Investigating Uncertainty and Sensitivity in Integrated, Multimedia Environmental Models: Leveraging PC-Based Supercomputing Through Hardware and Software Tools

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Why Research Uncertainty and Sensitivity in EPA Models?

- We are called upon to establish a model's validity, trustworthiness, and relevance in performing a prospective task of prediction. *(Chen and Beck, 1999)*
- Compared to efforts we place into model development and model applications, our current knowledge, capability and guidance is severely limited, especially for complex, high-order problems.
- The development of sound science in uncertainty and sensitivity analyses (UA/SA) for EPA models is as crucial an endeavor as is the development of sound science underpinning these models and their governing equations.

Client Analysis: Who Needs Sound Science and Tools To Facilitate Proper Model Evaluations Via Uncertainty/Sensitivity Analyses?

Essentially, a question of who needs Quality Assurance in model development and model application.

- **Regulators** (e.g. Office of Solid Waste: 3MRA use for HWIR)
- **Industry** (e.g. coalitions typically resist model applications based on lack of completeness, relevance, adequacy, comparative data; proffer status quo over uncertainty)
- **Congress** (e.g. calls for full model evaluation, uncertainty analyses before regulating via models → i.e. HWIR, TMDL)
- **Public** (…. our ultimate responsibility in delivering better Quality Assurance in models by succeeding in this work)

Research Objectives & Strategy

- **Immediate Picture: Develop Generic Hardware and Software Tools for Conducting Model Evaluation Research & Model Simulation Tasking**
  - Design & Construct PC-Based Supercomputer (i.e. SuperMUSE) (i.e. Hardware)
  - Create Distributed Parallel Computing Program Management Toolset (i.e. Software)
- **Big Picture: Develop/Expand Underlying Science & Tools for Model Evaluation Tasks**
  - Model Uncertainty Analysis Methods & Guidance
  - Model Sensitivity Analysis Methods & Guidance
  - Tool Integration into Framework for Environmental Modeling
    - Facilitate Multiple-Model Integration, Model Comparisons
    - (i.e 3MRA, 3MRA vs. TrimFATE, 1-D vs. 3-D)
    - Facilitate UA/SA Model Evaluation Tasks, Interpretation
- **Application Migration Strategy**
  - Become a Key Component of EPA's Future Modeling Frameworks (e.g. FRAMES)
    - *…the ultimate medium for convergence of core science, applied science, technology, and regulation.*

Problem Background

❑ Elucidating uncertainty and sensitivity structures in environmental models can be a difficult task, even for low-order, single-media constructs driven by a unique set of site-specific data.

❑ Quantitative assessment of integrated, multimedia models that simulate hundreds of sites, spanning multiple geographical and ecological regions, will ultimately require a comparative model evaluation approach using several techniques, coupled with sufficient computational power.

❑ The Framework for Risk Analysis in Multimedia Environmental Systems - Multimedia, Multipathway, and Multireceptor Risk Assessment (FRAMES-3MRA) is an important software code being developed by EPA for use in assessment of hazardous waste management facilities.

❑ The 3MRA model encompasses over 700 variables, 185 of which are explicitly stochastic. A characteristic of uncertainty and sensitivity analyses for very high order models (VHOMs) like 3MRA is their need for significant levels of computational capacity to perform massively redundant model simulations (millions upon millions of simulations needed to adequately assess).

❑ While UA/SA is emerging as a critical area for environmental model evaluation, resources for Windows-based, PC-based modeling have often been limited by an associated lack of supercomputing capacity. Equally, higher-order UA/SA algorithms warrant investigation.
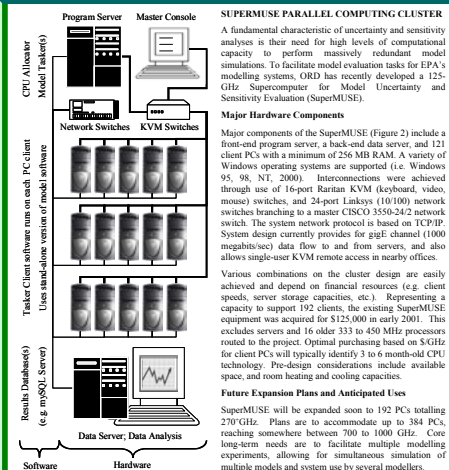
Modeling: A Bridge Between Science and Regulation

Environmental Science/Engineering — Environmental Regulation

Hardware Tool Development: SuperMUSE (Supercomputer for Model Uncertainty and Sensitivity Evaluation)

SUPERMUSE PARALLEL COMPUTING CLUSTER

A fundamental characteristic of uncertainty and sensitivity analyses is their need for high levels of computational capacity to perform massively redundant model simulations. To facilitate model evaluation tasks for EPA's modelling systems, ORD has recently developed a 125-GHz Supercomputer for Model Uncertainty and Sensitivity Evaluation (SuperMUSE).
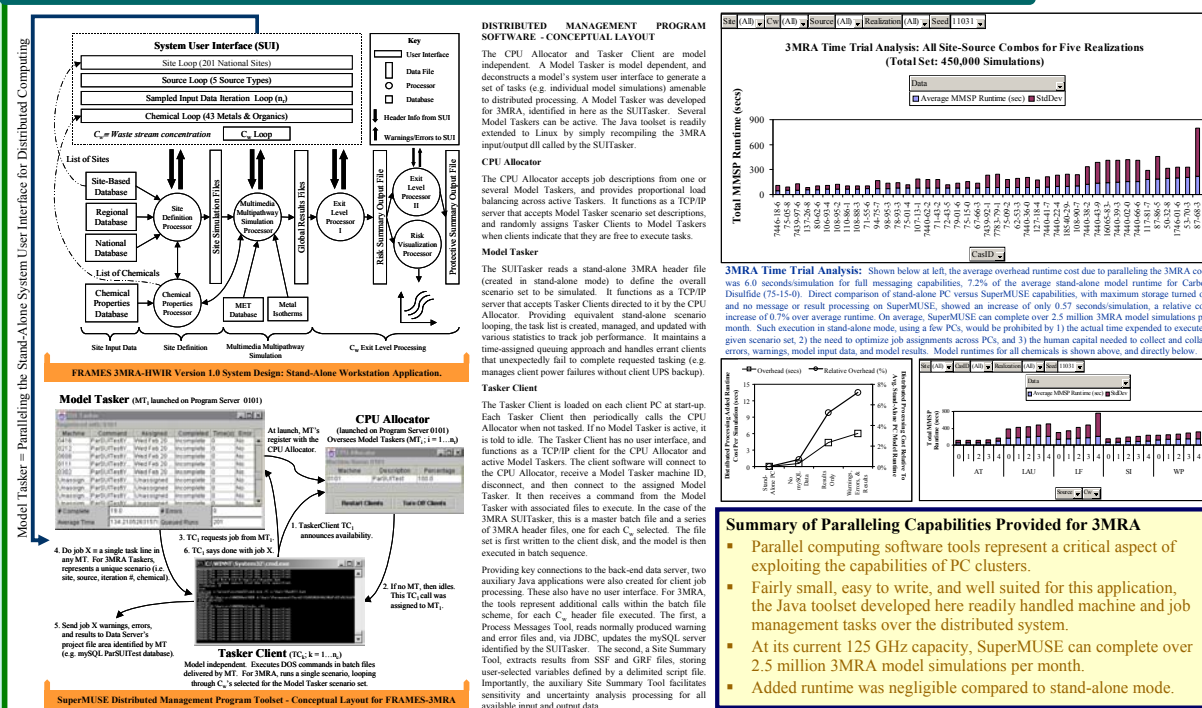
Major Hardware Components

Major components of the SuperMUSE (Figure 2) include a front-end program server, a back-end data server, and 121 client PCs with a minimum of 256 MB RAM. A variety of Windows operating systems are supported (i.e. Windows 95, 98, NT, 2000). Interconnections were achieved through use of 16-port Raritan KVM (keyboard, video, mouse) switches, and 24-port Linksys (10/100) network switches branching to a master CISCO 3550-24/2 network switch. The network protocol is based on TCP/IP. System design currently provides for gigE channel (1000 megabits/sec) data flow to and from servers, and also allows single-user KVM remote access in nearby offices.

Various combinations on the cluster design are easily achieved and depend on financial resources (e.g. client speeds, server storage capacities, etc.). Representing a capacity to support 192 clients, the existing SuperMUSE equipment was acquired for $125,000 in early 2001. This excludes servers and 16 older 333 to 450 MHz processors routed to the project. Optimal purchasing based on $/GHz for client PCs will typically identify 3 to 6 month-old CPU technology. Pre-design considerations include available space, and room heating and cooling capacities.

Future Expansion Plans and Anticipated Uses

SuperMUSE will be expanded soon to 192 PCs totalling 270'GHz. Plans are to accommodate up to 384 PCs, reaching somewhere between 700 to 1000 GHz. Core long-term needs are to facilitate multiple modelling experiments, allowing for simultaneous simulation of multiple models and system use by several modellers.

Software Tool Development: Paralleling Typical Stand-Alone Model Application for Distributed Computing

Model Tasker = Paralleling the Stand-Alone System User Interface for Distributed Computing

System User Interface (SUI)

- Site Loop (201 National Sites)
- Source Loop (5 Source Types)
- Sampled Input Data Iteration Loop (n_s)
- Chemical Loop (43 Metals & Organics)
- C_w = Waste stream concentration C_w Loop

Key: User Interface, Data File, Processor, Database, Header Info from SUI, Warnings/Errors to SUI

FRAMES 3MRA-HWIR Version 1.0 System Design: Stand-Alone Workstation Application.

Model Tasker (MT₁ launched on Program Server 0101)

At launch, MT₁'s register with the CPU Allocator. Oversees Model Taskers (MT₁, i = 1...n₄)

CPU Allocator

1. TaskerClient TC₁ announces availability.
2. If no MT, then idle. This TC₁ will run assigned to MT₁.
3. TC₁ requests job from MT₁
4. Do job X in a single task line in any MT. For 3MRA Taskers, represents a unique scenario (i.e. site, source, iteration #, chemical).
5. Send job X warnings, errors, and results to Data Server's project file area identified by MT (e.g. mySQL ParSUITest database).
6. TC₁ says done with job X.

Tasker Client (TC₁; k = 1...n₄)

Model independent. Executes DOS commands in batch files delivered by MT. For 3MRA, runs a single scenario, looping through C_w's selected for the Model Tasker scenario set.

SuperMUSE Distributed Management Program Toolset - Conceptual Layout for FRAMES-3MRA

DISTRIBUTED MANAGEMENT PROGRAM SOFTWARE - CONCEPTUAL LAYOUT

The CPU Allocator and Tasker Client are model independent. A Model Tasker is model dependent, and deconstructs a model's system user interface to generate a set of tasks (e.g. individual model simulations) amenable to distributed processing. A Model Tasker was developed for 3MRA, identified in here as the SUITasker. Several Model Taskers can be active. The Java toolset is readily extended to Linux by simply recompiling the 3MRA input/output dll called by the SUITasker.

CPU Allocator

The CPU Allocator accepts job descriptions from one or several Model Taskers, and provides proportional load balancing across active Taskers. It functions as a TCP/IP server that accepts Model Tasker scenario set descriptions, and randomly assigns Tasker Clients to Model Taskers when clients indicate that they are free to execute tasks.
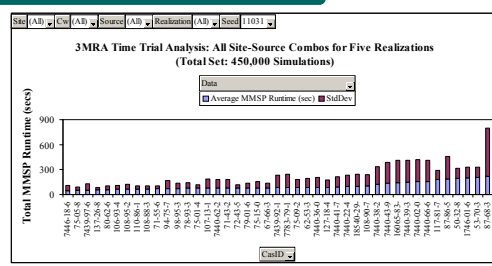
Model Tasker

The SUITasker reads a stand-alone 3MRA header file (created in stand-alone mode) to define the overall scenario set to be simulated. It functions as a TCP/IP server that accepts Tasker Clients directed to it by the CPU Allocator. Providing equivalent stand-alone scenario looping, the task list is created, managed, and updated with various statistics to track job performance. It maintains a time-assigned queuing approach and handles errant clients that unexpectedly fail to complete requested tasking (e.g. manages client power failures without client UPS backup).
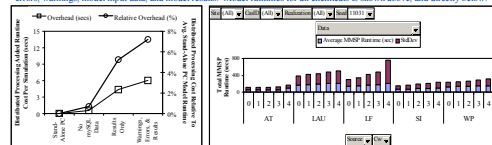
Tasker Client

The Tasker Client is loaded on each client PC at start-up. Each Tasker Client then periodically calls the CPU Allocator when not tasked. If no Model Tasker is active, it is told to idle. The Tasker Client has no user interface, and functions as a TCP/IP client for the CPU Allocator and active Model Taskers. The client software will connect to the CPU Allocator, receive a Model Tasker machine ID, disconnect, and then connect to the assigned Model Tasker. It then receives a command from the Model Tasker with associated files to execute. In the case of the 3MRA SUITasker, this is a master batch file and a series of 3MRA header files, one for each C_w selected. The file set is first written to the client disk, and the model is then executed in batch sequence.

Providing key connections to the back-end data server, two auxiliary Java applications were also created for client job processing. These also have no user interface. For 3MRA, the tools represent additional calls within the batch file scheme, for each C_w header file executed. The first, a Process Messages Tool, reads normally produced warning and error files and, via JDBC, updates the mySQL server identified by the SUITasker. The second, a Site Summary Tool, extracts results from SSF and GRF files, storing user-selected variables defined by a delimited script file. Importantly, the auxiliary Site Summary Tool facilitates sensitivity and uncertainty analysis processing for all available input and output data.

Summary of Paralleling Capabilities Provided for 3MRA

- Parallel computing software tools represent a critical aspect of exploiting the capabilities of PC clusters.
- Fairly small, easy to write, and well suited for this application, the Java toolset developed here readily handled machine and job management tasks over the distributed system.
- At its current 125 GHz capacity, SuperMUSE can complete over 2.5 million 3MRA model simulations per month.
- Added runtime was negligible compared to stand-alone mode.

3MRA Time Trial Analysis: All Site-Source Combos for Five Realizations (Total Set: 450,000 Simulations)

3MRA Time Trial Analysis: Shown below at left, the average overhead runtime cost due to paralleling the 3MRA code was 6.0 seconds/simulation for full messaging capabilities, 7.2% of the average stand-alone model runtime for Carbon Disulfide (75-15-0). Direct comparison of stand-alone PC versus SuperMUSE capabilities, with maximum storage turned off and no message or result processing on SuperMUSE, showed an increase of only 0.57 seconds/simulation, a relative cost increase of 0.7% over average runtime. On average, SuperMUSE can complete over 2.5 million 3MRA model simulations per month. Such execution in stand-alone mode, using a few PCs, would be prohibited by 1) the actual time expended to execute a given scenario set, 2) the need to optimize job assignments across PCs, and 3) the human capital needed to collect and collate errors, warnings, model input data, and model results. Model runtimes for all chemicals is shown above, and directly below.

Uncertainty & Sensitivity Analysis Research Aspects

- **Initial Focus on Uncertainty Attributed to Model Parameterization and Input Data**
- **Extend to Evaluate:**
  - Scenario Uncertainty (scenario description, aggregation, incomplete analysis)
  - Modeler & Model Uncertainty (model simplification, misspecification, misuse).
- **Investigate Varying Degrees of Effort in Sensitivity Analysis:**
  - Screening methods (simplified local, global)
  - Local methods (small portion of input parameter space)
  - Global methods ("all" possible input combinations)

Initial 3MRA Model Evaluation Tasking

- **Regression/Correlation-Based Global Methods for Sensitivity & Uncertainty Analysis:**
  - Utilize scatter plots, regression and stepwise regression, correlation and partial correlation; with and without use of rank transformations
  - Examine non-monotonic and non-random patterns
  - Evaluate dominance in media, pathway, receptors for various chemicals and/or groups (e.g. VOC, metals)
- **Screening Methods for Sensitivity Analysis:**
  - Morris' OAT Design
  - Andres' Iterated Fractional Factorial Design (IFFD)

Current/Future Algorithm Investigations

- **Adding Parameter Sampling Schemes to Framework:**
  - Random √, LHS, OAT, Factorial, Winding Stairs, etc.
- **VHOM Methods to be Researched:**
  - Regional Sensitivity Analysis (RSA) *(underway)*
  - Tree Structured Density Estimation (TSDE) *(underway)*
  - Uniform Coverage by Prob. Rejection (UCPR) *(underway)*
  - Sobol's Total Effect Method
  - Fourier Amplitude Sensitivity Test
  - High Dimensional Model Representations
  - Bayesian Analysis
  - NUSAP Scheme

Impact Analysis: Who Benefits and How?

- The Java-based paralleling software toolset developed here is platform-independent, and can be readily extended to other NERL and EPA exposure and risk assessment models and modelling systems.
- EPA is using hundreds of models to assess environmental issues.
- With migration in mind, our tool set concept represents a key component of future modelling frameworks that the Agency is moving towards.
- For regulators, industry, congress, and the public, UA/SA tools will ultimately strengthen their ability to properly evaluate regulatory-based modelling efforts, and to protect human health and the environment.

References

- Chen, J., and M.B. Beck, Quality Assurance of Multi-Media Model For Predictive Screening Tasks, USEPA, EPA/600/R-98-106, 1999.
- Saltelli, A., K. Chan, and E.M. Scott, *Sensitivity Analysis*, John Wiley & Sons, West Sussex, England, 475 pp., 2000.