# 3MRA Modeling System Technology

Science Advisory Board
Review of the 3MRA Modeling System

Presented by:
Karl Castleton, DoE/PNNL

August 26, 2003

# System Technology

- Need for the 3MRA technology
- Overview of the 3MRA technology
  - Science-based requirements
  - Software/Hardware requirements
- Design Features
  - Software system challenges
  - Description of 3MRA software
  - 3MRA modeling system outputs

# Science-Based Requirements

- Provide comprehensive human and ecological risk
- Accommodate 2 stage Monte Carlo
- Accommodate site-based modeling
- Provide for multimedia mass balance
- Provide for appropriate aggregation of risk results
- Provide a modeling tool for research in sensitivity analyses and variability and uncertainty assessments

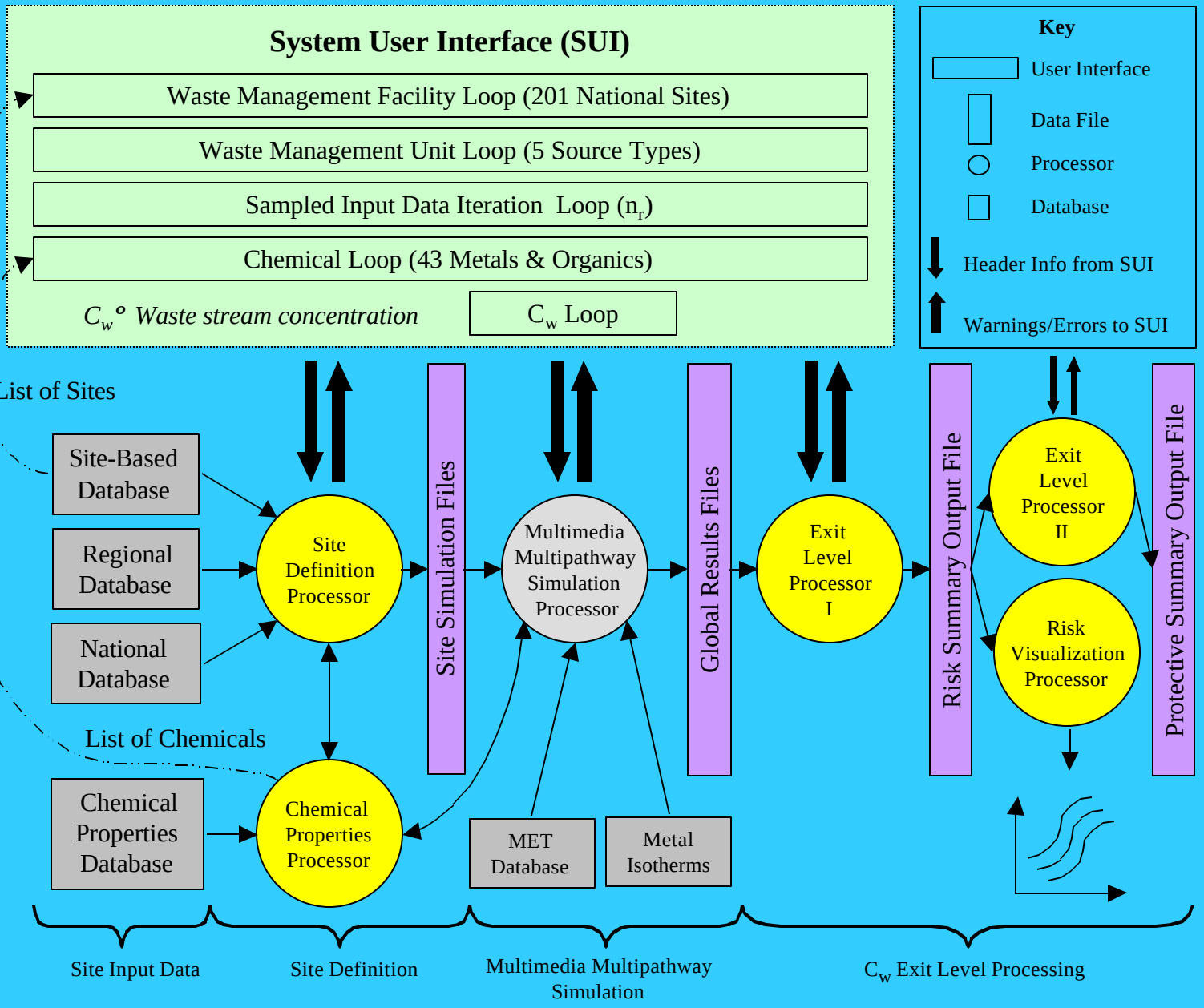
# Software Requirements

- Implementation on Windows-based PC environment (Pentium or higher)
- Object Oriented Design (with respect for the “real world”)
- Accommodate legacy codes
- Accommodate multiple programming languages (FORTRAN, C++, Java)
- Automatic QA/QC
- 100% Distributable

# Design Features

- Overview of the system design
- 3MRA module data exchange
- Potential dimensionality
- Actual dimensionality

# FRAMES 3MRA Modeling System



# Software System Challenges

- 3MRA Complexities
  - Hardware/Software Requirements
  - Diversity of Software Development Team
  - Software System Solutions
    - Standardizing the way model developers communicate data to each other
    - Standardizing the impacts one media/object on another

# Meta Data & Data Transfer Protocols

**Data Dictionaries (DIC files)**

- Sufficient dimensionality
- Designed as “data packets”, i.e., logical grouping of data

**Application Program Interface (API/IOdll)**

- Facilitates data transfer throughout system
- Conducts QA checks on data (e.g., units, range)
- Accesses Model Meta Data to check validity of CSM and inform models regarding locations of incoming data

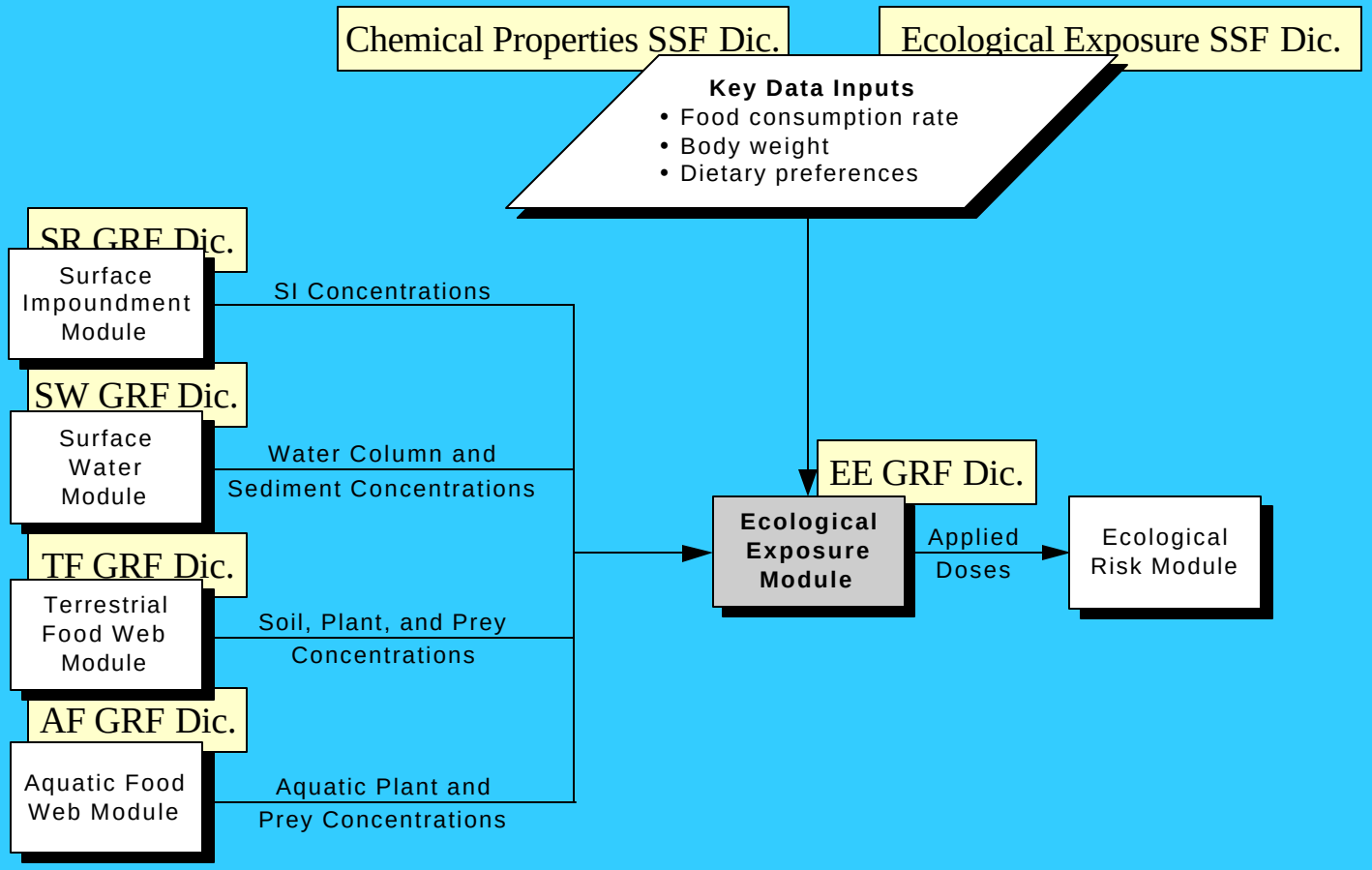
# Relationship Between Dictionary Files and Data Files

Data Files : Contain simulation-based values per variable

Dictionary Files : Contain information about variables found in Data Files (Meta Data of the data)

# Meta Data : Dictionary Files

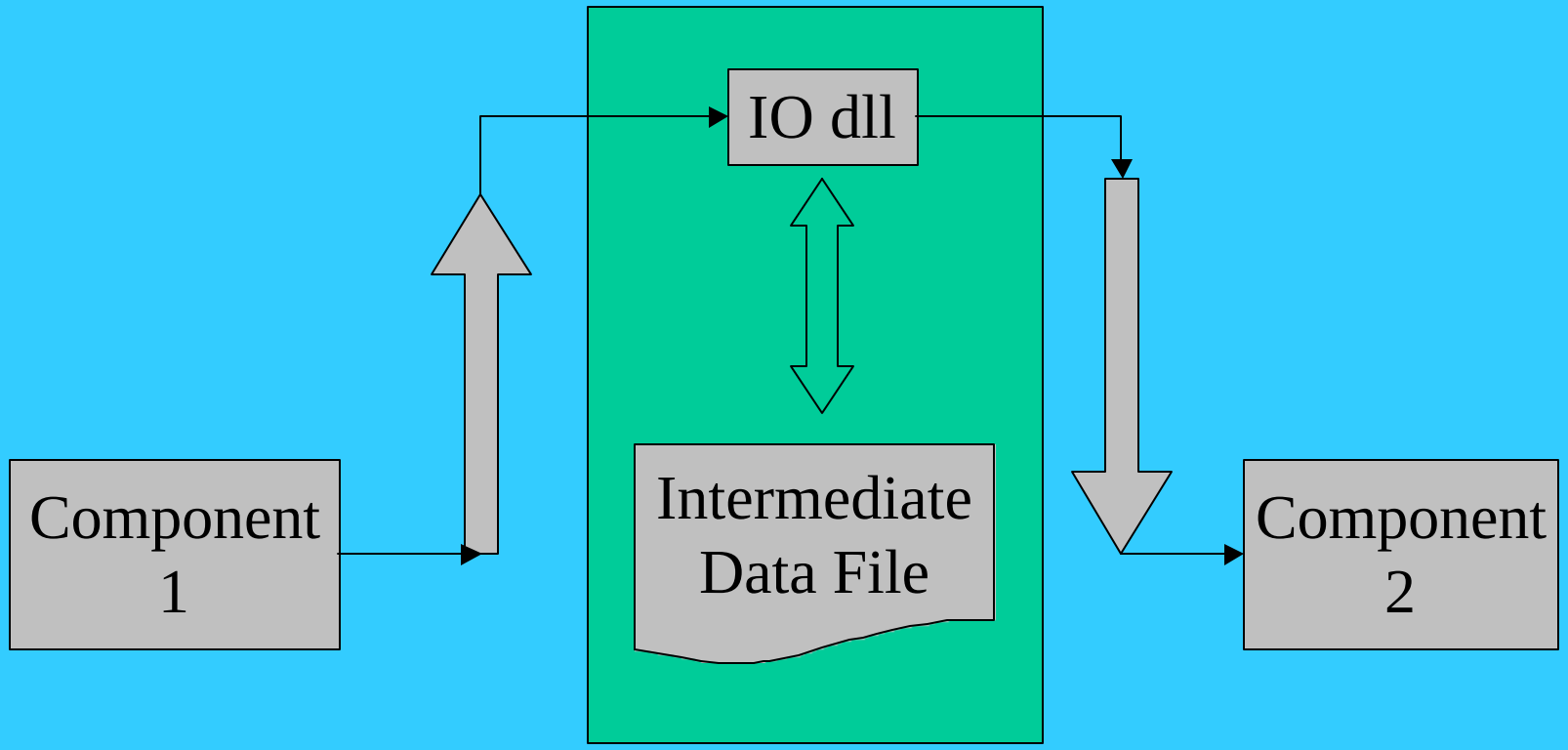
## Ecological Exposure Example



# Some Entries From a Dictionary

| 39 | source | | | | | |
|---|---|---|---|---|---|---|
| Code | Dim | Type | Min | Max | Units | Description |
| AnnInfil | 2 | float | 0 | 0.03 | m/d | leachate infiltration rate (annual avg., WMU subarea(s) only) |
| CE | 1 | float | 0 | 1E+08 | g/m2/d | constituent mass emission rate-PM30 |
| CENY | 0 | integer | 0 | 10000 | | number of years in outputs |
| CEYR | 1 | integer | 1 | 10000 | year | year associated with output |
| CTda | 3 | float | 0 | 1000000 | ug/g | depth averaged soil concentration (from zava to zavb) |
| CTdaNY | 2 | integer | 0 | 10000 | | number of years in outputs |
| CTdaYR | 3 | integer | 1 | 10000 | year | year associated with output |
| CTss | 3 | float | 0 | 1000000 | ug/g | soil concentration (annual average, all subareas) |
| CTssNY | 2 | integer | 0 | 10000 | | number of years in outputs |
| CTssYR | 3 | integer | 1 | 10000 | year | year associated with output |

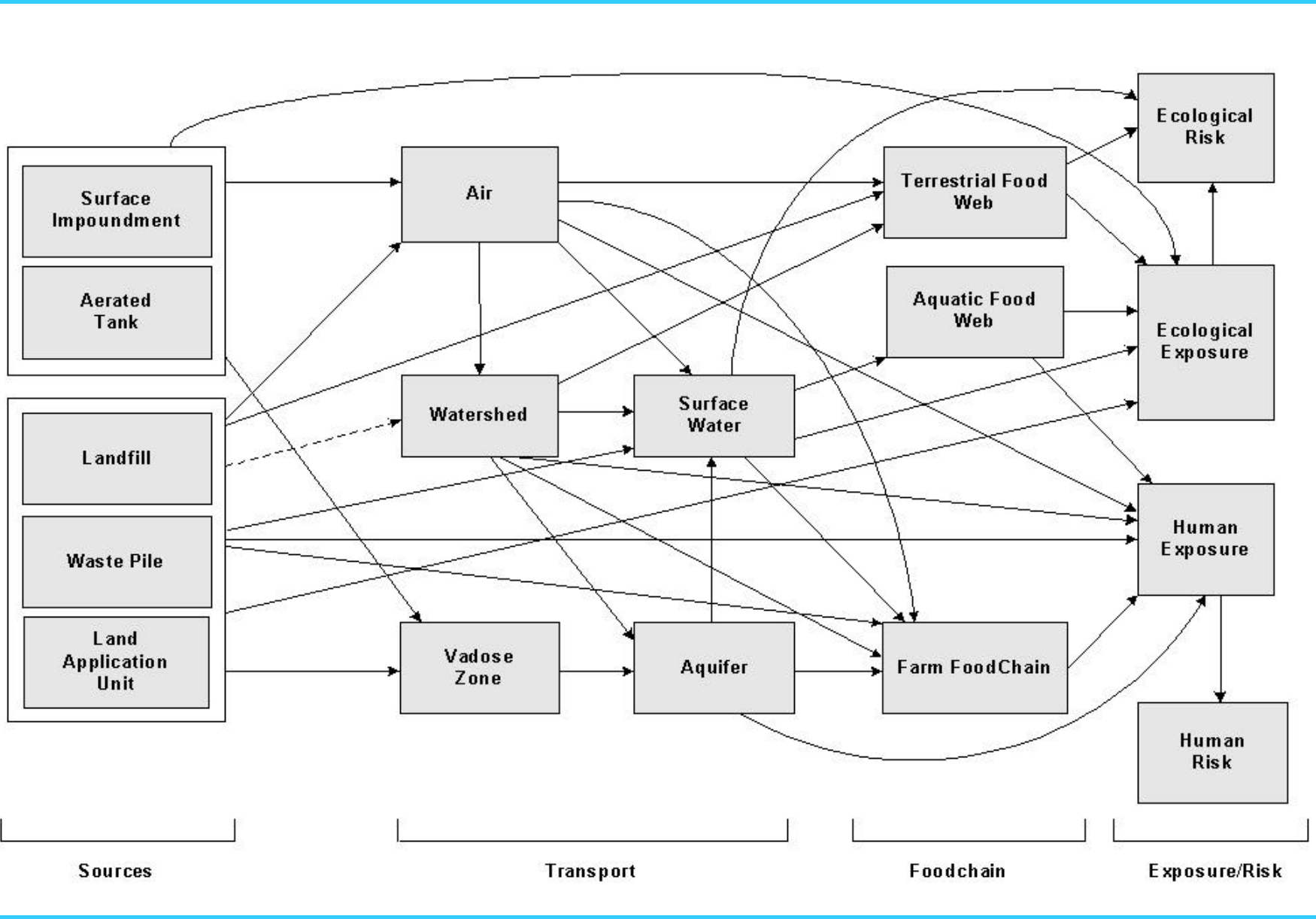
# IO DLL in SYSTEM CONTEXT



# Description of 3MRA Software

- Multiple Environmental Modules
  - 13 different modules to be invoked per run
- Multi-pathway
  - 4 types of releases (air, surface water, watershed, and vadose zone)
- Multi-receptor
  - 4 receptors, with 5 cohorts (4 used for decision making)
- Software system that allows you to run both production runs as well as answer science questions

# Integrating Environmental Models



# 3MRA Modeling System Outputs

- Requirements of ELP I, ELP II and RVP
- Human Risk Outputs
- Human Risk Roll Ups
- Ecological Risk Outputs
- Ecological Risk Roll Ups

# Potential Dimensionality for 3MRA National Assessment

| Simulations | Storage | |
|---|---|---|
| Realization (10000) | Receptor Type (9) | Time (10000) |
| Source Types (5) | Risk Bins (7) | Receptor Locations (677) |
| Site (201) | Pathways (13) | |
| Waste Level (5) | Cohort (6) | |
| Chemical (43) | Distances (3) | |
| | Risk Measure (2) | |

| | |
|---|---|
| Total Simulations (900,850,000) | Total Numbers Potentially Stored (1.8e20)<br>Total Bytes (1.8 Billion 10 GB hard drives) |

# Actual Dimensionality for 3MRA National Assessment

| Simulations | Storage | |
|---|---|---|
| Realization (1) | Receptor Type (5) | Time (1) |
| Source Types (5) | Risk Bins (7) | Receptor Locations (1) |
| Site (201) | Pathways (13) | |
| Waste Level (5) | Cohort (4) | |
| Chemical (43) | Distances (3) | |
| | Risk Measure (2) | |

| | |
|---|---|
| Total Simulations (90,085) | Total Numbers Stored (.96 Billion)<br>Total Bytes (Single 10 GB hard drives) |

# Conclusions 3MRA Software System

- Achieves balance
  - Between modern software (Object Oriented) and legacy
  - Complexity and simplicity
  - Runtime versus storage requirements
- Allows for testing at multiple levels and at different times
  - Modules and system
  - During development and running

# Future System Enhancements

- Support more programming languages
- Develop the ability to use different modules, module dictionaries and data-sets more easily
  - A user interface for checking/updating a site-based simulation
- Automated testing for module and system components
  - Cost of manual testing is restrictive