RESEARCH & DEVELOPMENT

Building a scientific foundation for sound environmental decisions

Parallel Computing and Model Evaluation for Environmental Systems:

An Overview of the SuperMUSE and FRAMES Software Technologies

Justin Babendreier

USEPA/ORD/NERL

ISCMEM Workshop on Environmental Modeling

Rockville, Md

October 14, 2009

RESEARCH & DEVELOPMENT

Building a scientific foundation for sound environmental decisions

Model Evaluation Science (UA/SA/PE) Research Program

Research Questions:

How can model evaluation science and integrated modeling technologies be extended, packaged, and delivered to directly support EPA's needs related to exposure & risk assessments for problems of national significance?

- Dealing with the Big problems == Big systems, Big spaces, and Big time horizons
- Everyone who models faces similar operational problems, even if <big^4

Why is this research important?

- Helps EPA form the needed technical basis to:
  - Identify needs for improved science and data;
  - More accurately assess uncertainties of science and data.

Need to facilitate improved models and regulatory programs through better characterization of UA/SA/PE and higher levels of quality assurance.

Approach:

- Provide methods/tools for simplifying the computational burdens of QA.
- Develop methods/tools for uncertainty analysis and parameter estimation; methods/tools for screening, local, and global-based sensitivity analyses.
- Demonstrate model evaluation abilities through various applications.

Discussion Points on Parallel Computing

Quantitative Aspects of UA/SA/PE:

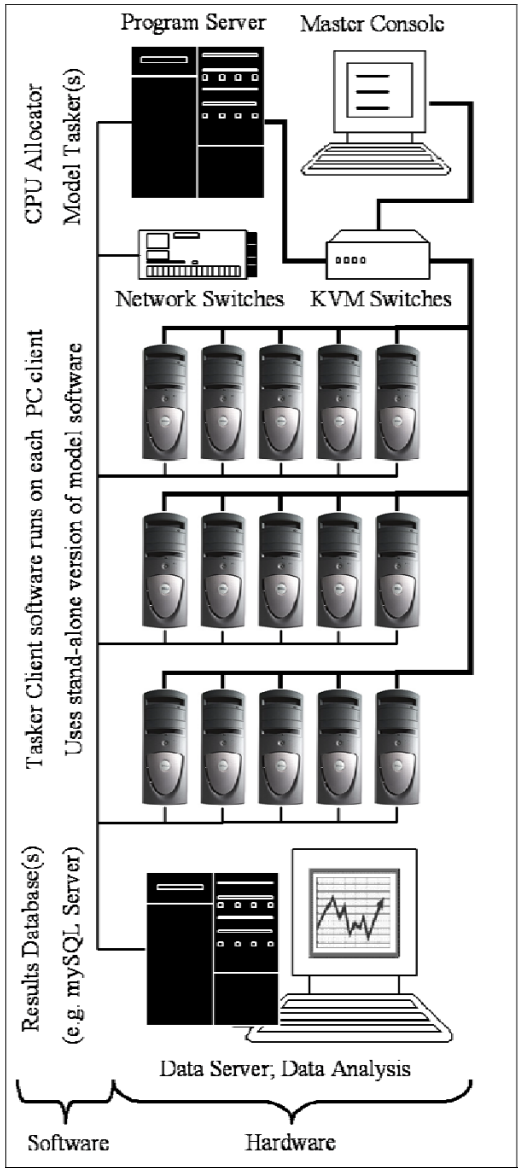
- Many techniques and methods available, improving constantly.
- Current knowledge and execution capabilities usually limited to a select few, out of reach from most model developers and model users.
- An "**embarrassingly parallel**" computational problem; solutions involve running a model over and over with slightly different inputs.
- Many EPA models written for Windows, but most supercomputing solutions today require "mainframes" or Linux-based PC clusters.

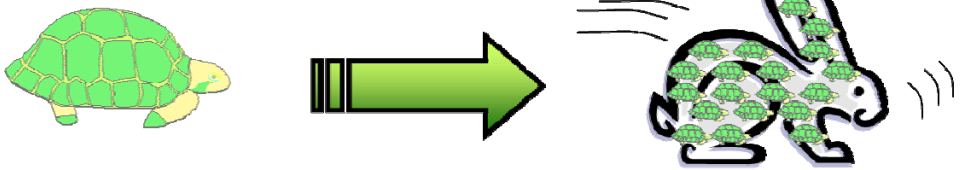
Parallel Computing and You

The UA/SA/PE Runtime Problem

- As model complexity, time & space grid density, or types of uncertainty and sensitivity analyzed increases, computational burden (runtime) typically increases geometrically.
- UA/SA/PE techniques not widely applied to EPA models due to lack of Windows based computer processing capacity.
- General trend → PC-based model developers increase model complexity over time, offsetting concurrent gains in CPU speed.
- Depending on the EPA model/application, need 100's to 10's of millions of simulations.

SuperMUSE: Hardware & Software





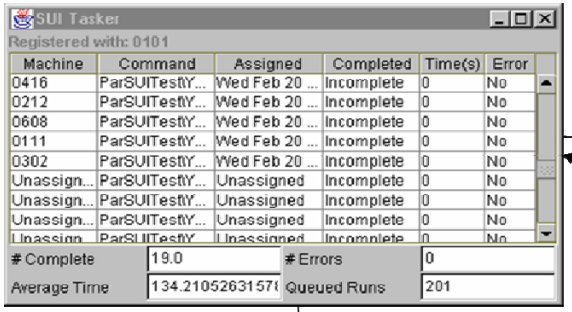
….tools to parallelize stand-alone PC-based models

Clustering to Increase Computational Capacity

Model Tasker

Model Dependent – Create an MT for each modeling system

Parallelizes a stand-alone PC-Model's System User Interface



CPU Allocator

Model Independent

Oversees Multiple Active Model Taskers

At launch, MT's register with the CPU Allocator.

1. TaskerClient TC_1 announces availability, one of many client PCs.

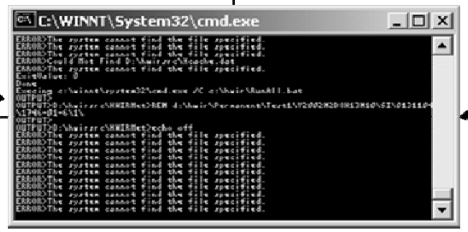
2. If no active MT, idles. This TC_1 call was assigned to MT_1.

3. TC_1 requests job from MT_1.

4. Do job X = a single task line in any MT (e.g., single model run)

5. Send job X warnings, errors, and results to Data Server's project file area identified by MT.

6. TC_1 says done with job X.



Tasker Client (TC_k; $k = 1 \ldots n_c$)

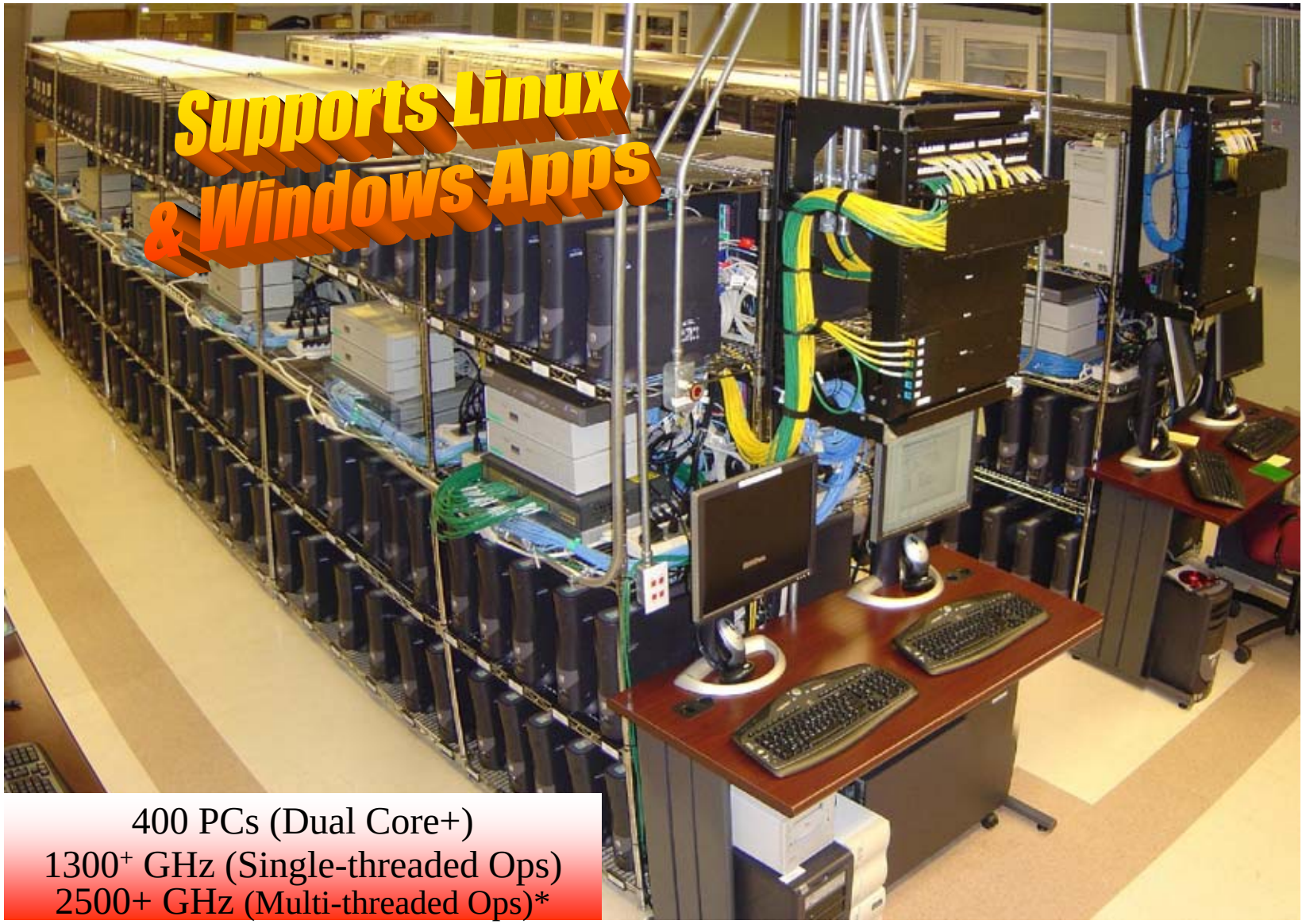
Model independent.

Executes DOS commands in batch files delivered by MT.

OO-JAVA design app.

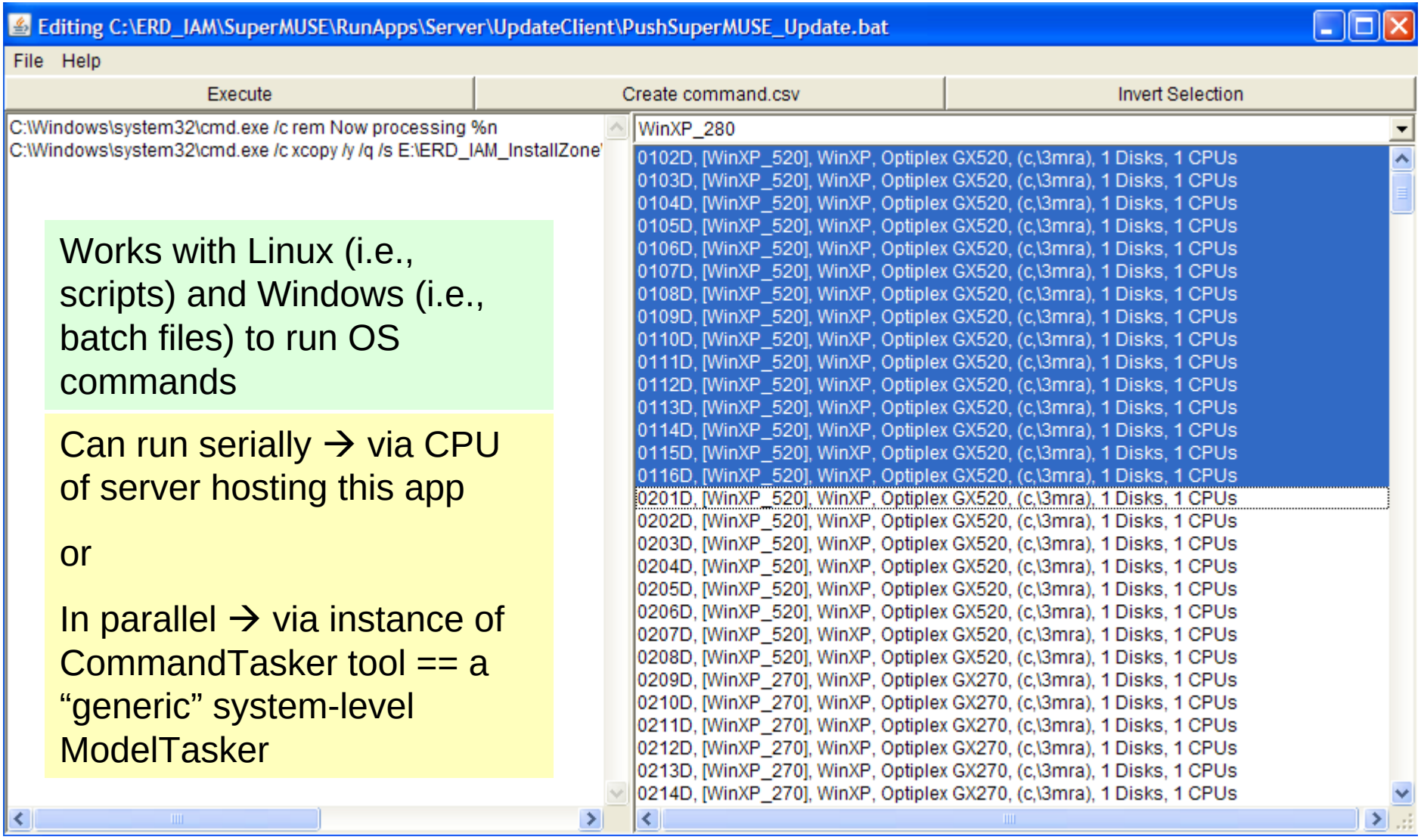
3MRA 1.x SUITasker, CPU Allocator, and TaskerClient shown

EPA's SuperMUSE Cluster, Athens GA



Example SuperMUSE Tool: UpdateClient

Managing files and PC settings across your cluster via OS



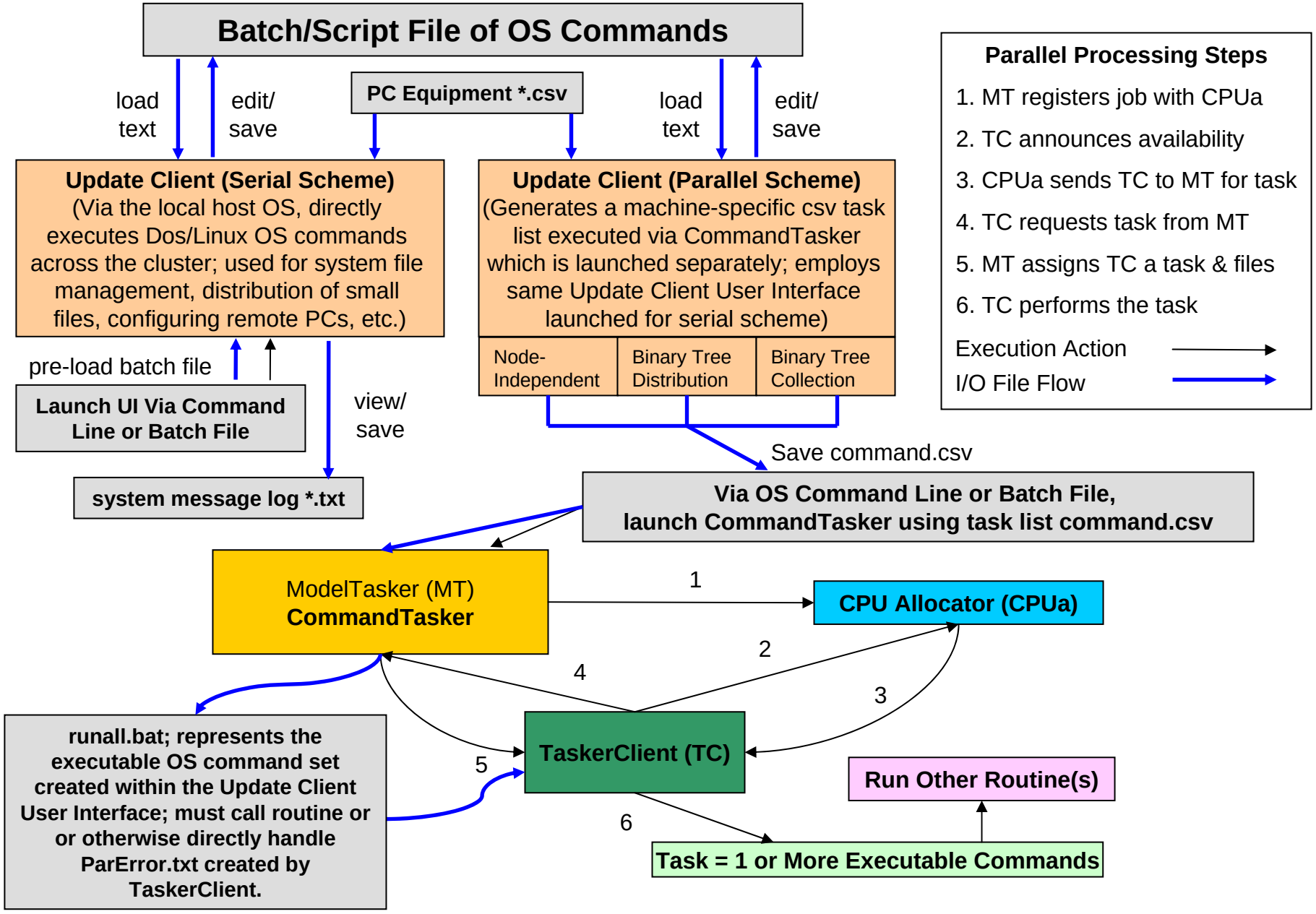
Works with Linux (i.e., scripts) and Windows (i.e., batch files) to run OS commands

Can run serially → via CPU of server hosting this app

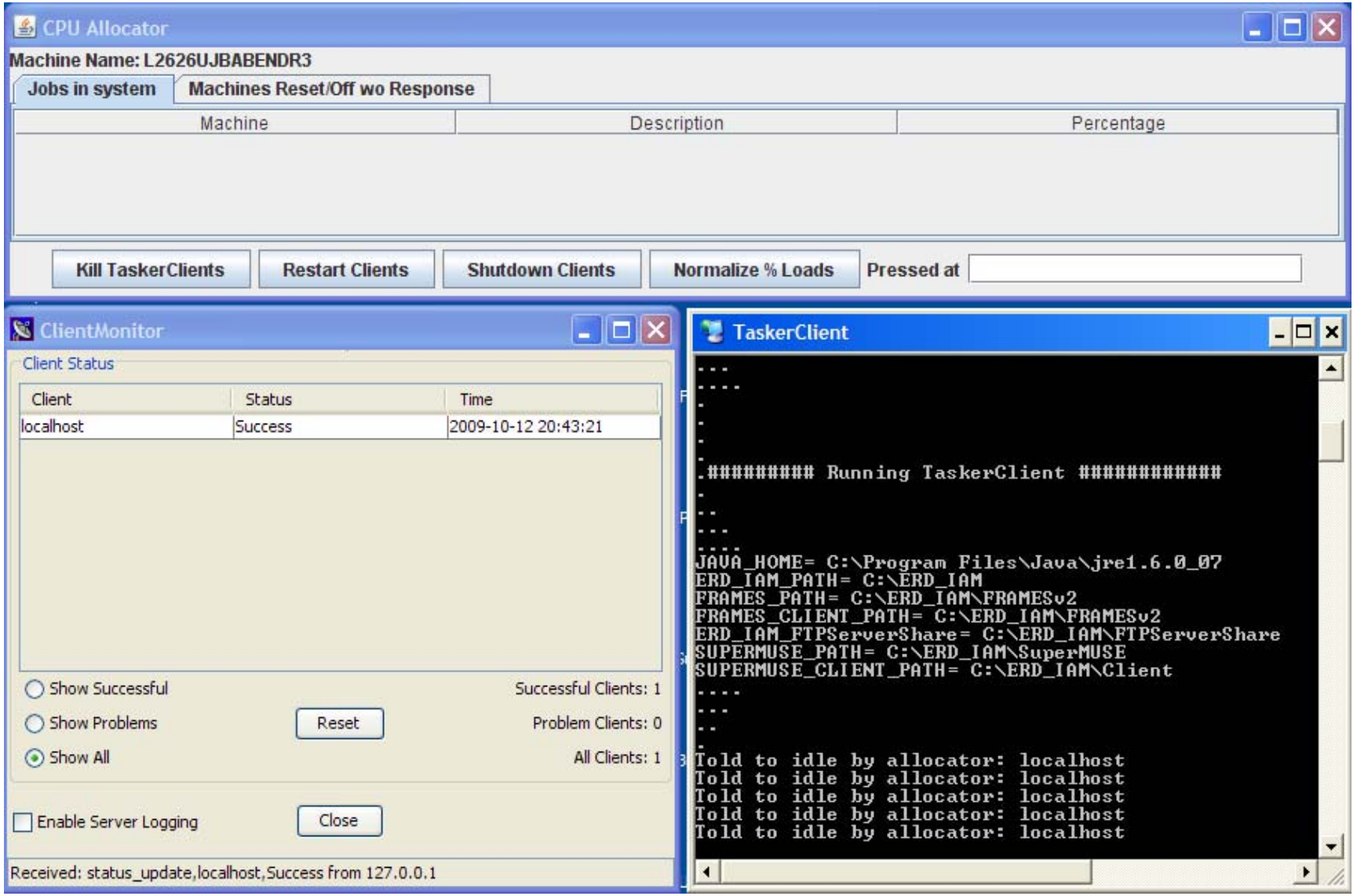
or

In parallel → via instance of CommandTasker tool == a "generic" system-level ModelTasker

SuperMUSE 1.0 UpdateClient Tool Detail

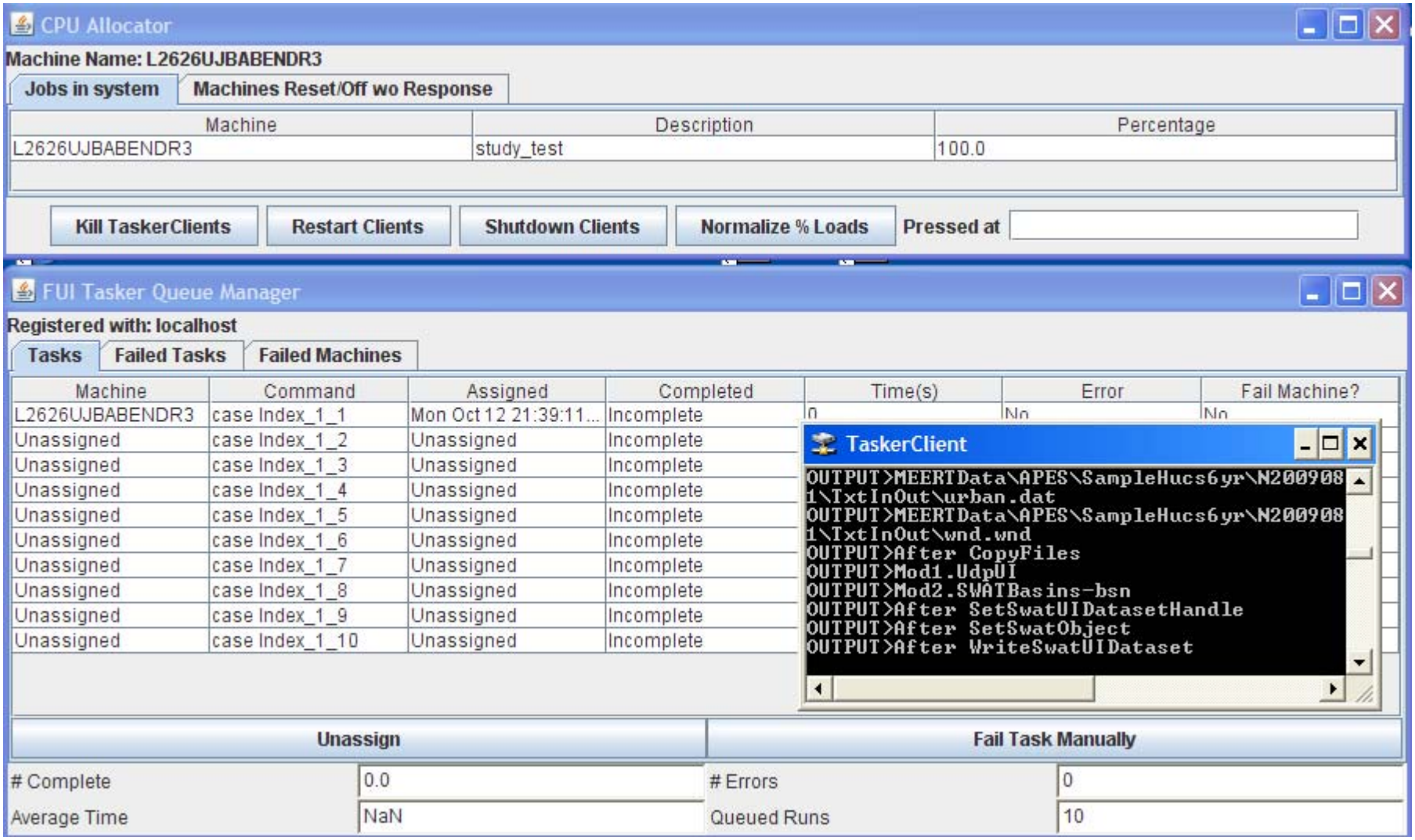


SuperMUSE CPU Allocator, TaskerClient, & ClientMonitor Tools



SuperMUSE ClientMonitor, CPU Allocator, and TaskerClient shown

Example Model Tasker → F2 FUITasker



CPU Allocator, TaskerClient shown with FRAMESv2 FUITasker Interface Example

Discussion Points on Model Evaluation

For a given class of problems (e.g., spatially explicit exposure/risk modeling) captured by a modeling system, decision support boils down to …

- **An ability to manage the modeling system input vector at two distinct levels: Decision and Non-decision Subspaces**

- **An ability to allow users to explore system I/O relations:**
  - **Decision input space of a given problem statement (e.g., scenarios)**
    - **Setting permutations of decision variable values to "run".**
  - **Non-decision input space of a given problem statement (i.e., data)**
    - **Managing the uncontrolled inputs to be set by nature or others**
    - **Dealing with variability and epistemic uncertainty in these inputs**
  - **Via science (i.e., models) used to translate an input vector (comprised of decision and non-decision subvectors) to an output vector.**
    - **Providing context for accuracy and precision of "outcomes" by scenario.**
    - **Providing an ability to compare 2 or more scenarios.**

Discussion Points on the Processes of Modeling and Decision-Making

Decision-Making Under Uncertainty Is "All About" Information and Integration

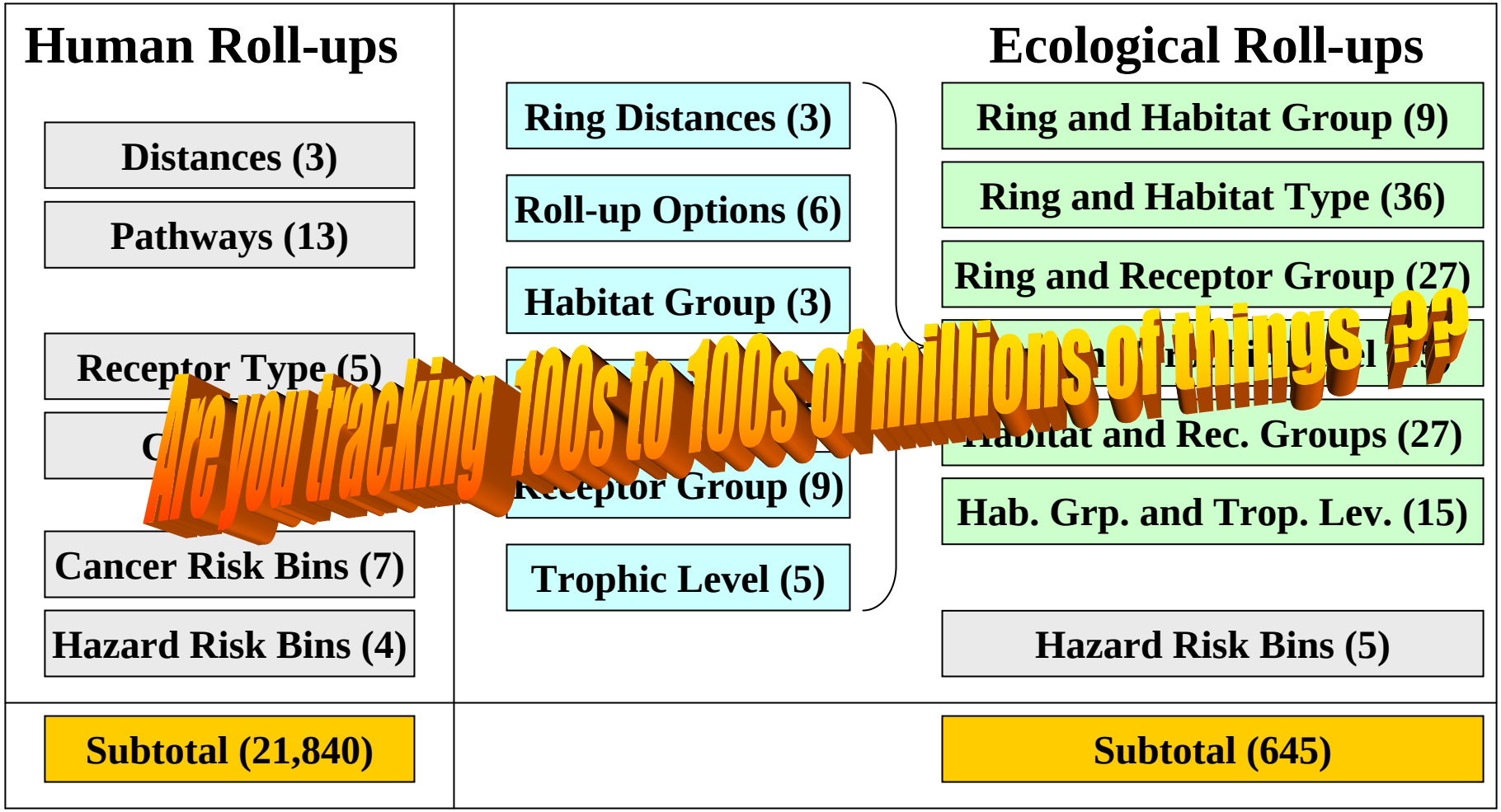
- **In the end….it is "all about" data and dimensionality reduction -- best decision.**

Modeling Under Uncertainty Is "All About" Indexing Data and Integration

- **In the end ….it is also "all about" data and dimensionality reduction, with a known (reproducible) level of quality -- best answer.**

Indexing is the engine room of science-based data reduction and decisions.....

Example Population-Based Risk Profiles Possible in 3MRA 1.0/1.x/2.0



Total (22,485) X Population % (10) Risk Measures (2^{+}) X Chemical (43^{+}) Source Type (5)

~ 10^{8+} permutations

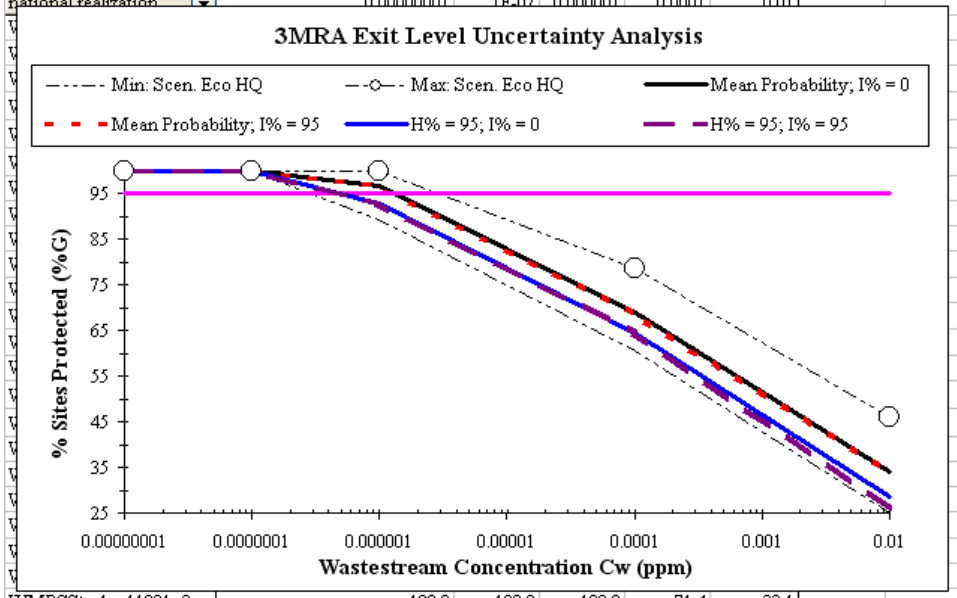
Example FRAMES-3MRA Uncertainty Analysis

source	LAU	<<Select to view output for different waste management units.
class/category/pathway	Eco HQ	<<Select to view output for different Receptor Class/Risk Category/Pathway profiles ("Risk" = Human Cancer; "HQ" = Human Hazard; "Eco HQ" = Eco Hazard).
scenario	1a	<<Select to view scenarios: (a) Human and Eco-terrestrial, (b) Human and Eco-aquatic; (c) Human and Eco-wetland. For (b) & (c) only Eco data are unique; for Human, alw
pop. percentile protected	99	<<Select to view output at different population percentiles.

Graphic Operates on Selections for %G, %H and %I in Orange

GRAPH

Table Data: %Gk	Cw (ppm)					
national realization	0.00000001	1E-07	0.000001	0.0001	0.01	
WMPCStudy_11031_3	100.0	100.0	100.0	71.4	32.1	



Monte Carlo Empirical Uncertainty Analysis (Accuracy*)

Interpolation Scheme Solution >>		Log-linear				Linear	
User Selected %Ge	%Ge	95	95	95			
User Selected %He	%He	95	80	Median	Mean	Mean	
Log-linear interpolation scheme for $y = m*Ln(x) + b$	x_1	1E-07	0.000001	0.000001	0.000001	0.000001	%H, %I = 0
	x_2	0.000001	0.0001	0.0001	0.0001	0.0001	
	y_1	100.0	96.4	96.4	96.8	96.8	
	y_2	92.9	64.3	67.9	68.8	68.8	
	b	50.0	0.0	10.7	12.9	97.1	
	m	-3.10	-6.98	-6.20	-6.07	########	
Exit Level (ppm) at H% Confidence		**5.01E-07**	1.23E-06	1.26E-06	1.34E-06	7.33E-06	

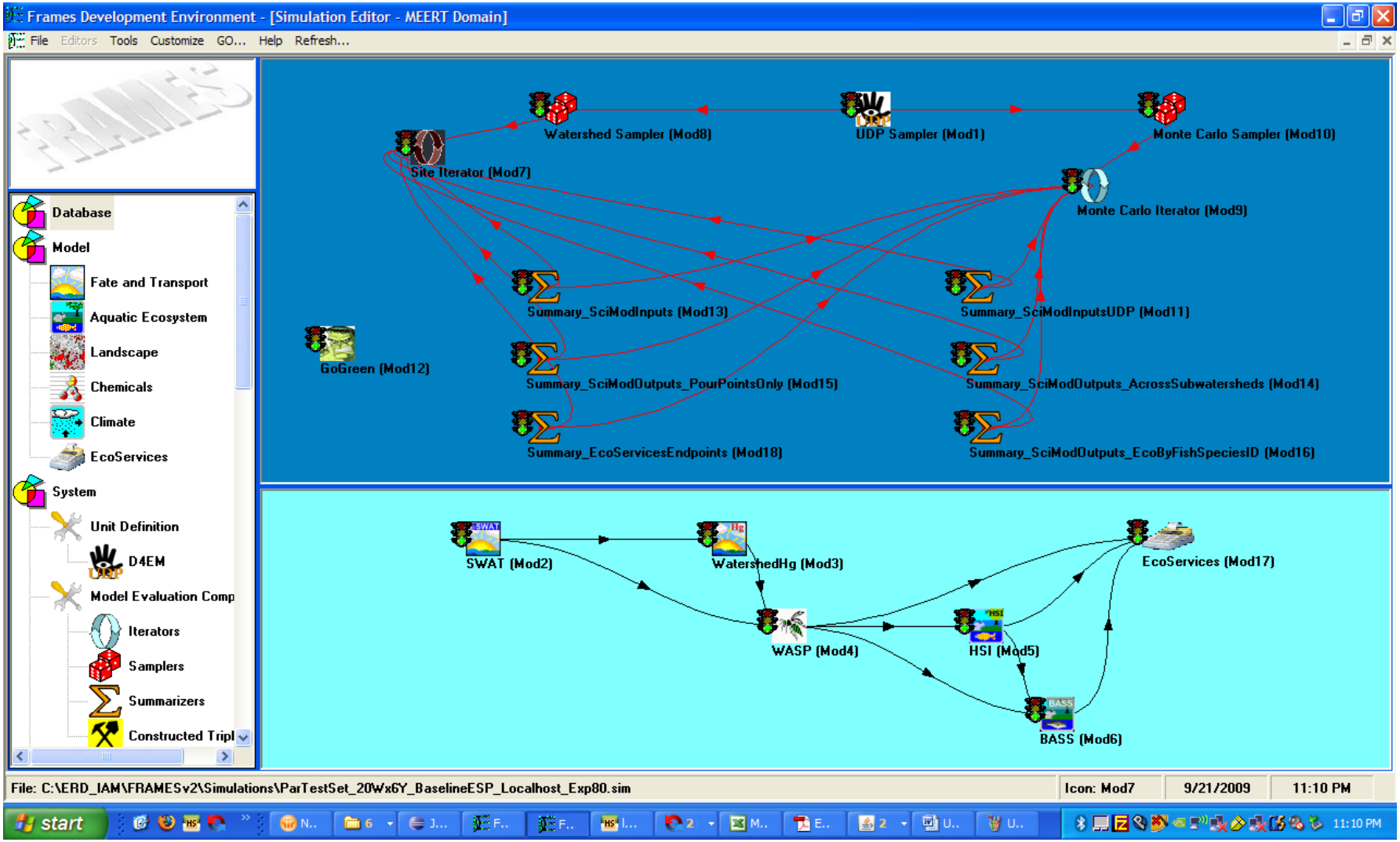
Monte Carlo Simulation Error Analysis (Precision*)

User Selected %Ie	%Ie	95	95	95			
Log-linear interpolation scheme for $y = m*Ln(x) + b$	x_1	1E-07	0.000001	0.000001	0.000001	0.000001	%H, %I
	x_2	0.000001	0.0001	0.0001	0.0001	0.0001	
	y_1	100.0	96.4	96.4	96.6	96.6	
	y_2	92.9	64.3	67.9	68.5	68.5	
	b	50.0	0.0	10.7	12.3	96.9	
	m	-3.10	-6.98	-6.20	-6.10	########	
Exit Level (ppm) at H%, I% Confidence		**5.01E-07**	1.23E-06	1.26E-06	1.31E-06	6.74E-06	

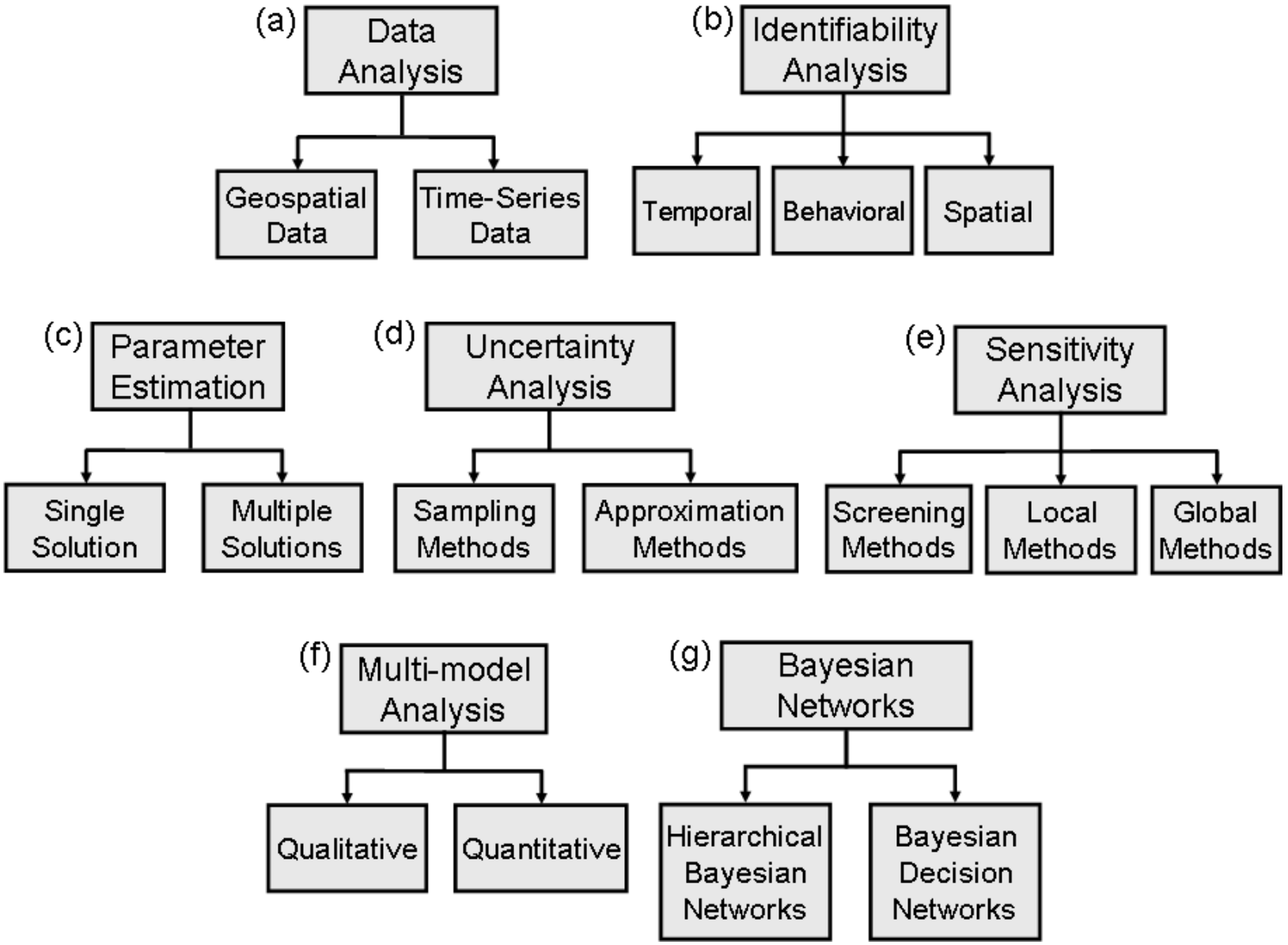
If shown, #NUM! typically indicates that the Exit Level >= maximum Cw simulated.

do you need to do it with accuracy & precision ??

FRAMESv2-MEERT App. Simulation Design with Cyclic System-level Model Evaluation Components



Model Evaluation Framework Implementation Plan



Recent and Ongoing Objectives

Develop FRAMESv2 capabilities for:

- Parallel-PC computations (100%),

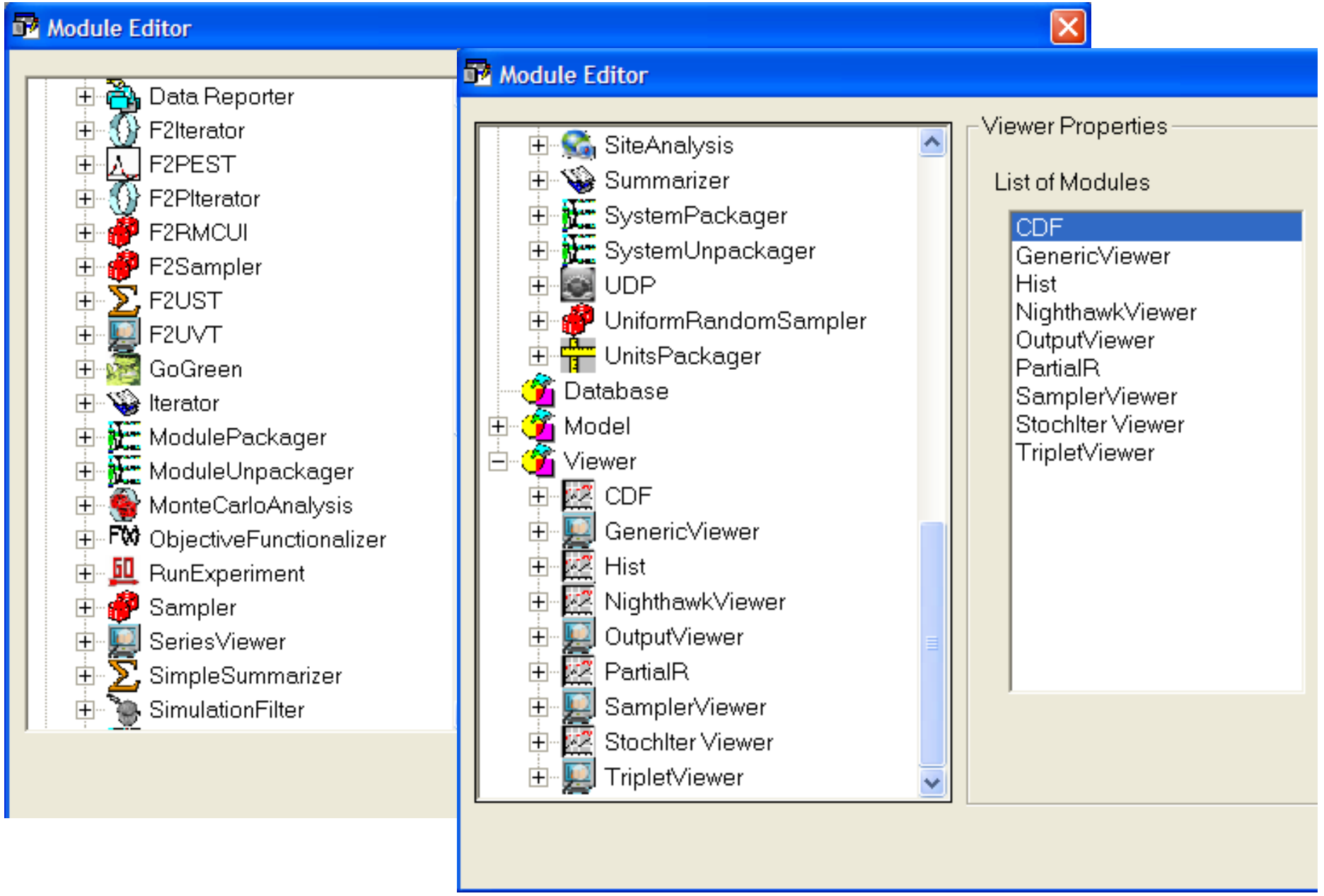
- Multi-threading jobs on single PC to leverage multiple CPU cores (95%),

- Generic multi-"unit" assessment capability within base F2 API architecture (100%)

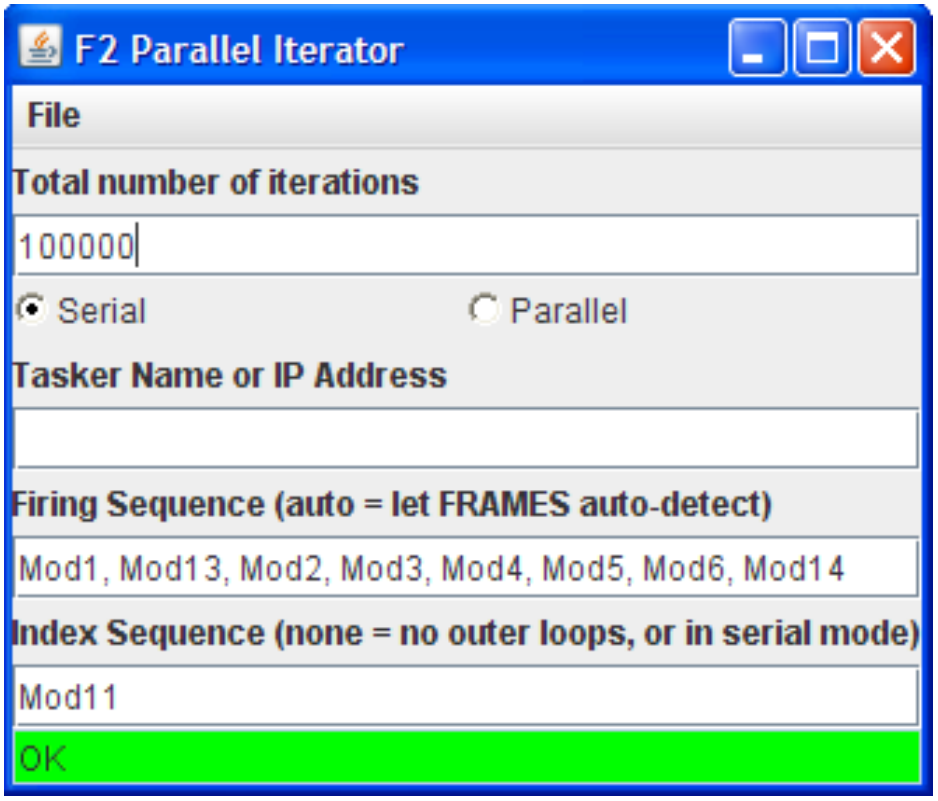
- Wide range of tools and pre/post-processing utilities for conducting UA/SA/PE, and data analysis/mining. (90%)

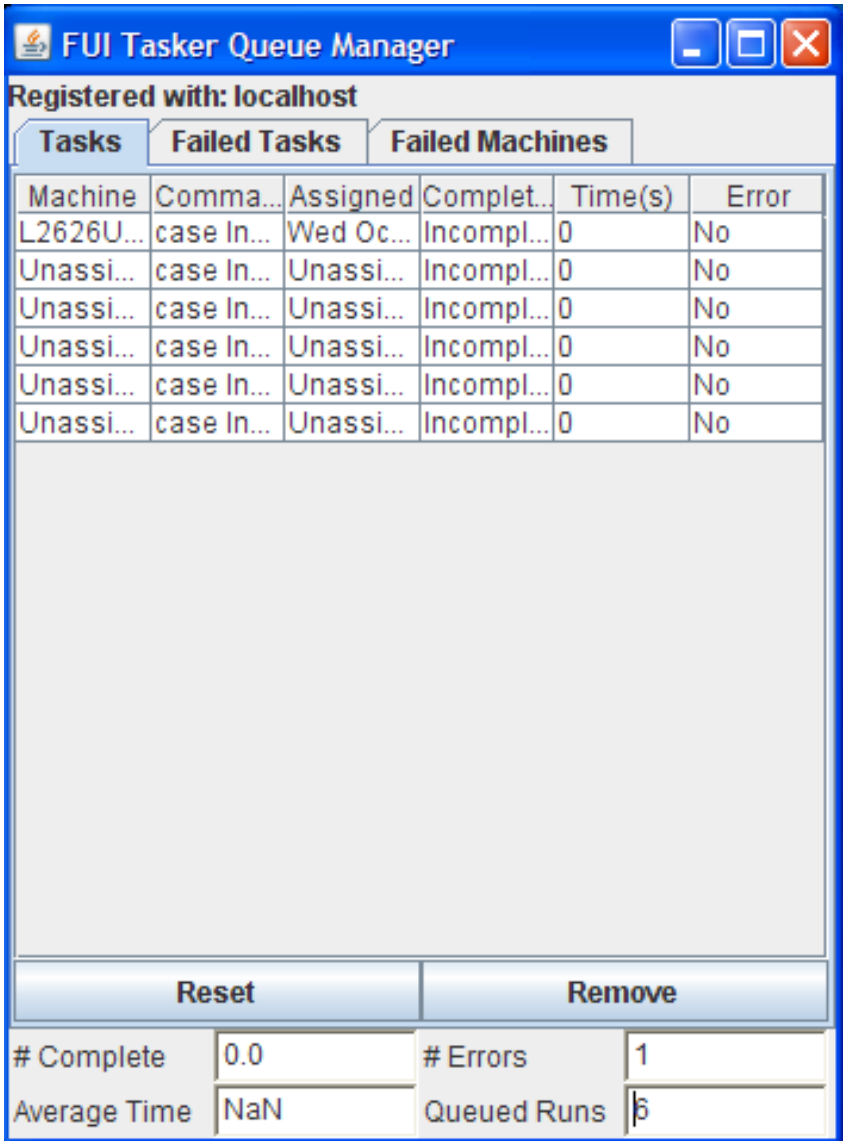
20+ iterators, samplers, summarizers, viewers, processors, tools - operational for the most part, undergoing beta testing

Systems Tools Development & Organization

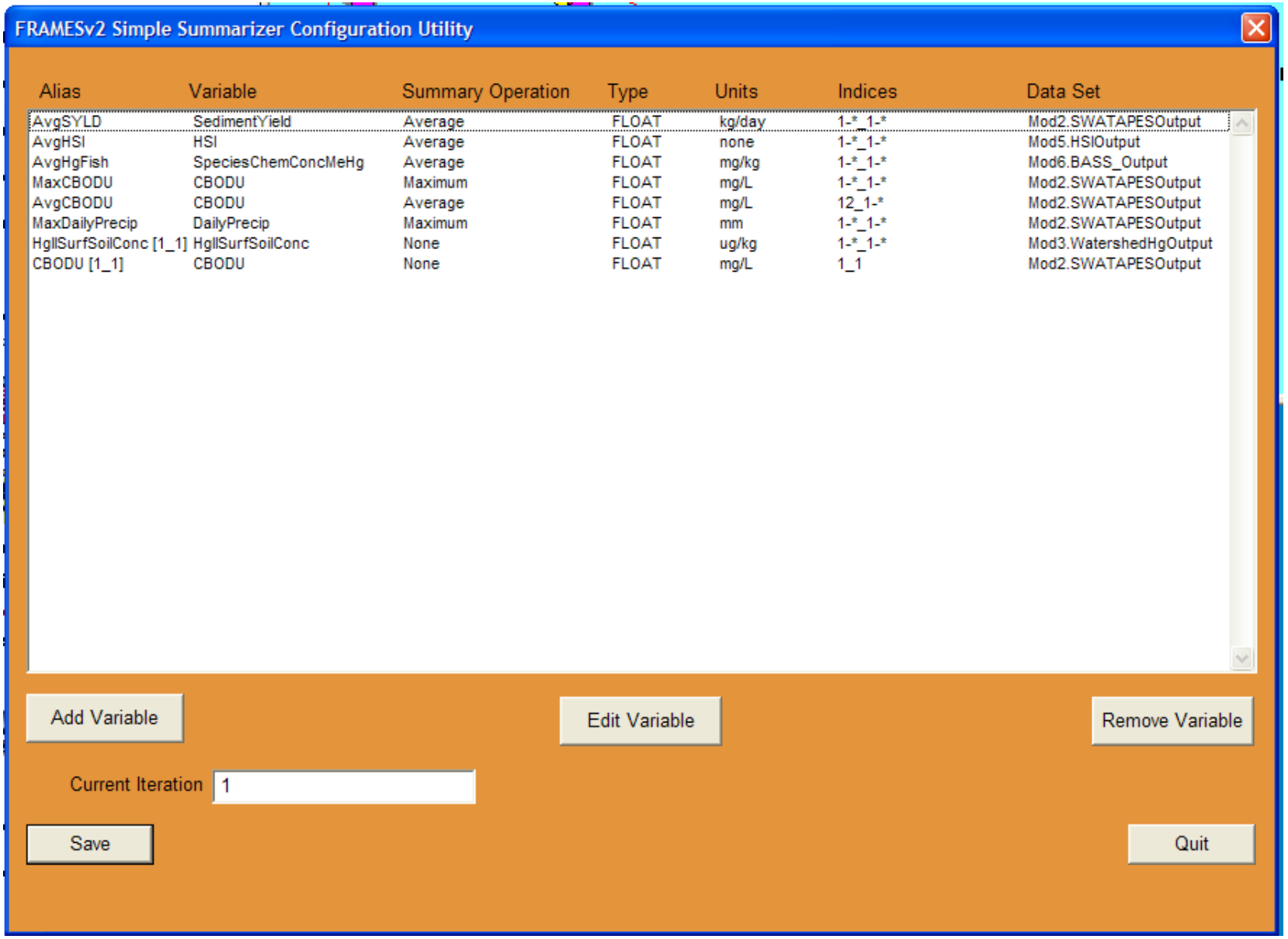


FRAMESv2 Parallel Processing Elements

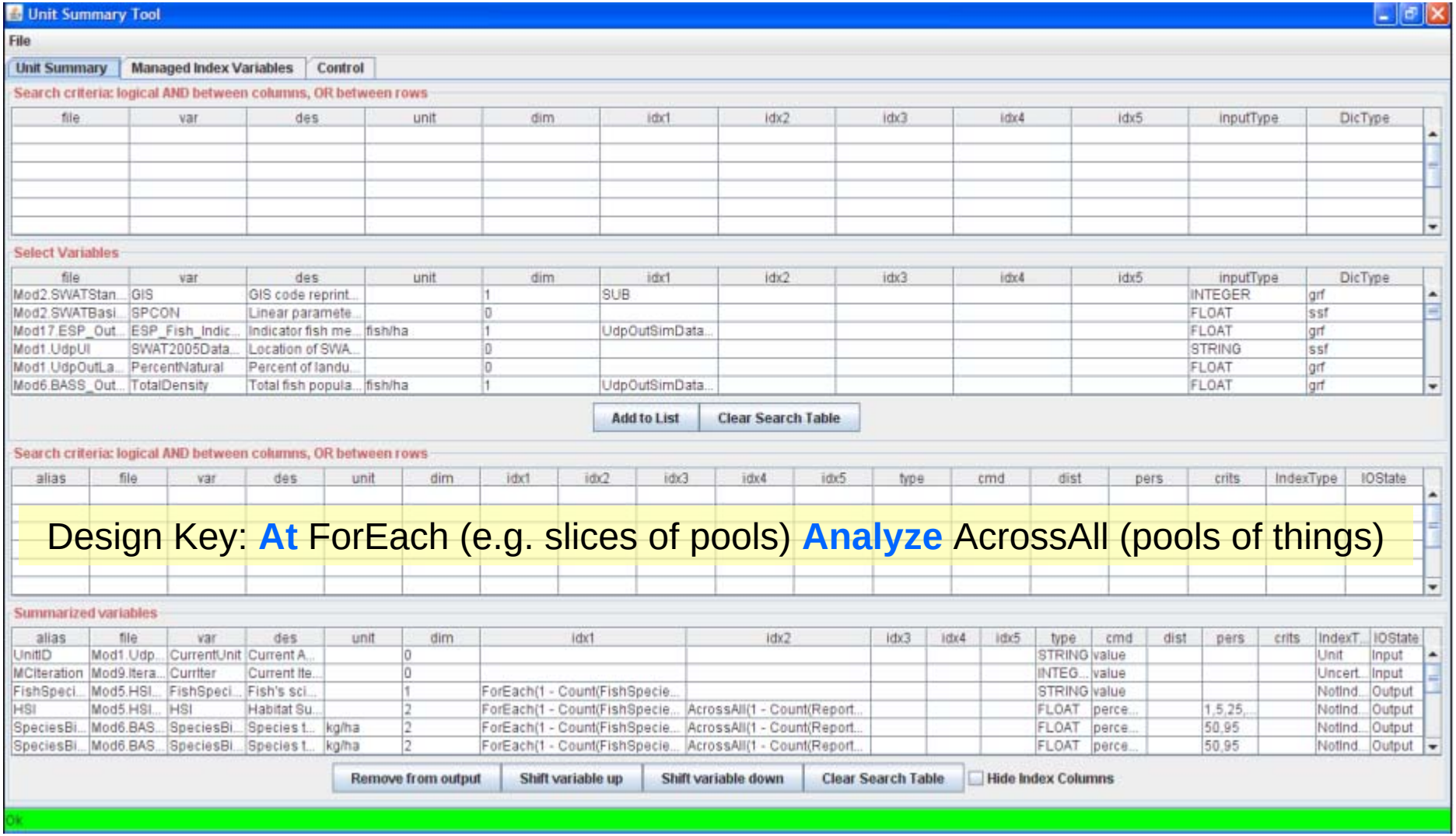




Example Summarizer Desktop F2 Summarizer



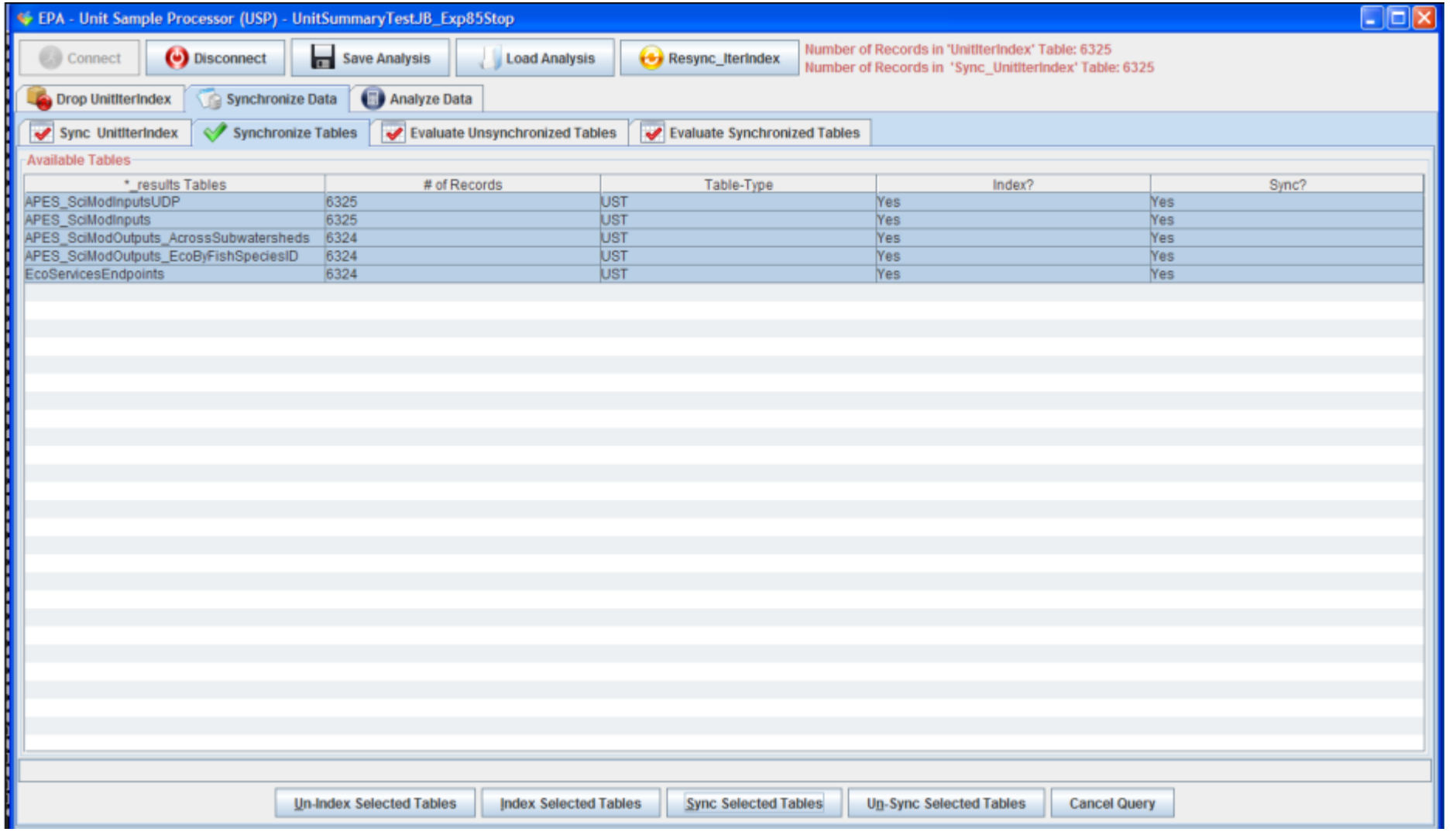
Unit Summary Tool User Interface



Design Key: **At** ForEach (e.g. slices of pools) **Analyze** AcrossAll (pools of things)

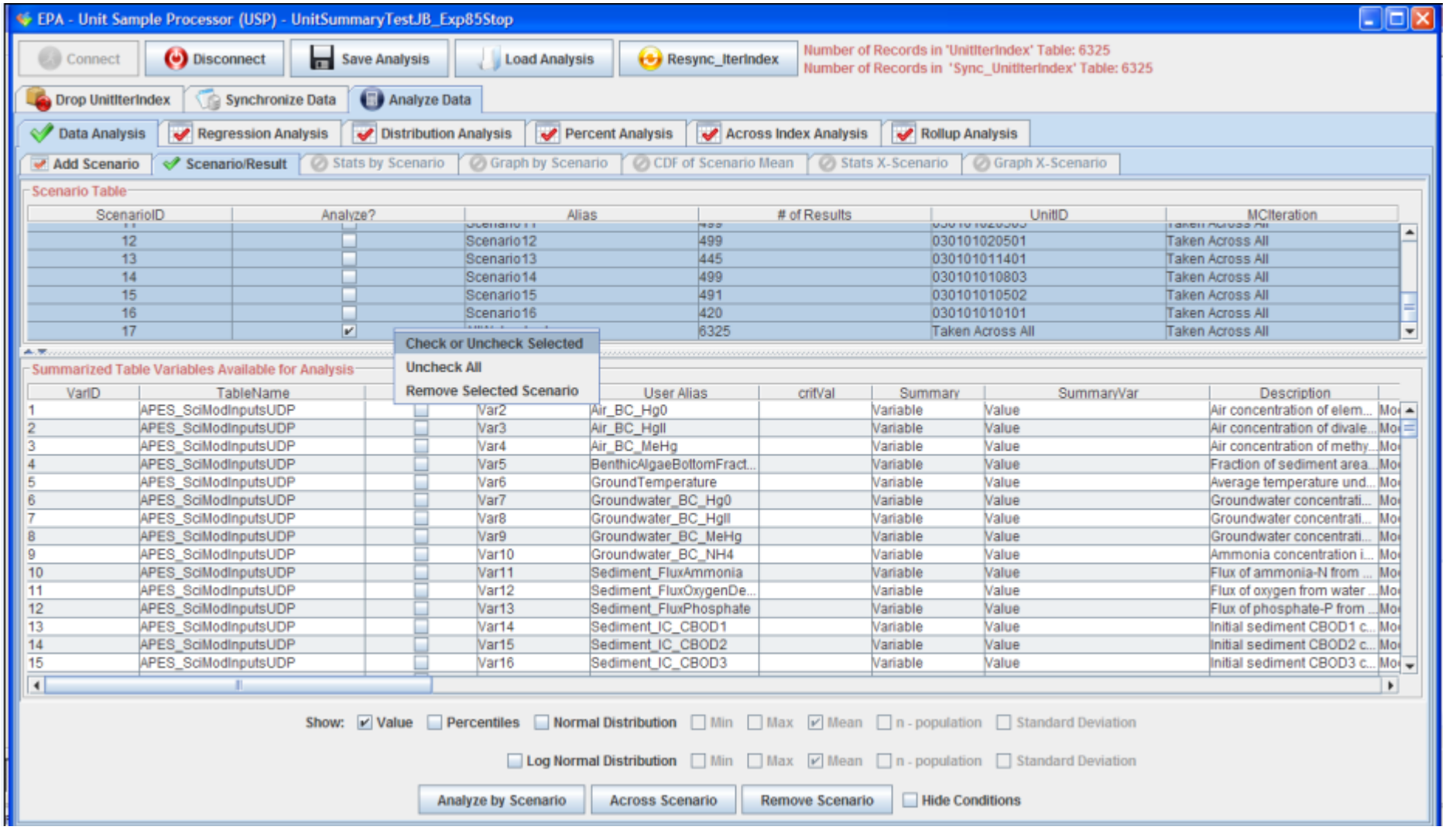
Choosing how and what model system I/O data you want indexed & summarized…

Unit Sample Processor Tool User Interface



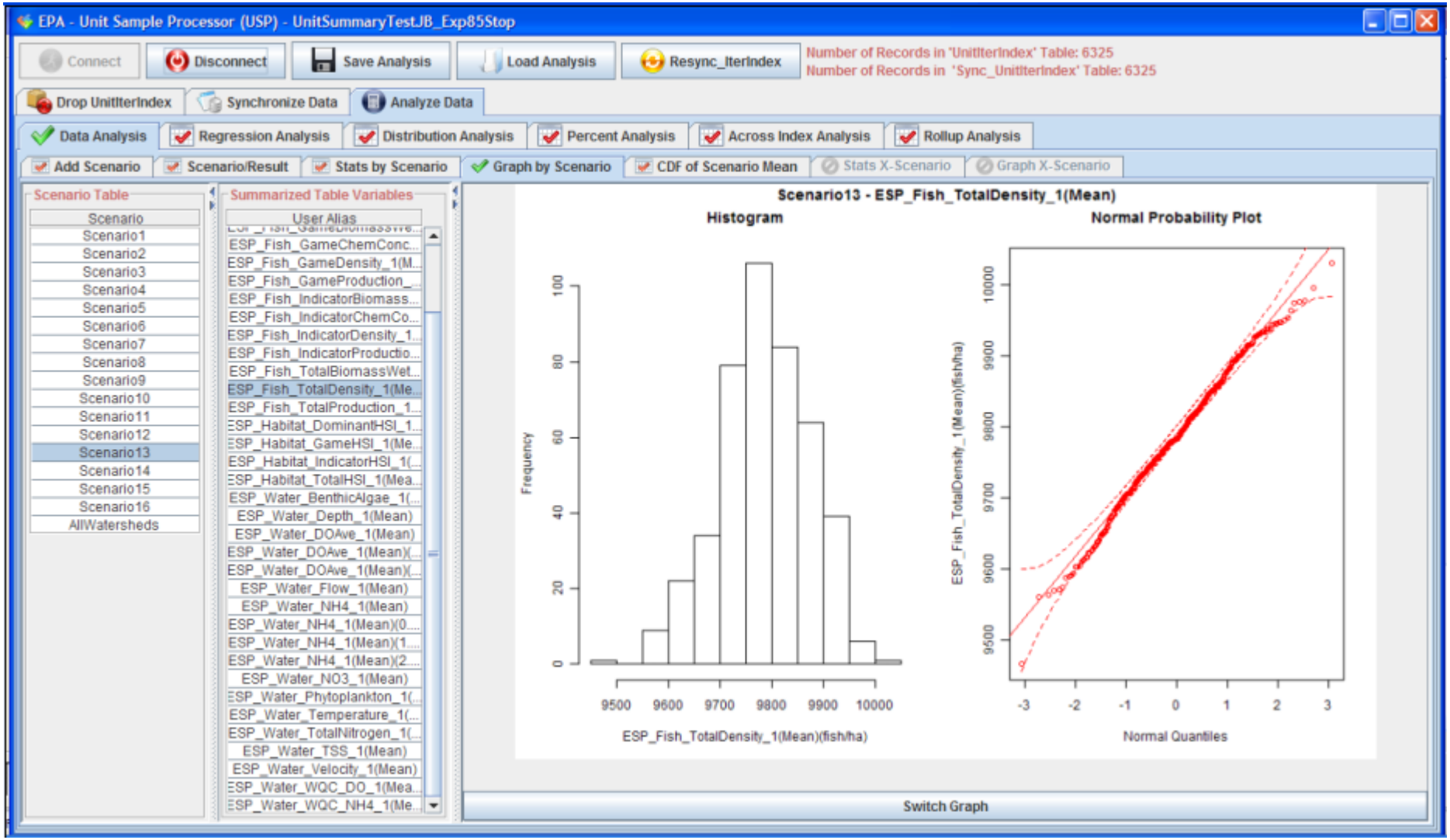
Consumes UST Tool Output (mysql format option)…allows multiple tables, etc

USP Tool: Setting-up Data Analysis



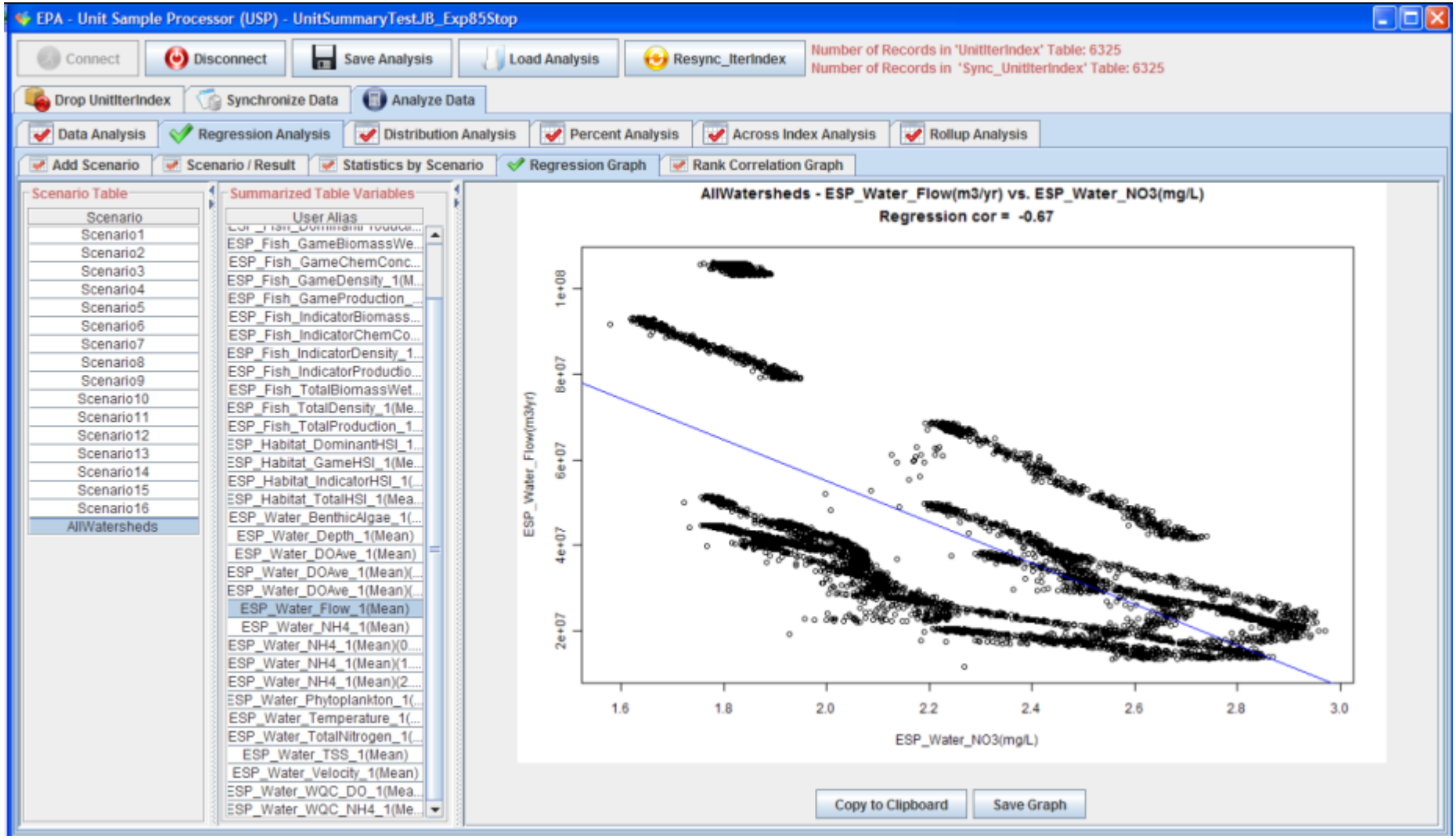
Example of choosing scenarios previously added, and variables of interest in analysis

USP Tool: Another Data Analysis Example



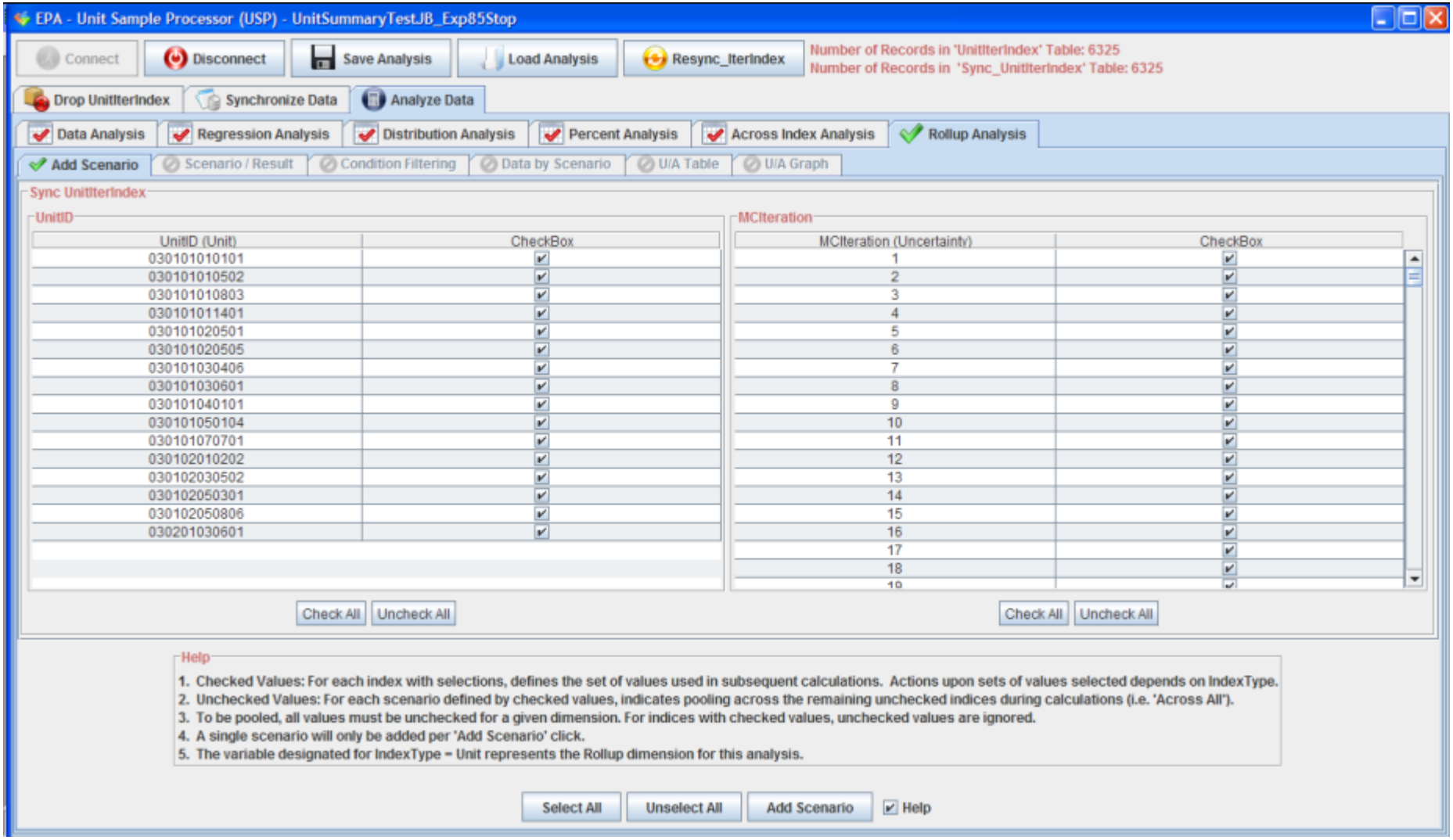
Example of graphical output in data analysis section…..

USP Tool: Regression Example



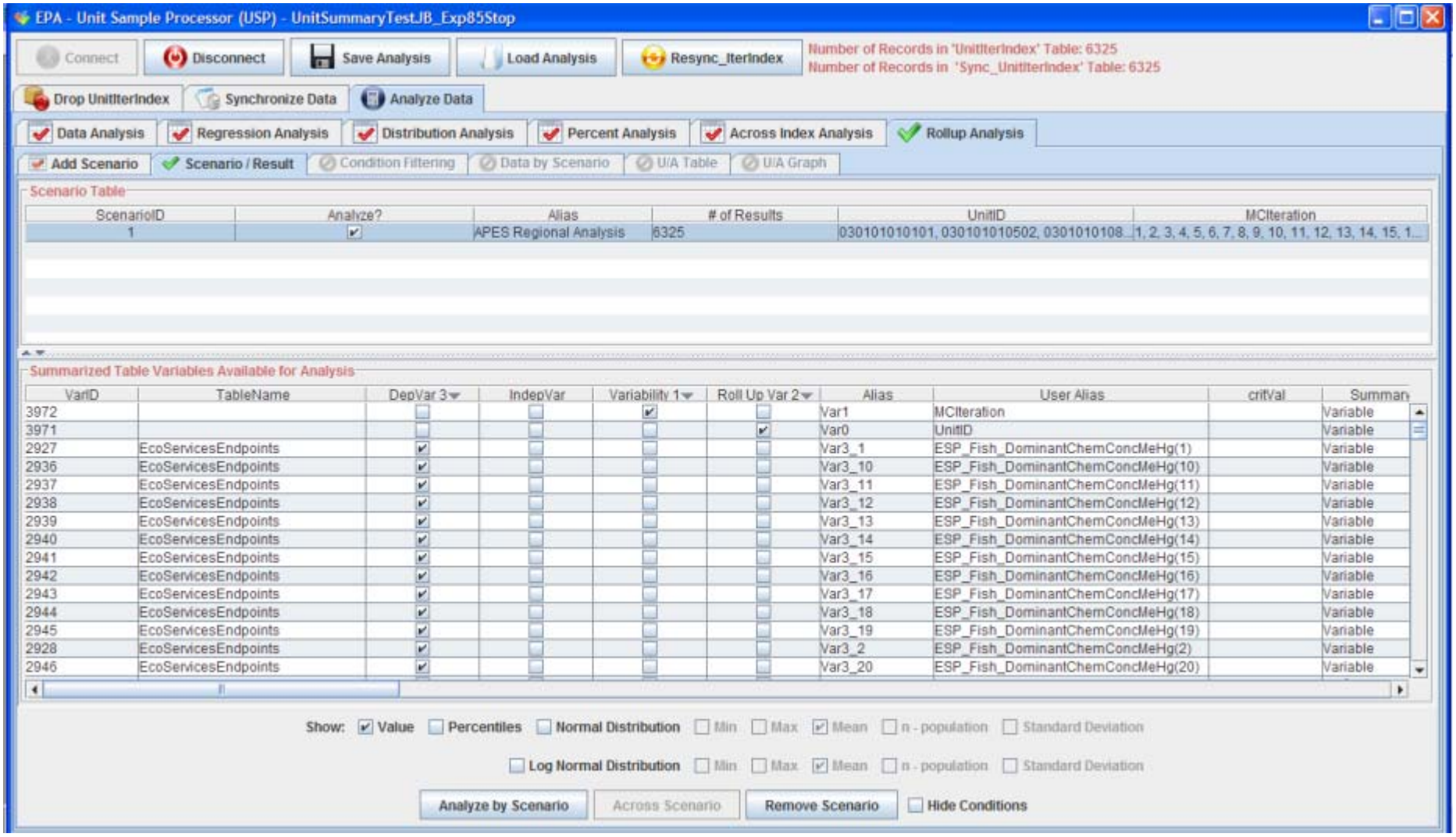
Example of graphical output in regression analysis section…..

USP Tool: Setting-up Rollup Analysis



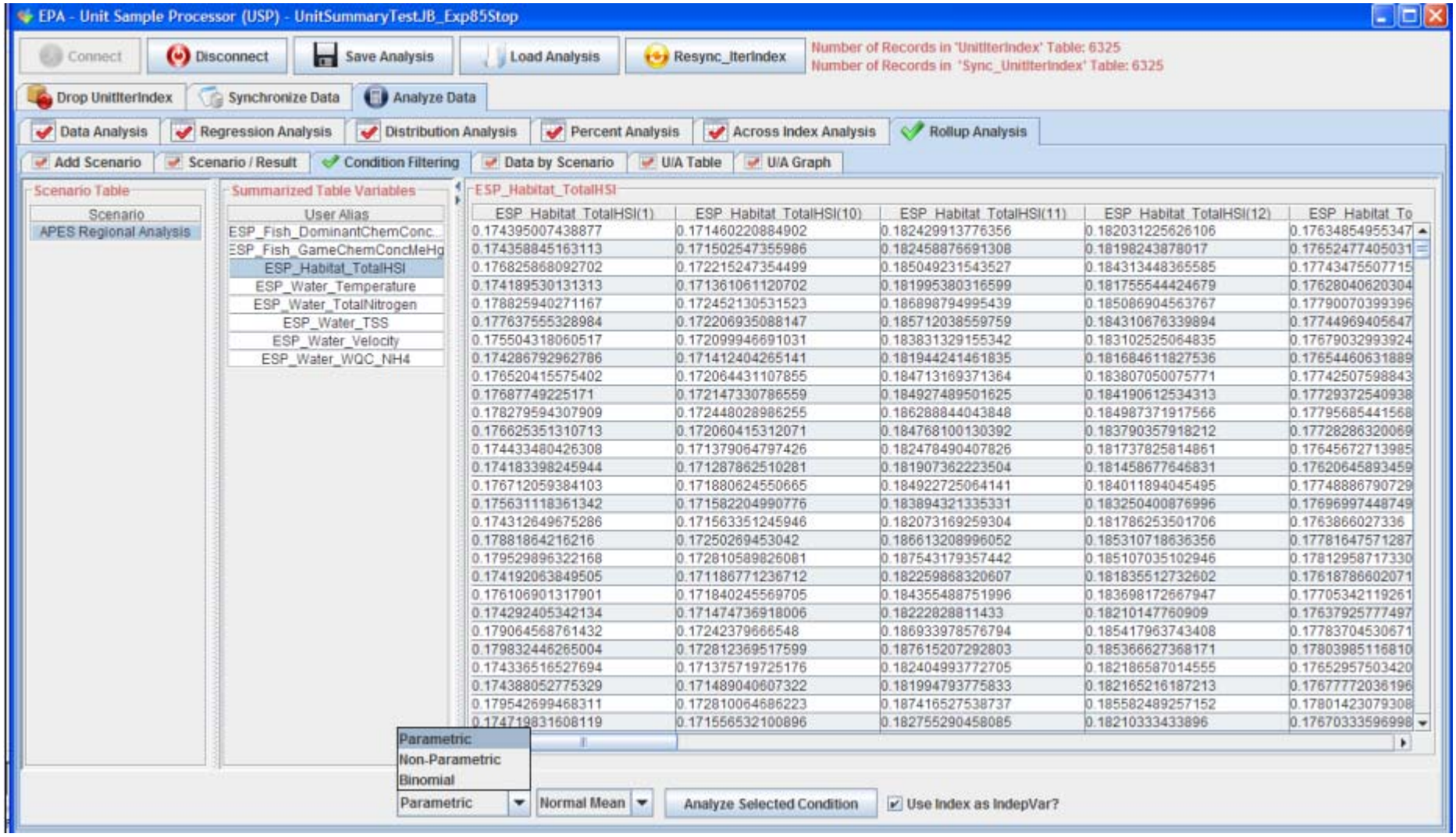
Choosing from “U/V”, “Unit”, and “ExtDecVars” (latter not shown) available in the data structure which was generated by the UST tool…

USP Tool: Setting-up Rollup Analysis



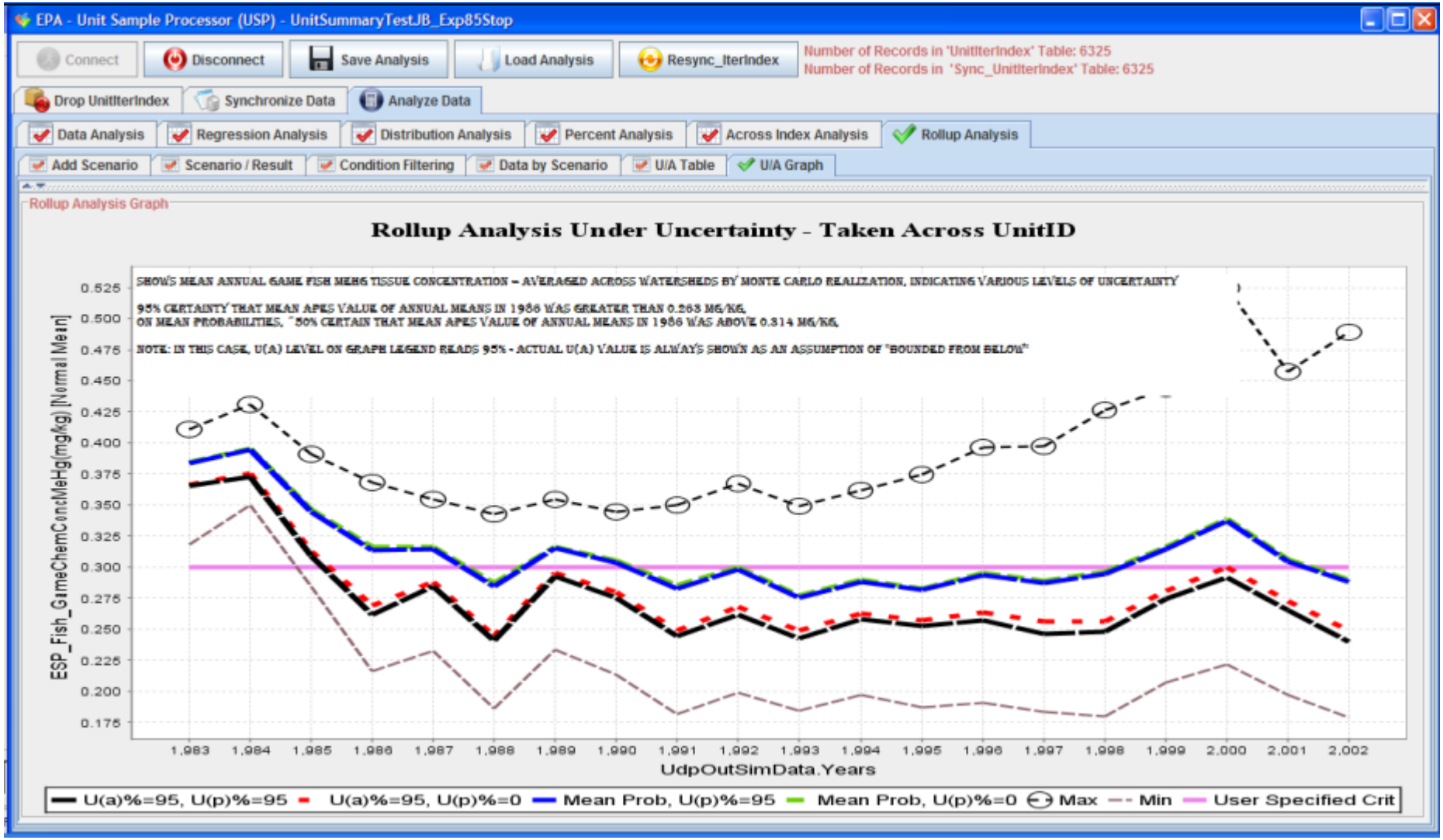
Choosing dependent and independent variables (e.g., ExtDecVars) for the rollup….

USP Tool: Setting-up Rollup Analysis



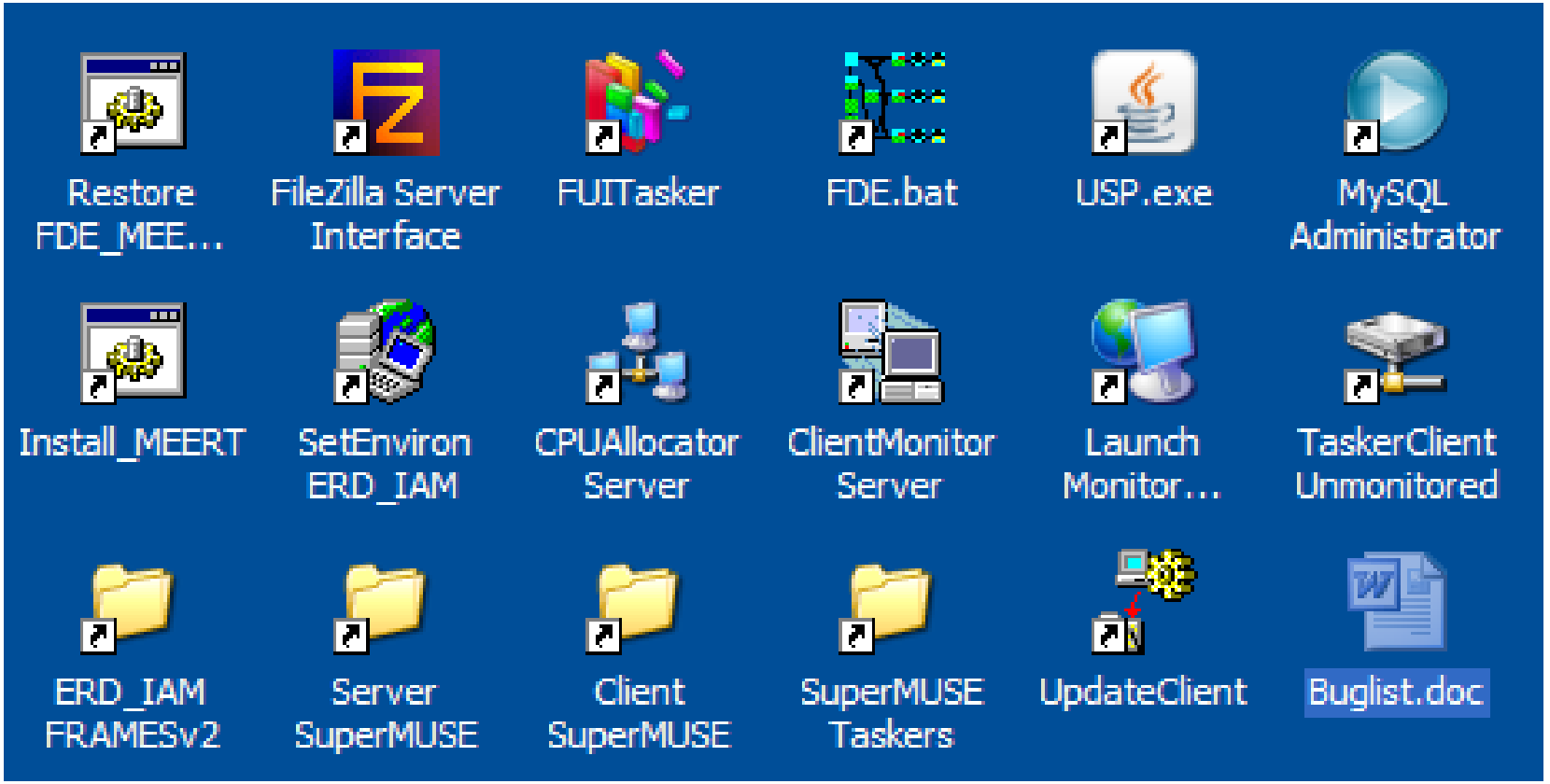
Choosing how you want the “unit” rollup dimension summarized…..i.e. pick a statistic

USP Tool: Rollup Analysis Example



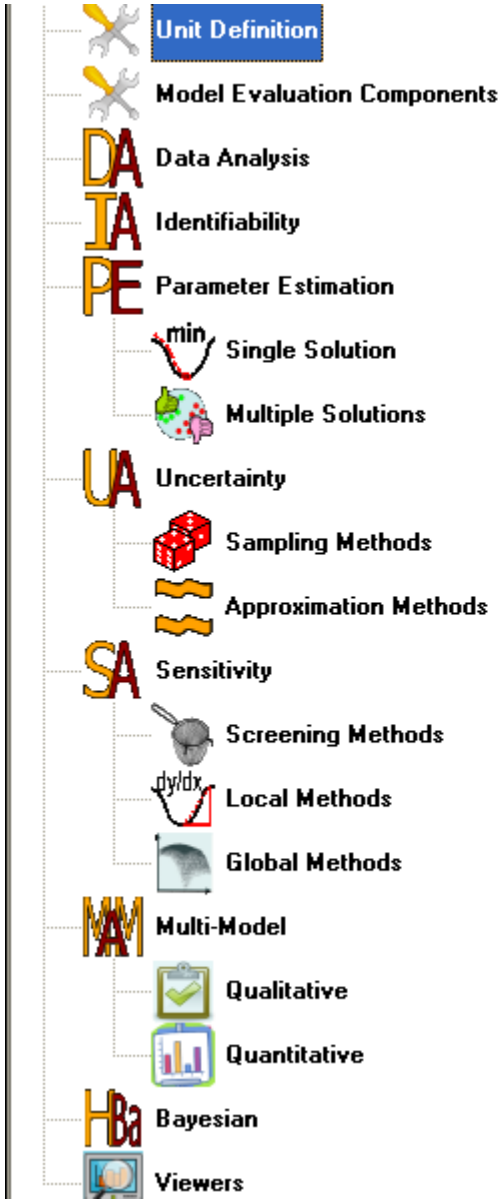
Example Rollup Analysis graphical output showing “population” analysis of units w/ UA

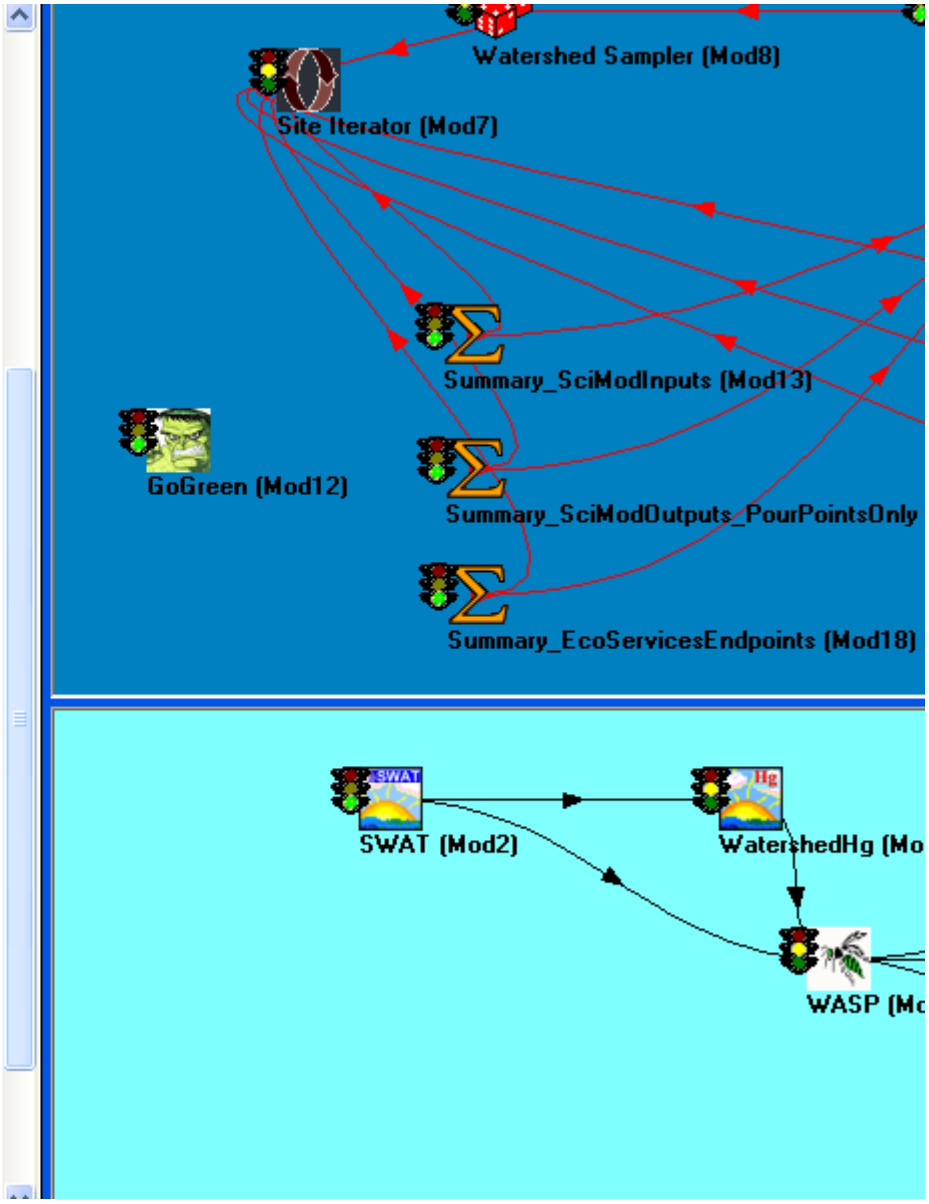
Simple Desktop Palette For Organizing & Launching F2 Stand-Alone PC, and Related SuperMUSE Ops



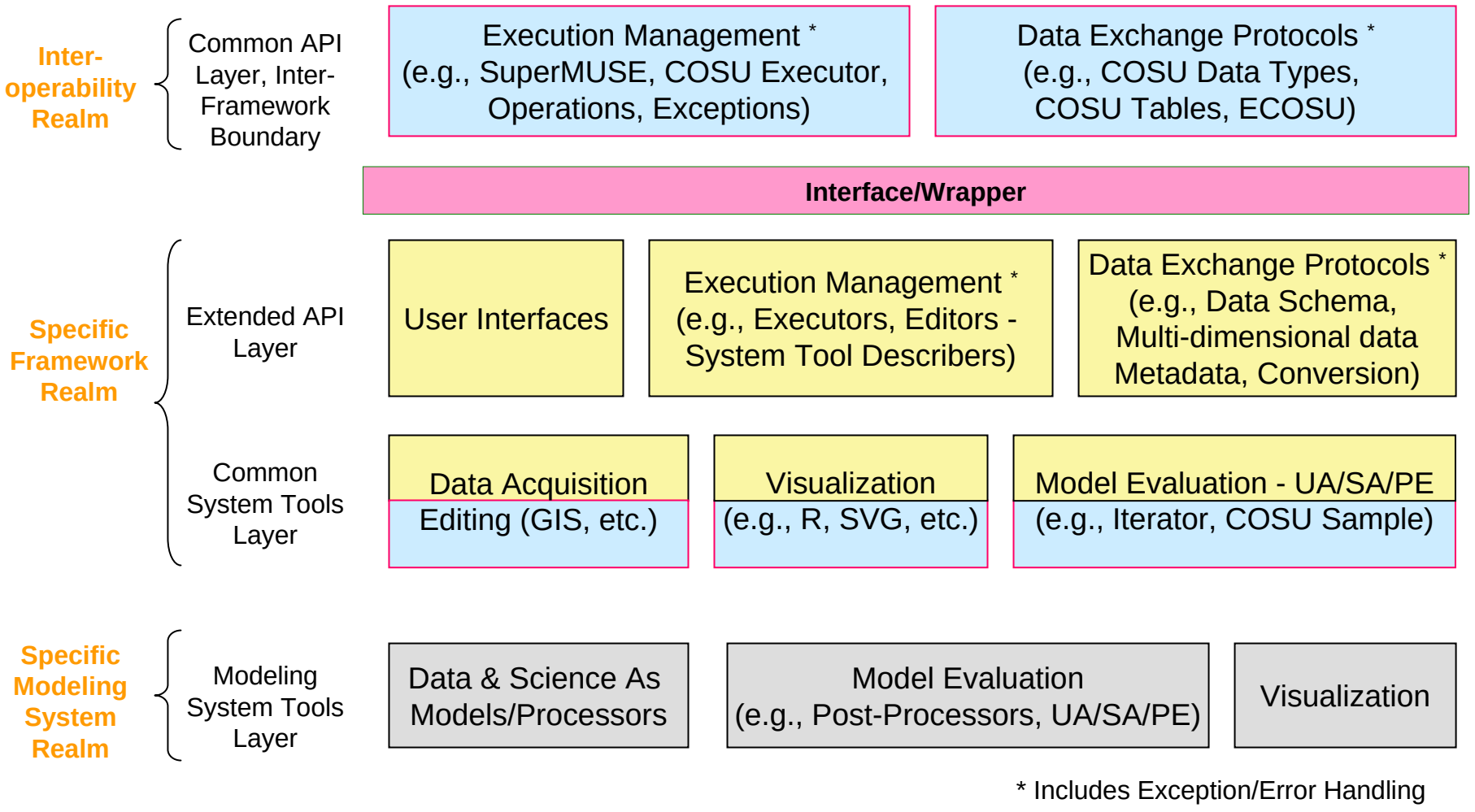
SuperMUSE 1.0 Software Status: beta form undergoing documentation & testing…. supporting multiple modeling systems, including now F2

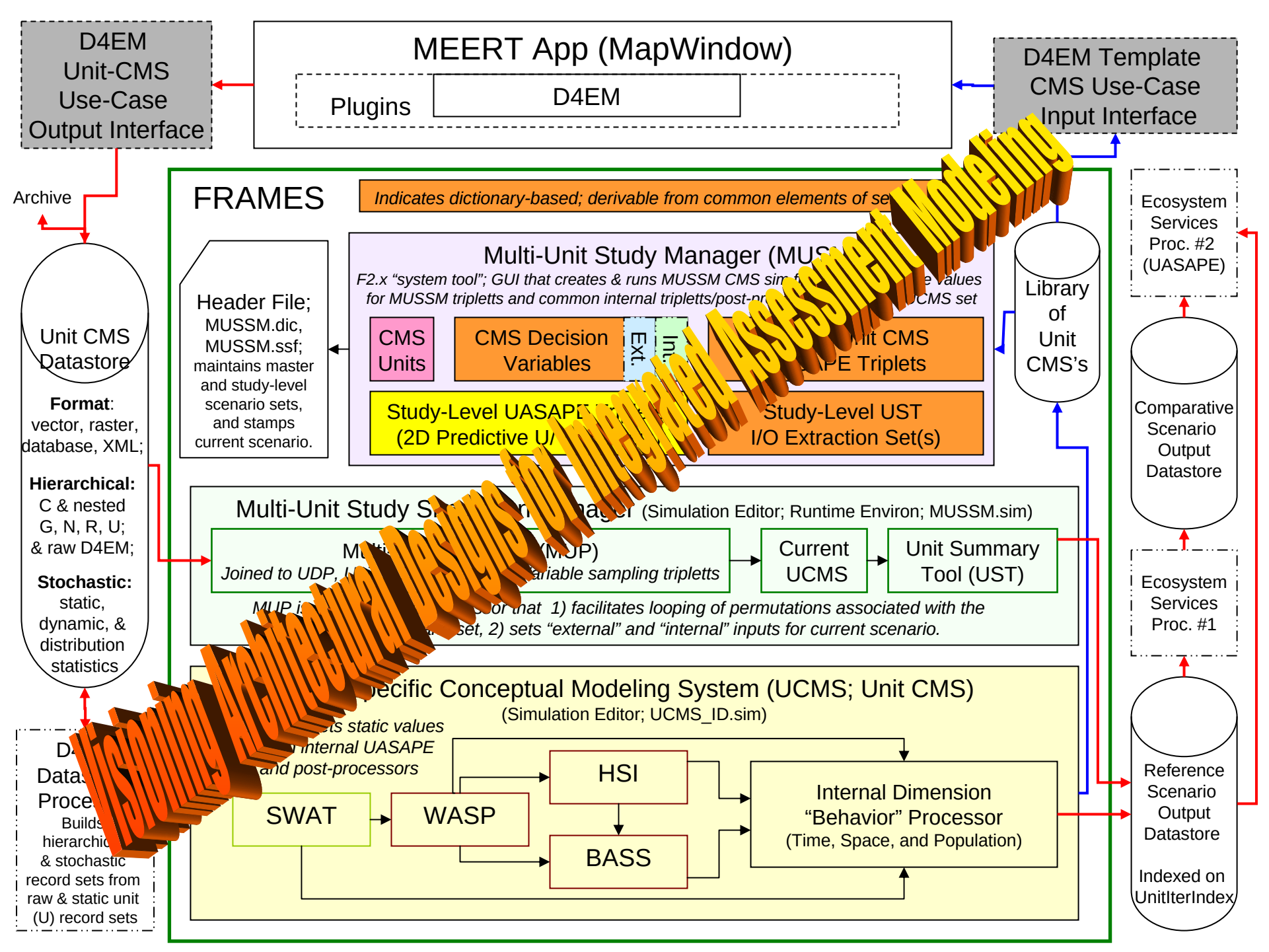
FRAMESv2 Envisioned Model Evaluation Palette





Generalized Inter-Framework Architecture Detail




D4EM Unit-CMS Use-Case Output Interface
MEERT App (MapWindow)
Plugins
D4EM
D4EM Template CMS Use-Case Input Interface
Archive
FRAMES
Indicates dictionary-based; derivable from common elements of se
Ecosystem Services Proc. #2 (UASAPE)
Multi-Unit Study Manager (MUS
F2.x "system tool"; GUI that creates & runs MUSSM CMS sim
for MUSSM tripletts and common internal tripletts/post-pr
CMS set
Header File; MUSSM.dic, MUSSM.ssf; maintains master and study-level scenario sets, and stamps current scenario.
CMS Units
CMS Decision Variables
Ext.
Int.
Unit CMS
PE Triplets
Study-Level UASAPE
(2D Predictive U
Study-Level UST
I/O Extraction Set(s)
Library of Unit CMS's
Unit CMS Datastore
Format: vector, raster, database, XML;
Hierarchical: C & nested G, N, R, U; & raw D4EM;
Stochastic: static, dynamic, & distribution statistics
Multi-Unit Study S
n Manager (Simulation Editor; Runtime Environ; MUSSM.sim)
M
(MUP)
Joined to UDP, I
riable sampling tripletts
Current UCMS
Unit Summary Tool (UST)
MUP i
or that 1) facilitates looping of permutations associated with the
set, 2) sets "external" and "internal" inputs for current scenario.
Comparative Scenario Output Datastore
Ecosystem Services Proc. #1
ecific Conceptual Modeling System (UCMS; Unit CMS)
(Simulation Editor; UCMS_ID.sim)
ts static values
internal UASAPE
and post-processors
HSI
SWAT
WASP
BASS
Internal Dimension "Behavior" Processor
(Time, Space, and Population)
Reference Scenario Output Datastore
Indexed on UnitIterIndex
Builds hierarchic & stochastic record sets from raw & static unit (U) record sets
Visually Architectural Designs for Integrated Assessment Modeling

Related Websites and Papers

http://www.epa.gov/ceampubl/mmedia/3mra/index.htm

- **CEAM Model Download Example: 3MRA Modeling System Files**
  - Source Code
  - Documentation
  - Installation procedures
  - Example Uncertainty Analysis of Seven Chemicals

http://www.epa.gov/athens/research/modeling/supermuse/supermuse.html

- **SuperMUSE**: Supercomputer for Model Uncertainty and Sensitivity Evaluation
  - Babendreier, J.E., Castleton, K.J.. (2005). Investigating Uncertainty and Sensitivity in Integrated Multimedia Environmental Models: Tools for FRAMES-3MRA. Journal of Environmental Modelling and Software, 20(8) pp: 1043-1055.

http://www.epa.gov/athens/research/modeling/modelevaluation/

- **EPA/ORD/NERL/ERD Model Evaluation Tools Website**
  - Matott, L. S., J. E. Babendreier, and S. T. Purucker (2009). Evaluating uncertainty in integrated environmental models: A review of concepts and tools, Water Resour. Res., 45, W06421, doi:10.1029/2008WR007301.

SuperMUSE Technical Support

Beta SuperMUSE Version 1.0

- Currently available in the F2 development community
  - Beta is beta, so users should use appropriate caution in disseminating results
  - Generally works pretty well, but specific network restrictions can apply
  - Software can be made available upon request
  - Can be used in desktop and cluster mode (e.g., 1 to 1000^{+} PCs)
- Documentation currently limited but in production, available 2010
  - Installation procedures with some discussion can be provided for now as feasible
  - Technical support and on-site installation help can be made available in a limited number of cases, as time, resources, and priorities allow
- Use and feedback by EPA is encouraged
  - Contact Justin Babendreier, EPA/ORD/NERL/ERD/RSB

Beta FRAMES Version 2

- Currently also available in the F2 development community
- Contact Gerry Laniak or Kurt Wolfe, EPA/ORD/NERL/ERD/RSB

SuperMUSE facilitates model evaluation functionality for both single desktop and cluster operations….multi-threaded F2 desktop ops soon - needs enhanced F2-API.