CBP CODE INTEGRATION GOLDSIM DLL INTERFACE

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FOREWORD

The Cementitious Barriers Partnership (CBP) Project is a multi-disciplinary, multi-institutional collaboration supported by the United States Department of Energy (US 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 multi-disciplinary partnership of federal, academic, private sector, and international expertise has been formed to accomplish the project objective. In addition to the US DOE, the CBP partners are the Savannah River National Laboratory (SRNL), Vanderbilt University (VU) / Consortium for Risk Evaluation with Stakeholder Participation (CRESP), Energy Research Center of the Netherlands (ECN), and SIMCO Technologies, Inc. The Nuclear Regulatory Commission (NRC) is providing support under a Memorandum of Understanding. The National Institute of Standards and Technology (NIST) is providing research under an Interagency Agreement. Neither the NRC nor NIST are signatories to the Cooperative Research and Development Agreement (CRADA).

The periods of cementitious performance being evaluated are up to or longer than 100 years for operating facilities and longer than 1000 years for waste management. The set of simulation tools and data developed under this project will be used to evaluate and predict the behavior of cementitious barriers used in near-surface engineered waste disposal systems, e.g., waste forms, containment structures, entombments, and environmental remediation, including decontamination and decommissioning analysis of structural concrete components of nuclear facilities (spent-fuel pools, dry spent-fuel storage units, and recycling facilities such as fuel fabrication, separations processes). Simulation parameters will be obtained from prior literature and will be experimentally measured under this project, as necessary, to demonstrate application of the simulation tools for three prototype applications (waste form in concrete vault, high-level waste tank grouting, and spent-fuel pool). Test methods and data needs to support use of the simulation tools for future applications will be defined.

The CBP project is a five-year effort focused on reducing the uncertainties of current methodologies for assessing cementitious barrier performance and increasing the consistency and transparency of the assessment process. The results of this project will enable improved risk-informed, performance-based decision-making and support several of the strategic initiatives in the DOE Office of Environmental Management Engineering & Technology Roadmap. Those strategic initiatives include 1) enhanced tank closure processes; 2) enhanced stabilization technologies; 3) advanced predictive capabilities; 4) enhanced remediation methods; 5) adapted technologies for site-specific and complex-wide D&D applications; 6) improved SNF storage, stabilization and disposal preparation; 7) enhanced storage, monitoring and stabilization systems; and 8) enhanced long-term performance evaluation and monitoring.

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LIST OF ACRONYMS AND ABBREVIATIONS

CBP  Cementitious Barriers Partnership
CRES P Consortium for Risk Evaluation with Stakeholder Participation
DLL  Dynamic-link library
DOE  Department of Energy
ECN  Energy Research Centre of the Netherlands
GTG  GoldSim Technology Group
NIST  National Institute of Standards and Technology
NRC  Nuclear Regulatory Commission
SRNL  Savannah River National Laboratory
STADIUM  Software for Transport and Degradation in Unsaturated Materials
XML  eXtensible Markup Language
CBP Code Integration GoldSim DLL Interface

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1 INTRODUCTION

A general dynamic-link library (DLL) interface has been developed to link GoldSim with external codes\(^1\). The overall concept behind this development is to use GoldSim as top level modeling software with interfaces to external codes for specific calculations. The DLL that performs the linking function is designed to take a list of code inputs from GoldSim, create an input file for the external application, run the external code, and return a list of outputs, read from files created by the external application, back to GoldSim. Instructions for creating the input file, running the external code, and reading the output are contained in an instructions file (DLL.dat) that is read and interpreted by the DLL. As an example, a prototype model linking GoldSim with the STADIUM® code used to predict concrete service life has been developed and successfully run. While the example is for an interface between GoldSim and STADIUM (Brown & Flach 2009), the DLL is designed to be general and should be readily adaptable to interfacing other codes to GoldSim.

2 DLL DESIGN

Design of the DLL assumes that the external application reads an input file that controls the calculations performed and writes an output file of results. The exact formatting of the input and output does not matter as long as the location of information in each file can be uniquely identified. The input can then be modified as needed to make different calculations and the results of these calculations can be processed for further use. The DLL also assumes that the external code can be automatically run as either an executable or through a

\(^1\) According to Microsoft (http://msdn.microsoft.com/en-us/library/ms682589(VS.85).aspx), a DLL is a module that contain functions and data that can be used by another module (application or DLL).
batch file (calling the executable) without user intervention. Minimal user intervention could be tolerated but defeats the purpose of code automation especially in the context of probabilistic analysis.

To some extent, the DLL design was based on information provided in Appendix C of the GoldSim User’s Guide (Volume 2 GoldSim Technology Group, Version 10.0 February 2009 (GTG 2009)). The User’s Guide specifies, in general, how the external interface must be constructed to be compatible with GoldSim’s calling conventions and gives a list of parameters that must be used. Within these constraints, the user can add additional functionality as desired. It is this additional functionality included in the DLL interface that is primarily the subject of this document.

The DLL code was written in Fortran 90 and is modularized into five files and 20 subroutines. A brief explanation of the function of each subroutine is provided in Appendix A. Operation of the DLL interface is controlled by instructions provided by the user in a DLL.dat file. An example instruction file is shown in Figure 1. This file is tab delimited (required format) into 13 fields. The first field starts in the first column. Continuation lines are marked by an "&" in the first column. The following key words initiate specific actions in the DLL interface:

1. PUT – Put data specified within the block into the named file.
2. GET – Get data specified within the block from the named file.
3. EXE – Perform the system calls specified within the block.
4. RPL – Replace complete lines in the named file.
5. SUP – Create a “super” file containing the commands or file names listed within the block.
6. LOG – Write a log file in XML format containing the input and output data.
7. END – Termination of a command block.

The actions are processed in the order that they appear in the DLL.dat file and each of the actions can be used more than once. Typically, the user would want to enter data into an input file using the PUT command, run an external application that reads from the input file using the EXE command, and retrieve output from the external application using the GET command. The DLL performs some error checking as it processes the instructions it receives. For example, if a GET or PUT instruction points to a file location that does not exist, the code will trap this error, send an error message back to GoldSim, and cleanly exit from the DLL interface. However, this error checking is not as extensive as it could be and will be expanded in future releases.
Figure 1: Example DLL.dat file

```
!                                                                                     !
!  ! #2 #3 #4 #5 #6 #7 #8 #9 #10 #11 #12 #13 (comment)                                 !
!-------------------------------------------------------------------------------  !
FUT Stadium\stad09d-cbp-task7-template.inp white
14 row 123 col 3  11 1 inputs 014-024
25 row 123 col 4  11 1 inputs 025-035
45 row 138 col 3  9 1 inputs 045-053
54 row 138 col 4  9 1 inputs 054-062
80 row 27 col 3  17 1 inputs 080-096
97 row 27 col 4  17 1 inputs 097-113
114 row 12 col 3  2 1 inputs 114-115
116 row 19 col 3  3 1 inputs 116-118
119 row 96 col 2  1 1 input 119
119 row 119 col 2  1 1 input 119
END
!-------------------------------------------------------------------------------  !
RPL stad09d-cbp-task7-template.inp
2 ..\..\Stadium\20cm-50cm-mesh01.cor
4 ..\..\Stadium\20cm-50cm-mesh01.ele
END
!-------------------------------------------------------------------------------  !
EXE ..\..\Codes\Stadium\stadium_2009d_CBP
& GUI=YES
& stad09d-cbp-task7-template.inp
& CBP002BATCH
& stad09d-cbp-task7-template.out
END
!-------------------------------------------------------------------------------  !
GET stad09d-cbp-task7-template.out.xls space ignore
1 value 1.0 1 -0.1 col 4  101 11 outputs 0001-1111
3312 value 1.0 1 -0.1 col 18  101 9 outputs 3312-3410
END
!-------------------------------------------------------------------------------  !
LOG stadium.xml
END
!-------------------------------------------------------------------------------  !
```
3 USER GUIDE

This section provides a guide to using the DLL by describing the commands that can be entered into the DLL.dat file.

3.1 PUT and GET

The PUT and GET commands are functionally similar and will be described together. The name of the file to be processed by the PUT or GET command is listed on the same line as the command in the column (next tab position) immediately following the key word. Following the file name, the delimiter used to separate data fields in the file is given in the next column. Recognized delimiter names are: colon, comma, semicolon, space, tab, and white. The delimiter “white” indicates any combination of tabs and/or spaces which will appear as “white” space in the file. When identifying delimiters in the files, it is assumed that the delimiter appears only one time following each field with the exception of spaces which can be inserted multiple times. For “white” space, tabs are replaced with spaces during file processing. If the delimiter name is followed by the key word “ignore,” any delimiters appearing before the first data entry are stripped out and ignored.

Between the PUT or GET command and the END statement, that indicates the termination of this command block, the instructions on each of the lines that direct the command operations are entered in Fields 2 – 12. These fields contain the information listed below.

Field 2: Input arguments are passed from GoldSim to the external interface in the array inargs(), and output arguments are passed from the external interface back to GoldSim in the array outargs(). Following Fortran 90 convention, the starting index of each array is 1 (rather than 0 in the C language). The number in Field 2 indicates the position in the one-dimensional array that begins the command. PUT commands use the inargs() array while GET commands use the outargs() array.

PUT commands must start with inargs(3). The first two entries in the inargs() array have been reserved to pass two special parameters from GoldSim to the DLL interface. The first parameter, isave passed in inargs(1), is set by the user within GoldSim to indicate whether results from individual GoldSim Monte Carlo realizations are to be saved (isave>0) or not (isave=0). If isave=0, a subdirectory named realization_0 is setup to hold results from the GoldSim run. If GoldSim is then run in Monte Carlo mode with multiple realizations, results saved in the subdirectory would be overwritten with each realization and only results from the final realization will be saved. If isave>0 and GoldSim is run with multiple realizations 1 … n, individual subdirectories realization_1 through realization_n are setup to save results from each realization. The second parameter passed from GoldSim in inargs(2) is the realization number.

Field 3 – Field 6: These entries specify how the row in either the input or output files where the data values are located is identified. The key words that can appear in Field 3 are listed in Table 1. The information that must appear in Fields 4 – 6 depends on the key word in Field 3 as explained in the Table 1.
Table 1. Row Specification in Field 3

<table>
<thead>
<tr>
<th>Key Word</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>row</td>
<td>The row (record) number where the data is located is entered in Field 4.</td>
</tr>
<tr>
<td>record</td>
<td>The record (row) number where the data is located is entered in Field 4.</td>
</tr>
<tr>
<td>label</td>
<td>An alphanumeric label identifying the row where the data is located is entered in Field 4 and the column where the label is to be read is entered in Field 5.</td>
</tr>
<tr>
<td>value</td>
<td>A numerical value that identifies the row where the data is located is entered in Field 4, the column where the label is to be read is entered in Field 5, and a tolerance on the value is entered in Field 6. A positive tolerance in Field 6 specifies that an absolute difference is used to test if the numerical value in Field 5 has been found while a negative tolerance specifies a relative difference. The DLL reads numerical values in the specified column and in all rows starting with the first row of data until the specified value is found. The data entry at this location is then used in the PUT or GET command.</td>
</tr>
<tr>
<td>string</td>
<td>A character (alphanumeric) string identifying the row where the data is located is entered in Field 4. The string can appear in any column. The DLL reads record entries as text strings in the file starting with the first row until the specified label is found. The data entry at this location is then used in the PUT or GET command.</td>
</tr>
</tbody>
</table>

Field 7 – Field 10: These entries specify how the column in either the input or output files where the data values are located is identified. The key words that can appear in Field 7 are listed in Table 2.
Table 2. Column Specification in Field 7

<table>
<thead>
<tr>
<th>Key Word</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>col</td>
<td>The column (field) number where the data is located is entered in Field 8.</td>
</tr>
<tr>
<td>field</td>
<td>The field (column) number where the data is located is entered in Field 8.</td>
</tr>
<tr>
<td>heading</td>
<td>An alphanumeric label identifying the column where the data is located is entered in Field 8 and the row where the label is located is entered in Field 9. The DLL reads entries in the specified row starting with the first column as text until the specified label is found. The data entry at this location is then used in the PUT or GET command.</td>
</tr>
<tr>
<td>value</td>
<td>A numerical value that identifies the column where the data is located is entered in Field 8, the row where the value is located is entered in Field 9, and a tolerance on the value is entered in Field 10. A positive tolerance in Field 10 specifies that an absolute difference is used to test if the numerical value in Field 8 has been found while a negative tolerance specifies a relative difference. The DLL reads numerical values in the specified row and in all columns starting with the first column of data until the specified value is found. The data entry at this location is then used in the PUT or GET command.</td>
</tr>
</tbody>
</table>

Field 11: This field contains the number of rows to be used for data processing; this allows entering or reading a row vector with a single command. For example, if a PUT command has the number \( n \) entered in Field 2 and the number \( m \) in Field 11, \( \text{inargs}(n) \) will be written into the data file row and column identified by the information in Fields 3 – 10. The values \( \text{inargs}(n+1) \) through \( \text{inargs}(n+m-1) \) will be written into the next \( (m-1) \) rows in the same column.

Field 12: This field contains the number of columns to be used for data processing; this allows entering a column vector with a single command or, in conjunction with Field 11, entering a matrix of values with a single command. For example, if a GET command has the number \( n \) in Field 2, the number \( m \) in Field 11 and the number \( p \) in Field 12, \( \text{outargs}(n) \) will be read from the data file row and column identified by the information in Fields 3 – 10. The values of \( \text{outargs}(n+1) \) through \( \text{outargs}(n+p-1) \) will be read from the next \( (p-1) \) columns in the same row and the values of \( \text{outargs}(n+p) \) through \( \text{outargs}(n+2p-1) \) will be read from the same columns in the next row down. This process will continue over \( m \) rows of data until a total of \( m \times p \) values have been read.

Field 13: This field can be used to enter an optional comment that is not read by the DLL or used by GoldSim.
3.2 RPL

The RPL command can be used to replace entire lines in an existing input file. GoldSim passes double precision numerical values in the inargs() and outargs() arrays. The only exception to this is that the external function can return an error message to GoldSim in the outargs() array using a special function supplied by GoldSim Technology Group (GTG). Passing only numerical values can be restrictive because input files may contain text strings with, for example, file names, and it may be desirable to change these file names for different simulations. As a simple work around to this limitation, the DLL interface was given the capability of replacing entire lines of input with text using the RPL command. Within the RPL command block, the entry in Field 2 identifies the line of input that will be replaced. The text starting in Field 3 will be used to replace the current entry in the line.

3.3 EXE

The EXE command block specifies DOS commands to be executed by the Windows operating system. The feature is primarily used to give the name and relative location of the file (or files) that must be run to execute the external code. This command could be used to run a batch file or an executable. Any arguments that must be passed to the executable are included in the command. Additional commands can be specified to perform other operations, such as copying or renaming output files.

3.4 SUP

The SUP command writes the specified text to the specified file. The file name must be provided in the second column on the same line as the SUP command. The file is created if not found, or overwritten if existing. The keyword can be used to create a “super” file of file names and instructions that can then be accessed by the external application.

3.5 LOG

The LOG command is used to give the name of a file where arrays of the GoldSim input and output data used in the simulation will be written in XML format. The log file name must be provided in the second column on the same line as the LOG command. The realization number is written to the log file followed by an array of the input data and an array of the output data.

4 EXAMPLES

4.1 PUT/GET Example

To test whether the various options available to PUT and GET values from the input and output arrays function correctly, a simple test run was made using the DLL.dat file shown in Figure 2 with the starting test.inp file shown in Figure 3. The PUT instructions should replace the values in test.inp along a diagonal from value (2,2) to value (6,6) with zeros. The test was made by running the GoldSim model intended for use with the STADIUM code with this DLL.dat instruction file. As the modified test.inp file in Figure 4 shows
the PUT operations worked correctly. The GET instructions were designed to read these zero values. Examination of the test.xml file (not provided) showed that the first six output arguments returned from the DLL to GoldSim were zero as intended.
Figure 2. DLL.dat file used to test DLL PUT and GET options

<table>
<thead>
<tr>
<th>PUT</th>
<th>test.inp</th>
<th>white</th>
<th>ignore</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>row</td>
<td>2</td>
<td>field</td>
</tr>
<tr>
<td>2</td>
<td>record</td>
<td>3</td>
<td>col</td>
</tr>
<tr>
<td>2</td>
<td>label</td>
<td>line3</td>
<td>headingfield</td>
</tr>
<tr>
<td>2</td>
<td>value</td>
<td>123</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>value</td>
<td>456</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>string</td>
<td>myStr</td>
<td>col</td>
</tr>
</tbody>
</table>

END

<table>
<thead>
<tr>
<th>GET</th>
<th>test.inp</th>
<th>white</th>
<th>ignore</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>row</td>
<td>2</td>
<td>field</td>
</tr>
<tr>
<td>2</td>
<td>record</td>
<td>3</td>
<td>col</td>
</tr>
<tr>
<td>3</td>
<td>label</td>
<td>line3</td>
<td>headingfield</td>
</tr>
<tr>
<td>4</td>
<td>value</td>
<td>123</td>
<td>2</td>
</tr>
<tr>
<td>5</td>
<td>value</td>
<td>456</td>
<td>2</td>
</tr>
<tr>
<td>6</td>
<td>string</td>
<td>myStr</td>
<td>col</td>
</tr>
</tbody>
</table>

END

| LOG | test.xml | END |

END
Figure 3. Input file used to test DLL PUT and GET options

```
!field1 field2 field3 field4 field5 field6 field7
line1  -111 -222 -333 -444 -555 -666
line2   -11  -22  -33  -44  -55  -66
line3   -999 -999 -999 -999 -999 -999
line4    123 -999 -999 -999 -999 -999
line5    456 -999 -999 -999 -999 -999
line6   -999 -999 -999      myStr -999 -999
line7   -999 -999 -999 -999 -999 -999
line8   -999 -999 -999 -999 -999 -999
```

Figure 4. Modified input file after running GoldSim

```
!field1 field2 field3 field4 field5 field6 field7
line1  0   -222 -333 -444 -555 -666
line2   -11   0  -33  -44  -55  -66
line3   -999 -999   0  -999 -999 -999
line4    123 -999 -999   0  -999 -999
line5    456 -999 -999 -999   0  -999
line6   -999 -999 -999    myStr -999   0
line7   -999 -999 -999 -999 -999 -999
line8   -999 -999 -999 -999 -999 -999
```
4.2 STADIUM Example

This example uses the DLL.dat file shown in Figure 1 to make a one year run of the STADIUM code with three realizations. Because the DLL replaces values in the input file, the user must supply a template file for the DLL to manipulate. As shown in Section 3.1, the DLL provides some flexibility for locating data within the template file. However, the user must either know the exact location of input parameters within the input file or know the basic structure of the input so that the methods described in Section 3.1 can be applied. The example DLL.dat file in Figure 1 locates data by giving specific row and column positions. The template file used for the STADIUM code is shown in Figure 5. After the DLL executes the RPL and PUT commands shown in Figure 1, the modified template file that was used as the actual input file for STADIUM is shown in Figure 6. The current version of the model did not try to replace the entire input file; the values actually replaced by the DLL are highlighted in Figure 6.

The GET command shown in Figure 1 was used to retrieve concentrations of the 11 chemicals and nine minerals used by the STADIUM code at each of the 101 node locations at time one year. The GET command can be interpreted as follows:

Look for a value of 1.0 in the first column of output data with a relative tolerance of 0.1 year. When this value is found, starting in column 4, retrieve 101 rows of data over 11 columns, then, starting in column 18, retrieve 101 rows of data over 9 columns. The first block of data retrieved is placed in the outargs() array starting with element one. The second block of data is placed in the outargs() array starting with element 3312.

The outargs() array that returns output to GoldSim has been dimensioned large enough to return concentrations at one time step for a mesh as large as 301 nodes. The gap between the two blocks of output data retrieved in this example allows blank spaces for the data that would have appeared in nodes 102 through 301.
Figure 5. Template input file for STADIUM
Database_file  CHM-DB-STADIUM.txt

<table>
<thead>
<tr>
<th>Element</th>
<th>Nb_cycles</th>
<th>Sequences_days</th>
<th>OH</th>
<th>Na</th>
<th>K</th>
<th>SO4</th>
<th>Ca</th>
<th>Al(OH)4</th>
<th>Cl</th>
<th>H2SiO4</th>
<th>CO3</th>
<th>NO3</th>
<th>NO2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>0 365.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>OH</td>
<td>1</td>
<td>0 0 0 0.0 0.0 0.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Na</td>
<td>1</td>
<td>0 0 0.0 0.0 0.0 0.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>K</td>
<td>1</td>
<td>0 0 0.0 0.0 0.0 0.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SO4</td>
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CONV

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<th>CO3</th>
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**Figure 5. Template input file for STADIUM (Cont’d)**
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**INIT**

external_file 0

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| Portlandite   | 13.6  | 41.9   |
| CaH2SiO4      | 37.9  | 103.3  |
| Ettringite    | 0.0   | 28.6   |
| Monosulfate   | 19.4  | 0.0    |
| C4AH13        | 14.8  | 0.0    |
| Thaumasite    | 0.0   | 0.0    |
| Calcite       | 0.0   | 4.8    |
| Monocarboaluminate | 0.0   | 11.0  |
| Gypsum        | 0.0   | 0.0    |

**IMPR**

number_print_times 31

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**Figure 5. Template input file for STADIUM (Cont’d)**
Figure 5. Template input file for STADIUM (Cont’d)

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2500.0
3000.0
4500.0
5000.0
5500.0
6000.0
6500.0
7000.0
7500.0
8000.0
8500.0
9000.0
9500.0
10000.0
print_before_chm 0
level_1_2 1
imp_flux_0_1_2 0
STOP
```
Figure 6. STADIUM input file after execution of PUT and RPL commands
Database_file   CHM-DB-STADIUM.txt

OH
Na
K
SO4
Ca
Al(OH)4
Cl
H2SiO4
CO3
NO3
NO2

Portlandite
CaH2SiO4
Ettringite
Monosulfate
C4AH13
Thaumasite
Calcite
Monocarboaluminate
Gypsum

COND
Nb_cycles           1
Sequences_days      0 365.0

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CONV
Nb_cycles           1
Sequences_days      0 365

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</table>

Figure 6. STADIUM input file after execution of PUT and RPL commands (Cont’d)
Figure 6. STADIUM input file after execution of PUT and RPL commands (Cont’d)
Figure 6. STADIUM input file after execution of PUT and RPL commands (Cont’d)

5 REFERENCES


APPENDIX A

LISTING AND EXPLANATION OF SUBROUTINES IN GOLDSIM DLL INTERFACE
The DLL interface code was written in Fortran 90 and is modularized into the five files and 19 subroutines listed below.

**DllExternalCode_g95.f90**
- DllExternalCode

**Filework.f90**
- ReadSup
- ReadRpl
- RunExe
- WriteLog
- GetOrPut
- ReadRow
- ReadCol
- ReadRecords
- setDelim
- checkField
- Continuation

**GSUtilities.f90**
- gs_parameters
- copy_msg_to_outputs

**Params.f90**

**putget.f90**
- putField
- getField
- FindDelim
- IostatCheck
- logstring

Module **Params** contains a list of parameters common to all of the other modules. **Params** also contains the two parameters **NINPUTS** and **NOUTPUTS** that give the number of inputs passed from GoldSim to the DLL and the number of outputs passed back from GoldSim to the DLL. These values must agree with the number of inputs and outputs defined in the GoldSim interface. The current version of the DLL has **NINPUTS = 119** and **NOUTPUTS = 6020**. The number of inputs is exactly the number of values that GoldSim uses to set up a STADIUM input file. The number of outputs is set large enough to hold data for 20 chemical and mineral concentrations at up to 301 nodes. If fewer nodes are present, the output array can still be organized correctly so that individual chemical and mineral species can be separated. However, it may be necessary to manually change these parameter values and recompile the DLL for different simulations. **Params** also contains names for the file containing the DLL instructions (generically referred to as **DLL.dat** in this document) and a log file where information primarily of interest for debugging purposes is written. The user may wish to change the default names of these files and recompile the DLL for specific simulations.
DLL SUBROUTINES

gs_parameters

This module specifies parameters used by GoldSim as a part of its DLL external interface. These parameters indicate the phase of the simulation currently in progress and provide return codes to GoldSim indicating the completion status of the external calculation. This subroutine was provided in Appendix C of the GoldSim User’s Guide (Volume 2 GoldSim Technology Group, Version 10.0 February 2009 (GTG 2009)) and was used without change.

Parameters used to indicate the phase of the simulation are:

- **INITIALIZE** - Called after DLL is loaded and before each realization.
- **REPORT_VERSION** - Called after DLL load to report the external function version number.
- **REPORT_ARGUMENTS** - Called after DLL load to report the number of input and output arguments.
- **CALCULATE** - Called during the simulation, each time the inputs change.

Parameters providing return codes to GoldSim are:

- **CLEANUP** - Called before the DLL is unloaded.
- **SUCCESS** - Call was completed successfully.
- **CLEANUP_NOW** - Call was successful, but GoldSim should clean up and unload the DLL immediately.
- **FAILURE** - Failure (no error information returned).
- **FAILURE_WITH_MSG** - Failure, with DLL supplied error message available. Address of error message is returned in the first element of the output arguments array.
- **INCREASE_MEMORY** - Failed because the memory allocated for output arguments is too small. GoldSim will increase the size of the output argument array and try again.

Subroutine to pass error message to GoldSim:

```c
void copy_msg_to_outputs (char *smsg, double outargs[]);
```

- `smsg` - String variable containing output message
- `outargs` - Array of output arguments returned to GoldSim

To help GoldSim users debug problems with DLL external functions, GoldSim allows users to send an error message from the DLL back to GoldSim through the external element interface when the call to an external function fails. The error message is displayed to the user in a pop-up dialog. The subroutine that performs this task was provided by GoldSim in Appendix C of the User’s Guide (GTG 2009) and was used without change. An example of the use of this subroutine is shown in Figure A-1.
subroutine DllExternalCode (method_id, status, inargs, outargs) BIND (C)

!Variable typing statements

select case (method_id)
  case (INITIALIZE)
    outargs(1) = NINPUTS
    outargs(2) = NOUTPUTS
    status = SUCCESS
  case (REPORT_VERSION)
    outargs(1) = VERSION
    status = SUCCESS
  case (REPORT_ARGUMENTS)
    outargs(1) = NINPUTS
    outargs(2) = NOUTPUTS
    status = SUCCESS
  case (CALCULATE)
    !Set working directory
    !Open file for logging processing of DLL instructions
    !Make subdirectory for run(s)
    !Make subdirectory for realization
    !Read in instructions
    call ReadRecords (datfile, instructions, nInstructions, msg)
    !Put inargs(*) into input file(s)
    call GetOrPut (streamlined, nStreamlined, subdir, "PUT", inargs, msg)
    !Create superfile per instructions
    call ReadSup (streamlined, nStreamlined)
    !Replace lines in input file per instructions
    call ReadRpl (streamlined, nStreamlined)
    !Execute command per instructions
    call RunExe (streamlined, nStreamlined)
    !Get outargs(*) from output file(s)
    call GetOrPut (streamlined, nStreamlined, subdir, "GET", outargs, msg)
    !Create logfile
    call WriteLog (streamlined, nStreamlined, inargs, outargs, irealization)
    !Report success
    status = SUCCESS
  case (CLEANUP)
    status = SUCCESS
  case default
    msg = "Unknown method ID requested"
    call copy_msg_to_outputs(msg, outargs)
    status = FAILURE_WITH_MSG
end select
end subroutine DllExternalCode

Figure A-1. Outline of Subroutine DllExternalCode
**DllExternalCode (method_id, status, inargs, outargs)**

- **method_id**... Parameter indicating phase of simulation
- **status**........ Return code to GoldSim indicating status of external calculation
- **inargs** .......... Array of input arguments received from GoldSim
- **outargs** .......... Array of output arguments returned to GoldSim

This is the main subroutine called by the external link and, as such, controls the flow of the file processing. The basic structure that must be followed for this subroutine was given in Appendix C of the GoldSim User’s Guide (GTG 2009). An outline version of this subroutine with many of the detailed statements removed is shown in Figure A-1. This outline illustrates the use of the parameters listed above and calls to some of the primary subroutines in module Filework.

**ReadSup (records, nRecords)**

- **records**......... Array of records in SUP block
- **nRecords** ........ Number of records in SUP block

Subroutine ReadSup reads the instructions in the SUP block and writes them into a “super” file that can then be used by external applications. This feature would typically be used to provide a list of files and their relative locations required by the external application.

**ReadRpl (records, nRecords)**

- **records**......... Array of records in RPL block
- **nRecords** ........ Number of records in RPL block

Subroutine ReadRpl reads the instructions in the RPL block and replaces the identified lines in the input file with the text supplied in the records. The first entry in each record is the number of the line in the file that is to be replaced and the second entry in each record is the text string that will be placed in the file.

**RunExe (records, nRecords)**

- **records**......... Array of records in EXE block
- **nRecords** ........ Number of records in EXE block

Subroutine RunExe reads the instructions in the EXE block and makes system calls to execute each of the commands listed within the block. More than one external application can be executed. Any command-line arguments required by the executables must be included in the commands.
WriteLog (records, nRecords, inargs, outargs, irealization)

records ................. Array of records in LOG block
nRecords ............... Number of records in LOG block
inargs ................. Array of input arguments received from GoldSim
outargs................ Array of output arguments returned to GoldSim
irealization .......... Number of the realization being run

Subroutine WriteLog writes an XML formatted log file containing the realization number and the input and output data used for this particular calculation.

GetOrPut (DLLdat, nDLLdat, subdir, action, args, msg)

DLLdat ............. Array of records in GET or PUT block
nDLLdat............ Number of records in GET or PUT block
subdir ............ For a PUT command, the name of the subdirectory where the input file is to be written
action .............. Key word GET or PUT
args.................. For PUT command inargs() array, for GET command outargs() array
msg.................... Text containing error message

Subroutine GetOrPut implements the GET or PUT commands entered into the DLL.dat file. These commands are described in Section 3.1.

ReadRow (vctr, iloc, array, nRecords, delim, msg)

vctr .................. Vector containing row specifications from Fields 3 – 6 in the PUT or GET command
iloc .................. Row number where PUT or GET command should start operating
array ................. Array of records in file where PUT or GET command is operating
nRecords .......... Number of records in file where PUT or GET command is operating
delim .............. Delimiter used in file where PUT or GET command is operating
msg .................... Text string containing error message

Subroutine ReadRow reads the row specifications in a PUT or GET command (see Section 3.1, Field 3 – Field 6) and uses the specifications to find the row within the data file where the command should start operating.

ReadCol (vctr, iloc, array, nRecords, delim, msg)

vctr .................. Vector containing column specifications from Fields 7 – 10 in the PUT or GET command
iloc .................. Column number where PUT or GET command should start operating
array ................. Array of records in file where PUT or GET command is operating
nRecords .......... Number of records in file where PUT or GET command is operating
delim .............. Delimiter used in file where PUT or GET command is operating
msg .................... Text string containing error message
Subroutine **ReadCol** reads the column specifications in a **PUT** or **GET** command (see Section 3.1, Field 7 – Field 10) and uses the specifications to find the column within the data file where the command should start operating.

**ReadRecords** *(file, array, nRecords, msg)*

```plaintext
    file.................. Text string with name of file to read
    array.............. Array of records in file
    nRecords .......... Number of records in file
    msg.................. Text string containing error message
```

Subroutine **ReadRecords** reads the data records in the specified file and returns an array containing the records and the number of records found. If a read error is encountered, an error message is returned in text string **msg**.

**setDelim** *(field, delim, msg)*

```plaintext
    field.............. Text string with name of file delimiter
    delim............. Text character representing delimiter used in file
    msg.................. Text string containing error message
```

Subroutine **setDelim** reads the name of the delimiter specified in the **DLL.dat** file and returns the delimiter character. If an incorrect delimiter name is encountered, an error message is returned in text string **msg**. Valid delimiters are: colon, comma, semicolon, space, tab, and white (a combination of tabs and spaces).

**Strip** *(records, nRecords, delim)*

```plaintext
    records.......... Array of records
    nRecords ........ Number of records
    delim............. Text character representing delimiter used in file
```

Subroutine **Strip** removes leading blank spaces from the set of records passed to the subroutine.

**checkField** *(field, check, toler, found)*

```plaintext
    field............. Text string holding data that is to be checked
    check............. Value that is being searched for
    toler............... Tolerance allowed in identifying value
    found............... Logical variable indicating whether the numerical value of the data in the field is within the tolerance of the value of check.
```

Subroutine **checkField** implements the option to search for a numerical value to identify either the row or column in a data file that a **PUT** or **GET** command is manipulating.
Continuation (nInput, input, continuationCharacter, nOutput, output)

- nInput: Number of records in original DLL.dat file
- input: Array of records in original DLL.dat file
- continuationCharacter: Text character used to identify a continuation line
- nOutput: Number of records in processed DLL.dat file
- output: Array of records in processed DLL.dat file

Subroutine Continuation collapses continued lines in the DLL.dat file into a single record, removes comment lines, and returns an array of processed DLL.dat command lines.

putField (line, lineLength, nField, field, fieldLength, delim, new_line, lerr)

- line: A text string containing the record to be modified
- linelength: Maximum length of the record
- nField: The field in the record to be replaced
- field: A text string containing the value to be inserted into the record
- fieldlength: Maximum length of the field
- delim: The delimiter used in the record
- new_line: Logical variable indicating if the record is a new line of the data file
- lerr: Logical variable indicating an error in the PUT operation

Subroutine putField is called to insert a data value into a data record replacing the old value at the same position. Only new lines need to have delimiter positions located. That is, when the subroutine is inserting another value into the same line used previously it already knows the delimiter positions.

getField (line, lineLength, nField, field, fieldLength, delim, new_line)

- line: A text string containing the record to be used
- linelength: Maximum length of the record
- nField: The field in the record to be extracted
- field: A text string containing the value extracted from the record
- fieldlength: Maximum length of the field
- delim: The delimiter used in the record
- new_line: Logical variable indicating if the record is a new line of the data file

Subroutine getField is called to extract a data value from a data record. Only new lines need to have delimiter positions located. That is, when the subroutine is reading another value from the same line used previously it already knows the delimiter positions.

FindDelim (line, linelength, delim, position)

- line: A text string containing the record to be searched
- linelength: Maximum length of the record

Subroutine FindDelim is called to find the position of a delimiter in a data record.
delim................. The delimiter to search for
position ............ An array of delimiter positions

Subroutine FindDelim is called to locate delimiter positions in a data record and return a list of the positions to the calling routine.

*** IostatCheck (iostat_flag, exit_flag, msg) ***

  iostat_flag..... Integer variable indicating status of read
  exit_flag ........ Logical variable signaling exit from read
  msg................. Text string containing error message

Subroutine IostatCheck is called to check the status of an attempted read statement. If an error or end of file is detected, exit_flag is set to false. If an error is detected, the error message “***READ ERROR ***” is returned to the calling program.

*** logstring (iunit, label, value) ***

  iunit.............. Output unit where label and value will be written
  label ............. Text string containing label to be output
  value ............. Text string containing value to be written

Subroutine logstring is called to write a labeled value to an output file. This subroutine is used to write messages to file DLL.log indicating the status of operations the DLL is performing to assist the user in debugging applications.