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TITLE: Coupling Legacy and Contemporary Deterministic Codes to Goldsim® for Probabilistic Simulations

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I. ABSTRACT:

Sandia National Laboratories (Sandia), a U.S. Department of Energy National Laboratory, has over 30 years experience in radioactive waste disposal and is providing assistance internationally in a number of areas relevant to the safety assessment of radioactive waste disposal systems. This international technology transfer effort is often hampered by small budgets and a lack of experienced personnel in countries without large waste disposal programs. In an effort to surmount these difficulties, Sandia has developed a system that utilizes a combination of commercially available codes and existing legacy codes for probabilistic safety assessment modeling that facilitates the technology transfer and maximizes limited available funding. Numerous codes developed and endorsed by the United States Nuclear Regulatory Commission and codes developed and maintained by United States Department of Energy are generally available free of charge to foreign countries after addressing any import/export control and copyright requirements. From a programmatic view, it is easier to utilize existing codes than to develop new codes. From an economic perspective, it is not possible for most countries to maintain complex software, which meets the rigors of both domestic regulatory and international peer review. Therefore, re-vitalization of deterministic legacy codes, as well as an adaptation of contemporary deterministic codes, provides a creditable and solid computational platform for constructing probabilistic safety assessment models. External model linkage capabilities in Goldsim® and the techniques applied to facilitate this process will be presented using example applications, including Breach, Leach, and Transport-Multiple Species, a U.S. NRC code simulating release and transport of contaminants from a subsurface low-level waste disposal facility.

II. Introduction

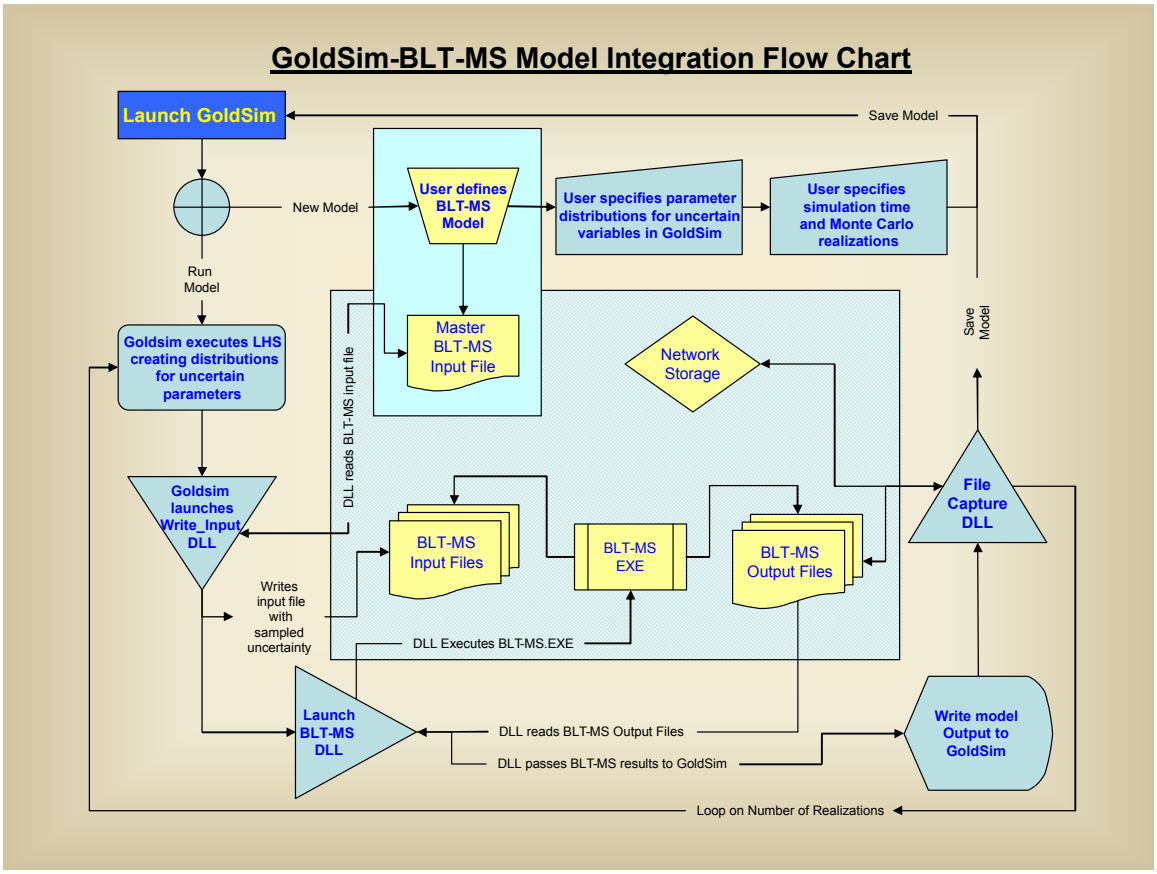
- To methods can be employed by using GoldSim external DLL element or external pathway element
    - External Pathway Elements External Pathways provide a mechanism by which external program modules for contaminant transport (e.g., analytical, finite element or finite difference solute transport models) can be directly integrated into GoldSim. These modules (referred to as *External pathway functions*) are linked into GoldSim as DLLs (Dynamic Link Libraries) at run time. External pathways are specialized extensions of the External element.
    - External Elements (DLL): The modules are linked into GoldSim as DLLs (Dynamic Link Libraries) at run time. Integrating these external modules into GoldSim requires that you develop a "wrapper" (or "shell") around your existing function, and compile it into a DLL. In most cases, this will require only a limited number of programming modifications.
- The example problem uses a external DLL element rather than external pathway, even though the selected code is used for a mass transport calculation.
- This choice was made to preserve the original code (e.g. no modification were made to change the exe to a DLL) to maintain the QA pedigree.

III. Benefits of coupling existing commercial and legacy codes to GoldSim

- Can utilize deterministic codes for probabilistic analysis with no modifications to the original code
- Modernization of DOS based exe's utilizing GoldSim's graphical features for pre and post processing
- Numerous codes developed by established government programs (like the U.S. DOE & NRC) are generally available for nominal costs
- Use of recognizable codes with an established QA pedigree
- Can utilize existing validation and verification test suite
- Can establish internationally creditable probabilistic safety assessment results
- Lower program costs for emerging international programs

IV. An Example of a Coupled Modeling System: A coupled model using BLT-MS and GoldSim

- Since the BLT-MS.EXE was not modified for this application we had to develop a small code that interfaces between BTL-MS.EXE and GoldSim
- This application requires a suite of codes that contains the logic for launching the EXE and reading the output back into GoldSim and functionality for capturing output files when running a multiple realization model using the distributed processing module.
- Figure 1 outlines the logical flow of information and identifies the individual codes used for this application.



- **Note:** When the coupled model is executed GoldSim executes the DLL calls in the order in which they are linked together. For example output from the first DLL (Read_BLTv1.1.001.DLL) feeds the second DLL (Launch_BLTMSv1.1.010) therefore the Read_BLTv1.1.001.DLL will execute before the Launch_BLTMSv1.1.010.DLL.

- In the example, the READ_BLTv1.1.001.DLL receives selected input data values from GoldSim. These inputs include which parameters should be replaced with uncertain values and the sampled value during each realization. The DLL writes these values to the BLTMS.EXE input file and tags the file with the current realization number.

- When the input file is written, the READ_BLTv1.1.001.DLL ends, and the Launch_BLTMSv1.1.010.DLL is launched. The Launch_BLTMSv1.1.010.DLL executes the current input file, then waits until the BLTMS.EXE has completed. When the BLTMS.EXE has completed the Launch_BLTMSv1.1.010.DLL reads the data from the BLTMS.EXE output files to GoldSim.

- The FileCapture.DLL is the last DLL in the sequence. It is a postprocessor called after the LAUNCH_BLT.DLL has completed to copy selected input and output files created by the BLT-MS.EXE during the simulation to a central location on a local LAN. Thus any input or output file can be captured, when the simulation is run locally or when using the distributed processing (i.e., multi-processor run) feature.

- These DLL's are executed for each realization during a Monte Carlo analysis.

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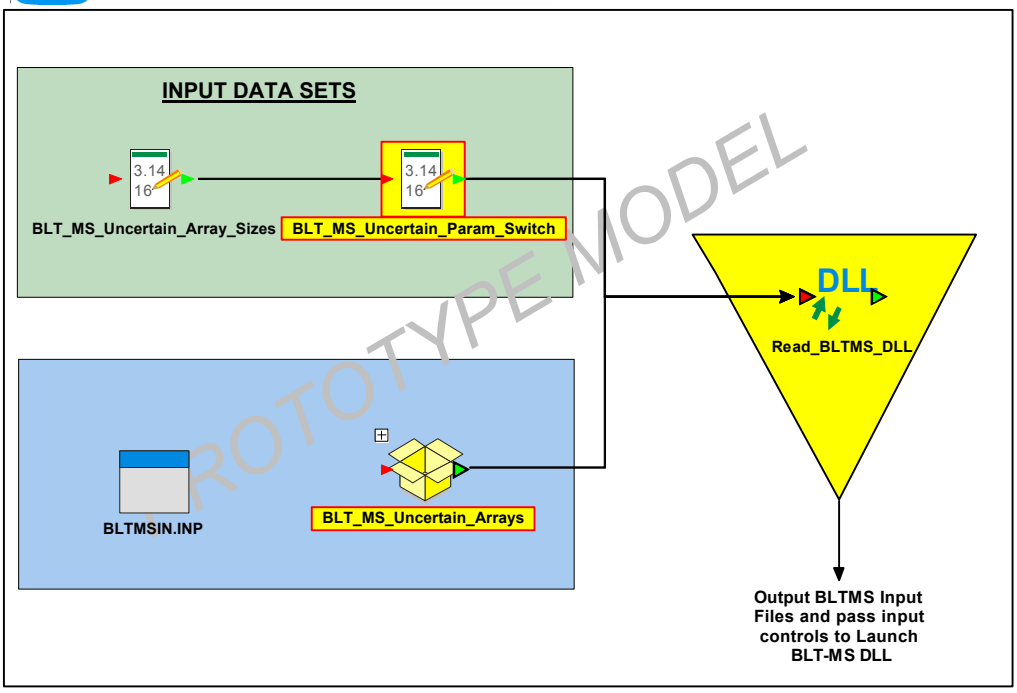

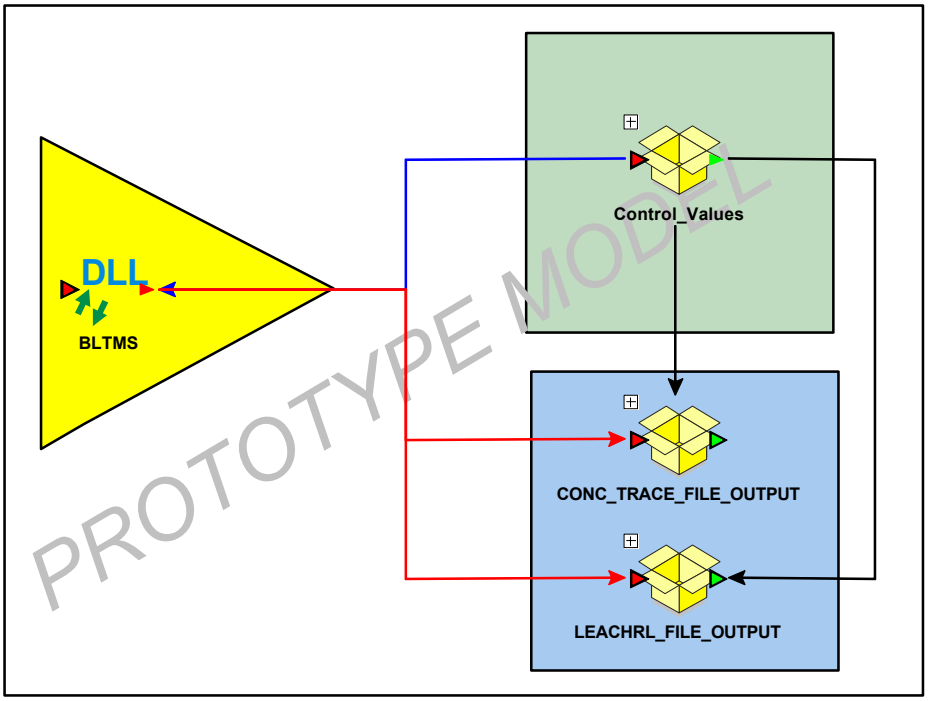

V. Examples of CODES Coupled to GoldSim: the following is a partial list of codes that have been successfully coupled using GoldSim external elements and external pathways.

BLT-MS (Breach, Leach, and Transport-Multiple Species – United States Nuclear Regulatory Comission 2-D finite element computer model for simulating release of contaminants from a subsurface Low-Level radioactive waste disposal facility. Developed by U.S. Department of Energy Brookhaven National Laboratory. NUREG/CR-6492

FEHM (Finite Element Heat and Mass Transfer Code): FEHM is a numerical simulation code for subsurface transport processes. It models 3-D, time-dependent, multiphase, multicomponent, nonisothermal, reactive flow through porous and fractured media. It can accurately represent complex 3-D geologic media and structures and their effects on subsurface flow and transport. FEHM has been used to simulate groundwater and contaminant flow and transport in deep and shallow, fractured and un-fractured porous media throughout the US DOE complex. Developed by the Hydrology, Geochemistry & Geology Group (EES-6) at U.S. Department of Energy Los Alamos National Laboratory.

INPAG-N (Near-Field Code for Total System Performance Assessment of Taiwanese Geological Disposal of Nuclear Spent Fuel) – INPAG-N is preliminary source-term (or the near-field) model, based on the Taiwanese disposal concept, for INER's first TSPA program. The computation of the source-term by INPAG-N uses a compartment modeling approach. A compartment model is a numerical method similar to finite-difference method. Developed by Monitor Scientific, LLC.

INPAG-F and INPAG-FL (Far-Field Code for Total System Performance Assessment of Taiwanese Geological Disposal of Nuclear Spent Fuel) - INPAG-N is preliminary source-term (or the far-field) model, based on the Taiwanese disposal concept, for INER's first TSPA program. The "Far Field" (geosphere) is a physical region representing the natural barrier in the concept of geological disposal of nuclear wastes.). The INPAG-F model explicitly solves transport equations in a single fracture and the surrounding matrix. Hence, the model can be classified as the "discrete fracture models".The INPAG-FL code uses a La Place transform solution. Developed by Monitor Scientific, LLC.

VI. Conclusions

- Emerging programs can take advantage of existing codes and customize model input through the use of the GoldSim interface
- Using the GoldSim interface for model setup (preprocessing) and model analysis (post processing) a graphical representation of the model is created
- The graphical environment makes it easier to support management and decision making
- Robust legacy codes can be modernized easily, without time consuming and costly modifications to the source code
- Deterministic solutions can be exercised using GoldSim's Monte Carlo simulation capabilities.

VII. Sandia National Laboratories international radioactive waste disposal projects:

United States

- Lead Laboratory for United States Department of Energy's evaluation of the Yucca Mountain site for development as a repository for the disposal of spent nuclear fuel and high level radioactive waste.

- Lead Laboratory for United States Department of Energy's evaluation of the Waste Isolation Pilot Plant as a repository for the disposal of transuranic mixed waste.

- United States Department of Energy Office of Civilian Radioactive Waste Management (OCRWM) international program support

    - Sweden Nuclear Fuel and Waste Management Co (SKB) Aspö URL projects
    - OECD-Nuclear Energy Agency (NEA) review panel
    - Japan Nuclear Cycle Development Institute (JNC)
    - US-China Peaceful Use of Nuclear Technology
    - US-Taiwan Civil Nuclear Energy Cooperation

Republic of China (Taiwan)

- High Level Waste disposal safety assessment/site selection technology transfer to Taiwan research institutes including Taiwan's Atomic Energy Council's Institute of Nuclear Energy Research and Taiwan Power Corporation.

- Low Level Waste disposal safety assessment/site selection technology transfer to Taiwan research institutes including Taiwan's Atomic Energy Council's Institute of Nuclear Energy Research and Taiwan Power Corporation.

Japan

- Collaboration with the Nuclear Waste Management Organization of Japan (NUMO) on assessing their deep geological disposal program for high-level radioactive wastes

- Collaboration with Japan Atomic Energy Agency (JAEA)

International Atomic Energy Agency

- host IAEA Fellows from Republic of Solvika, Egypt, etc.

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