GROUNDWATER REMEDIATION EXPERIMENTS USING INTERACTIVE COMPUTATIONAL STEERING ON THE INTEL PARAGON

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OUTLINE

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  - Need for Steering and Tracking
- **Implementation Details**
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    - Numerical Implementation
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  - Graphical and Controller Library G3D
  - Coupling PGREM3D and G3D
- **Results**
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  - Some snapshots
- **Conclusions**

OBJECTIVE

- To produce an interactive groundwater remediation research and design tool that will utilize the computational power of an MPP machine (Intel Paragon) and the graphical capabilities of a graphics workstation (SGI workstation).

NEED FOR INTERACTIVE TRACKING AND STEERING

- Large scale groundwater remediation experiments either for research or design purposes can be costly in terms of time and effort.
- An interactive tool can greatly minimize the need to perform repeated simulations inorder to arrive at an optimal remediation design.
- The ability to perform effective interactive simulations depend on the following
  - Application Code – Speed of computations
    - High performance computing systems
    - Powerful computational algorithms
  - Graphical Interface Front–End
  - Effective communication between the Graphics Front–End and the application code

APPLICATION CODE PGREM3D

- **PGREM3D: Parallel Groundwater Transport and Remediation Code (*Mahinthakumar, 1997*)**
  - Primarily intended for large scale simulations
- **PGREM3D has three main modules:**
  - Finite Element Flow
  - Finite Element Transport
  - Particle Tracking Transport (not used in this study)
- **Finite Element Flow**
  - 3D steady state saturated flow
- **Finite Element Transport**
  - 3D advection–dispersion with first order kinetic and nonlinear bioremediation reactions

PGREM3D EQUATIONS

CONTAMINANT

$$\frac{\partial C}{\partial t} = \nabla \cdot (\boldsymbol{D} \cdot \nabla \boldsymbol{C}) - \nabla \cdot (C\,\boldsymbol{v}) - R_C$$

$$R_C = \mu_{\max} X \left(\frac{C}{K_C + C}\right)\left(\frac{N}{K_N + N}\right) + (\lambda + K_w)C + (\lambda + K_s)S_C + \frac{\rho}{\theta}\frac{\partial S_C}{\partial t} + \frac{q}{\theta}(C - C_0)$$

$$\frac{\partial S_C}{\partial t} = k_r\,(K_d\,C - S_C) - (\lambda + K_s)S_C$$

C = Dissolved Phase Contaminant Concentration

NUTRIENT

$$\frac{\partial N}{\partial t} = \nabla \cdot (\boldsymbol{D} \cdot \nabla \boldsymbol{N}) - \nabla \cdot (N\,\boldsymbol{v}) - R_N$$

$$R_N = \mu_{\max} X \left(\frac{C}{K_C + C}\right)\left(\frac{N}{K_N + N}\right) + f_{use} b X \left(\frac{N}{K_N + N}\right) + (\lambda + K_w)C + (\lambda + K_s)S_N + \frac{\rho}{\theta}\frac{\partial S_N}{\partial t} + \frac{q}{\theta}(N - N_0)$$

$$\frac{\partial S_N}{\partial t} = k_r\,(K_d\,N - S_N) - (\lambda + K_s)S_N$$

N = Dissolved Phase Nutrient Concentration

BIOMASS

$$\frac{\partial X}{\partial t} = \mu_{\max} X \left(\frac{C}{K_C + C}\right)\left(\frac{N}{K_N + N}\right) - bX\left(\frac{N}{K_N + N}\right)$$

X = Biomass Concentration

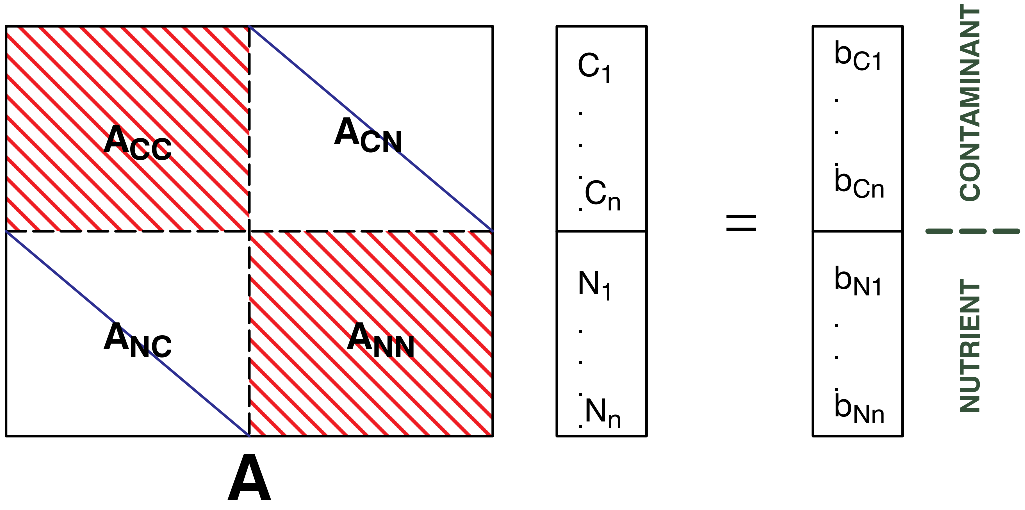
$$D_{ij} = \alpha_T |\boldsymbol{v}| \delta_{ij} + (\alpha_L - \alpha_T)\frac{v_i v_j}{|\boldsymbol{v}|} + D_m$$ *Disperisivity Tensor*

$$\nabla(\boldsymbol{K}\nabla h) = q \qquad \theta\,\boldsymbol{v} = -\boldsymbol{K}\nabla h$$ *Flow Equations*

MAIN FEATURES OF PGREM3D TRANSPORT

- **Three–dimensional advection–dispersion equation with first order kinetic and nonlinear bioremediation reactions.**
  - Flexible boundary conditions with options to use time–dependent and cyclic time–dependent cases.
- **Galerkin finite–elements with 8–node hexahedral elements.**
  - Logically rectangular grid structure (with ”natural ordering” of nodes and elements) with options to use uniform rectangular, non–uniform rectangular, and fully distorted grids.
- **Solution algorithms**
  - Non–linearity handled by picard iterations
  - Matrix solution performed by iterative Krylov solvers. Options available to use BiCGSTAB, GMRES(m), ORTHOMIN(k), and CGS.
- **Parallelization using 2–D domain decomposition**
  - explicit message passing using NX or MPI
  - portability has been tested on Intel Paragons, SGI Power Challenge Arrays, Cray/SGI Origin–2000, Convex Exemplar SPP–1200, and IBM SP.

COUPLED MATRIX SYSTEM

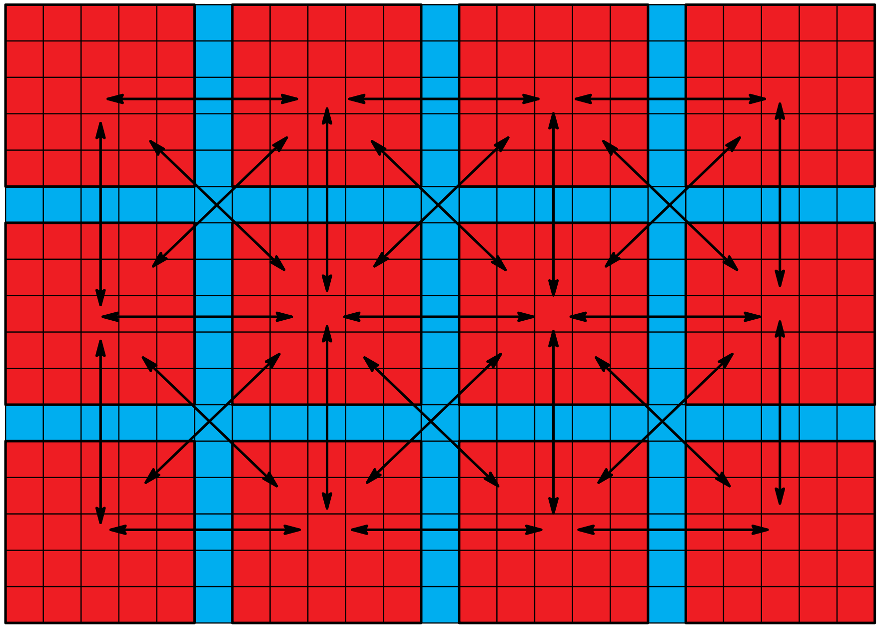


- **A lumped formulation is used for all zeroth derivative and time derivative terms including non–linear coupling terms**
  - **this in turn greatly simplifies the implementation by making the off–diagonal coupling blocks to be unit diagonal**

PARALLEL IMPLEMENTATION OF PGREM3D

- Two–dimensional domain decomposition
  - communication with at most 8 neighboring processors
  - natural node ordering for individual processor regions
- Explicit message passing required to exchange information at processor boundaries especially during finite–element assembly and matrix–vector product stages
  - NX communication library for Intel architectures
  - MPI for other architectures
- Scalability has been demonstrated up to 1024 processors of the Intel Paragon

PARALLEL DOMAIN DECOMPOSITION



🟦 overlapping processor regions

🟥 individual processor regions

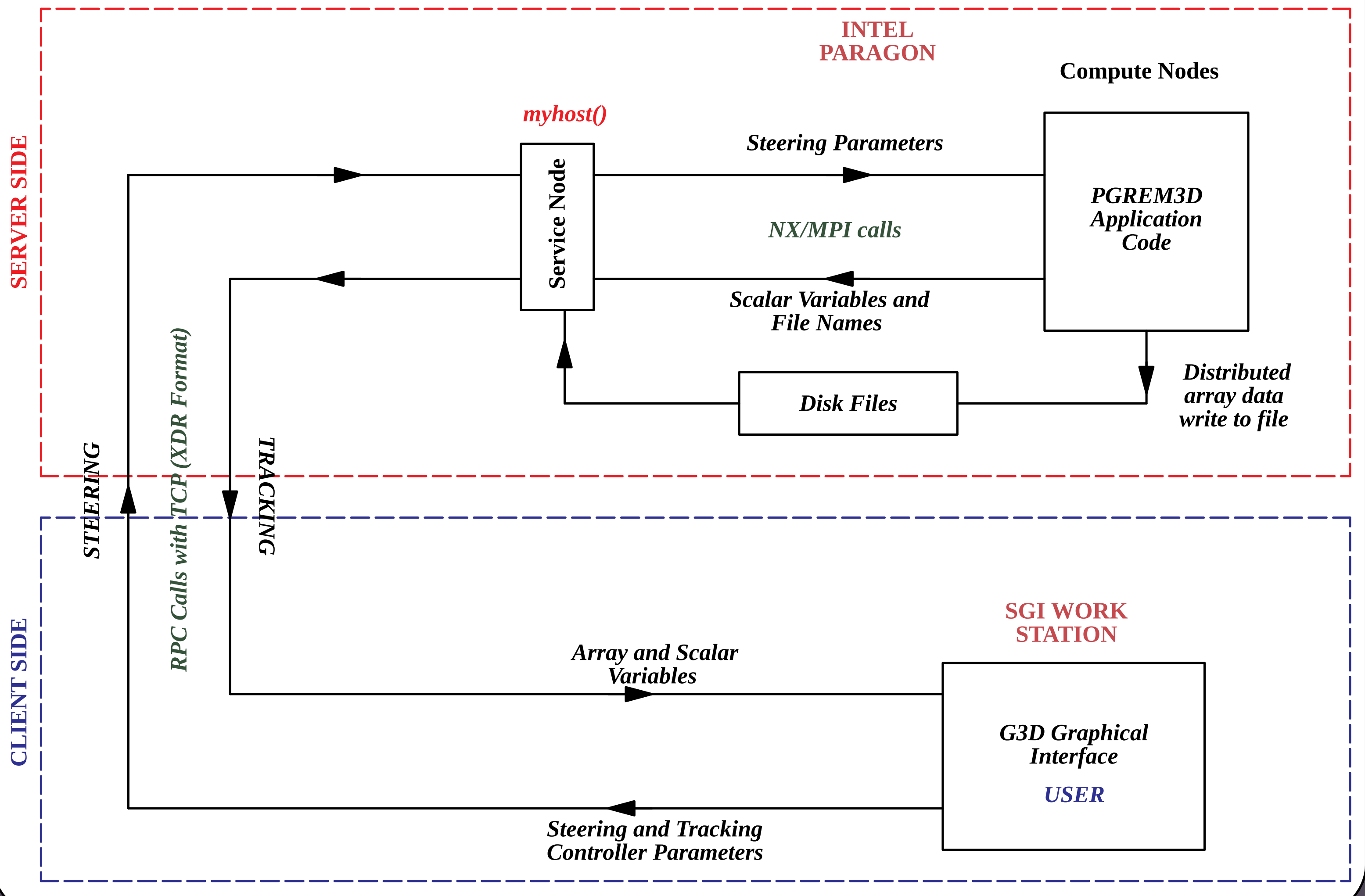
(arrows show communication pattern)

Plan View of Two–Dimensional Domain Decomposition
(showing a 4x3 processor decomposition)

MAIN FEATURES OF G3D AND CONTROLLER LIBRARY

- **Graphical User Interface G3D (*Johnson et al., 1997*)**
  - pre–processing capabilities
    - grid and boundary condition specification/editing
    - material properties and initial conditions
  - post–processing capabilities
    - multiple orthogonal slices
    - multiple isosurfaces (both opaque and semi–transparent)
    - time animations
- **Controller library (*Kaulgud et al.,* 1997)**
  - uses RPC calls with TCP to exchange data between the Client (SGI workstation) and the Server (Intel Paragon)
    - XDR library is used to handle byte–ordering between machines
  - Tracking (Server to Client)
    - interactively visualize progress of a simulation
  - Steering (Client to Server)
    - interactively steer the computation

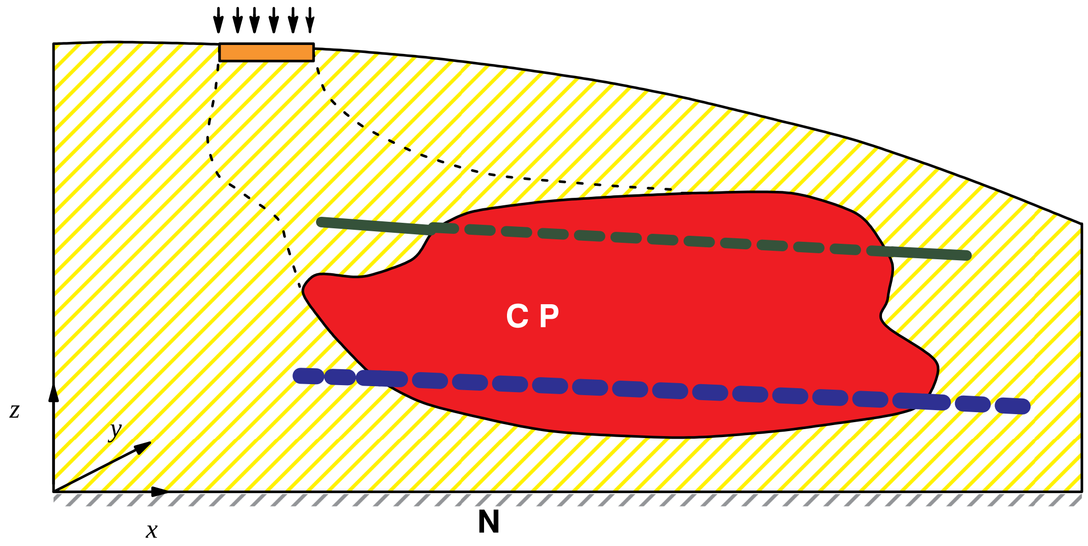
SCHEMATIC LAYOUT OF INTEGRATED USER ENVIRONMENT



COUPLING G3D AND PGREM3D

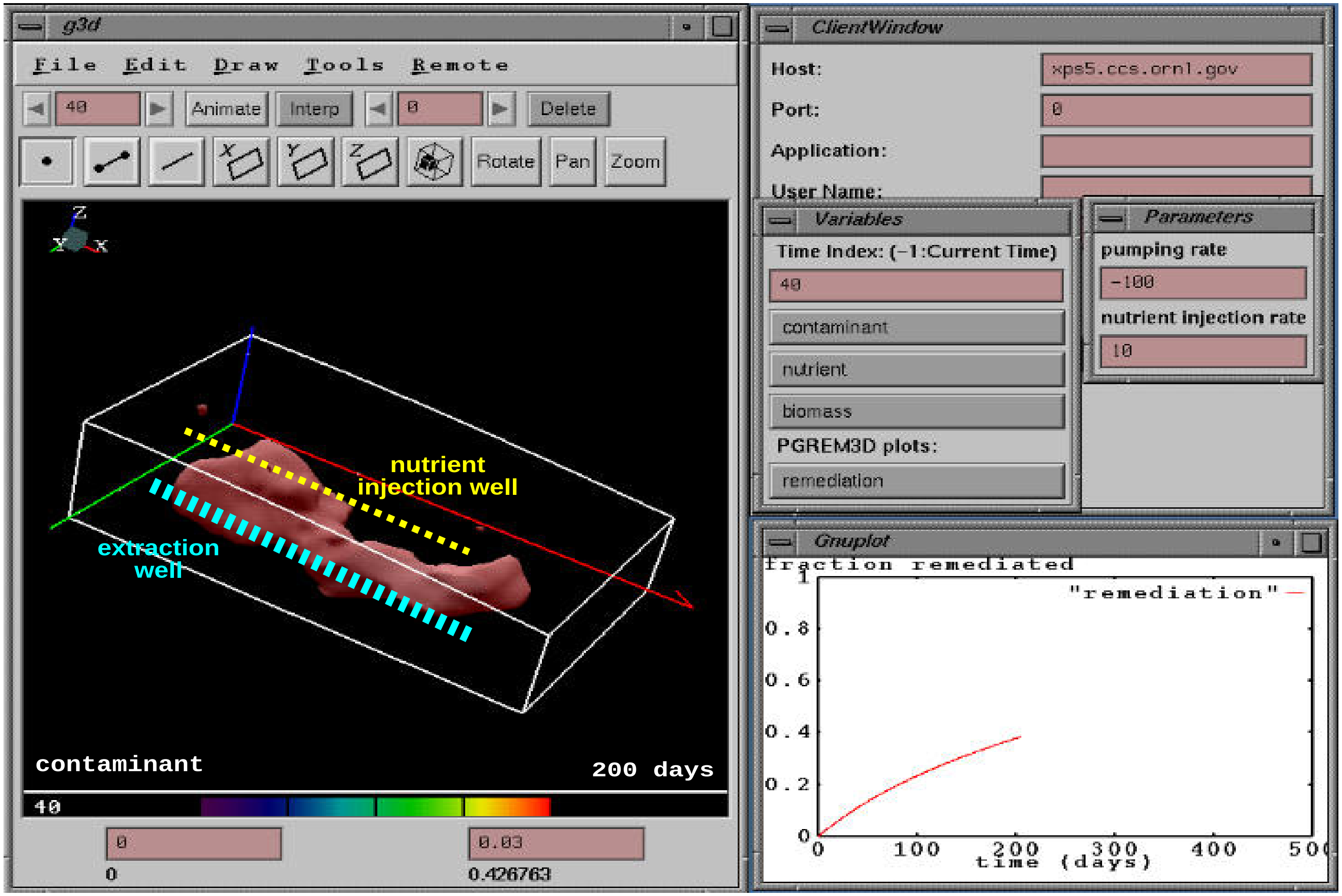
- user will write a few routines on the server side which will be used to communicate with the server library examples are provided with the library
  - register all variables (for initialization)
  - send variables (for tracking)
    - concentrations, remediation efficiency etc.
  - get parameters (for steering)
    - pumping rates, injection rates etc.
- these routines will then be called from the application code at desired break points

TEST PROBLEM FOR REMEDIATION EXPERIMENT



- The test problem is a slight modification of the Waterloo Problem (*Segol, 1994*).
- Fully heterogeneous hydraulic conductivity field generated by the turning bands algorithm (*Tompson et al., 1989*).
- contaminant plume is generated from a naturally leaching source which is capped after a certain duration.

SNAPSHOT OF REMEDIATION EXPERIMENT (CONTAMINANT)



ClientWindow

Host: xps5.ccs.ornl.gov

Port: 0

Application:

User Name:

Variables

Time Index: (-1:Current Time) 40

contaminant

nutrient

biomass

PGREM3D plots:

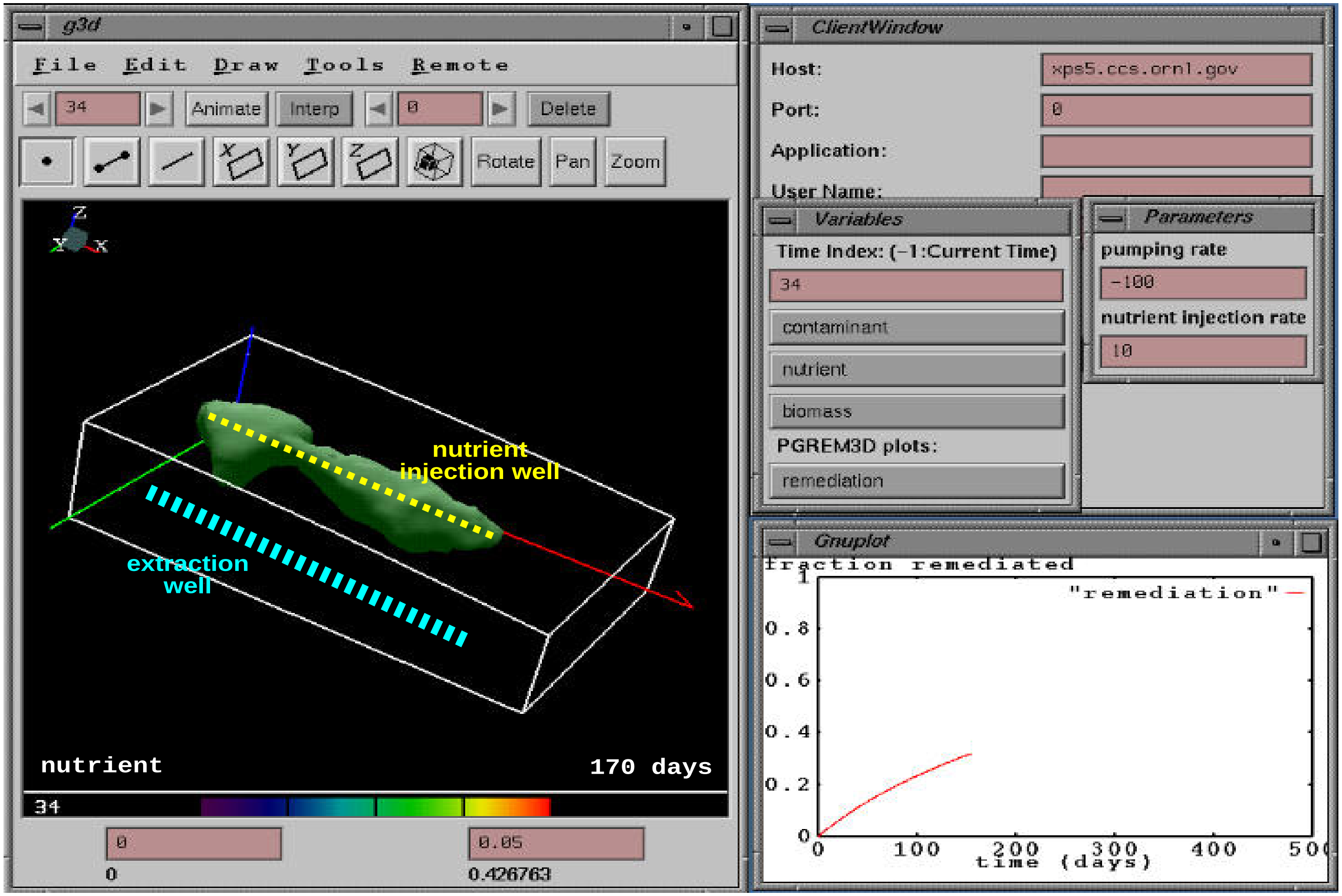
remediation

Parameters

pumping rate -100

nutrient injection rate 10

SNAPSHOT OF REMEDIATION EXPERIMENT (NUTRIENT)



Host: xps5.ccs.ornl.gov

Port: 0

Application:

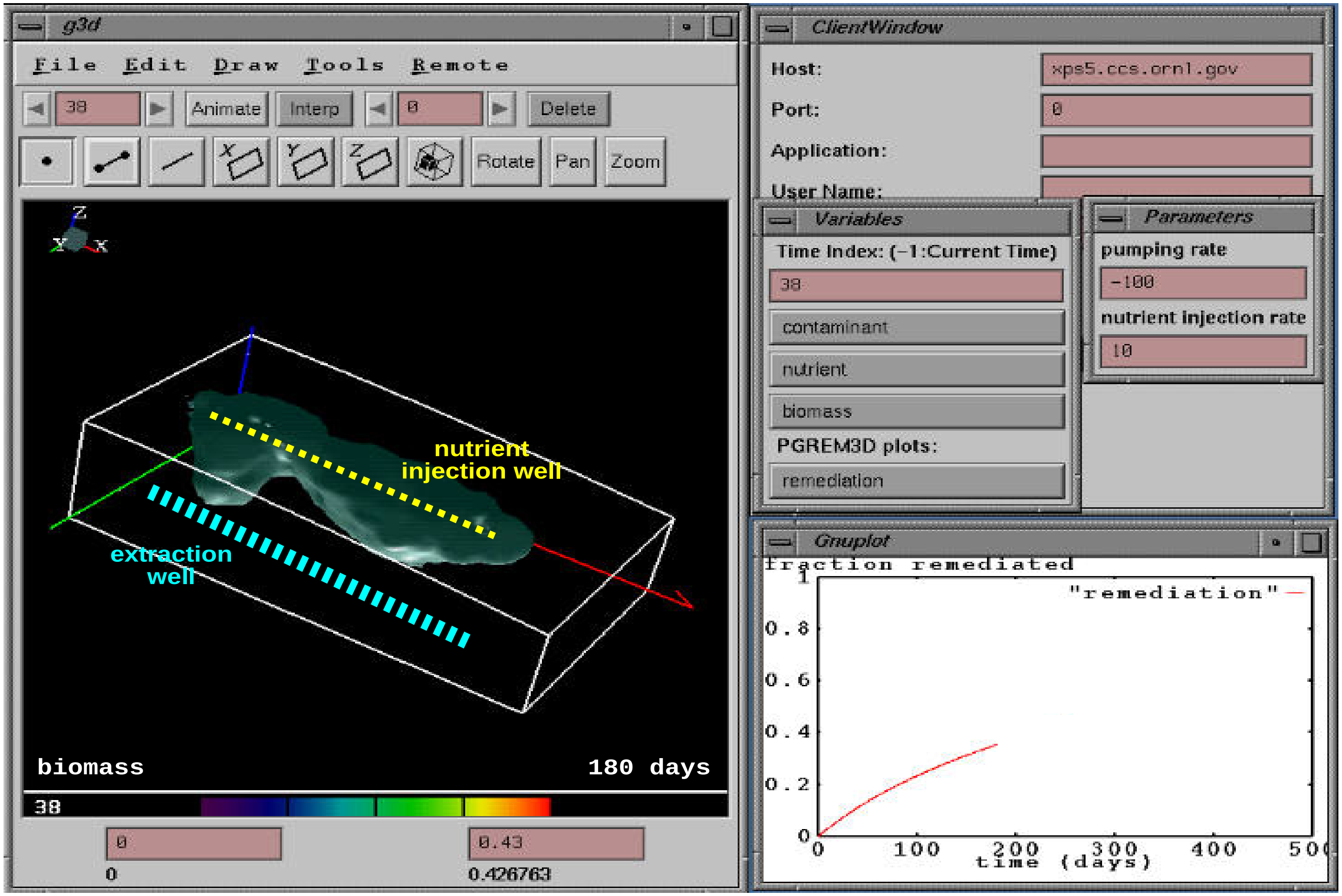
User Name:

Time Index: (-1:Current Time) 34

pumping rate -100

nutrient injection rate 10

SNAPSHOT OF REMEDIATION EXPERIMENT (BIOMASS)



Host: xps5.ccs.ornl.gov

Port: 0

Application:

User Name:

Time Index: (-1:Current Time) 38

pumping rate -100

nutrient injection rate 10

CONCLUSIONS

- **An integrated user environment for groundwater remediation designs has been created by coupling an application code with a graphical controller library**
  - **Both tracking and steering capabilities have been tested**
  - **A groundwater remediation experiment involving coupled bioremediation and pump–and–treat system has been tested**
- **Future work needs to be done inorder to bring this to an industrial strength production environment**
  - **The application code PGREM3D needs future work to handle unsaturated and multi–phase flow, flow in fractured media, geochemical reactions, bacterial transport etc.**
  - **New hooks need to be built into both the application code and the library to handle well positioning, simultaneous visualization of multiple variables, automatic display of remediation curves etc.**

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