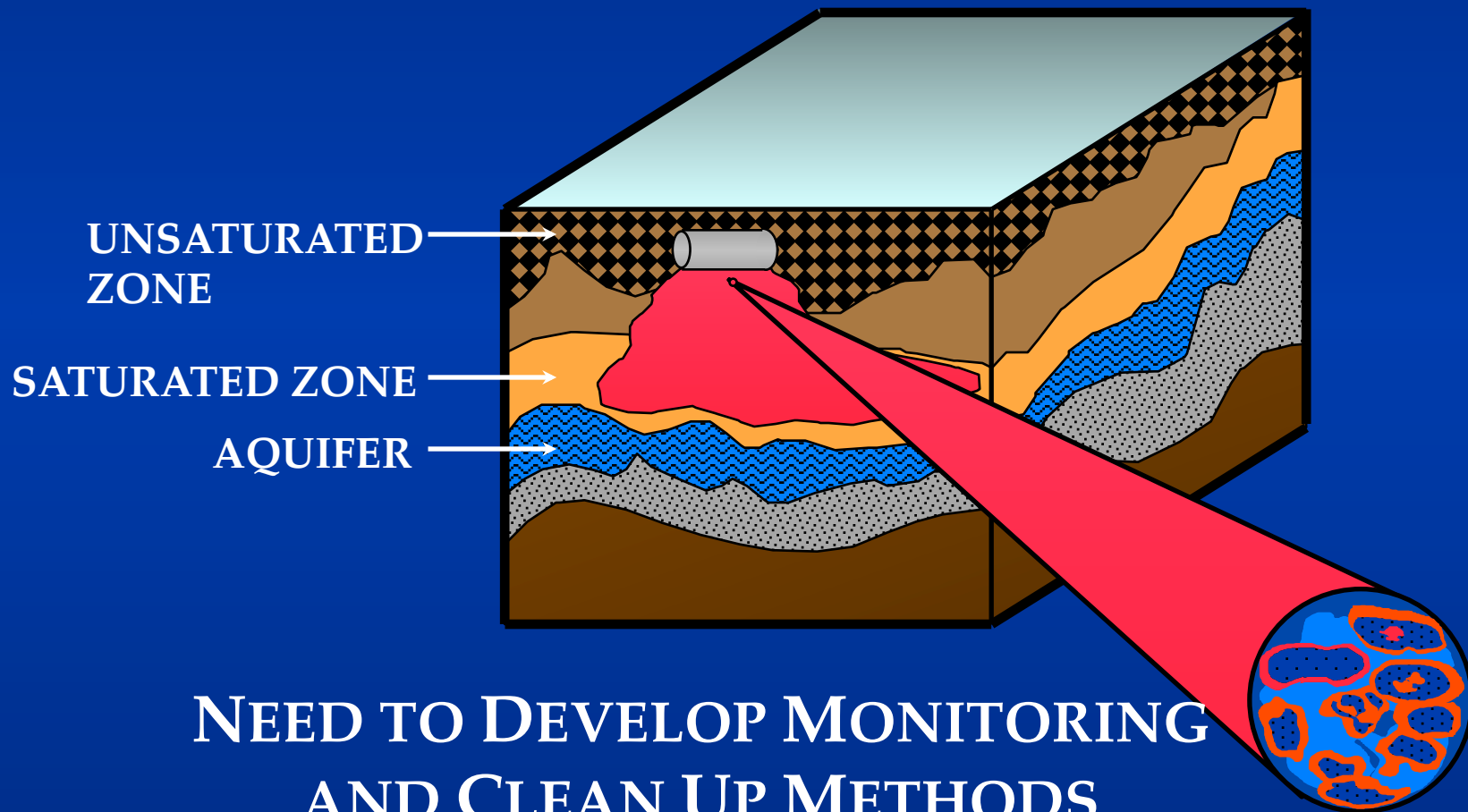


INTERACTIVE CONTROL OF LARGE-SCALE SIMULATIONS

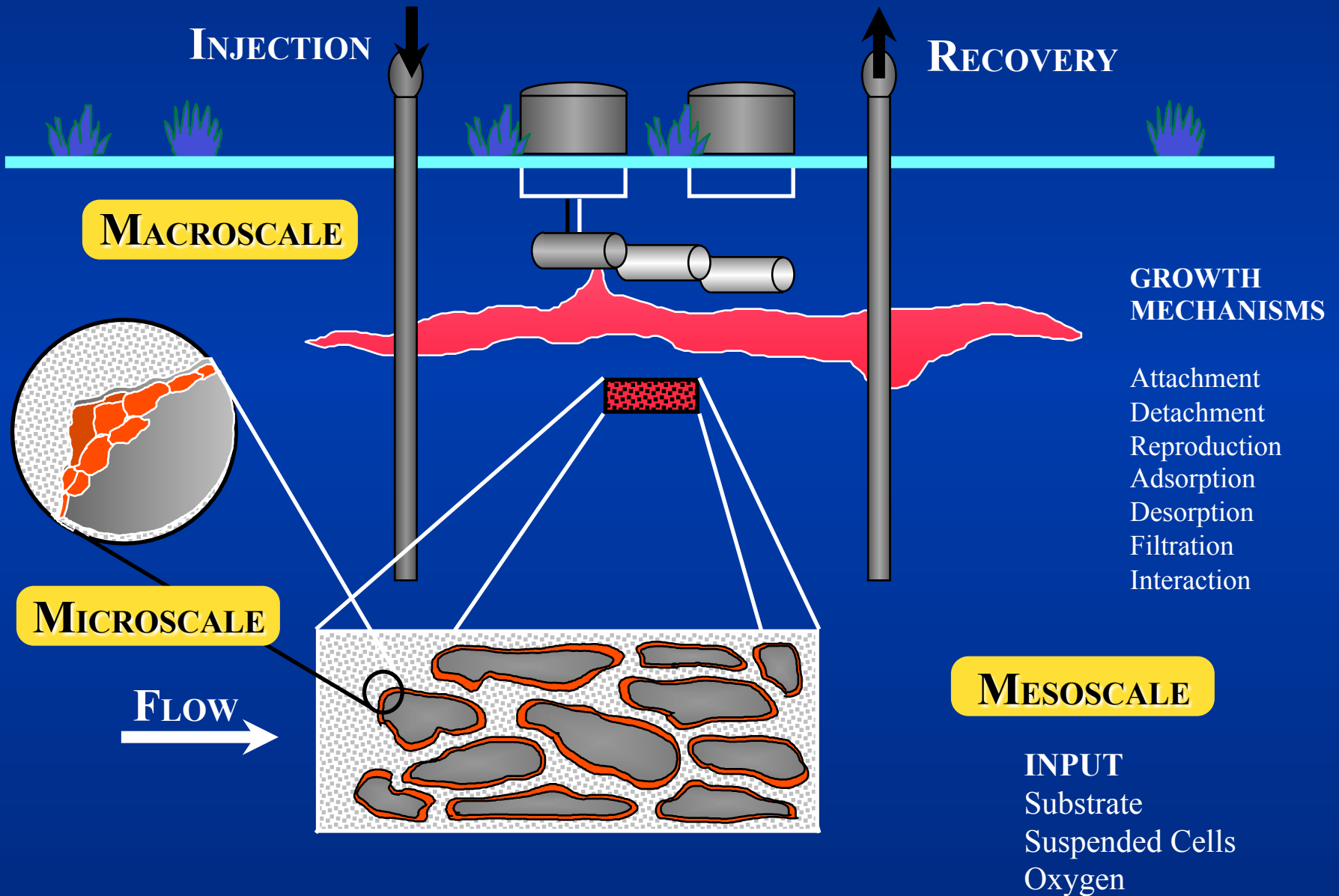
**Richard E. Ewing
Institute for Scientific Computation
Texas A&M University**

**Robert C. Sharpley
Industrial Mathematics Institute
University of South Carolina**

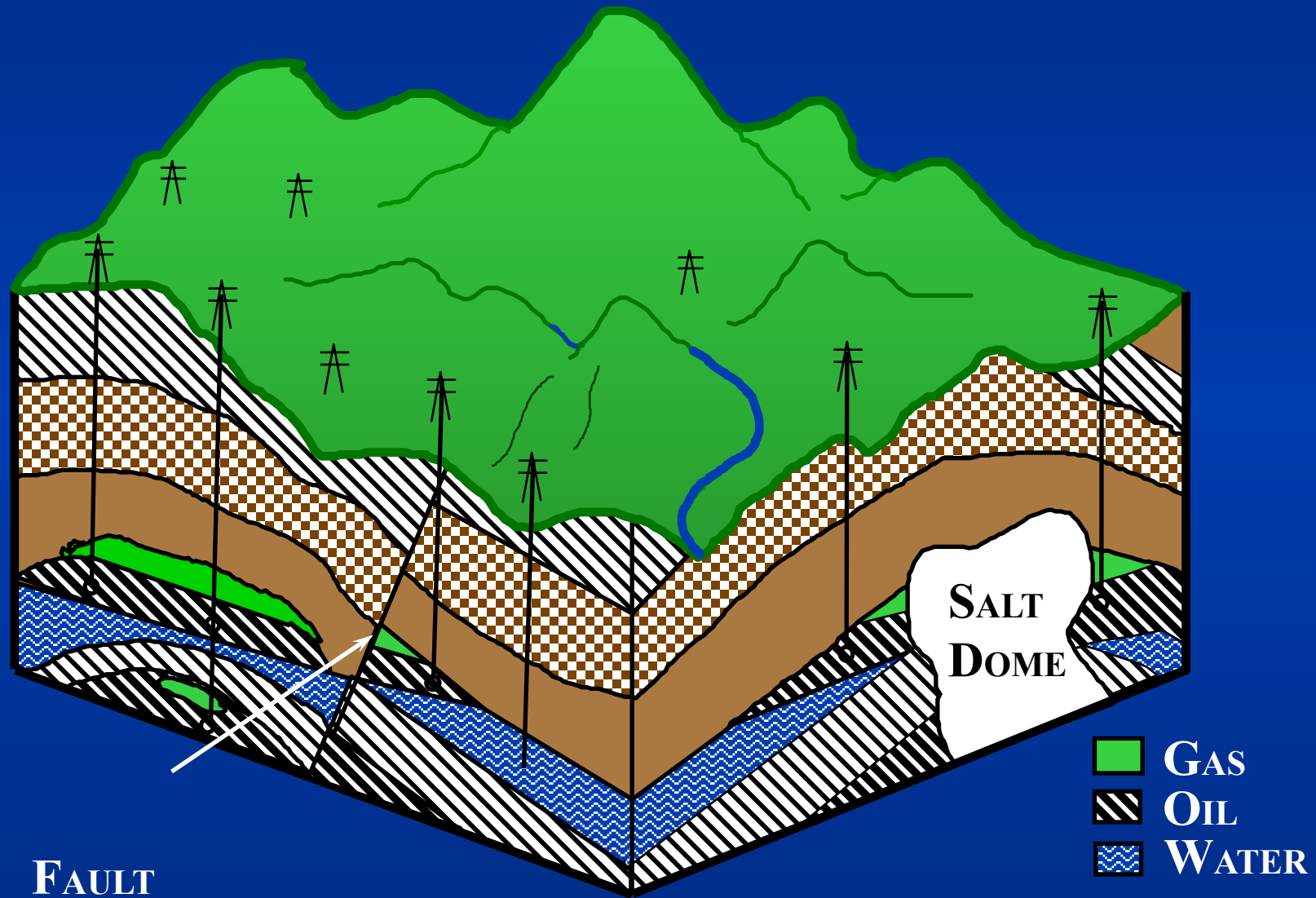
LEAKY UNDERGROUND STORAGE TANKS



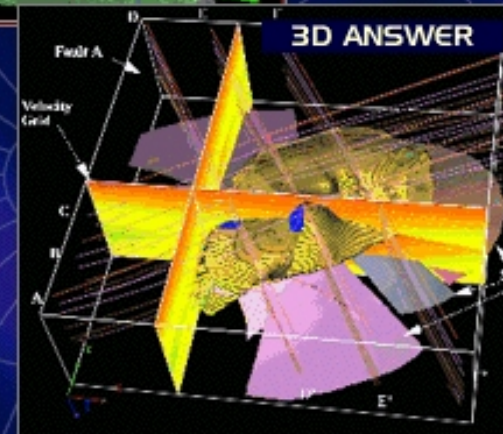
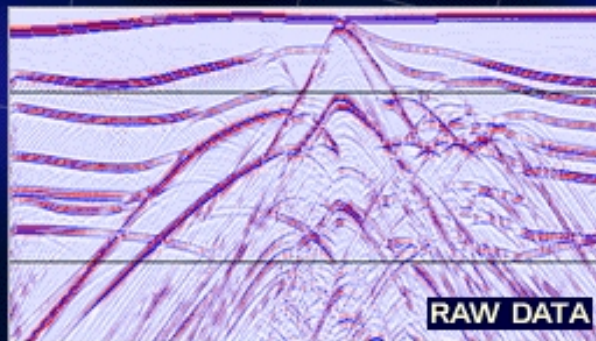
BIOREMEDIATION STRATEGIES

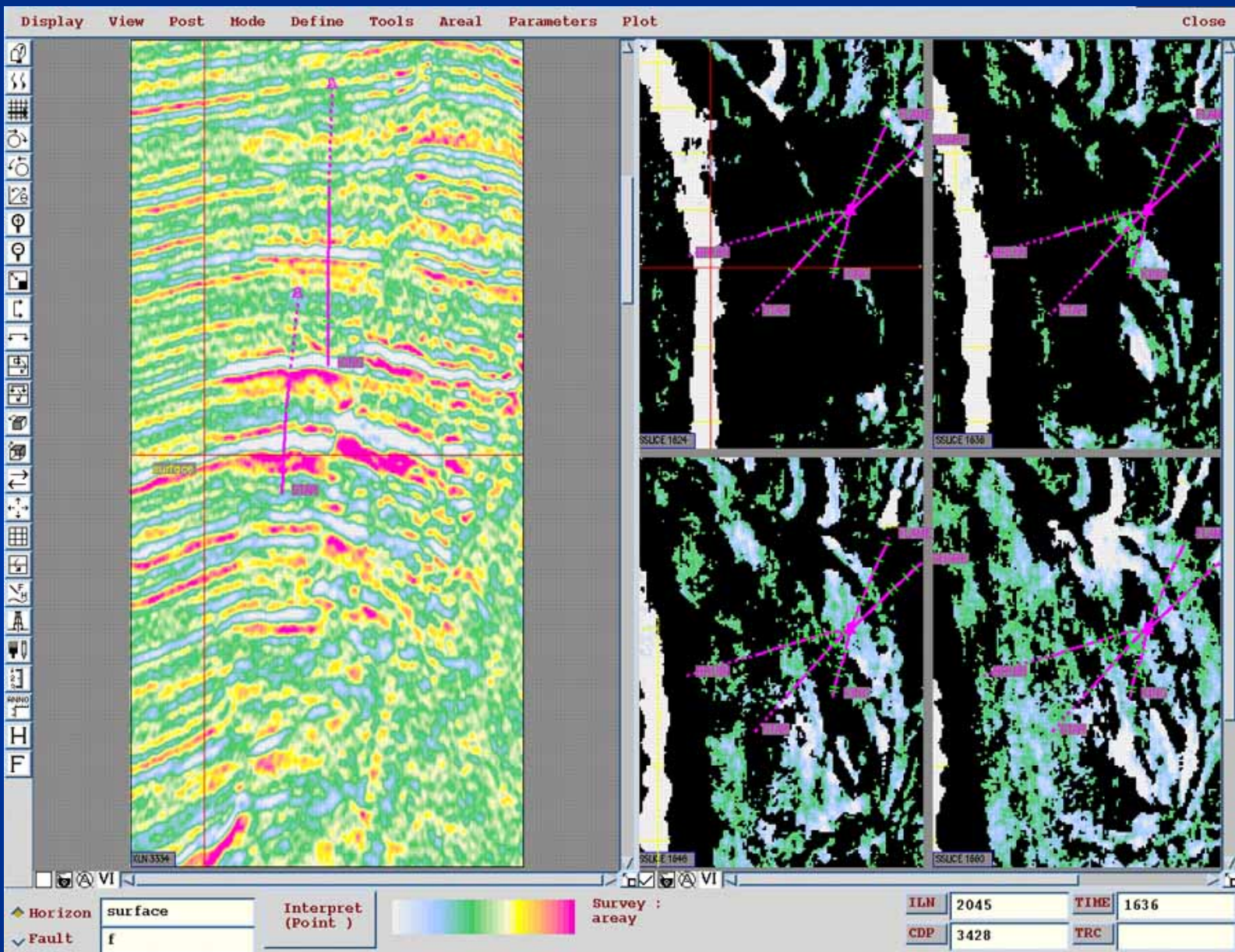


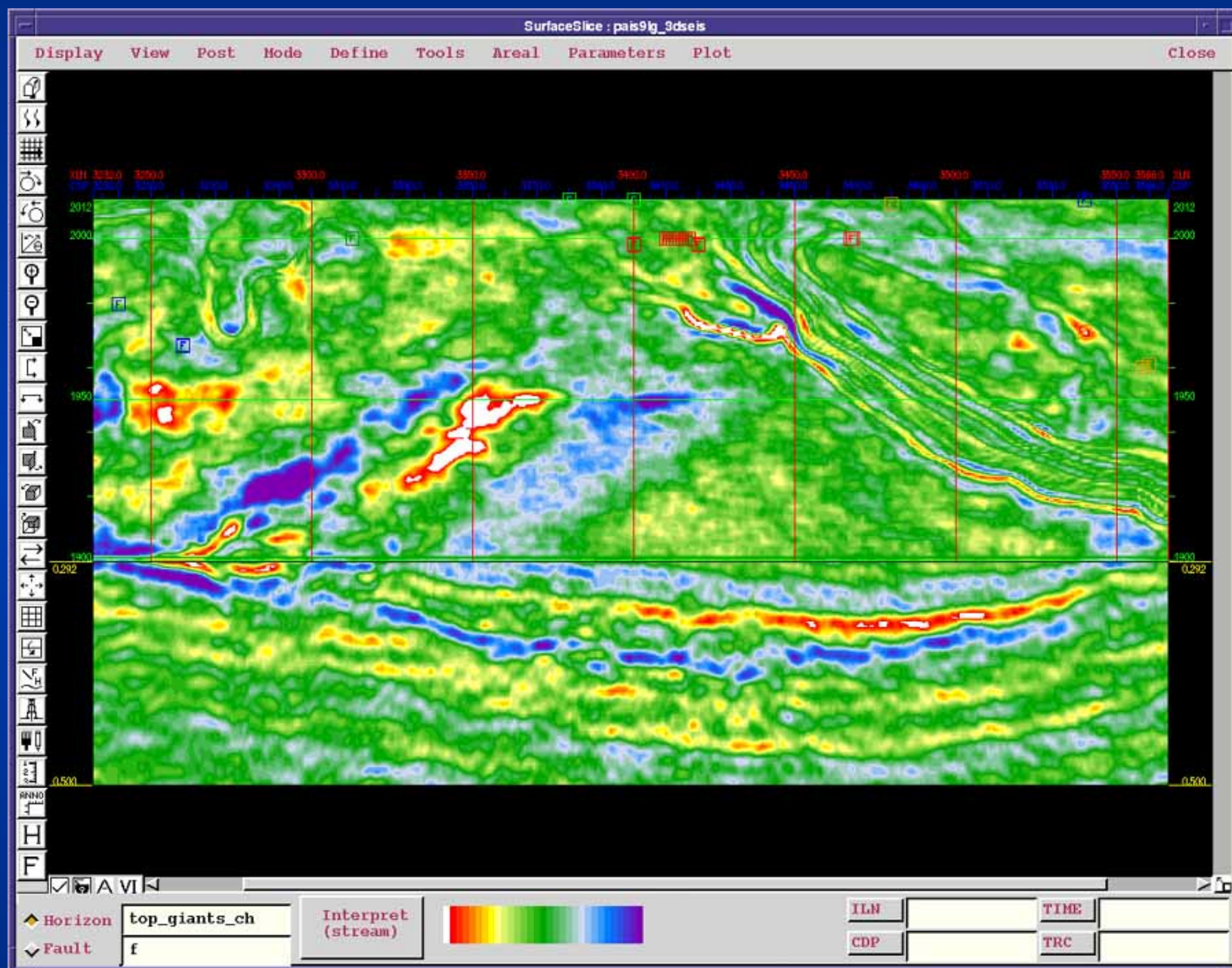
PETROLEUM APPLICATIONS

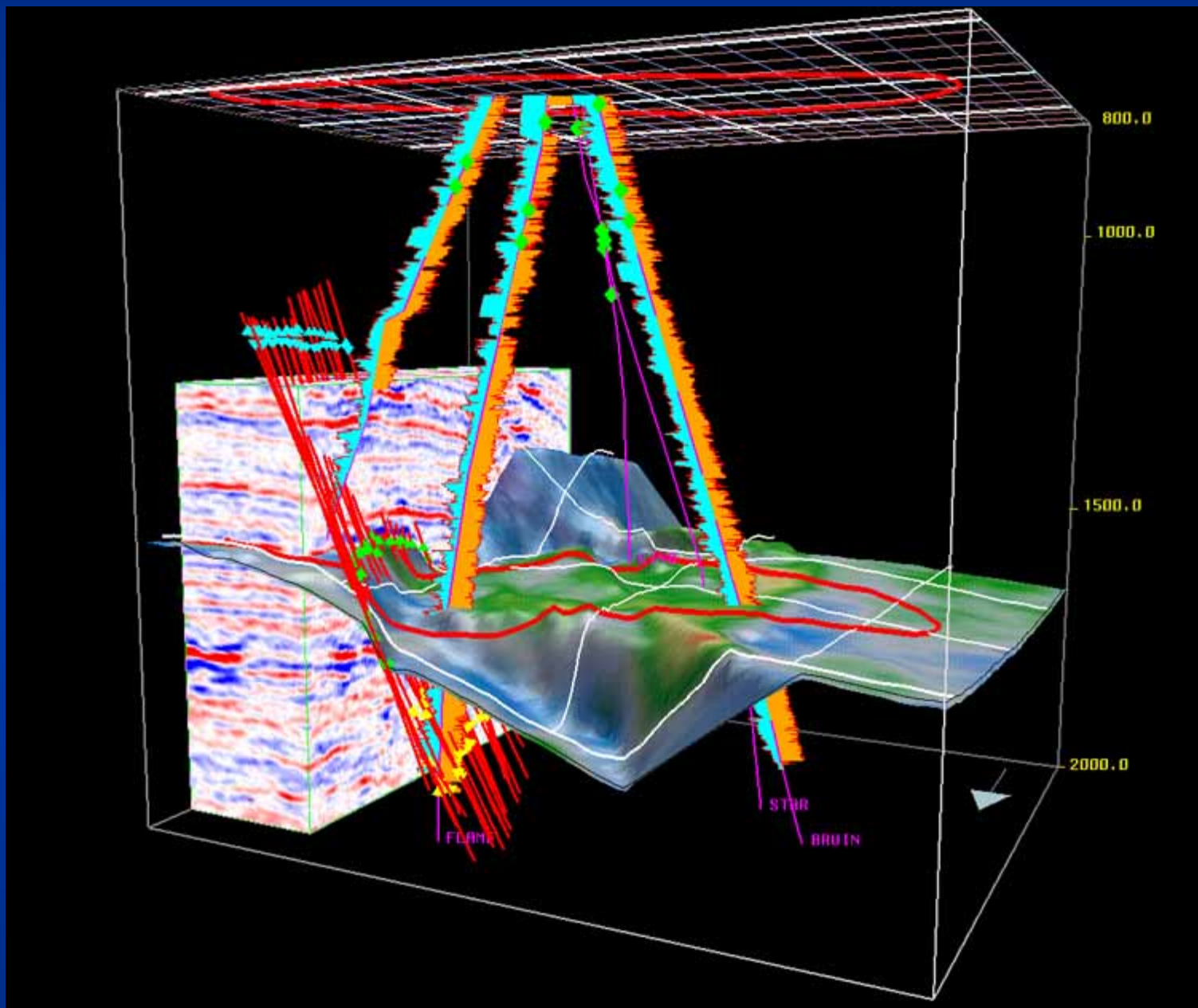


DATA PROCESSING

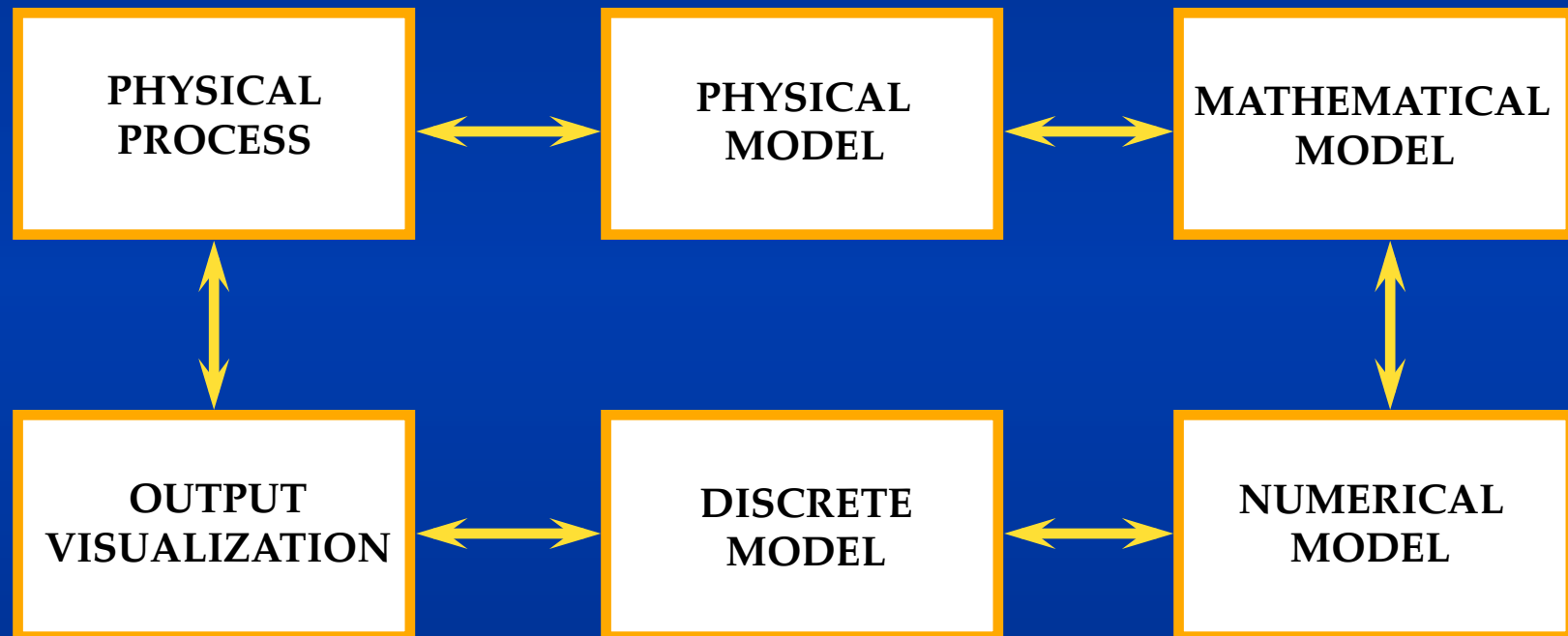








MODELING PROCESS



NEED FOR SIMULATION

- ◆ **DEVELOP BETTER UNDERSTANDING OF NONLINEAR BEHAVIOR**
 - COMPUTATIONAL LABORATORY $\longleftrightarrow$ EXPERIMENTS
 - UNDERSTAND SENSITIVITIES OF PARAMETERS
 - ISOLATE PHENOMENA THEN COMBINE
- ◆ **SCALE-UP INFORMATION AND UNDERSTANDING**
 - PORE $\longrightarrow$ LABORATORY $\longrightarrow$ FIELD
- ◆ **OBTAIN BOUNDING CALCULATIONS**
- ◆ **DEVELOP PREDICTIVE CAPABILITIES**
 - OPTIMIZATION AND CONTROL

TRANSPORT IN POROUS MEDIA

◆ PHYSICAL RELATIONS:

CONSTITUTIVE LAW (**D'** ARCY)

$$\mathbf{u} = -T \nabla \Phi$$

CONSERVATION OF MASS

$$-\operatorname{div} \mathbf{u} = \frac{\partial}{\partial t} (\phi S(\Phi)) + q$$

COMPONENT BALANCES

$$\frac{\partial}{\partial t} (\phi f_1(c)) + \operatorname{div}(\mathbf{u} f_2(c)) = \nabla \bullet (D \nabla c) + q(c)$$

EQUATIONS OF STATE

THERMAL BALANCE

TRANSPORT IN POROUS MEDIA (CONTINUED)

- ◆ ϕ, T, S, f_1, f_2, D ARE USUALLY UNKNOWN
 - PARAMETER ESTIMATION / INVERSE PROBLEMS
- ◆ PARAMETERS ARE HETEROGENEOUS AT VARIOUS LENGTHS
 - NEED EFFECTIVE PARAMETERS / EQUATIONS
- ◆ NEED ACCURATE FLUID VELOCITIES
 - MIXED FINITE ELEMENT METHODS
- ◆ IMPORTANCE OF TRANSPORT
 - EULERIAN - LAGRANGIAN METHODS
- ◆ COUPLED NONLINEAR SYSTEMS
 - EFFECTIVE LINEARIZATION / SOLUTION METHODS

TWO-PHASE FLOW

D' ARCY'S LAW:

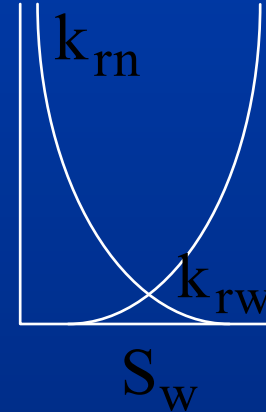
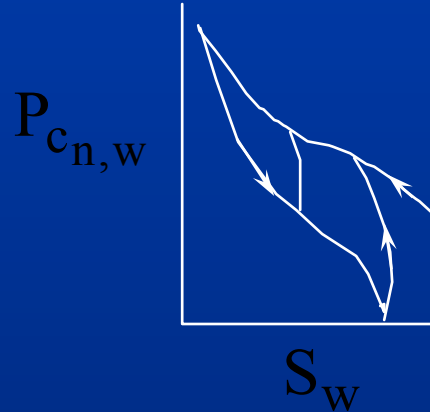
$$u_i = -\frac{K k_{ri}}{\mu_i} (\nabla p_i - \rho_i g \nabla z), \quad i = w, n$$

MASS BALANCE:

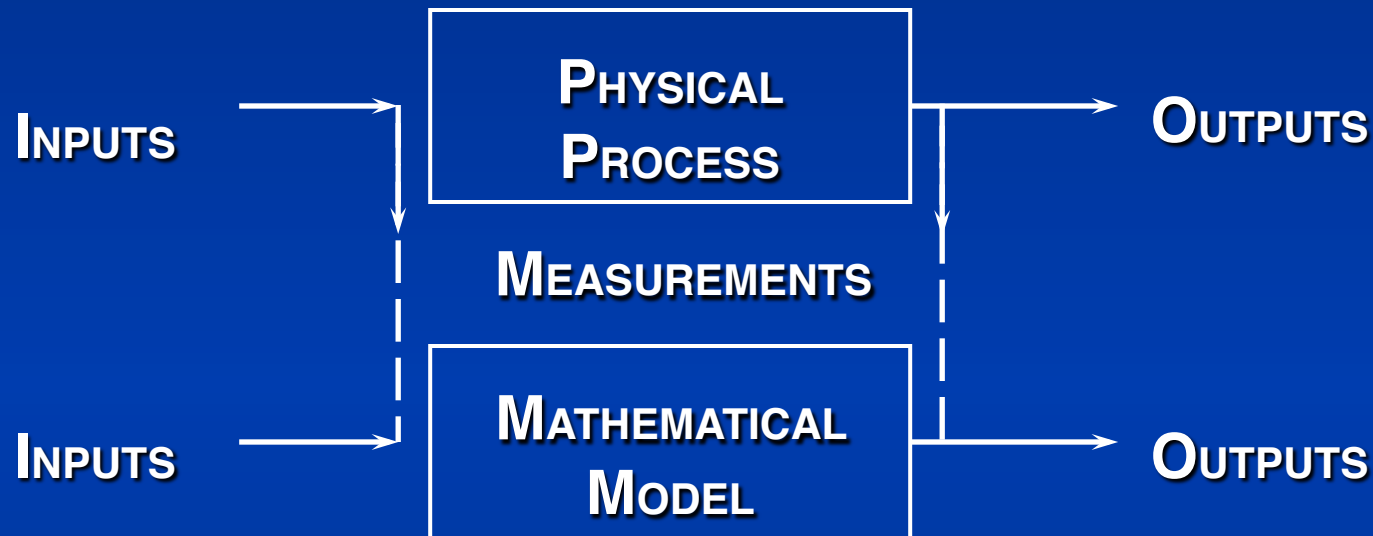
$$\frac{\partial}{\partial t} (\phi \rho_i S_i) + \nabla \cdot (\rho_i u_i) = q_i \rho_i, \quad i = w, n$$

$$p_{c_{n,w}} = p_n - p_w, \quad S_n + S_w = 1$$

w = Wetting Phase
n = Nonwetting Phase

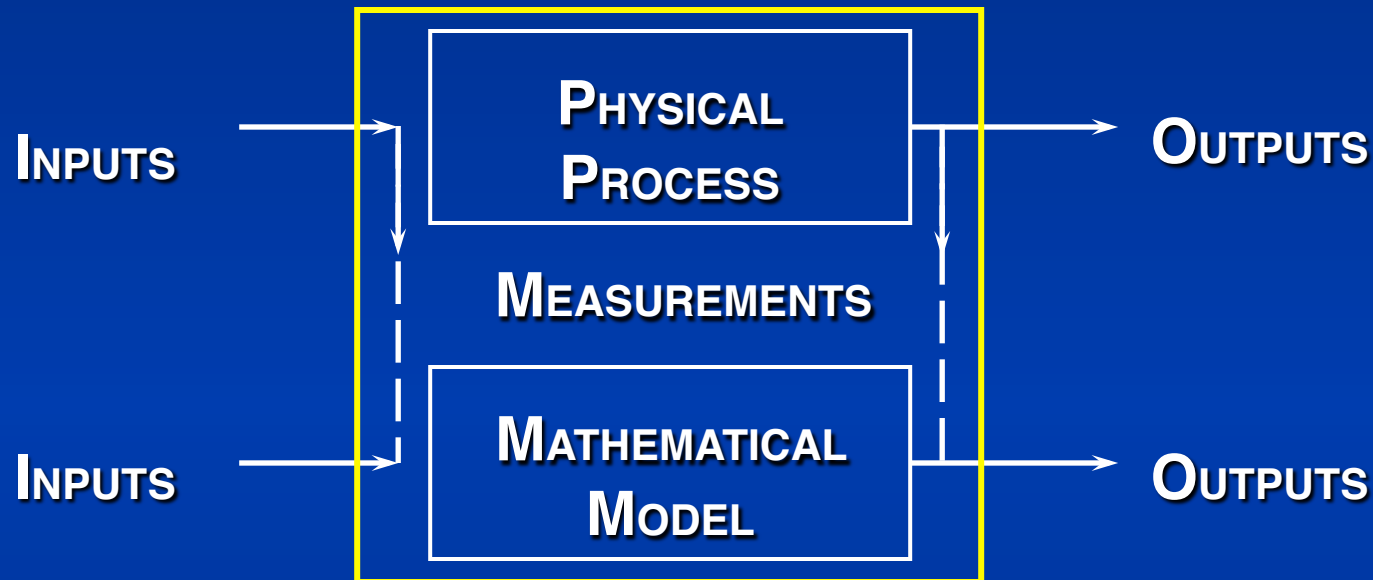


IDENTIFICATION (INVERSE) PROBLEM



- ◆ DETERMINE SUITABLE MATHEMATICAL MODEL
- ◆ ESTIMATE PARAMETERS WITHIN MATHEMATICAL MODEL

IDENTIFICATION (INVERSE) PROBLEM



- ◆ DETERMINE SUITABLE MATHEMATICAL MODEL
- ◆ ESTIMATE PARAMETERS WITHIN MATHEMATICAL MODEL

LARGE SCALE INTERACTIVE APPLICATIONS ON REMOTE SUPERCOMPUTERS

- ◆ **Model Development and Formulation**
- ◆ **Coupled Flow and Transport Codes with Complex Boundary Conditions**
- ◆ **Numerical Discretization and Parallel Algorithm Development**
- ◆ **MPP Code Development**
- ◆ **Field Testing and Production Runs**
- ◆ **User Environments and Visualization Tools**

Need for Interactive tracking and steering

PRIMARY RESEARCH TEAM

◆ Texas A&M

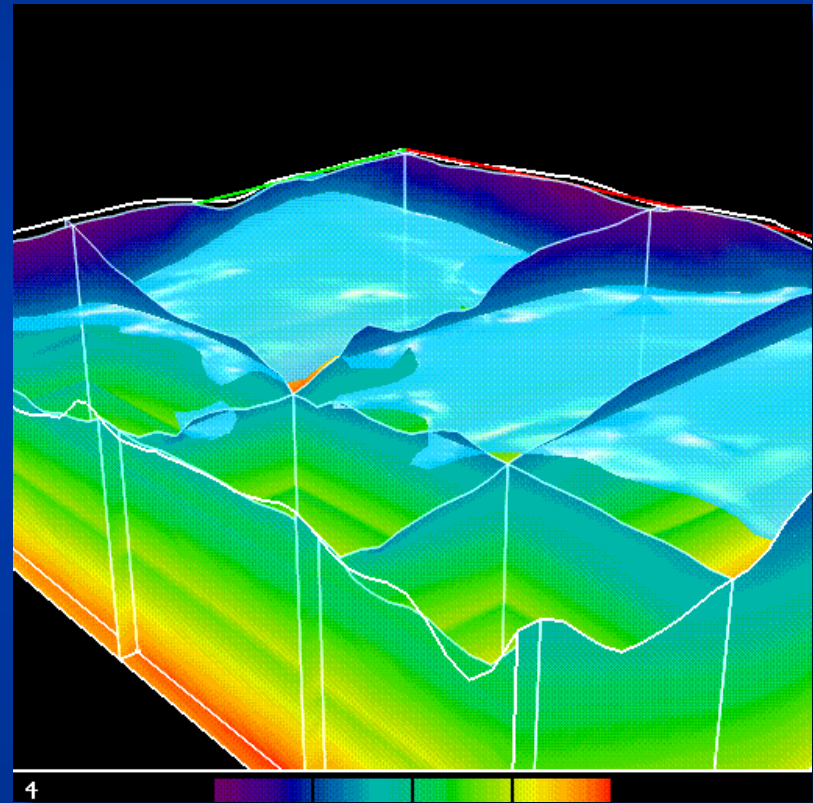
- Richard Ewing
- Steve Johnson
- Hao Lu
- Joseph Pasciak

◆ South Carolina

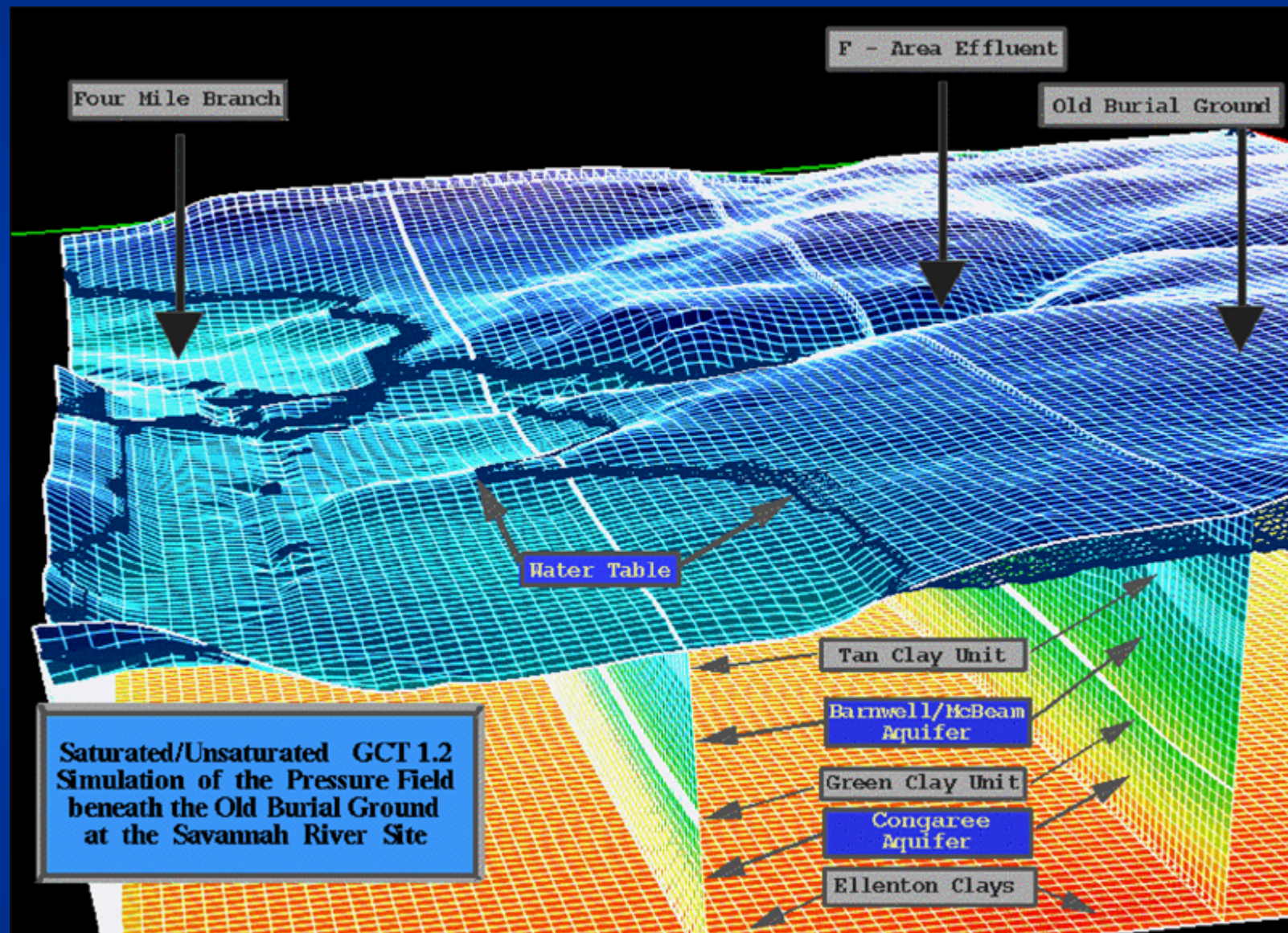
- Robert Sharpley
- Ronald DeVore
- L. Scott Johnson

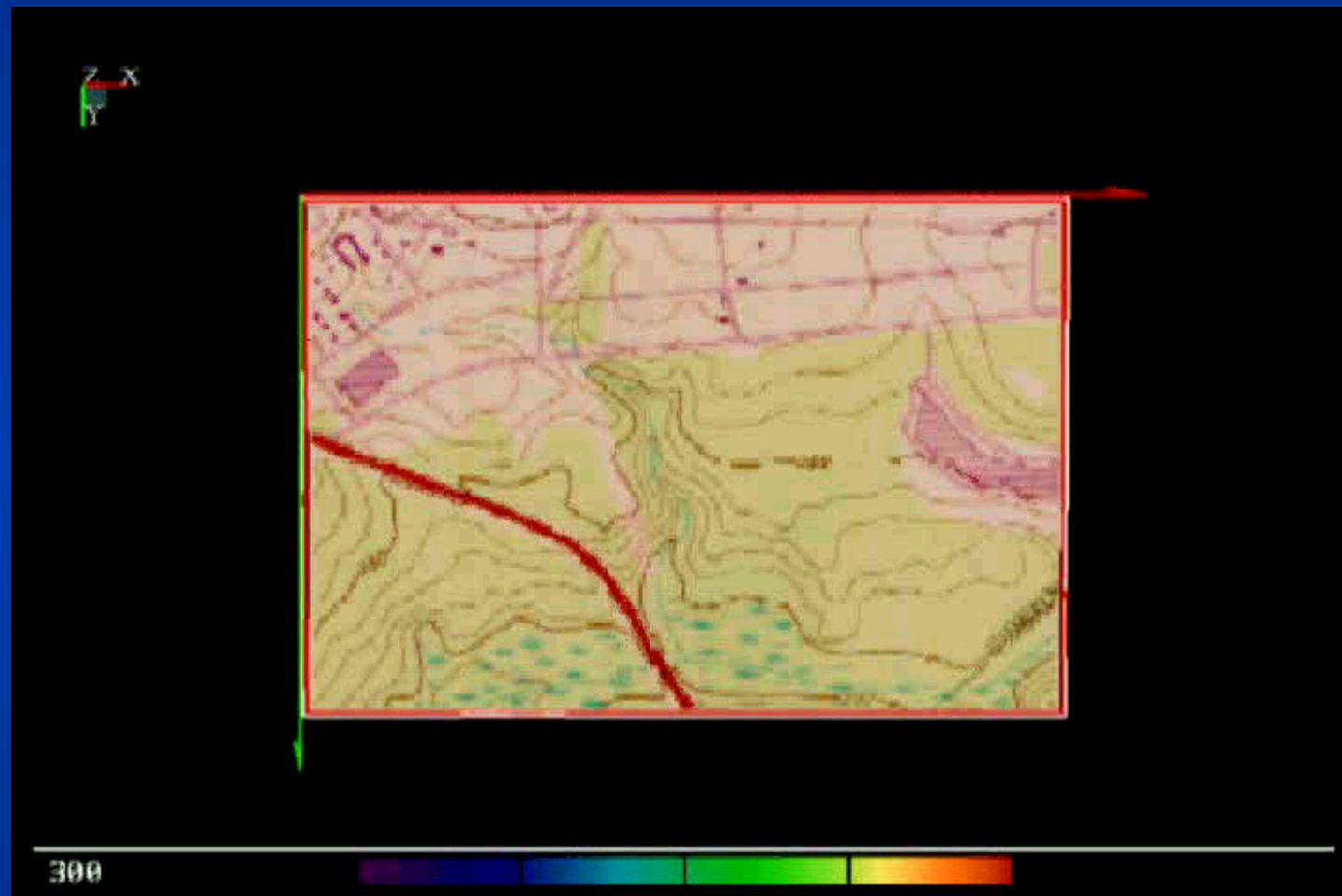
SAVANNAH RIVER SITE

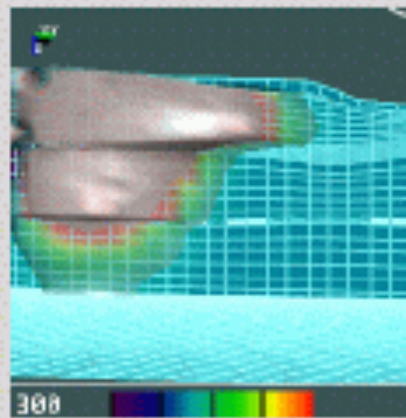
- ◆ Difficult topography
- ◆ Highly Heterogeneous Soils
- ◆ Saturated and Unsaturated Flows
- ◆ Reactions with disparate time scale
- ◆ Transient/Mixed Boundary Conditions



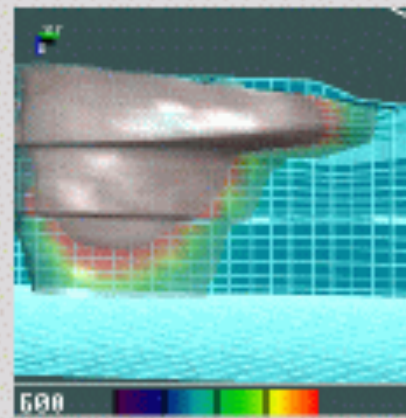




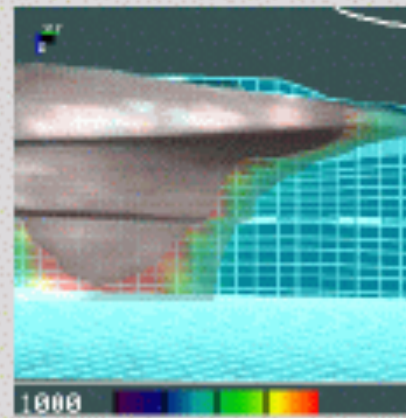
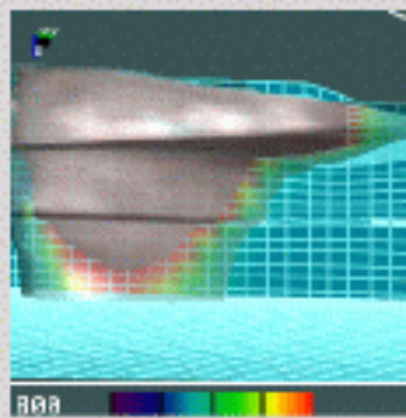


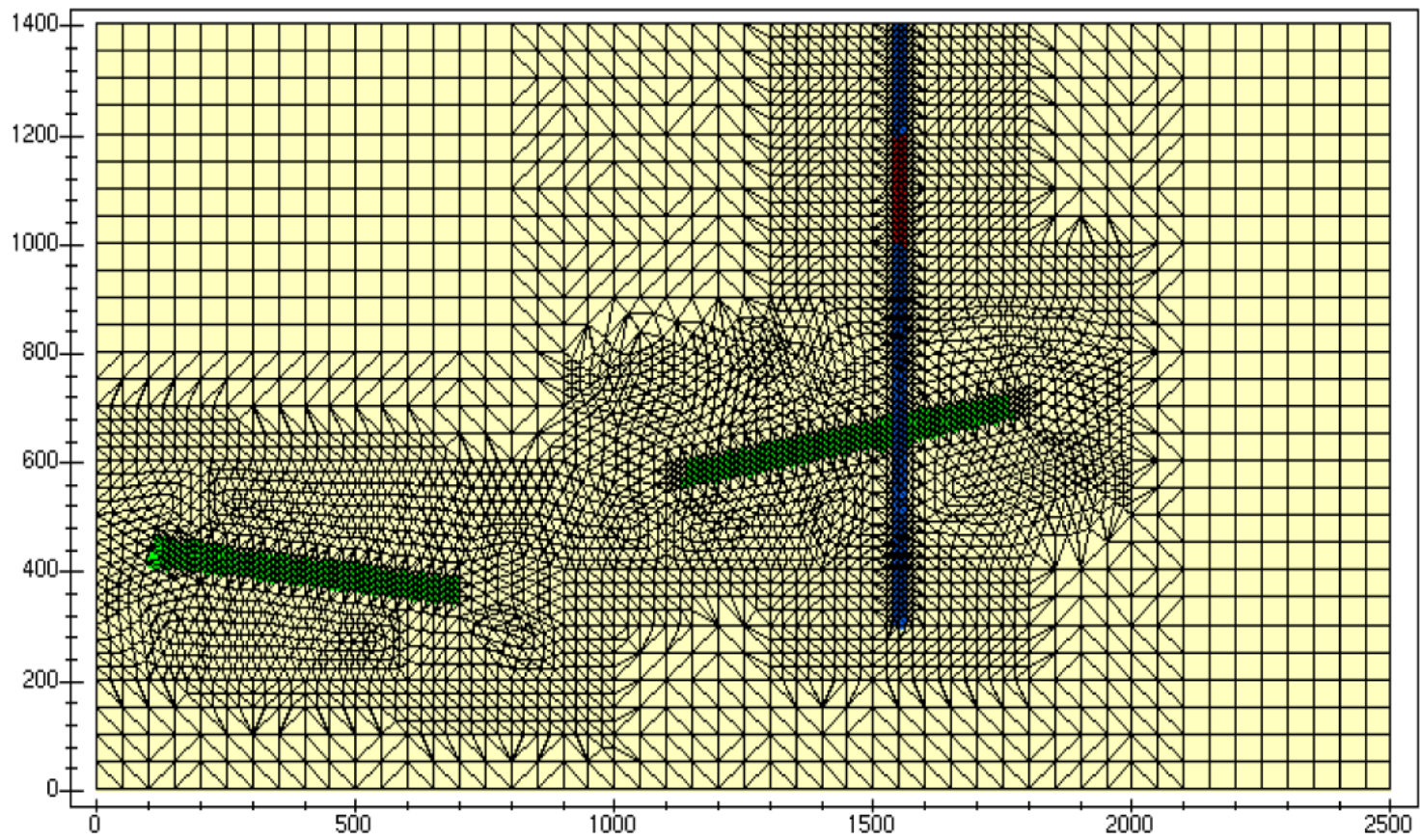


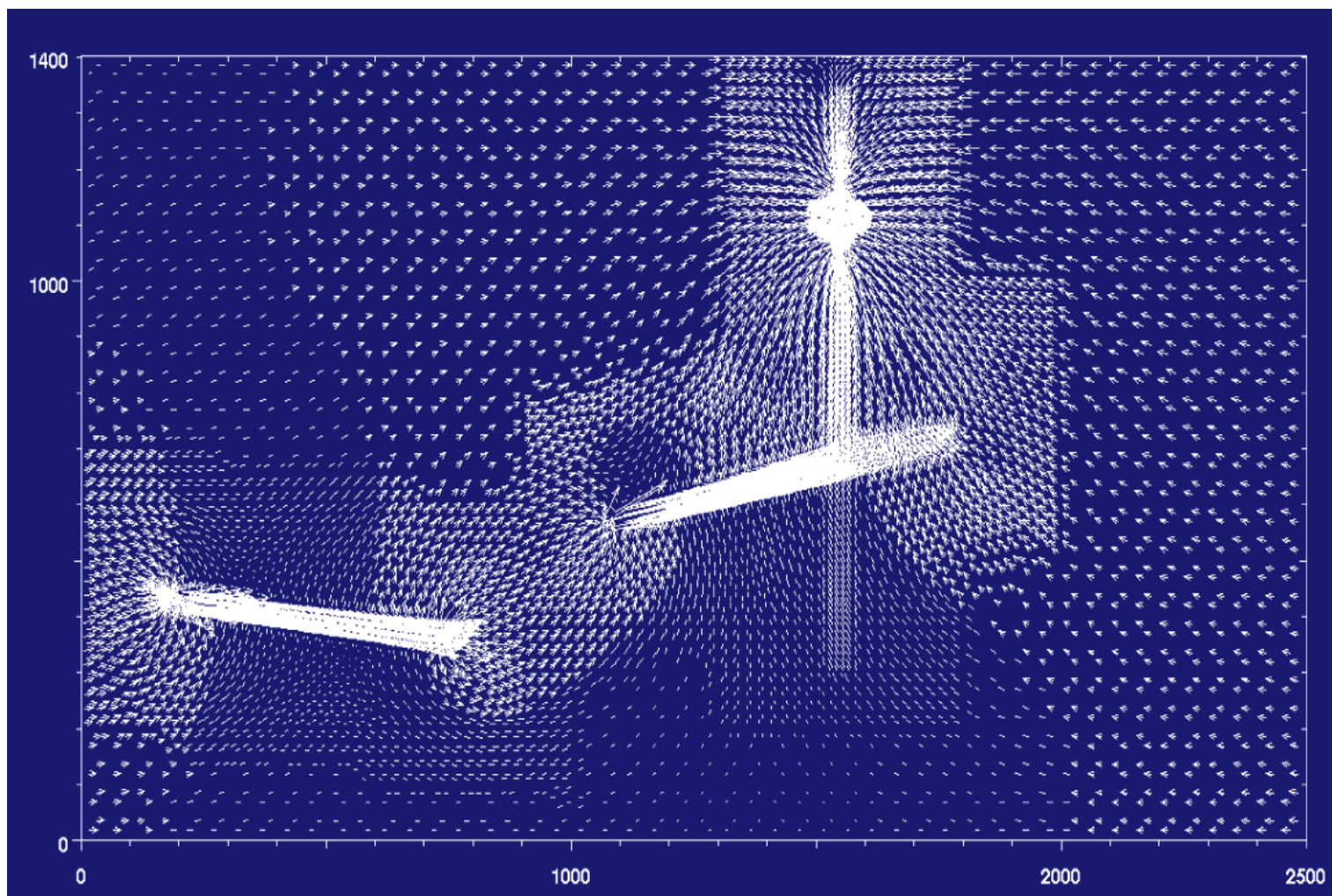
(a)

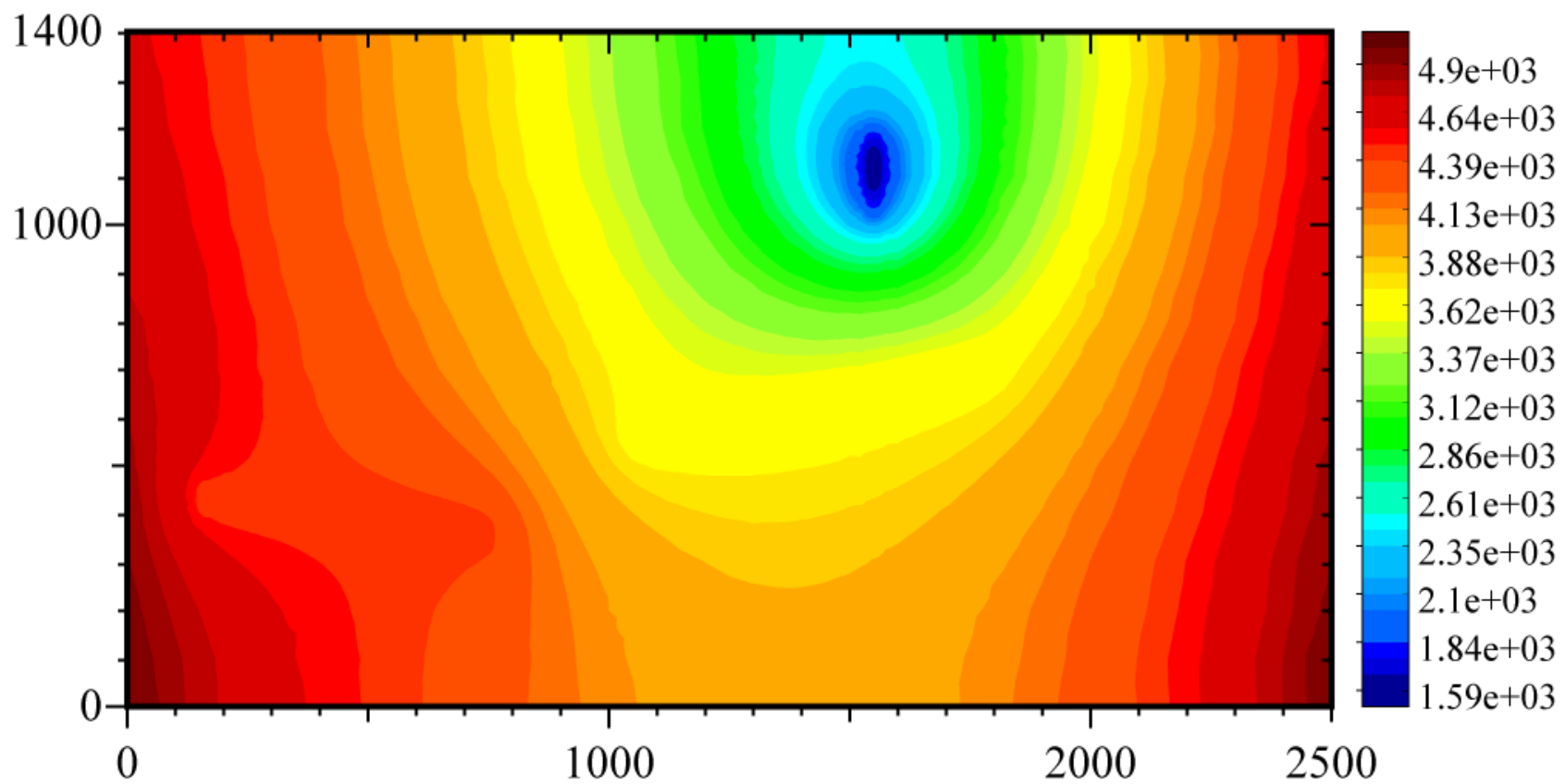


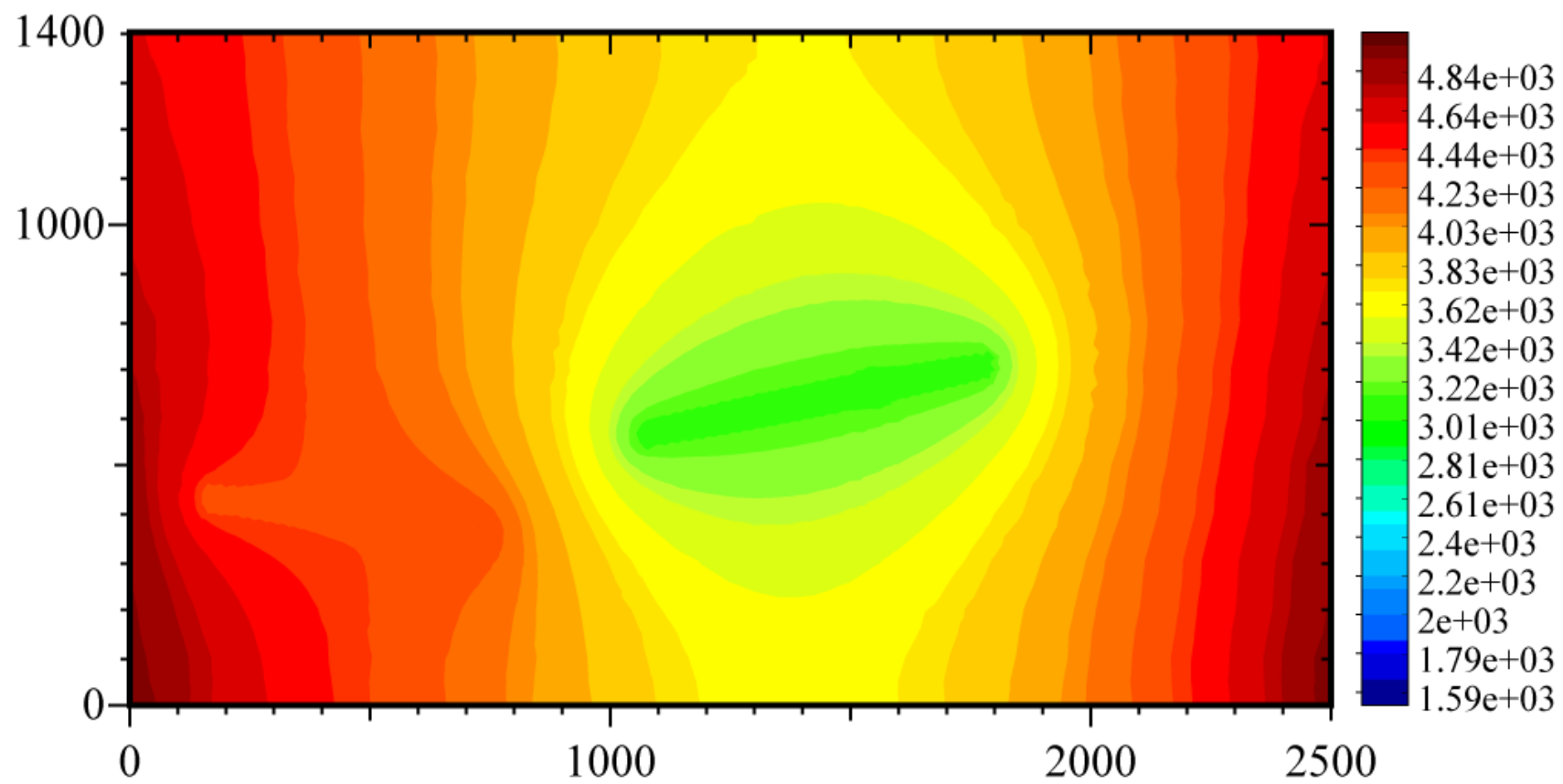
(b)

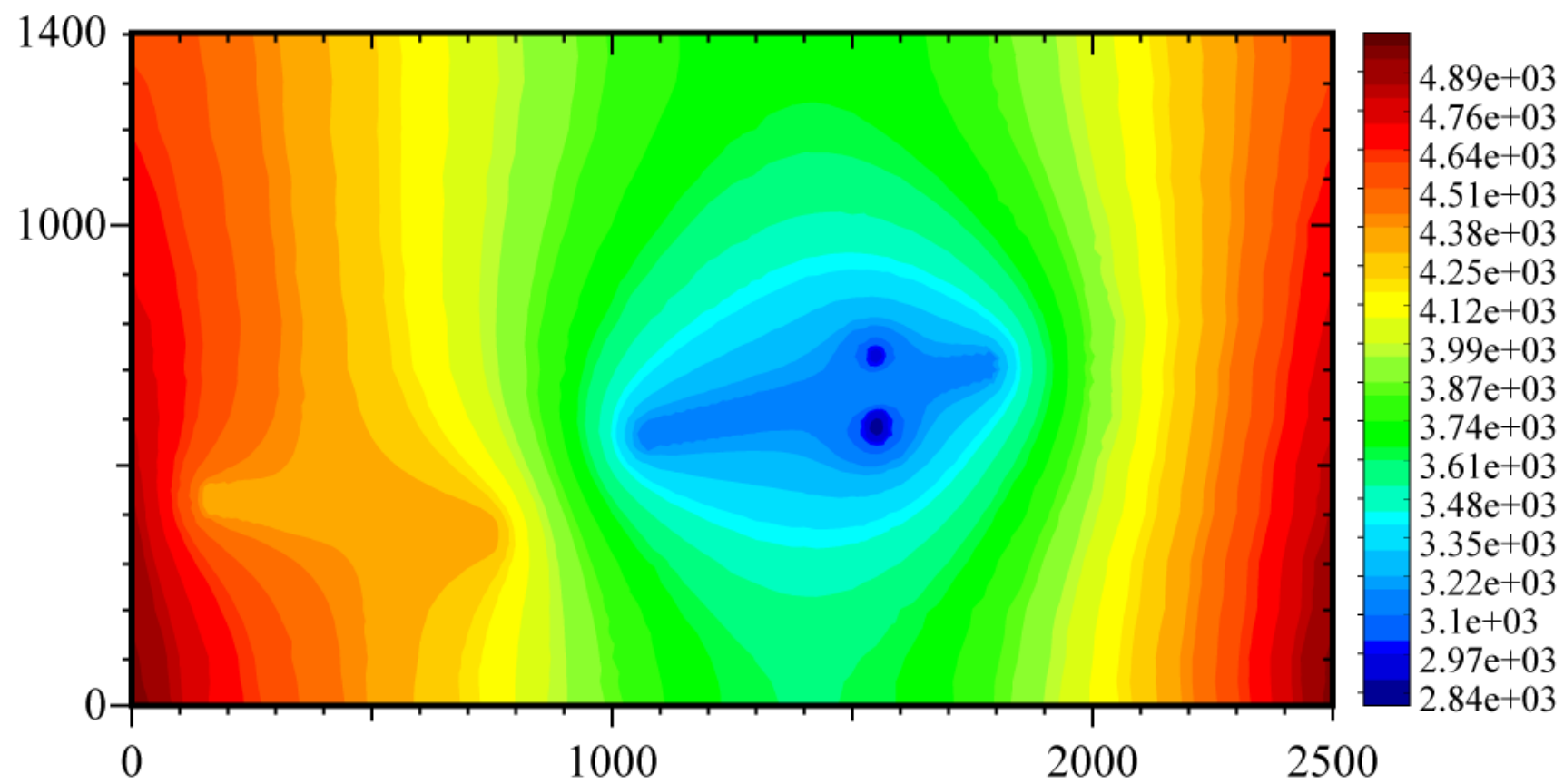










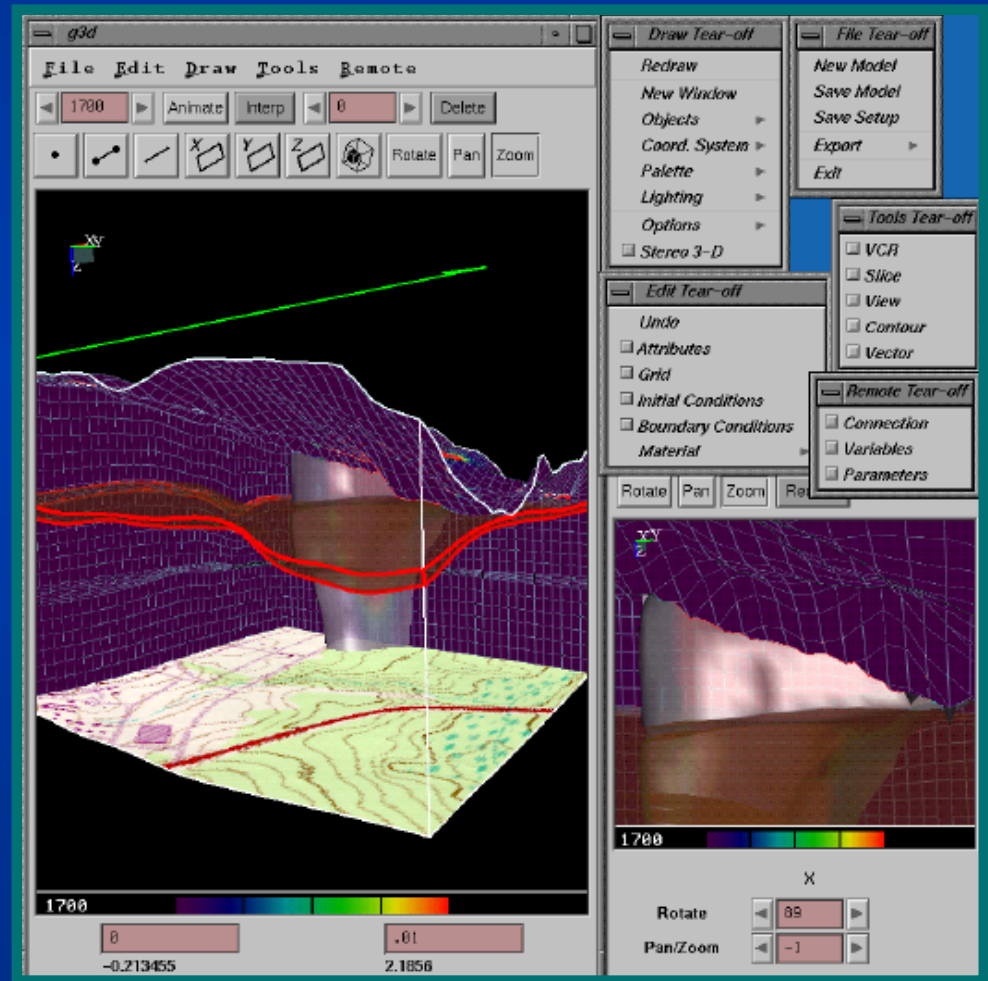


G3D - GRAPHICS FRONT-END

- ◆ **Software Engineering**
 - Motif with OpenGL / MESA rendering areas
 - Self-Interrupting Work Stack
- ◆ **3D Pre-processing**
 - Data set construction
 - GIS Import of Field Data
 - Data Verification
- ◆ **Post-processing**
 - Data Verification
 - Model and Algorithm Verification
- ◆ **Controller library coupling**

GRAPHICS PRE-PROCESSING

- ◆ 3D grid creation and editing
- ◆ Material properties
- ◆ Initial conditions
- ◆ Time dependent boundary conditions
- ◆ Multiple views



GRAPHICS POST-PROCESSING

- ◆ Multiple vector/scalar fields
- ◆ Time animation
- ◆ Multiple slices/Iso-surfaces
- ◆ Stereo rendering, lighting models
- ◆ Overlay images for orientation
- ◆ Volume rendering

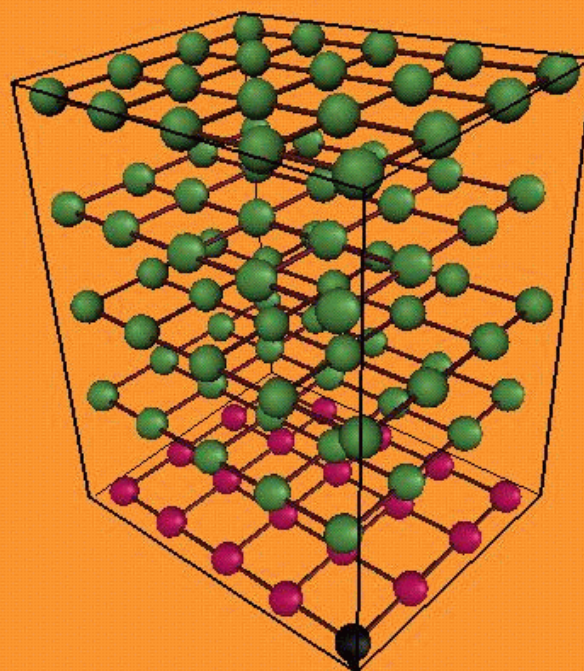
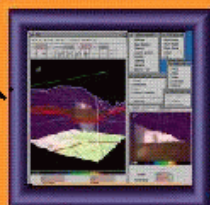
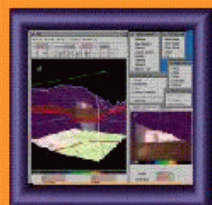
Hierarchical Representations

CONTROLLER LIBRARY

- ◆ User callable
- ◆ Client - Server
 - server MPP - client workstations
- ◆ Non-interrupt approach
- ◆ Controller - “Graphics” Node
 - processes client requests and performs scale analysis/compression
- ◆ MPI Message passing
- ◆ Remote procedure calls

PICS : Interactive Steering and Visualization

Remote
Graphics
Workstation



**P
A
R
A
G
O
N**



System
Node



Compute
Node



Graphics
Node

COMPRESSION MODULE FOR ENCODED TRANSMISSION OVER CONGESTED NETWORKS

- ◆ Wavelet based processing
 - Fast decomposition/reconstruct
 - Nonlinear approximation in various metrics
 - Compression
 - Feature identification at various scales
 - Scale up/scale down
- ◆ Progressive transmission
 - Lossy to lossless
 - Adaptive local spatial resolution
- ◆ Scattered data assimilation and denoising

INTERACTIVE CONTROL OF LARGE-SCALE SIMULATIONS

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