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

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ISCMEM Workshop on Environmental Modeling Rockville, Md

RESEARCH & DEVELOPMENT

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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 <big⁴

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:

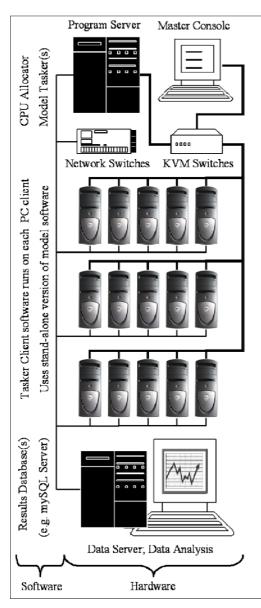
- Many techniques and methods available, improving constantly.
- Current knowledge and execution capabilities usually limited to a select few, out of reach from most model developers and model users.
- An "**embarrassingly parallel**" computational problem; solutions involve running a model over and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

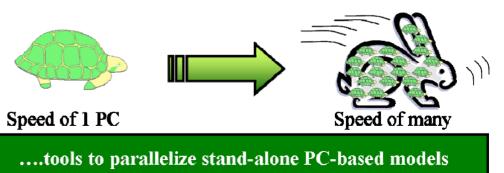
Parallel Computing and You

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 <u>&</u> Software

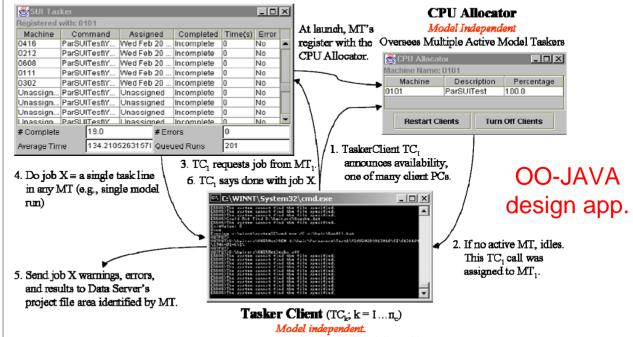




Clustering to Increase Computational Capacity

Model Tasker

Model Dependent - Create an MT for each modeling system Parallelizes a stand-alone PC-Model's System User Interface



Executes DOS commands in batch files delivered by MT.

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

EPA's SuperMUSE Cluster, Athens GA

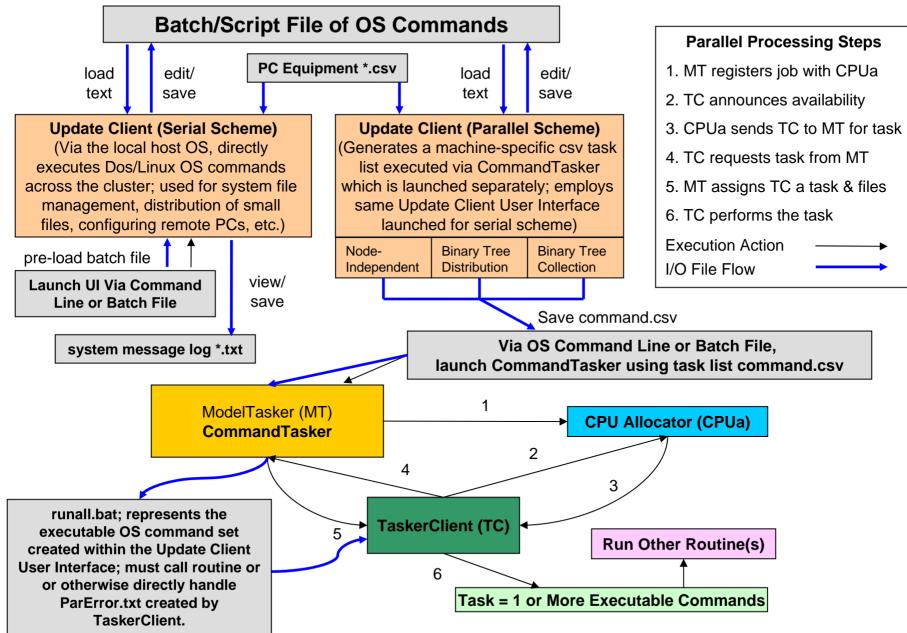


Example SuperMUSE Tool: UpdateClient

Managing files and PC settings across your cluster via OS

Editing C:\ERD_IAM\SuperMUSE\RunApps\Server\Upd	lateClient\PushSuperMUSE_Update.bat	
File Help Execute	Create command.csv	Invert Selection
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Can run serially → via CPU of server hosting this app or	0114D, [WinXP_520], WinXP, Optiple 0115D, [WinXP_520], WinXP, Optiple 0116D, [WinXP_520], WinXP, Optiple 0201D, [WinXP_520], WinXP, Optiple 0202D, [WinXP_520], WinXP, Optiple 0203D, [WinXP_520], WinXP, Optiple	x GX520, (c,\3mra), 1 Disks, 1 CPUs x GX520, (c,\3mra), 1 Disks, 1 CPUs
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SuperMUSE 1.0 UpdateClient Tool Detail



SuperMUSE CPU Allocator, TaskerClient, & ClientMonitor Tools

🛃 CPU Allocator						_ 🗆 🗙
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🔀 ClientMonitor			🦉 TaskerClient			- 🗆 🗙
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Client	Status	Time				
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SuperMUSE ClientMonitor, CPU Allocator, and TaskerClient shown

Example Model Tasker → F2 FUITasker

🖆 CPU Allocator								_ 🗆 🛛
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Kill TaskerClie	ents Restart	Clients Sh	utdown Clients	Normalize	% Loads	Pressed at		
🕌 FUI Tasker Queu	ie Manager							
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Tasks Failed Tas	sks Failed Macl	nines						
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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

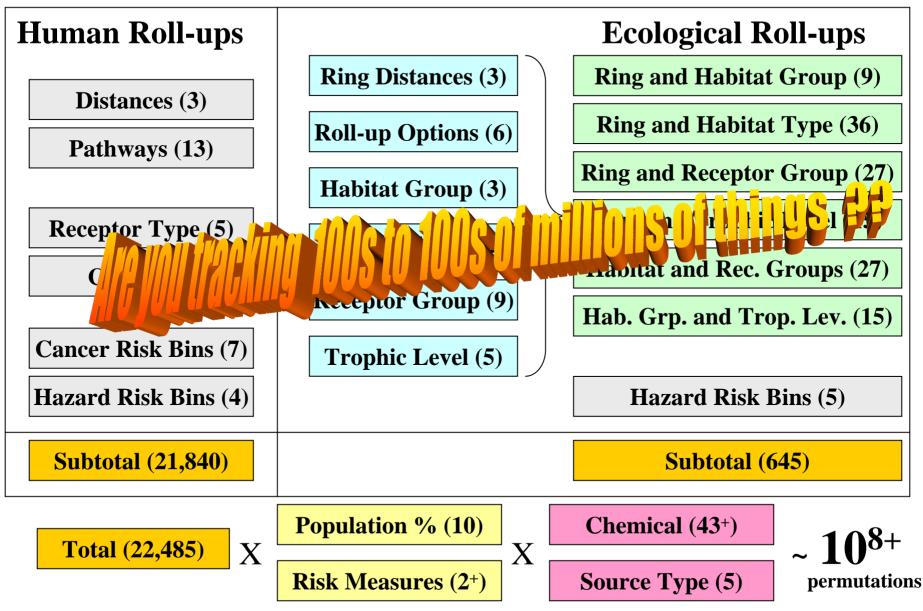
 In the end....it is "all about" data and dimensionality reduction -- best decision.

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

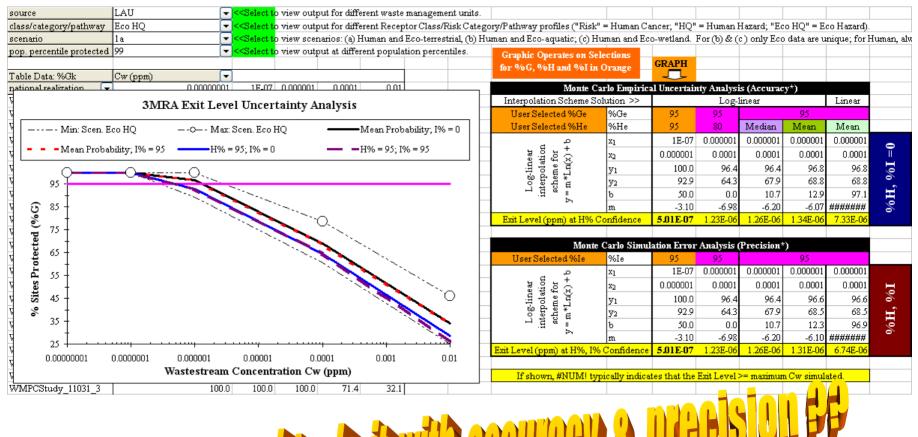
 In the endit is also "all about" data and dimensionality reduction, with a known (reproducible) level of quality -- best answer.

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

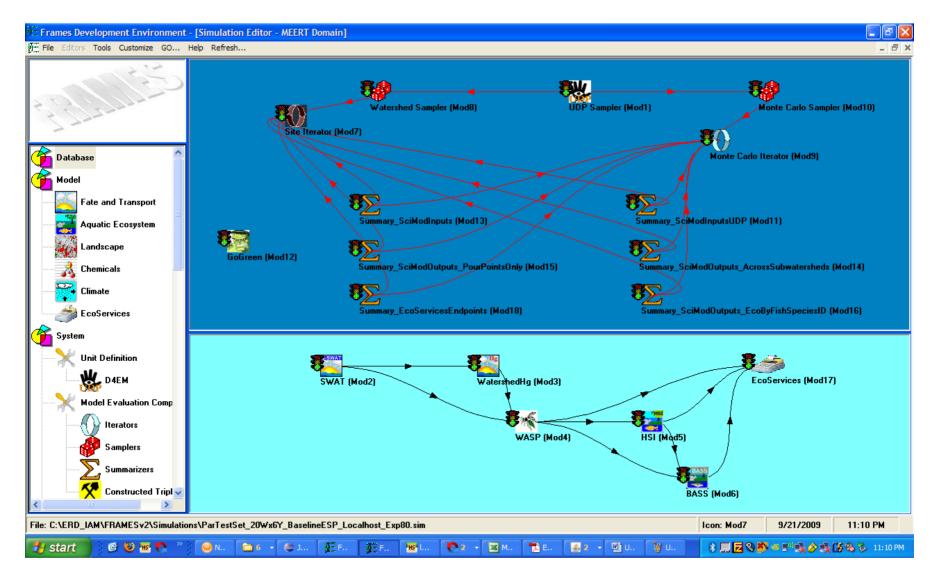


Example FRAMES-3MRA Uncertainty Analysis

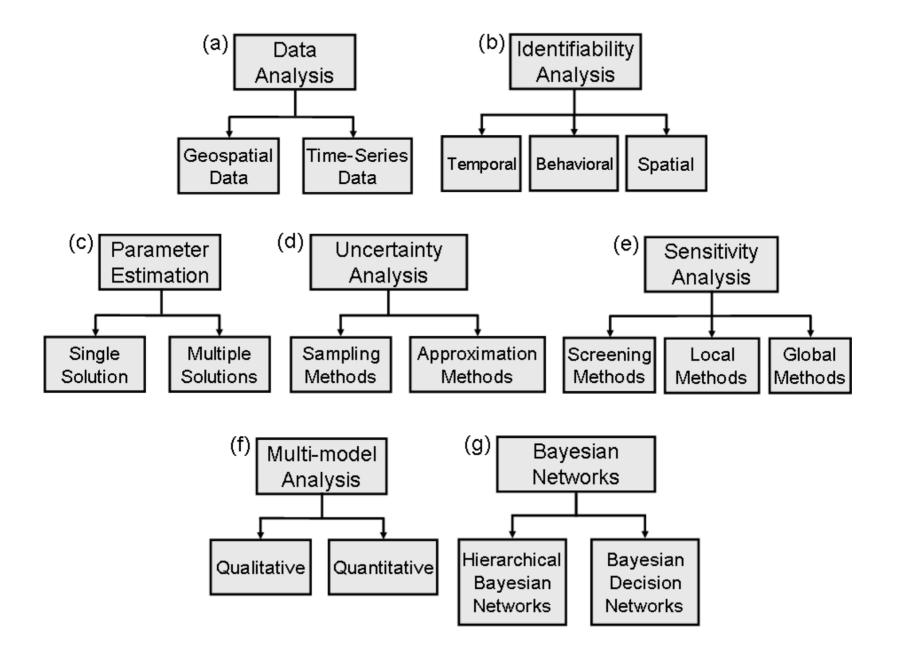




FRAMESv2-MEERT App. Simulation Design with Cyclic System-level Model Evaluation Components



Model Evaluation Framework Implementation Plan



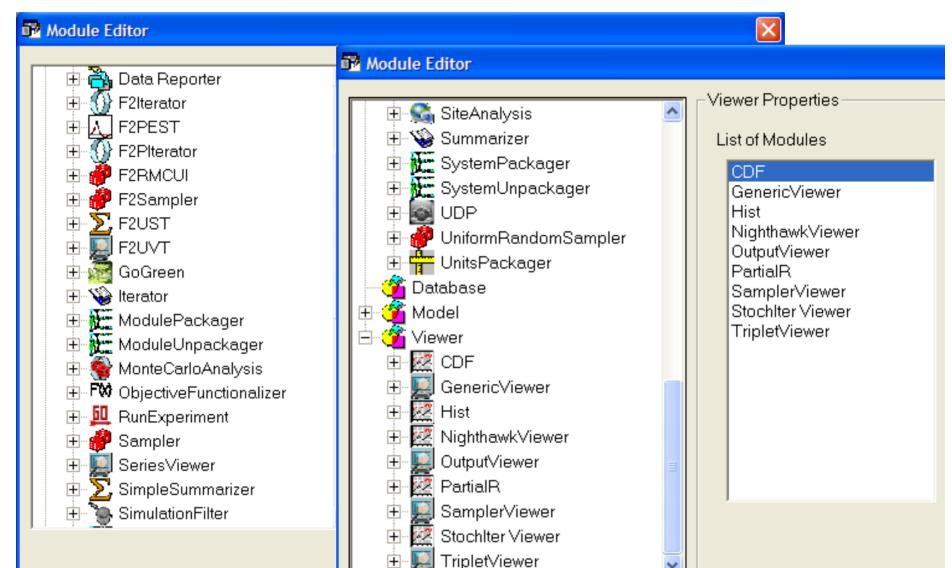
Recent and Ongoing Objectives Develop FRAMESv2 capabilities for:

- 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/postprocessing 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

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lod1, Mod13, Mod2, Mod3, Mod4, Mod5, Mod6, Mod14					
dex Sequence (none = no outer loops, or in serial mode)					
lod11					
NK					
		Reset		Rer	nove
	# Complet	te 0.0		# Errors	1
	Average Ti	ime NaN		Queued Runs	6

Example Summarizer Desktop F2 Summarizer

×

FRAMESv2 Simple Summarizer Configuration Utility

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Add Variable			Edit Variable			Remove Variable
Current Iterati	ion 1					
Save						Quit

Unit Summary Tool User Interface

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

Unit Sample Processor Tool User Interface

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Connect Oisconne	ct Save	Analysis		😔 Resync_IterIndex		Records in 'UnitIterIndex' Table: 6325 Records in 'Sync_UnitIterIndex' Table: 63	125
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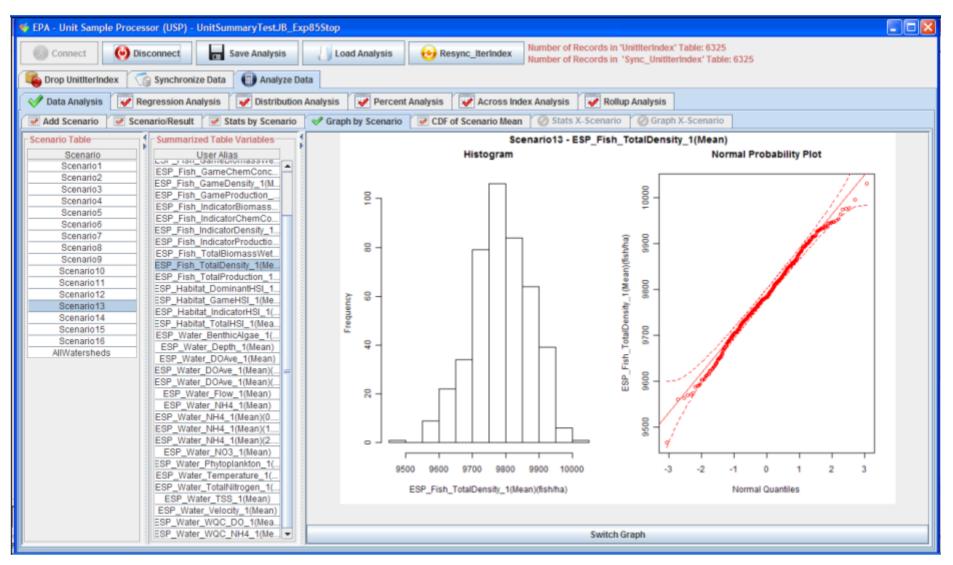
Consumes UST Tool Output (mysql format option)...allows multiple tables, etc

USP Tool: Setting-up Data Analysis

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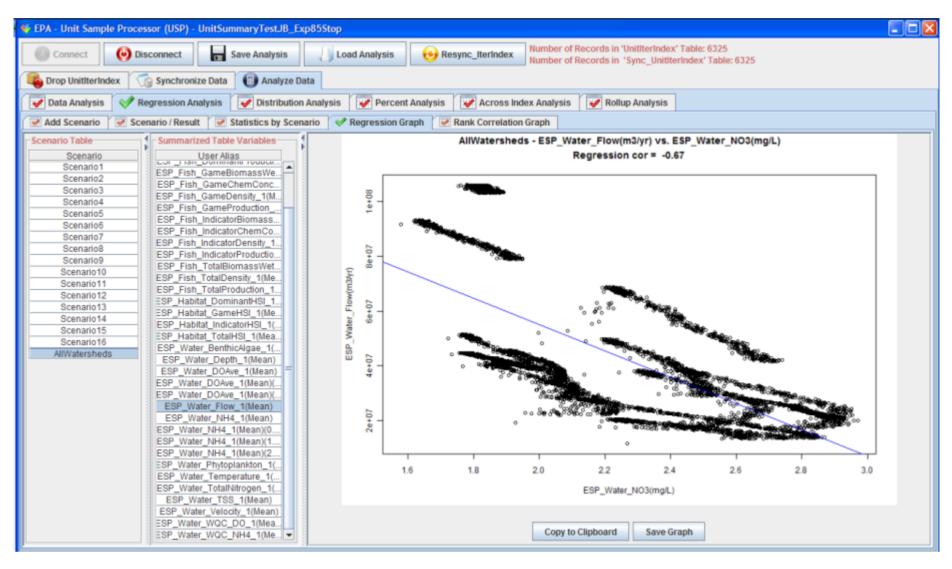
Example of choosing scenarios previously added, and variables of interest in analysis

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

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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

💗 EPA - Unit San	mple Processor (USP) - UnitSu	mmaryTestJB_Exp8	5Stop						
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VariD	TableName	DepVar 3-	IndepVar	Variability 1-	Roll Up Var 2-	Alias	User Alias	critVal	Summan
3972	2 and a contraction			2		Vart	MCIteration	arrist ar	Variable +
3971			1 N N		v .	Var0	UnitID		Variable =
2927	EcoServicesEndpoints	×				Var3_1	ESP_Fish_DominantChemConcMeHg(1)		Variable
2936	EcoServicesEndpoints	2				Var3_10	ESP_Fish_DominantChemConcMeHg(10)		Variable
2937	EcoServicesEndpoints	2				Var3_11	ESP_Fish_DominantChemConcMeHg(11)		Variable
2938	EcoServicesEndpoints	2				Var3_12	ESP_Fish_DominantChemConcMeHg(12)		Variable
2939	EcoServicesEndpoints	V				Var3_13	ESP_Fish_DominantChemConcMeHg(13)		Variable
2940	EcoServicesEndpoints	2				Var3_14	ESP_Fish_DominantChemConcMeHg(14)		Variable
2941	EcoServicesEndpoints	~				Var3_15	ESP_Fish_DominantChemConcMeHg(15)		Variable
2942	EcoServicesEndpoints	¥	2		1 1	Var3_16	ESP_Fish_DominantChemConcMeHg(16)		Variable
2943	EcoServicesEndpoints	r				Var3_17	ESP_Fish_DominantChemConcMeHg(17)		Variable
2944	EcoServicesEndpoints	×.				Var3_18	ESP_Fish_DominantChemConcMeHg(18)		Variable
2945	EcoServicesEndpoints	2				Var3_19	ESP_Fish_DominantChemConcMeHg(19)		Variable
2928	EcoServicesEndpoints	×.				Var3_2	ESP_Fish_DominantChemConcMeHg(2)		Variable
2946	EcoServicesEndpoints	r .				Var3_20	ESP_Fish_DominantChemConcMeHg(20)		Variable 👻
4	1	1 220	24 - CAN	61 1020	10 - 1103	2	- A		
	Show] Min 🗌 Max [🛛 Mean 🔲 n	- population Standard Deviation - population Standard Deviation Hide Conditions		

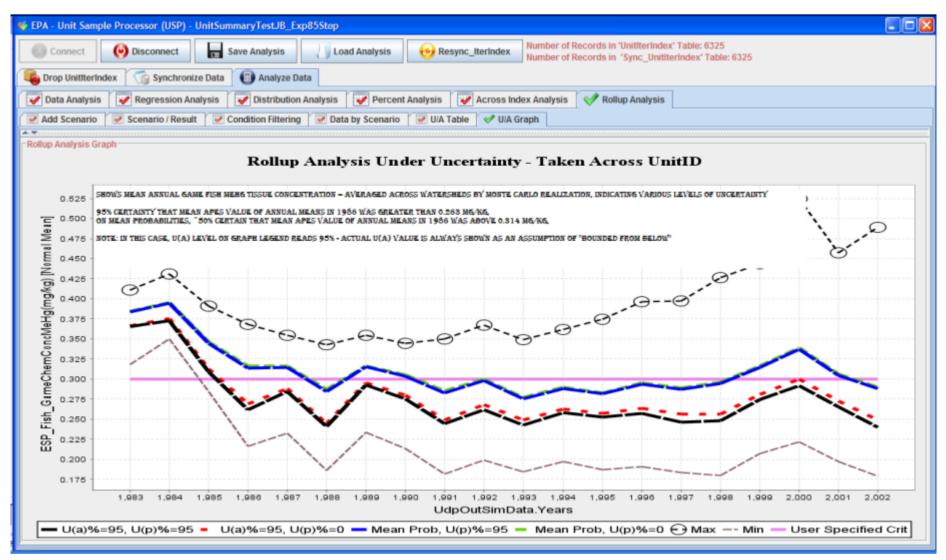
Choosing dependent and independent variables (e.g., ExtDecVars) for the rollup....

USP Tool: Setting-up Rollup Analysis

🥑 Data Analysis 🛛 🛃 I		ze Data ution Analysis				
		ution Analysis				
🦉 Add Scenario 🎽 💽 Sc	1	anon reading and	ysis 🛛 😺 Across Index Analys	is 🔗 Rollup Analysis		
and the second se	enario / Result 🛛 🥩 Condition Filt	ering 🖉 Data by Scenario 🏾	UIA Table 📝 UIA Graph			
icenario Table	Summarized Table Variables	ESP_Habitat_TotalHSI				
Scenario	User Alias	ESP Habitat TotalHSI(1)	ESP Habitat TotalHSI(10)	ESP Habitat TotalHSI(11)	ESP Habitat TotalHSI(12)	ESP Habitat To
APES Regional Analysis	ESP Fish DominantChemCon		0.171460220884902	0.182429913776356	0.182031225626106	0.17634854955347
	ESP_Fish_GameChemConcMe	Hg 0.174358845163113	0.171502547355986	0.182458876691308	0.18198243878017	0.17652477405031
	ESP_Habitat_TotalHSI	0.176825868092702	0.172215247354499	0.185049231543527	0.184313448365585	0.17743475507715
	ESP_Water_Temperature	0.174189530131313	0.171361061120702	0.181995380316599	0.181755544424679	0.17628040620304
	ESP_Water_TotalNitrogen	0.178825940271167	0.172452130531523	0.186898794995439	0.185086904563767	0.17790070399396
	ESP_Water_TSS	0.177637555328984	0.172206935088147	0.185712038559759	0.184310676339894	0.17744969405647
	ESP_Water_Velocity	0.175504318060517	0.172099946691031	0.183831329155342	0.183102525064835	0.17679032993924
	ESP_Water_WQC_NH4	0.174286792962786	0.171412404265141	0.181944241461835	0.181684611827536	0.17654460631889
		0.176520415575402	0.172064431107855	0.184713169371364	0.183807050075771	0.17742507598843
		0.17687749225171	0.172147330786559	0.184927489501625	0.184190612534313	0.17729372540938
		0.178279594307909	0.172448028986255	0.186288844043848	0.184987371917566	0.17795685441568
	1	0.176625351310713	0.172060415312071	0.184768100130392	0.183790357918212	0.17728286320069
		0.174433480426308	0.171379064797426	0.182478490407826	0.181737825814861	0.17645672713985
		0.174183398245944	0.171287862510281	0.181907362223504	0.181458677646831	0.17620645893459
		0.176712059384103	0.171880624550665	0.184922725064141	0.184011894045495	0.17748886790729
		0.175631118361342	0.171582204990776	0.183894321335331	0.183250400876996	0.17696997448749
		0.174312649675286	0.171563351245946	0.182073169259304	0.181786253501706	0.1763866027336
		0.17881864216216	0.17250269453042	0.186613208996052	0.185310718636356	0.17781647571287
		0.179529896322168	0.172810589826081	0.187543179357442	0.185107035102946	0.17812958717330
		0.174192063849505	0.171186771236712	0.182259868320607	0.181835512732602	0.17618786602071
		0.176106901317901	0.171840245569705	0.184355488751996	0,183698172667947	0.17705342119261
		0.174292405342134	0.171474736918006	0.18222828811433	0.18210147760909	0.17637925777497
		0.179064568761432	0.17242379666548	0.186933978576794	0.185417963743408	0.17783704530671
		0.179832446265004	0.172812369517599	0.187615207292803	0.185366627368171	0.17803985116810
		0.174336516527694	0.171375719725176	0.182404993772705	0.182186587014555	0.17652957503420
		0.174388052775329	0.171489040607322	0.181994793775833	0.182165216187213	0.17677772036196
		0.179542699468311	0.172810064686223	0.187416527538737	0.185582489257152	0.17801423079308
		0.174719831608119	0.171556532100896	0.182755290458085	0.18210333433896	0.17670333596998
		metric n		M	-19 -19	•
		Parametric				
	Bino	mial metric 💌 Normal Mean 💌		Use Index as IndepVar?		

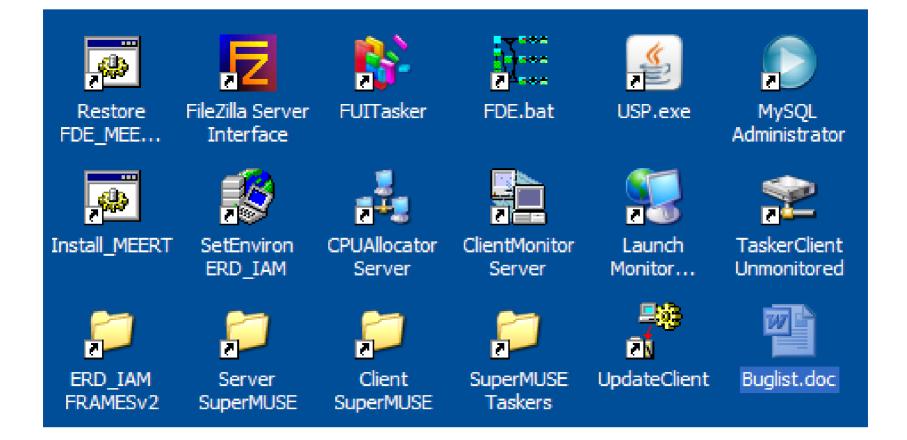
Choosing how you want the "unit" rollup dimension summarized.....i.e. pick a statistic

USP Tool: Rollup Analysis Example



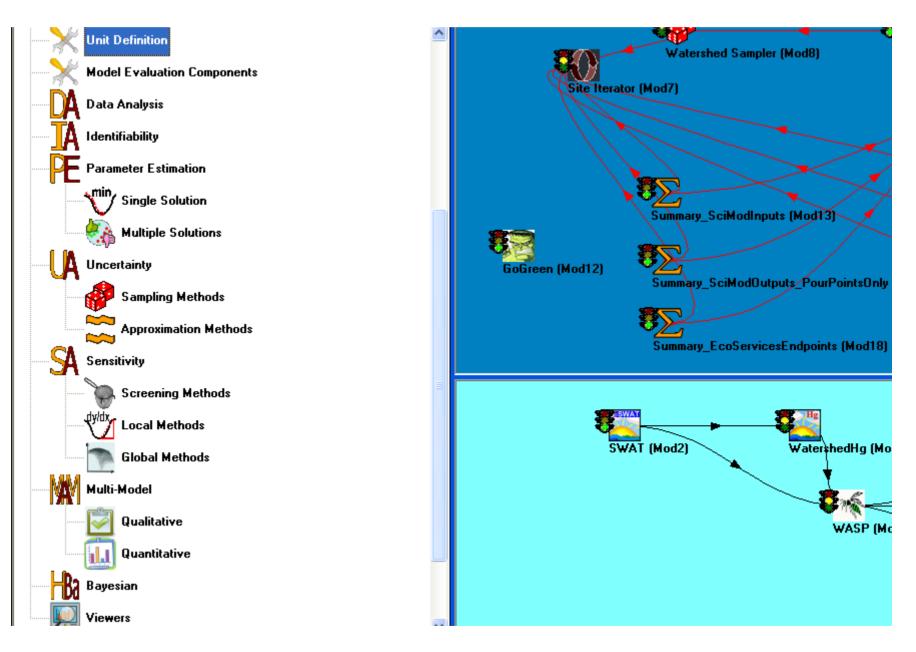
Example Rollup Analysis graphical output showing "population" analysis of units w/ UA

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

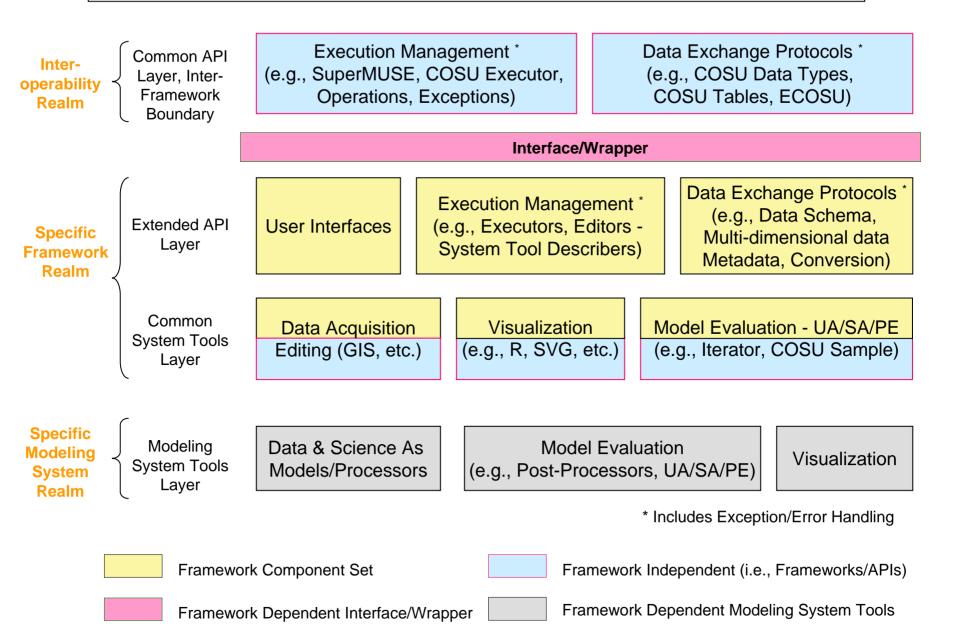


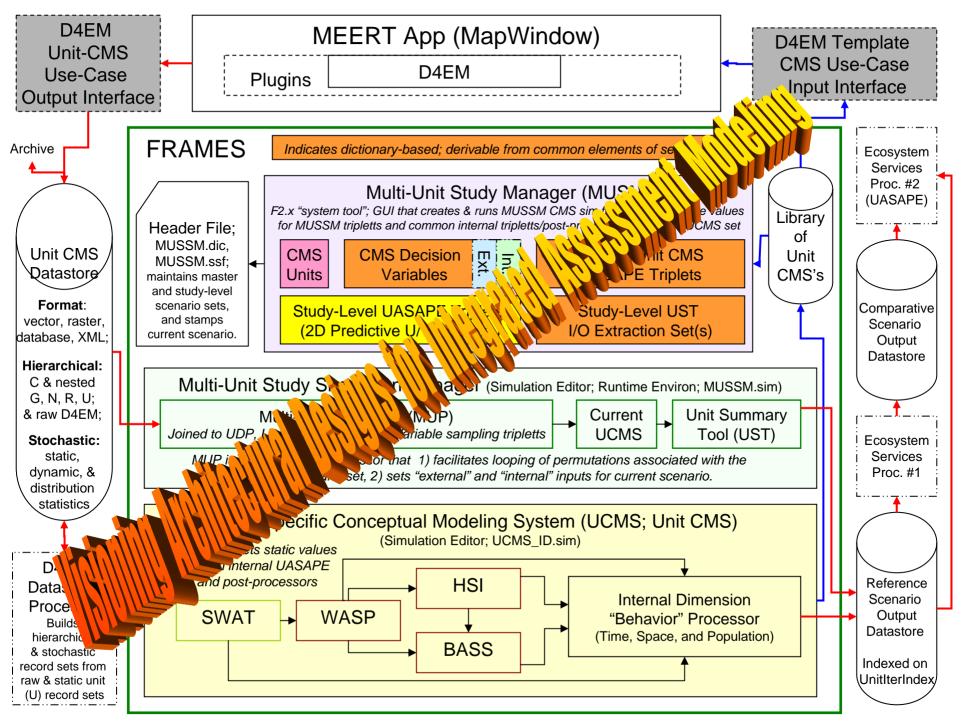
SuperMUSE 1.0 Software Status: beta form undergoing documentation & testing.... supporting multiple modeling systems, including now F2

FRAMESv2 Envisioned Model Evaluation Palette



Generalized Inter-Framework Architecture Detail





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.

Disclaimer: Although this work was reviewed by EPA and approved for publication, it may not necessarily reflect official Agency policy. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

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.