

# Large Irregular Datasets and the Computational Grid

Joel Saltz

University of Maryland College Park

Computer Science Department

Johns Hopkins Medical Institutions

Pathology Department

# Computational grids and Irregular Multidimensional Datasets

- Spatial/multidimensional multi-scale, multi-resolution
- Applications select portions of one or more datasets
- Selection of data subset makes use of spatial index (e.g. R tree or quad tree)
- Data not used “as-is”, generally preprocessing is needed
- *Databases to carry out spatial queries and data aggregation in irregular multidimensional datasets*

# Querying Irregular Multidimensional Datasets

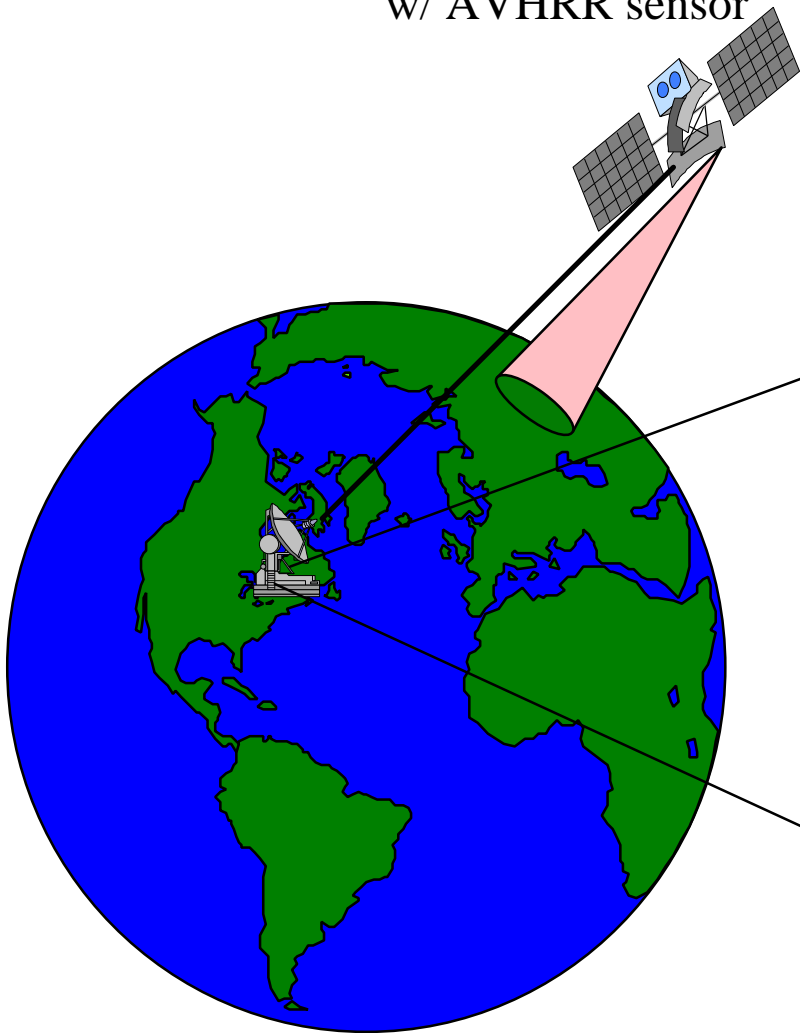
- Irregular datasets
  - Think of *disk based* unstructured meshes, data structures used in adaptive multiple grid calculations
    - indexed by spatial location (e.g. position on earth, position of microscope stage)
  - Spatial query used to specify iterator
    - computation carried out on data obtained from spatial query
    - computation aggregates data - resulting data product size significantly smaller than results of range query

# Application Scenarios

- Ad-hoc queries or data products from satellite sensor data
- Sensor data, fluid dynamics and chemistry codes to predict condition of waterways (e.g. Chesapeake bay simulation) and to carry out reservoir simulation
- Browse or analyze (multiresolution) digitized slides from high power light or electron microscopy (1-50Gbytes per digitized slide - 1000's of slides per day per hospital)
- Predict materials properties using electron microscope computerized tomography sensor data
- Post-processing, analysis and exploration of data generated by large scientific simulations

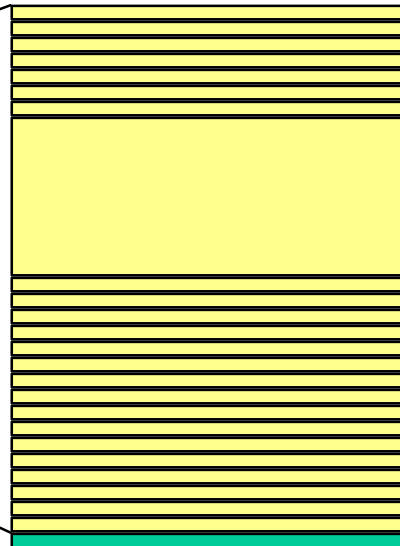
# Processing Remotely Sensed Data

NOAA Tiros-N  
w/ AVHRR sensor



## AVHRR Level 1 Data

- As the TIROS-N satellite orbits, the *Advanced Very High Resolution Radiometer* (AVHRR) sensor scans perpendicular to the satellite's track.
- At regular intervals along a scan line measurements are gathered to form an *instantaneous field of view* (IFOV).
- Scan lines are aggregated into Level 1 data sets.



A single file of *Global Area Coverage* (GAC) data represents:

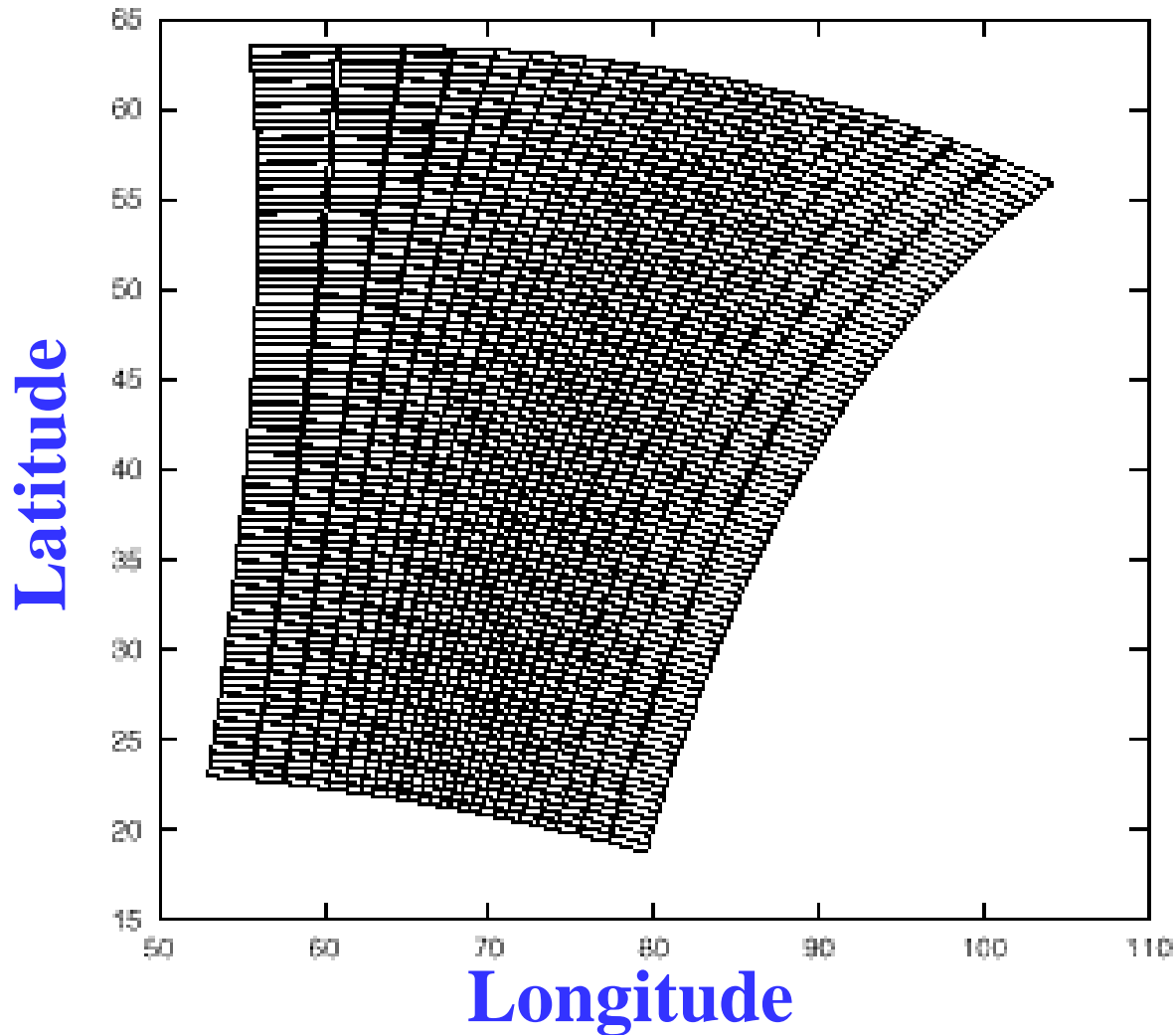
- ~one full earth orbit.
- ~110 minutes.
- ~40 megabytes.
- ~15,000 scan lines.

One scan line is 409 IFOV's

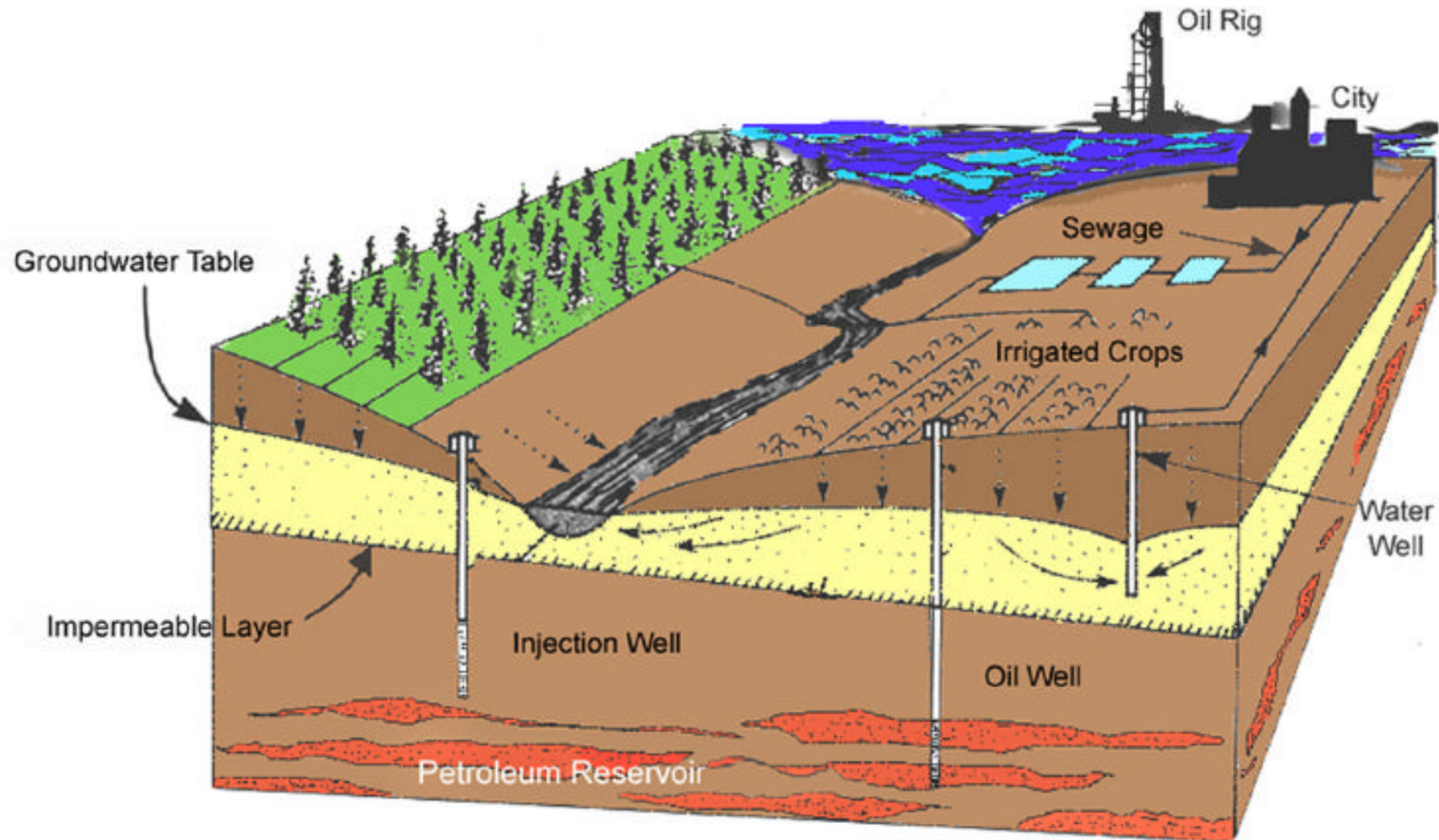


# Spatial Irregularity

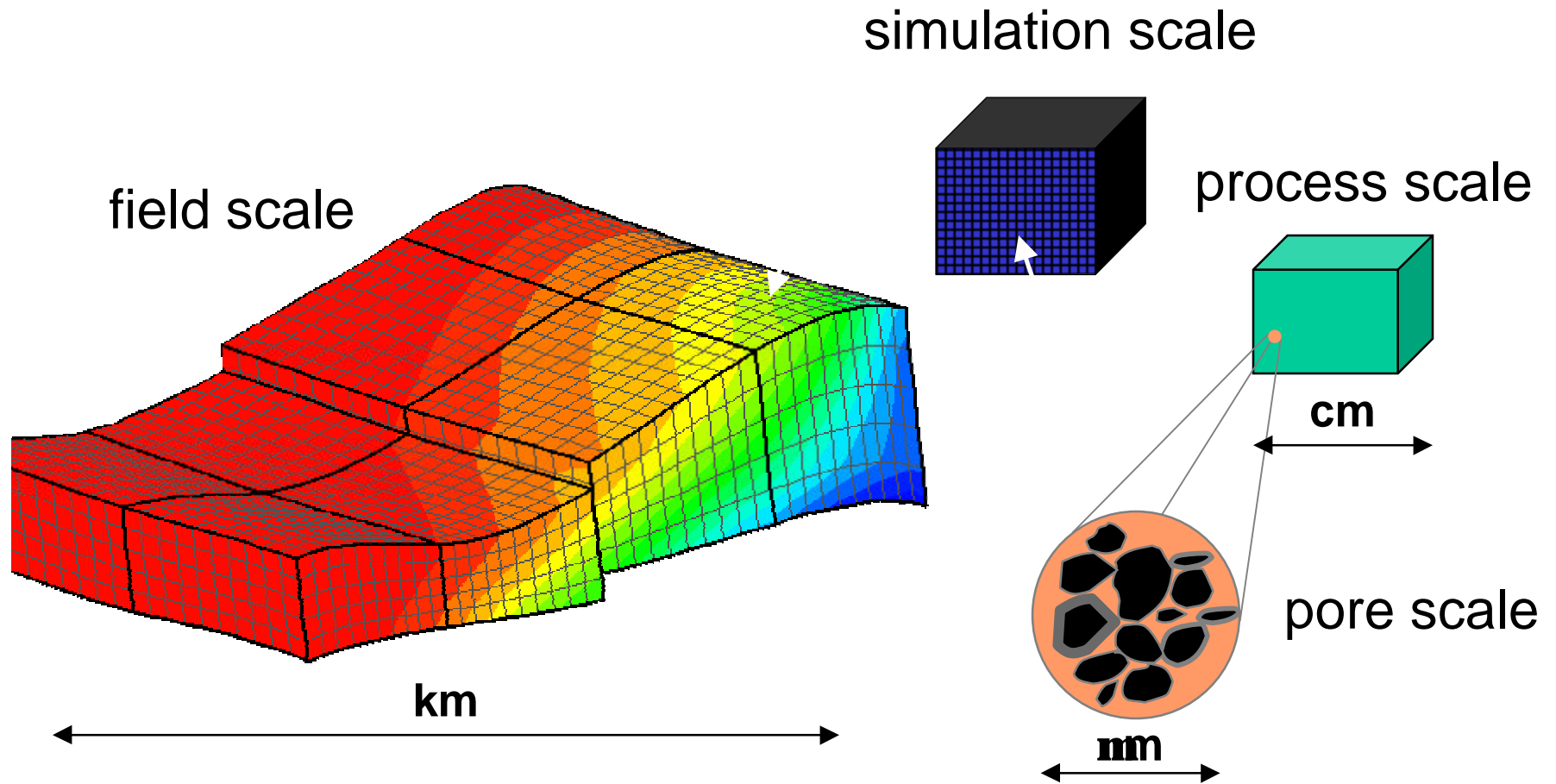
AVHRR Level 1B NOAA-7 Satellite 16x16 IFOV blocks.



# Multiscale Physics Based Simulation of Fluid Flow for Energy and Environment



# The Tyranny of Scale





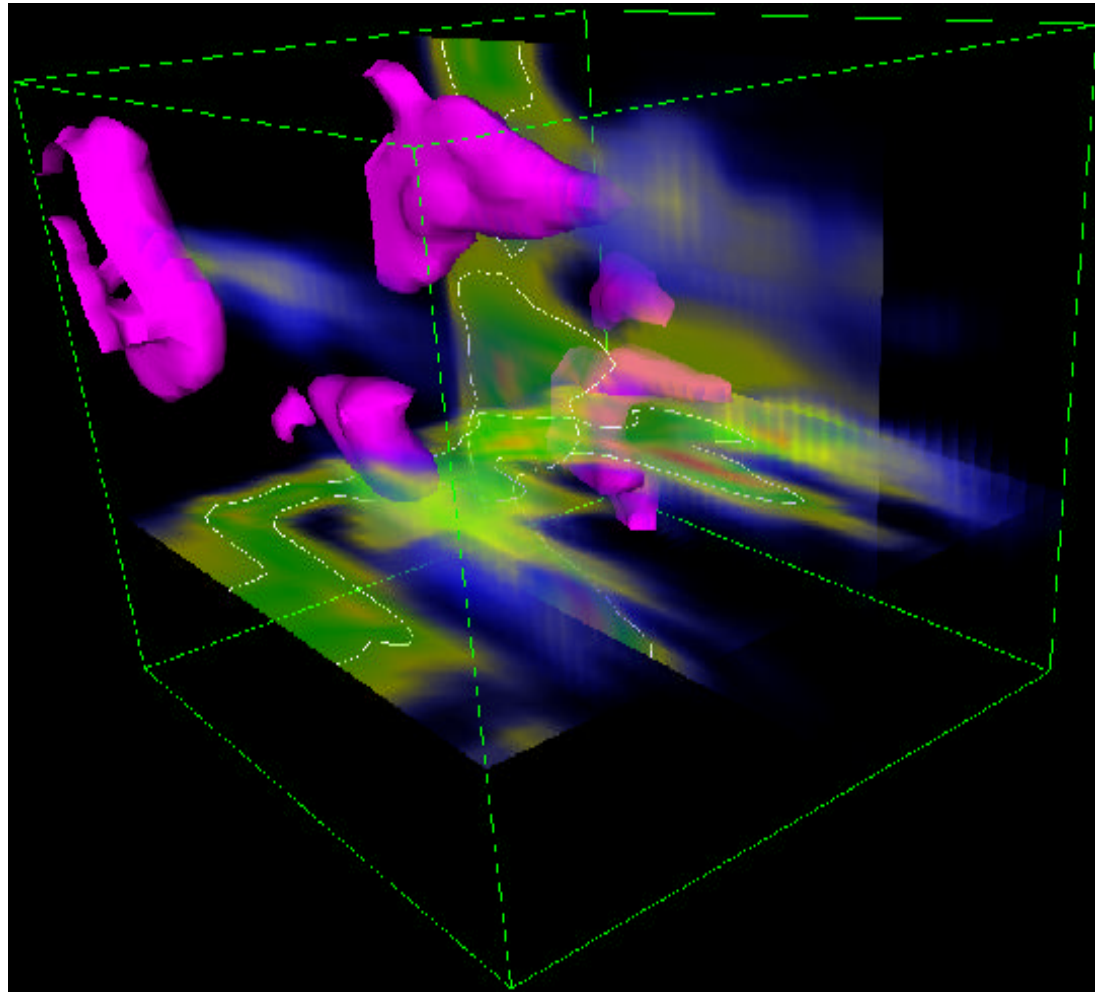
# Bioremediation Simulation

**abiotic  
reactions  
compete with  
microbes,  
reduce extent of  
biodegradation**

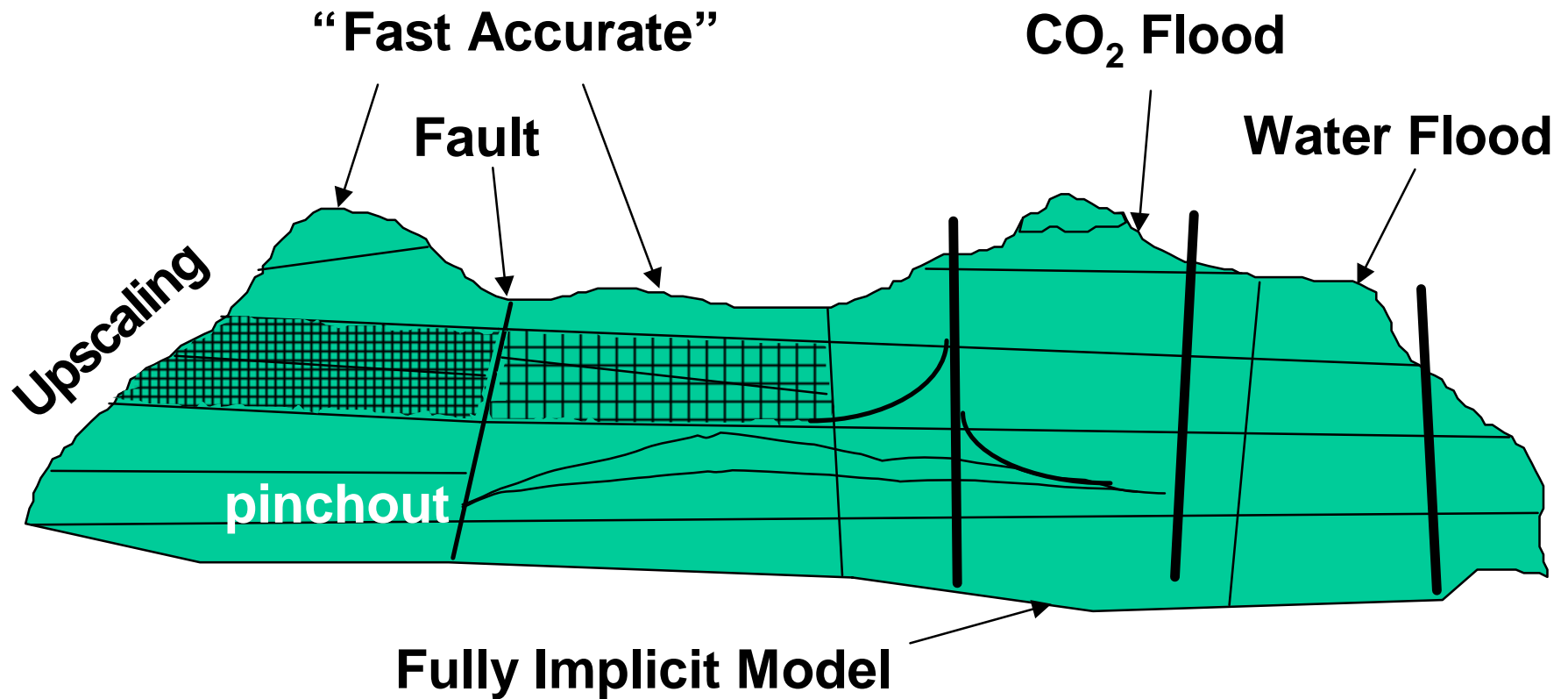
Microbe colonies  
(magenta)

Dissolved NAPL (blue)

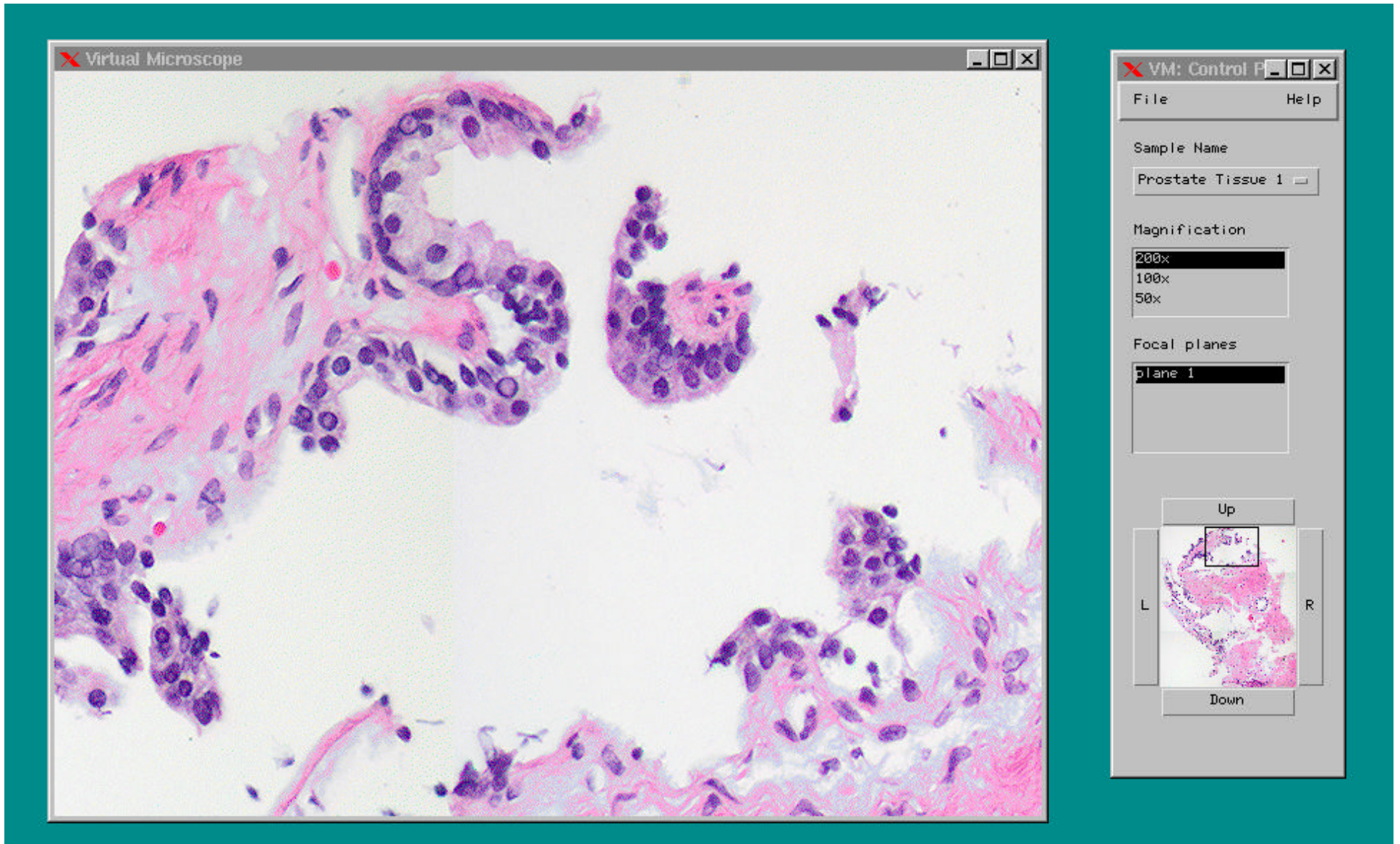
Mineral oxidation  
products (green)



# Multiblock Methods Lead to Irregular Datasets

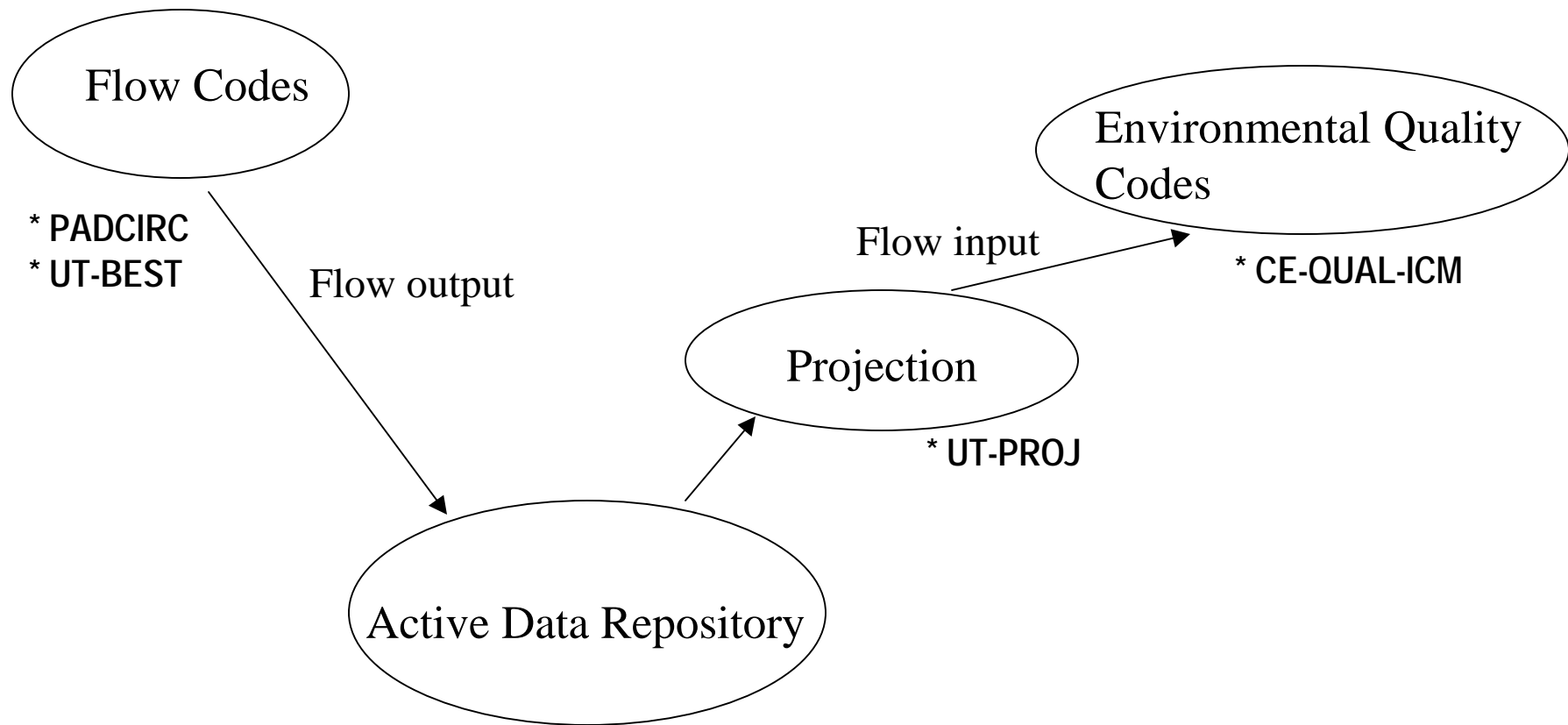


# Virtual Microscope Client



# Coupling of Different Models

(Coupling of Flow Codes with Environmental Quality Codes)



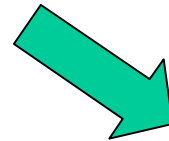
*\* Storage, retrieval, processing of multiple datasets from different flow codes*

# Active Data Repository and MetaChaos

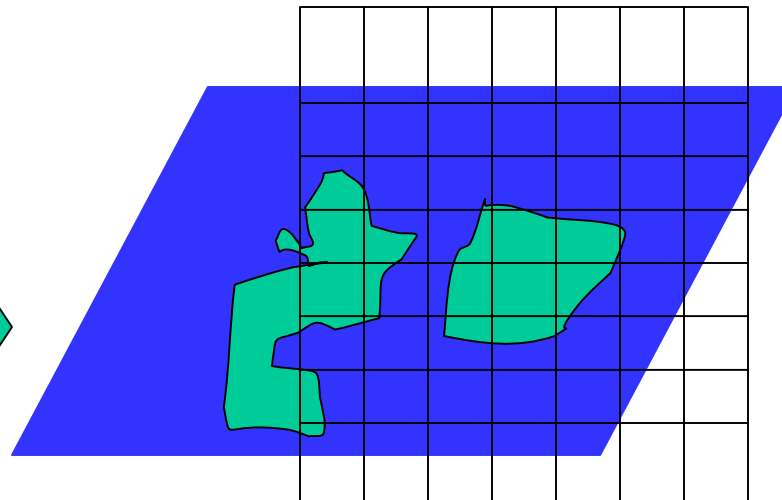
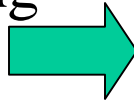
- Active Data Repository -- Parallel database infrastructure to query and preprocess multi-scale multiresolution datasets
  - Projections, interpolations, combining data from different timesteps, single value of new variable from multiple existing variables
  - Performance prediction techniques for database configuration, query optimization, software and hardware design
- MetaChaos -- Tools to couple parallel databases, parallel and distributed application programs

# Typical Query

Output grid onto  
which a projection  
is carried out



Specify portion of raw  
sensor data corresponding  
to some search criterion

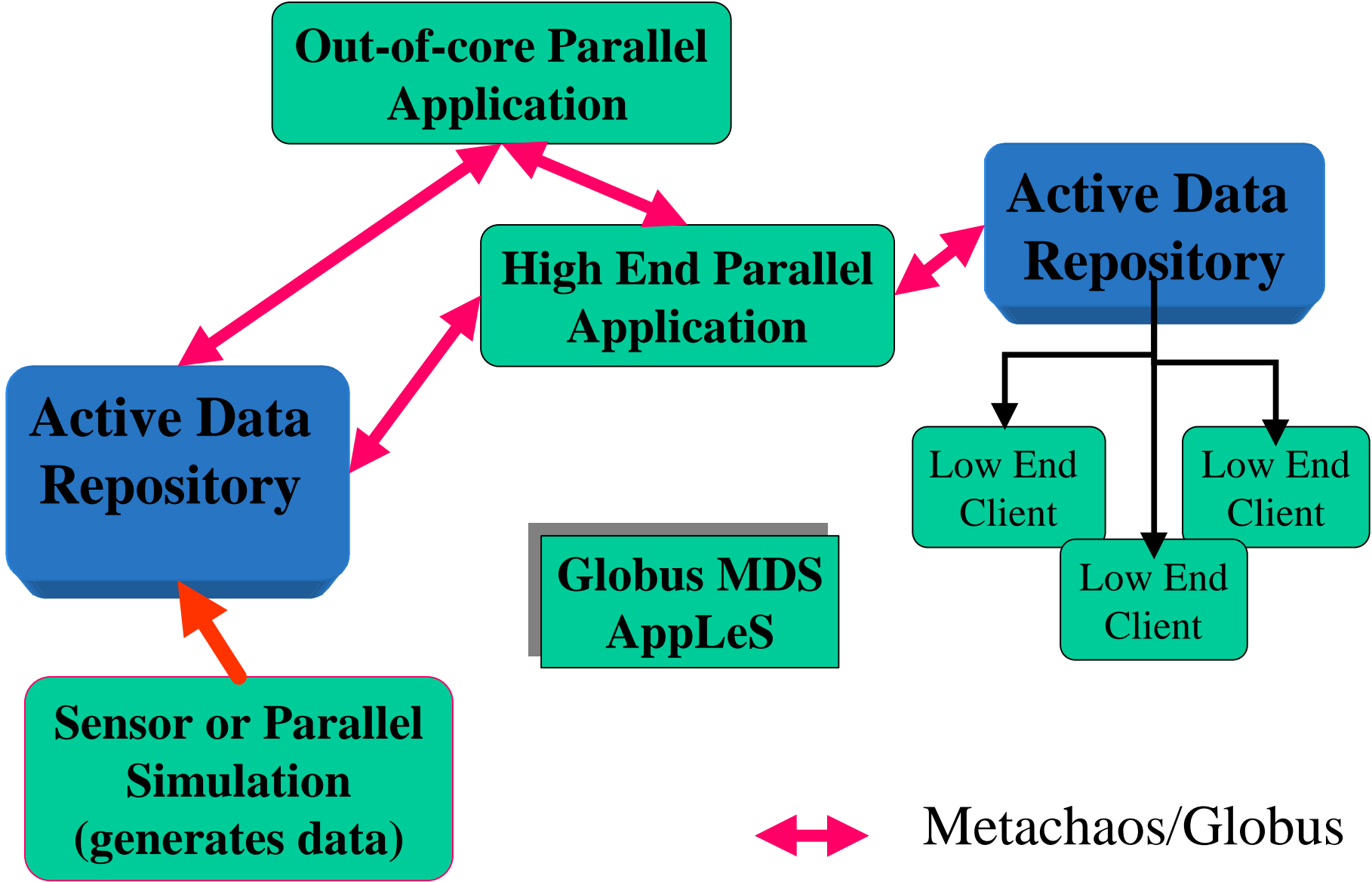




# Active Data Repository Design Objectives

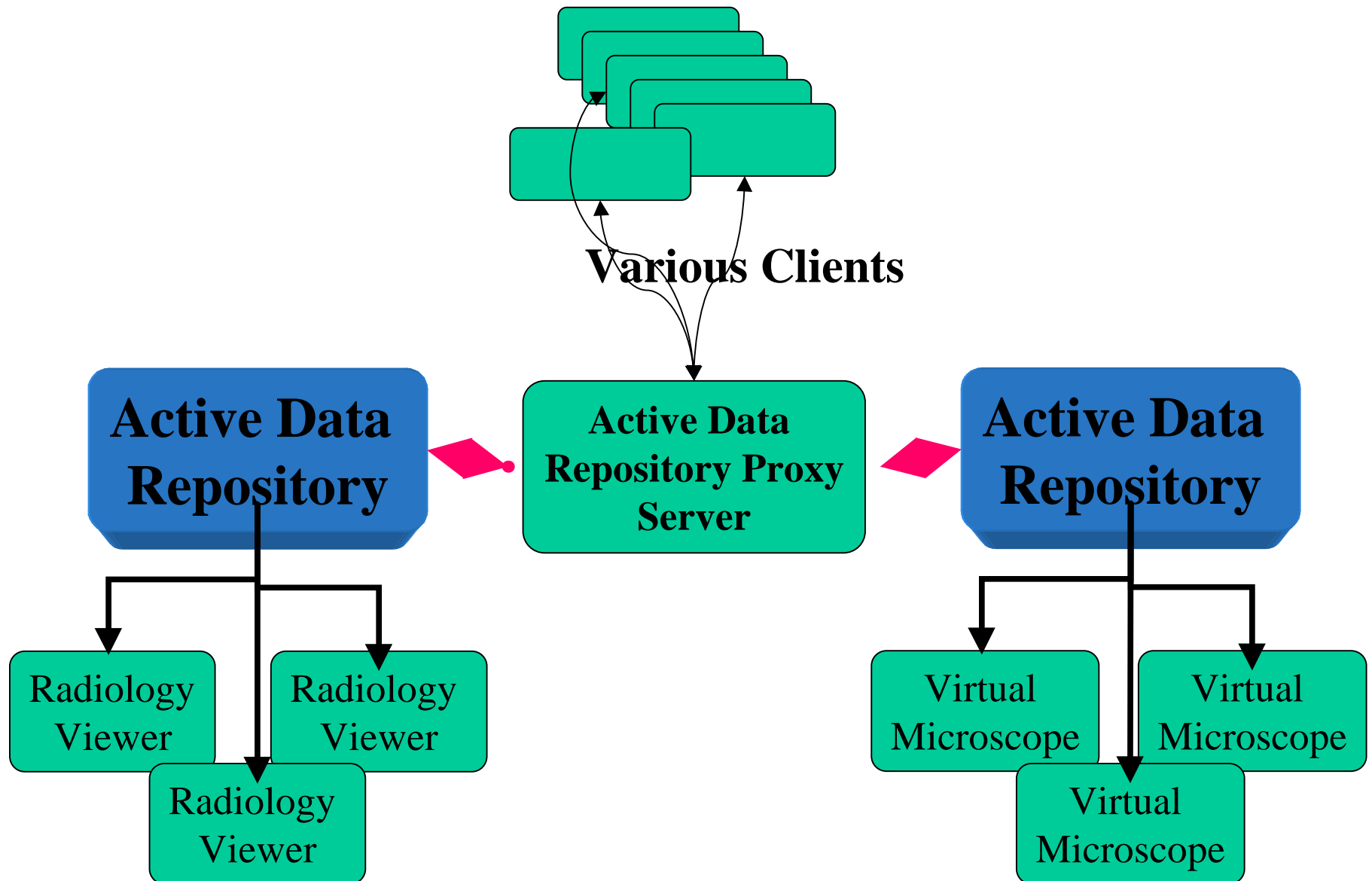
- *Support optimized associative access and processing of multiresolution and irregular persistent data structures*
- Integrate and overlap a wide range of user-defined operations, in particular, order-independent operations with the basic retrieval functions
- Targets *parallel and distributed architectures* that have been configured to support high I/O rates
- Applications -- Titan: Satellite sensor data; Virtual Microscope Server, Bay and Estuary Simulation

# Active Data Repository, MetaChaos Grid Scenarios

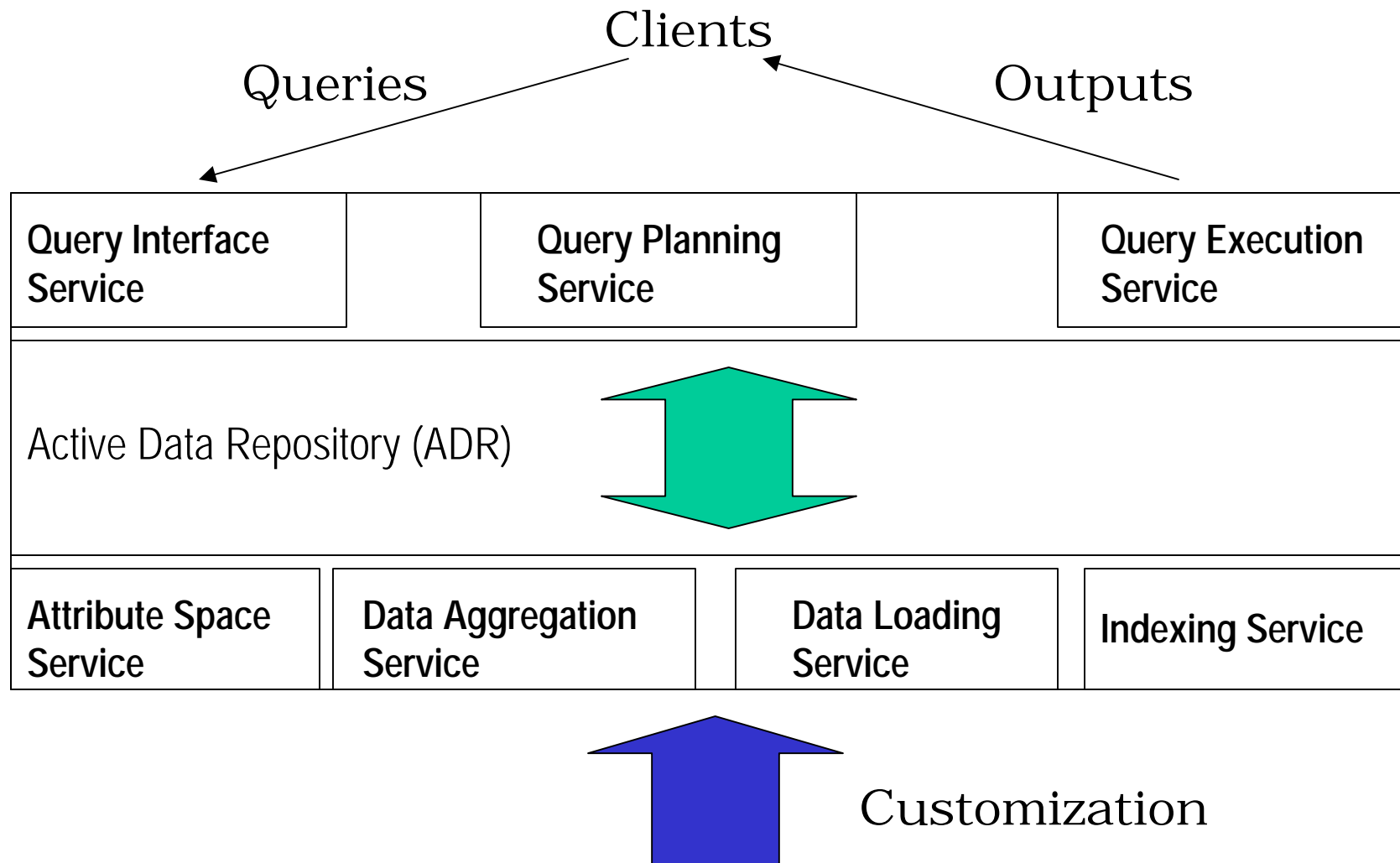




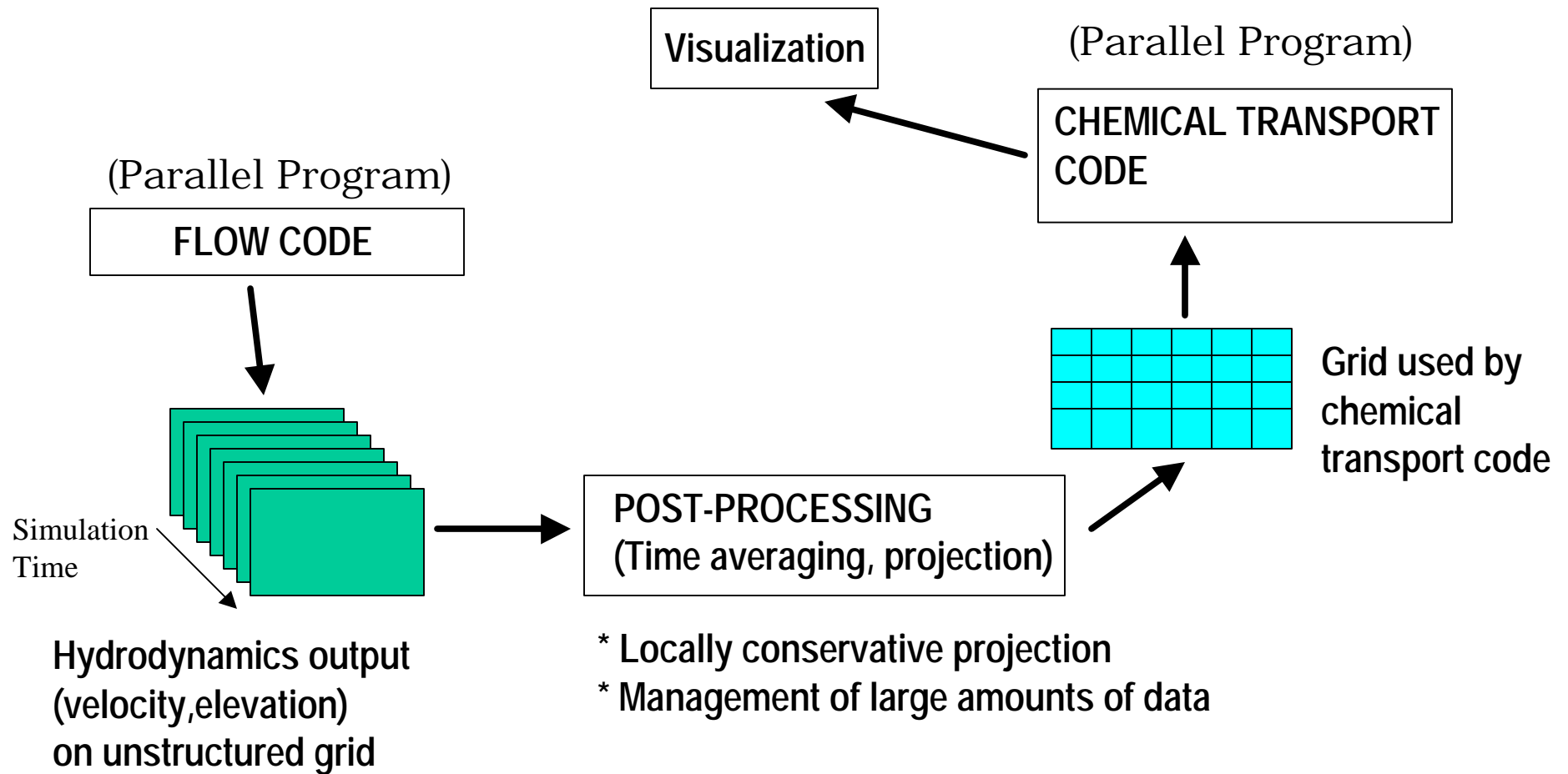
# Grid Scenarios



# Architecture of Active Data Repository



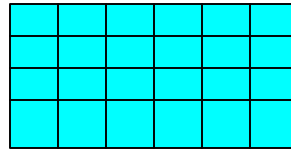
# Water Contamination Studies





# Water Contamination Studies

## Output Grid

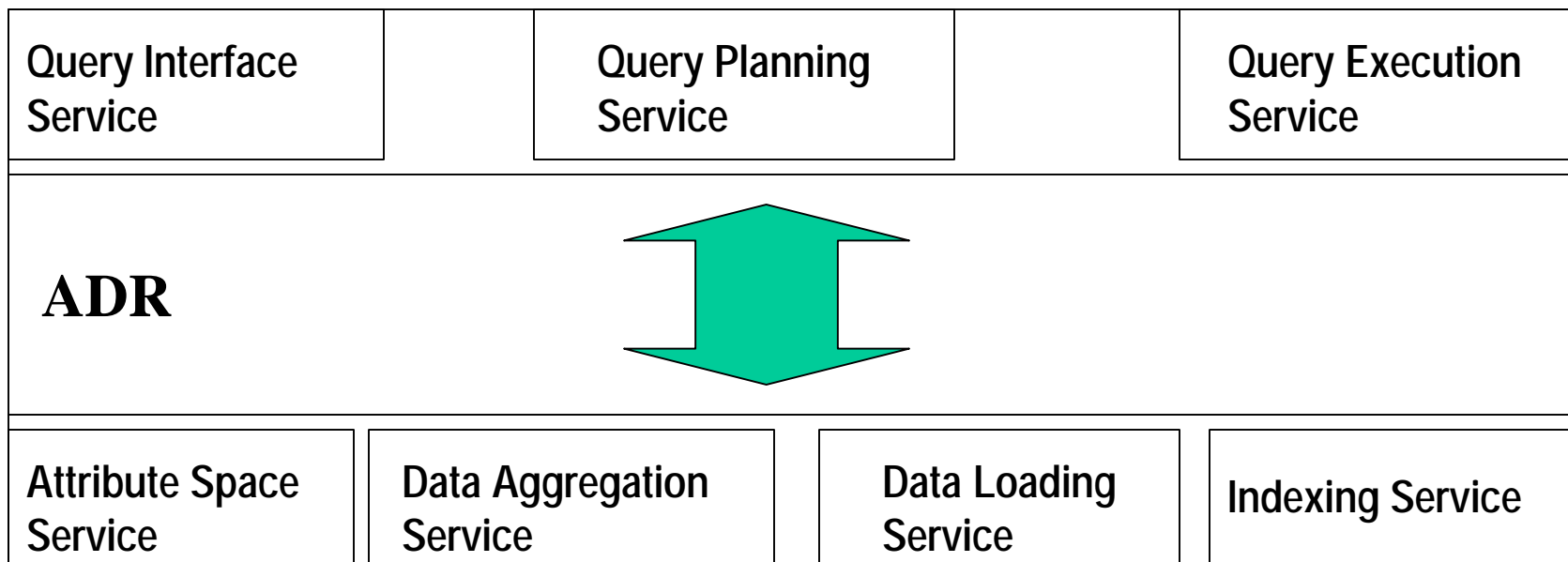


TRANSPORT CODE

Query:

- \* Time period
- \* Input grid
- \* Output grid
- \* Post-processing function (Time Averaging)

POST-PROCESSING  
(Projection)



# Performance Prediction -- Application Emulators

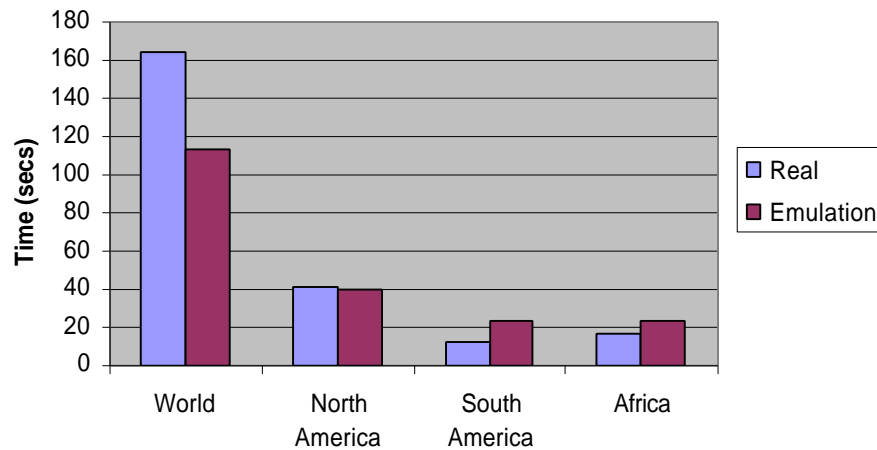
- Performance prediction:
  - How to configure database
    - data partitioning
    - how many compute processes and where should they run
  - Performance of database various possible architectures
    - standard architectures, petaflop, active disks
  - Insight into how to improve software design to optimize performance

# Performance Prediction -- Application Emulators

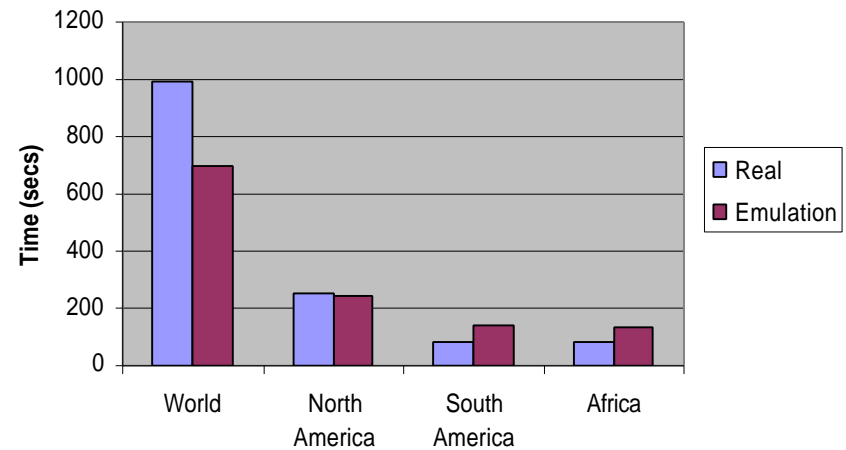
- Application Emulators:
  - Parameterized program designed to mimic application computation and data movement patterns
  - Focus is on lower layers of memory hierarchy, computational details, cache behavior are abstracted
  - Coarse grained, executable description of patterns of data movement and computation
- Simulator suite to project performance to varying levels of accuracy

# Comparison of Real Application and Emulator (Maryland 16 Processor SP-2)

## Execution Times, 10-day data



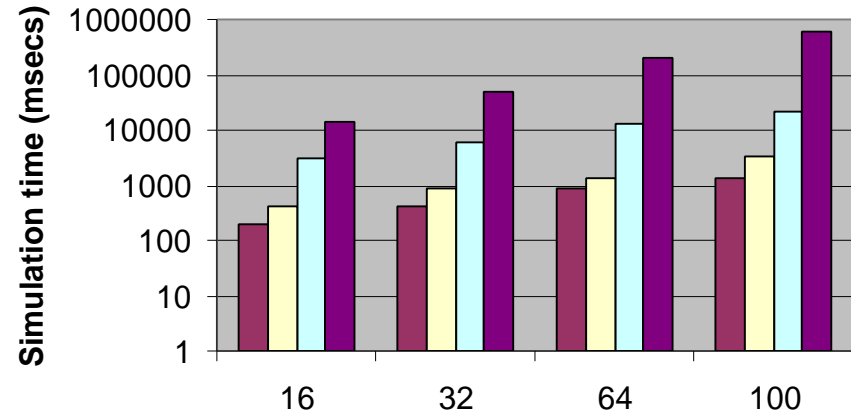
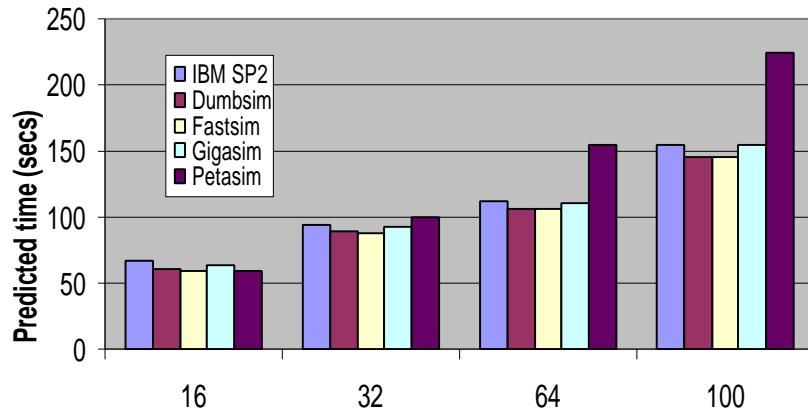
## Execution Times, 60-day data



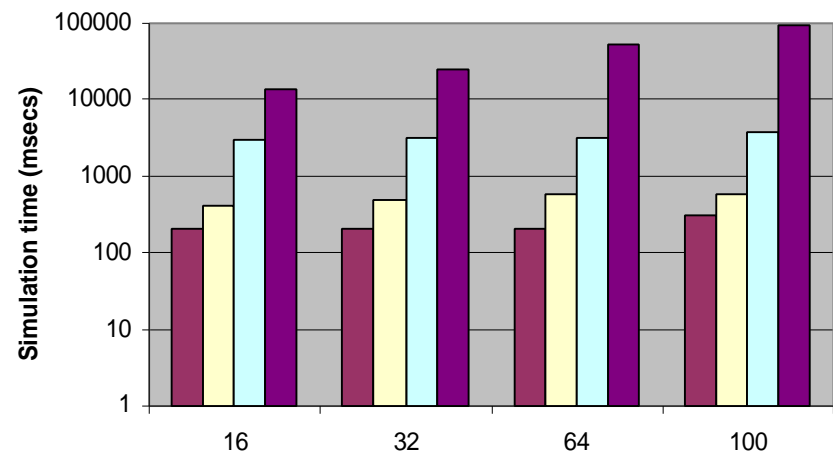
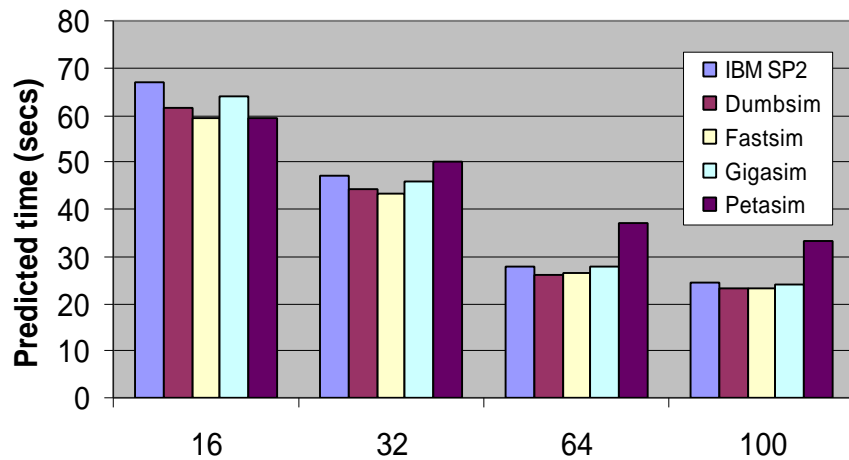


# Satellite Data Processing (SP-2)

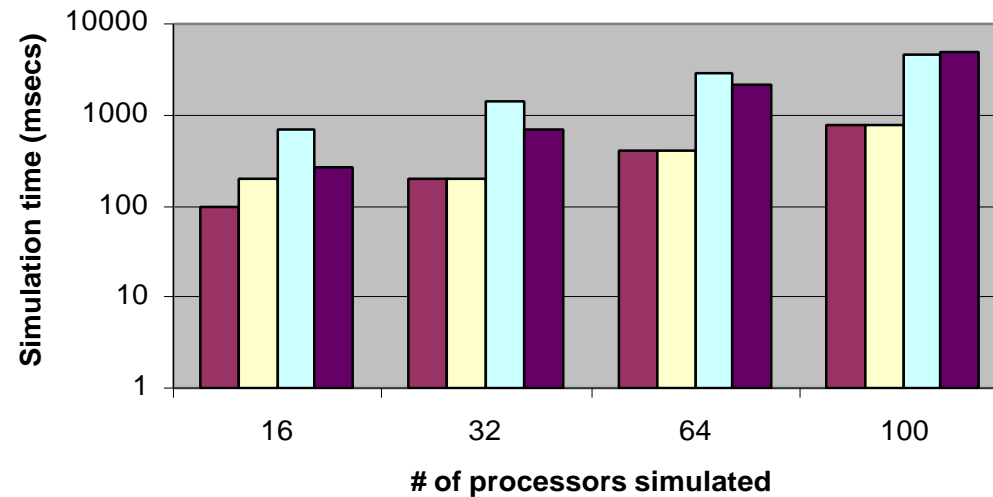
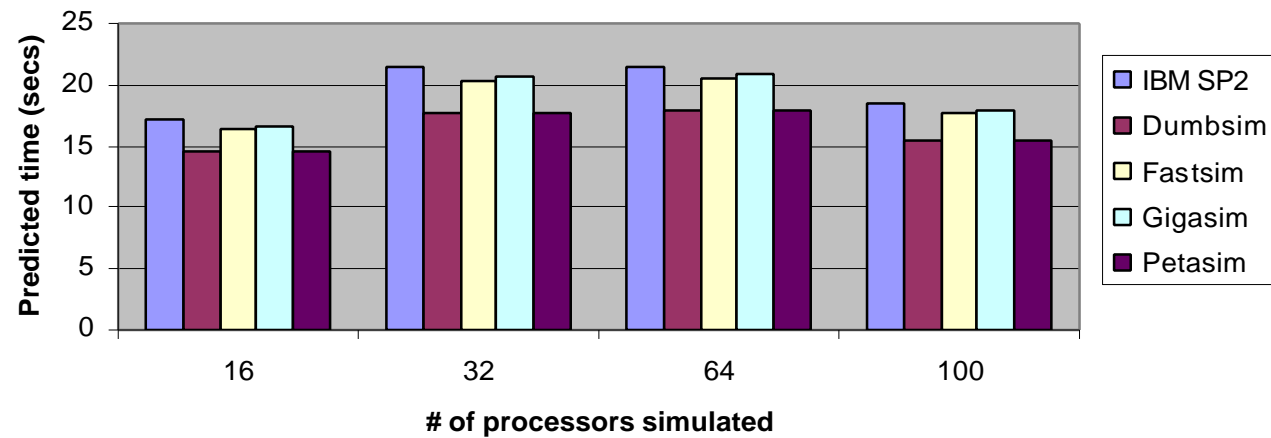
## Scaled Input



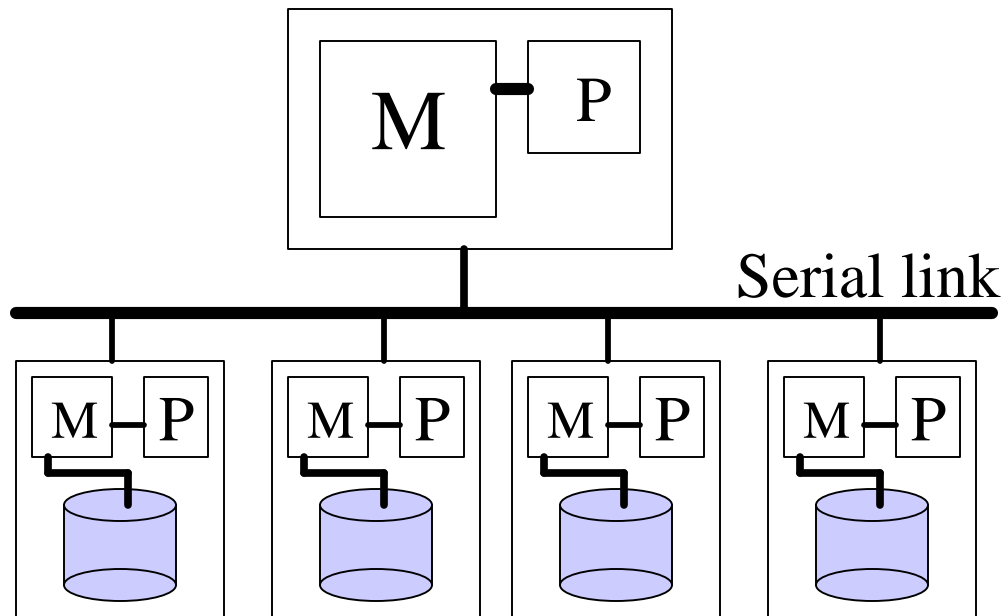
## Non-scaled Input



# Virtual Microscope (SP-2)



# Active Disk Architecture



- Restructure apps
- Disk-resident code
  - bulk processing
  - *disklet*
- Host-resident code
  - coordination
  - communication
  - combination

- Processing power scales naturally with storage capacity
- Processing power evolves with storage

# Experiments

- Compared algorithm-architecture combinations
  - current and future configurations
- Evaluated scalability
  - configuration: 4-32 disks
  - dataset size
- Evaluated impact of host upgrades

# Conclusion

- Large irregular datasets are coming to your computational grid
- Database software can hide complexity of exploiting large irregular datasets
- Performance methodology for configuring database, for choosing target architectures and in predicting cost of queries

# Ongoing and Open Issues

- Integration into metacomputing environment
  - ADR metadata to be stored in NPACI SRBs and Globus MDS
  - Process placement and communication coordinated by Globus, scheduled by AppLeS (Generalization of SARA!)
  - Coupling ADR with parallel programs coordinated by MetaChaos
- Integration into object-relational framework
  - Appropriate query language
  - Compile-time/runtime optimizations
    - intermodule tiling