Uncertainty Analysis: Parameter Estimation

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Outline

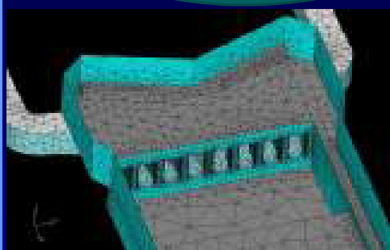
- ADH
- Optimization Techniques
- Parameter space
- Observation data
- PEST Application
- Surrogate models

Department of Defense Environmental Concerns

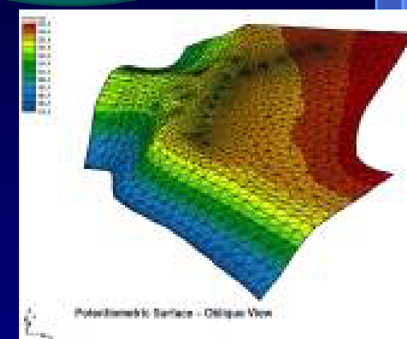
- estuaries
- coastal regions
- river basins
- reservoirs
- groundwater
- heat transport

ADH

Navier-Stokes
Equations

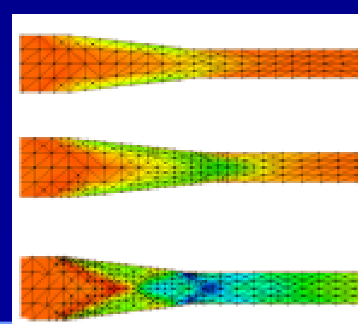


Unsaturated
Groundwater
Equations

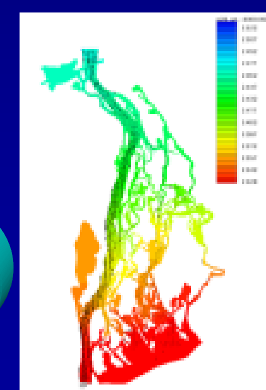


Computational Engine
*(finite element utilities,
generic PDE integration routines,
mesh adaption and coarsening,
preconditioners and solvers,
I/O to GUIs)*

**Heat Transport
Equations**



Shallow Water
Equations



Advantages

- Code Reuse
  - Takes advantage of large investment in element adaption and parallelization.
- Code Consolidation
  - Maintain a single code.
  - Advances are felt immediately across multiple hydrologic applications.
- Interchange of fluid and constituents among previously-separate hydraulic systems.

Challenges

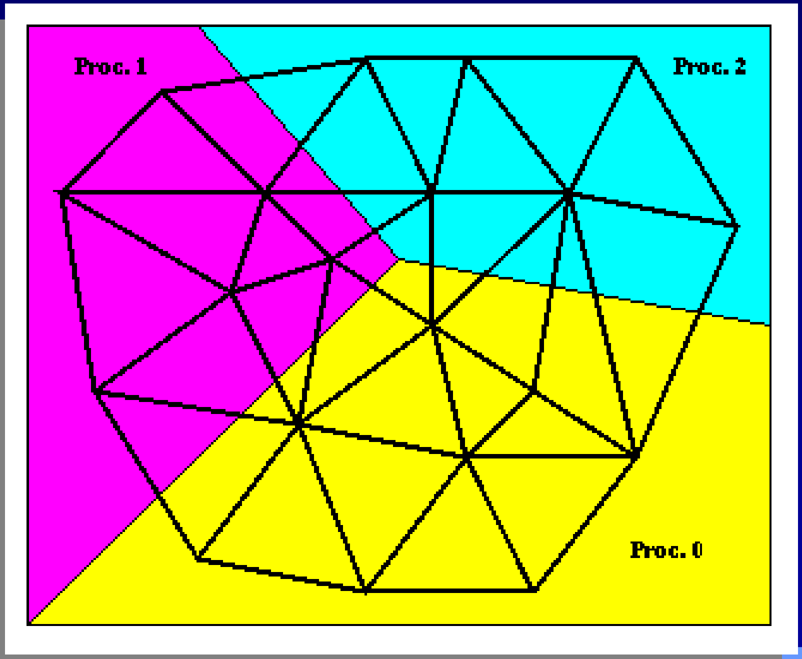
- Single solver for many types of problems
- Overhead
  - Extra baggage can make the combined simulator larger and slower than problem-specific code.
- Maintenance
  - Must retain compartmental, structured code or the model becomes unwieldy.
  - Revision control --- many cooks in the kitchen.

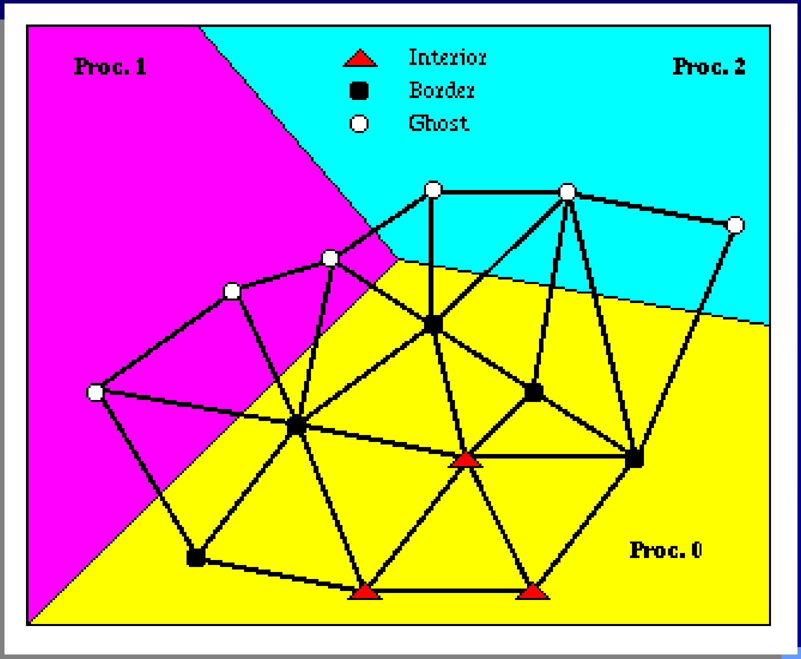
ADH Model

- Linear, simplex, continuous finite elements (tetrahedra, triangles, lines)
- Dynamic mesh adaption
- Written in C using dynamic memory allocation
- MPI message-passing model
- Bi-CGSTAB linear solver
- Variety of pre-conditioners (Jenkins)
- Inexact Newton nonlinear solver
- Dynamic load balancing
- Galerkin Least Squares-like stabilization
- CVS and SVN revision control

Parallel Finite Element Approach

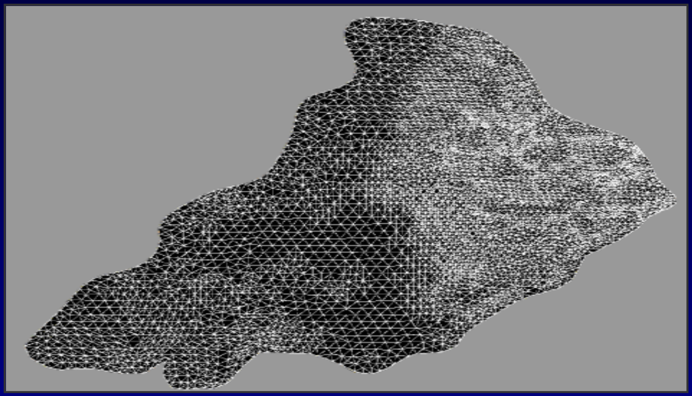
- Partition grid and distribute partitions to processors.
  - Assign nodes to processors.
  - Share elements along processor boundaries.

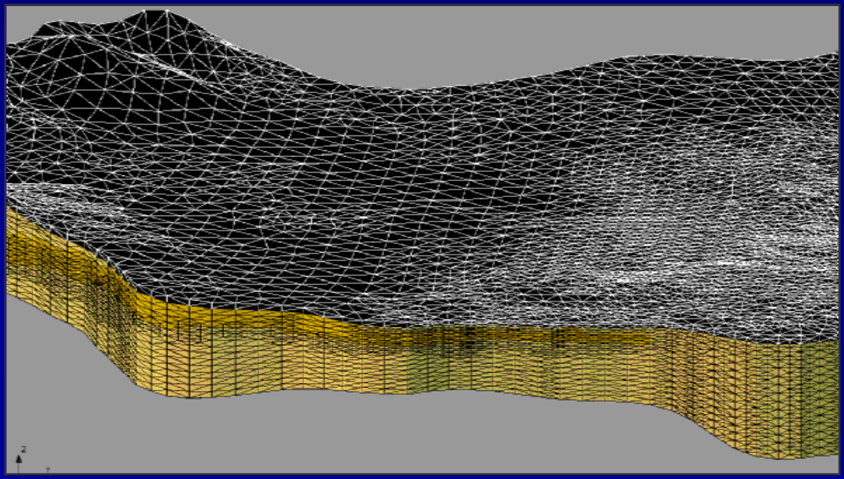




Adaption Details

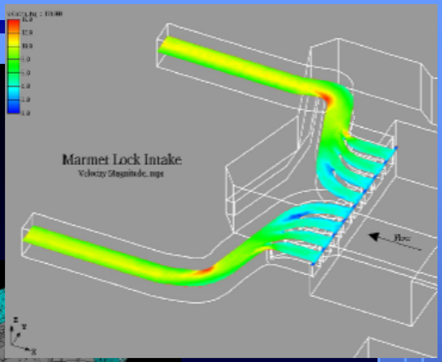
- Refinement
  - Error Indicator
  - Splitting Edges
  - Closure
- Coarsening
  - Finding duplicates

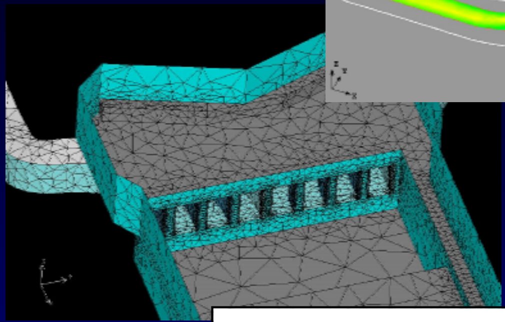


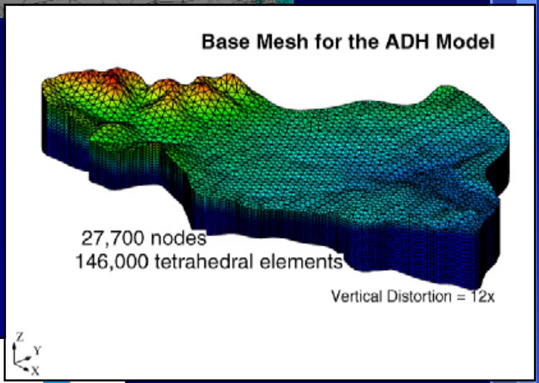


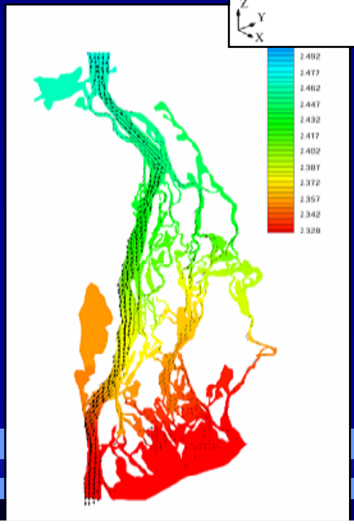
Problems Addressed

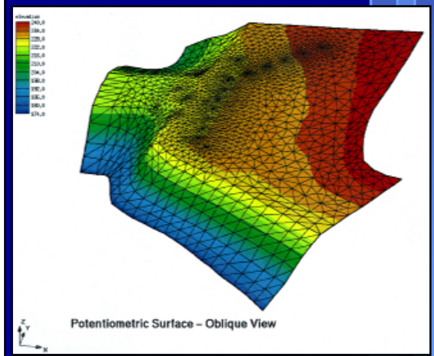
- Physical Systems
  - Partially saturated groundwater
  - Shallow water (with wave stresses)
  - Navier-Stokes (hydrostatic and non-hydrostatic)
  - Non-cohesive and cohesive sediment erosion/deposition and transport
  - Turbulence effects
  - Multi-constituent transport
  - Heat transport
- Internal coupling of groundwater and surface water simulations.



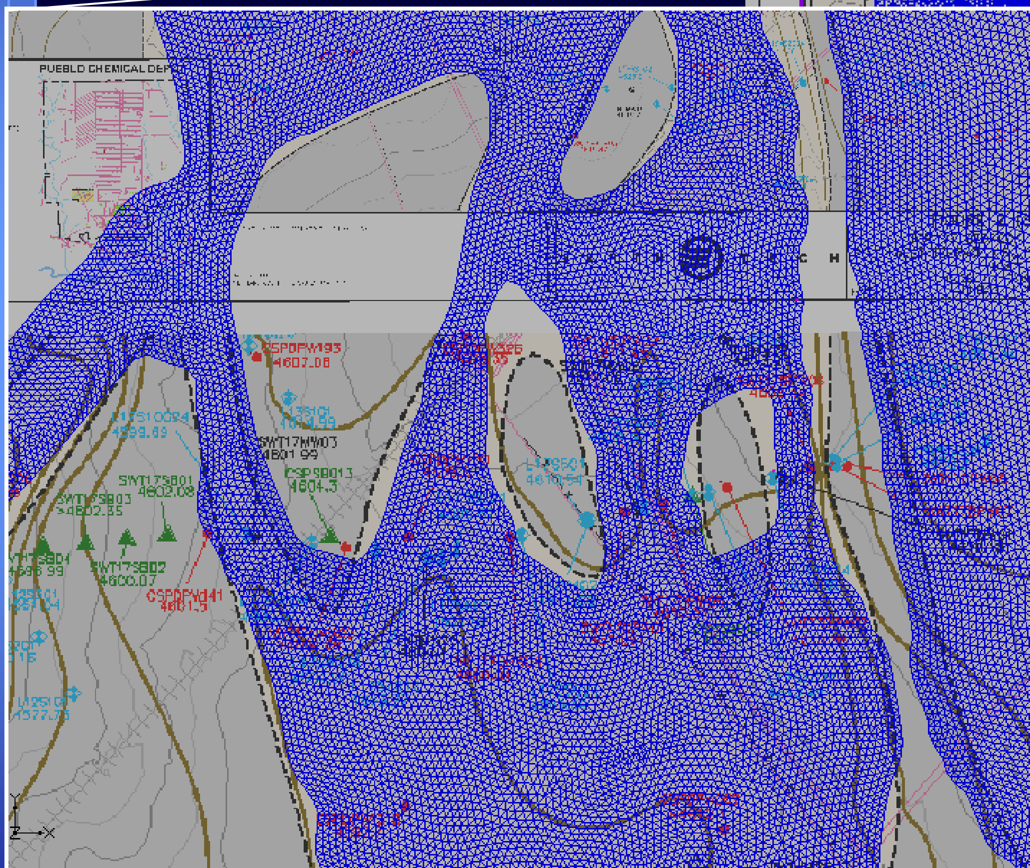


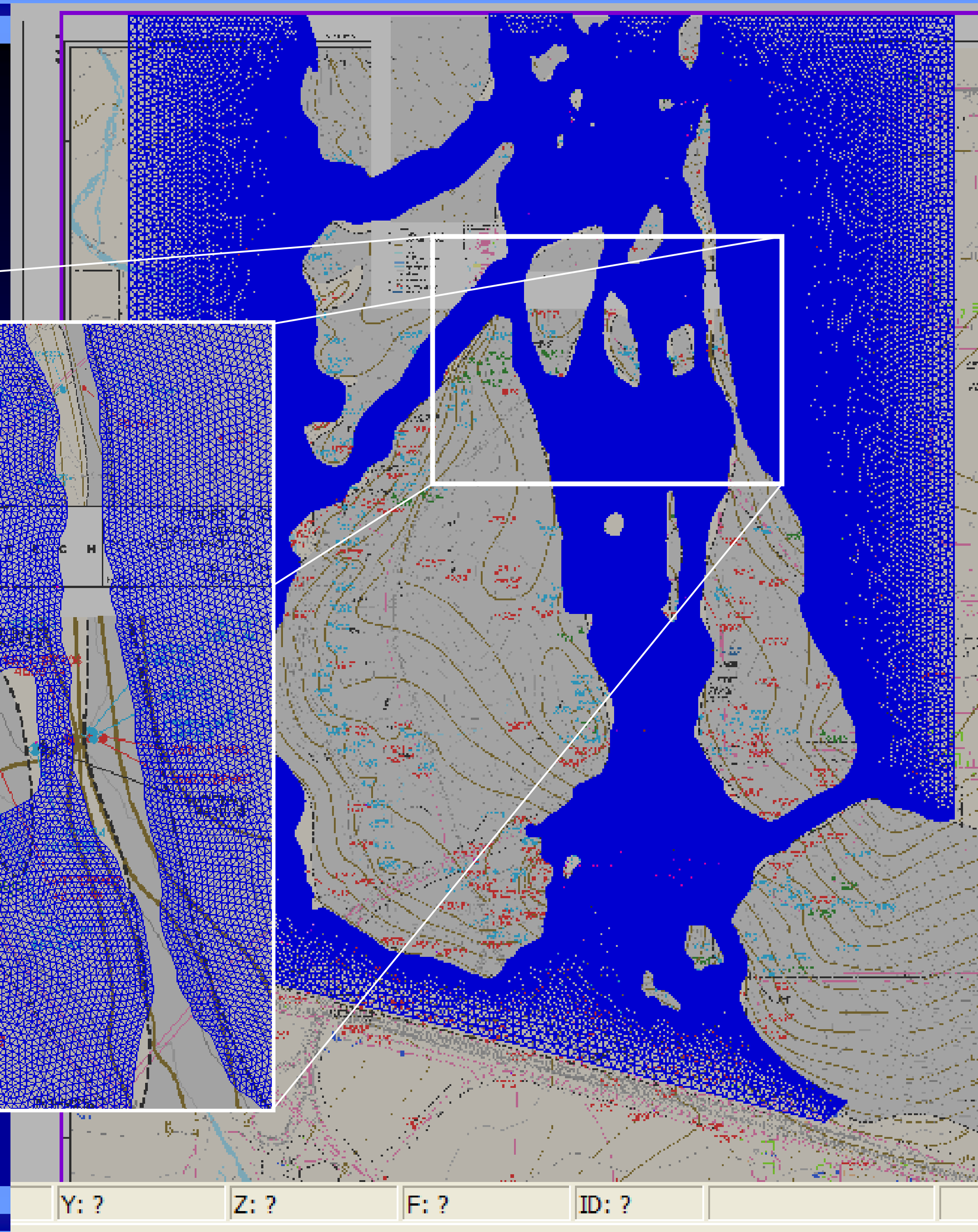






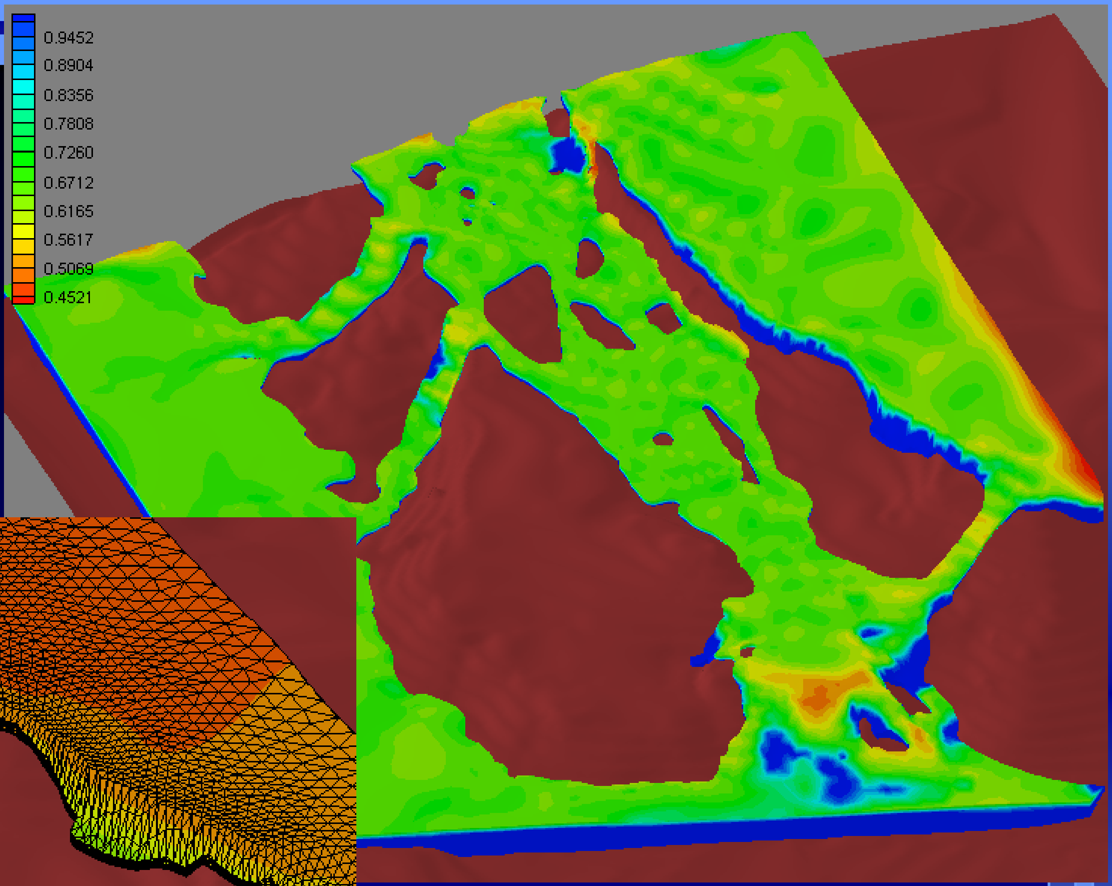
Pueblo Chemical Depot Fine Mesh

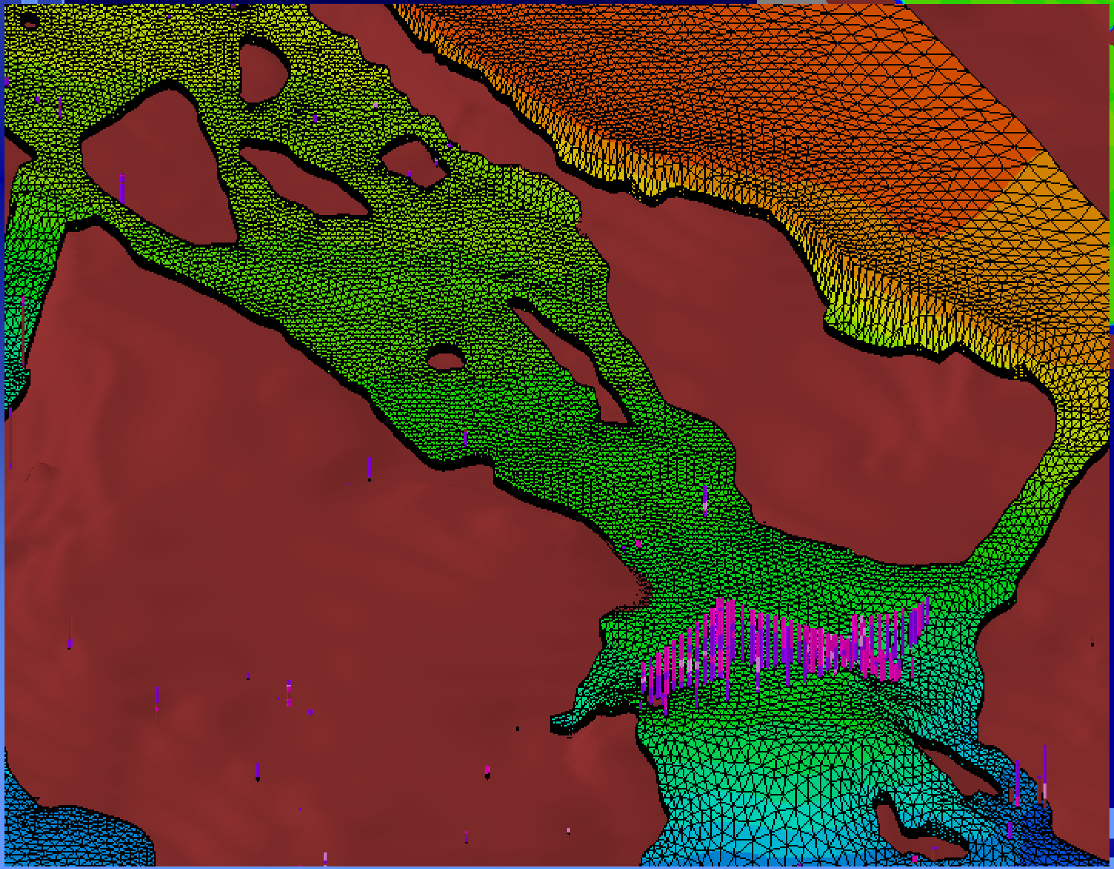




318,000 nodes, 2M elements

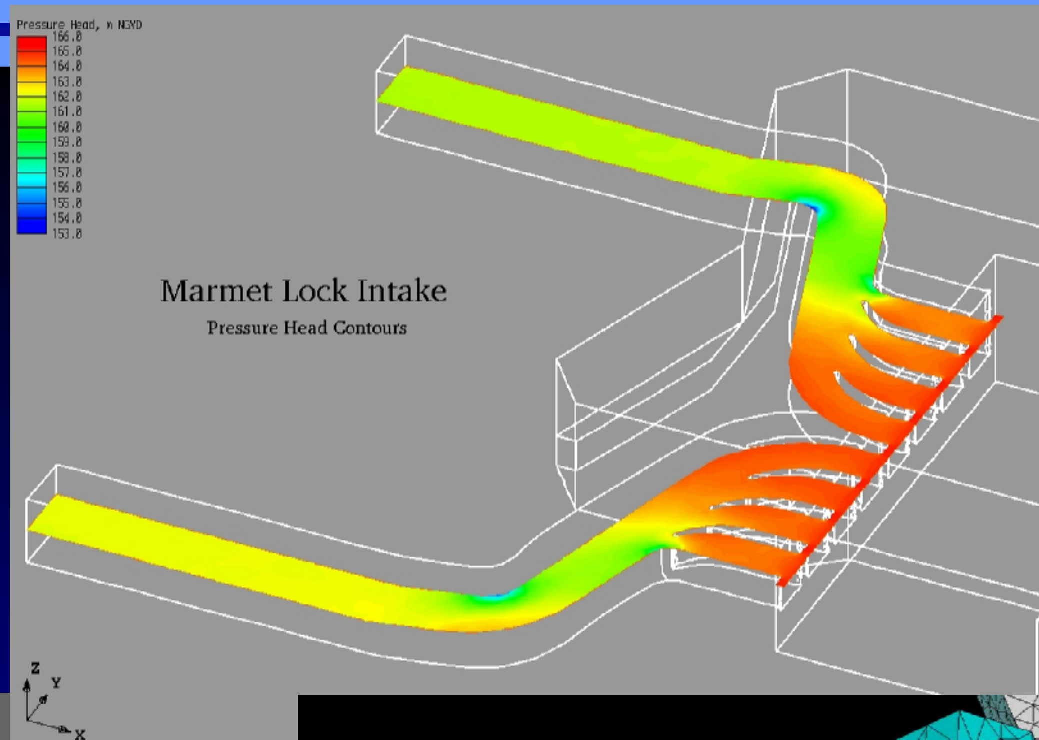
Pueblo Chemical Depot Coarse Mesh

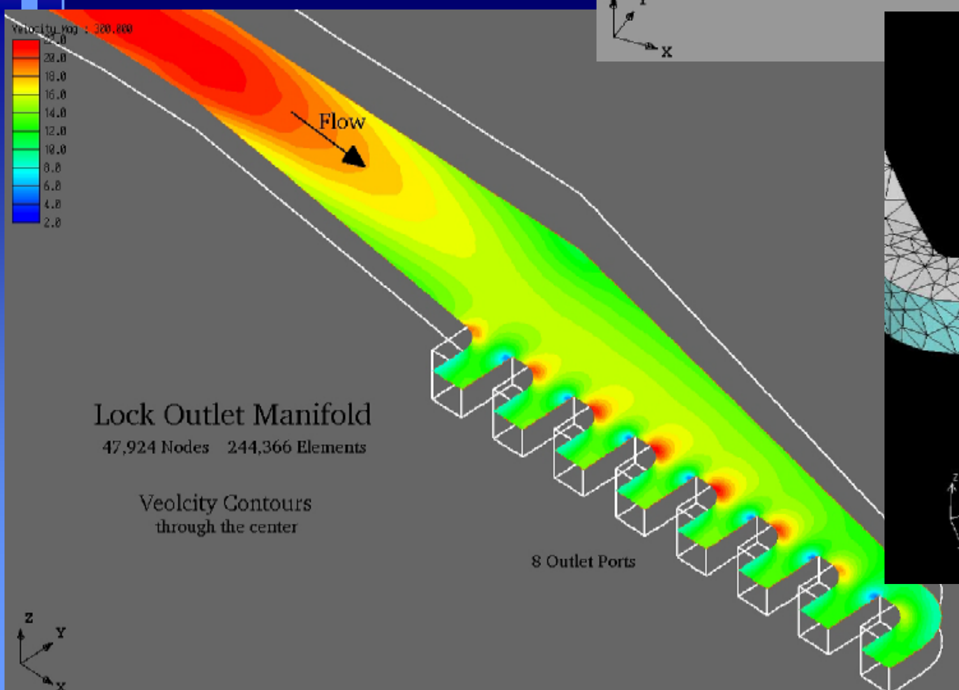


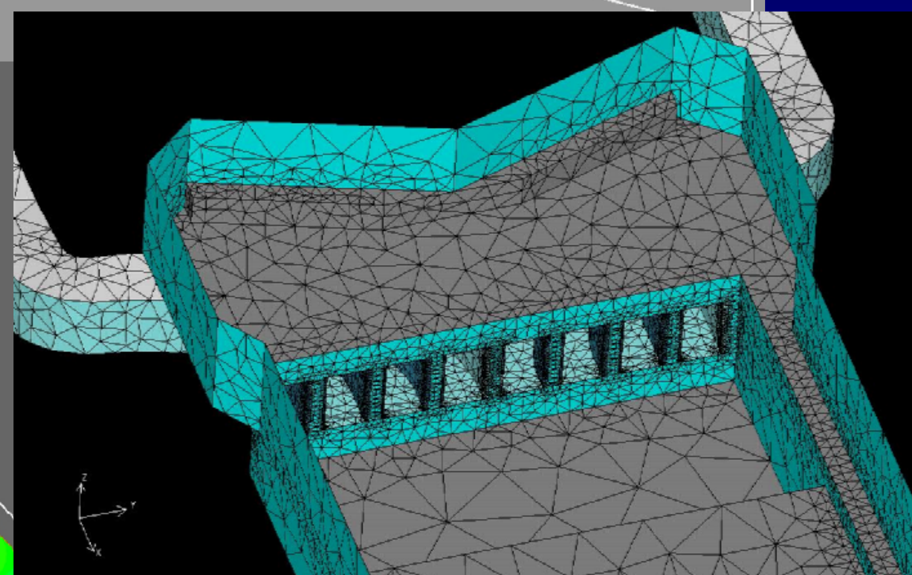


89,000 nodes,
420,000 elements

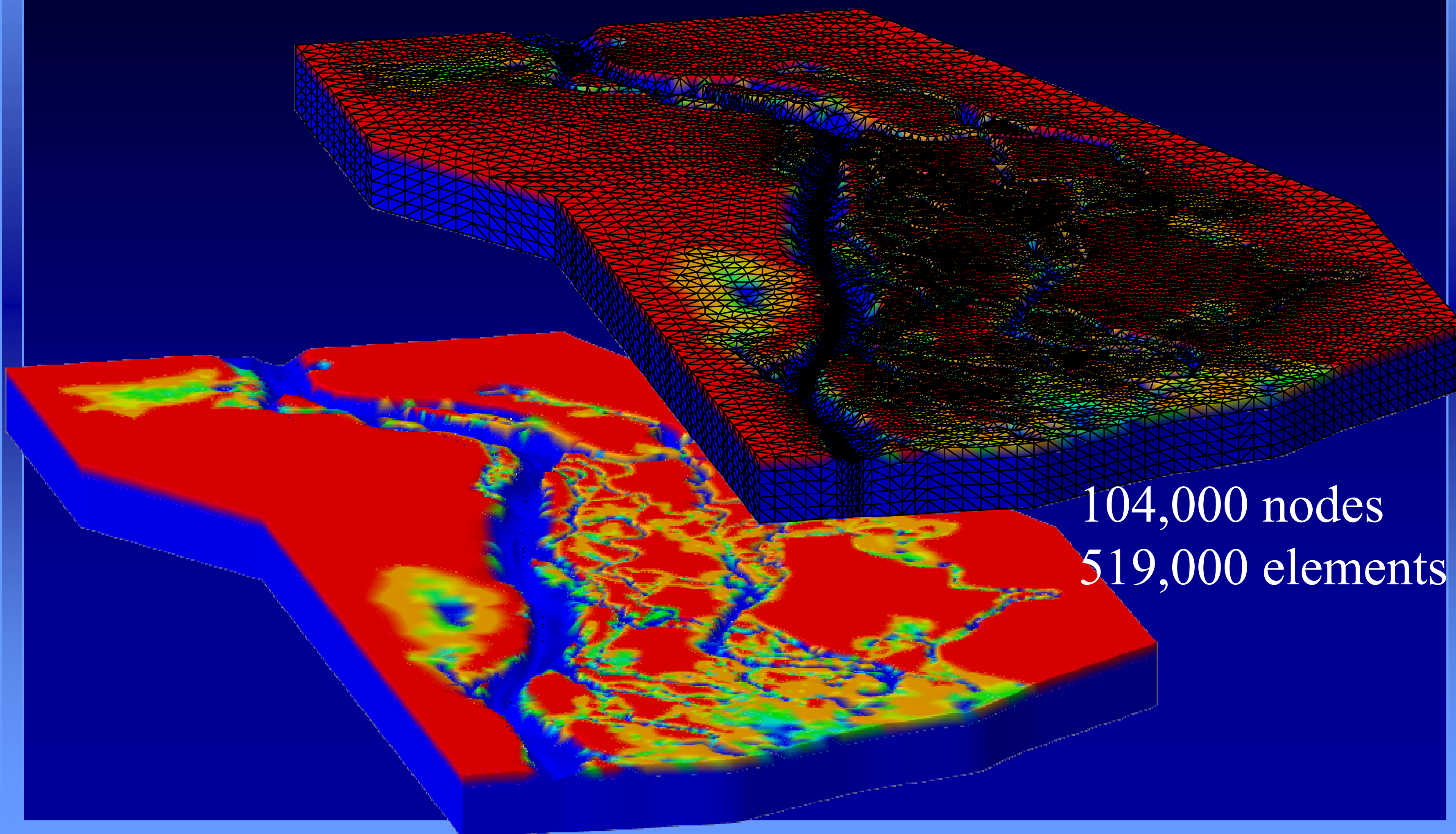
Lock Intake and Outlet







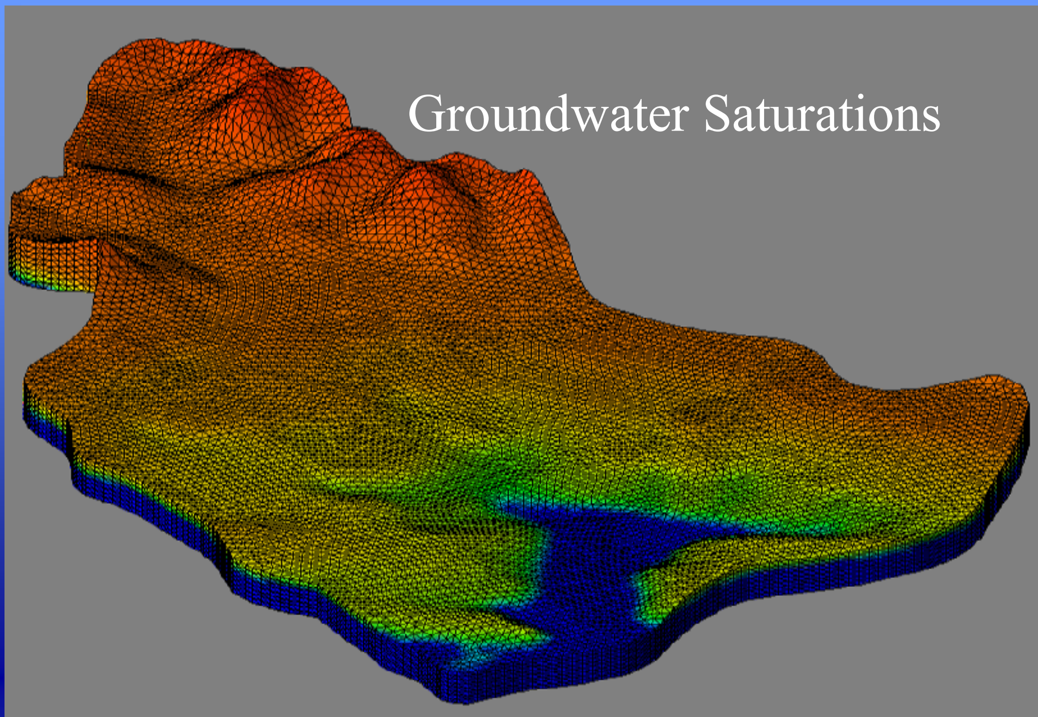
Pool 8 Mississippi River
Groundwater Surface Water Interaction

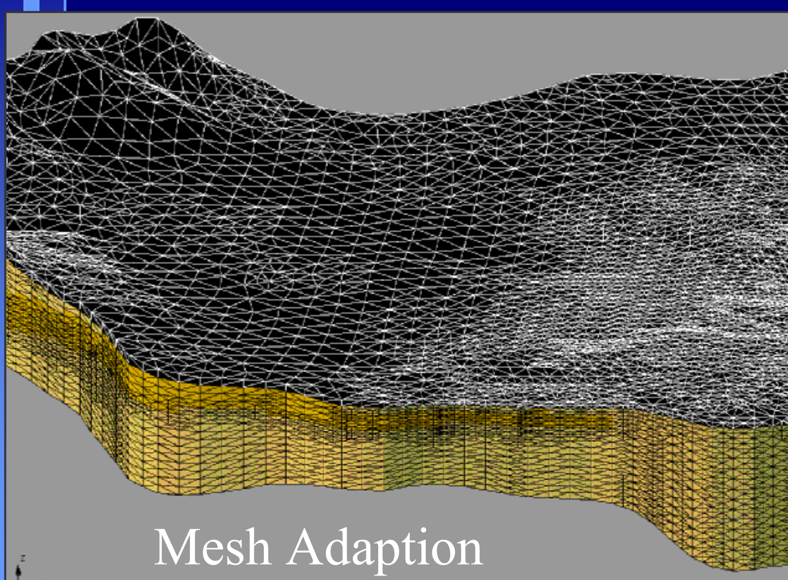


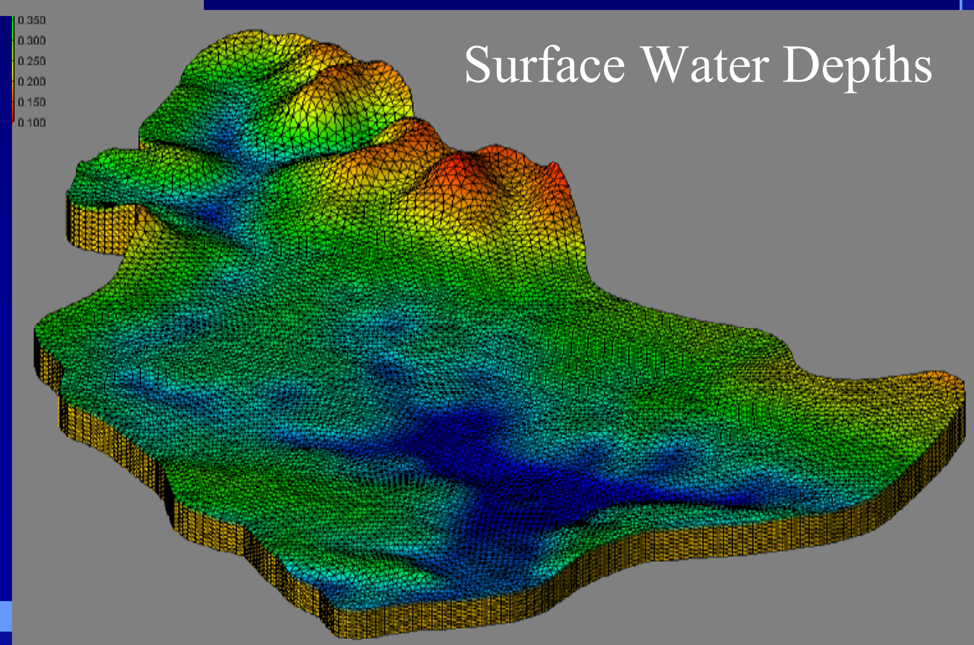
Goose Prairie Creek Watershed

72,000 nodes

375,000 elements







Optimization in Engineering

- Aerospace Applications
  - Airfoil design
  - Design of aerodynamic structures
- Groundwater Applications
  - Design of pump-and-treat remediation system
  - Location of wells for monitoring
- Surface Water Applications
  - Design of open channel structures
  - Location and scheduling of dredging
  - Multi-reservoir systems operation
  - Control of contaminant releases in rivers

Optimization Techniques

- Nonlinear constrained optimization problem

Minimize: $F(x)$ objective function

Subject to:

$$g_j(X) \le 0$$ j=1,m inequality constraints

$$h_k(X) = 0$$ k=1,*l* equality constraints

$$X_i^l \le X_i \le X_i^u$$ i=1,n side constraints

Optimization Techniques

$$\text{where} \qquad X = \begin{Bmatrix} X_1 \\ X_2 \\ X_3 \\ . \\ . \\ . \\ X_n \end{Bmatrix} \qquad \text{design variables}$$

Optimization Method	Type of Problem	Advantages	Disadvantages
Inverse Methods	Analytic Formula	Highly Efficient	Not Generally Applicable
Genetic Algorithm (Probabilistic Methods)	Discontinuous, Discrete, Cheap Simulations, Multi-Model	Avoids Local Minim, No Gradient Needed	Many Function Evaluation
Finite Difference	Any	Easiest To Use	Large Computer Cost, Accuracy
ADIFOR, CTSE	Any	Highly Accurate Derivative, Easy to Use	Large Computer Cost, Accuracy
Continuous Sensitivity Analysis	Explicit High-Fidelity	Computationally Efficient	Derive and Solve Adjoint Equations
Discrete Sensitivity Analysis	Implicit High-Fidelity	Accurate Derivatives, Efficient	Jacobian Matrix Needed

Burg 2001

Parameter Space

- Groundwater
  - Hydraulic conductivity
  - Constitutive Equations
- Surface Water
  - Roughness
  - Elevation of wetlands
- Overland Flow
  - Roughness
  - Runoff coefficients
- Heat Transport
  - Heat capacity
  - Heat conductivity

Observation Data

- Groundwater
  - Head values
  - Flux from/to surface water
- Surface Water
  - Tidal data
  - Fluxes
- Overland Flow
  - Hydrograph
- Heat
  - Temperature

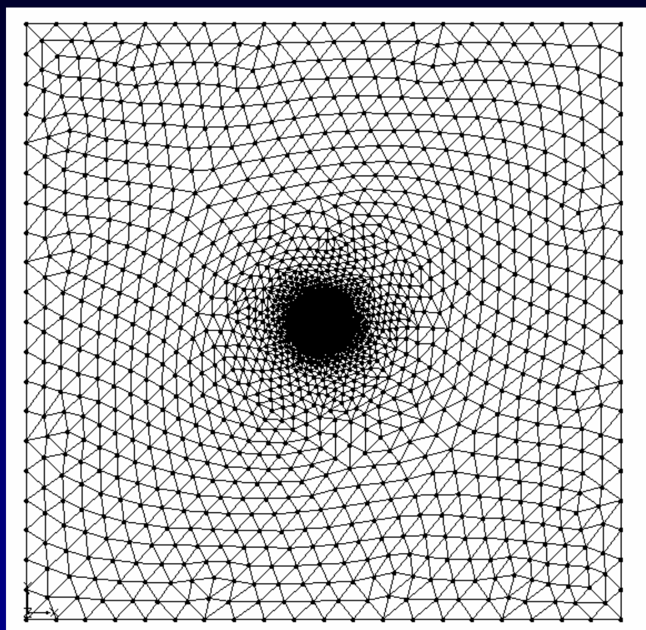
Treatment of Observation Data

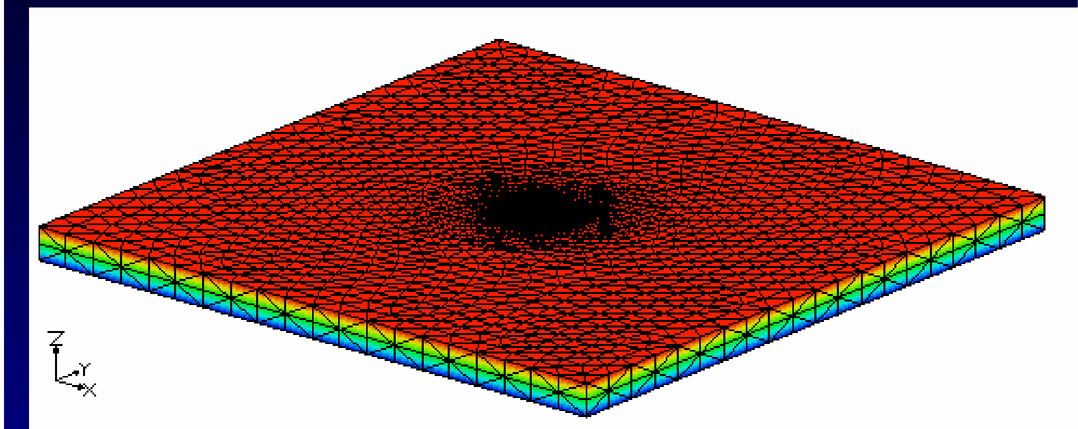
- Sufficient data to properly define the problem
- Data that is sparse spatially, but dense temporally
- How do you deal with tidal data when matching the range, max, and min is the objective?

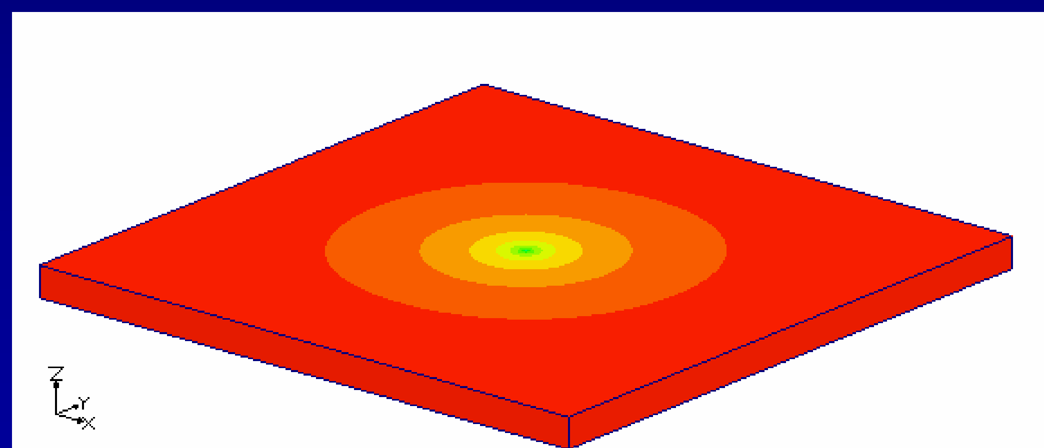
PEST

- based on Gauss-Marquardt-Levenberg (GML) method
- facilitates the use of multi-component objective functions
- performs three model operations
  - parameter estimation
  - regularization
  - predictive analysis

Theis Problem







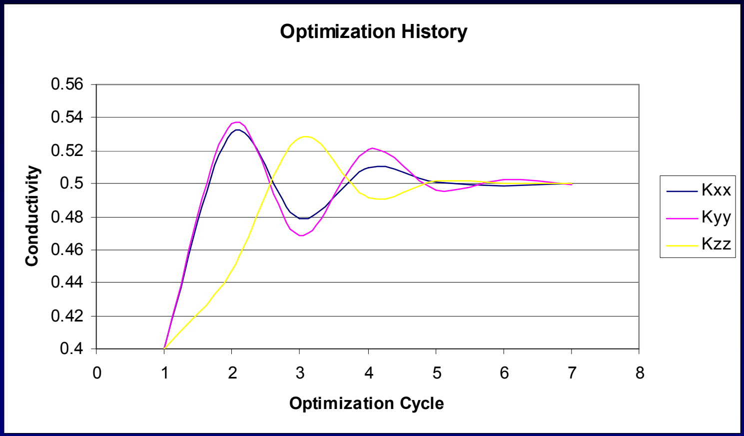
9483 nodes

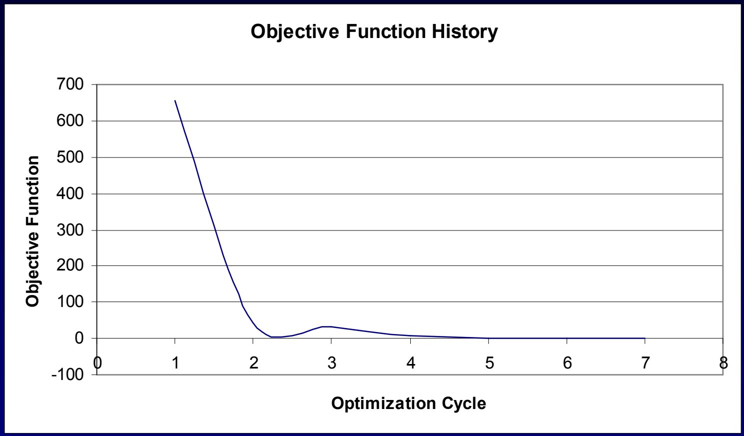
37440 elements

1 material

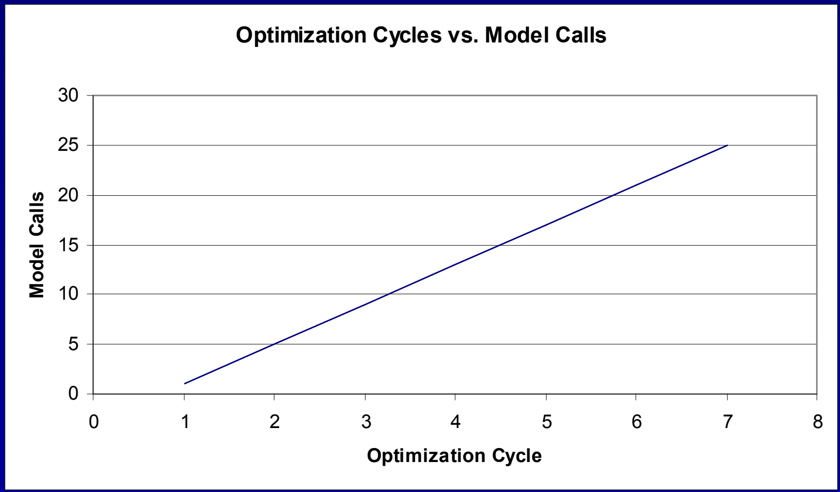
1 extraction well

Optimization History





- 9 observation points with head values
- 3 parameters varied Kxx, Kyy, Kzz
- Kxx = 0.500462
  - 95% confidence interval = 0.499112 to 0.501812
- Kyy=0.499490
  - 95% confidence interval = 0.498167 to 0.500814
- Kzz = 0.499969
  - 95% confidence interval = 0.459354 to 0.540585
- Computational time per function call = 4.6 minutes



Surrogate Models

- Model built from function values to represent the original model with less computational cost
- Accomplished, for example, by neural nets or reducing the underlying physical equations
- May not be possible to build surrogate due to complexity of the model

Summary

- ADH solves multi-physics problems
- Major component of uncertainty analysis is parameter estimation
- PEST can be used with ADH for parameter estimation