xLPR

PROBABILISTIC FRACTURE MECHANICS CODE

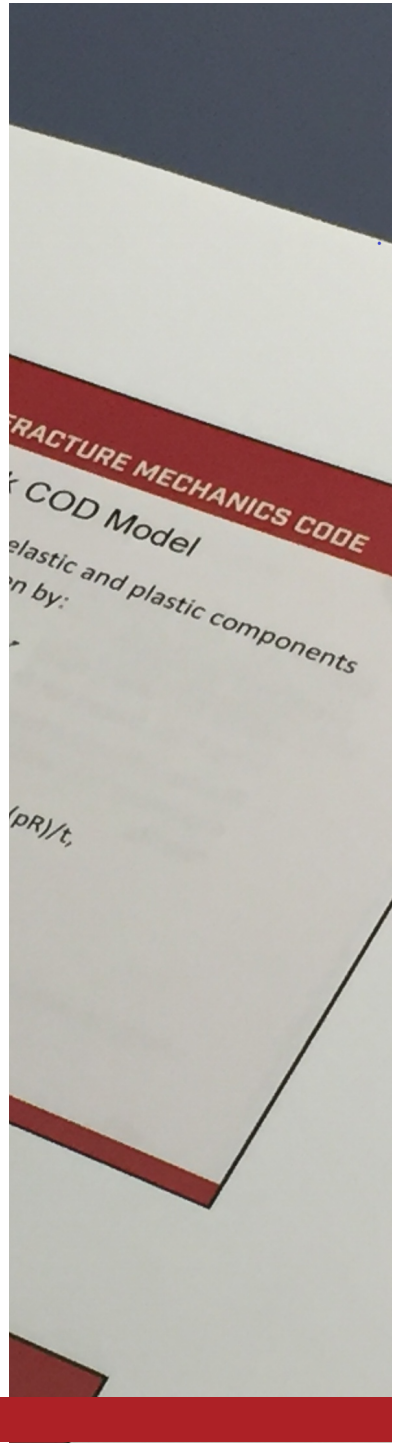
EVENTS

1. **Models Overview**
   June 3rd | 10-12 EDT

2. **Setting Up the Inputs**
   July 15th | 10-12 EDT

3. **Running the Simulation and Retrieving Results**
   July 29th | 10-12 EDT

4. **Advanced Methods**
   August 5th | 10-12 EDT



Seminar 4: Advanced Methods Agenda

Introduction and Opening Remarks

Inputs – Advanced Methods

Sampling – Advanced Methods

Results and Outputs – Advanced Methods

Improving Efficiency

Questions and Answers

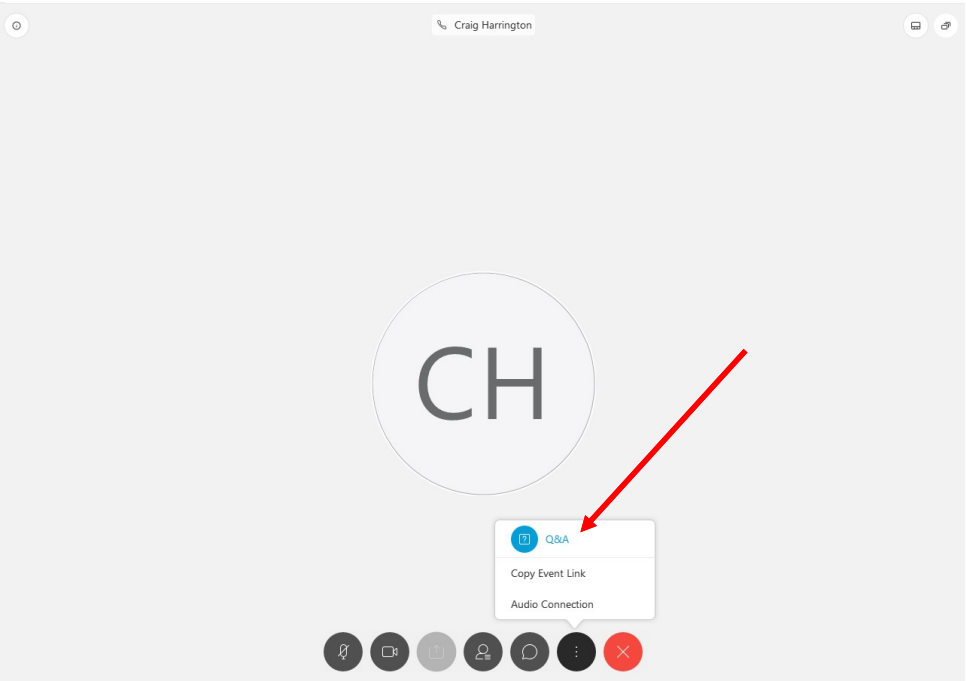
Closing Remarks

PRIOR WEBINARS

- Recordings of the Extremely Low Probability of Rupture (xLPR) webinars are, or will soon be, available on YouTube.com
  - Public Release
    https://www.youtube.com/watch?v=McVVFriy7wQ
  - Seminar 1: Models Overview
    https://www.youtube.com/watch?v=vsOOtdXYxoY&
  - Seminar 2: Setting up the Inputs
    https://youtu.be/nRk5VBAT8ww
  - Seminar 3: Running the Simulation and Retrieving Results
  - Seminar 4: Advanced Methods
- Search for "xLPR" on YouTube.com, or go to the U.S. Nuclear Regulatory Commission (NRC)'s YouTube Channel (https://www.youtube.com/user/NRCgov)

WEBEX Q+A

Webex Internet Browser



Webex Desktop Client

REFERENCES

- xLPR-GR-FW, “Computational Framework Development, Testing, and Analysis,” Version 1.0, January 2020.*
- xLPR-UM-2.1, “User Manual for xLPR Version 2.1,” Version 1.0, May 2020.

*To be released at a later date

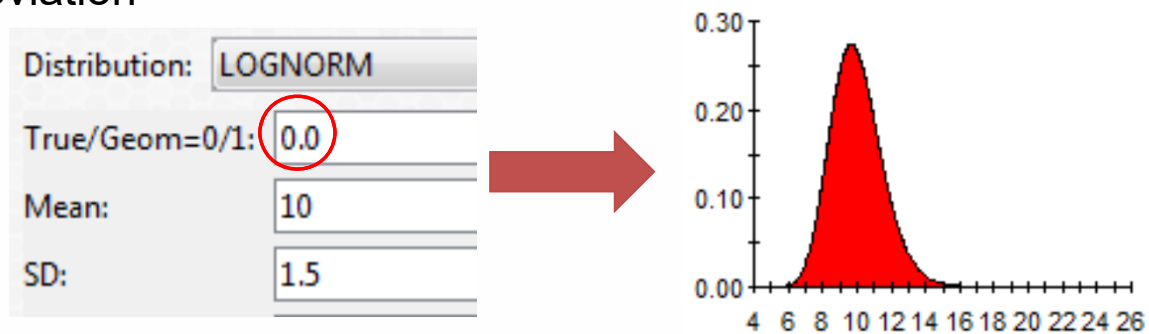
Inputs

Advanced Methods

ENTERING LOG-NORMAL DISTRIBUTIONS

- In xLPR Version 2.1 (V2.1), the log-normal distribution may be based on either the true (arithmetic) mean and standard deviation, or the geometric mean and geometric standard deviation
  - True (arithmetic) mean ($=e^{\mu+\frac{\sigma^2}{2}}$)
  - True (arithmetic) standard deviation ($=\sqrt{\left(e^{\sigma^2}-1\right)\left(e^{2\mu+\sigma^2}\right)}$)

μ (mean of log-transformed data) and σ (standard deviation of log-transformed data) are the traditional parameters of the log-normal distribution



  - Geometric mean ($=e^{\mu}$)
  - Geometric standard deviation ($= e^{\sigma}$)

CORRELATED VARIABLES

- Correlation is applied pairwise for select pairs of inputs
  - Applies to certain inputs on the Properties and material (i.e., Left Pipe, Right Pipe, Weld, and Mitigation) tabs of the Input Set
  - Applied as a rank correlation
- Strength of correlation is input by the user

CORRELATIONS

ID	name	ID	name	location	(rank) correlation
5012	c	5013	d	general	0
5101	Intercept, B0 (circ)	5102	Slope, B1 (circ)		0
5103	Intercept, B0 (axial)	5104	Slope, B1 (axial)	pre-mitigation	0

CORRELATIONS

ID	name	ID	name	location	(rank) correlation
2594	Peak-to-Valley ECP Ratio, P-1	2595	Charact Width of Peak vs ECP, c	PWSCC growth properties	0.714
2551	Weibull Vertical Intrcpt Error, EpsC	2552	General Weibull Slope, Beta	PWSCC initiation	0
2525	Strain Threshold, STH	2528	Co	Fatigue Initiation	1
2592	Comp-to-Comp Variab Factor, fcomp	2543	Multiplier proport. Const. A (DM1)		0

DETERMINING IF INPUTS ARE OUTSIDE RANGE OF APPLICABILITY (1/2)

- Automated checks are included within the Input Set
  - Allowable input range is shown in left-most column
  - Values out of allowable range are highlighted in red
- Sim Editor performs the same allowable input range checks as the input set
  - Demonstrated in the “Setting Up the

Range	Global ID	
	OPTIONS / CONSTANTS	
	General Options (0001	
(0.08333, nomax)	0001	Plant (
Z[2, 30]	0002	Numb
Z[0,3]	0003	Crack (
	Looping / Sampling Op	
Z[1, 1e7]	0101	Sampl
	0102	Rando
Z[0,1]	0103	Imp Sa
Z[0,0]	0104	Use Ac
Z[0,1]	0105	Use Di
Z(nomin, nomax)	0106	Numb
Z[2, 1e8)	0107	Sampl
	0108	Rando
Z[0,1]	0109	Imp Sa
Z[0,0]	0110	Use Ac
Z[0,1]	0111	Use Di
Z(nomin, nomax)	0112	Numb

Range	Global ID	Property Name	Unit	Data Source	Importance Sampling	Region of importance	Deterministic Value
	General Properties (1000)						
		General (1001-1099)					
(0, 60]	1001	Effective Full Power Years (EFPY)	yr	Constant	no	0.5	70

DETERMINING IF INPUTS ARE OUTSIDE RANGE OF APPLICABILITY (2/2)

- xLPR-UM-2.1, Appendix E, includes module-specific input limits
  - Physical limits / range of validity

Table E.6-1: CGR Subroutine Arguments List ([E.6-1], [E.6-9]) (cont'd)

#	Description	Symbol Used in this SRD	Required Units	Range of Validity [1]	Data Type	Sample Frequency
Fatigue CGR Model Inputs (required only for Mechanism Type 1 or 3)						
General Fatigue CGR Model Inputs (required for all Material Groups)						
16	Number of transient components during time step	NTS	-	1 - 20 (inclusive)	integer	-
17	Duration of integration time step	Δt	EFPY	> 0	real	-
18	Number of cycles array	N_{cyc}	-	≥ 0	real array	-
19	Minimum stress intensity factor array	K_{min}	MPa√m	$\leq K_{max,i}$	real array	-
20	Maximum stress intensity factor array	K_{max}	MPa√m	$\geq K_{min,i}$	real array	-
21	Rise time array	τ_R	s	>0	real array	-
22	Threshold stress intensity factor range scaling factor	C_{Kth}	-	≥ 0	real	per heat

- Module subgroup reports* include additional details on range of validation for each module

Table 5-2. Range of Applicability for Coalescence Inputs

Input Description	Range of Applicability	Technical Basis
Number of cracks represented	0-200	Engineering judgment; any number of cracks can be evaluated by the coalescence module, provided other configuration inputs satisfy those ranges described below.
Crack Type array	All crack types	Two surface cracks as well as two idealized TW cracks are explicitly validated in the coalescence MVR. Engineering judgment applied to extend validity to all crack type combinations.

*To be released at a later date

TOOLS FOR COMPARING INPUT SETS

- Microsoft Spreadsheet Compare
  https://support.microsoft.com/en-us/office/compare-two-versions-of-a-workbook-by-using-spreadsheet-compare-0e1627fd-ce14-4c33-9ab1-8ea82c6a5a7e
  - Included with some Microsoft Office licenses
  - Application is separate from Excel
- xlCompare
  https://www.xlcompare.com/product.asp
  - 30-day free trial, then need to register
- Conditional Formatting or Boolean logic in Excel
- Many other options

Sampling

Advanced Methods

SAMPLING

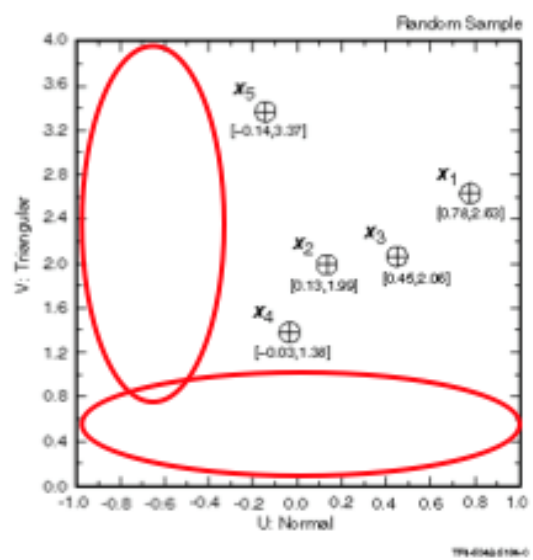
- There are many ways to sample inputs in xLPR V2.1 for uncertainty propagation:
  - Simple Random Sampling (SRS)
  - Latin Hypercube Sampling (LHS)
  - Importance Sampling
    - Can be used with LHS or SRS
  - Discrete Probability Distribution (DPD)
    - Can be used with LHS or SRS

CHOOSING A SAMPLING SCHEME

- **SRS** is simplest – easy to analyze, combine results across runs, and calculate sampling uncertainty
- **LHS** is an improvement on simple random sampling without increasing the computation time or complexity of post-processing
- **Importance sampling** helps estimate very small probabilities in reasonable computing times
  - Chosen after preliminary sensitivity analyses have been conducted
- **DPD** results in samples that are always uniformly distributed over the sample space, but take on fewer unique values
  - Can be useful when simulation sample size is limited. However,

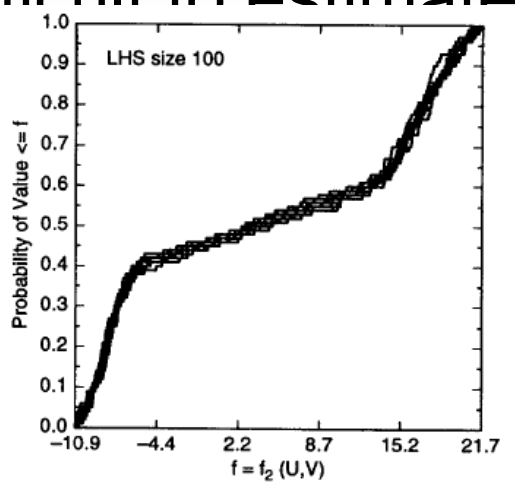
SIMPLE RANDOM SAMPLING

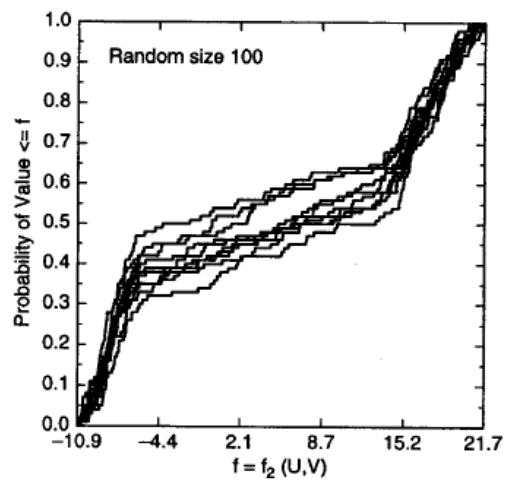
- The simplest Monte Carlo sampling scheme is SRS
  - All inputs are randomly sampled from their input distributions
  - **Pros:** Easy to implement, easy to explain, and easy to analyze data
  - **Cons:** Sufficiently large samples may not be possible to achieve reasonably low sampling uncertainty



LATIN HYPERCUBE SAMPLING

- "Force" samples to be spread across domain of the input distributions using dense stratification across range of each variable
- **Pros:** Lower sampling uncertainty than SRS, easy to analyze
- **Cons:** Difficult to estimate sampling uncertainty





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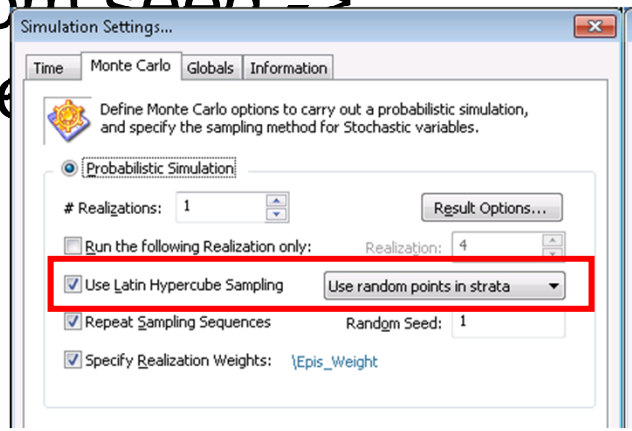
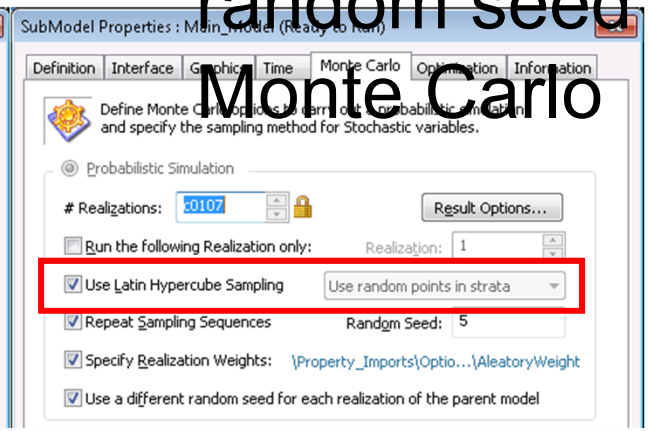
SWITCHING BETWEEN SIMPLE RANDOM AND LATIN HYPERCUBE SAMPLING

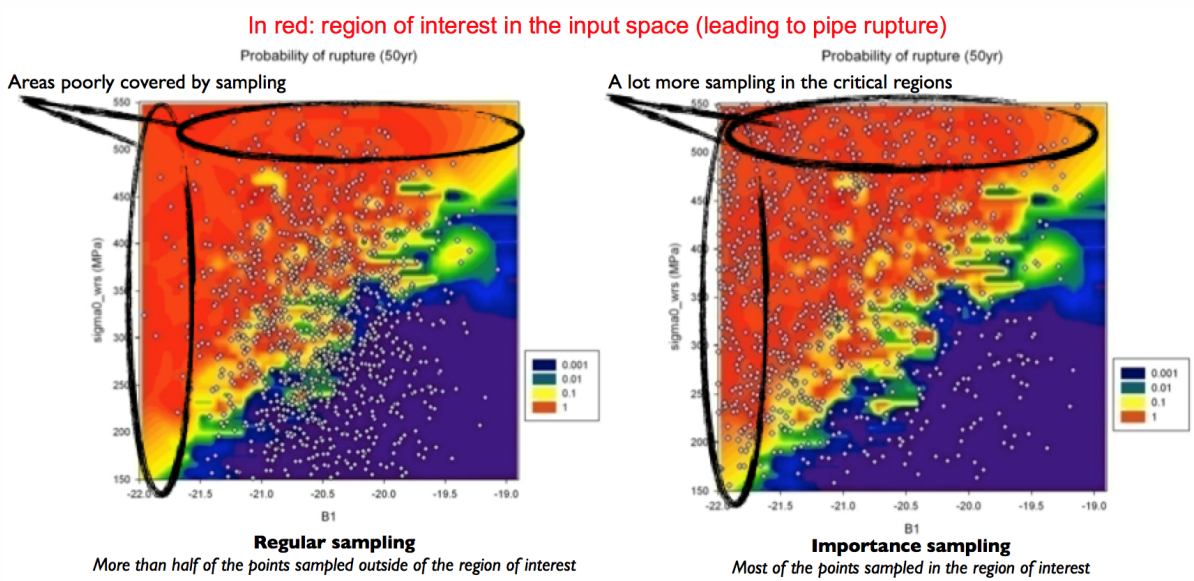
- Epistemic (outer) loop
  - Run -> Simulation Settings -> Monte Carlo
  - Set up epistemic sample size and random seed -> Monte
- Aleatory (inner) loop
  - From model root, right-click "Main_Model" –Monte Carlo
  - Set up aleatory random seed -> Monte Carlo





IMPORTANCE SAMPLING (1/3)

- Over-sample ‘important’ parts of the input space
- **Pros:** Better estimation of rare event probabilities
- **Cons:** Harder to implement, more difficult to analyze data, poor implementation can increase sampling uncertainty



IMPORTANCE SAMPLING (2/3)

- Applying importance sampling in xLPR V2.1
  - User has to select whether to apply importance sampling on each variable
  - Importance sampling concentrates half of the samples taken for a given input within a region about a user-selected quantile
    - Width of this region depends on the number of inputs selected for importance sampling

IMPORTANCE SAMPLING (2/3)

Global ID	Brief Description	Unit	Value	Input Description
OPTIONS / CONSTANTS (0000)				
General Options (0001-0099)				
0001	Plant Operation Time	yr	60	Unit must be "yr" or "mon" for input range validation
0002	Number of Subunits	-	19	
0003	Crack Orientation	-	3	0: none, 1: Circumferential, 2: Axial, 3: Circumferential + Axial
Looping / Sampling Options (0101-0199)				
0101	Sample Size (Epistemic)	-	1	Number of outer loops in the simulation (NEEDS TO BE SET IN GOLDSIM FROM GLOBAL SETTINGS DASHBOARD)
0102	Random Seed (Epistemic)		1	Random Seed for outer loop (NEEDS TO BE SET IN GOLDSIM FROM GLOBAL SETTINGS DASHBOARD)
0103	Imp Sampling (Epistemic)	-	1	Imp sampling setting for outer loop 0: None, 1: Internal
0104	Use Adaptive (Epistemic)	-	0	0 = no, 1 = yes (not implemented yet)
0105	Use Discretization (Epistemic)	-	0	0 = no, 1 = yes
0106	Number of Strata (Epistemic)	-	1	Strata for discretization (integer >1 and < epistemic sample size (0101))
0107	Sample Size (Aleatory)	-	20	Number of inner loops in the simulation
0108	Random Seed (Aleatory)	-	3	Random Seed for inner loop (NEEDS TO BE SET IN GOLDSIM FROM GLOBAL SETTINGS DASHBOARD)
0109	Imp Sampling (Aleatory)	-	0	Imp sampling setting for inner loop 0: None, 1: Internal
0110	Use Adaptive (Aleatory)	-	0	0 = no, 1 = yes (not implemented yet)
0111	Use Discretization (Aleatory)	-	0	0= no , 1 = yes
0112	Number of Strata (Aleatory)	-	10	Strata for discretization (integer >1 and < aleatory sample size (0107))

Global ID	Property Name	Unit	Data Source	Importance Sampling	Region of importance
2542	Proportionality Const, A (DM 1)	yr-1-MPa-1	Aleatory	no	0.5
2543	Multiplier proport. Const. A (DM1)		Epistemic	yes	0.995

DISCRETE PROBABILITY DISTRIBUTION

- Discretizes the domain in as many equiprobable strata (or levels) as selected by the user
- After partitioning the sample space, DPD uses the conditional mean of the stratum
  - If 5 levels are defined, any quantile value in [0, 0.2] will be set to distribution mean over [0, 0.2], but not necessarily q=0.1
  - Similarly for subsequent quantiles [0.2,0.4], [0.4,0.6], …
- When DPD is selected, discretization is applied to all variables within the loop (epistemic (outer) or aleatory (inner))

Global ID	Brief Description	Unit	Value	Input Description
OPTIONS / CONSTANTS (0000)				
General Options (0001-0099)				
0001	Plant Operation Time	yr	60	Unit must be "yr" or "mon" for input range validation
0002	Number of Subunits	-	19	
0003	Crack Orientation	-	3	0: none, 1: Circumferential, 2: Axial, 3: Circumferential + Axial
Looping / Sampling Options (0101-0199)				
0101	Sample Size (Epistemic)	-	1	Number of outer loops in the simulation (NEEDS TO BE SET IN GOLDSIM FROM GLOBAL SETTINGS DASHBOARD)
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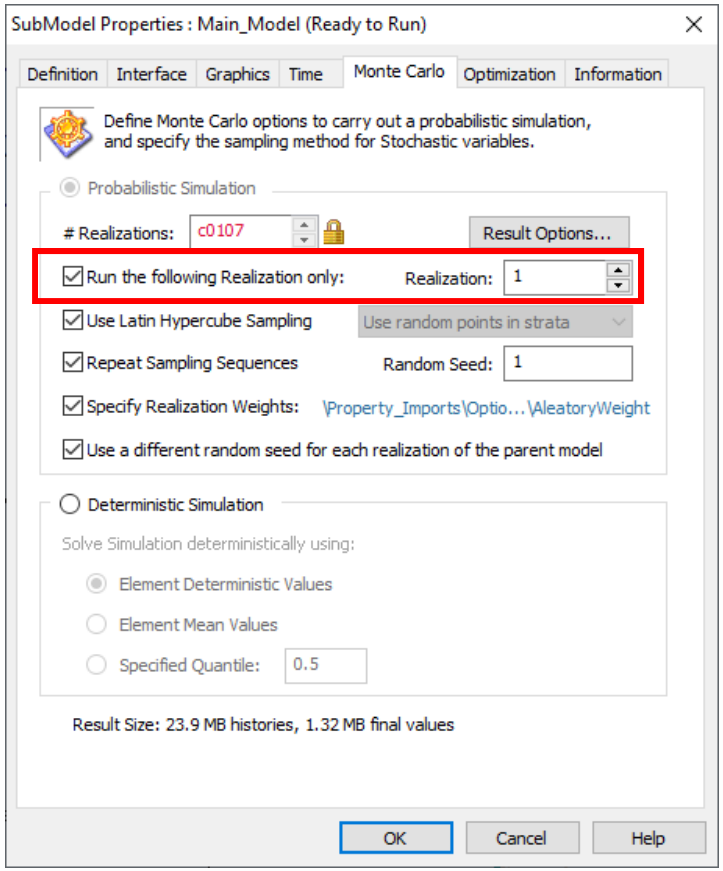
0105	Use Discretization (Epistemic)	-	0	0 = no, 1 = yes
0106	Number of Strata (Epistemic)	-	1	Strata for discretization (integer >1 and < epistemic sample size (0101))
0107	Sample Size (Aleatory)		20	Number of inner loops in the simulation
0108	Random Seed (Aleatory)	-	5	Random Seed for inner loop (NEEDS TO BE SET IN GOLDSIM FROM GLOBAL SETTINGS DASHBOARD)
0109	Imp Sampling (Aleatory)	-	0	Imp sampling setting for inner loop 0: None, 1: Internal
0110	Use Adaptive (Aleatory)		0	0 = no, 1 = yes (not implemented yet)
0111	Use Discretization (Aleatory)	-	0	0= no , 1 = yes
0112	Number of Strata (Aleatory)	-	10	Strata for discretization (integer >1 and < aleatory sample size (0107))

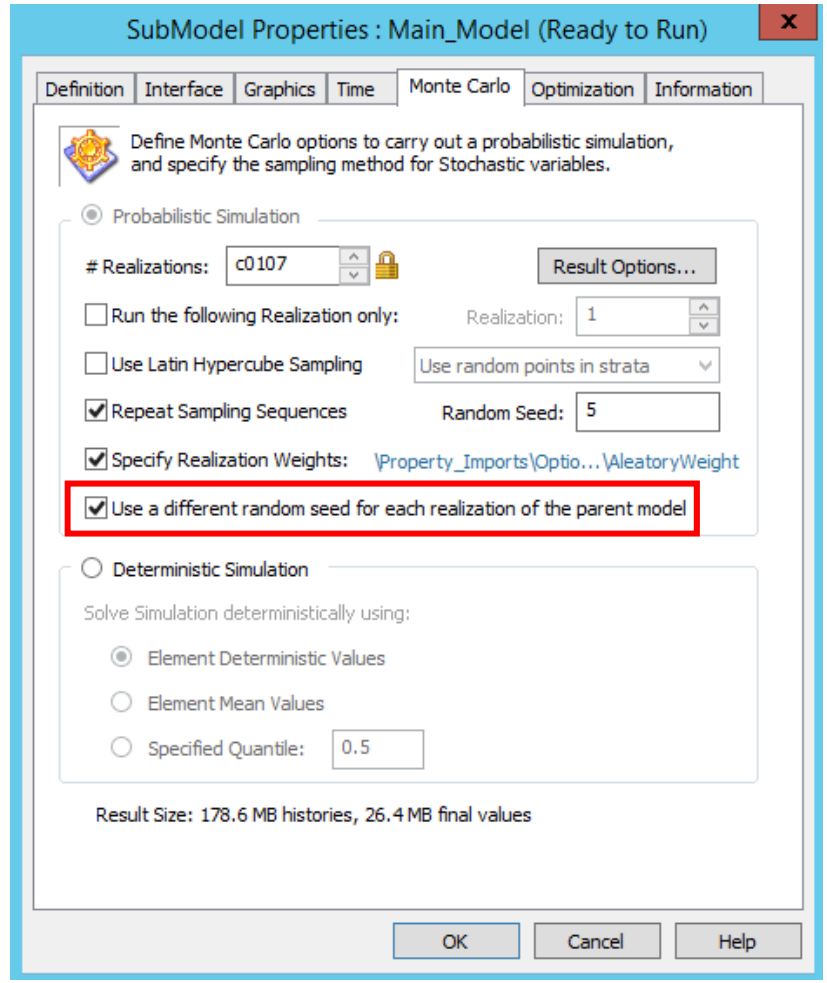
SINGLE-LOOP SIMULATIONS (1/2)

- To sample all variables in the epistemic (outer) loop
  - Set all sampled inputs to epistemic in the Input Set
  - The submodel requires at least two realizations within the aleatory (inner) loop
    - Can adjust settings to run only one realization
  - Run only one realization in the aleatory (inner) loop
    - "Set up aleatory random seed" -> Monte Carlo
- Epistemic (outer) loop allows for larger sample sizes using LHS



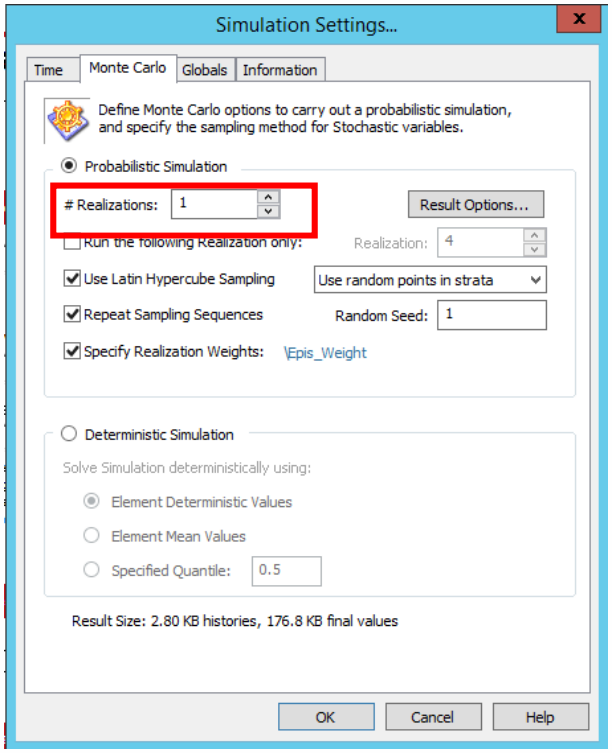
SINGLE-LOOP SIMULATIONS (2/2)

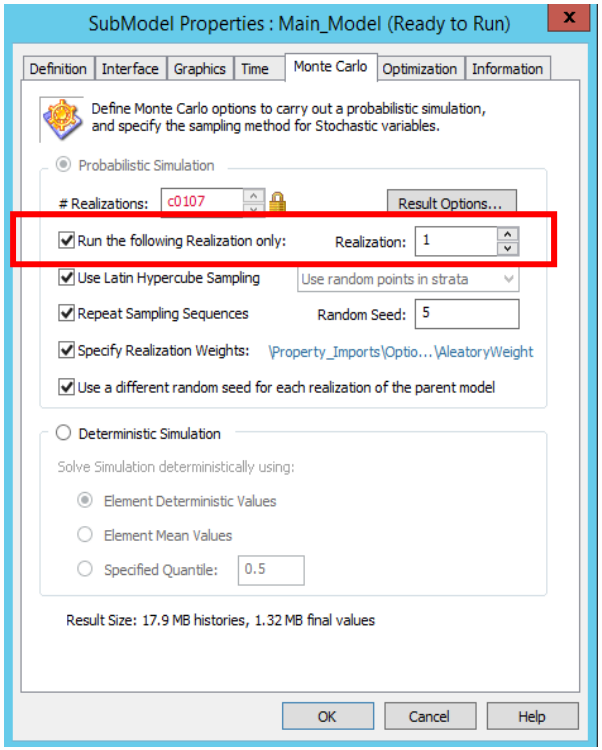
- To sample all variables in the aleatory (inner) loop
  - <u>Set all sampled inputs to aleatory</u> in the Input Set
  - Use different random seed for new instance of parent model
    - "Set up aleatory random seed"
      -> Monte Carlo
- Aleatory (inner) loop allows for larger sample sizes using SRS



DETEMINISTIC SINGLE-REALIZATION SIMULATION

- For a deterministic, single-realization run, run only one realization in both the epistemic (outer) and aleatory (inner) loops
- Set all inputs to constant





Demo – Simulation Settings

Questions?

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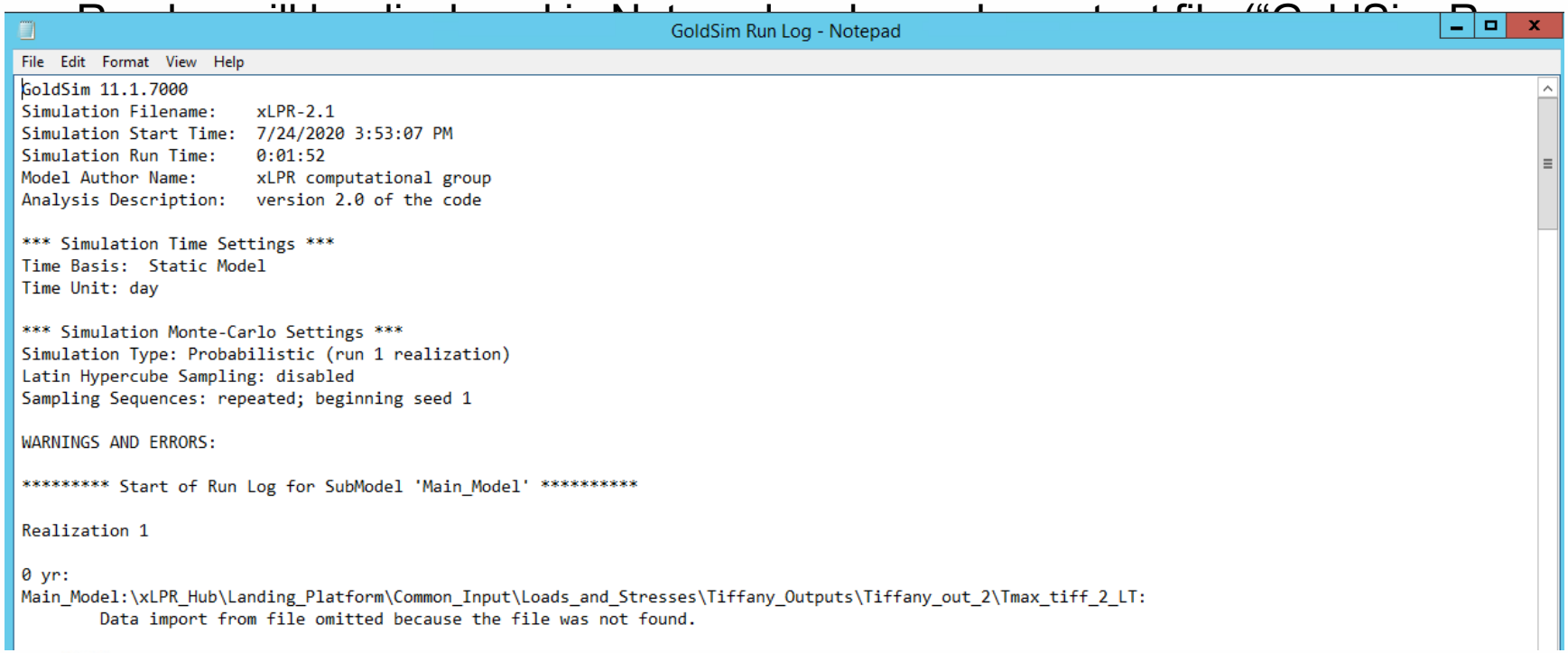
for Additional Information

Results and Outputs

Advanced Methods

INTERPRETING THE RUN LOG

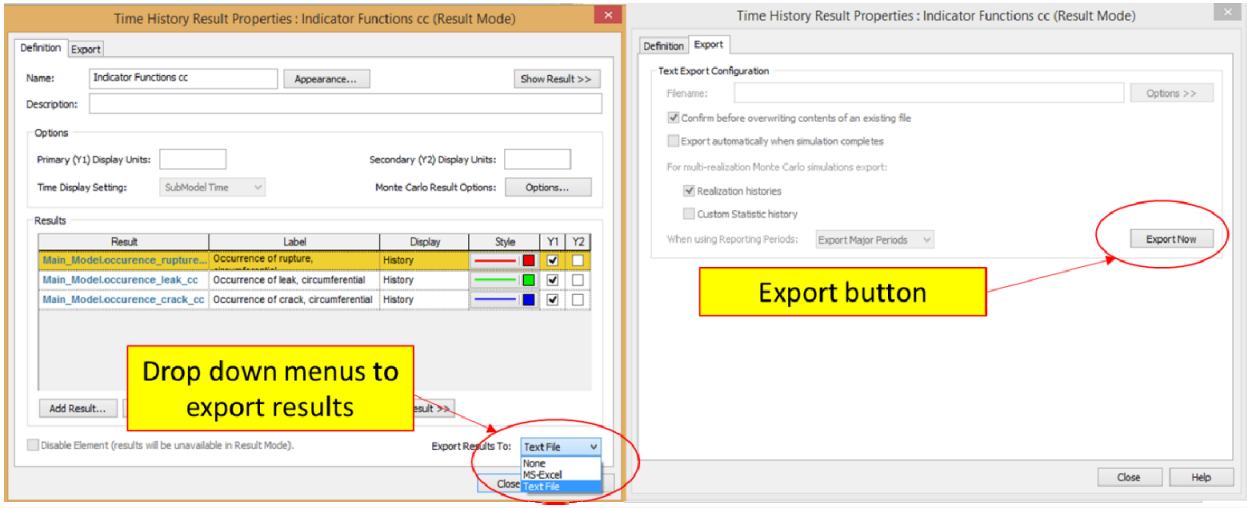
- The GoldSim environment creates a run log
  - User should inspect the run log for warnings and error messages
  - The Framework writes a message to the run log every time a module has an error
- To open the run log:
  - In GoldSim, click Run -> “View Run Log”




```
GoldSim 11.1.7000
Simulation Filename:    xLPR-2.1
Simulation Start Time:  7/24/2020 3:53:07 PM
Simulation Run Time:    0:01:52
Model Author Name:      xLPR computational group
Analysis Description:   version 2.0 of the code

*** Simulation Time Settings ***
Time Basis:  Static Model
Time Unit: day

*** Simulation Monte-Carlo Settings ***
Simulation Type: Probabilistic (run 1 realization)
Latin Hypercube Sampling: disabled
Sampling Sequences: repeated; beginning seed 1

WARNINGS AND ERRORS:

********* Start of Run Log for SubModel 'Main_Model' **********

Realization 1

0 yr:
Main_Model:\xLPR_Hub\Landing_Platform\Common_Input\Loads_and_Stresses\Tiffany_Outputs\Tiffany_out_2\Tmax_tiff_2_LT:
        Data import from file omitted because the file was not found.
```

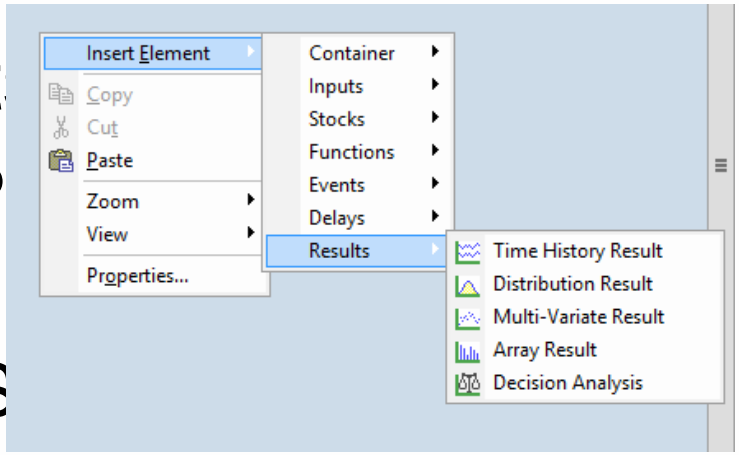
EXTRACTING RESULTS FROM GOLDSIM

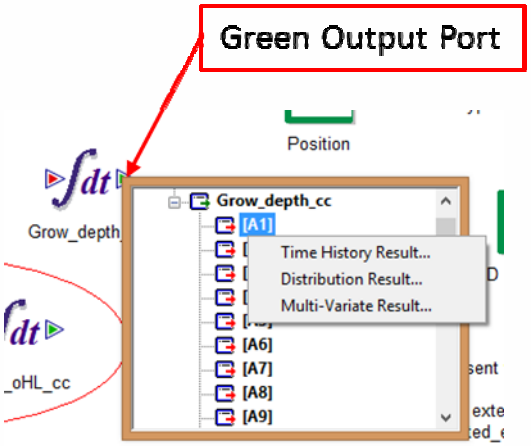
- By default, xLPR V2.1 does not export results to external files
- The results from Time History result elements (located in the model root) can be exported to a specific Excel or text file
  - Use the “Export Results To” pull down menu of the result elements



ADDING INTERMEDIATE OUTPUT VARIABLES (1/2)

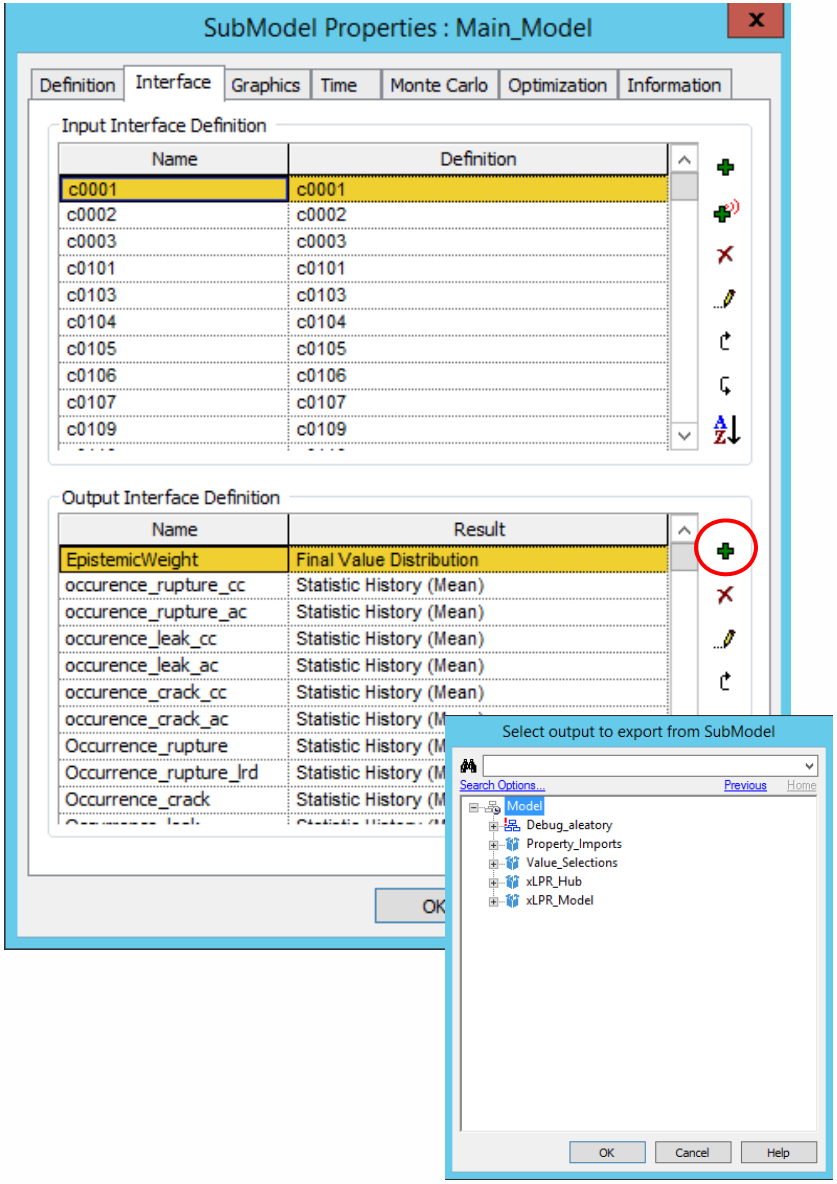
- Creating new result element
  - Only possible with GoldSim P
  - Can view results of existing GoldSim elements with GoldS Player
  - Frequently used result elements include:
    - Time History Result
    - Distribution Result
    - Array result





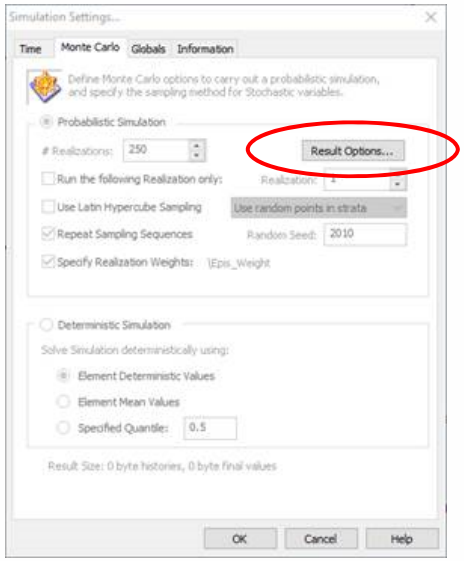
ADDING INTERMEDIATE OUTPUT VARIABLES (2/2)

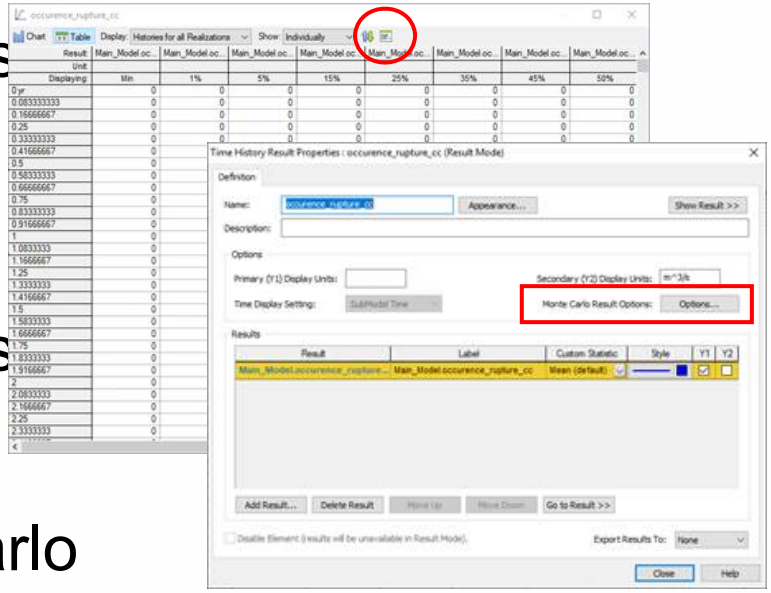
- Getting results out of the main model
  - Only possible with GoldSim Pro
- The submodel has an interface to the model root (or epistemic (outer) loop)
  - Right-click “Main_Model” -> Properties -> Interface
  - Additional output variables are added using green plus-sign



SCREENING RESULTS (1/3)

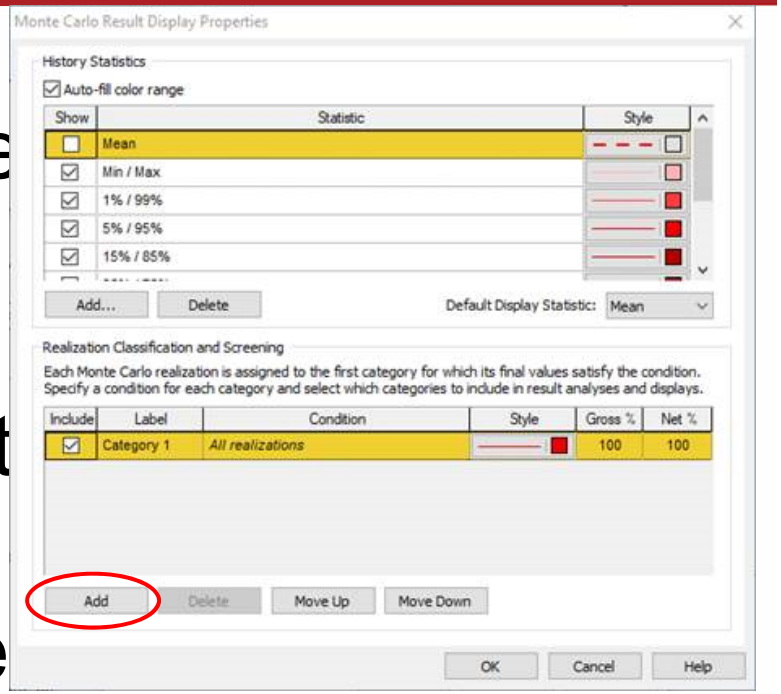
- When running a large sample size, it may be difficult to extract all of the results
- While GoldSim only displays the first 1,000 values, a screening feature allows other values to be seen
  - See page 533 of the GoldSim User Manual, Volume 2, Version 11.1
- Two ways to access screening settings:
  - Go to Run -> Simulation Settings -> Monte Carlo -> Result Options
  - In result element, click on “Edit Properties” icon, then “Monte Carlo Result Options”

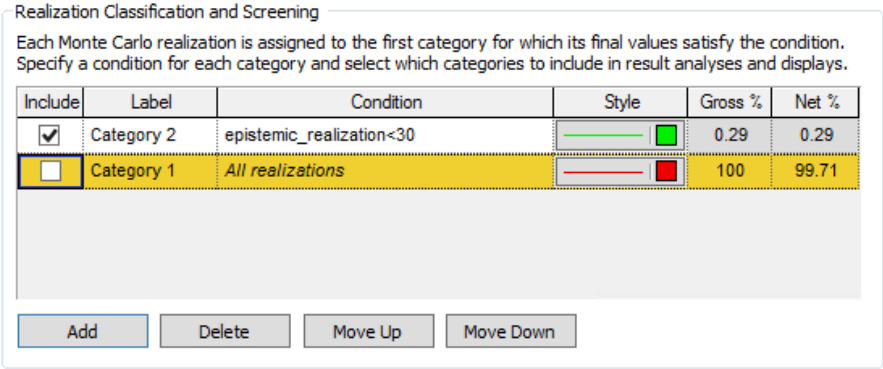




SCREENING RESULTS (2/3)

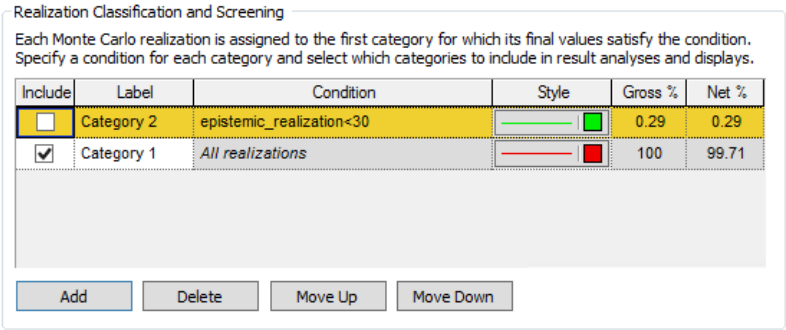
- Screening is controlled unde
  "Realization Classification
  and Screening"
- By default, screening is set t
  "All realizations"
- Additional conditions can be
  added and applied for
  screening
  - Click on "Add"
  - Enter a new condition
  - Uncheck Category 1 ("All
    realizations")

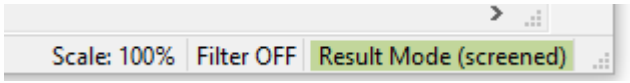


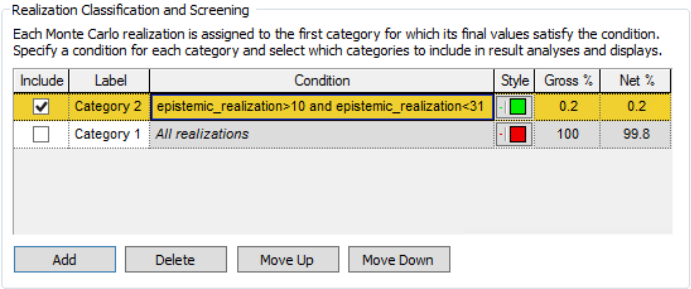


SCREENING RESULTS (3/3)

- It is important to note:
  - Conditions can also be used to screen out results (e.g., check Category 1 and uncheck Category 2)
  - When screening is applied, the status of the file is changed to “Result Mode (screened)”
  - Unchecking all categories may lead to GoldSim crashing. It is recommended to always save once a calculation is performed, before any screening.
  - Multiple conditions can be applied, such as: “epistemic_realization>10 and epistemic_realization<31”

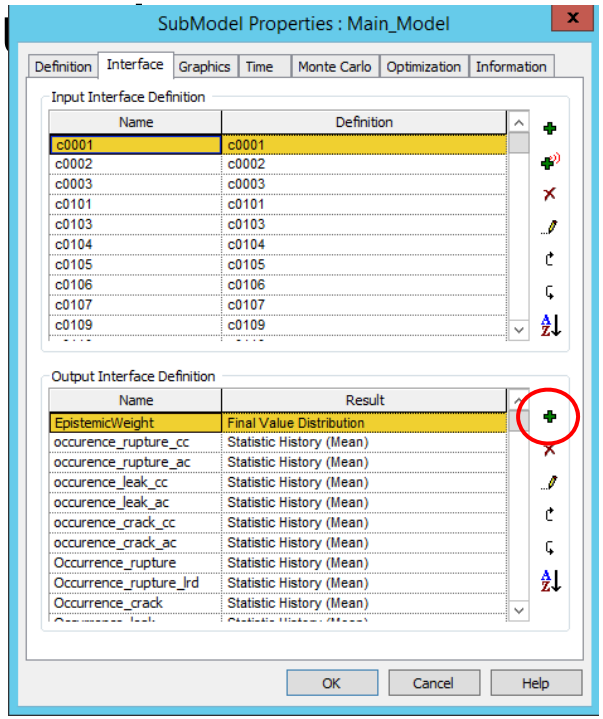


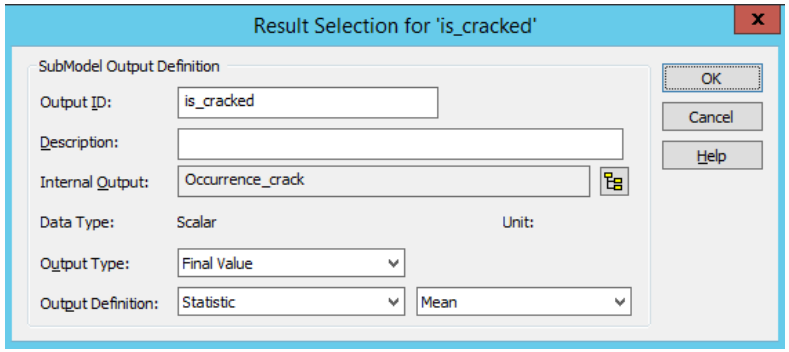




SCREENING RESULTS EXAMPLE – REALIZATIONS WITH INITIATED CRACKS (1/2)

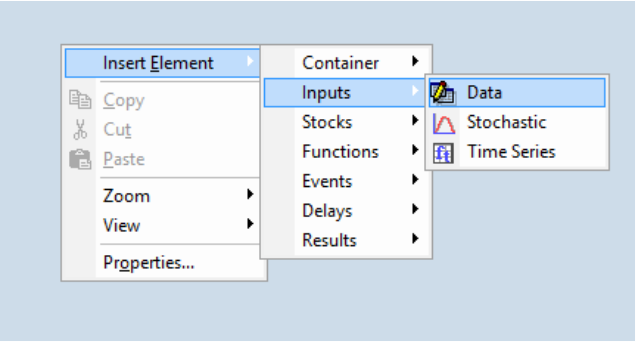
- Additional output “is_cracked” is added to Main Model interface
  - Right-click “Main_Model” -> Properties -> Interface
  - Additional output variables are added using green pl

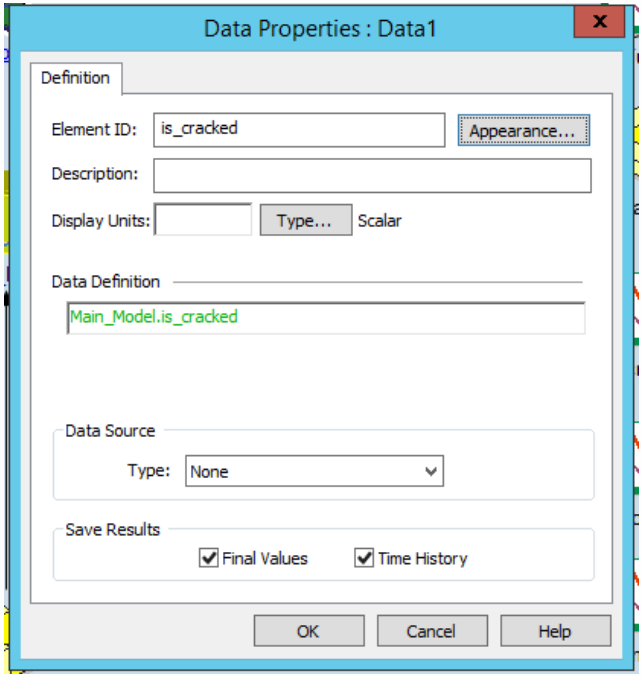


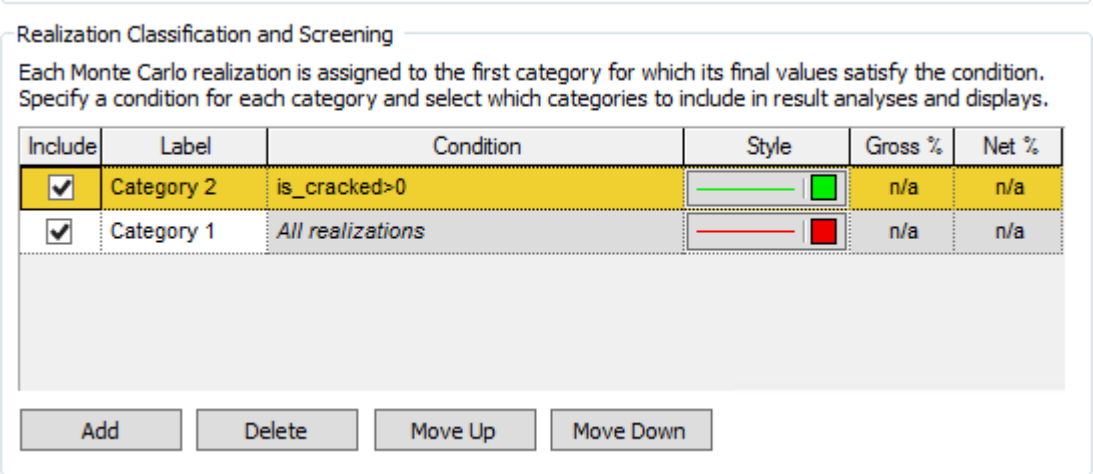


SCREENING RESULTS EXAMPLE – REALIZATIONS WITH INITIATED CRACKS (2/2)

- Insert a Data element that links to “Main_Model.is_cracked”
  - Right click -> Insert Element -> Inputs -> Data
- Can then apply screening with the newly added output, is_cracked







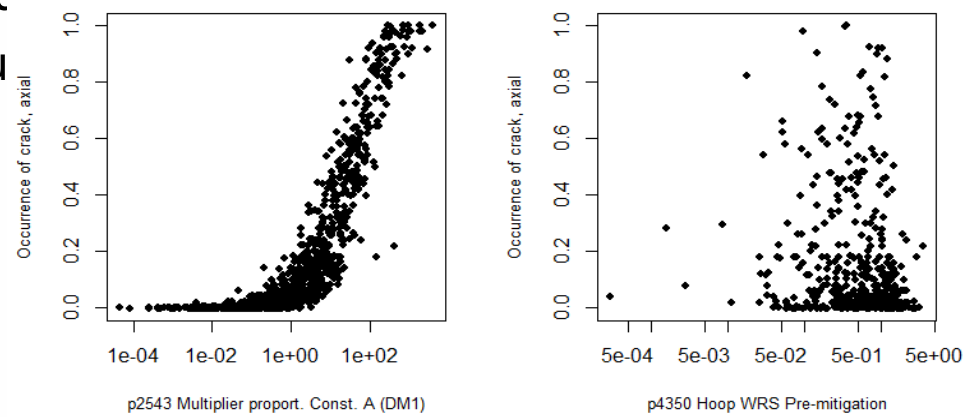
POST-PROCESSING

- After extracting results from GoldSim, can perform post-processing to calculate outputs not directly calculated in xLPR V2.1
  - Examples
    - Leak-before-break ratio
      - Ratio between critical crack size and crack size at detectable leakage
    - Time from detectable leakage to rupture
  - Use tool of choice
    - Excel, R, Python, etc.

SENSITIVITY ANALYSIS

- Sensitivity analysis is used to:
  - Understand the relationship between model inputs and outputs
  - Identify the inputs that have the most significant impact on the results of the model
- Knowledge of the most important inputs can be used to:
  - Target inputs where more information could be collected to decrease uncertainty
  - Identify inputs for importance sampling to increase precision in estimating rare probabilities
- Many statistical methodologies exist to determine which sampled inputs have the greatest influence on simulation outputs of interest
  - Need to also save all sampled inpu

Example: In xLPR V2.1, the Direct Model 1 (DM1) multiplier is highly correlated with the probability of crack, while the hoop weld residual stress (WRS) pre-mitigation is not highly correlated with the probability of crack



Demo – Screening Results

Questions?

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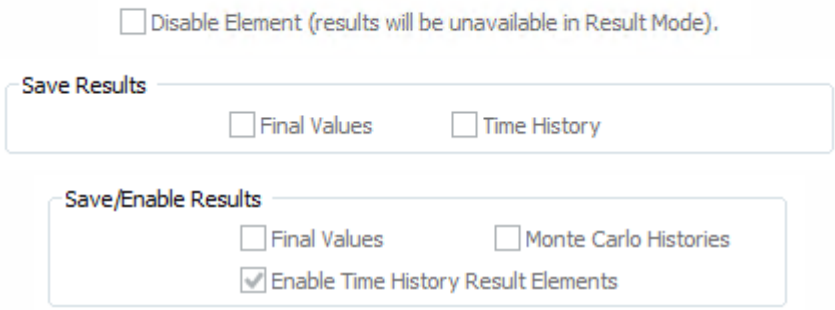
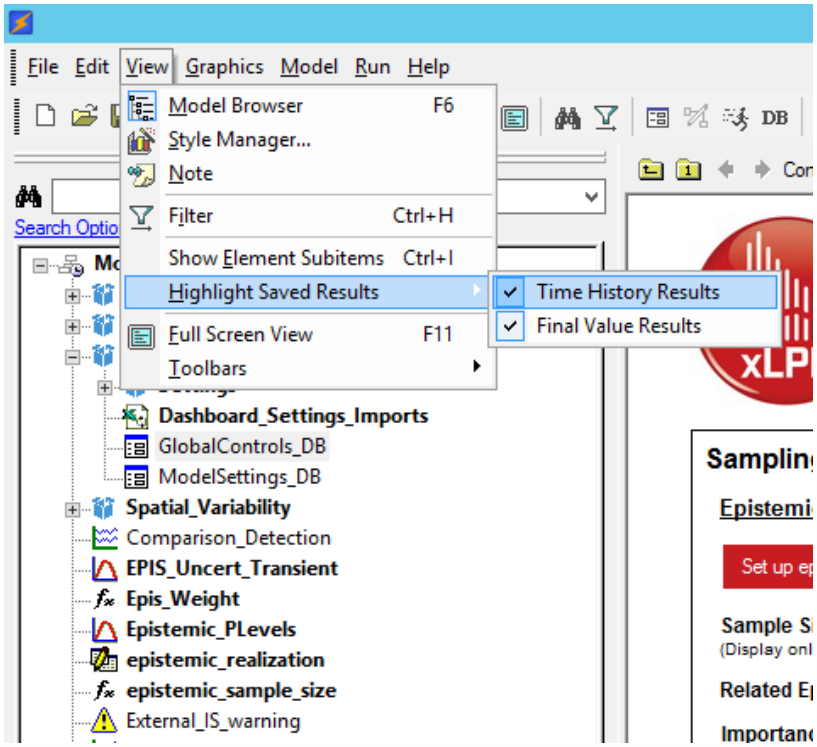
for Additional Information

Improving Efficiency

DISABLING OUTPUTS (1/2)

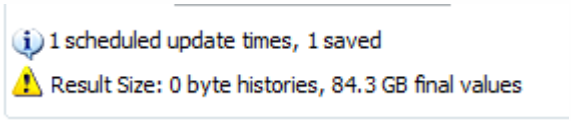
- Many of the GoldSim elements have options to save time history or final values
  - Can disable result elements in GoldSim Player
  - Can edit settings using GoldSim Pro
- When highlighting saved results, GoldSim shows saved variable names in bold text
- Simulation settings and "Main_Mod
  Result Size: 178.6 MB histories, 26.4 MB final values
  show saved result size

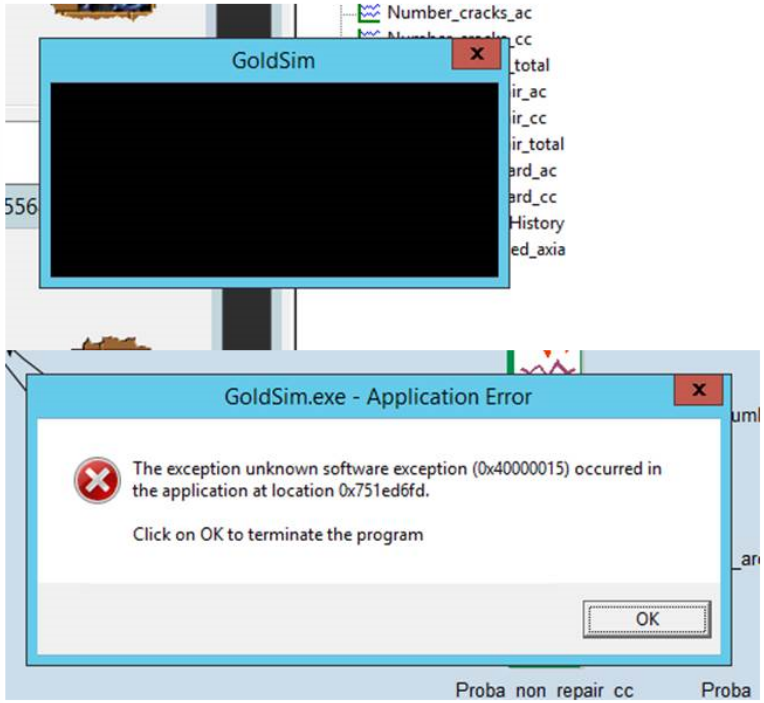




DISABLING OUTPUTS (2/2)

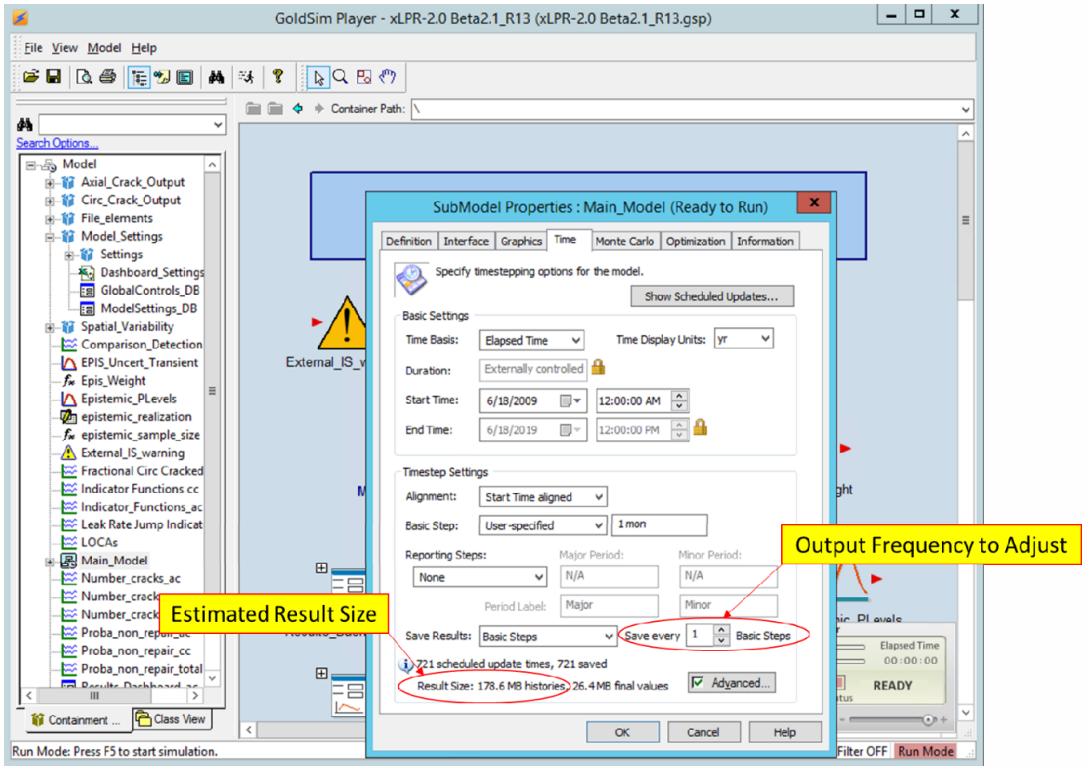
- Several errors may occur if GoldSim memory limits are reached
- Errors include, but are not limited to:
  - Warning in “Simulation Settings”
  - Errors occur (as shown on right)
  - GoldSim crashes during run





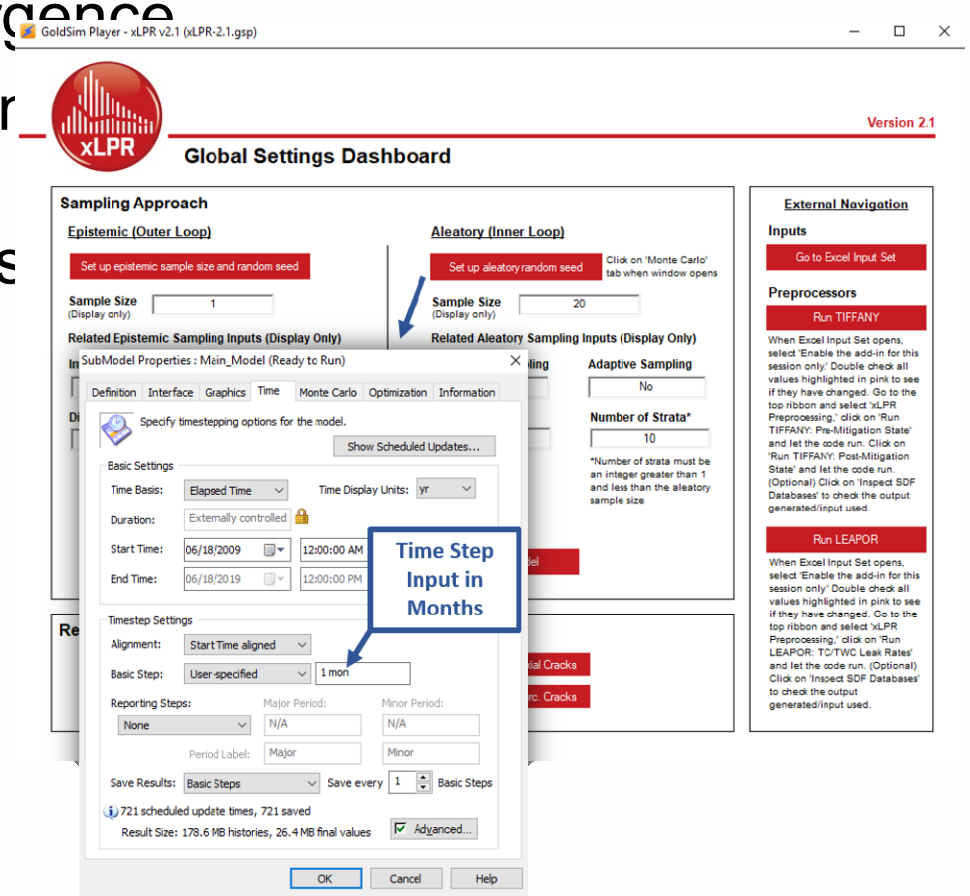
TIME SETTINGS – SAVING FREQUENCY

- GoldSim stores and saves the results of each realization
- GoldSim provides the ability to estimate the final size of the model and adjust the output saving frequency to adjust the size of the results
  - "Main Model" properties, "Time" tab



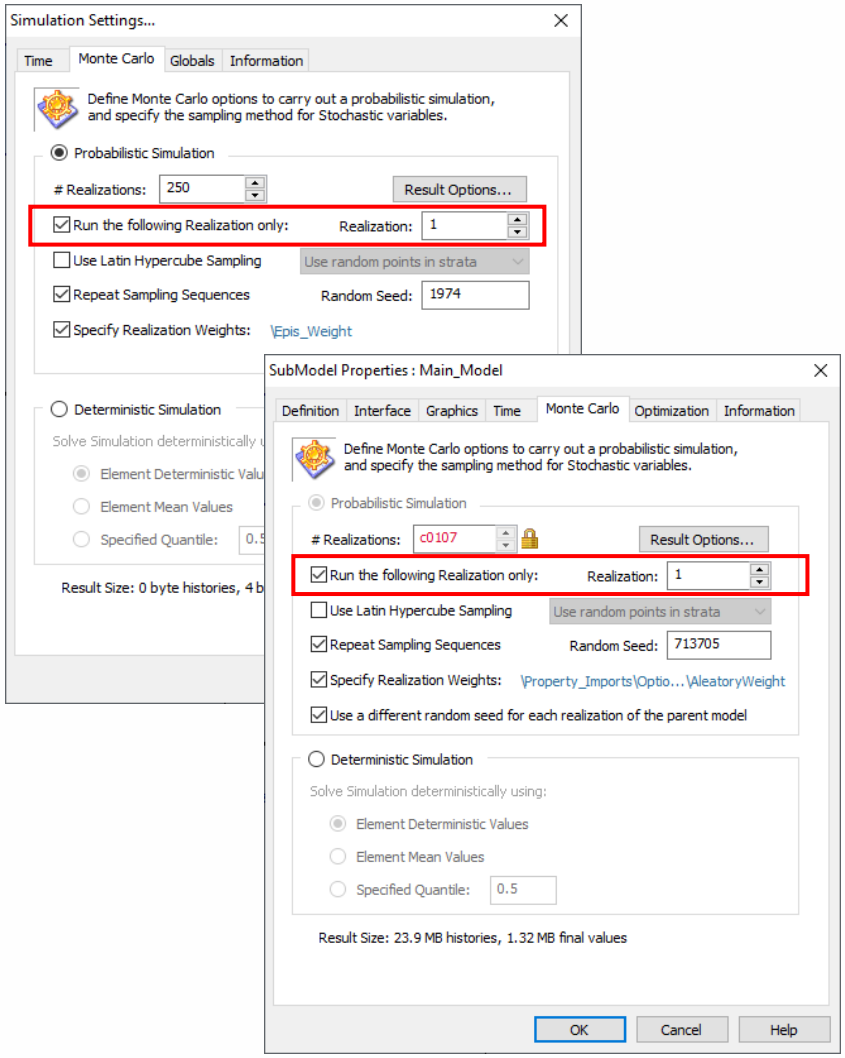
TIME SETTINGS – TIME STEP

- In xLPR V2.1, the default time step is set to 1 month
- This time step can be modified if needed, e.g., to investigate temporal convergence
- The simulation time step can only be adjusted from the aleatory (inner) loop settings dashboard



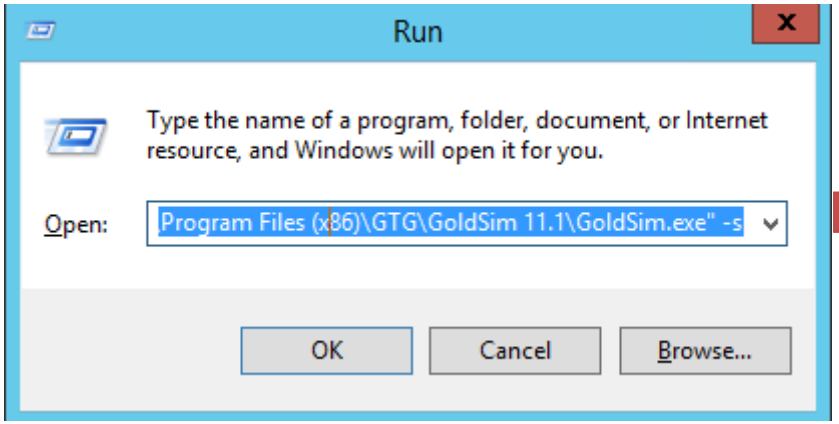
DISTRIBUTED PROCESSING (1/4)

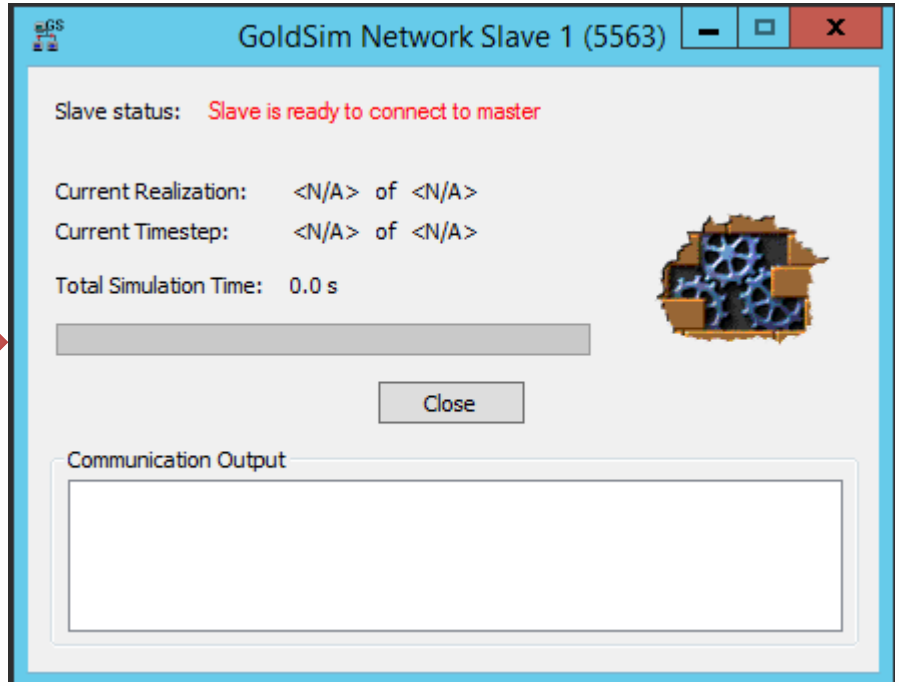
- To run xLPR V2.1 in parallel (up to 4 slave processes), GoldSim Pro is required
- GoldSim Distributed Processing Plus Module allows for more than 4 slave processes
- First run the code with a small sample size to confirm all values from the Input Set have been updated
  - While this should be done automatically, some issues have been found with input data not being updated when running xLPR V2.1 in parallel
- Then, run in parallel on up to N-1 slave processes (per next slide)
  - N = number of cores in the computer's processor



DISTRIBUTED PROCESSING (2/4)

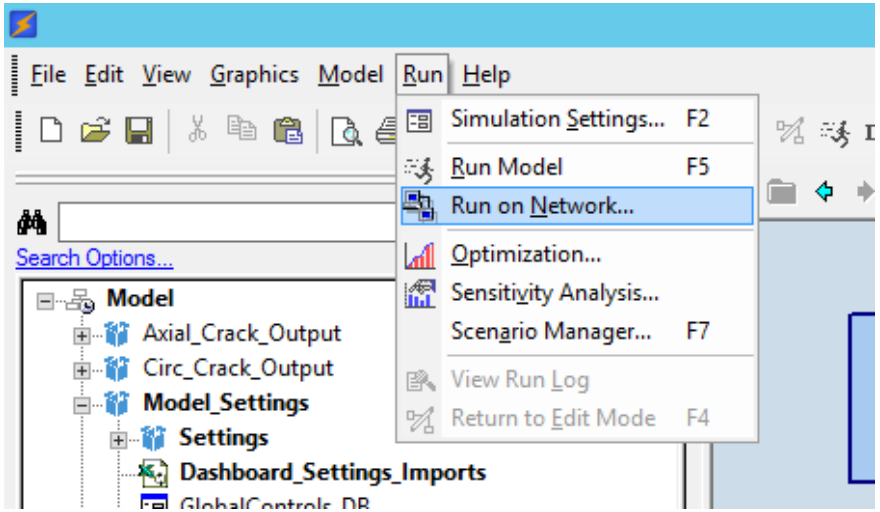
- GoldSim Slave processes can be started using the Windows "Run" utility (Windows key + R)
- Inside the "Run" utility, enter the following:
  - "C:\Program Files (x86)\GTG\GoldSim 11.1\GoldSim.exe" –s
- Each time this command is run, one slave process is started
  - Repeat for as many slave processes that you would like to run

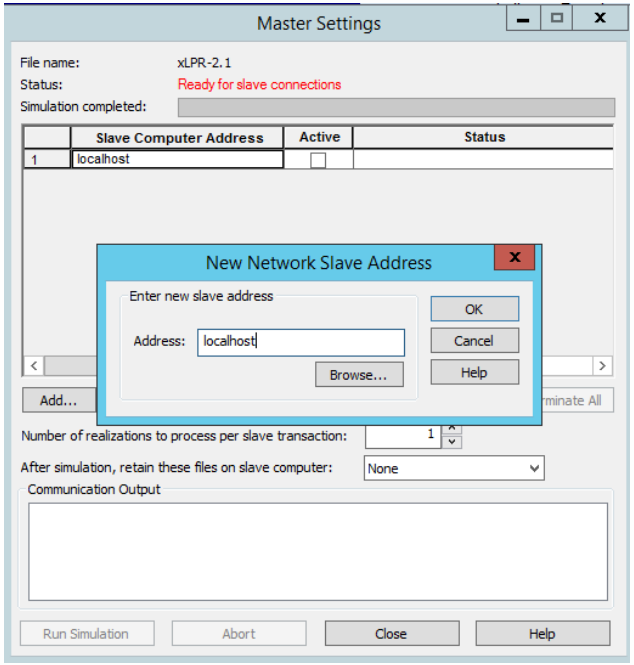




DISTRIBUTED PROCESSING (3/4)

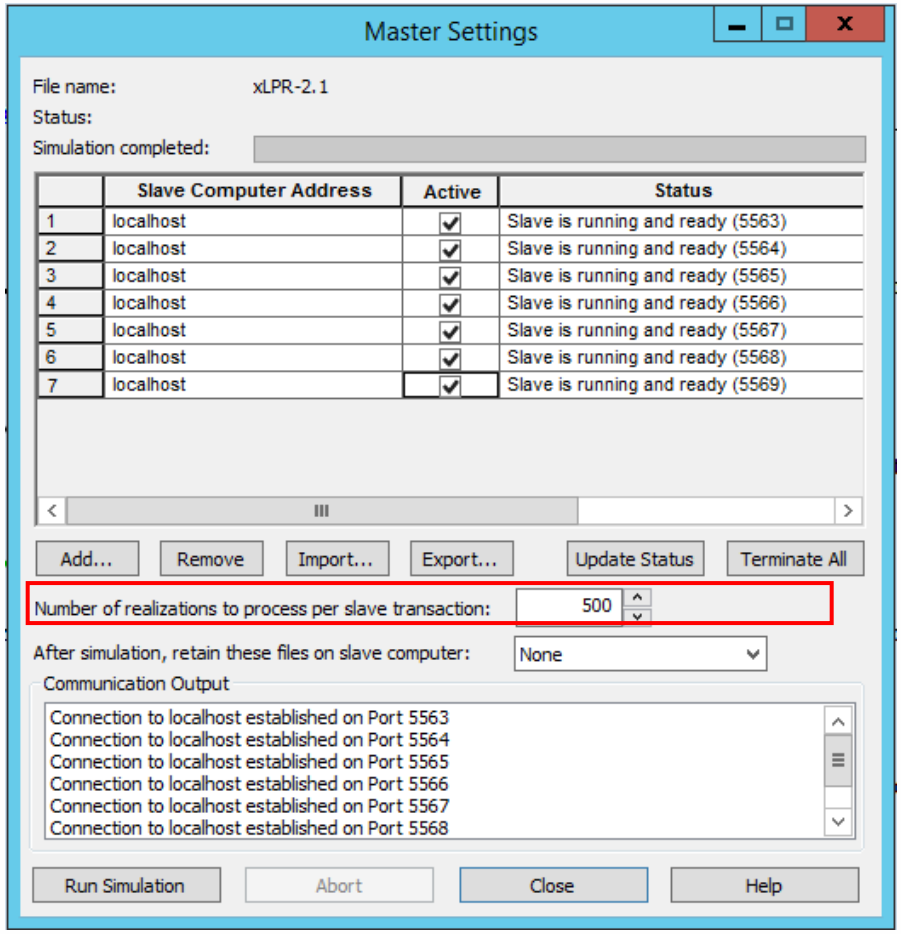
- User selects: Run -> Run on Network
- Connect GoldSim “master” with “slave” processes
  - For “slave” processes on the same computer, can use the “localhost” address
  - Can click “update status” to confirm the link between the master and the slaves





DISTRIBUTED PROCESSING (4/4)

- Parallel execution is only applied to the epistemic (outer) loop
- Adjusting the number of realizations per slave transaction can improve runtimes
  - Rule of thumb: 100 to 1,000 realizations per transaction
  - Too small: requires more data transfer
  - Too large: reduces benefits of parallel execution, longer times for data transfer
- Press “Run Simulation” button to run xLPR V2.1



Demo – Distributed Processing

Closing Remarks

LOOKING FORWARD

- Development of an xLPR user group is underway
- Stay tuned for further communications
  - Survey will be distributed to users

Questions?

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for Additional Information