Introduction to GoldSim Interface and CBP Software Communications Bridge

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Overview

• Design philosophy
• GoldSim software bridge
• GoldSim Dashboard GUI
• Hands-on tutorials
Segment 1 – Design Philosophy

CBP Custom DLL

LX LEACH

THAMES
Software integration objectives

- Provide a common, unified, interface to CBP partner codes through a GoldSim Dashboard GUI
- Provide a wrapper for probabilistic analysis (e.g. Monte Carlo)
- Create pre-defined scenarios (e.g. sulfate attack)
- Connect to system level PA models
- Couple LeachXS/Orchestra, STADIUM, and THAMES in a synergistic manner
• Phenomena best coupled **between stand-alone codes**
  – lower numerical stability constraints
  – capability exists in component codes (collectively)

• Phenomena best coupled **within component code**
  – higher numerical stability constraints
  – capability does not yet exist
Three Natural Development Phases

• Phase I: Couple existing CBP partner codes "as is"
  – minimal coupling

• Phase II: Couple through functions (e.g. of time)
  – modest coupling
  – enhanced I/O needed in partner codes
  – use spreadsheet and/or "system call" DLLs

• Phase III: Couple at each GoldSim timestep
  – strongest coupling / synchronization
  – partner codes as DLL subroutines
Some Design Principles

• Influence, but stay within, CBP partners' main code development path

• Accept duplication of function, but require or monitor for adequate consistency
  – e.g. bulk chemistry

• Common repository for common data

• Common data formats, so an output can be an input

• Common graphics format

• Common mesh generator
GoldSim Merits

• Can function as an integrating platform by calling external programs and databases

• Built-in probabilistic analysis
  – Monte Carlo, Latin Hypercube Sampling uncertainty
  – sensitivity analysis for phenomenological and parameter importance

• Significant and growing market share in PA community

• GoldSim Player available free of charge

• Well developed Graphical User Interface (GUI)
  – model construction occurs at high/conceptual level
Segment 2 – GoldSim Software Bridge

CBP Custom DLL

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Simulation for the Real World
GoldSim Links to External Functions

Three basic methods:

• Lookup table
• Spreadsheet
• DLL subroutine
DLL External Element

Input Interface Definition:

<table>
<thead>
<tr>
<th>#</th>
<th>Name</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Input1</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Input2</td>
<td></td>
</tr>
</tbody>
</table>

Output Interface Definition:

<table>
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<tr>
<th>#</th>
<th>Name</th>
<th>Data Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>sum</td>
<td>Value (m)</td>
</tr>
<tr>
<td>2</td>
<td>product</td>
<td>Value (m2)</td>
</tr>
</tbody>
</table>
5 standard functions:
  • Initialize
  • Report version
  • Report number of inputs and outputs
  • Calculate
  • Cleanup

```fortran
subroutine add_mult_scalars(method_id, status, inargs, outargs) BIND(C)
! The following attributes are used specify this function name and arguments
! for "export" from the DLL.
! These attributes are specific to Intel Visual Fortran.
! Other compilers may require different code to declare the "export" information.

!DEC$ ATTRIBUTES dlllexport,c :: add_mult_scalars
!DEC$ ATTRIBUTES value :: method_id
!DEC$ ATTRIBUTES reference :: status
!DEC$ ATTRIBUTES reference :: inargs
!DEC$ ATTRIBUTES reference :: outargs

use gs_parameters
implicit none
real(8), parameter :: VERSION = 1.03
integer(4), parameter :: NINPUTS = 2 ! Two scalar inputs expected
integer(4), parameter :: NOUTPUTS = 2 ! Two scalar outputs returned

integer(4) method_id, status
real(8) inargs(*), outargs(*)

integer(4), value :: method_id
integer(4) :: status

select case (method_id)
case (INITIALIZE)
  status = SUCCESS
  outargs(1) = VERSION
  status = SUCCESS
  outargs(2) = NINPUTS
  outargs(2) = NOUTPUTS
  status = SUCCESS
  outargs(1) = inargs(1) + inargs(2) ! return the sum
  outargs(2) = inargs(1)*inargs(2) ! return the product
  status = SUCCESS
  outargs(3) = status
  outargs(4) = VERSION
  status = SUCCESS
end case
!
end subroutine add_mult_scalars
```
DLL is "middle-man" between GoldSim and External Function

```fortran
select case (method_id)
  case (INITIALIZE)
    status = SUCCESS
  case (REPORT_VERSION)
    outargs(1) = VERSION
    status = SUCCESS
  case (REPORT_ARGUMENTS)
    outargs(1) = NINPUTS
    outargs(2) = NOUTPUTS
    status = SUCCESS
  case (CALCULATE)
    string = 'cat input.dat >output.dat'
    call system(trim(string))
    outargs(1) = VERSION
    status = SUCCESS
  case (CLEANUP)
    status = SUCCESS
  case_default
    call copy_msg_to_outputs('Unknown method ID requested', outargs)
    status = FAILURE_WITH_MSG
end select
end subroutine makeSysCall
```
Design Objectives for CBP DLL

• Avoid need for low-level programming by typical user
  – put generic content in pre-compiled subroutine (DLL)
  – put application-specific content in "instructions" file read at run-time

• Provide flexible, user-friendly, access to CBP partner code input and output files via the instructions file
  – row selection by number, label, value within a tolerance, string anywhere
  – field selection by number, heading, value within a tolerance
CBP DLL Subroutine Design

- CBP DLL written / compiled in Fortran 90 (g95)
  - Instructions file describes actions to be taken based on six pre-defined keywords
  - Actions processed in order where each action can be called multiple times

- Instructions file keywords (and corresponding actions)
  - PUT / GET – Put/get data specified within block into/from file
  - EXE – Perform the system-level calls specified within block
  - RPL – Replace complete lines in named file
  - SUP – Create a “super” file containing commands or file names
  - LOG – Write a log file (XML) containing all input and output data
### DLL Language – Instructions Example

```plaintext
! !
#2 #3 #4 #5 #6 #7 #8 #9 #10 #11

**PUT** Stadium\SRS_Vault2_Saltstone_01.inp space

3 row 124 field 3 11 1 inargs03-13
14 row 139 field 3 9 1 inargs14-22
23 row 124 field 4 11 1 inargs23-33
34 row 139 field 4 9 1 inargs34-42
43 row 124 field 5 11 1 inargs43-53
54 row 139 field 5 9 1 inargs54-62

**END**

**EXE**

copy ..\..\Stadium\PITZER-STADIUM.dat *.*
..\..\Codes\Stadium\stadium_2009c_CBPOk GUI=YES SRS_Vault2_Saltstone_01.inp CBP002BATCH

**GET** SRS_Vault2_Saltstone_01.out.xls space

1 value 1.0 2 field 19 51 1 outargs001-051
52 value 0.74 2 field 20 51 1 outargs052-102
103 value 0.246 2 field 21 51 1 outargs103-153

**END**

**LOG** stadium.log

**END**

---

SRNL-STI-2012-00382
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Summary of External Linking

Inputs

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<th>Definition</th>
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<tbody>
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<td>MineralComps</td>
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<td>7</td>
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Outputs

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<th>Name</th>
<th>Data Type</th>
</tr>
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<tbody>
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<td>Matrix[Nodes,Chemicals] of Values (mmol/L)</td>
</tr>
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<td>Mineral_Conc</td>
<td>Matrix[Nodes,Minerals] of Values (dimensionless)</td>
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</table>

stadium_2layers.xml

```xml
<CBPDataLog Realization="0">
  <DataSet Name="Input">
    <Values Number="119">
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      0.0000
      670.08
      4420.0
      120.00
      130.70
      0.41000
      0.14000
      ...
      1575.0
      ...
      101.00
    </Values>
  </DataSet>
  <DataSet Name="Output">
    <Values Number="6020">
      0.0000
      0.0000
      0.0000
      0.0000
      0.0000
      0.0000
      ...
      0.0000
      ...
      0.0000
    </Values>
  </DataSet>
</CBPDataLog>
```
• GoldSim graphical user interface to STADIUM

• Monte Carlo analysis:
  - 50 realizations
  - 8 Intel Xeon CPUs
  - 4 simultaneous realizations
  - 8.0 to 15.6 hrs per realization
  - 6+ days overall
Cementitious Barriers Partnership (CBP)

DLL Link to STADIUM® and LeachXS™/ORCHESTRA Codes

The Cementitious Barriers Partnership (CBP) Project is a multi-disciplinary, multi-institutional collaboration supported by the US Department of Energy (DOE) Office of Waste Processing. The objective of the CBP project is to develop a set of tools to improve understanding and prediction of the long term structural, hydraulic, and chemical performance of cementitious barriers used in nuclear applications.

A Dashboard is a user interface employed in GoldSim to control a simulation. Double-click links in GoldSim to activate.
Segment 4 – Hands Ons Demo

CBP Custom DLL

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Tutorial #1

• Tutorial 1- Make deterministic Stadium run w/default settings
  – Make copy of "Template" folder first
  – Delete "...\Runs" folder
  – Run simulation
Tutorial #2

- Tutorial 2 - Modify scenario definition; Monte Carlo
  - 2 layer saltstone+concrete (omit soil)
    - GoldSim dashboard switch
    - comment out layer in mesh file
  - Increase saltstone thickness to 0.5 meters
    - GoldSim dashboard field
    - modify mesh file
  - Decrease elements to 50, 25 in each material (51 nodes)
    - GoldSim dashboard field
    - modify mesh file
    - make mesh
    - modify GET instructions for DLL
  - Run 3 probabilistic simulations
    - Change GoldSim Monte Carlo simulation settings