Title
Unit 130 - Process Modeling and Simulations

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Unit 130 - Process Modeling and Simulations

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Advanced Organizer

Topics covered in this unit

- definition of process modeling and simulations
- types of processes relevant to GIS
- approaches to process modeling and simulations
- calibration, error propagation and sensitivity analysis
- integration of process models and GIS
- application examples

Intended learning outcomes

- after learning the material covered in this unit, students should be able to
  - characterize types of processes and simulations relevant to GIS
  - identify methods and their suitability for various processes
  - explain the integration of GIS and models at different levels
  - discuss GIS relevant issues with a modeling specialist
  - write simple process modeling tools using map algebra

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Unit 130 - Process Modeling and Simulations

1. Introduction

- **Definition of process modeling and simulation**: theoretical concepts and computational methods that describe, represent and simulate the functioning of real-world processes;
  - computer simulations are becoming a 'third way' of performing research, expanding thus traditional experimental and theoretical approaches:
    - simulation can be regarded as a numerical experiment, but it often requires advancements in theory
    - simulations can provide information which is impossible or too expensive to measure, as well as insights which are not amenable or too complicated for analytical theory methods
  - models are simplified abstractions of reality representing or describing its most important/driving elements and their interactions
  - simulations can be regarded as model runs for certain initial conditions (real or designed)

- **Purpose of modeling and simulations**:
  - analysis and understanding of observed phenomena
  - testing of hypotheses and theories
  - prediction of spatio-temporal systems behavior under various conditions and scenarios (both existing and simulated, often performed to support decision making)
  - new discoveries of functioning of geospatial phenomena enabled by unique capabilities of computer experiments

- **Role of GIS**:
  - storing and managing input data and results
  - pre-processing of input data (editing, transformation, interpolation, derivation of parameters, etc.)
  - analysis and visualization of results (Mitas et al 1997)
  - providing computational environment and tools for simulations

2. Types of process models

- based on **area of application**, models represent:
  - natural processes
    - atmospheric (global and regional circulation, air pollution)
    - hydrological (water cycle and related processes, see unit 179)
    - geological, geomorphological (solid earth processes)
- biological and ecosystem (see unit 171)
- interactions between hydrosphere, atmosphere, lithosphere and biosphere
  - socio-economic/anthropogenic processes
    - transportation
    - urban, population
    - production (manufacturing, farming (see unit 181)
    - distribution and services (see unit 174)
    - interactions between socio-economic processes
  - interaction of natural and anthropogenic phenomena (e.g., environmental models, food production, forestry, mining)

- based on the **type of spatial distribution**, process models describe the behavior of phenomena represented by:
  - homogeneous or spatially averaged units, e.g. subwatersheds, counties, polygons (sometimes referred to as *lumped models*) with processes described by ordinary differential equations
  - fields/multivariate functions discretized as rasters, grid cells or meshes (*distributed models*) with processes described by partial differential equations or cellular automata (see unit 054)

- Table 1. Representation of phenomena as multivariate fields.

- based on the **nature of spatial interactions**, (see unit 021 and unit 123) models involve:
  - no spatial interaction, only location dependent behavior
  - short-range, close neighborhood interaction
  - long-range/expanding interaction

- based on the **type of underlying physical or social process**, models simulate
  - fluxes (over a surface, through network, in 3D space), including: diffusion, dispersion, advection, convection, reaction, radiation and heat transfer
  - proliferation and decay (chemical processes, radioactive decay)
  - population dynamics (birth/death, competition, predator/prey, epidemics)
  - intelligent agents (systems of independent entities which interact between themselves and with environment with a certain degree of decision making capabilities)

- based on the **spatial extent** of modeled phenomena models are
  - local
  - regional
  - global
  - multiscale or nested models (Steyaert 1993 in Goodchild et al. 1993), with
    - high resolution models used to calibrate the large scale, low resolution models,
    - output of large scale models used as an input for small scale models

3. Approaches to modeling and simulations
• real processes are complex and often include non-linear behavior, stochastic components and feedback loops over spatial and temporal scales, therefore models can represent the processes only at a certain level of simplification
• **empirical models** are based on statistical analysis of observed data, and they are usually applicable only to the same conditions under which the observations were made (for example the Universal Soil Loss Equation for modeling annual soil loss based on terrain, soil, rainfall and land cover factors, Renard et al. 1991)
• **process based models** are based on understanding of physical, chemical, geological, and biological processes and their mathematical description (for example, hydrologic and erosion models SIMWE: Mitas and Mitasaova 1998, CASC2D: Saghafian 1996 in Goodchild et al 1996)
• models of complex systems often use combination of empirical and process based approaches

### 3.1 Deterministic models

• model processes which are often described by differential equations, with a unique input leading to unique output for well-defined linear models and with multiple outputs possible for non-linear models;
• equations can be solved by different **numerical methods** (after discretization: modification to run on a grid or a mesh, and parametrization: setting parameters to account for subgrid processes):
  - **finite difference**
    - principle (Press et al 1992)
    - example (Saghafian 1996 in Goodchild et al 1996: CASC2d)
  - **finite element**
    - principle, meshes (Burnett 1987)
    - example (Vieux 1996 in Goodchild et al 1996: r.water.fea)
  - **path simulation**
    - principle: based on random walker representation, *note: not to be confused with stochastic simulations*
    - example: Figure 1 - path simulation solution of sediment flow continuity equation and resulting spatial distribution of erosion (red) and deposition (blue) (SIMWE model, *animation*, Mitas and Mitasaova 1998).
• models describe processes at various **levels of temporal variation**
  - **steady state**, with no temporal variations, often used for diagnostic applications
  - **time series of steady state** events, computed by running a steady state model with time series of input parameters, this approach is commonly used for estimation of long term average spatial distributions of modeled phenomena
  - **dynamic**, describing the spatio-temporal variations during a modeled event, used for prognostic applications and forecasting

### 3.2 Stochastic models

• model spatio-temporal behavior of phenomena with **random components**
• unique input leads to different output for each model run, due to the random component
of the modeled process, single simulation gives only one possible result

- multiple runs are used to estimate **probability distributions**
- conditional simulations combine stochastic modeling and geostatistics to improve characterization of geospatial phenomena
- behavior of dynamic stochastic systems can be described by different types of stochastic processes, such as Poisson and renewal, discrete-time and continuous-time Markov process, matrices of transition probabilities, Brownian processes and diffusion (Nelson 1995, Molchanov and Woyczynski 1997)

### 3.3 Rule based models

- model processes governed by local rules using **cellular automata**: non-linear dynamic mathematical systems based on discrete time and space (Wolfram 1984)
- principles
  - cellular automaton evolves in discrete time-steps by updating its state according to a transition rule which is applied universally and synchronously to each cell at each time step.
  - value of each cell is determined based on a geometric configuration of neighbor cells which is specified as a part of the transition rule.
  - complex global behavior may emerge from application of simple local rules, thus useful for simulating systems that are not fully understood but for which their local processes are well known.
- examples
  - urban growth simulation models: diffusion-limited aggregation (Batty and Longley 1994), innovation diffusion model (Clarke 1996, Park and Wagner 1997)
  - spatially explicit ecological models
  - forest fire simulation (Clarke et al 1994)

### 3.4 Multi-agent simulation of complex systems

- model movement and development of groups of many **interacting agents**
- agent is any actor in a system, that can generate events that affect itself and other agents, a typical agent is modeled as a set of rules, responses to stimuli
- **individual-based models** represent movement/development of individual entities over space and time based on local rules
- hierarchical models can be built by nesting multiple collections of agents with their schedule of activity
- example:
  - SWARM - multiagent simulation of complex systems (Minar et al 1996, Booth 1997)

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### 4. Models and reality

- calibration
the role of parameters and their limits are evaluated by parameter scans (Clarke 1996 in Goodchild et al 1997 CDROM, Mitas et al. 1997)
  - Figure 2 - parameter scan for sediment flow and erosion/deposition for detachment capacity coefficient changing from 0.001-10, animation
  - model results are compared with experiments and parameters are set to values which ensure the best reproduction of the experimental data
- sensitivity analysis, error propagation and uncertainty is performed to estimate impact of errors in input data on the model results (2.10: u096)
- causes of inconsistency between models and reality (Steyaert 1993 in Goodchild et al 1993)
  - only limited number of interacting processes can be treated
  - process may not be well understood or is treated inadequately
  - resolution and/or scale may be inadequate
  - numerical solution can be too sensitive to initial conditions
  - model can be incorrectly applied to conditions when its assumptions are not valid
  - errors in input data

5. GIS implementation

- simple modeling is supported by most commercial GIS, especially within the raster subsystems (ARCGRID, ArcView Spatial Analyst, Intergraph ERMA, IDRISI, GRASS, ERDAS)
- full integration of complex models may require extensions of standard GIS functions such as support for temporal and 3D/4D data and meshes for finite element methods
- opening of data formats and incorporation of customization and application development tools stimulate coupling of commercial GIS and modeling
- use of object oriented technology facilitates more efficient GIS implementation and merges the different levels of coupling.

5.1 Full integration - embeded coupling

- model is developed and implemented within a GIS using the programing and development tools of a given GIS (Application Programming Interface (API), scripting tools, map algebra operations)
- model is run as a GIS command,
- inputs and outputs are in a GIS database and no data transfer is needed,
- computation is efficient for adequately coded models, models written with scripting tools may be slower,
- portability is restricted because of dependence on a GIS within which the model was developed and implemented,
- examples
  - embeded coupling
    - r.hydro.CASC2d, r.water.fea in GRASS (Saghafian 1996, Vieux 1996 in Goodchild et al 1996)
    - Darcyflow, Particletrack in ARCGRID (ESRI 1994)
  - map algebra implementation
- water flow (example in GRASS r.mapcalc, Shapiro and Westervelt 1992)
- dispersion: simple fire spread model (example in ARCGRID, ESRI 1994)
- model development is supported by customization and application development tools
  and extensions to map algebra (for example, Wesseling et al. 1996: DYNAMITE for

5.2 Integration under a common interface - tight coupling

- model is developed outside GIS and has its own data structures with exchange of data
  between model and GIS hidden from user, although in some cases the data files can be
  shared
- GIS and model are linked through a common interface
- interface often supports integration of GIS and several different models for simulation
  of complex systems with interrelated processes
- portability is restricted
- examples: (see Web references)
  - SWAT, AGNPS, ANSWERS coupled with GRASS
  - SWAT, IDOR3D, BASIN-2 coupled with ArcView

5.3 Loose coupling

- model is developed and run independently of GIS
- input data are exported from GIS and results are imported to GIS for analysis and
  visualization
- portability - model can be used with different GIS
- examples:
  - PAYSAGE-forest and habitat change (Hansen et al. 1996), coupled with
    Arcview/ArcInfo
  - SIMWE-erosion and deposition (Mitas and Mitasova 1998), coupled with
    GRASS, but can run with any GIS which supports raster data

5.4 Modeling environments linked to GIS

- aimed at modular, reusable model development
- modeling environment is linked to GIS through interface or data import/export
- examples:
  - SME: Spatial Modeling Environment (Maxwell and Constanza 1997)
  - SWARM: Multi-agent simulation of complex systems (Minar et al. 1996)
  - MMS-Modular Modeling System (Leavesley 1993 in Goodchild et al. 1993)

6. Application examples and future trends

6.1. Natural resources

- water, sediment and contaminants (see unit 179):
• **SWAT: Soil and Water Assessment Tool**
• IDOR2D,3D: Hydrodynamic Pollutant Transport Simulation
• Hydrology models in GRASS
• solid earth processes
  • **SAND: conditional simulations for mining**
  • landscape evolution
• atmospheric modeling
• spatially explicit ecological models (see unit 171)
  • Dynamic ecological simulations
  • Forest dynamics
  • SWARM: multiagent simulation of complex systems
  • Mallard production models

### 6.2 Socio-economic

• transportation
  • Transportation management with GIS
• population growth and migration
• urban growth (see unit 163)
  • Clarke Urban Growth Model
• food production
  • Interfacing crop growth models with GIS
• military

### 6.3 Integrated models of complex systems

• atmospheric+hydrologic+plant growth+erosion/sedimentation
  • Modular Modeling System
• economic-ecological systems
  • Integrated Ecological Economic Modeling And valuation of Watersheds: Patuxten watershed model

### 6.4 Future trends

• real-time simulations
• distributed on-line modeling
• complex systems: integrated models of interacting processes
• dynamic systems in 3D space
• object oriented reusable model development environments

### 7. Summary

• process modeling is aimed at improving our understanding and predicting the impact of natural and socio-economic processes and their interactions
• GIS provides supporting tools for modeling, especially spatial data management,
analysis and visualization

- process models describe the behavior of phenomena represented by fields, networks and individual agents with various types of spatial interactions at local, regional or global scale
- models can be rule based, deterministic, stochastic, multiagent
- issues of calibration, error propagation and scale are important for realistic simulations
- GIS and models can be fully integrated or linked through data and interface
- well developed applications are in hydrology, sediment and contaminants transport, ecosystem modeling and urban growth

8. Review and study questions

- find examples of process models using phenomena represented by fields, networks and points
- name the type of processes and disciplines where deterministic models are often used
- give examples of models when GIS implementation as a script would be the most effective
- write a simple diffusion model using map algebra

9. Reference materials

9.1 Print References


_Urban growth modeling by cellular automata_

_Individual based simulation system for multiple species at multiple trophic levels_
- Burnett D. S. 1987, Finite Element Analysis: From Concepts to Applications, Addison-Wesley, Reading, MA.
- ESRI 1994, Cell-based Modeling with GRID, ESRI, Redlands, CA.
- ESRI 1996, Avenue: Customization and application development for ArcView, ESRI, Redlands, CA
- Goodchild, M.F, L. T. Steyaert, and B. O. Parks, eds., 1993, Geographic Information...

Proceedings from a conference in Boulder, CO, 1991 includes numerous excellent examples of environmental models linked or integrated with GIS

Proceedings from a conference in Breckenridge, CO, 1993 reflects progress in integration of GIS and modeling

Proceedings from a third conference held in Santa Fe 1996

Excellent description of multi-agent simulation principles using the SWARM simulation system

Example of process-based distributed model SIMWE with loose coupling to GRASS

Paper from a special issue devoted to visualization illustrates use of visualization at different stages of modeling from data processing through model development and application

Good description of cellular coupling automata with GIS in IDRISI with useful spatial dynamic modeling examples
description of finite difference methods and algorithms, including programs


description of an empirical erosion model commonly used with GIS


9.2 Web references

- government web sites and organizations
  - Geographic Information Science and Technology Group, Oak Ridge National Laboratory (Department of Energy)
  - Environmental Protection Agency BASIN-2, watershed and water quality analysis models integrated within an ArcView GIS environment.
  - IDRISI - raster based GIS and its applications
- on-line tutorials
  - Tutorial for ecosimulations from University of Oregon
- case study examples: Modeling environments
  - Spatial Modeling Environment:SME
  - SWARM
  - case study examples: Models
  - Dynamic Landscape Simulation Modeling
  - Forest dynamics
  - SWAT: Soil and Water Assessment Tool
  - IDOR2D,3D: Hydrodynamic and pollutant transport simulations
  - Hydrologic modeling integrated with GIS at EMGIS Laboratory, University of Oklahoma
  - Environmental Modeling Research Laboratory - hydrologic models GMS, SMS, WMS linked to ArcView
  - Hydrologic models linked to GIS
  - Clarke Urban Growth Model

Includes link to research by Batty (see print references) and cellular automata
bibliography
- Transportation management with GIS
- Stochastic modeling of petrophysics
- Geographic Modeling Systems Laboratory, including link to Environmental modeling and visualization and GRASS5.0

- commercial web sites
  - ESRI-GRID, Avenue, Spatial Analyst
  - Intergraph ERMA

Citation

To reference this material use the appropriate variation of the following format:


Unit 130

Metadata and Revision History

1. About the main contributors

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2. Details about the file

   • unit title: Process modeling and simulations
   • unit key number 130

3. Key words

   • spatio-temporal modeling, GIS and model integration, landscape processes

4. Index words

   • integration, coupling, flux, diffusion, deterministic, stochastic, rule-based models, path
     simulation, calibration, multiscale;

5. Prerequisite units

   • representation of fields, rasters, networks, map algebra

6. Subsequent units
- hydrologic applications, ecosystem applications, cellular automata, error propagation

7. Other contributors to this unit

- none at this time

8. Revision history

- 9 February, 1998 - unit originally created
- 27 March, 1998 - new material added
- 12 November, 1998 - text revised and references added
- 2 December, 1998 - posted to NCGIA website

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<th>phenomenon (field)</th>
<th>point data</th>
<th>3D dynamic map</th>
</tr>
</thead>
<tbody>
<tr>
<td>elevation: $z=f(x,y)$; single surface</td>
<td></td>
<td></td>
</tr>
<tr>
<td>precipitation: $p_i=f(x,y)$; $i=1,...,12$; time series of surfaces</td>
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<td></td>
</tr>
<tr>
<td>soil horizons: $z_i=f_i(x,y)$; $i=1,...,5$; vertical series of surfaces</td>
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<tr>
<td>soil pH: $pH=f(x,y,z)$; single volume</td>
<td></td>
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<tr>
<td>concentrations of nitrogen in water: $w=f(x,y,z,t)$; volume evolving in time (jan-dec)</td>
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</tr>
</tbody>
</table>
Detail of a DEM interpolated from data points on contours. Size of the cylinder represents a deviation of terrain model from the given data. (The deviation is 4x exaggerated, the area is 2.6x3.7km)
3D soil samples with measured pH