Introduction to GoldSim Interface and CBP Software Communications Bridge

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CBP
Cementitious Barriers Partnership

SRNL-STI-2012-00382

Overview

- Design philosophy
- GoldSim software bridge
- GoldSim Dashboard GUI
- Hands-on tutorials

Segment 1 – Design Philosophy

CBP Custom DLL

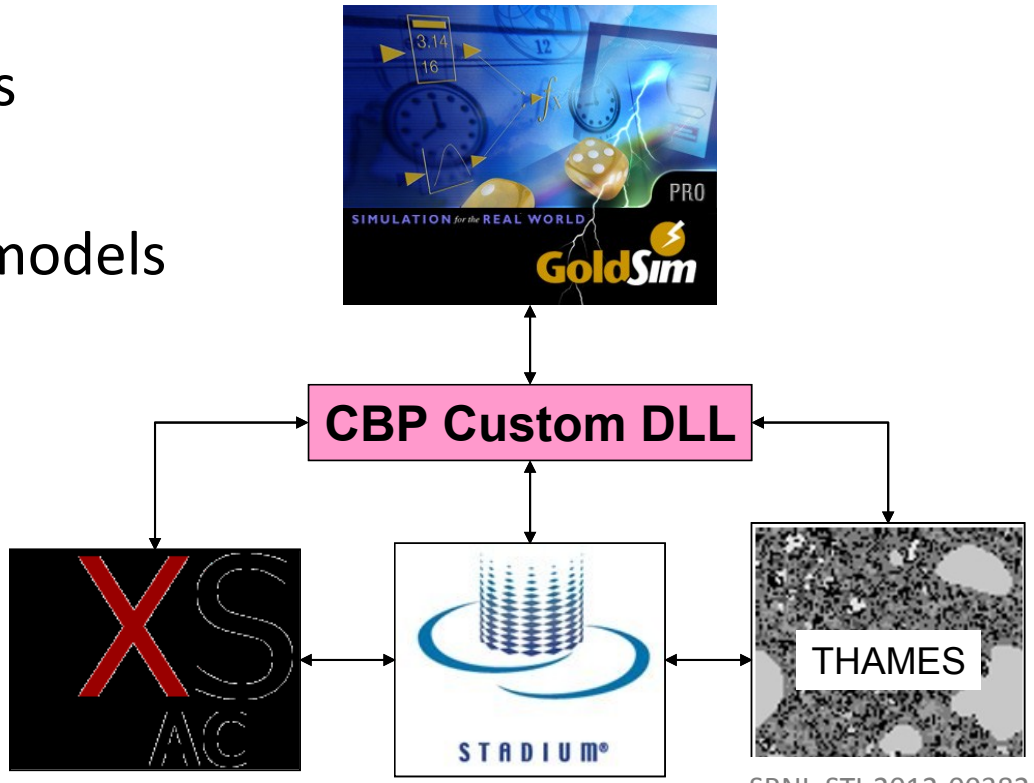
LXS LEACH

STADIUM®

CBP Partner Code Integration

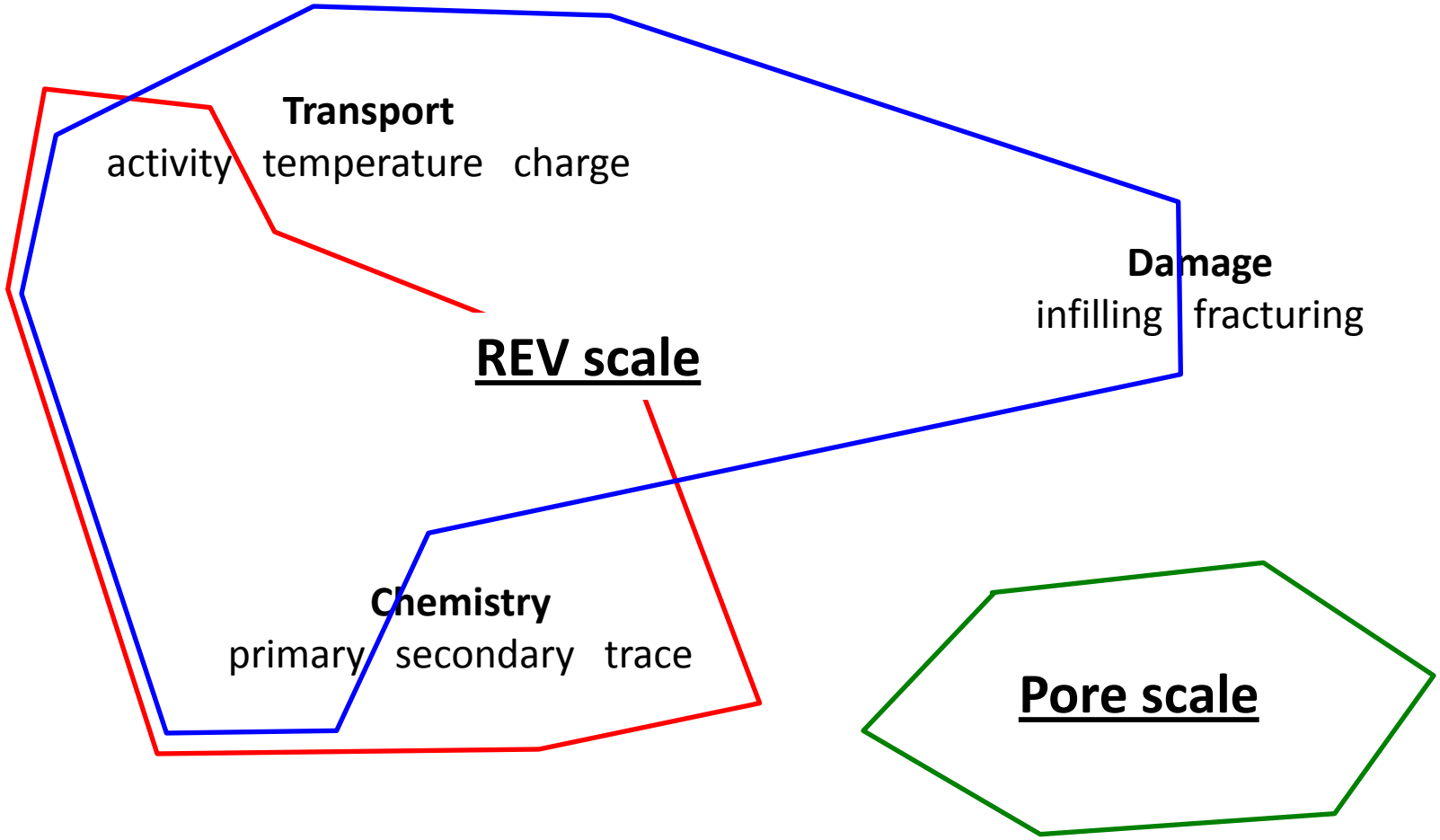
Software integration objectives

- 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



CBP Partner Codes

~LeachXS/Orchestra ~STADIUM ~THAMES



Coupling Decisions

- **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**

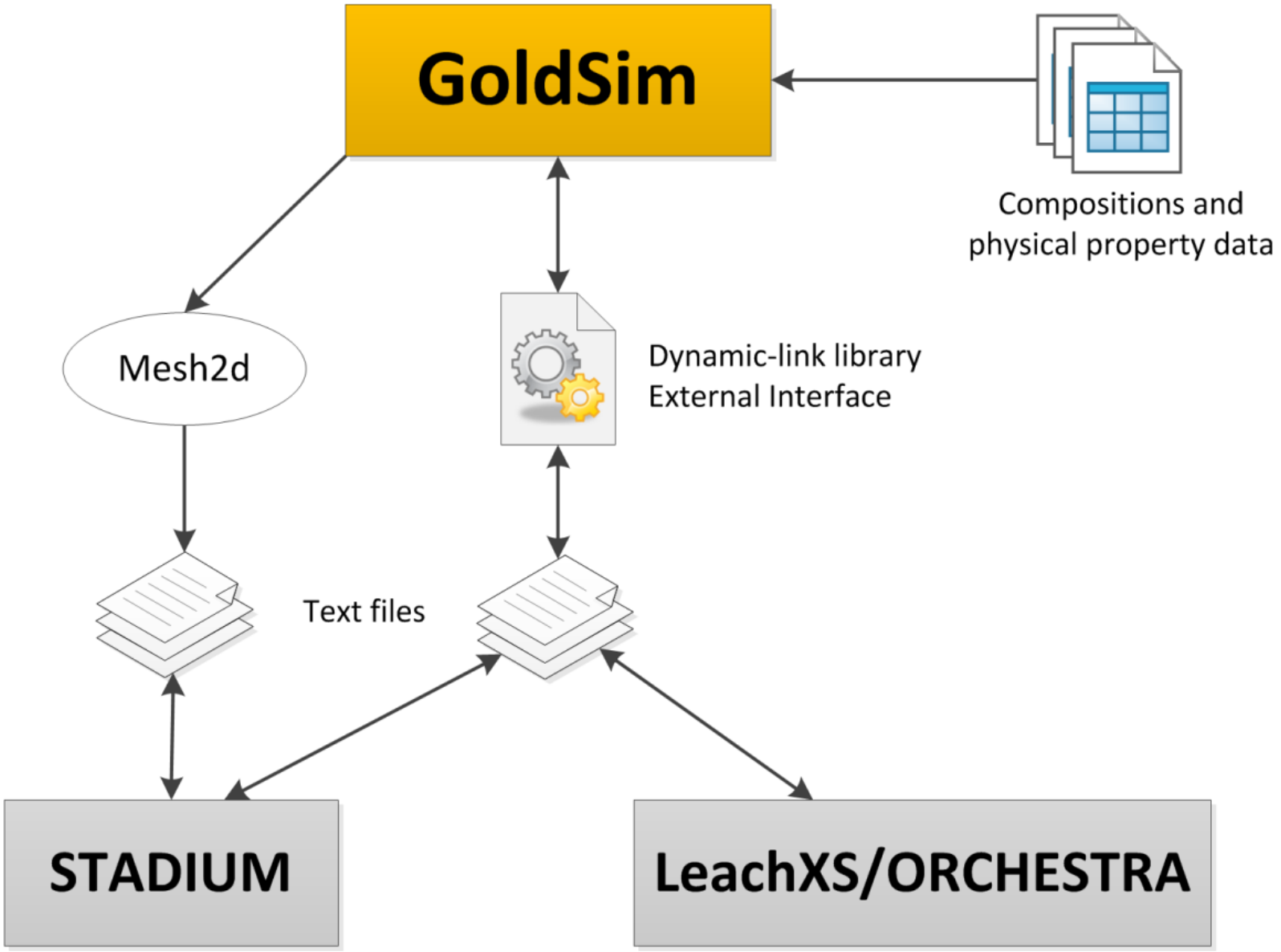
Some Design Principles

- 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

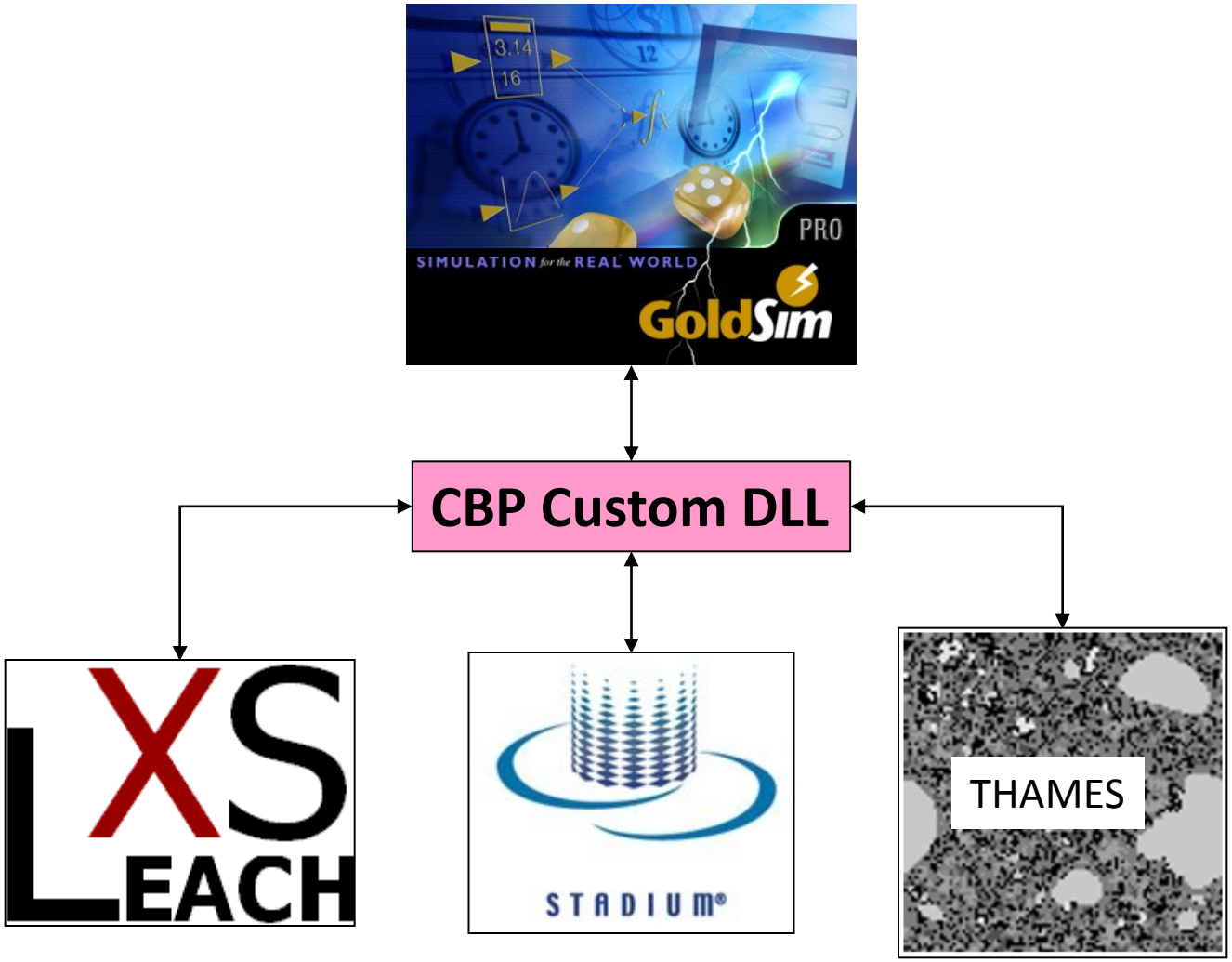
GoldSim Merits

- **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**

Phase I Progress



Segment 2 – GoldSim Software Bridge

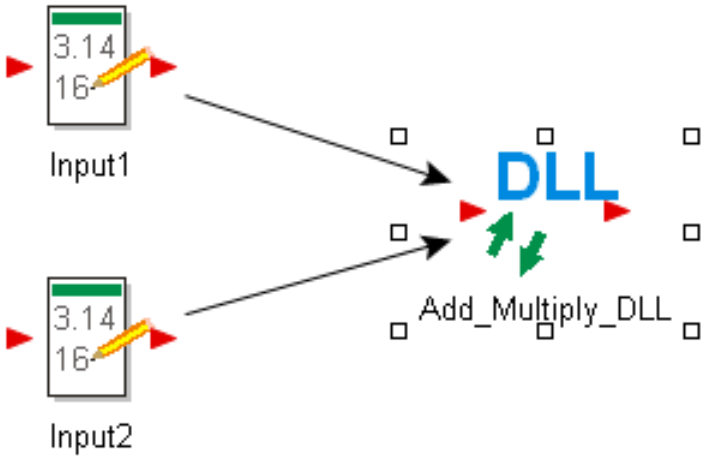


GoldSim Links to External Functions

Three basic methods:

- **Lookup table**
- **Spreadsheet**
- **DLL subroutine** 

DLL External Element



External Properties : Add_Multiply_DLL

Definition | Interface

Element ID: Add_Multiply_DLL — Appearance...

Description:

Options

DLL Path: add_mult_scalars.dll

Function Name: add_mult_scalars

☐ Lock onto this file ☐ Run in separate process

☐ Unload DLL after each use

☐ Run Cleanup after each realization

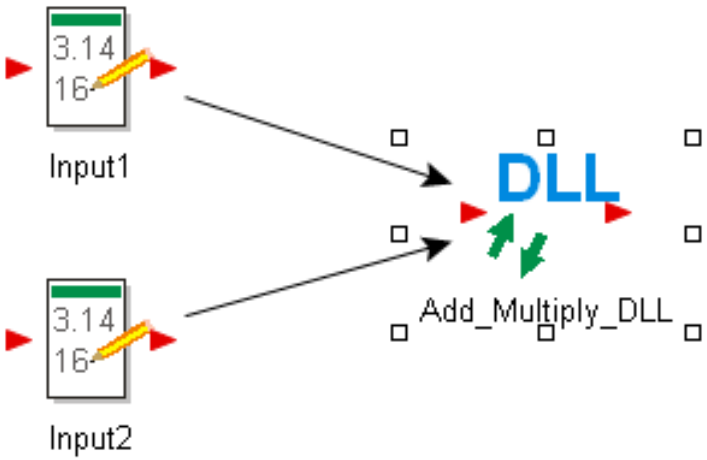
The element defines 2 inputs and 2 outputs.

Save Results

☑ Final Values ☐ Time Histories

OK | Cancel | Help

DLL External Element



External Properties : Add_Multiply_DLL

Definition | Interface

Input Interface Defintion

#	Name	Definition
1	Input1	Input1
2	Input2	Input2

Output Interface Definition

#	Name	Data Type
1	sum	Value (m)
2	product	Value (m2)

OK | Cancel | Help

Corresponding DLL Subroutine

5 standard functions:

- Initialize
- Report version
- Report number of inputs and outputs
- Calculate
- Cleanup

```
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 dllexport,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
    case (REPORT_VERSION)
        outargs(1) = VERSION
        status = SUCCESS
    case (REPORT_ARGUMENTS)
        outargs(1) = NINPUTS
        outargs(2) = NOUTPUTS
        status = SUCCESS
    case (CALCULATE)
        outargs(1) = inargs(1) + inargs(2)      ! return the sum
        outargs(2) = inargs(1)*inargs(2)        ! return the product
        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 add_mult_scalars
```

DLL That Makes System Call

DLL is "middle-man“ between GoldSim and External Function

```
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

```
!
!       #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_CBP  GUI=YES  SRS_Vault2_Saltstone_01.inp  CBP002BATCH
END
!-------------------------------------------------------------------------------------
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
!-------------------------------------------------------------------------------------
```

Input Placement (PUT)

```
INIT
    external_file          0

    OH                     0.00      400.00      487.00
    Na                     0.00      282.10      4419.20
    K                      0.00      138.00      120.10
    SO4                    0.00      8.00        120.00
    Ca                     0.00      0.50        0.90
    Al(OH)4                0.00      0.10        0.10
    Cl                     0.00      5.00        9.00
    H2SiO4                 0.00      0.00        0.00
    CO3                    0.00      0.00        115.00
    NO3                    0.00      0.00        2000.00
    NO2                    0.00      0.00        1575.00
    Rel_Humidity           1.00      1.00        1.00
    Potential              0.00      0.00        0.00
    Temperature            23.00     23.00       23.00

    Portlandite            0.00      13.60       32.90
    CaH2SiO4               0.00      37.90       91.80
    Ettringite             0.00      0.00        5.00
    Monosulfate            0.00      19.40       0.00
    AFm-OH                 0.00      14.80       0.00
    Thaumasite             0.00      0.00        0.00
    Calcite                0.00      0.00        4.00
    Monocarboaluminate     0.00      0.00        20.00
    Gypsum                 0.00      0.00        0.00
```

Output Retrieval (GET)

	A	B	P	Q	R	S	T	U	V	W	X	Y
1	*2*	*3*	*17*	*18*	***19***	***20***	***21***					
2	Years	Node	Potential	Temperature	Portlandite	CaH2SiO4	Ettringite	Monosulfate	AFm-OH	Thaumasite	Calcite	Monoca
27	0.246575	25	1.92E-03	1.43E+01	1.29E+01	3.79E+01	0.00E+00	1.87E+01	1.46E+01	0.00E+00	0.00E+00	0.00E
28	0.246575	26	-2.96E-04	1.43E+01	1.29E+01	3.79E+01	0.00E+00	1.87E+01	1.46E+01	0.00E+00	0.00E+00	0.00E
29	0.246575	27	-2.49E-03	1.44E+01	1.29E+01	3.79E+01	0.00E+00	1.87E+01	1.46E+01	0.00E+00	0.00E+00	0.00E
30	0.246575	28	-4.99E-03	1.44E+01	1.29E+01	3.79E+01	0.00E+00	1.87E+01	1.46E+01	0.00E+00	0.00E+00	0.00E
31	0.246575	29	-7.81E-03	1.44E+01	1.29E+01	3.79E+01	0.00E+00	1.87E+01	1.46E+01	0.00E+00	0.00E+00	0.00E
32	0.246575	30	-4.18E-03	1.44E+01	1.30E+01	3.79E+01	0.00E+00	1.86E+01	1.46E+01	0.00E+00	0.00E+00	1.88E
33	0.246575	31	1.12E-03	1.45E+01	2.89E+01	8.68E+01	1.49E+01	0.00E+00	0.00E+00	0.00E+00	1.06E+01	1.45E
34	0.246575	32	1.26E-03	1.45E+01	2.91E+01	8.68E+01	1.39E+01	0.00E+00	0.00E+00	0.00E+00	1.05E+01	1.50E
35	0.246575	33	1.18E-03	1.46E+01	2.91E+01	8.68E+01	1.39E+01	0.00E+00	0.00E+00	0.00E+00	1.05E+01	1.50E
36	0.246575	34	1.11E-03	1.47E+01	2.91E+01	8.68E+01	1.38E+01	0.00E+00	0.00E+00	0.00E+00	1.05E+01	1.50E
37	0.246575	35	1.05E-03	1.48E+01	2.91E+01	8.68E+01	1.37E+01	0.00E+00	0.00E+00	0.00E+00	1.05E+01	1.51E
38	0.246575	36	9.79E-04	1.48E+01	2.92E+01	8.68E+01	1.36E+01	0.00E+00	0.00E+00	0.00E+00	1.05E+01	1.51E
39	0.246575	37	9.13E-04	1.49E+01	2.92E+01	8.68E+01	1.36E+01	0.00E+00	0.00E+00	0.00E+00	1.05E+01	1.52E
40	0.246575	38	8.48E-04	1.50E+01	2.92E+01	8.68E+01	1.35E+01	0.00E+00	0.00E+00	0.00E+00	1.05E+01	1.52E
41	0.246575	39	7.82E-04	1.51E+01	2.92E+01	8.68E+01	1.34E+01	0.00E+00	0.00E+00	0.00E+00	1.05E+01	1.52E
42	0.246575	40	7.17E-04	1.51E+01	2.92E+01	8.68E+01	1.33E+01	0.00E+00	0.00E+00	0.00E+00	1.05E+01	1.53E
43	0.246575	41	6.51E-04	1.52E+01	2.92E+01	8.67E+01	1.32E+01	0.00E+00	0.00E+00	0.00E+00	1.05E+01	1.53E
44	0.246575	42	5.86E-04	1.53E+01	2.92E+01	8.67E+01	1.32E+01	0.00E+00	0.00E+00	0.00E+00	1.05E+01	1.53E
45	0.246575	43	5.21E-04	1.54E+01	2.93E+01	8.67E+01	1.31E+01	0.00E+00	0.00E+00	0.00E+00	1.05E+01	1.54E
46	0.246575	44	4.56E-04	1.55E+01	2.93E+01	8.67E+01	1.30E+01	0.00E+00	0.00E+00	0.00E+00	1.05E+01	1.54E
47	0.246575	45	3.91E-04	1.55E+01	2.93E+01	8.67E+01	1.29E+01	0.00E+00	0.00E+00	0.00E+00	1.04E+01	1.54E
48	0.246575	46	3.26E-04	1.56E+01	2.93E+01	8.67E+01	1.28E+01	0.00E+00	0.00E+00	0.00E+00	1.04E+01	1.55E
49	0.246575	47	2.61E-04	1.57E+01	2.93E+01	8.67E+01	1.27E+01	0.00E+00	0.00E+00	0.00E+00	1.04E+01	1.55E
50	0.246575	48	1.96E-04	1.58E+01	2.93E+01	8.67E+01	1.27E+01	0.00E+00	0.00E+00	0.00E+00	1.04E+01	1.56E
51	0.246575	49	1.32E-04	1.58E+01	2.93E+01	8.67E+01	1.26E+01	0.00E+00	0.00E+00	0.00E+00	1.04E+01	1.56E
52	0.246575	50	6.72E-05	1.59E+01	2.94E+01	8.67E+01	1.25E+01	0.00E+00	0.00E+00	0.00E+00	1.04E+01	1.56E
53	0.246575	51	-2.86E-152	1.60E+01	2.94E+01	8.67E+01	1.24E+01	0.00E+00	0.00E+00	0.00E+00	1.04E+01	1.57E
54												

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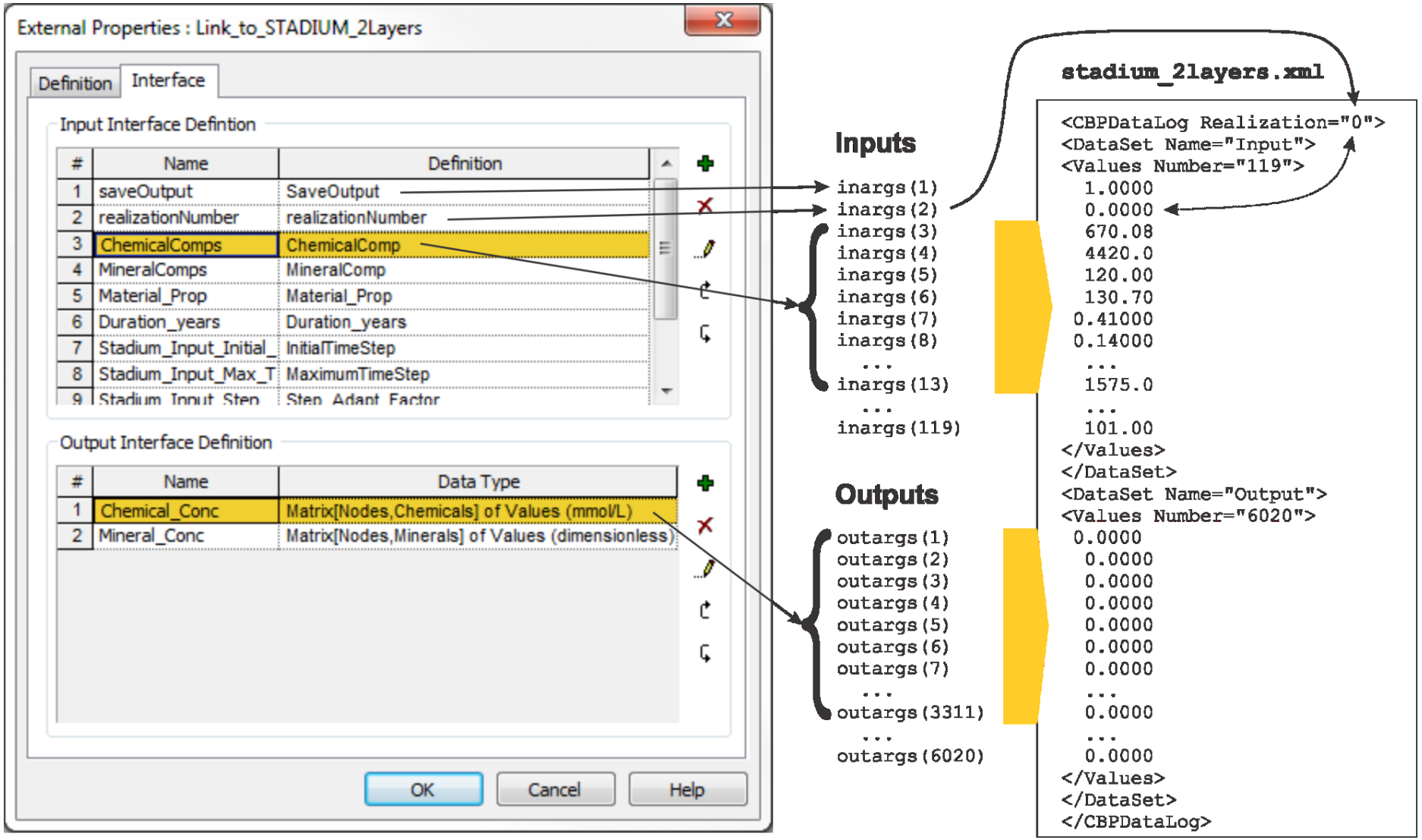
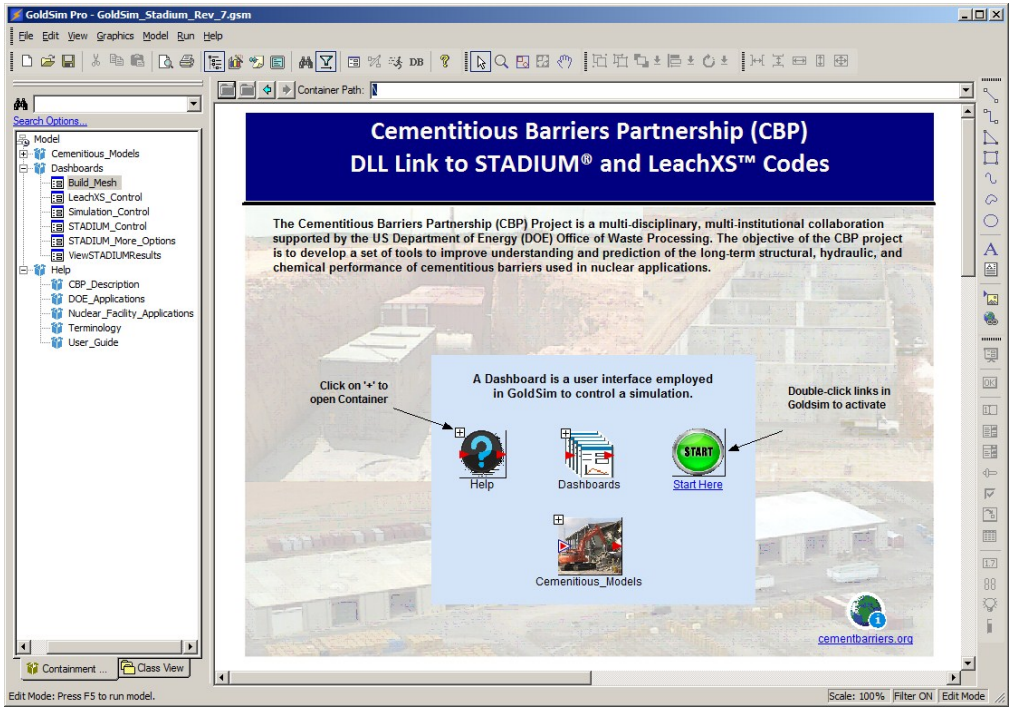
Summary of External Linking

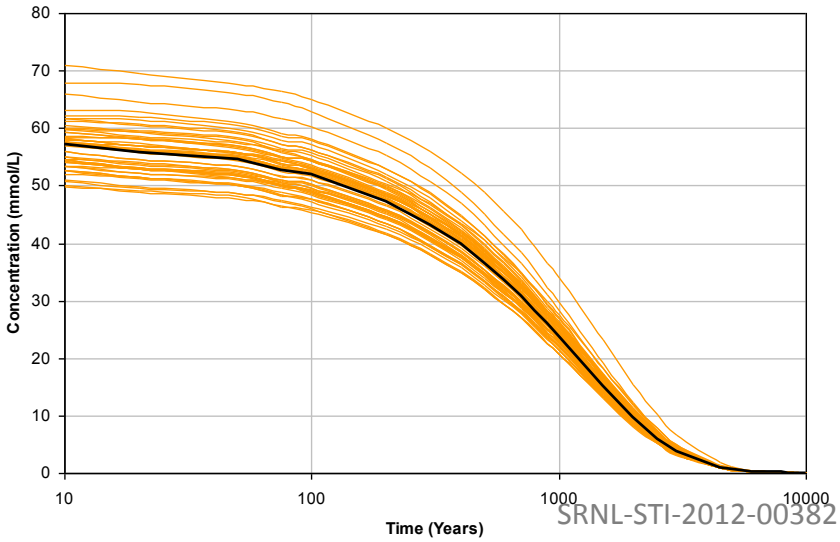


DLL Robustness Test

- **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



Segment 3 – GoldSim Dashboard

CBP Custom DLL

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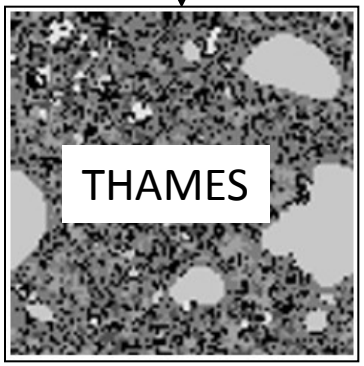

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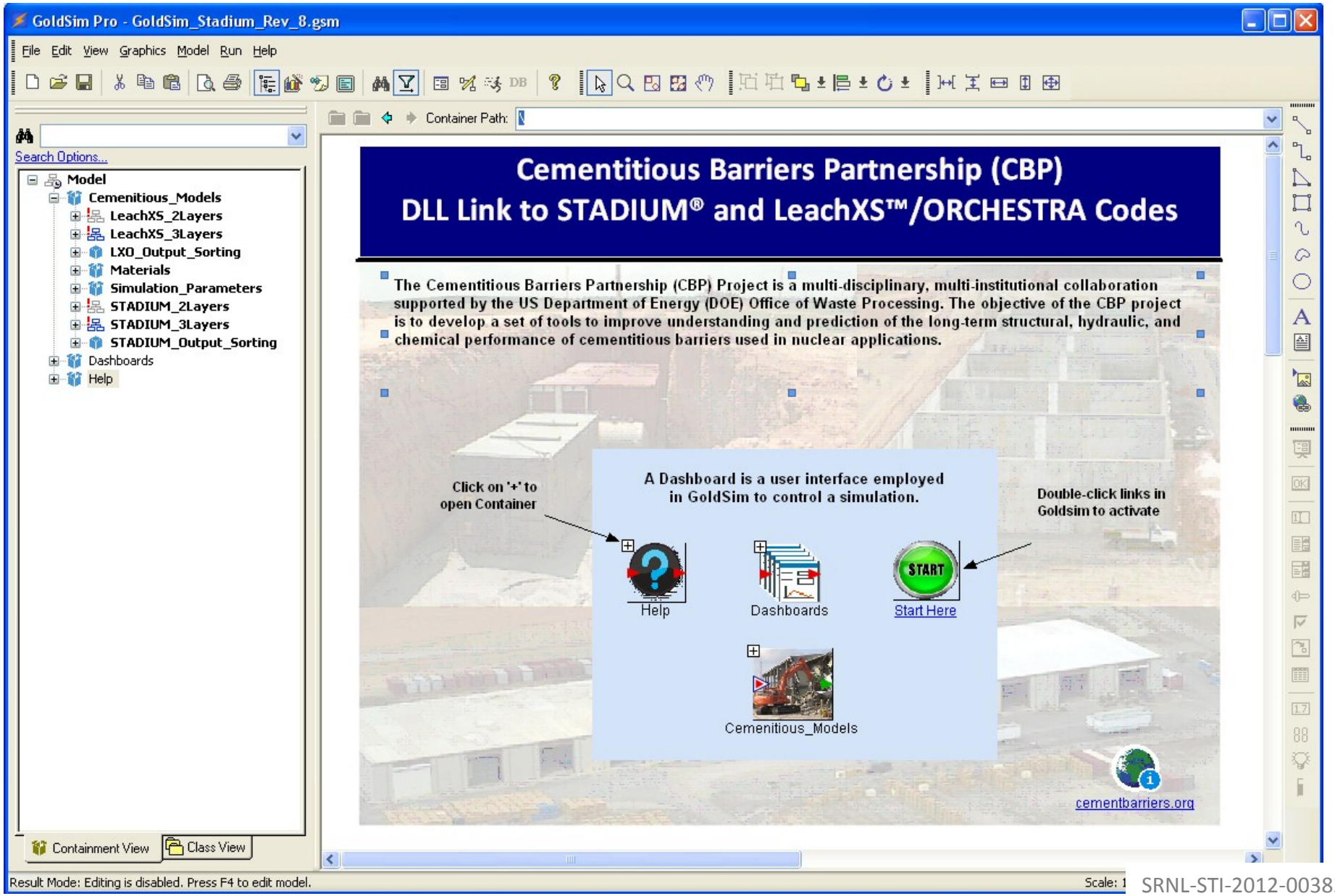
GoldSim Dashboard – Top Level



Segment 4 – Hands Ons Demo

CBP Custom DLL

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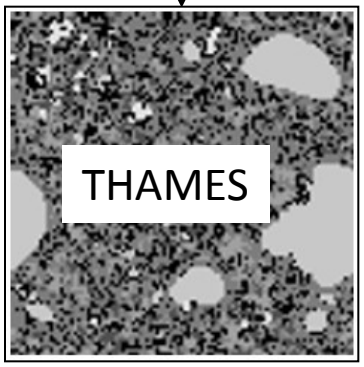

Tutorial #1

- **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**