# The Containment Assurance Risk Framework of the Mars Sample Return Program



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The decision to implement Mars Sample Return will not be finalized until NASA's completion of the National Environmental Policy Act process. This document is being made available for information purposes only.

### **Planned MSR Campaign Architecture Overview**



Mars Sample Return – Capture, Containment and Return System



### **ERO-CCRS** mission overview

- Mission objectives:
  - Capture the OS and bring it back to Earth
  - Relay support for Mars assets
- Nominal mission ("28/27/33"):
  - Launch and near-Earth commissioning [30 days]
  - Outbound transfer with heliocentric parking orbit [3 years]
  - Mars orbit insertion [2 weeks]
  - Spiral down [<1 year]</li>
  - Low Mars orbit (relay support, OS rendezvous, OS containment) [1-1.5 years]
  - Spiral up [<1 year]</li>
  - Inbound transfer [1 year]
  - EES delivery phase [few days]
  - Retirement [few days]





### What is planetary protection?



# FORWARD PLANETARY PROTECTION (FPP)

From NASA Procedural Requirement NPR 8715.24:

"Planetary protection is the practice of **protecting solar system bodies** from harmful contamination by terrestrial materials to enable scientific exploration and **protecting the Earth-Moon system** from possible harmful extraterrestrial contamination that may be returned from other solar system bodies."

### BACKWARD PLANETARY PROTECTION (BPP)

#### Also see:

1. Article IX, UN Space Treaty (UNOOSA 2017, Report of the Committee on the Peaceful Use of Outer Space, 60<sup>th</sup> Session, A/72/20, United Nations, New York)

2. Planetary Protection Policy, Committee on Space Research (COSPAR), 2021

### The 5 primary paths of Mars material that can enter Earth's biosphere



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- Break-the-chain of contact (BTC)
  - Ensure all Mars material and hardware that contacted Mars material is sterilized or contained inside externally clean vessels.
- **Containment Not Assured** (CNA)
  - The state in which one or more requirements for ensuring containment of Mars material have not been met.
  - CNA does not necessarily equate to Mars material release.
  - If the CNA probability exceeds a target probability, additional analyses and/or mitigation measures *may* be undertaken.
- Probability Target
  - Values used in engineering requirements to drive robust containment capabilities.
  - Targets are used to understand if the path to demonstrating PP compliance is quantitative or qualitative.
- Risk elements
  - MSR's BPP requirements are organized in three risk elements, each with a 10<sup>-6</sup> CNA probability target.



CNA probability targets specify both median (50<sup>th</sup> percentile) and upper bound values (90<sup>th</sup> percentile) to protect against non-normal distributions.

### Outline

**TASK:** Develop a **framework for verification of containment assurance (CA) requirements** through analysis with input from all relevant phases, including on-orbit assembly, pre-release, approach (A), entry (E), descent (D), and landing (L).

This analytical framework, briefly called Containment Assurance Risk Framework (CARF), is intended to **integrate models from several domains** and requires **extensive coordination among all the teams**.

**GOAL:** This presentation will guide the reader through a conception of this framework and its implementation in terms of **methodologies**, resources, and preliminary results.

Some technical aspects of this framework are described in some detail and are to be seen as proposed tools or methodologies with potential benefits.

### AGENDA

- 1. CARF Overview
- 2. CARF Implementation
- 3. Example of application
- 4. Conclusions



# CARF Overview





# NASA

## Fault tree analysis – What can go wrong and how?



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- 1. Identify **failure modes** and **fault conditions** that cause CNA.
- 2. Combine them in **fault trees** down to the initiating/basic events.
- Determine failure rates, i.e., probabilities of occurrence, of initiating/basic events.
  - Note these can be either point estimates or probability density functions (PDFs).
- 4. Roll up following fault tree logic.
- **NOTE:** Given the non-Gaussian nature and interdependence of several of these PDFs, proper statistical methods are needed to combine them as they are rolled up.

(Credit: Kyle Grello)

### **Outcome – Quantified CNA**

 The ultimate product will be a PDF that allows verifying CNA performance against the requirements.



The following slides will show the **computational methods** proposed to calculate the required (very low) probabilities <u>at the</u> <u>bottom of the fault</u> <u>tree</u>, as well as how to perform the roll-up.

As an example to guide the reader through the process, a landing model that was used as a pathfinder will be briefly described and results from it will be shown.





# **CARF** Implementation

Modeling and simulation strategies with preliminary test results



### Fault tree analysis – General process





- 1. Define CNA metrics.
- 2. Generate distributions at the bottom associated with such metrics.
- 3. Sample from them.
- 4. "Add/multiply" as prescribed by fault logic.
  - More mathematical details in following slides.

NOTE: Probability density functions are expected to be different in nature (i.e., non-Gaussian). Their combinations will lead to non-analytical forms that will require advanced sampling techniques, e.g., Markov Chain Monte Carlo.

### **STEP 1 – Define CNA metrics**



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- Some of these metrics may be defined in terms of:
  - Point estimates (literature data, vendor manuals, etc.)
    - Failure rates
  - Probability density functions (model outputs, design of experiments)

• Statistics & UQ do the rest!

## **STEP 2a – Generate CNA estimates**

- Data readily available:
  - 1. Literature data
  - 2. Vendor manuals/datasheets
  - 3. Previous missions
  - 4. Tests/Experiments
  - 5. Etc.

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- Data not readily available:
  - Collect test hardware data
  - Use mathematical models
    - If the limit state is a point estimate, use one of the following:
      - 1. Cumulative distribution functions
      - 2. Monte Carlo
      - 3. Importance sampling
      - 4. Subset simulations
      - 5. First/Second-order reliability methods (FORM/SORM)
      - 6. Multifidelity importance sampling
      - If the limit state is a probability distribution:
        - Design of experiments with synthetic data and overlap area



### STEP 2a – Point estimates (1): Cumulative Distribution Functions



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#### **EXAMPLE**

#### Peak landing acceleration > set critical value

The Cumulative Distribution Functions (CDFs) shown in this plot is come from a high-fidelity (HF) and a low-fidelity (LF) model.

- CDFs from expensive HF model with few runs have very poor resolution, especially in the tails.
- CDFs from **LF models** may be **smooth** but suffer from **additional uncertainties** due to the models' low fidelity.



### STEP 2a – Point estimates (2): Monte Carlo and others



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MCS - Convergence of  $P_{CNA}$  $imes 10^{-5}$ This plot is only for illustrative purposes and is based CIon a LF model that approximates the HF landing model. MATLAB UQLab's Reliability module provides several algorithms to compute probabilities of failures, e.g., Monte Carlo, Importance Sampling, Subset P<sub>CNA</sub> Simulations, FORM/SORM, etc. [1] 0 P(COS Accel ≥ 3000 G) = 1 – P(COS Accel < 3000 G) = 5.50e-6 23 8 5 9 104  $\times 10^{6}$ 

Regular Monte-Carlo approaches may require thousands/millions of runs before reaching convergence, which is impossible with expensive HF models.

Using LF models implies working with additional uncertainties due to the models' low fidelity.

- Challenge: it only works with HF models (expensive) or LF models (biased, inaccurate).
- Focus should be on improving knowledge of CDF tails through a multifidelity approach (faster and more accurate) as shown on the next slide.

[1] S. Marelli, R. Schobi, B. Sudret, UQLab user manual
Structural reliability (Rare event estimation), Report
#UQLab-V1.4-107, Chair of Risk, Safety and Uncertainty
Quantification, ETH Zurich, Switzerland, 2021

### Multifidelity approach to computationally expensive models



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## Multifidelity approach to computationally expensive models



### Simplified models

Early-stopping criteria

Natural problem hierarchies (e.g., in CFD: DNS -> LES -> RANS)

Coarse-grid approximations

Linearized models

### Data-fit models

Interpolation

- Polynomial interpolation
- Radial basis functions
- Kriging

Regression

- Polynomial Chaos Expansion
- Support Vector Machines

### **Projection-based models**

Proper Orthogonal Decomposition (POD)

Reduced-basis method

Krylov subspace methods

### Information sources beyond models Expert opinions

Experimental data

Historical data

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- Low-fidelity (LF) models should be of different type, approximation quality and cost to inform different aspects of the HF model.
- This is better than using only LF models that are accurate but lack a rich diversity [2,3].
- Successfully applied to JWST [4].

[2] Ng, Willcox, Multifidelity approaches for optimization under uncertainty, *Int. J. Numer. Meth. Engng.* 2014; **100**:746–772
[3] Peherstorfer, Willcox, Gunzburger, Optimal model management for multifidelity Monte Carlo estimation, *SIAM J. Sci. Comput.* 2016; **38**(5):A3163-A3194
[4] Cataldo, Qian, Auclair, Multifidelity uncertainty quantification and model validation of large-scale multidisciplinary systems, *J. Astron. Telesc. Instrum. Syst.*, **8**(3), 038001 (2022)



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### **IMPORTANCE SAMPLING**

Variance reduction strategy for Monte Carlo estimation

that samples from a problem-dependent biasing distribution

- TWO STEPS:
  - 1. The biasing distribution is constructed.
  - 2. Samples are drawn from the biasing distribution and the estimate is derived [6, 38].

#### **CHALLENGE:**

Construction of a **suitable biasing distribution** that leads to **variance reduction** 

#### SOLUTION: MULTIFIDELITY PRECONDITIONING OF THE CROSS-ENTROPY METHOD

Chosen such that **fewer samples** are necessary to obtain an acceptable estimate of the rare event probability than with standard Monte Carlo

The bias introduced by the sampling from the biasing distribution is **corrected** by reweighing the samples in the importance sampling estimator.

[5] Peherstorfer, Kramer, Willcox, Multifidelity Preconditioning of the Cross-Entropy Method for Rare Event Simulation and Failure Probability Estimation, *J. Uncertain. Quant.* 2018; **6**(2):737–761

by



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### **Cross-entropy (CE) method**

Provides a practical way to approximate the zero-variance density

**HOW?** By optimizing for a density that minimizes the Kullback-Leibler divergence from the zero-variance density in a set of feasible densities

#### **CHALLENGE:**

Even though solving for a biasing density with the CE method typically requires fewer high-fidelity model evaluations than estimating the rare event probability with a standard Monte Carlo approach, the cost of the optimization problem in the CE method can still be significant

if the high-fidelity model is expensive to evaluate

#### **SOLUTION:**

Multifidelity method that leverages a hierarchy of low-cost, low-fidelity models to reduce the costs of constructing a CE-optimal biasing density

[5] Peherstorfer, Kramer, Willcox, Multifidelity Preconditioning of the Cross-Entropy Method for Rare Event Simulation and Failure Probability Estimation, J. Uncertain. Quant. 2018; 6(2):737–761



- The bound on the number of iterations of the CE method depends on the density with which the CE method is initialized.
- The method developed in [5] exploits the fact that the bound on the number of CE iterations can be reduced by a suitable choice of the density with which the CE method is initialized.
- The MFCE method iterates through the different models (1,...,L).
  - L identifies the high-fidelity model.
  - At level 1, the MFCE method constructs a biasing density with the classical CE method, initialized with the nominal density and using low-fidelity model 1.
  - At level 2, the MFCE method uses the CE method to derive a density with model 2.
    - However, the CE method is initialized with the density of the previous level, instead of the nominal density as in the classical CE method.
  - This hierarchical process is continued until level L, where the final estimate uses the high-fidelity model.
- Numerical examples show ability to estimate probability of failures as low as 10<sup>-9</sup>!

[5] Peherstorfer, Kramer, Willcox, Multifidelity Preconditioning of the Cross-Entropy Method for Rare Event Simulation and Failure Probability Estimation, J. Uncertain. Quant. 2018; 6(2):737–761 And references therein.



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### P(COS Accel ≥ 3000 G) = 8.1062e-6 ± 2.0331e-5

Convergence achieved with 1 HF model, 2 LF models and **only 6 total iterations**!

Multifidelity importance sampling uses both HF/LF models to recover probability of failures as low as 1e-9! [5]

The result accuracy is guaranteed by keeping the HF model in the loop.

PROPOSED METHODOLOGY for expensive models with run times ≥ 1 min

[5] Peherstorfer, Kramer, Willcox, Multifidelity Preconditioning of the Cross-Entropy Method for Rare Event Simulation and Failure Probability Estimation, *J. Uncertain. Quant.* 2018; **6**(2):737–761

### **STEP 2b – Generate input data for distributions**

- Design of experiments with numerical models or test hardware
  - Monte Carlo
  - Latin Hypercube
  - Quasi-random
    - Halton
    - Sobol
  - Response surface
    - Box-Behnken
    - Central composite
  - D-Optimal
    - Seeks to minimize the covariance of the parameter estimates for a specified model
    - Good for non-linear models, constrained factors, correlated parameters
  - Maximum projection
    - Maximizes the product of the distances between potential design points with the goal of providing good space-filling properties on projections of factors.





23

Containment Metric — Limit State

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– Etc.

### **STEP 3 – Combine all distributions**



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### **STEP 3 – Combine all distributions**



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### **STEP 3 – Combine all distributions**



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### **CARF – First demonstration**

- Propagation of CNA probabilities through requirements tree
  - Leaf nodes (green hexagons) represent basic events
  - Distribution of leaf-node success probabilities from stochastic simulations using physical models
  - Compute distributions of success probabilities of interior-nodes' (blue) events sequentially down the tree to the root
- Code written in Julia using Graphs.jl and Metagraphs.jl packages.
  - Create ProbabilityGenerator objects to model univariate or joint distributions for leaf nodes based on Monte Carlo results.
  - And/Or logic tests for independence among interior nodes, and manages dependence if needed.
  - Carries whole distributions (as histograms) down the tree, and can report any desired statistics of the distribution in the node label.

15 (0 491306 (0 509 19 (0.489) 18 (0.4713) 12 (0.499 6 (0.5127) 17 (0.2241) 5 (0.5156) 13 (0.4992) 11 (0.5041) 14 (0.7473) 7 (0.5089 3 (0.516) 10 (0.9748) 9 (0.4929) 4 (0.8848 3 (0.9994) 23 (0 4898 22 (0.5202) 2 (0.5078 21 (0.2519)

**Figure**: Small example tree with node labels as node identification number and mean of the distribution (in parentheses) of probabilities. Green hexagons are leaves; blue nodes are interior nodes. AND gates are circles, OR gates are rectangles.



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### **Final product – Requirement verification**



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### Conclusions



- To demonstrate compliance with the strict requirements of MSR, a statistical framework was developed to assess the likelihood of containment loss posed by each sample return phase and make a statement about the total combined mission probability of containment not assured.
- The framework considers failure modes or fault conditions that can initiate propagation sequences ultimately leading to a containment not assured.
- Given the multidisciplinary nature of the problem and the different types of mathematical models used, the statistical tools needed for analysis are required to be computationally efficient.
  - While standard Monte Carlo approaches are used for fast models, a multi-fidelity approach to rare event
    probabilities is proposed for expensive models. In this paradigm, inexpensive low-fidelity models are developed for
    computational acceleration purposes while the expensive high-fidelity model is kept in the loop to retain accuracy in
    the results.
  - This work presented an example of end-to-end application of this framework highlighting the computational benefits of a multi-fidelity approach and the overcoming of several complexities inherent to the computation of very low (<1e-6) probabilities.</li>



- Update process to handle joint and conditional distributions
  - Both in design of experiments and fault tree "roll-up"
- Continue research on sampling techniques for extreme values
- Perform analysis with latest mathematical models and test data as the mission progresses toward more mature designs





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### **Variance-based Sensitivity Analysis**





- Determine the amount of variance that would disappear in the outputs if the uncertainty in one or more input parameters were reduced
- Prioritize parameters by identifying those which, on average, once reduced their uncertainty, would cause the greatest reduction in the output variance

### Multifidelity approach to computationally expensive models





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- A multifidelity (MF) approach leads to more accurate
   results and cheaper
   computational costs
- The example shown here is from JWST [5]
- What it takes:
  - MATLAB
  - UQLab toolbox (freely available) to develop low-fidelity models
  - mfGSA code (freely available) to run MF analysis
  - A number of samples from HF model

[4] Cataldo, Qian, Auclair, Multifidelity uncertainty quantification and model validation of large-scale multidisciplinary systems, *J. Astron. Telesc. Instrum. Syst.*, **8**(3), 038001 (2022).