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Statistical Methods for Subsurface Surveys to Support Decommissioning

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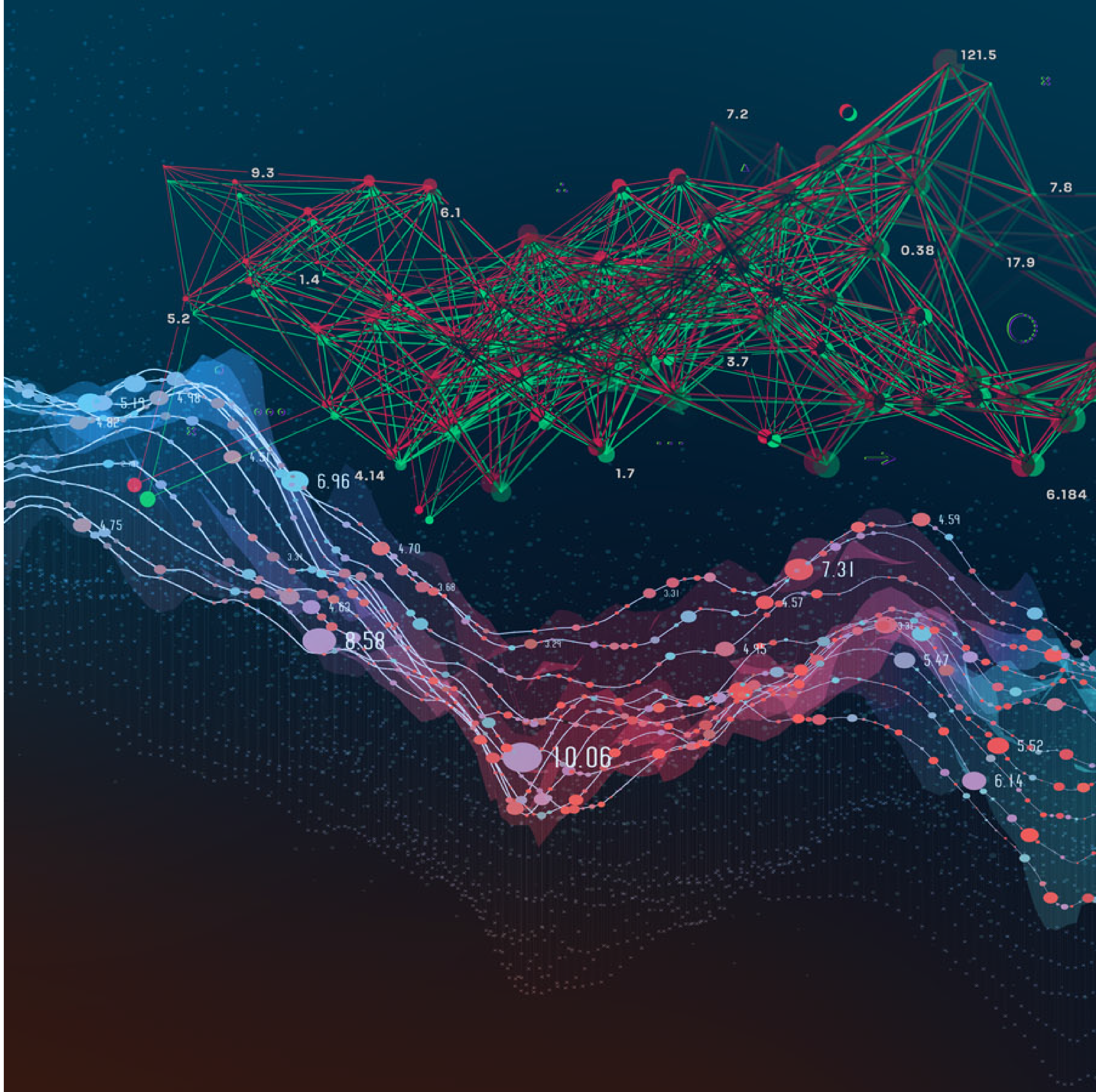


Topics

- Scope & assumptions
- Subsurface data
- Survey planning & analysis
- Discussion

SCOPE & ASSUMPTIONS

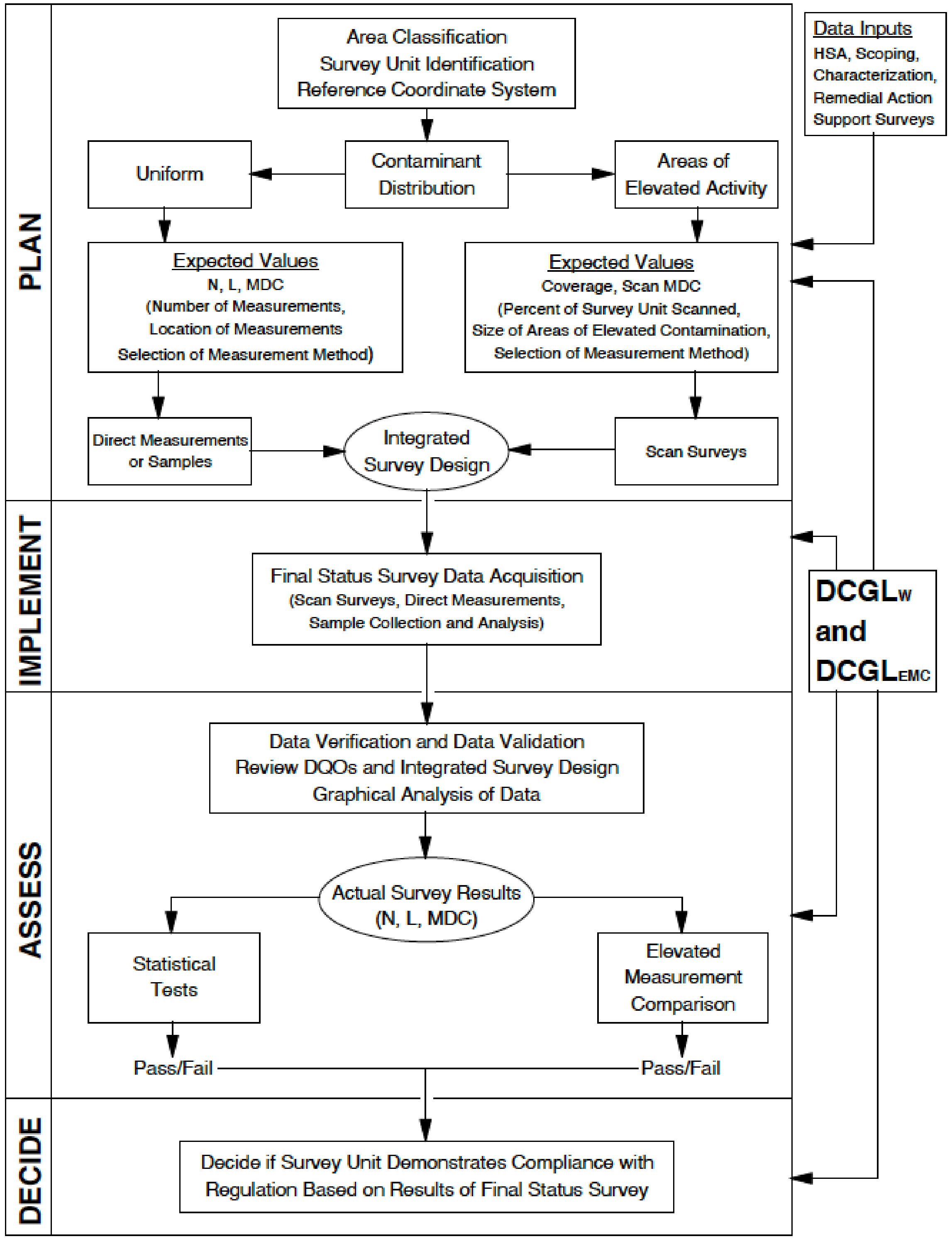
MARSSIM Roadmap for the Surface

PLANNING
Data Quality Objectives Process
Quality Assurance Project Plan Development

IMPLEMENTATION
Field Data Collection and Associated
Quality Assurance/Quality Control Activities

ASSESSMENT
Data Validation/Verification
Data Quality Assessment

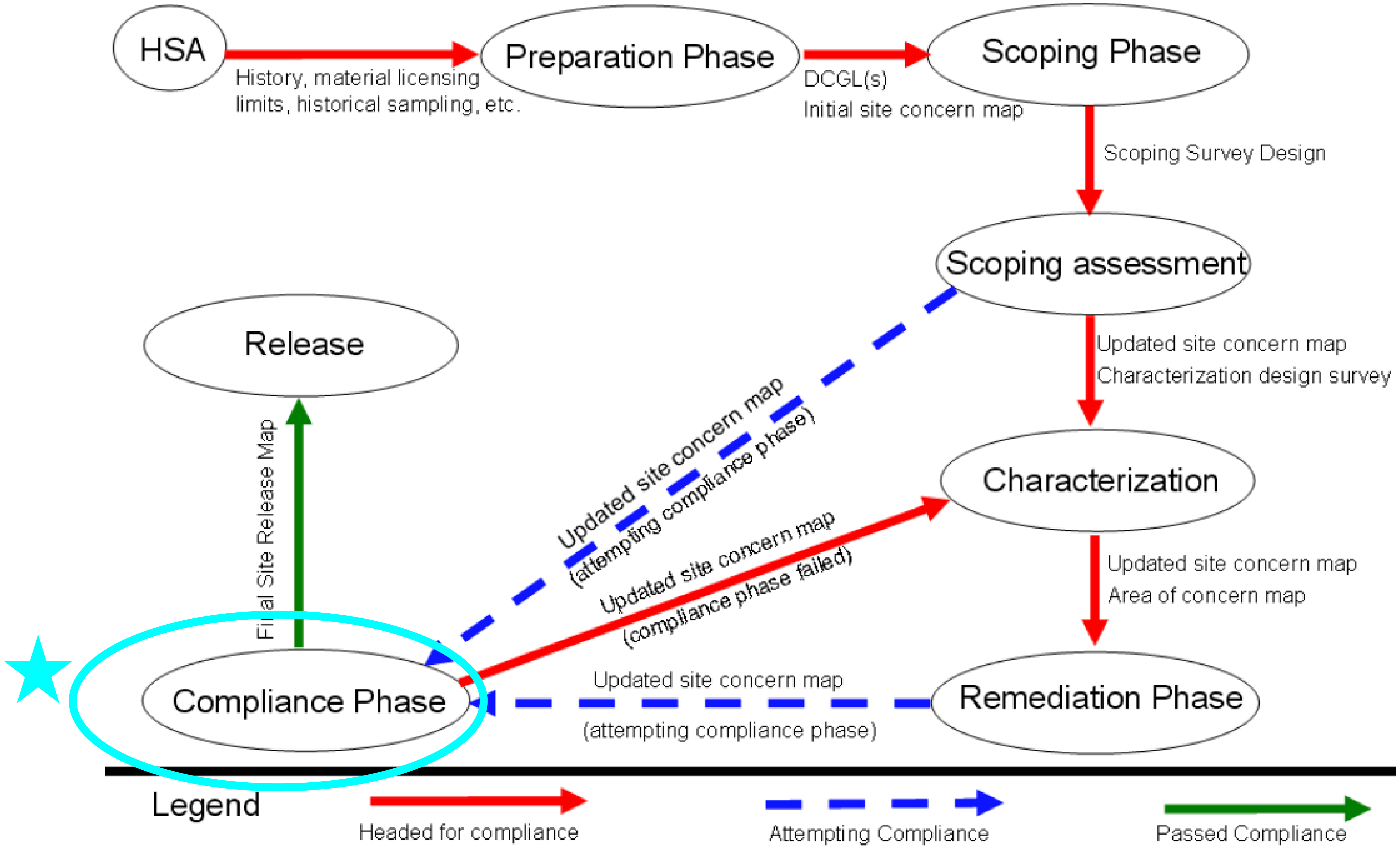
Data Life Cycle



NUREG-1575, Rev 1

MARSSIM provides detailed guidance for planning, implementing, and evaluating environmental and facility radiological surveys conducted to demonstrate compliance with a dose- or risk-based regulation.

Subsurface Flow Diagram



NUREG-7021

Preparation through Remediation Phases

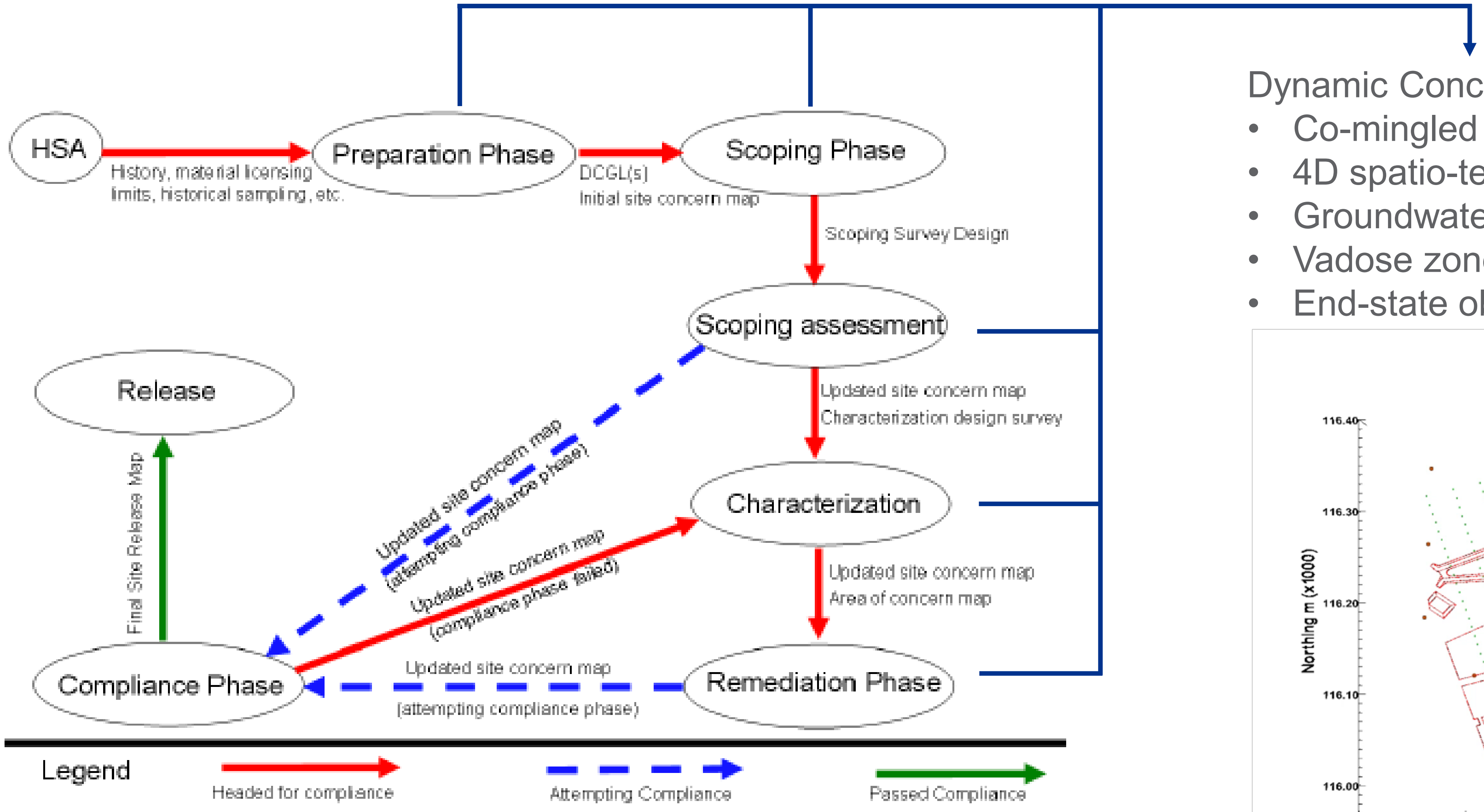
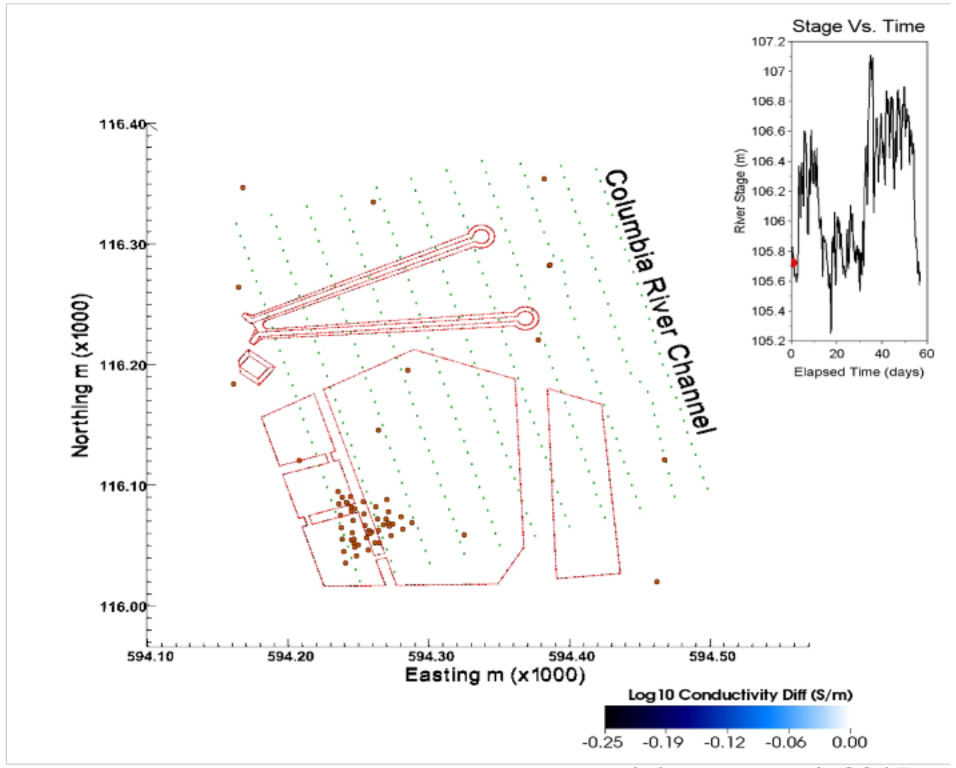


Figure 3.3 from NUREG/CR-7021

Dynamic Conceptual Site Model

- Co-mingled COPCs
- 4D spatio-temporal dynamics
- Groundwater/surface water interactions
- Vadose zone/groundwater interactions
- End-state objective



Johnson, et al, 2015

Compliance Phase

Information needed to show end-state is achieved

- Surface & subsurface matrix samples showing
- Fate & transport of COPCs on-/off-site are understood
- COPC spatio-temporal concentrations meet release criteria

Assumptions

- Data from HSA, preparation, and scoping phases will be available
- Data from characterization and remediation phases may be available
- Variation in how much/what type

What tools are needed in the compliance phase?

- Visualization
- Data collection planning
- Data analysis
- Uncertainty quantification/confidence bounds and hypothesis testing for end-state decisions

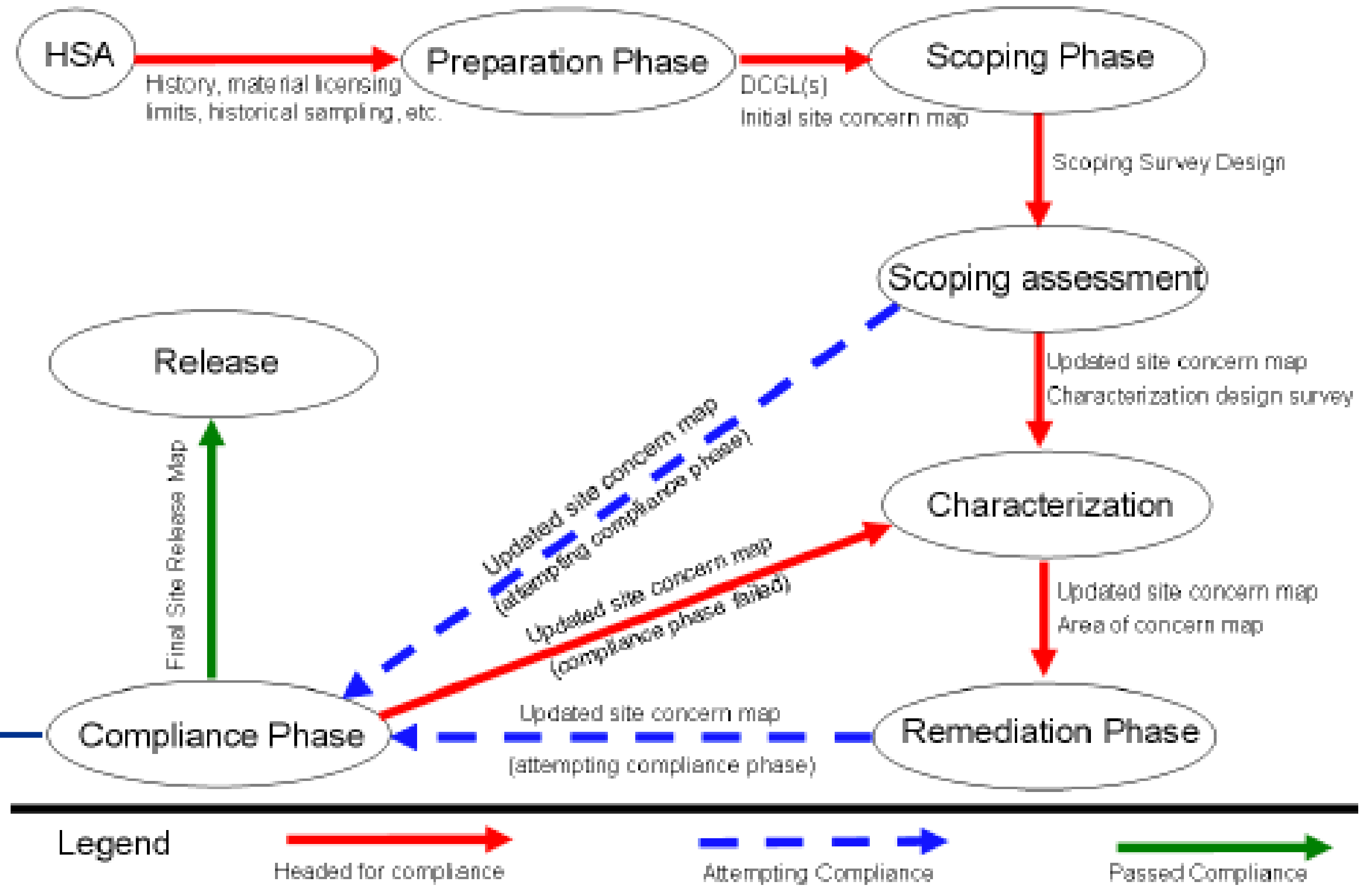


Figure 3.3 from NUREG/CR-7021

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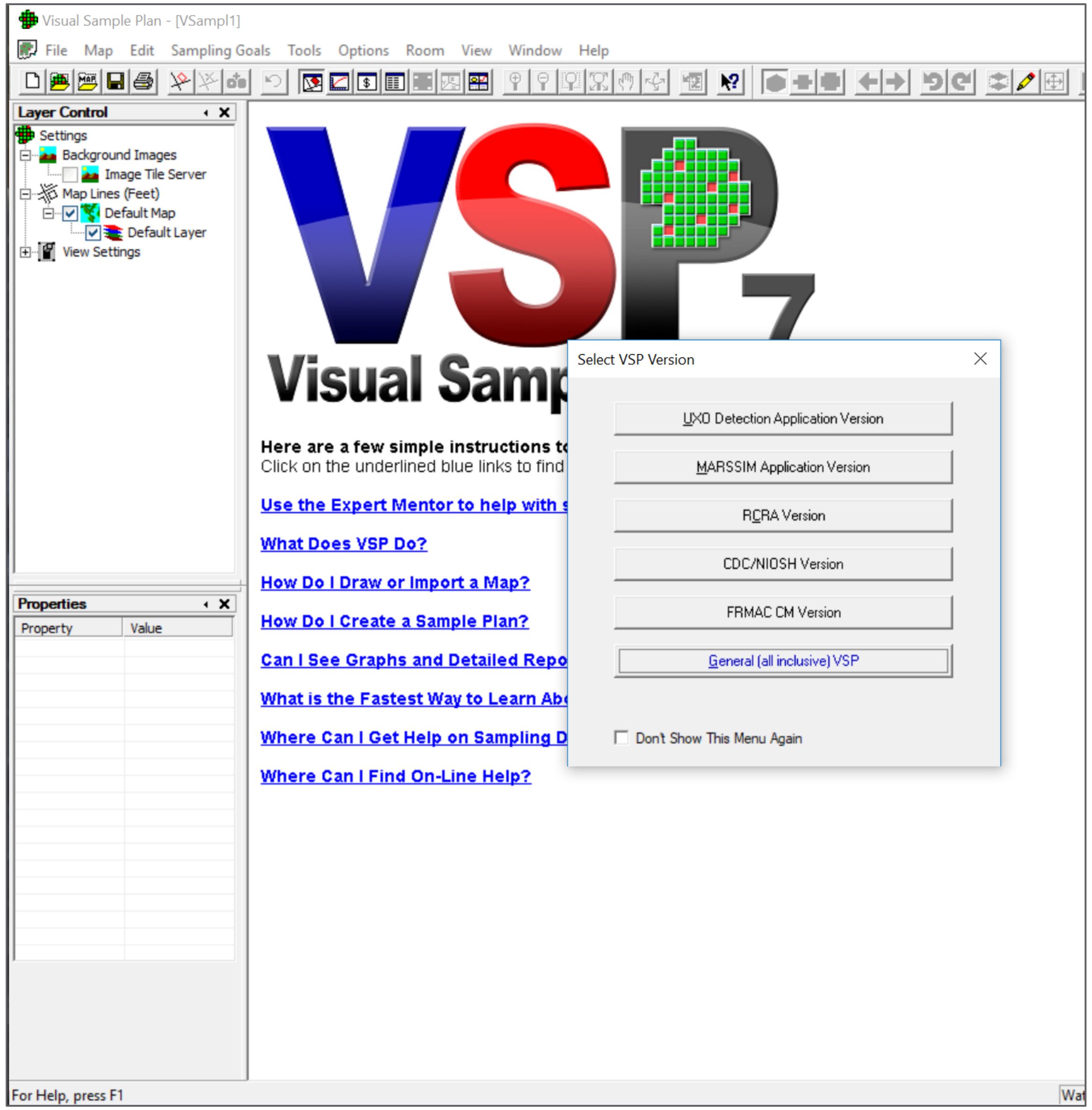
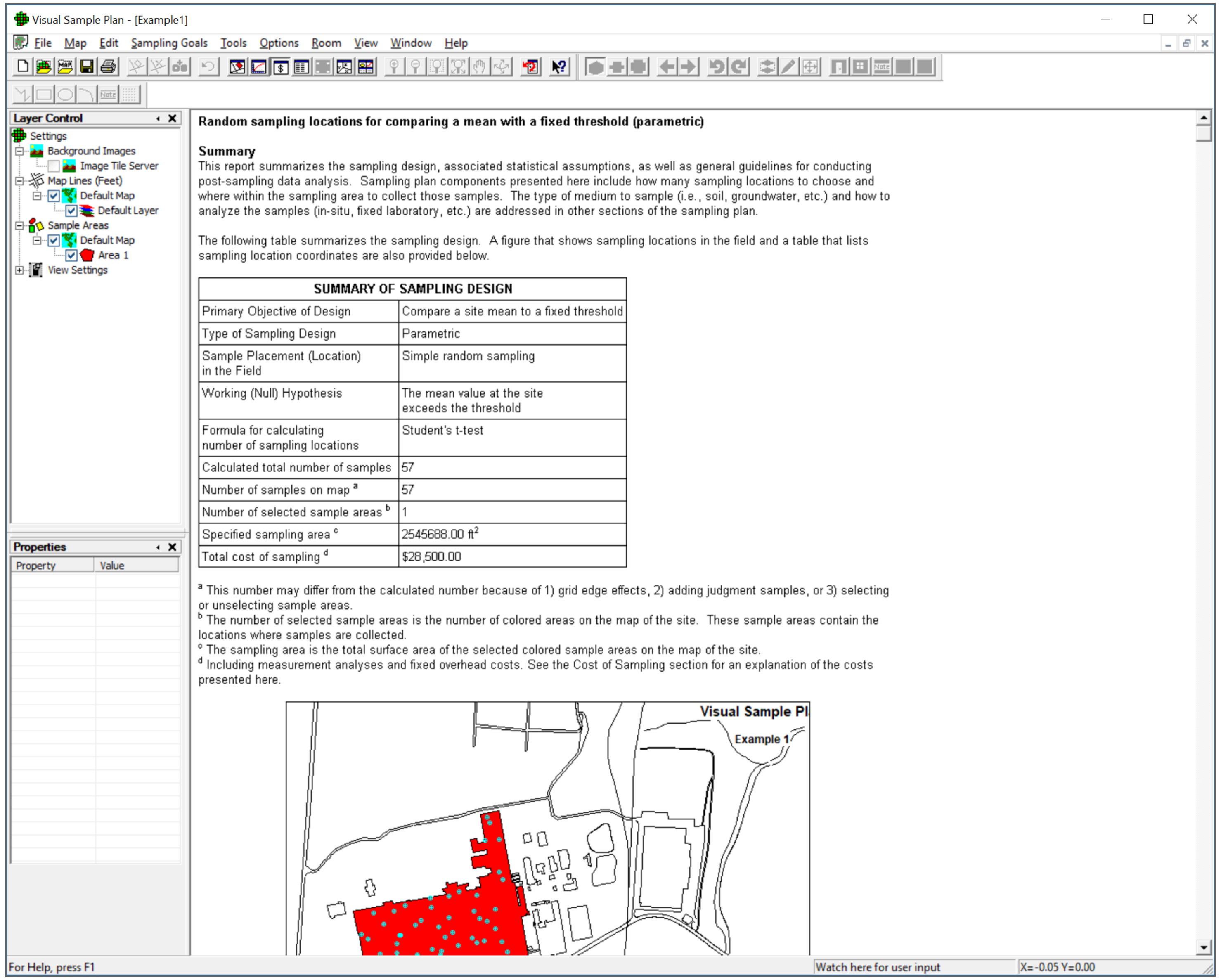
Visual Sample Plan (VSP)

VSP available on
NRC RAMP website (link)
& PNNL website (link)





SUBSURFACE DATA

Data Available for Compliance Survey Planning

Data source	Data set description(s)
Previous to RSSI	Engineering drawings (facilities, structures, etc.), operations logs, GIS maps, background geophysical data (surface/subsurface), water resource characterization and climate data for Conceptual Site Model (CSM) development
HSA	Risk assessment, hazard assessment, RCRA/CERCLA documentation (including soil/rock core sample data as appropriate), NEPA documentation (as appropriate), Source term quantification modeling/estimates for relevant sites, Contaminant fate and transport modeling
Scoping	RI/FS or FI/CM reports, updated CSMs, specification of sampling types/design/media/location, proposed statistical methods, identification and characterization of potential contaminant plumes
Characterization	Geologic maps, soil maps, drillers logs, maps of site infrastructure, collection of groundwater levels, hydraulic tests, soil or rock cores, and development of a GIS, visualizations, and maps for the site, Surveillance monitoring data from previous remediation activities (if applicable), geophysical and hydrogeological modeling results,
Remediation	Characterization of plume structure and composition, conceptual site model, possibly computer models of flow and transport for the site, feasibility studies or prior relevant work demonstrating the feasibility of amendments, ongoing monitoring data to assess performance of the remedy, including routine sampling of contaminant concentration and signatures of the remedy and its effects.
Geophysical data	Borehole, cross-hole, surface, or remote sensing collection of data through electrical techniques (e.g., electrical resistivity tomography, induced polarization), electromagnetic methods (e.g., frequency and time domain electromagnetic induction, magnetotellurics, ground penetrating radar), seismic methods (e.g., reflection seismology, seismic refraction, seismic tomography), gravity techniques (e.g., gravimetry and gravity gradiometry), magnetic techniques (e.g., magnetometers), thermal methods (e.g., infrared, fiber-optic distributed temperature sensing) or multi-spectral/hyperspectral methods.
Groundwater model	Deterministic or stochastic subsurface numerical models of flow and transport in the vadose zone, saturated zone, or a combination, including input files, model calibration results, and predictive results. Geo-framework model describing the hydrogeology and forming the basis for a Conceptual Site Model.
Authorized limit data	Authorized limit(s) based on DOE Order 458.1 (DOE 2011, 2017) or data required to translate regulatory limits to authorized limit(s), including hydrologic parameters (i.e. soil density, precipitation, irrigation) human health based from pre-described risk approach, and other default params in the RESRAD computer code.

Data Quality Assurance (DQA)

- Combining 3D spatial/4D spatiotemporal data from disparate sources & of varying formats, quality, and resolutions expected to be a major undertaking and formidable challenge
- However, much will have been performed prior to compliance survey
- Therefore, a major component of data wrangling required for the compliance phase will include data quality assurance (DQA)

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Discussion Topics

- What DQA activities must be performed on each data set?
  - Determining representativeness of timeframe over which data were collected
  - Identifying seasonal effects
  - Validation of fate & transport models
- Expect to use convenience sampling (e.g. existing boreholes). What methods will be required to determine/verify existing boreholes, say, provide representative data for the larger subsurface volume?
- What will resulting compliance survey data sets look like at the outset of compliance survey process?

SUBSURFACE SURVEY PLANNING & ANALYSIS

Compliance Survey Planning Approaches

- Historical locations should be leveraged into compliance survey design
  - Convenience, judgmental, geophysical model-based locations
  - Additional locations based on classical or geostatistical models
- Classical approaches (parametric or non-parametric)
  - Stratified random/systematic: use conceptual site model to allocate samples across strata
    - ✓ Sampling unit representativeness based on risk or geophysical modeling
    - ✓ Strata definitions:
      - Vertical for geophysical layers
      - Horizontal (vertical) based on risk model
  - Check & cover: convenience + random
    - ✓ Specify the number of convenience locations, VSP provides random locations

Compliance Survey Planning Approaches

- Geostatistical approaches
  - Determine mathematically where to locate samples based on geostatistical uncertainty
  - Geophysics input through
    - ✓ Bayesian methods
    - ✓ geospatial methods that combine data with different fields of view or uncertainties
    - ✓ Identification of strata, sample allocation across strata

Compliance Survey Planning Approaches

- Ellipgrid and Bayesian ellipgrid (characterization surveys)
  - Must specify size and shape of elevated area
  - Elevated zone assumed to exist *with some probability* (specified by user)
  - Applicability depends on availability and type of data collected in prior phases
  - Pros: reduced number of samples to achieve same false-negative rate
  - Cons: how to check reliability of prior?
- Markov Bayes and Bayesian Ellipgrid (characterization surveys)
  - Model for the compliance survey, given data on belief of exceeding threshold and Bayesian ellipgrid
  - Estimates variogram between "hard data“ (measurements) and "soft data” (prior belief) captures correlation between prior beliefs and measurements
  - Co-krige to predict hard data at unobserved locations
  - Pros: combines hard and soft data into updated estimate of the probability of exceeding a threshold
  - Cons: no uncertainty estimate associated with the posterior probability (How confident should we be in the "posterior" estimate?)

Compliance Survey Planning (cont.)

- Ranked set sampling (characterization surveys)
  - Fast/cheap coarse measurements to obtain (approximate) stratification of population
  - MARSSIM Rev 2 Appendix E: *augment* final status surveys involving HTD radionuclides
  - Pros: more statistical power and increased probability of detecting elevated areas
  - Cons: measurement may not sufficiently rank (stratify) the population, restrictions on sample size (multiples of 3,4, or 5) extending to subsurface

Statistical Analysis Approaches

- Approaches
  - 3D estimation and hypothesis testing to compare estimates to a threshold
  - Geostatistical methods/kriging/prediction to determine boundaries of potential residual contamination
- Dimensionality of approach
  - Layered: apply methods to individual 2D layers of the 3D volume
  - Volume: apply methods to 3D volume

Statistical Analysis Approaches

- 3D estimation and hypothesis testing to compare estimates to a threshold
  - "Classical" approaches (e.g., compare a mean to a threshold)
    - ✓ Independence assumption is violated
    - ✓ Increases Type II error if spatial correlation is not incorporated
      - Type II error = incorrectly assuming a clean site is dirty
  - Mathematically model the spatial correlation – if it is not present, outcome is "classical"
- Parametric and non-parametric methods to model spatial correlation

Statistical Analysis Approaches

- Determine boundaries of elevated residual activity
  - Moran's I
    - ✓ LISA statistic (local indicator of spatial association)
  - Kriging
    - ✓ Indicator
    - ✓ Empirical Bayes
    - ✓ FRK
  - Inverse distance weighting
- Parametric and non-parametric methods to model spatial correlation

Discussion Topics

- Methods for 3D kriging
- New statistical methods needed for
  - Improving Markov-Bayes framework to characterize uncertainty & provide confidence levels
  - Incorporating information from geophysical layer/model (e.g., transport between layers, anisotropy)
  - Ensuring computational tractability
- What about censored data in kriging? Indicator kriging?

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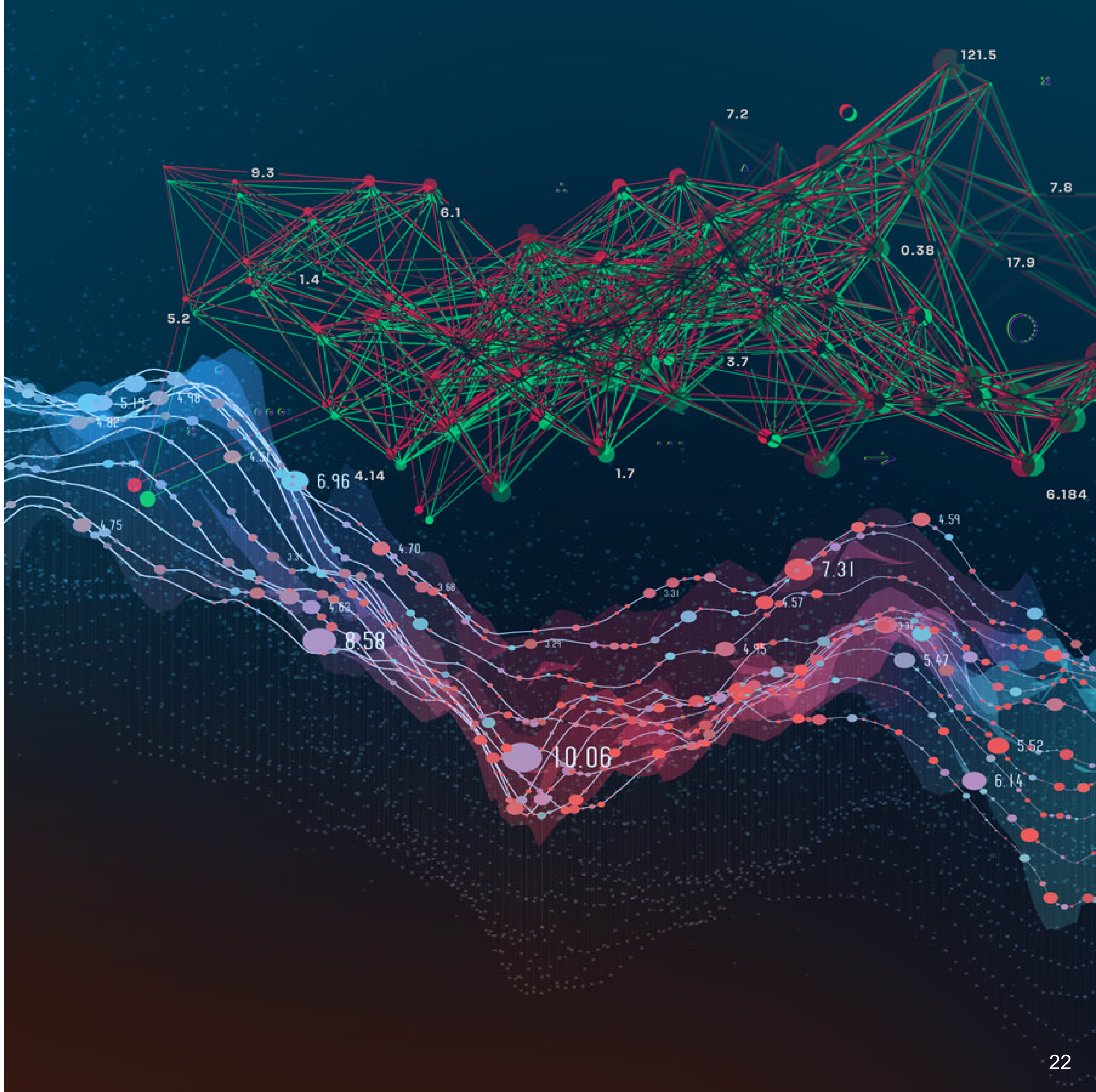
Thank you



ADDITIONAL DISCUSSION

Additional Discussion Topics

- How does the number of samples change for estimation versus prediction?
- Are there advantages or disadvantages to using a 2D layered versus 3D approach?
- How would a stratified sampling design effectively estimate a statistic to compare to a dose threshold? Can a stratified design be used with kriging?
- Using a layered approach, how should survey/sampled data be processed to perform kriging more effectively (e.g., average, maximum)?
- What are the temporal considerations for estimation and prediction?

Estimation versus Prediction

- Estimation used to compare estimate to threshold and is based on a statistic (e.g. average, percentile) calculated from observed data
  - Point estimate and confidence bounds
  - Statistical hypothesis testing
- Prediction relates to interpolation between observed data at sampled points (i.e. using kriging) and is typically used to characterize a surface or volume
  - Kriged surface or volume of measurement at and between sample locations
  - Elevated region (hot spot) detection
  - Tolerance bounds

2D Layered versus 3D Volume Approach

2D layered approach

- Pros
  - Use existing methods, software, reports for each layer
  - Familiarity → ease → efficiency & communication
- Cons
  - Requires methodology to define/identify layers
  - If interactions/correlations between layers exist, ignores those
  - Could increase total sample size

3D volume

- Pros
  - Capture interactions/correlations between layers
  - Could require fewer samples than layered approach
- Cons
  - Could require new statistical methods
  - Requires new guidance, training, vocabulary & communication