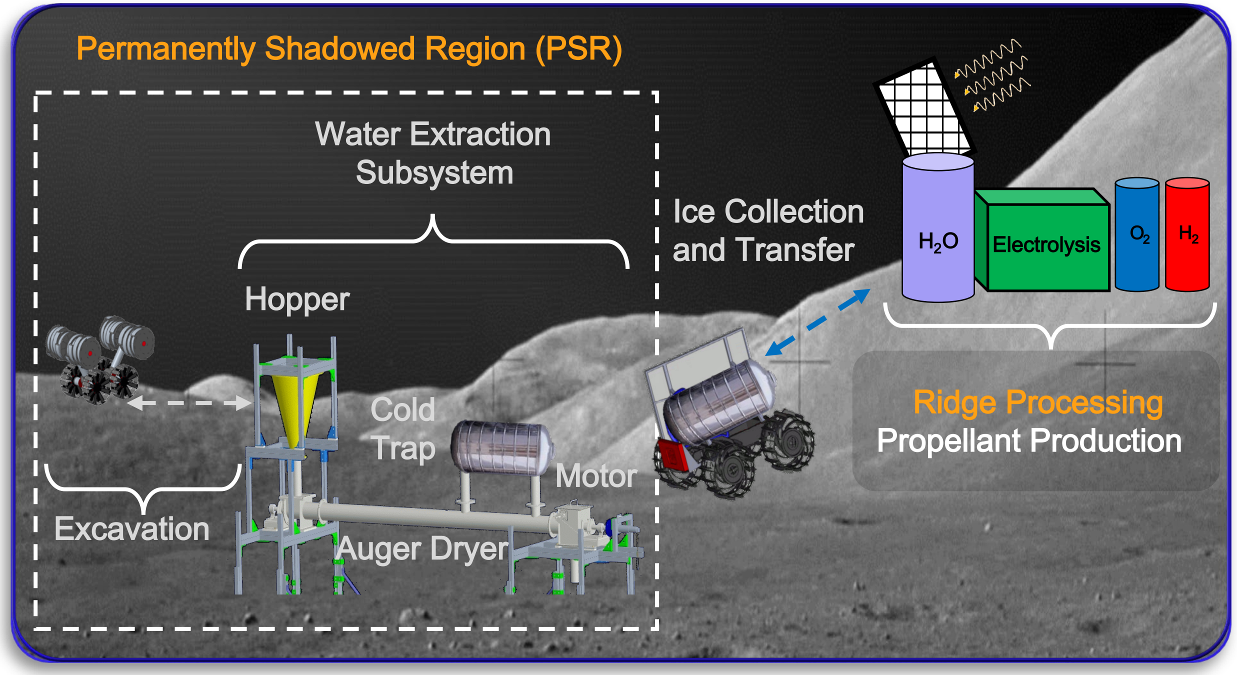
Jacobs Challenging today. Reinventing tomorrow.

In-Situ Resource Utilization Modeling of Lunar Water Processing System

Avery Carlson, Noah Andersen, Jacob Collins

SIMA tool facilitates ISRU architecture planning

- **SIMA is an integrated & flexible framework of connected ISRU-related subsystem models**
  - Enables point solutions, optimization, and parametric studies at system level
  - Supports infusion of model and integration early in NASA’s technology development lifecycle



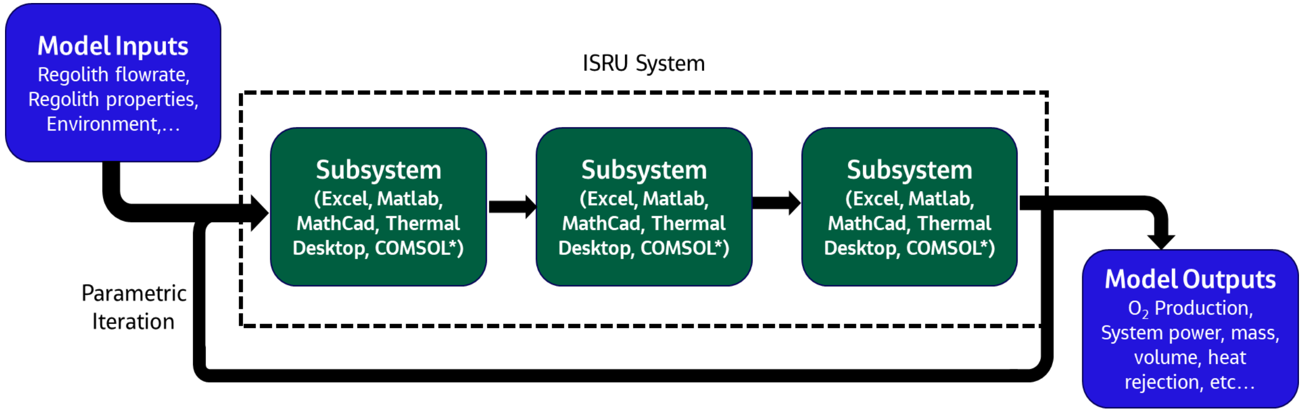
Simple Lunar Water Processing Plant[1]

SIMA tool facilitates ISRU architecture planning

- SIMA is an integrated & flexible framework of connected ISRU-related subsystem models
  - Enables point solutions, optimization, and parametric studies at system level
  - Supports infusion of model and integration early in NASA's technology development lifecycle
- **Establishes a modular, end-to-end modeling & analysis capability**
  - Leverages prior & on-going research and development, subsystem models and data
  - Rapid analysis turnaround as needs change or more data becomes available
  - Communicates with widely available software (Matlab, Excel, Thermal Desktop,Comsol*)

*API currently being developed

SIMA Simple Process Flow Diagram



Model Inputs
Regolith flowrate, Regolith properties, Environment,…

ISRU System

Subsystem
(Excel, Matlab, MathCad, Thermal Desktop, COMSOL*)

Subsystem
(Excel, Matlab, MathCad, Thermal Desktop, COMSOL*)

Subsystem
(Excel, Matlab, MathCad, Thermal Desktop, COMSOL*)

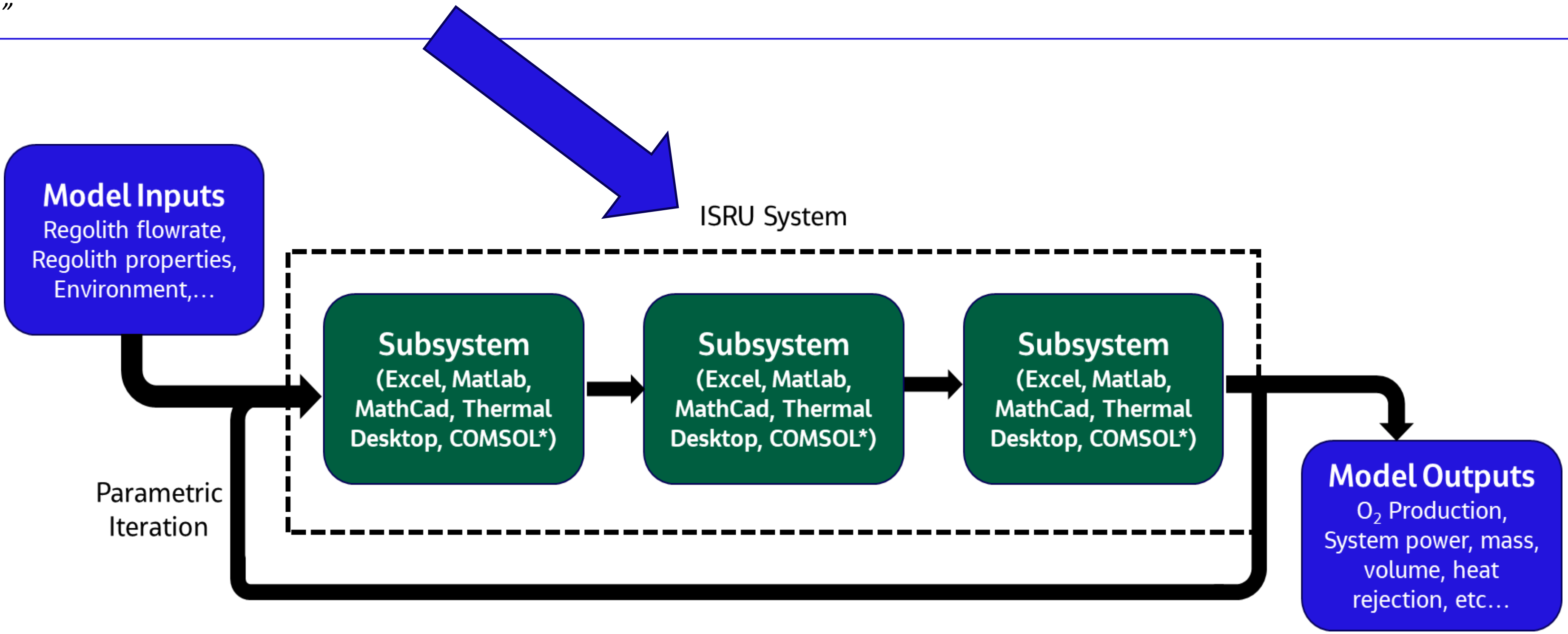
Parametric Iteration

Model Outputs
O_2 Production, System power, mass, volume, heat rejection, etc…

SIMA Project Addresses ISRU Modeling Shortfalls

STMD Shortfall 581 – ISRU System Modeling[2]

"ISRU systems involve many components/subsystems; ***interface conditions between these are key to design of viable system hardware.*** *Components/subsystems are often modeled with physics-based models and empirical test data to facilitate hardware scaling, con-ops planning, and optimization. These models must be pulled together into* ***a full ISRU system model to enable scaling studies, concept of operations, and optimization at the system level;*** *as well as getting* ***system level mass/power predictions for mission architecture planning. Flexible****, widely available platforms are needed that allow* ***for subsystems to be input as modules and swapped*** *to evaluate different technology options in trade studies. These trade studies are critical to architecture definition activities.* ***Validating the models with integrated system tests*** *(subsystems and end to end) is also a key aspect of this shortfall."*



Model Inputs
Regolith flowrate,
Regolith properties,
Environment,…

ISRU System

Subsystem
(Excel, Matlab, MathCad, Thermal Desktop, COMSOL*)

Subsystem
(Excel, Matlab, MathCad, Thermal Desktop, COMSOL*)

Subsystem
(Excel, Matlab, MathCad, Thermal Desktop, COMSOL*)

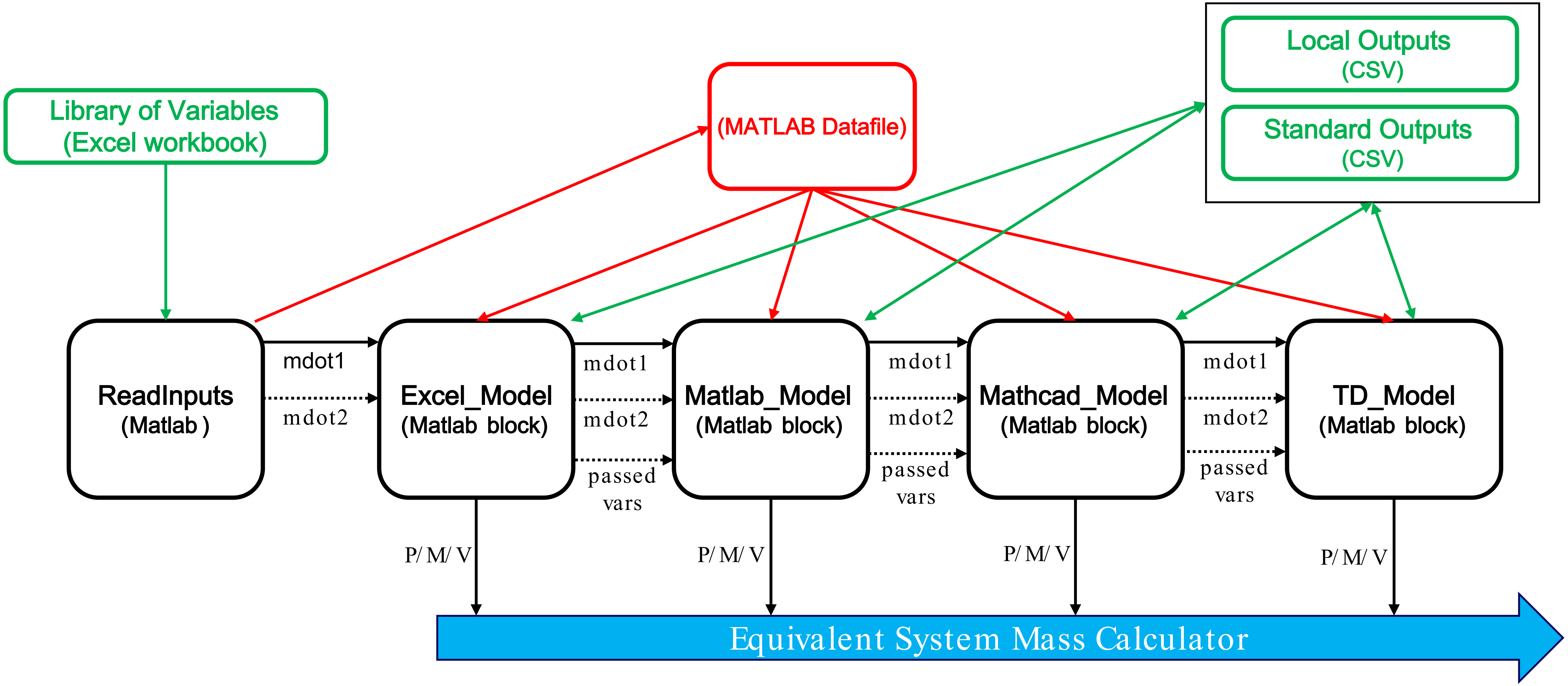
Parametric Iteration

Model Outputs
O_2 Production,
System power, mass, volume, heat rejection, etc…

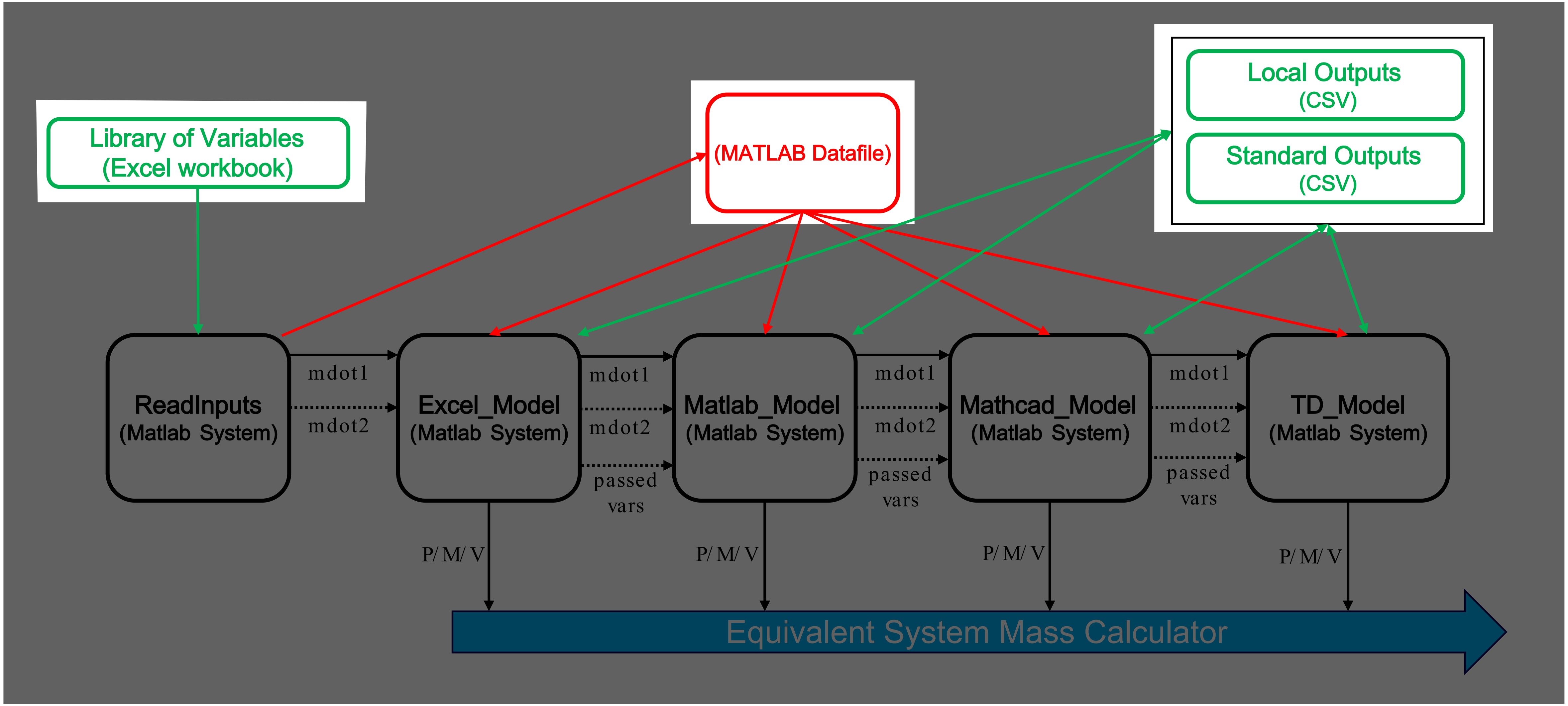
Brief Overview of SIMA Model Framework

ISRU Case Study: Water Processing on Lunar Surface

Overview of SIMA Framework



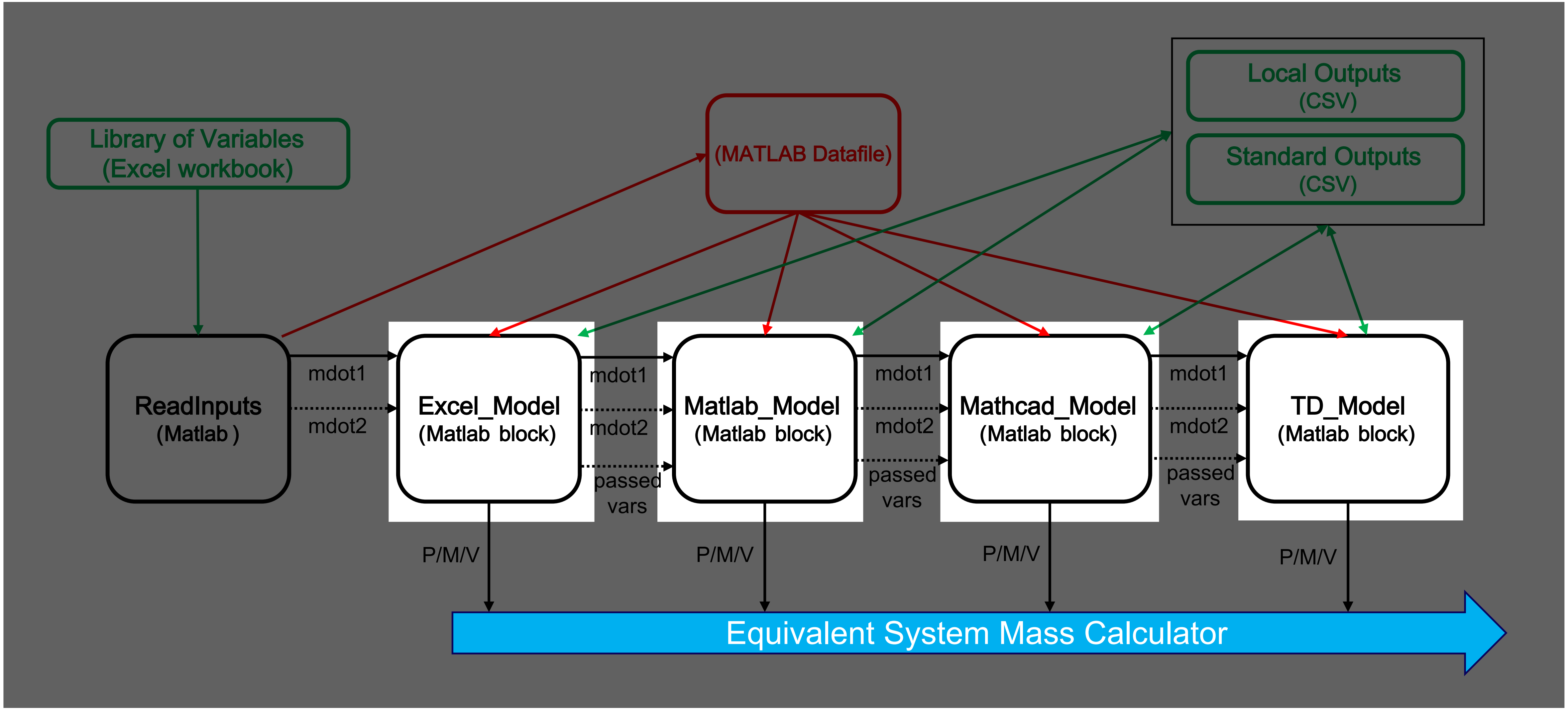
How does SIMA track Inputs and Outputs?



How does SIMA track Inputs and Outputs?

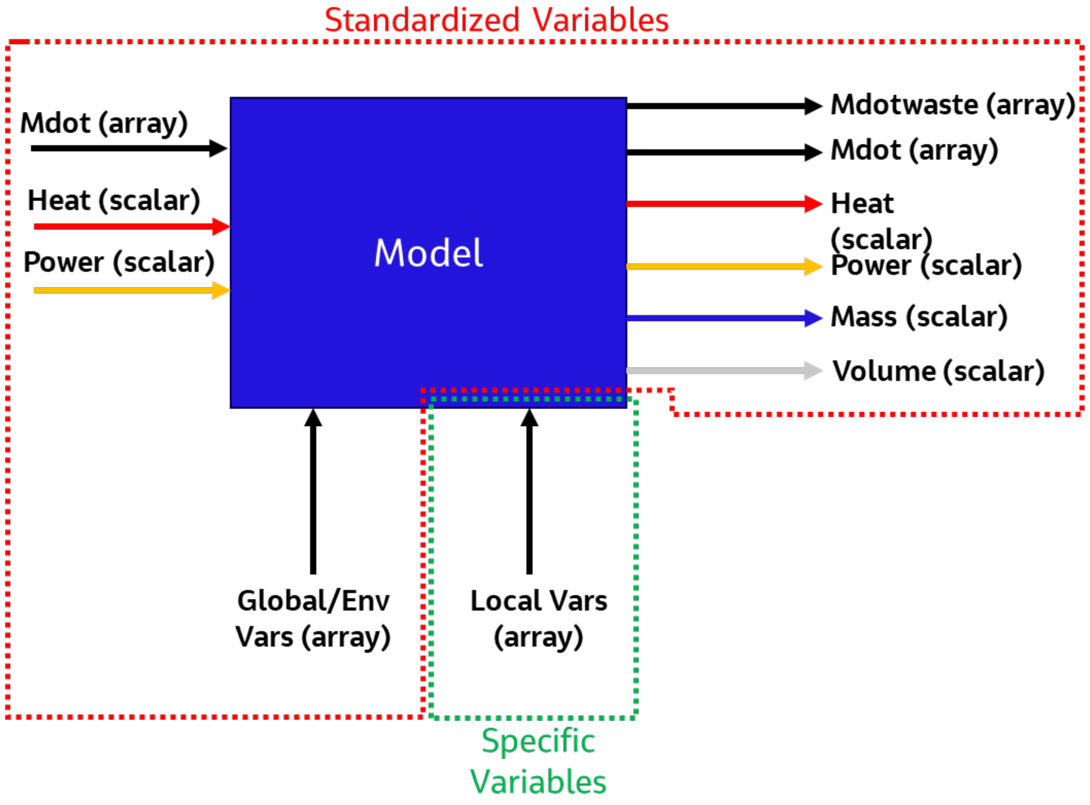
- **Library of Variables:** Multipage Excel workbook that contains all information needed to run model:
  - Global Variables: Contains all variables describing environment. All models will have access to these variables and must use the same naming convention and units
  - Passed Variables: Defines all standard variables to be passed between models (e.g. pressure, temperature, mass flowrate, P/M/V)
  - Local Variables: Process-specific variables
- **Parametrics:** User-defined variables that will change step-wise during a parametric sweep
- **MATLAB Datafile:** Internal structure that contains variables for a **specific** parametric case and can be quickly read by all models.
- **Local Outputs & Standard Outputs:** CSVs that have organized inputs and outputs for every parametric run
  - This file is also read by the subsystem models at each step prior to running to check if the specific model run does not need to be rerun.

How does SIMA run a Subsystem Block?



How does SIMA run a Subsystem Block?

- Read local variables from MATLAB data file
- Logic to check if model needs to be run (important for making parametric sweeps more efficient)
  - Compare current iteration inputs to previous run inputs
  - If there is a previous run with same inputs as current, skip the run, using data from previous run
- Send all inputs to model, Run, Read outputs
  - Develops API to communicate with subsystem file software
  - Modifies to specific software requirements
- Write output files



How does SIMA run a Subsystem Block?

- Read local variables from MATLAB data file
- Logic to check if model needs to be run (important for making parametric sweeps more efficient)
  - Compare current iteration inputs to previous run inputs
  - If there is a previous run with same inputs as current, skip the run, using data from previous run
- Send all inputs to model, Run, Read outputs
  - Develops API to communicate with subsystem file software
  - Modifies to specific software requirements
- Write output files
- **Parametric Sweeps:**
  - Method of testing boundaries in a complex system
  - Iteratively submit inputs to the model based on discrete step-changes
- **ESM Calculator:**
  - Subsystem mass, power, volume, & heat rejection calculated within the model
  - Passes to a post-processing script for optimization analysis

$ESM = \sum \text{Subsystem Mass} + K_{p,VSAT} * \text{Total Power} + \text{Cable} \sim f(\text{PSR Power})$

*Total Volume considered for module deployment vehicles (work TBC)

**Heat Rejection factored as a subsystem radiator component

Brief Overview of SIMA Model Framework

ISRU Case Study:

Water Processing on Lunar Surface

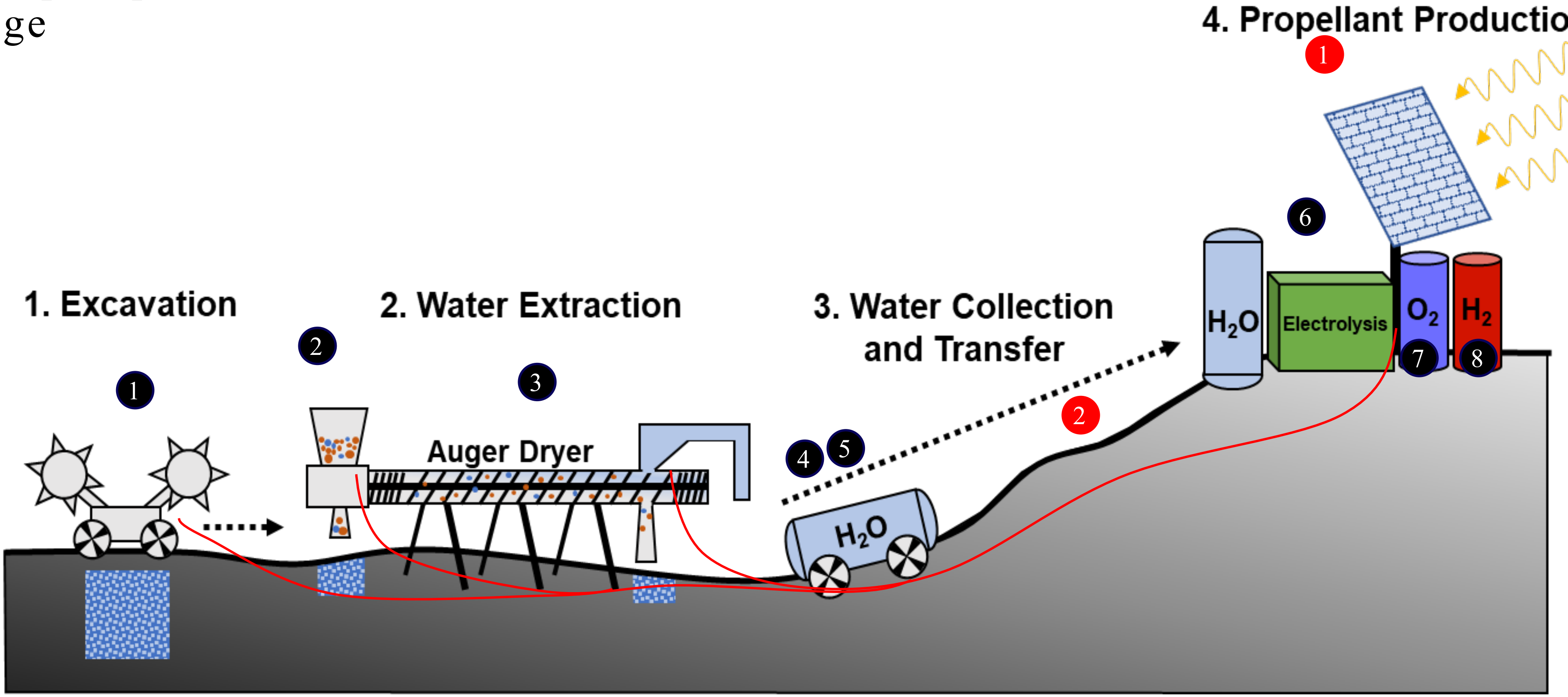
Lunar Water Processing– High level architecture [3]

ISRU Infrastructure Physical-Chemical Processes

1. Icy regolith is excavated
2. Regolith is loaded into a hopper
3. Regolith passes through auger dryer, which heats regolith and sublimates water vapor
4. Water vapor is frozen in cold trap, deposited as ice
5. Ice is transported to crater ridge
6. Water is split into H_2 and O_2
7. O_2 gas is liquefied and stored
8. H_2 gas is liquefied and stored

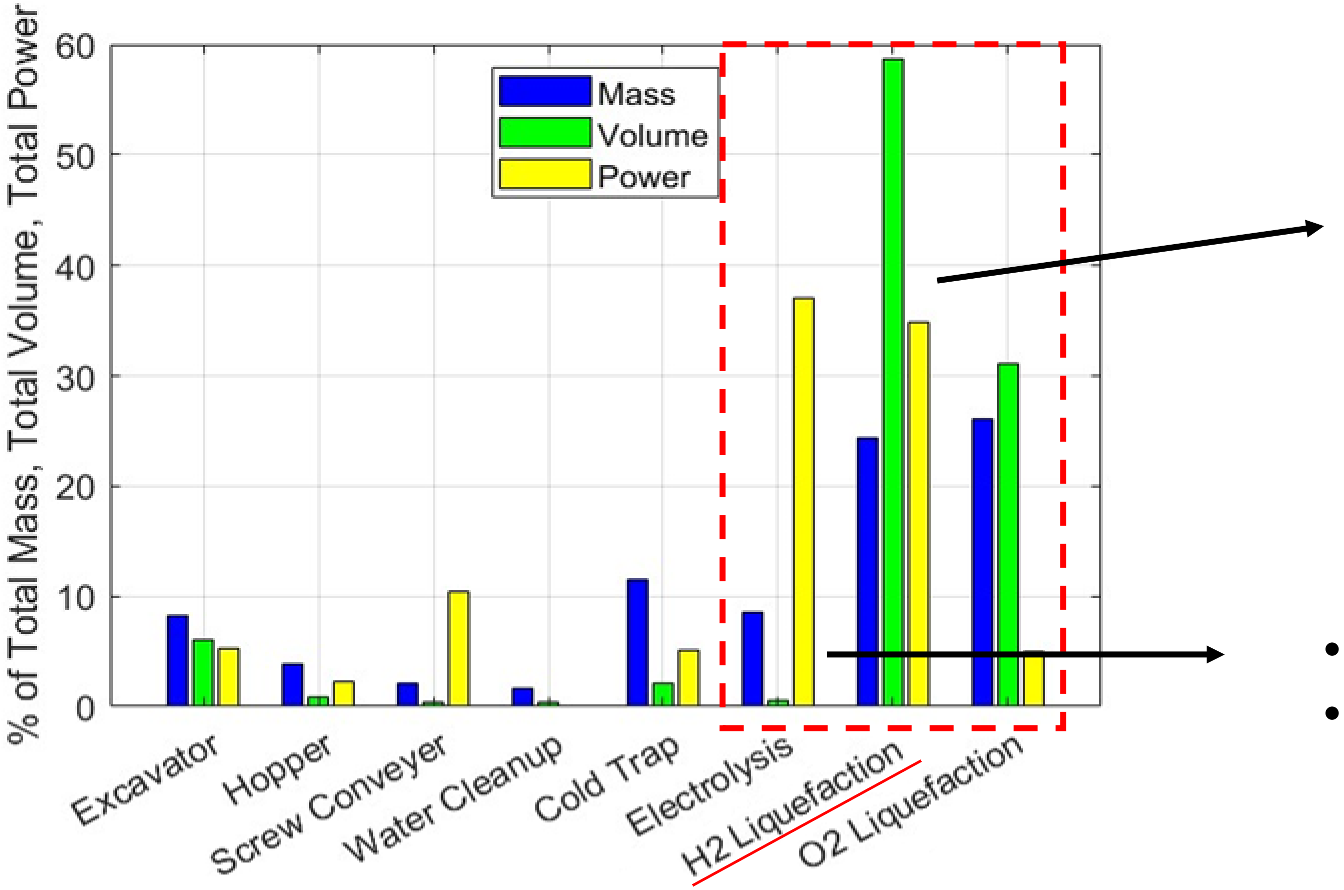
Power Generation & Distribution

1. Power is captured via vertical solar array (VSAT)
2. Power is transmitted to processes in PSR through cables



Takeaway 1: Demonstrating System-Level Inefficiency

- Hydrogen liquefaction is a power intensive process and requires substantial storage mass & energy
- Electrolysis trade-offs with process type & operating temperature



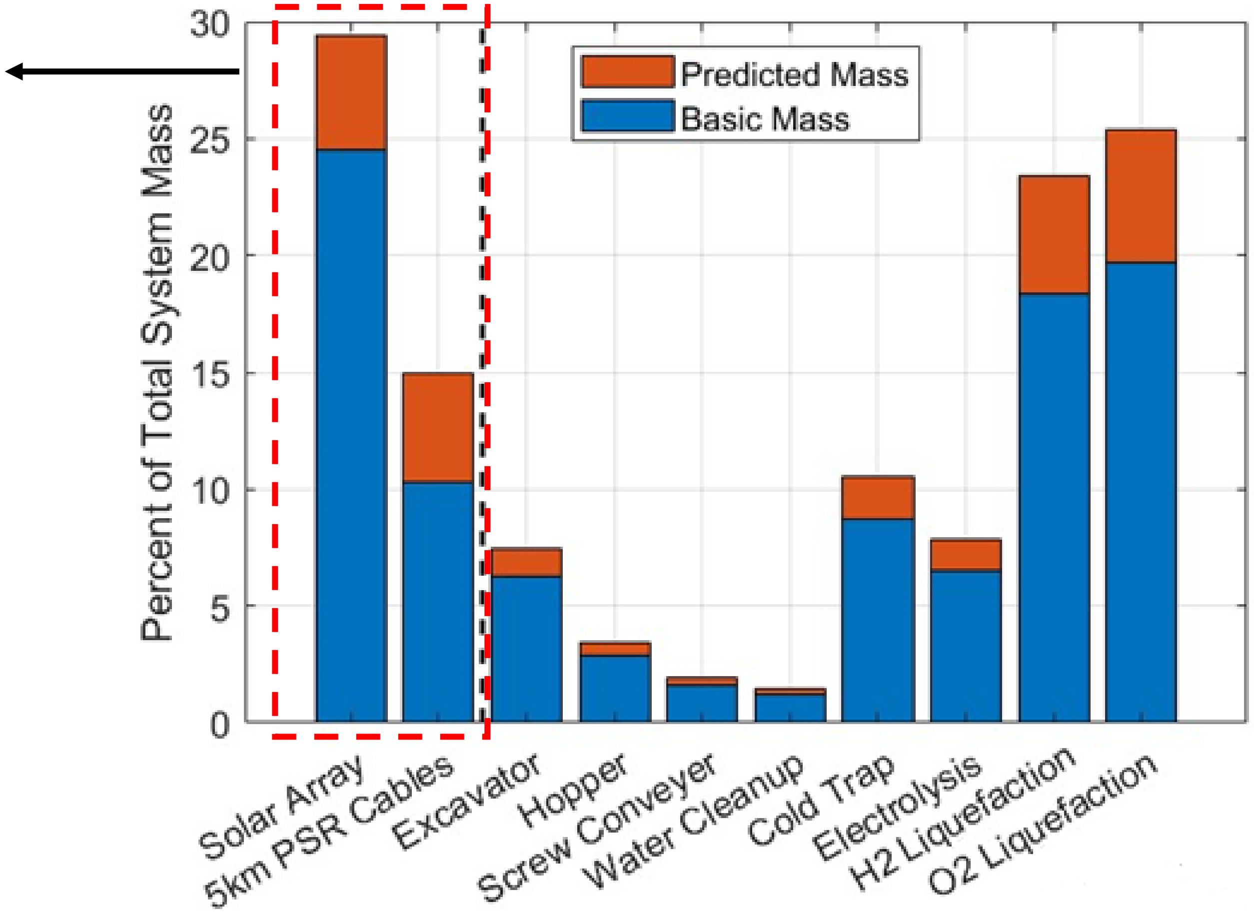
- Trade venting vs. storage
  Can specific R&D investments facilitate a breakeven point?
- Is there a viable alternative storage option or configuration?

- Trade PEM vs other electrolyzer types
- Options to reduce operating temperature, ensure power efficiency

Takeaway 2: Importance of Integrating Power/Transmission into the Architecture

- The power generation technology and transmission contributes a significant portion of the overall system mass and must be appropriately accounted for.

- Power generation (on ridge) and transmission (from ridge to PSR) makes up a substantial portion of the total system mass
- More freedom with PSR systems especially at scale, recommend optimizing thermal loading
- Power distribution alternatives?

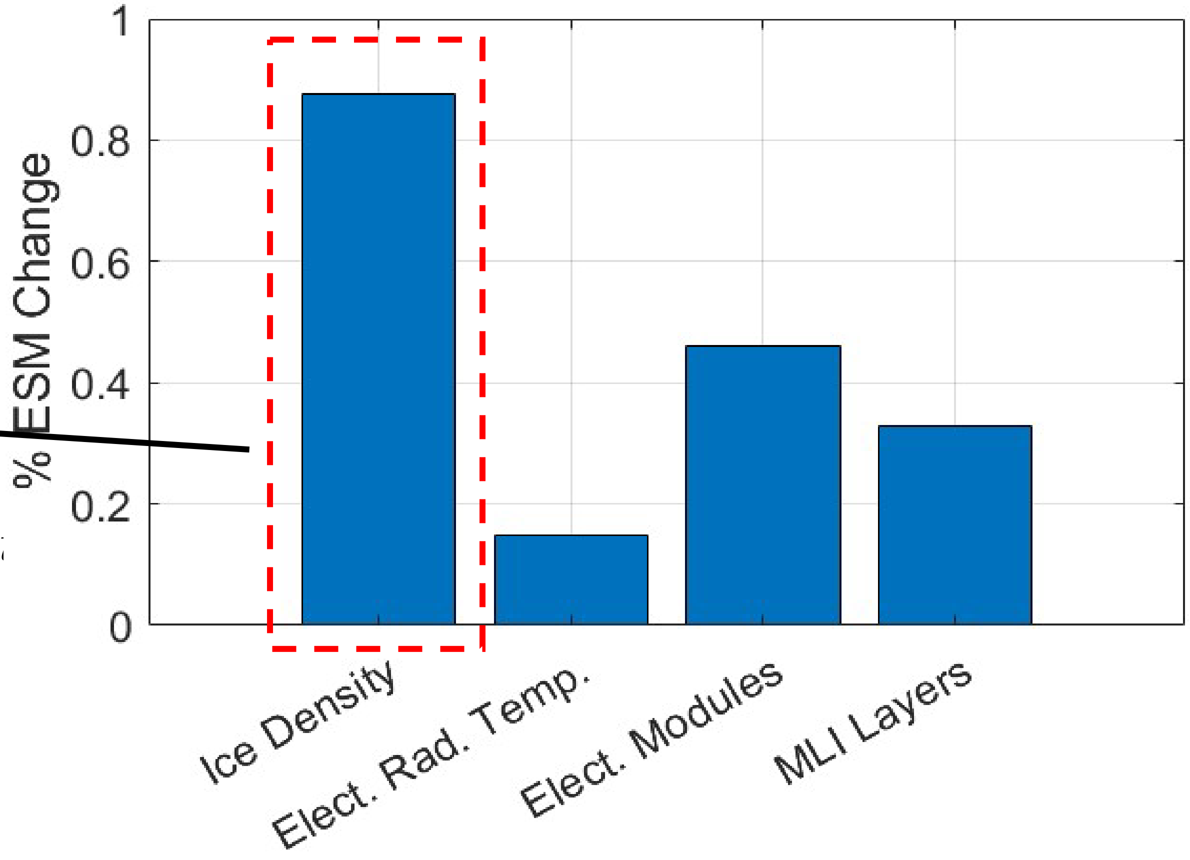


Takeaway 3: Sensitivity of System Mass to Parametric Variables

- SIMA can be used to determined the sensitivity of the system mass to specified variables.
- Example Parametric variables shown on x-axis
  - Parametric System mass ~ f(Input + Step Change)
- Ice Density characteristics have the largest impact on system mass.

Low Density→ High Density Ice ≈ 10% Increase
System Mass

  - Recommended to focus near-term research goals on finding consistent value



ΔSystem mass after 10% change to variable input

SIMA Tool Rapid Turnaround for Other ISRU Architectures

- Current FY Technology Comparison
  - Keep upstream/downstream subsystems and easily swap technology groups
    - Exp: water electrolysis types
    - Exp: Molten Regolith Electrolysis (MRE) subsystems
  - We want to leverage research & development, collaboration with other NASA centers
- Martian ISRU for Oxygen and Methane Production
  - Simulation under different environmental conditions to produce additional products
  - Compiling new subsystems from government & commercial partners, taking advantage of previous studies

Summary of SIMA Tool

- SIMA is a modeling tool developed to service STMD shortfalls
  - Flexible framework for integrating technology developed subsystem models
  - Rapidly turns around trade studies, configuration optimization & analysis
- Modeling framework built to:
  - Integrate & pass data between individual subsystems
  - Allow different types of solver methods and techniques for optimization
  - Accommodate multiple layers of subsystems & components, various complex configurations
  - Be software “agnostic”
- Analyses on high-quality architectures using subsystem models from technology developers
  - Technology developers write their model in a convenient and appropriate software language
  - Future high-fidelity models may not be hand calculations, rather more complex thermal models in accordance with upward TRL trajectory
  - SIMA can fit in the hardware development lifecycle

Conclusions & Major Takeaways from Inaugural Trade Study

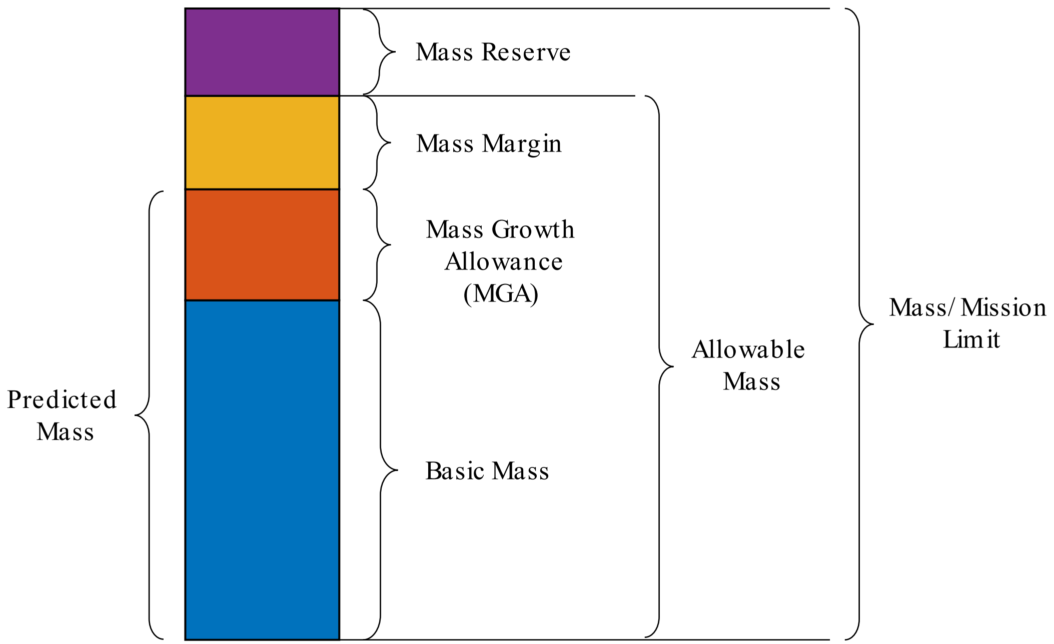
- Major Takeaways from Inaugural Lunar Water Processing Trade Study

  1. <u>Choice of power source and integrating power transmission</u> into the PSR should not be neglected.
  2. Hydrogen Liquefaction represents a <u>system-level inefficiency</u> made apparent from model mass, power, & volume estimates.
  3. <u>Sensitivity analysis around parametric data</u> reveals cold trap ice density to be important parameter affecting plant ESM at larger scales.

Backup Slides

Mass Property Control (AIAA S-120-2006)

- **Basic mass** is model-calculated mass of the system without any margin
  - Sometimes called "current best estimate"
- **Predicted Mass** is estimated final mass at system delivery operation.
  - Determined by adding the Mass Growth Allowance (MGA) for each **subsystem**
  - Accounts for design maturity, and hardware category (more mature designs will have a smaller MGA)
- **Allowable Mass** is the mass against which the mass margins are compared. If mass



MATLAB/Simulink Model Environment

- Uses MATLAB/ Simulink to link various subsystem models into an overall system model
  - MATLAB can create Application Program Interface (API) to communicate with other software (e.g., MathCad, COMSOL, Thermal Desktop)
  - Simulink environment is designed to handle time-dependent signals (ideal for parametric/ iterative sweeps)

Why not develop model framework completely in Excel?

- Feedback from similar modeling efforts in the past: Issues with maintaining models in different versions, solver and optimization capabilities, and intensive effort required to code all functionality
- Variable library is in Excel for easier setup
  - MATLAB can automate any Excel files via COM server