

Printed from: Interstate Technology & Regulatory Council (ITRC). 2016. *Geospatial Analysis for Optimization at Environmental Sites (GRO-1)*. Washington, D.C.: Interstate Technology & Regulatory Council, Geostatistics for Remediation Optimization Team. www.itrcweb.org/gro-1.

Software Descriptions

ArcGIS Tools—Geostatistical Analyst and Spatial Analyst

VRead more

The Geostatistical Analyst and Spatial Analyst extensions to ESRI's ArcGIS software provide spatial interpolation and surface modeling tools. These extensions allow geospatial methods to be performed within the broader Geographic Information System (GIS) environment, so that input data can be queried and filtered, and models can be built and assessed for quality before results are exported.

In general, the Spatial Analyst extension is designed for automated modeling and analysis to create surfaces and contours and perform grid calculations such as slope/terrain and cut/fill. Spatial Analyst is also useful for data conversion, such as turning topographic contours lines or points into rasters and vice versa. Spatial Analyst, however, provides only basic interpolation methods and does not allow the user to easily manipulate model parameters. For example, Spatial Analyst has a kriging tool for spatial interpolation, but variography cannot be performed to determine model parameters, and it is not possible to incorporate data transformations, anisotropy, or cross-validation.

More advanced spatial data analysis and interpolation in the ArcGIS environment can be performed with the Geostatistical Analyst extension. Exploratory spatial data analysis tools within Geostatistical Analyst include: histogram and Q-Q plots to evaluate data distribution and summary statistics, Voronoi maps and trend analysis to evaluate spatial variability and stationarity, and semivariogram and cross-variance clouds to evaluate spatial dependence within and between data sets, respectively. Data interpolation tools within Geostatistical Analyst include methods such as polynomial interpolation and inverse distance weighted functions, and many forms of kriging such as: ordinary, simple, universal, indicator, probability, disjunctive, and co-kriging. Geostatistical Analyst allows the user to detrend and transform data to approach stationarity and normality, and to fit model parameters such as anisotropy, nugget, range, and sill. The user can perform model diagnostics such as cross-validation and calculation and visualization of prediction standard error. Geostatistical Analyst also supports more advanced analysis such as moving window kriging, Gaussian Geostatistical Simulation, and Empirical Bayesian Kriging (EBK). EBK automates aspects of the kriging process and accounts for error related to estimation of the semivariogram.

These ArcGIS tools are not custom made for environmental monitoring and remediation; rather, they provide a platform for performing many different types of spatial analysis and interpolation to understand and visualize data sets, quantify uncertainty, and inform decisions regarding optimization of remedial systems. The surfaces generated using Geostatistical Analyst and Spatial Analyst can be integrated into a 3D model using the 3D Analyst extension to ArcGIS. 3D visualizations are often components of CSMs used to optimize remedial systems. There is some redundancy in geoprocessing tools between Spatial Analyst and 3D Analyst, so that if a user has the 3D Analyst extension enabled, Spatial Analyst may not add significant capability. Additionally, although 3D visualization of surfaces such as topography is possible, 3D interpolation of data is not. With respect to optimization, although ArcGIS tools are able to perform geospatial analysis, users must manipulate and interpret the results manually for optimization applications such as monitoring well redundancy analysis.

For more detailed information about the software program and methodology, see <u>Tables 7, 8, and 9</u>.

Case studies: using ArcGIS software include a radioactive site, a tidal site, and a lead-contaminated site.

Source: ESRI, Inc. (ESRI 2013) **Ease of Use:** Moderate

Training and Resources: Several free online training options are available. Program documentation is also available (ESRI

2015b).

EVS/MVS

TRead more

Environmental Visualization System (EVS) and Mining Visualization System (MVS) represent two versions of earth science software with advanced gridding, geostatistical analysis, and full 3D visualization tools developed by C Tech. As the names suggest, EVS/MVS has been developed and optimized to work with environmental and subsurface data (air, water, soil, and

lithology). Two new versions of EVS/MVS, Earth Volumetric Studio (EVS) and EnterVol are available. While similar in core functionality, the new versions are new applications. The new EVS ultimately will replace EVS/MVS. EnterVol is a version of EVS, which operates with ESRI's ArcGIS. The Earth Volumetric Studio supports cross-validation.

The user interacts with the module-based software through a GUI. Modules are selected for a particular task and can be combined in a network with other modules to build an application that enables the user to save the ordered modules as an application for reuse. For example, a simple application may consist of a few modules to apply kriging to a data set, create 2D isoconcentration lines, and export to a GIS or CAD file.

EVS/MVS analyzes the input data, constructs best-fit multidimensional variograms, and performs kriging in the domain to be visualized. User options include input of values for parameters controlling the variogram and kriging procedure, display and analysis of the data, and comparison of the modeled and measured domains. While there are several options to adjust input variables and confidence levels, the underlying kriging methodology is unavailable to the user (which may be a drawback to users with advanced knowledge of geospatial methods). For project managers without advanced geospatial knowledge, EVS/MVS may enable them to perform more advanced analysis.

Volumetric analysis includes true 3D and volumetric objects. For example, a kriged plume can be queried for volume and with user-supplied values for soil porosity, soil density, and chemical density, estimates of contaminant mass and volume can be calculated. For optimization, spatial analyses include capabilities for well network optimization and decommissioning, a drilling guide, as well as confidence and uncertainty maps. The volumetrics and overburden modules can assist with cost analyses

Principal modules and capabilities include:

- 3D and 2D data interpolation and extrapolation with kriging, inverse distance weighting, or natural neighbor
- 3D geology interpolation and extrapolation with kriging, inverse distance weighting, or natural neighbor
- user-defined anisotropy, detection limits, kriging confidence and uncertainty
- spatial and temporal interpolation and extrapolation (for example, animate a plume through time)
- volumetric estimates and excavation estimations
- monitoring well network optimization and decommissioning
- ability to distribute models as video files, 3D PDF or interactive read-only models
- 3D subsetting (for example, user defined isoconcentration or cross section subsets)
- EDA tools

For more detailed information about the software program and methodology, see Tables 7, 8, and 9.

Source: C Tech Development Corporation (C Tech Development Corporation 2015a), www.ctech.com

Ease of Use: Complex

Training and Resources: EVS/MVS - Environmental Visualization System and Mining Visualization System provides information on available documentation (including workbooks), training videos, scheduled and in-person training classes, and technical support (<u>C Tech Development Corporation 2015b</u>).

Global Mapper

TRead more

Global Mapper software is a GIS data processing application originally developed by the USGS in 1998 for viewing their DLG (Digital Line Graph) vector data products. The software is used in the oil and gas industry for siting drill pads. Global Mapper analyzes and maps spatial data. While Global Mapper is not specifically designed for optimization and does not have a cost evaluation function, it may be a visual aid to help with optimization analysis.

Global Mapper can perform distance/area and cut/fill calculations, generate contours from surface data, and grid 3D point data. Global Mapper works in 3D, gridded elevation, raster (scanned maps/imagery) or vector formats. The software supports many different spatial data formats. Repetitive tasks can be accomplished using the built-in scripting language or comprehensive batch conversion functionality. Optional LiDAR and GEM (dual cameral GPS imagery system software) modules are available for advanced processing for extra cost.

Disclaimer: Geospatial functions and capabilities presented for this software have not been reviewed or verified by Blue Marble Geographics.

For more detailed information about the software program and methodology, see Tables 7, 8, and 9.

Source: Blue Marble Geographics (<u>Blue Marble Geographics 2015b</u>)

Ease of Use: Moderate

Training and Resources: Several training options are available, including live and recorded online training, self-study, and certification courses. Most online training is free. Training modules are also available for free to academic institutions (<u>Blue Marble Geographics 2015a</u>).

GMS

TRead more

Groundwater Modeling System (GMS) is 3D groundwater modeling and simulation software based on the USGS MODFLOW finite-difference flow model. For model building in GMS, data can be imported from several file types including raster images, topography, MODFLOW, ArcGIS shapefiles, and CAD (.dwg, .dwn and .dxf). Cross sections can be generated using site data. Geospatial methods include kriging, inverse distance weighting, and natural neighbor. GMS kriging functions are based upon GSLIB routines. Modeling visualization output includes photo-realistic figures, layered images over model outputs, animations for presentations, with the ability to add site and company detail to the output.

GMS does not include functions and trend analyses to evaluate sufficiency of well networks or costs of optimization. Transition Probability Geostatistical Software (T-PROGS), a stochastic subsurface modeling program that can allow for spatial variability of hydraulic properties, can be linked to GMS as a user interface for visual output.

Disclaimer: Geospatial functions and capabilities presented for this software have not been reviewed or verified by Aquaveo.

For more detailed information about the software program and methodology, see <u>Tables 7, 8, and 9</u>.

Source: Aquaveo (Aquaveo 2015b)

Ease of Use: Moderate

Training and Resources: The vendor website offers a <u>learning center</u>. Training modules are available for free in PDF format to download (<u>Aquaveo 2015a</u>).

GRASS

TRead more

Geographic Resources Analysis Support System (GRASS) was developed by the U.S. Army Construction Engineering Research Laboratory as a land management and environmental planning software for military use. GRASS is an open source GIS software that is generally used for geospatial data management. Commonly used spatial interpolation methods are built-in and include inverse distance weighting and smoothing spline interpolation.

GRASS can perform geospatial modeling (with add-on packages) and can interface with other geospatial software such as $\underline{\mathbb{R}}$ and $\underline{\mathsf{Matlab}}$. GRASS does not include functions and trend analyses to evaluate sufficiency of well networks or to evaluate costs for optimization.

Disclaimer: Geospatial functions and capabilities presented for this software have not been reviewed or verified by the developers.

For more detailed information about the software program and methodology, see Tables 7, 8, and 9.

Source: GRASS GIS (GRASS GIS Team 2013)

Ease of Use: Complex

Training and Resources: User manuals are updated and available and linked support is available in email groups or blogs (<u>GRASS GIS Team 2015</u>). Support can also be obtained from businesses that offer support for a fee.

GS+

▼Read more

GS+ is a geospatial modeling software developed by Gamma Design Software LLC in 1988 as the first such program for desktop computers. GS+ includes a comprehensive range of 2D geospatial functions from variogram analysis to mapping. GS+ does not include functions and trend analyses to evaluate sufficiency of well networks or costs for monitoring optimization.

The software has an easy-to-use, menu-driven GUI and has 2D and 3D plotting capabilities. Users can directly enter spatial data into data worksheets and perform spatial geospatial analyses. The software can also interface with several standard formats including text, HTML tables, spreadsheets, and databases (Microsoft Excel, Access). GS+ can export output into several formats including Surfer, ArcView, and GSLIB formats.

Geospatial modeling capabilities of GS+ include univariate data analysis, variogram analysis and interpolation using ordinary and simple kriging, co-kriging, and inverse distance weighting methods. Available variogram models are spherical, exponential, Gaussian and linear isotropic, and similar anisotropic models. Additional capabilities include kriging-based conditional simulation, and cross-validation of the interpolated results. The software also provides a convenient method to exclude or include zones and polygons during interpolation.

For more detailed information about the software program and methodology, see <u>Tables 7, 8, and 9</u>. **Source:** Gamma Design Software (<u>Gamma Design Software 2014</u>) and RockWare (<u>Rockware 2015a</u>)

Ease of Use: Moderate

Training and Resources: The software comes with a user manual. Training information is available at (<u>Gamma Design Software 2015</u>). Vendor training is available, including webinars and workshops in Colorado.

GTS Optimization Software

TRead more

GTS (Geostatistical Temporal-Spatial) software is an open-domain application that was developed with technical oversight and funding by the AFCEC. The software was developed to optimize long-term monitoring programs for both individual sites and entire installations, some having over 500 wells and sampling events spanning over 30 years.

This software is designed to reduce monitoring redundancy by determining optimal sampling frequencies, identifying the optimal number and placement of wells, proposing new sampling locations in areas of high spatial uncertainty, and evaluating optimization costs. State-of-the-art statistical and geostatistical analytical routines are built in and perform nonlinear trend analysis (locally weighted quadratic regression, LWQR) and generate concentration-based plume maps (quantile local regression) over multiple sampling events. A quasi-genetic algorithm identifies redundancy in the monitoring network and determines essential well locations. Optimal sampling intervals are determined by a process known as iterative thinning or by analyzing temporal variograms. The software includes basic GIS capability and imports shape files of infrastructure, installation boundaries, or potentiometric data. Formal tests for trend (using LWQR, or Thiel-Sen nonparametric methods) are performed on all wells spanning: (1) the entire historical sampling record; (2) the last four years; and (3) the last four sampling events. One of the unique features of the software is its ability to generate and analyze concentration maps over time (time slices) and vertical space. This analysis is helpful for developing CSMs and analyzing concentration patterns with respect to changing site conditions.

GTS is bundled with other open-source programs such as R, MatLab runtime libraries, and SQLite, to perform statistical computing, data visualization, interface modules, and database management. The software is limited to evaluating up to four chemicals per run and up to five horizons. Visualization and tabular output is mostly HTML format, but some reports are output as ASCII files.

For more detailed information about the software program and methodology, see Tables 7, 8, and 9.

Case Study: using GTS software includes a former ordnance site.

Source: AFCEC (AFCEC 2011)

Ease of Use: Moderate

References: Hunter, Cameron, and Stewart 2011

Training and Resources: Limited training resources are available. Case study examples are available as well (Hunter,

Cameron, and Stewart 2011).

GWSDAT

▼Read more

The Groundwater Spatiotemporal Data Analysis Tool (GWSDAT) was developed by Shell Global Solutions as an open-source tool for analysis and reporting of groundwater monitoring data. GWSDAT software uses nonparametric statistical methods for trend analysis of simple time-series groundwater concentration and elevation data, and can plot nonaqueous phase liquid (LNAPL) thickness. GWSDAT also calculates temporal plume changes. The quantities of plume mass, average concentration, area and location of the center of mass are calculated by spatial integration of the plume concentration above a predefined concentration threshold.

Geospatial modeling calculations are made with the open-source R statistical program. Data are entered into a standardized Microsoft Excel spreadsheet template. Site base map information can be imported in GIS shapefile format. GWSDAT applies a spatio-temporal model smoother (based on <u>penalized splines</u>) for a more coherent and smooth interpretation of the

groundwater concentration, elevation, and LNAPL trend data. GWSDAT assumes homogeneous concentrations across the aquifer depth.

Output for reporting can be exported to Microsoft Word or PowerPoint. GWSDAT does not include functions and trend analyses to evaluate sufficiency of well networks or costs for monitoring optimization.

For more detailed information about the software program and methodology, see Tables 7, 8, and 9.

Case Study: using GWSDAT includes groundwater monitoring at a research facility. **Source:** American Petroleum Institute website, Shell (Shell Global Solutions 2014)

Ease of Use: Easy

References: Jones et al. 2014; Evers et al. 2015; Jones, Spence, and Bonte 2015

Training and Resources: Training or other support is not available. A user manual is included in the downloaded software. A FAQ document can be downloaded from the Shell website (<u>Shell Global Solutions 2015</u>).

Hydro GeoAnalyst

TRead more

Hydro GeoAnalyst (HGA) is an environmental data management system for groundwater and environmental data developed by Waterloo Hydrogeologic. HGA integrates a wide range of tools for data interpretation, statistical analysis, GIS mapping, data charting, and 2D and 3D visualizations. Some typical applications for HGA include (<u>Waterloo Hydrogeologic 2015a</u>):

- regional water well management
- contaminant site inventory
- regulatory compliance
- geologic cross sections
- public access to information
- environmental site assessment
- monitored natural attenuation
- regional aquifer characterization and management
- cross-boundary data sharing
- aguifer vulnerability mapping

HGA does not include functions and trend analyses to evaluate sufficiency of well networks or costs for monitoring optimization.

For more detailed information about the software program and methodology, see <u>Tables 7, 8, and 9</u>.

Source: Waterloo Hydrogeologic 2015a

Ease of Use: Moderate

Training and Resources: Tutorials and user manual are available (Waterloo Hydrogeologic 2015b).

Isatis

▼Read more

Isatis is software created by the Mining School of Paris, France, and is currently developed by GEOVARIANCES, a French company founded in 1986 by three engineers from this school. Isatis is a general-purpose geostatistical toolbox. The main application for Isatis is in the mining and oil and gas industries, but the software has applications in environmental data evaluation.

Isatis can be used for soil and groundwater characterization studies, air quality, and nuclear contamination projects. Data integration is performed through multiple import/exports formats: ASCII, Excel, DXF, ArcView Shapefiles, NetCDF, GSLIB, ODBC, and image files (PNG, GIF, BMP).

Software modules commonly used for environmental studies include:

- general tools including a calculator, Gaussian transformations, and geology modeling
- graphic interactive exploratory data analysis, including quick statistics and various linked graphics: base maps, scatter diagrams, variogram maps (for anisotropy analysis), and experimental variogram construction (multivariate, multidirectional, multistructure)
- interactive and automatic variogram fitting and cross-validation tool
- geospatial interpolation methods such as co-kriging, indicator kriging, collocated co-kriging, external drift (trend)

kriging, and conditional co-simulations (discrete and continuous variable)

- simulation postprocessing tool allow construction of probability maps for distribution of contamination (concentrations higher than the remediation threshold) and risks curve defining the overall degree of contamination on the site
- uncertainty maps allowing the evaluation of well network sufficiency
- 2D and 3D calculations and visualization (Boreholes, surfaces, polygons, faults, wireframes)
- batch capabilities, enabling the automatic reproduction of complex workflows

Isatis does not include functions and trend analyses to evaluate sufficiency of well networks or costs for monitoring optimization, but can identify data duplication.

For more detailed information about the software program and methodology, see <u>Tables 7, 8, and 9</u>.

Case Study: using Isatis software includes PAH contaminated sediments.

Source: Geovariances (Geovariances 2015a)

Ease of Use: Complex

Training and Resources: Technical support is included with purchase of the software. Single or multiple-day training courses, or online and individualized training are available at cost from Geovariances (Geovariances 2015b)

Kartotrak

TRead more

In 2005, the Kartotrak software was created jointly by CEA (French Atomic Energy Commission) and GEOVARIANCES, a French software vendor founded in 1986 by three engineers from Paris School of Mines. Kartotrak was designed to locate and estimate contaminated soil volumes. It is a comprehensive software solution providing an integrated work flow for the characterization of sites contaminated with chemical or radioactive substances.

Principal software modules commonly used for environmental studies include:

- GIS-based Interface which can load standard geo-referenced file formats such as DXF,
- GeoTiff
- Mapinfo
- shapefiles, as well as scanned maps and screen shots
- Its interactive data georeferencing and customizing display features in a 3D viewer or 2D map.
- data handling, which allows for real-time data acquisition by connecting with GPS and other measuring devices, management of geographic projections, lithology interpolation, multilevel database (acquisition, raw, and validated), simple data validation, and EDA
- statistics, which includes a sampling design module, 2D sampling optimization based on criteria such as confidence interval, risk of getting a false negative, and under-sampled areas
- geostatistical processing, which includes variography, co-kriging, and 2D or 3D co-simulations, risk assessment
 mapping (quantiles, confidence intervals, probability to exceed thresholds), computation of surfaces or volumes,
 data flattening according to a reference surface (such as topography), pollutant mass computation
- geporting and export, with an integrated word processor that store in pdf, odf, and html formats, and can export result with georeferencing (geoTIFF)

For more detailed information about the software program and methodology, see Tables 7, 8 and 9.

Source: Geovariances (Geovariances 2015c)

Ease of Use: Moderate

Training and Resources: Technical support is included with purchase of the software. Single or multiple-day training courses, or online and individualized training are available at cost from Geovariances (<u>Geovariances 2015b</u>).

Leapfrog Hydro

▼Read more

Leapfrog Hydro is software created and distributed by ARANZ Geo Limited of New Zealand. This program is a comprehensive 3D geological modeling tool designed to solve problems related to both contaminated sites and groundwater allocation. Different hydrogeological hypotheses can be analyzed with this program in rapid succession; numerical fate and transport modeling is supported with dynamic modeling and 3D graphics support visualization.

Leapfrog Hydro can integrate large data sets into its rapid grade contouring and integrate GIS data. This program can also produce Windows Media Video files with its movie editor (including High Definition). The user can determine how the software handles nondetects. Issatis and GSLIB software modules can be integrated with Leapfrog Hydro. For optimization, the software includes an add-in interpolation model, spatial sampling analysis, and remedy components. Cost analysis is not available on Leapfrog Hydro.

Principal software features include:

- dynamic geological modeling using a rapid 3D geological modeling tool enabling field data to be transformed into 3D models, which can be dynamically updated with additional source information
- MODFLOW and FEFLOW from both legacy models, which can be imported for comparison to current data sets
 and used as a basis for the construction of dynamic models, and can also be created from geological models.
- output visualization in 3D using MODFLOW transient simulation outputs
- dynamic interpolation engine for numeric modeling, which can aid in analyzing and visualizing large numerical data sets
- interpolation using linear and spheroidal interpolants, which is similar to linear and spheroidal variogram models used in kriging (fast radial basis functions (RBFs) as primary computation engine, with advanced algorithms to evaluate the estimates quickly)

Disclaimer: Geospatial functions and capabilities presented for this software have not been reviewed or verified by ARANZ. For more detailed information about the software program and methodology, see <u>Tables 7, 8, and 9</u>.

Source: ARANZ (ARANZ Geo Limited 2015a)

Ease of Use: Moderate

Training and Resources: A user manual comes with the software. Support is available through Leapfrog Hydro (<u>ARANZ Geo Limited 2015b</u>). Training options range from phone and internet support services to standardized training classes to specific training designed to meet user needs.

MAROS

TRead more

Monitoring and Remediation Optimization System (MAROS) is public-domain software developed for the Air Force Civil Engineer Center (AFCEC, formerly AFCEE) by GSI Environmental Inc. MAROS was designed to evaluate and optimize groundwater long-term monitoring (LTM) programs. MAROS is constructed using Microsoft Access database as its platform, and can use all site spatial and temporal groundwater data to evaluate groundwater contaminant plumes, and to support LTM optimization. MAROS can be used for small sites with six or more wells, or large sites with as many as 100 wells and multiple sampling events. MAROS assumes a 2D and pseudo-2D aquifer.

Principal software modules include EDA tools, including <u>Kaplan Meier method</u>, outlier identification, data distribution, and trend analysis for individual well results. Geospatial analyses include estimation of total plume contaminant mass, center of mass and spread of mass over time using Delaunay triangle/Voronoi diagram mesh creation algorithms. Trends in the contaminant mass and distribution of mass are used to evaluate plume stability and remedy performance. The Delaunay/Voronoi geospatial algorithms are also used to prioritize wells for future sampling and optimize the spatial distribution of monitoring wells. MAROS provides recommendations for additional wells in locations of high spatial uncertainty and recommendations to eliminate redundant sampling locations. MAROS does not include a function to evaluate the cost of optimization.

For more detailed information about the software program and methodology, see Tables 7, 8, and 9.

Case Studies: using Maros software includes groundwater monitoring for the <u>State Road 114</u> and the <u>Stringfellow</u> Superfund sites.

Source: GSI (GSI Environmental Inc. 2013a)

Ease of Use: Easy

Training and Resources: A user manual comes with the software download. Limited <u>support</u> is available through GSI at. Training webinar slides are also available from GSI (<u>GSI Environmental Inc. 2013b</u>).

R

▼Read more

R is a programming language and environment for statistical computing developed under the GNU project by Robert

Gentleman and Ross Ihaka of the University of Auckland. R is available under the Free Software Foundation's GNU General Public License. The R environment is a statistical system that comes with a set of statistical packages, with other packages available through the Comprehensive R Archive Network (CRAN). The main geospatial packages include geoR and geoRglm. There are many other packages that could be useful in evaluating environmental data. You can run R either at the command line or through scripts.

geoR

The geoR package performs geospatial data analysis and spatial prediction developed by the Department of Mathematics and Statistics at Lancaster University, UK. The functions available in the package assume a basic Gaussian model and features include empirical variograms, likelihood-based estimation, variogram-based estimation, spatial interpolation (simple, ordinary, universal, and external trend kriging), cross-validation, Bayesian inference, and simulations. EDA is performed through R's graphical capabilities using functions plot.geodata and points.geodata.

geoRgIm

The geoRgIm package uses Markov-chain Monte Carlo methods for inference in generalized linear spatial models and was developed by the Department of Mathematical Sciences, Aalborg University, Denmark and the Department of Mathematics and Statistics, Lancaster University, UK. As an extension to geoR, the package uses several of geoR's internal functions. The distinction from geoR is that this package implements the spatial Poisson model and the spatial binomial model.

R does not include functions and trend analyses to evaluate sufficiency of well networks or costs for monitoring optimization.

Disclaimer: Geospatial functions and capabilities presented for this software have not been reviewed or verified by the developers.

For more detailed information about the software program and methodology, see Tables 7, 8, and 9.

Source:

R website (R Development Core Team 2008), geoR website (geoR website), geoRglm website (geoRglm website 2015)

Ease of Use: Complex

References: Chambers 2008; Ihaku and Gentleman 1996

Training and Resources: A user manual can be downloaded (<u>Hornik 2016</u>). Online tutorials can be found on youtube.com and r-statistics.com. Other publications can be found online (<u>Bivand, Pebesma, and Gomez-Rubio 2013</u>).

RockWorks

VRead more

RockWorks is a spatial data visualization software program that is designed for geologic, environmental, petroleum, and mining uses. The program provides a large list of tools for generating maps, borehole logging, cross sections, fence diagrams, solid models, and volumetrics from geologic, environmental, chemical, and hydrologic data. Data can be entered into RockWorks either by typing it in individually, or by importing spreadsheets or ASCII files that conform to a RockWorks-specific format. RockWorks does not include functions and trend analyses to evaluate sufficiency of well networks or costs for monitoring optimization.

Geospatial methods are available for generating 2D models of spatial data. The following methods are available for interpolating data over a grid:

- closest point
- cumulative
- dip/direction
- inverse distance model (with or without directional weighting)
- kriging (with variogram displays)
- sample density (for count data)
- trend surface regression
- trend surface residuals
- triangulation
- a hybrid method that allows the use of several gridding methods by applying a weighting factor to each

RockWorks also offers surface-based stratigraphic modeling with onlap and underlap rules, and provides multiple methods for 3D (solid) modeling, such as distance to point, inverse-distance weighting, lateral extrusion/blending.

For more detailed information about the software program and methodology, see Tables 7, 8, and 9.

Source: Earth Science and GIS Software (Rockware 2015a)

Ease of Use: Moderate

Training Resources: Manuals and tutorials are available (<u>Rockware 2015b</u>). Classroom workshops are offered several times per year and periodic webinars are scheduled.

Custom training, both web-based and in person, is available by contacting training@rockware.com.

SADA

▼Read more

Spatial Analysis and Decision Assistance (SADA) was developed by The Institute for Environmental Modeling at the University of Tennessee, Knoxville. SADA is designed for environmental site assessments and to support decision making. SADA software is used to characterize contaminated sites, including developing sampling designs, assessing risk, supporting remedial design, and performing cost/benefit analysis. SADA also can be used with the USEPA Triad field investigation method.

SADA contains integrated modules for visualization, geospatial analysis, statistical analysis, human health risk assessment, ecological risk assessment, cost/benefit analysis, sampling design, and decision analysis. The modules can be used independently or collectively.

SADA offers several tools to perform geospatial analysis that include 2D and 3D methods. The geospatial tools can model spatial correlation among data and produce maps for concentration, risk, probability, variance, and cleanup and also integrate geospatial models directly into decision frameworks such as spatial sampling and human/ecological risk. Geospatial analysis options include:

- ordinary kriging
- indicator kriging
- co-kriging
- inverse distance
- natural neighbor
- nearest neighbor
- Gaussian simulation
- indicator simulation
- import custom geospatial tool

SADA does not include functions and trend analyses to evaluate sufficiency of well networks or costs for monitoring optimization.

For more detailed information about the software program and methodology, see <u>Tables 7, 8, and 9</u>.

Source: University of Tennessee (University of Tennessee 2013a). A new version V.6 is expected to be released in 2016.

Ease of Use: Moderate

References: The University of Tennessee maintains a list of published references on SADA software (<u>University of Tennessee 2013b</u>).

Training and Resources: The user guide is extensive (<u>University of Tennessee 2013c</u>). Technical support is provided through a <u>Yahoo SADA user group</u> (<u>Tennessee 2016</u>). For archived past training on capabilities of SADA, see the USEPA Cluin website (<u>USEPA 2006c</u>). New training will be available through University of Tennessee after release of V.6.

SAS

TRead more

SAS is a suite of software for advanced analytics, data management, data visualization, and business intelligence. It is used in various fields including financial services, medicine, insurance, retail, manufacturing, and oil and gas. Although not designed specifically for environmental applications, SAS has a comprehensive range of statistical analyses that may be applicable. Statistical analyses include statistical intervals, hypothesis testing, nonlinear regression, correlation, outlier tests, spatial weighting, trend analysis, variograms, kriging, and a variety of graphical methods including contour plots, as well as time series analysis, forecasting, optimization, simulation, and process control. While these procedures are not necessarily available in a drop-down menu or as a specific pre-coded application, all of them can be coded into a SAS program by a proficient user. User-coded methods including nonparametric or nonnormal procedures, as well as those noted above, are available in additional purchased software. Free-form code can also be written to call statistical procedures and within one program regroup and revise data, perform multilayered analyses, output new data sets, and provide presentation-grade

graphical analyses.

The entry level offering, SAS Analytics Pro which includes Base SAS, SAS/STAT, and SAS/GRAPH, contains many general statistical procedures, as well as data handling, data manipulation, and graphics capabilities. It is useful for most standard groundwater monitoring applications. More complex matrix-based procedures are provided with SAS/IML, process control applications (such as Shewhart-Cusum charts) are specifically addressed in SAS/QC, optimization and simulation are provided in SAS/OR, and time series analysis in SAS/ETS. All of these are purchased separately.

SAS does not include functions to evaluate sufficiency of well networks or costs for monitoring optimization, although such functions can be created by the user in SAS code.

For more detailed information about the software program and methodology, see <u>Tables 7, 8, and 9</u>.

Source: SAS Institute (SAS Institute 2015a)

Ease of Use: Complex

Training and Resources: At-cost multiday training courses in a classroom or online venues are available (<u>SAS Institute 2015</u>). Books on SAS (<u>SAS Institute 2015</u>) and blog and other online chat support (<u>SAS Institute 2013</u>) are also available.

SGeMS

TRead more

The Stanford Geostatistical Modeling Software (SGeMS) is an open-source geostatistics software that was developed at Stanford University and is used in mining, petroleum engineering, and environmental fields. SGeMS offers a wide variety of geospatial estimation techniques including ordinary kriging, simple kriging, kriging with trend, indicator kriging, and co-kriging, as well as simulation techniques such as sequential Gaussian simulation. In addition, SGems is the only geostatistical package that contains a multiple-point simulation algorithm (snesim). This package also contains various preprocessing and postprocessing algorithms that operate on the results or data. SGeMS can model in both 2D and 3D based on uniform rectilinear grids as well as masked grids. The Python scripting language is embedded in SGeMS, which offers flexibility in automating complex tasks involving geospatial methods and data pre- and postprocessing.

SGeMS visualization output used outside of SGeMS is limited to screen shots. Input data must be supplied in a text file in the GSLIB format. SGeMS projects are saved in a binary file format that can only be opened in SGeMS.

SGeMS does not include functions to evaluate sufficiency of well networks or costs for monitoring optimization.

For more detailed information about the software program and methodology, see Tables 7, 8, and 9.

Source: SGeMS website (Stanford University 2015d)

Ease of Use: Complex

References: Remy, Boucher, and Wu 2009

Training and Resources: No technical support is offered. Information about training and support resources is available (<u>Stanford University 2015a</u>). A user forum (<u>Stanford University 2015b</u>) and user guide (<u>Stanford University 2015c</u>) are available.

Summit Envirosolutions

▼Read more

The Summit Envirosolutions Sample Optimizer/Sample Tracker software consists of two major modules: Sample Optimizer and Sample Tracker. An additional component of the Summit software is Model Builder, which is embedded in both Sample Optimizer and Sample Tracker.

Sample Optimizer identifies redundant sampling locations (spatial optimization) or redundant locations and frequencies (spatiotemporal optimization) in historical data. This module identifies redundancies using a multiobjective genetic algorithm to obtain monitoring designs that represent optimal tradeoffs among two or more monitoring objectives, such as minimizing the number of samples and minimizing the interpolation error at locations that are removed. The error generally increases as number of wells decreases, resulting in a tradeoff.

Sample Tracker allows current monitoring data to be reviewed against selected historical data (which is called the background data) to identify cases in which current data deviate from expectations that are based on the background data values and patterns.

Model Builder is an additional component within the software that is used by Sample Optimizer and, in some cases, by Sample Tracker. Model Builder has two sections: one for model fitting, visualization, and analysis (with kriging or inverse distance weighting) and another for visualizing relative uncertainty.

During initial optimization and periodic review, Model Builder constructs spatial or spatiotemporal models for the measurements of the primary contaminants. The model identified by Model Builder is then used by Sample Optimizer to identify optimal sampling plans for subsequent routine monitoring, with redundancies eliminated.

For more detailed information about the software program and methodology, see Tables 7, 8, and 9.

Case Study: using Summit Environmental Solutions software includes a former ordnance plant.

Source: Summit Inc. (<u>Summit Envirosolutions 2013</u>).

Ease of Use: Moderate

References: Harre et al. 2009

Training and Resources: A user manual is available on the Summit Envirosolutions website. Training is available for a fee. (Summit Envirosolutions 2013). See the Summit Envirosolutions website.

Surfer

TRead more

Surfer is a 2D contouring, gridding, and mapping software developed by Golden Software and first released in 1985. While not tailored specifically to remediation projects, Surfer's capabilities find many applications in environmental projects, primarily to generate and visualize contours and surfaces. Surfer can read input data from a variety of ASCII text file formats and can export surfaces and contours in formats compatible with ArcGIS and AutoCAD. Surfer is limited to 2D interpolation; it can interpolate surfaces but not solid volumes. Repetitive tasks can be automated with the Scripter program packaged with Surfer.

Surfer supports ordinary kriging and universal kriging in addition to several other interpolation methods including natural neighbor, inverse distance weighting and polynomial regression. A default linear variogram is used for kriging unless the user specifies otherwise. It is simple to generate contours and surfaces with Surfer; however, it is also quite simple for inexperienced users to generate erroneous results if the program's default settings are not appropriate. The Surfer interface is user friendly and the help topics are comprehensive.

Surfer can provide limited analysis of well networks using cross-validation but does not fully evaluate sufficiency of monitoring well networks or costs of monitoring optimization.

For more detailed information about the software program and methodology, see Tables 7, 8, and 9.

Source: Golden Software (Golden Software 2013) and also available from third-party vendors.

Ease of Use: Easy

Training and Resources: A variety of free support services are available (<u>Golden Software 2015</u>) including blogs, webinars, forums, and newsletters.

Voxler

▼Read more

Voxler 3D Data Visualization was developed by Golden Software LLC. to characterize subsurface geologic and groundwater conditions. The software creates a wide variety of 3D visualizations including: volumes, scatterplots, heightfields (such as elevation models), vectors, and wells. The software can also import data already gridded by Surfer, another Golden Software product. The Voxler software is stand-alone software that runs on the Windows operating system.

The primary modules of the software are: Data Sources, Computational, and Graphics Output. Data Sources can be imported from a variety of sources including text files, spreadsheets and Surfer grid files, or the data to be modeled can be created using mathematical functions. Computational modules process the data. Available processes include filtering, creating gradients, gridding, performing mathematical transformations, merging, resampling, slicing, and creating a subset or transforming coordinates.

Graphics Output Modules create the visualizations. There are several visualizations that are particularly relevant to remediation. Well boreholes can be depicted including paths of nonvertical and curving boreholes. The color and size of paths can be varied depending on input variable (for instance, lithology or chemical concentration). Subsurface volumes can be modeled to depict plume extent. Any volume modeled can be viewed and sliced from any direction and angle. Graphic Outputs can be combined from multiple data sets of different types to create complex visualizations. For instance, outputs from different types of data sets such as well data, groundwater elevations and chemical concentrations can be combined to show well paths and plume volumes with the water table and then viewed from any angle. Control over the graphic display is extensive, so most aspects of the visualization can be customized to suit the needs of the user. Visualizations can be

captured through still pictures or video.

The mathematics of the computational models is documented in the user manual. Methods available for interpolation are inverse distance, local polynomial, and data metric.

Voxler does not include functions to evaluate sufficiency of well networks or costs for monitoring optimization.

For more detailed information about the software program and methodology, see Tables 7, 8, and 9.

Source: Golden Software (Golden Software 2016)

Ease of Use: Easy

Training and Resources: With purchase of the Voxler software, Golden offers free technical support (<u>Golden Software</u> <u>2015</u>) in the form of direct assistance, online videos and tutorials, and discussion forums. A user manual comes with the software.

VSP

TRead more

VSP (Visual Sampling Plan) was developed by the Department of Energy's Pacific Northwest National Laboratory in Richland, Washington. The software tool determines the right number and location of environmental samples or transects based upon statistical sampling theory so that the results of statistical tests performed on the data collected by the sampling plan have the required confidence for decision making. VSP is unique in that the user can specify the criteria for how close the answer must be in order to determine the required sample size. The software also provides a module of geospatial analyses that is applied for radiological survey data in the mapping of anomaly density. VSP is applicable to characterization, remediation, and monitoring stages of the project life cycle.

The software uses geospatial analysis of existing data to improve estimates by adding sampling locations with the goal of reducing uncertainty. Spatial and temporal redundancy can also be analyzed with VSP based on geospatial analysis using global iterative thinning, kriging weights, and variograms. In a spatial analysis, the global kriging weight is associated with each sample and is determined by the addition of kriging weights for that data point for all locations in the kriging grid. Sample locations are ranked in terms of the contribution to the plume map through the global kriging weight, and the lowest ranked data location is removed from the data set. This process is iterative until the maximum number of samples is removed from the data set. The kriging algorithm uses a fitted model of spatial variability determined from a variogram. The newest release (2015) includes updates and enhancements to many program user functions such as toolbar displays, internal module functions, and interaction with other software.

An advantage of VSP is that it can be used to implement steps 6 and 7 of the USEPA DQO process (<u>USEPA 2006b</u>). The program uses the information provided by the user to compute the recommended minimum number of samples and sampling locations. Thus, the software provides support for USEPA's systematic planning process in the selection between clearly defined alternatives, studies in which a confidence interval or estimated parameter is needed, or determination of whether a hot spot or target exists.

VSP performs calculations for sample size and sample location and outputs a sampling design that can be displayed in multiple formats. The program also prompts for sampling costs and tests alternative designs against a fixed budget. Reports produced by VSP can be pasted directly into Microsoft Word files. For optimization, VSP allows for both spatial sample analysis and cost analysis, but it does not have a remedy component.

For more detailed information about the software program and methodology, see Tables 7, 8, and 9.

Source: Download from Pacific Northwest National Laboratory (PNNL 2011).

Ease of Use: Easy

References: Matzke et al. 2014

Training and Resources: The user guide for the most current version of VSP (and also for past versions) may be downloaded (<u>PNNL 2015c</u>). Information about free multiday training is available (<u>PNNL 2015b</u>). Custom on-site training is also available. Online help files are available (<u>PNNL 2015a</u>).

Custom Geospatial Applications

While prepackaged geospatial software applications can be convenient, many practitioners choose to program custom geospatial functions in other software applications. Geospatial algorithms can be programmed in applications or languages with existing underlying tools, graphics, and built-in math functions such as Microsoft Excel, Python, Mathematica (Wolfram), and MATLAB. Some users have incorporated programming from geospatial libraries such as GSLIB or GSTAT into custom

applications run on various platforms. Several open-source application languages (such as Python) have user communities that share geospatial code, which can form the basis of custom software applications.

The benefits of custom-programmed software include design for specific input file formats or data sets, and the programmer can include algorithms specific to the goals and scale of the analysis or the setting of the site. Output can be specified to coordinate with other software programs for visualization or further interpretation. The disadvantage of custom-designed software, aside from the cost of code development and maintenance, is that the results can be difficult to review for quality control.

Excel is a spreadsheet application commonly packaged with Microsoft Office. Excel was designed, primarily as a business spreadsheet program; however, several mathematical and visualization tools have been added over the years. Custom macros can be programmed in the Visual Basic for Applications (VBA) language. Various third-party applications that use Excel as a platform, such as the USEPA's 3PE flow directions tool, are also available. MS Access is the database application in MS Office, and can also support programming of geospatial algorithms in VBA. The benefit of MS applications is that, while not free, they are widely distributed, installed on most computers, and do not present an extra cost for most users. The disadvantage of programming in Excel is that MS software upgrades can alter how macros function, causing compatibility issues between versions.

Python is a scripting language designed to be highly readable and easy to use. Python implementations can be downloaded for free as open-source software, which can run in a variety of Windows, Macintosh, or Linux environments. Algorithms written in Python can be packaged as stand-alone applications that do not require Python to be installed locally. Python is often used in conjunction with ESRI ArcGIS software for custom analysis and visualizations. Python has an active user group developing geospatial tools and several resources are available to support custom geospatial applications.

MATLAB (Matrix Laboratory) is proprietary, commercial software developed by MathWorks as a numerical computing environment and programming language. As such, MATLAB requires a user license, and applications cannot be created to operate independently outside of the licensed domain. MATLAB is commonly used in academic settings and math and engineering students are often trained in its application. MATLAB does require a moderate to advanced level of training and an understanding of the underlying mathematics to operate. Geostatistical toolboxes such as mGstat have been developed by user communities for MATLAB and are downloadable from the web. Matlab can interact with the SGeMS.

Mathematica is a proprietary, commercial software developed by Wolfram Research based on the Wolfram programming language. The software includes many mathematical function libraries to support statistics, visualizations, computational geometry, and optimization routines. User groups have developed packages that include a number of geospatial operations. Mathematica requires a moderate to advanced level of training to operate.

Geostatistical Libraries are collections of scripts or codes that perform specific statistical or geostatistical functions and are used as add-ons to established geostatistical software, or can be used to develop custom-programmed software with programming platforms such as the four programs discussed above. Some examples of geostatistical libraries include GSLIB/WinGslib, GSTAT, GsTL, and HPGL Python Library. GSLIB consists of a group of 40 scripts that are run on the command line or through WinGslib. WinGslib serves as a graphic user interface and postscript viewer for GSLIB. GSLIB performs the kriging routines for the software Leapfrog Hydro, GMS, and T-PROGS and is compatible for output with other software such as GS+ and Isatis. GSTAT was developed in the late 1990s as C language source code for developing programs to carry out geostatistical computations but was eclipsed for further development with release of R software in 2003.

GSTAT performs variogram modeling using simple kriging, ordinary kriging, sequential Gaussian or indicator simulation, and has map plotting capability. GsTL is a generic programming library in C++ language with algorithms for kriging (simple, ordinary, and kriging with trend), and sequential simulation (Gaussian, indicator, and multiple point). GsTL performs the geostatistical calculations for the SGeMS software. High Performance Geostatistics Library (HPGL) is in C++/Python language and contains algorithms for kriging (simple, ordinary, indicator, and co-kriging) and simulations (sequential indicator and sequential Gaussian).