advection, reaction kinetics and similar types of equations.

4. *Constituent or state equations* which relate the constituents to physical conditions and parameters (e.g, equation which provides relation between detachment capacity of water flow, soil erodibility and topography). These equations are often based on a combination of physical and empirical approaches and may include a high level of uncertainty.

2.1 Duality between particles and fields

Most models of landscape processes are based on numerical solutions of governing partial differential equations by finite element [14], finite difference [10] or path sampling methods [8]. The path sampling method has several important advantages when compared with more traditional approaches. The method is very robust, can be easily extended into arbitrary dimension, is mesh-free and very efficient on parallel architectures. It is based on duality between the particle and field representation of spatially distributed phenomena. Within this concept, density of particles in space defines a field and vice versa, field is represented by particles with corresponding spatial distribution of their densities. Using this duality, processes can be modeled as evolution of fields or evolution of spatially distributed particles (Figure 1), with the solution obtained as follows.
Suppose that we have an equation:

$$L[c(\mathbf{r},t)] = S(\mathbf{r},t) \tag{1}$$

where L is an operator, $c(\mathbf{r},t)$ is the unknown quantity and $S(\mathbf{r},t)$ denotes sources-sinks. Suppose that L is linear (although weak non-linearities can be treated too). Symbolically, the solution can be written as

$$c(\mathbf{r},t) = L^{-1}[S(\mathbf{r},t)] \tag{2}$$

where L^{-1} is the operator inverse to L. That, of course, implies that the inverse operator is known, which is seldom the case. Nevertheless, we are able to simulate what is the action of L^{-1} on $S(\mathbf{r},t)$. This can be done by

a) sampling the source term field by a set of points in the configuration space,
b) applying the action of L^{-1} on $S(\mathbf{r},t)$ by using appropriate expression for the Green's function [11], making the points representing the source $S(\mathbf{r},t)$ evolve and create paths,
c) transforming the solution represented by the path samples to continuous field $c(\mathbf{r},t)$ by evaluating the path densities.

Averaging of path samples provides an estimation of the actual solution with statistical accuracy proportional to the inverse suqare root of the number of walkers. The solution is not restricted to the steady state and the state of the modeled quantity at any given time can be obtained by averaging the path samples at the selected time.

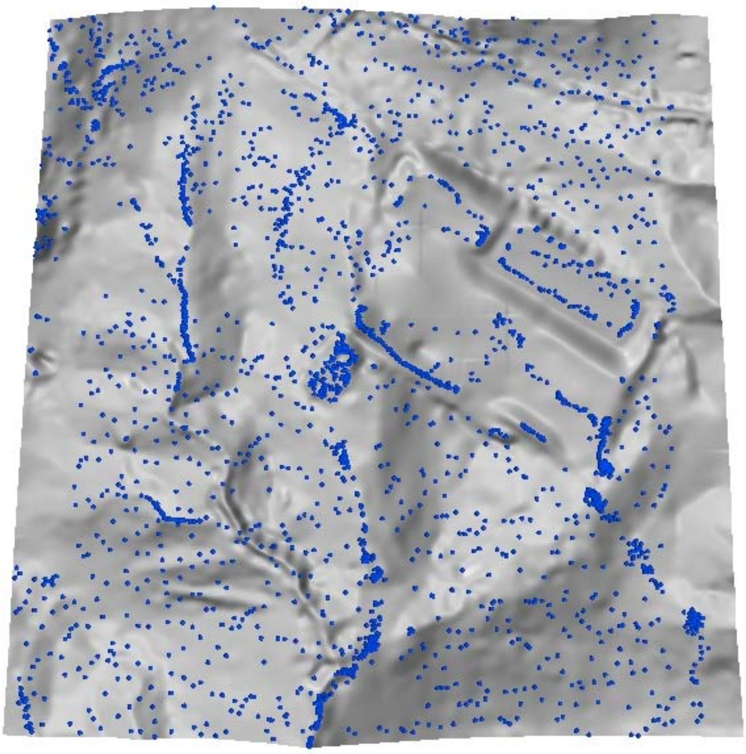

Figure 1: Evolution of St. Venant equation solution using path sampling technique. Density of points draped over a DEM represents water depth evolving under spatially variable land cover and topographic conditions (only 20% of particles are shown). (animation)

2.2 Application to water and sediment transport

Path sampling has been used for a number of environmental applications including simulation and transport of dissolved and suspended substances in water [1], [2], groundwater modeling [13] and soil erosion by overland flow [8]. This paper illustrates the implementation of the method for modeling shallow surface water flow and sediment transport, including net erosion and deposition.

Overland flow is based on the solution of bivariate St. Venant's continuity equation for steady state flow using approximate diffusive wave [8]. The source term represents rainfall excess while the modeled quantity is a function of water depth. No sinks are considered in the current version. Small diffusive term allows us to approximate some backwater effects.

Sediment transport is based on the hillslope erosion model used in the WEPP [4], [5] which was generalized to a bivariate form [8]. The basic relationship describing the sediment transport by overland flow is the continuity of sediment mass, which relates the change in sediment storage over time, and the change in sediment flow rate along the hillslope to effective sources and sinks (e.g., [6], [5]). The sediment flow rate is a function of water flow and sediment concentration. For shallow, gradually varied flow the storage term can be neglected leading to a steady state form of the continuity equation. The sources/sinks term is derived from the assumption that the erosion and deposition rates are proportional to the difference between the sediment transport capacity and the actual sediment flow rate [5]. The concept allows us to simulate the sediment transport between the *detachment limited case* when only erosion occurs, to *transport capacity limited case* with the greatest spatial extent of deposition. The sediment transport capacity and detachment capacity represent maximum potential sediment flow rate and maximum potential detachment rate, respectively, and are functions of a shear stress.The parameters and adjustment factors for the estimation of detachment and transport capacity are functions of soil and cover properties, and their values for a wide range of soils, cover, agricultural and erosion prevention practices can be obtained from the references to the WEPP model [4].

Equations for both water and sediment transport models are described in a number of papers and reports including [8], [9]. While the core governing equations remain as described in these references, some constituent or state equations can change in the released version to reflect the latest research. The most recent manual page should therefore be consulted for the latest updates.

3 Implementation in GRASS

The GRASS implementation of path sampling method is based on a library called *simlib* which includes functions needed for solving the continuity equations. This library can be used to develop specific modules for simulation of transport of various substances, such as sediment, nitrogen, bacteria, etc. The concept can be easily extended to 3D. In this paper we describe two modules, *r.sim.water* simulating overland water flow and *r.sim.sediment* for modeling soil erosion and sediment transport by water.

3.1 Overland flow simulation module *r.sim.water*

Overland water flow module *r.sim.water* is fully implemented for a steady state case with dynamic version under development. Input data representing the configuration space and source term are elevation [m], first-order partial derivatives of elevation surface *dx/dz, dy/dz*, Manning's surface roughness coefficient and rainfall excess (rainfall-infiltration rate, [m/s]). Elevation surface and its partial derivatives can be computed from contours or measured elevation points using *s.surf.rst* module. If elevation raster is already provided, partial derivatives can be computed using *r.slope.aspect* module. They can be also computed from slope and aspect using *r.mapcalc* and formulas described in [9]. Partial derivatives define the elevation surface gradient and determine the direction and magnitude of water flow. They can be combined with gradients representing channels or other features influencing water flow as described in the section 4.2. Mannings coefficient can be estimated based on the land cover data using published values for various types of surfaces and vegetation.

Rainfall excess is rainfall intensity - infiltration rate. Rainfall data are usually available from meteorological stations. Estimation of infiltration rate is more difficult and it is usually associated with high level of uncertainty, as it depends on the current state of soil properties and land cover and varies in both space and time. For saturated soil and steady-state water flow it can be estimated using saturated hydraulic conductivity rates based on field measurements or using reference values found in literature. Infiltration rate can be also computed using several available infiltration models (e.g. Green-Ampt, Holtan, etc.) implemented e.g. in *r.hydro.casc2d*.

Module outputs water depth [m] and water discharge [m^3/s] raster files. The spatial distribution of numerical error associated with path sampling solution can be analysed using the output error raster file [m]. This error is a function of the number of particles used in the simulation and can be reduced by increasing the number of walkers given by parameter nwalk. To analyze the relation between the particles and the resulting continuous field, the walkers can be saved in a site file at different times during the simulation. For practical purposes it us useful to save only a fraction of walkers which is controlled by output walker density parameter. The user can perform simulation for a given time and save the results as a time series by using *–t* flag and a time step for writing output files.

Simulation equations include a diffusion term (*diffc* parameter) controlling the ability to overcome elevation depressions or obstacles. When water depth exceeds a threshold water depth value (*hmax* parameter), a diffusion term can be increased at a rate given by *halpha* parameter. The direction of outflow from depressions is controlled by "prevailing" direction computed as average of flow directions computed from *hbeta* grid cells through which the walker has passed, approximating the water flow momentum.

3.2 Sediment transport simulation module *r.sim.sediment*

Sediment transport and net erosion/deposition is simulated by module *r.sim.sediment*, It is a landscape scale, bivariate model of sediment transport and net soil erosion/deposition by overland water flow designed for spatially variable terrain, soil, cover and rainfall excess conditions.

The inputs include raster files with elevation [m], first-order partial derivatives of elevation surface, overland water flow depth [m], detachment capacity coefficient [s/m], transport capacity coefficient [s], critical shear stress [Pa] and Manning's n surface roughness coefficient. Elevation, partial derivatives and Mannings coefficient can be computed as suggested in the previous section. The water depth can be estimated by the module *r.sim.water*, however, other models, such as *r.hydro.casc2d* can be used as well.

Detachment and transport capacity coefficients as well as critical sheer stress reflect the influence of soil properties and land cover. They can be estimated from soil and land use maps using published values in literature [4]. The ratio between the detachment and transport capacity coefficients determines how far the eroded sediment can be transported. For very small values of this ratio (transport capacity greatly exceeding detachment) erosion is close to detachment limited case and sediment can be transported over long distances (e.g. in case of non-aggregated clays). For ratio equal or greater than one (detachment rate at or exceeding sediment transport capacity) soil erodes quickly but it also deposits within short distances from the source (typical for heavier aggregates or sand). More details about the impact of various parameters on the resulting pattern of erosion and deposition can be found in [6], [8], [10].

Output includes raster files representing the sediment transport capacity (maximum possible sediment flow) [kg/(ms)], transport capacity-limited erosion/deposition computed as a divergence of transport capacity (maximum net erosion/deposition) [$kg/(m^2s)$], actual sediment flow rate [kg/(ms)], and net erosion/deposition (defined as a divergence of sediment flow) [$kg/(m^2s)$]. Duration of simulation is controlled by the number of iterations and time to steady-state can vary substantially depending on complexity of terrain, land cover, and size of the area. Output files can be saved during the simulation using time series flag *–t* and a time step parameter for writing output files.

4 Data preparation and model behavior

The path sampling technique has several unique advantages. Perhaps one of its most significant properties is robustness which makes it possible to solve the equations for complex cases, such as discontinuities in the coefficients of differential operators (in our case, abrupt slope or cover changes, etc). In more traditional models substantial part of the modelling effort is devoted to data preparation in order to avoid numerical instability or computational errors. In our case the time needed to get reasonable modeling results is minimized partly by GIS implementation and partly by the robustness of the path sampling method. The most common examples of possible modeling problems include:

- modeling overland flow in flat areas and depressions,
- abrupt changes in terrain or landcover,
- modeling at high resolutions,
- incorporation of man-made features (pipes, drainage lines...).

4.1 Flat areas and depressions

Flat areas and depressions often pose a problem because of the undefined water flow direction. In models based on solution of kinematic wave equations, elevation values must be changed to create an artificial terrain surface with well defined gradients. However, this modification greatly distorts the actual flow pattern by ignoring the impact of water standing in depressions. In *r.sim.water* this problem is adressed by incorporation of the spatially variable diffusion term. By defining the diffusion term as a function of water depth and the velocity of flow as a function of an approximate water flow momentum, the water fills the depressions or spreads in the flat area and flows out in the prevailing flow direction (Figure 2). The ability to overcome depressions and other obstacles in *r.sim.water* is represented by *diffc* parameter which value is used when water depth exceeds a threshold water depth value (*hmax).* When it is reached, diffusion term increases as given by *halpha*, advection term (direction of flow) is given as "prevailing" direction of flow computed as average of flow directions from the previous a number of grid cells defined by *hbeta*.

4.2 Preferential flow

For the situations when the flat areas or depressions are drained by natural or man-made swales, channels or even pipes, the water flow can be simulated by combining the gradient field derived from the DEM with the gradient of the drainage (Figure 3). The input vector field $s(\mathbf{r})$ representing the flow direction is then defined as:

$$s(\mathbf{r}) = (1-\delta_{ij})s_e(\mathbf{r}) + \delta_{ij}s_d(\mathbf{r}) \qquad (3)$$

where $s_e(\mathbf{r})$ is the vector in the steepest slope direction derived from a DEM and $s_d(\mathbf{r})$ is the vector representing the flow through the surface drainage which can be estimated, for example, from drainage line data using GIS tools and/or from field measurements. In GIS such cases can be handled quite easily merging data layers containing partial derivatives of terrain and features with preferential flow direction. Water in these areas will flow in the direction defined by feature gradient which can be easily derived from vector line data (in GRASS using *v.to.rast2* and *r.mapcalc* commands).

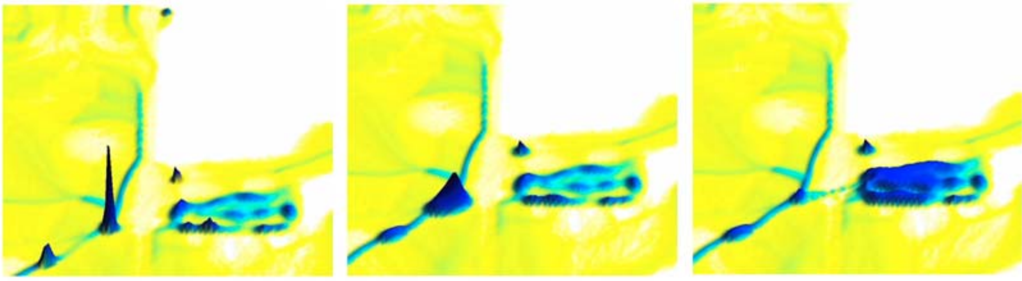

Figure 2: Water depth as a surface: left – without diffusion, middle – with diffusion, right - with diffusion and preferential flow

5 Example application

To demonstrate the model capabilities we present a study which uses a simulation of water and sediment flow to study the impact of development in the Centennial Campus area undergoing significant change in land cover and topography due to the transformation of a natural area to urban and recreational land use.The study area is located in Centennial Campus (CC) of North Carolina State University in Raleigh, U.S.A. (Figure 3).

During construction, soil erosion and water contamination pose serious problems when land cover is heavily disturbed removing land cover and exposing soil to rainfall. To reduce the negative effects, sediment control measures need to be installed. Current practice relies on selection, placement, design and scale of control measures during and after construction based on topographic maps using contributing area as a measure of flow. The presented example explores the use of GIS and simulations to better assess the need for sediment control measures and plan their most effective locations.

Figure 3: Study area (Data courtesy: Rob Austin)

5.1 Centennial Campus Southwest section development

The original land cover at the Southwest section of the CC area included secondary forest and open meadows. The topography is characterized by 3 watersheds with total area of 92.9 acres. In 1998 a school with a parking lot and outdoor athletic facility was built in the upper part of the area, along with 3 checkdams and several sedimentation ponds installed to control sediment transport and contamination during the school construction. In the near future, construction of golf course is planned in the area currently covered mainly by forest and open meadows.

The construction of golf course contains several phases, each characterized by changes in topography, land cover and soil properties. Available GIS data for each phase include topography (contours, golf course plans, survey), soil data (SSURGO), land cover data (orthotophotomap, golf course plans, survey). Rainfall data are measured at the nearby meteorological station and water and sediment discharge are monitored at the outlets of all 3 watersheds. Survey data were obtained by aerial photogrammetry, traditional and Real Time Kinematic surveys (RTKS).

Based on the available data three configuration spaces were defined in the GIS data base, with each one representing different stage of landscape development (Figure 4, 5, 6):

1.*Current state, before golf course construction*. Topography is represented by a 6 ft (2 m) resolution DEM interpolated using *s.surf.rst* from 2 ft (60 cm interval) contours based on 1993 photogrametry mapping, school construction plans and RTKS. Three check dams controlling the flow from the school's parking lot were added to the original DEM using r.mapcalc. Several pipes were defined to drain water under the roads. Land cover was derived using a color infrared digital orthophotography (1998) and Wake county GIS database. Soil data were taken from SSURGO database.

2.*Start of the golf course construction*. Topography is the same as in the previous case. Land cover data were modified according to golf course plans, however, bare soil conditions in the construction area were assumed.

3.*After the construction with finished golf course*. Topography is represented by the DEM data from previous state and terrain modification in the golf course area as defined by golf course plans. The original elevation site file was masked out in golf course area and new contours were added. The new DEM was re-interpolated using the same interpolation parameters. Land cover was changed reflecting the finished golf course.

5.2 Comparison of water and sediment transport for different stages of development

To evaluate the impact of development on water and sediment flow, to assess the efficiency of the installed control measures and to provide information for the golf course construction sediment control planning we simulated the overland flow, sediment transport and net erosion and deposition for all 3 stages using a rainfall event characterized by 43.2 mm/hr rainfall intensity and saturated soil conditions.

The overland flow and sediment transport parameters were defined using the soil, land cover data for each scenario. Water discharge and spatial pattern of erosion and deposition after 1-hr rainfall for all 3 scenarios is illustrated by Figures 4-6. The animations (Scenario 1, 2, 3) represent evolution of discharge during the rainfall event, illustrating the effectiness of sediment control measures (sedimentation basins and check dams, Figure 7) in reducing the flow at the watershed outlet. The comparison of discharge, sediment transport and erosion/deposition rates reveals the enormous impact of removing the current land cover. Reduced inflitration and increased water flow velocity dramatically increases water flow in the stream, leading to erosion rates, especially in areas with concentrated water flow. It is clear that the protecting buffer zones along the streams are not sufficient and additional erosion and sediment control measures will be necessary (such as ponds, check dams, spreaders, silt fences) in order to slow down the overland flow and sediment transport.

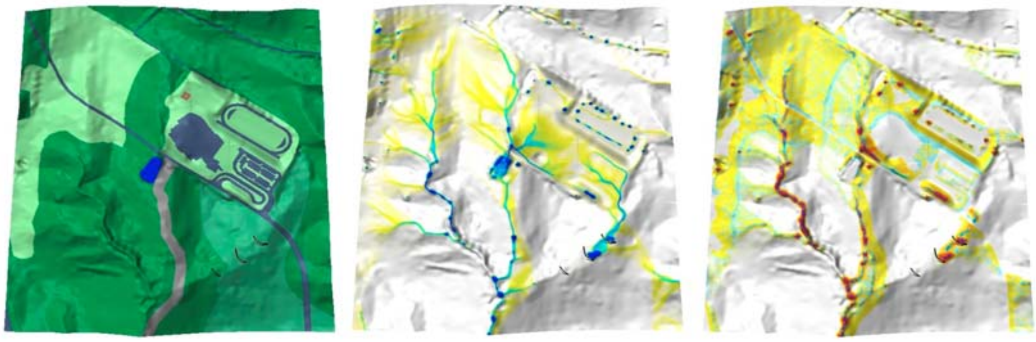

Figure 4: Before construction (land cover, water discharge, erosion/deposition)

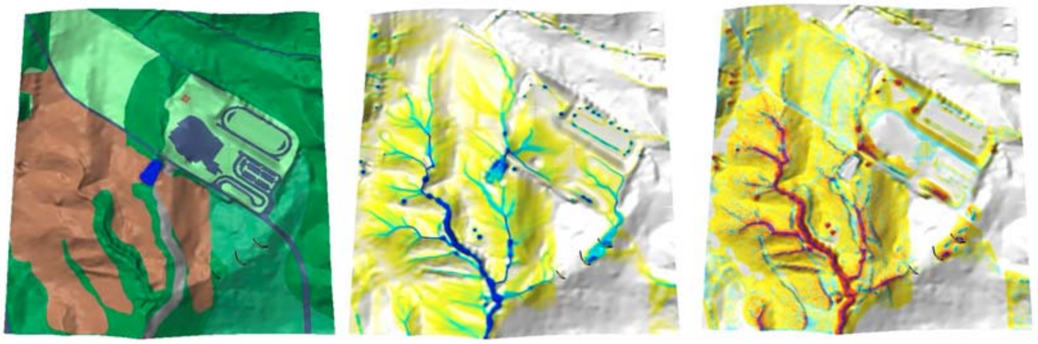

Figure 5: Start of the construction (land cover, water discharge, erosion/deposition)

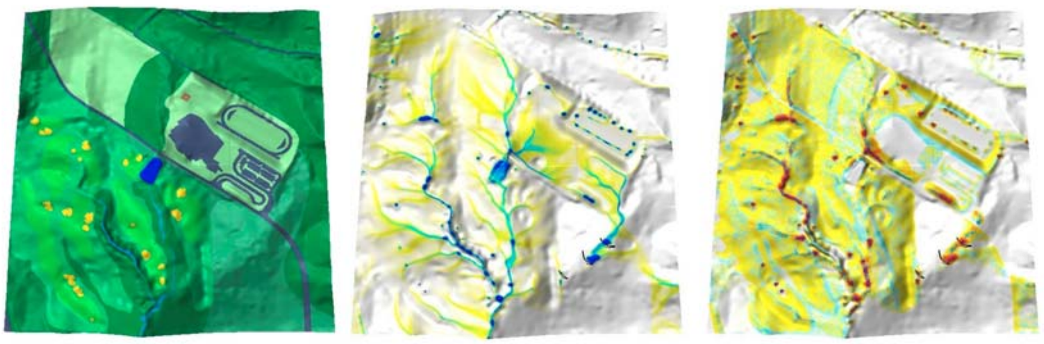

Figure 6: Finished golf course (land cover, water discharge, erosion/deposition)

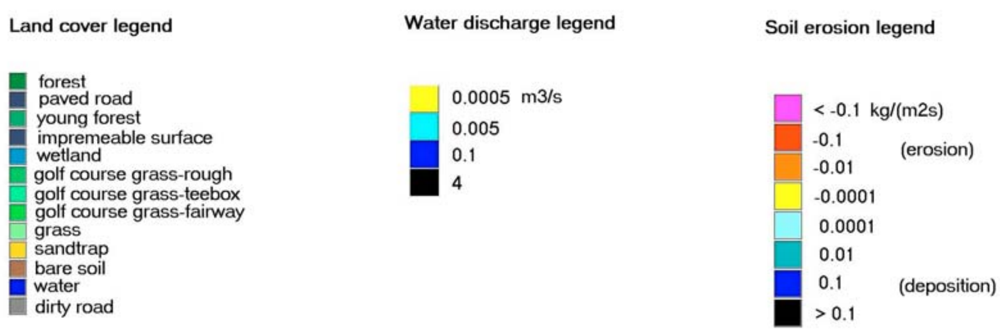

Figure 7: Sediment control measures (wetland, fence, check dam)

5.3 Communication of results - dynamic visualization

Both the water flow and sediment transport modules optionally output time series of raster maps representing evolution of the modeled phenomenon over time. Viewing these time series in the form of animation can provide valuable insight into the functioning of sediment control structures and conservation measures within a complex landscape.

The evolution of water flow at different stages of landscape development can be viewed and compared by simultaneosly animating the 3 time series of water discharge (or water depth) raster maps using *xganim*. Such animations clearly communicate the impact of impervious surfaces and disturbed areas on rapid increase in the amount of surface water flow and its velocity with serious consequnces for sediment transport. To better understand the interaction between water flow and sediment transport *xganim* can be used to simultaneously animate time series of water discharge, sediment flow rate and net erosion/deposition. The construction work often includes significant changes in local topography, especially when golf courses and similar developments are involved. Changes in topography due to development often tend to reduce the water flow velocity by reducing the elevation surface gradients, partially compensating for negative impacts of vegetation removal. Visualizing the evolution of water and sediment flow draped over 3D terrain can provide additional insights into the complex interactions between the spatially variable land cover and topography. The "File sequence tool" in the GRASS module *nviz* was used to create the animations representing the evolution of water discharge for each of the 3 studied stages of development. Automated display of time stamp, legend and scale directly within *nviz* would make creating such animations even more useful and effective.

6 Conclusions and future

The presented simulation model based on Green's function Monte Carlo method is a promising approach for modeling landscape processes (fluxes). Using this method, the modelling process is much more robust and flexible. GRASS GIS environment at the same time provides easy access and flexibility in input data and parameter preparation, scenario modification and model calibration.

Future development will be associated with enhancements in dynamics (temporal changes in fields) and parameter optimization.

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