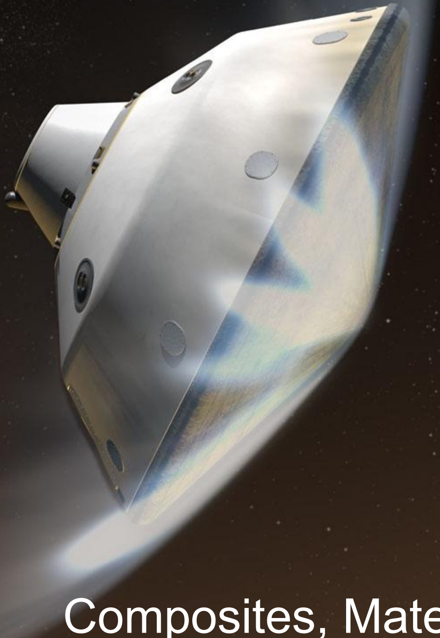
# Material Response Modeling of Ablative Thermal Protection Systems using PATO



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Composites, Materials, and Structures
Cocoa Beach, FL

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# Outline

- Overview of PATO and Applications
- Surface Modeling of Silicone Based Coatings (NuSil)
- Mechanical Erosion Modeling
- Loose Coupling with CFD Aerothermal Environment Computations

# Porous Material Analysis Toolbox based on OpenFOAM (PATO)

## OpenFOAM

- Finite Volume
- PETSc
- I/O management
- Numerical schemes
- Massive MPI
- Fluid solvers
- Moving geometry
- Chemistry
- Basic mesh gen.
- Thermo/Transp.

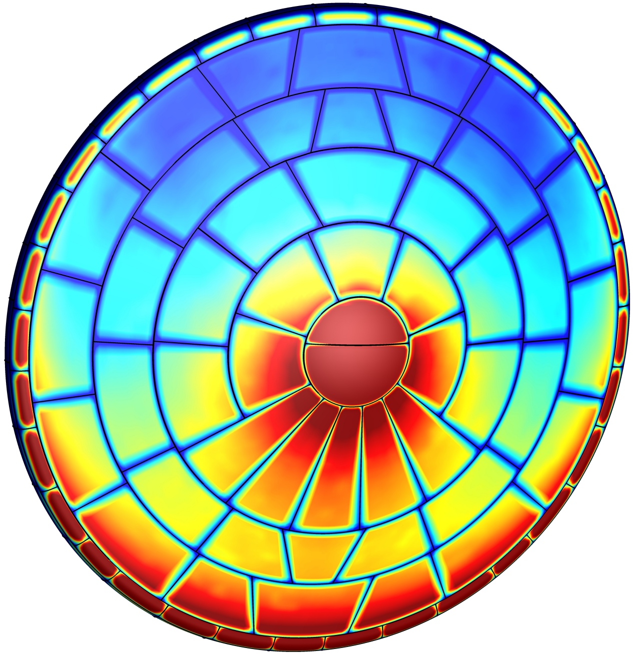
## PATO: material response

- ***PATOx exectuable***
- *Pyrolysis*
- ***libPATOx library***
- *Pure conduction*
- *Equilibrium chemistry*
- *1D/2D/3D mapping*
- *Finite-rate chemistry*
- *Multi-material*
- *Volume Ablation*
- *Fluid coupling*

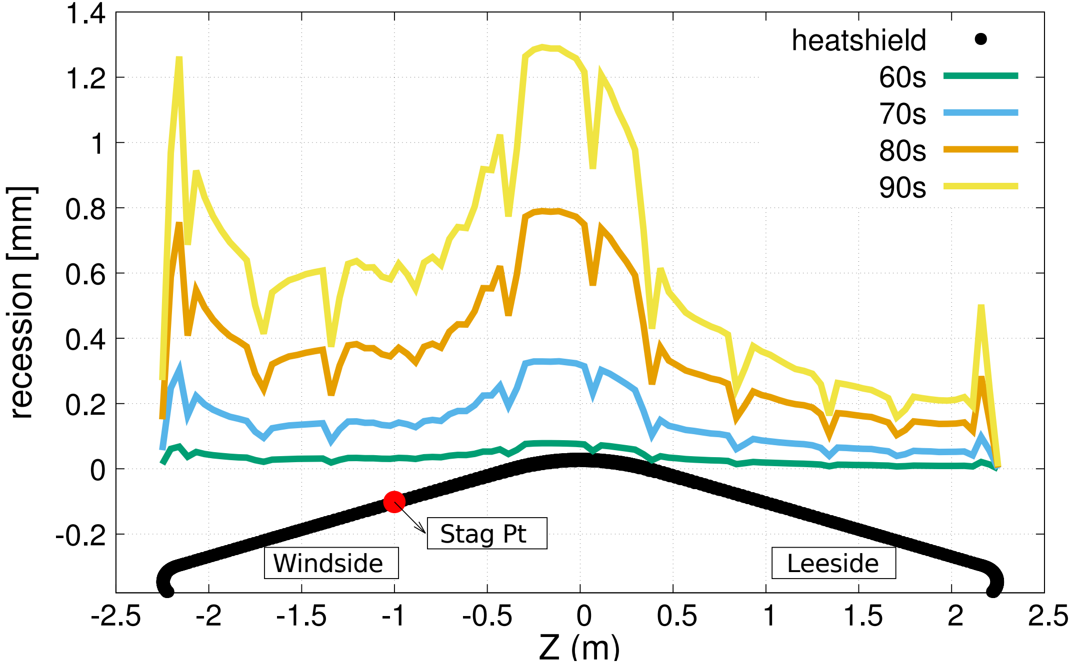
- Written in C++
- Utilizes finite volume solvers from OpenFOAM
- Mutation++ used in computing chemistry
- Open source release: [https://www.pato.ac/](https://www.pato.ac/)

Main Developer: Jeremie B. E. Meurisse

# Full Heatshield Material Response

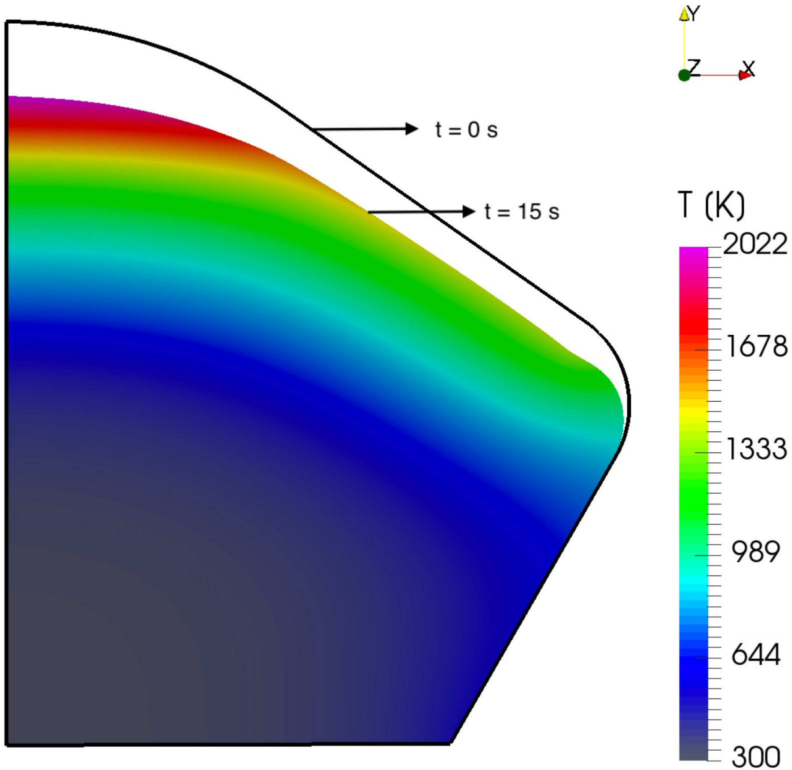


Recession computed using PATO for the Mars Science Laboratory Heatshield after atmospheric entry



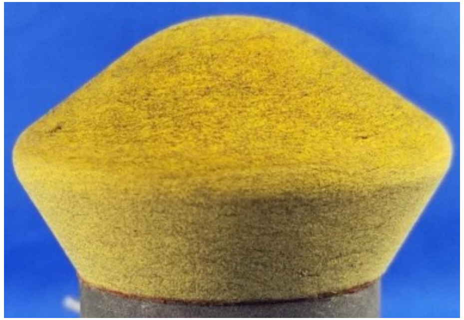
Centerline plot showing computed recession at multiple times after the entry interface

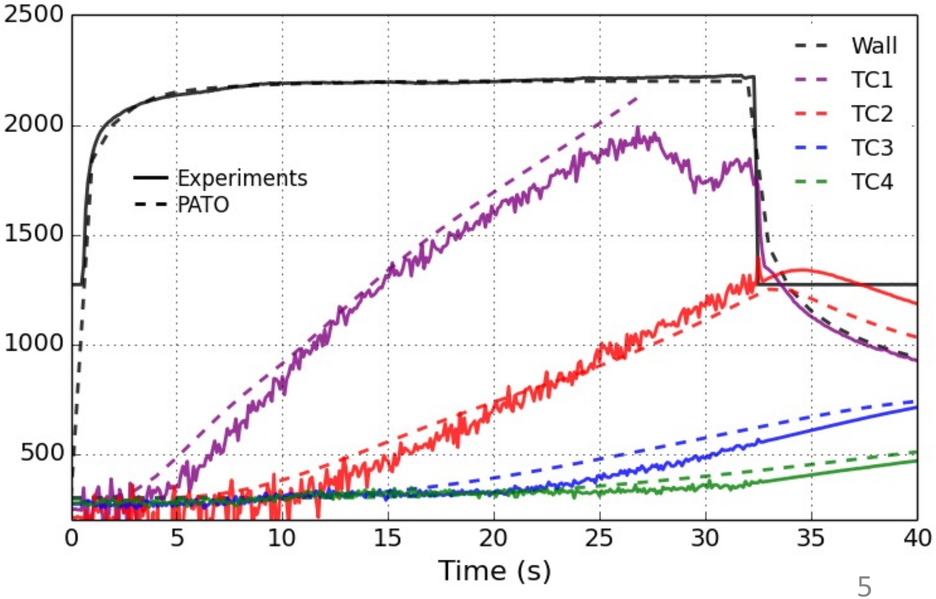
# Simulation of Arc Jet Tests



Temperature and recession at 15 sec.

sphere-cone sample





# Surface Modeling of Silicone Based Coatings (NuSil)

*Point of Contact: Jeremie Meurisse*

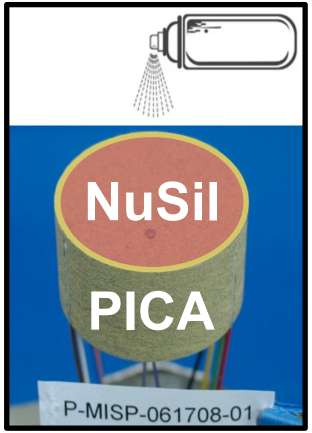
# PICA-NuSil Modeling

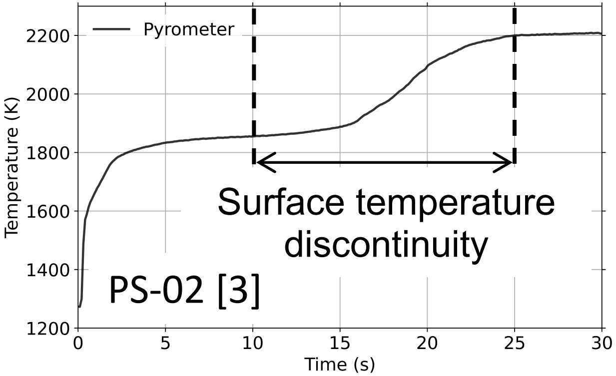
NuSil, a silicone-based overcoat, was sprayed onto the MSL and Mars 2020 heatshields including their in-depth temperature instruments (MISP) to mitigate the spread of phenolic dust from PICA.

The behavior and material response of the PICA-NuSil (PICA-N) system consists an open problem in the literature [1,2].

To better understand the behavior of the NuSil coating, dedicated experimental campaigns were conducted at NASA:

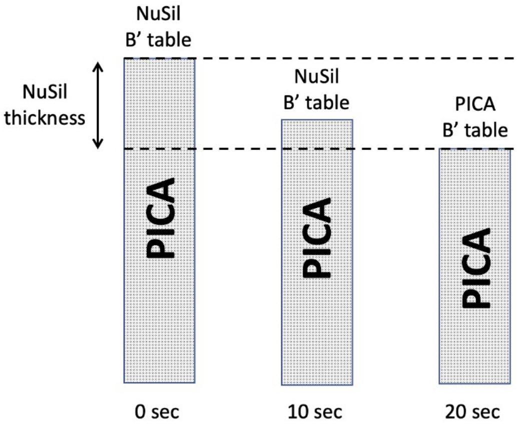
1. HyMETS at NASA LARC in March 2019 [3,4].
2. AHF at NASA ARC in November 2020.

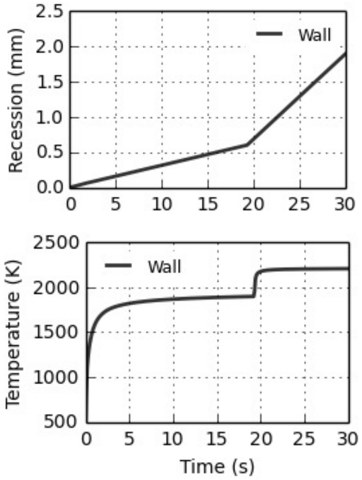


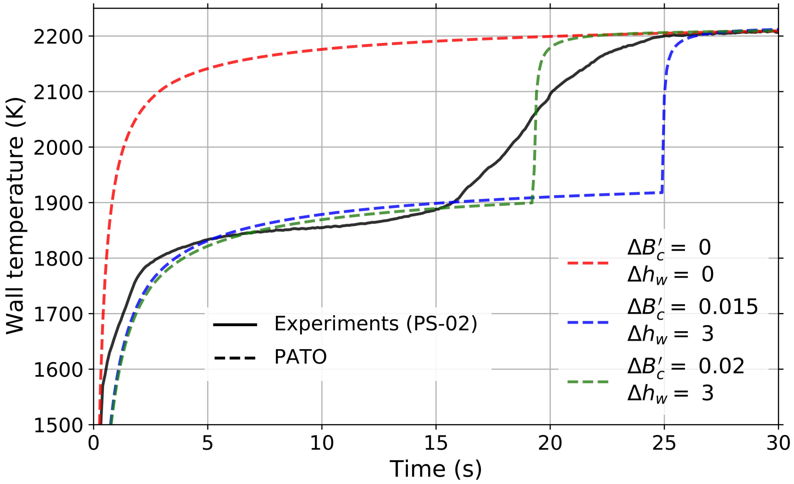


[1] Meurisse et. al, *Ablation Workshop. (2019).*
[2] Meurisse et. al, *submitted manuscript. (2021).*
[3] Bessire et. al, *IPPW. (2019).*
[4] Bessire et. al, *Ablation Workshop. (2019).*

# PICA-NuSil Modeling







A novel material response model of PICA-N was implemented in PATO. The charred NuSil surface was modeled as pure silica ($SiO_2$) based on the observations of a glassy layer on the coated samples post-test.

The surface mass and energy balance equations were modified by adding a constant offset to the char blowing rate ($\Delta B'_c$) and the wall enthalpy ($\Delta h_w$) to reproduce the HyMETS experimental results (temperature and recession).

**Meurisse et. al, Equilibrium model for the ablation response of silicone-coated PICA. *Manuscript submitted for publication. (2021).***

# PICA-N Material Response

| Material | Model | Atmosphere | Heat flux [W/cm$^2$] | Pressure [kPa] |
|---|---|---|---|---|
| PICA-N | PS-02 | Earth | 140 | 5.6 |

**Recession**: $r_{exp} = 1.93\ mm \ |\ r_{pato} = 1.98\ mm$

**NuSil B' table**: $\Delta B'_c = 0.0195 \ |\ \Delta h_w = 3\ \frac{MJ}{kg}$

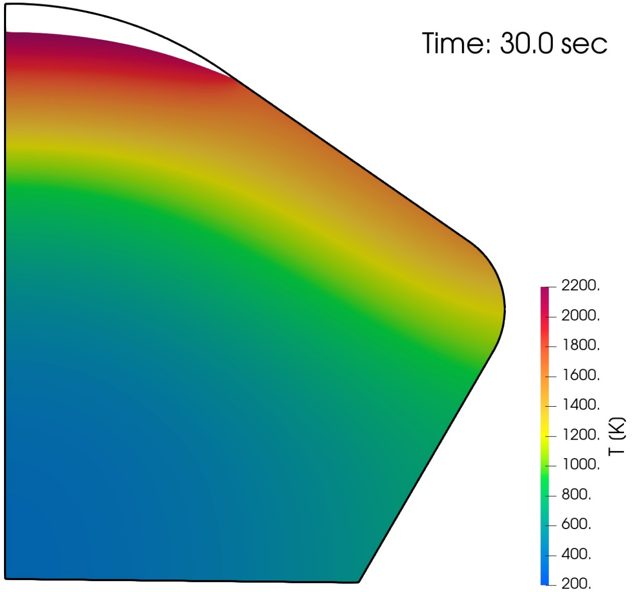


Fig. 1 Temperature at 30 sec

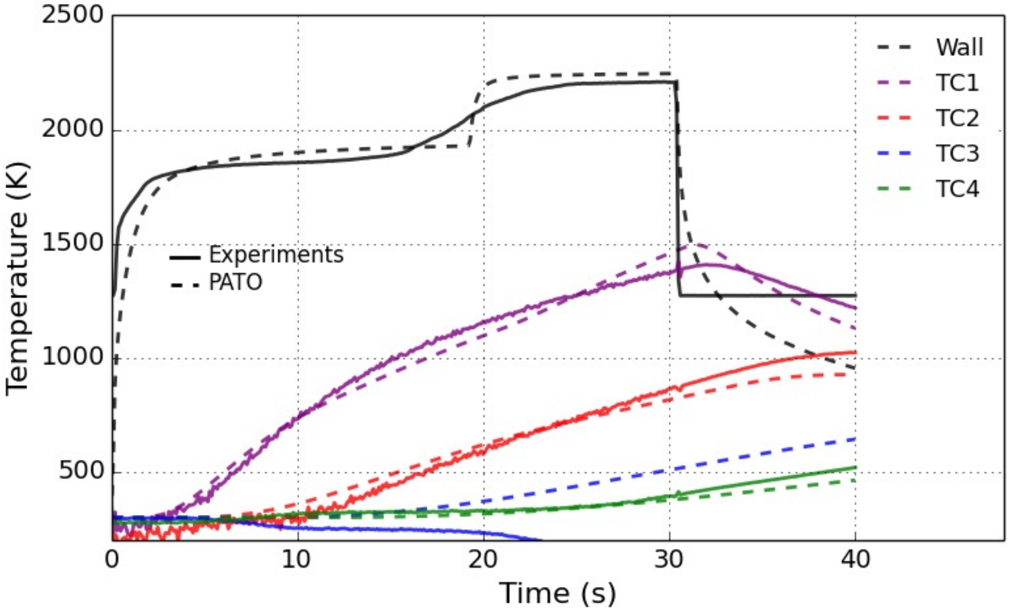
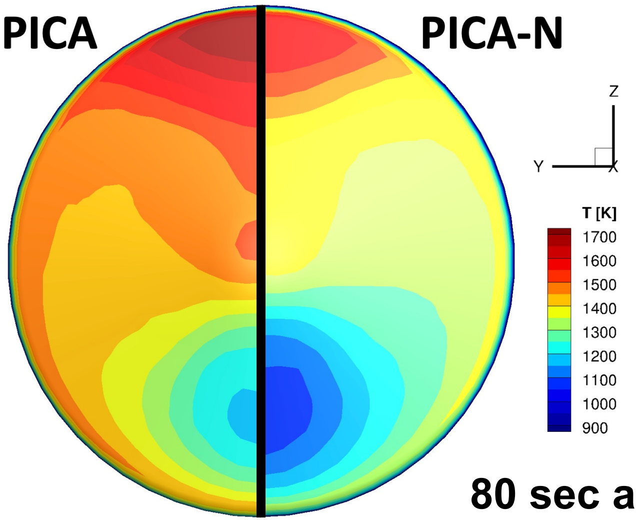


Fig. 2 Time evolution of the temperature

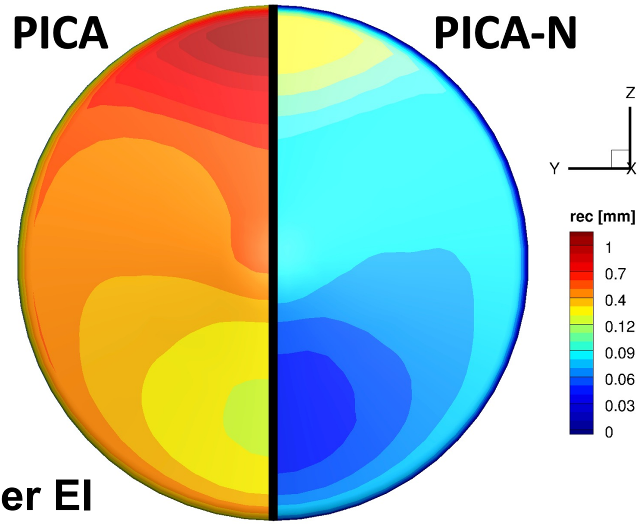
Meurisse et. al, Equilibrium model for the ablation response of silicone-coated PICA. *Manuscript submitted for publication. (2021).*

# PICA-N Material Response

Temperature from PATO



Recession from PATO



**80 sec after EI**

3D material response of the MSL heatshield using PICA and PICA-NuSil for a fully turbulent environment from DPLR. The NuSil layer thickness was estimated at 200 $\mu m$. The PICA-N model gave lower surface temperature and recession results than the PICA model. The NuSil coating still fully covered the MSL heatshield.

**Meurisse et. al, 3D material response of the MSL heatshield using NuSil-coated PICA. *IPPW. (2021).***

# Mechanical Erosion Modeling

*Point of Contact: Sergio Fraile Izquierdo*

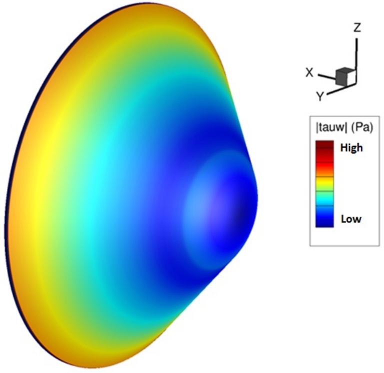
# Mechanical Erosion Modeling

Mechanical erosion may lead to additional mass removal of heatshield material during atmospheric entry, increasing the total surface recession.

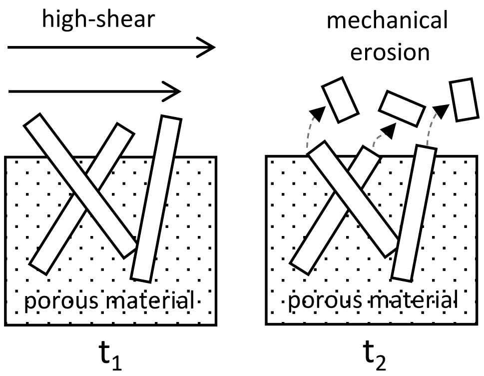
Three main mechanisms identified in the literature:

- Shear stress induced by the flow
- Normal stress induced by pyrolysis gas
- Thermal stress induced by the material's temperature field

The mechanical erosion model implemented in PATO accounts for the mass removal induced by high shear conditions.

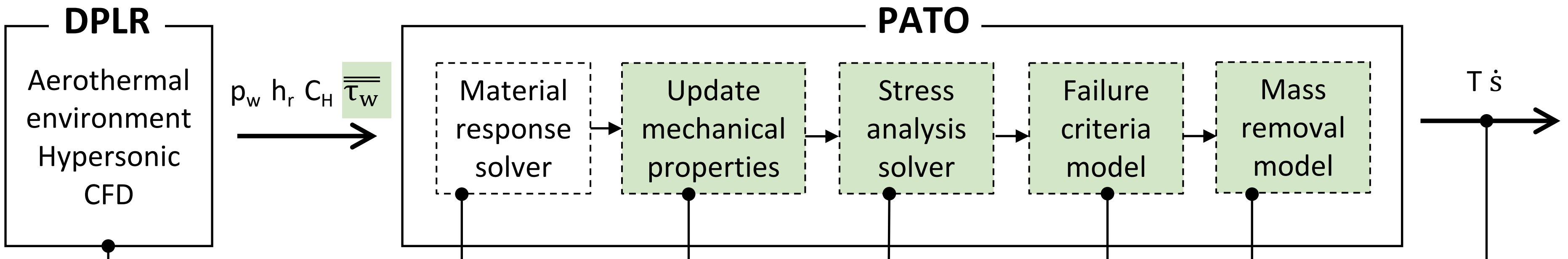


Shear stress for EEV entry



Schematic of the shear induced mass removal.

# Mechanical Erosion Modeling



Hypersonic CFD simulations are performed using the DPLR software [1]. The aerothermal environment (wall pressure [$p_w$], recovery enthalpy [$h_r$], heat transfer coefficient [$C_H$]) and wall shear stress tensor [$\overline{\overline{\tau_w}}$] are extracted.

PATO computes the pressure (Darcy's flow) and temperature inside the material as well as the surface recession.

The mechanical properties (E, G, nu and CTE) are updated as a function of the material temperature and orientation.

This solver computes the stress tensor and the displacement for orthotropic materials using the CFD wall shear stress tensor.

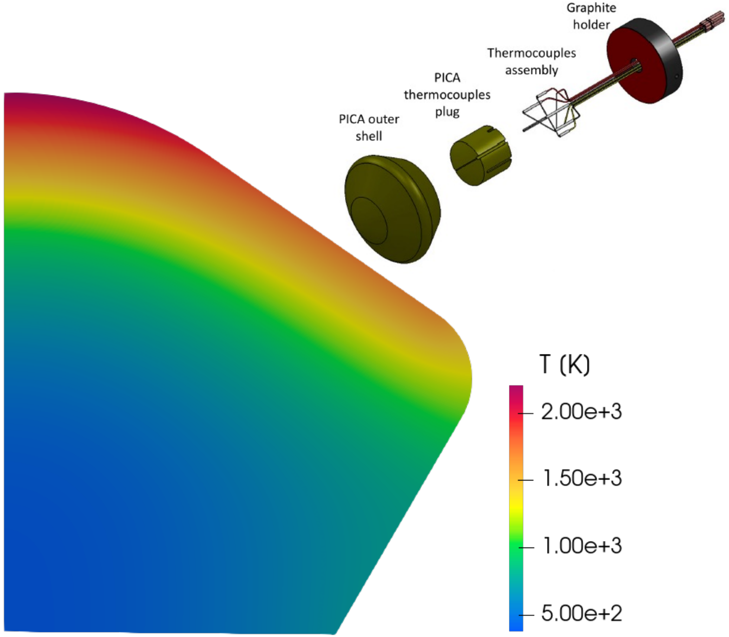
These models define the regions where the stress is higher than the ultimate strength and then move the mesh accordingly.

The model of high shear TPS mass removal coupled to material response was added to PATO. The total recession $\dot{s}$ accounts for the oxidation and the shear-induced erosion.

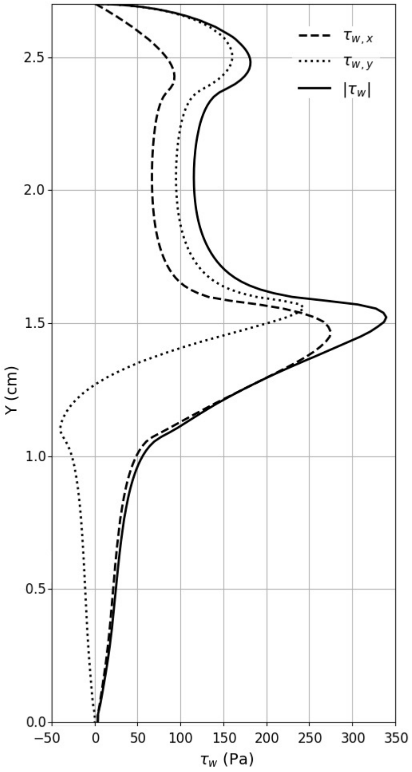
**[1] Wright et. al, DPLR Code User Manual: Acadia-Version 4.01.1. *(2009).***

# Mechanical Erosion Modeling

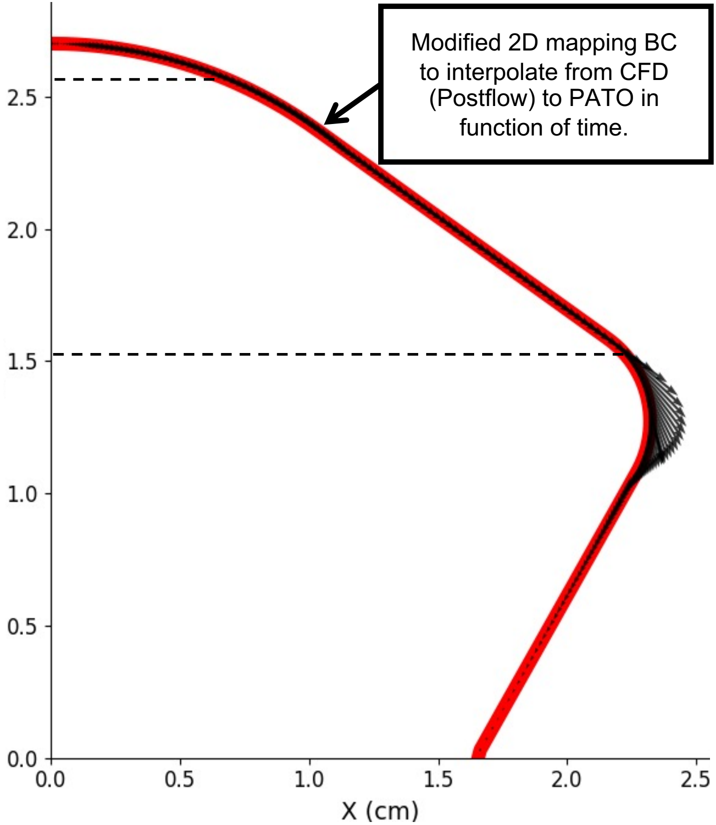
| Material | Model | Atmosphere | Heat flux [W/cm$^2$] | Pressure [kPa] |
|---|---|---|---|---|
| PICA | 12 | Mars | 126 | 5.3 |



PATO thermal response of baby-SPRITE geometry at 30 sec without recession

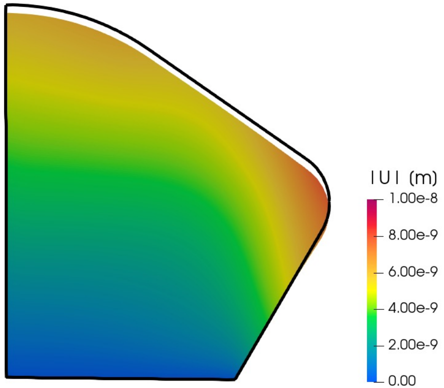


Components of the wall shear stress in function of the Y axis


Modified 2D mapping BC to interpolate from CFD (Postflow) to PATO in function of time.

Direction and magnitude of the wall shear stress

# Mechanical Erosion Modeling



Displacement using shear stress (x10) and shape scale factor (x$10^5$)

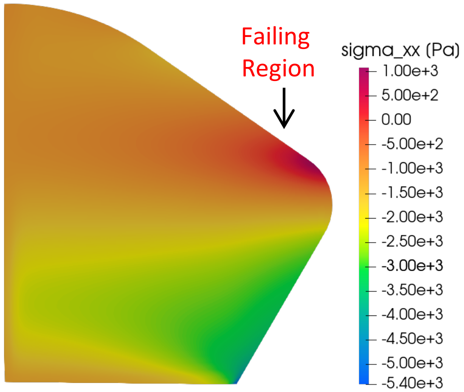
**Theoretical failure criteria**

$$\max\left(\frac{\sigma_{xx}}{\mathrm{F}_{\mathrm{tu},xx}}, \left|\frac{\sigma_{xx}}{\mathrm{F}_{\mathrm{cu},xx}}\right|, \frac{\sigma_{yy}}{\mathrm{F}_{\mathrm{tu},yy}}, \left|\frac{\sigma_{yy}}{\mathrm{F}_{\mathrm{cu},yy}}\right|, \left|\frac{\sigma_{xy}}{\mathrm{F}_{\mathrm{su},xy}}\right|\right) > 1$$

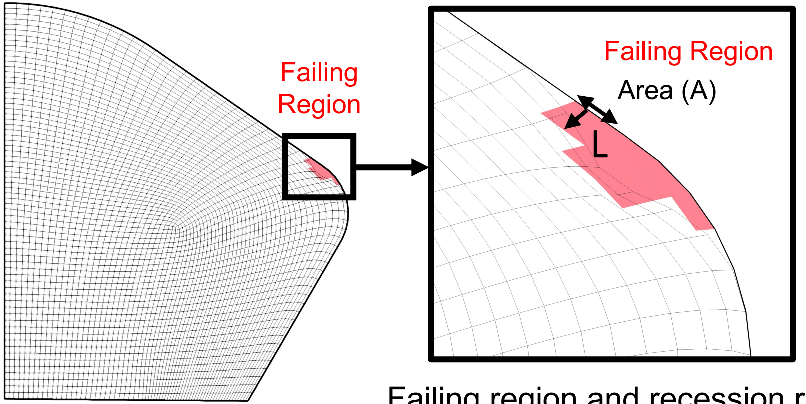
**Ultimate Strength**
tu: Traction
cu: Compression
su: Shear

$\mathrm{F}_{\mathrm{tu,\ xx}}$ = 500 Pa

$\mathrm{F}_{\mathrm{cu,\ xx}}$ = 1 MPa



Component X of the stress tensor and theoretical failure criteria



Failing region and recession rate

The recession rate and the mass loss are computed as follows:

$$M_{\mathrm{loss}} = \rho\ A\ \dot{s}\ \Delta t \qquad \dot{s} = \frac{L}{\Delta t}$$

The total mass loss and its ratio with the sample mass are:

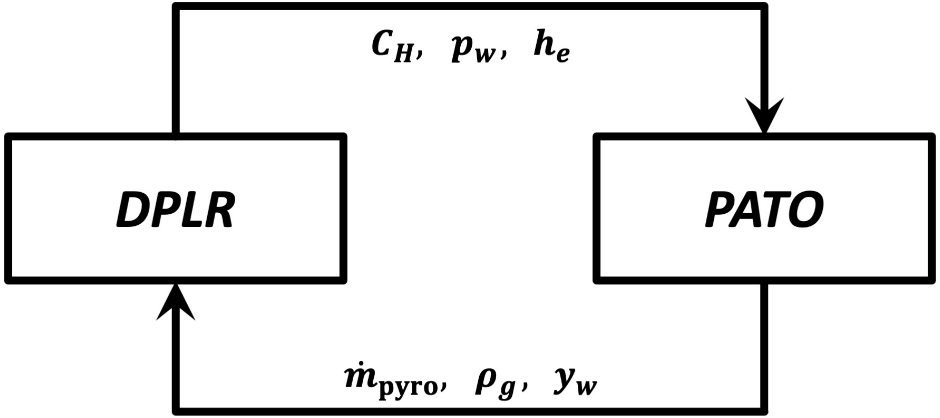
$$M_{\mathrm{loss}} = 6.33 \cdot 10^{-7}\ \mathrm{kg}$$
$$M_{\mathrm{loss}}/M_{\mathrm{sample}} = 0.70\%$$

# Loose Coupling with CFD

# Loose Coupling with CFD

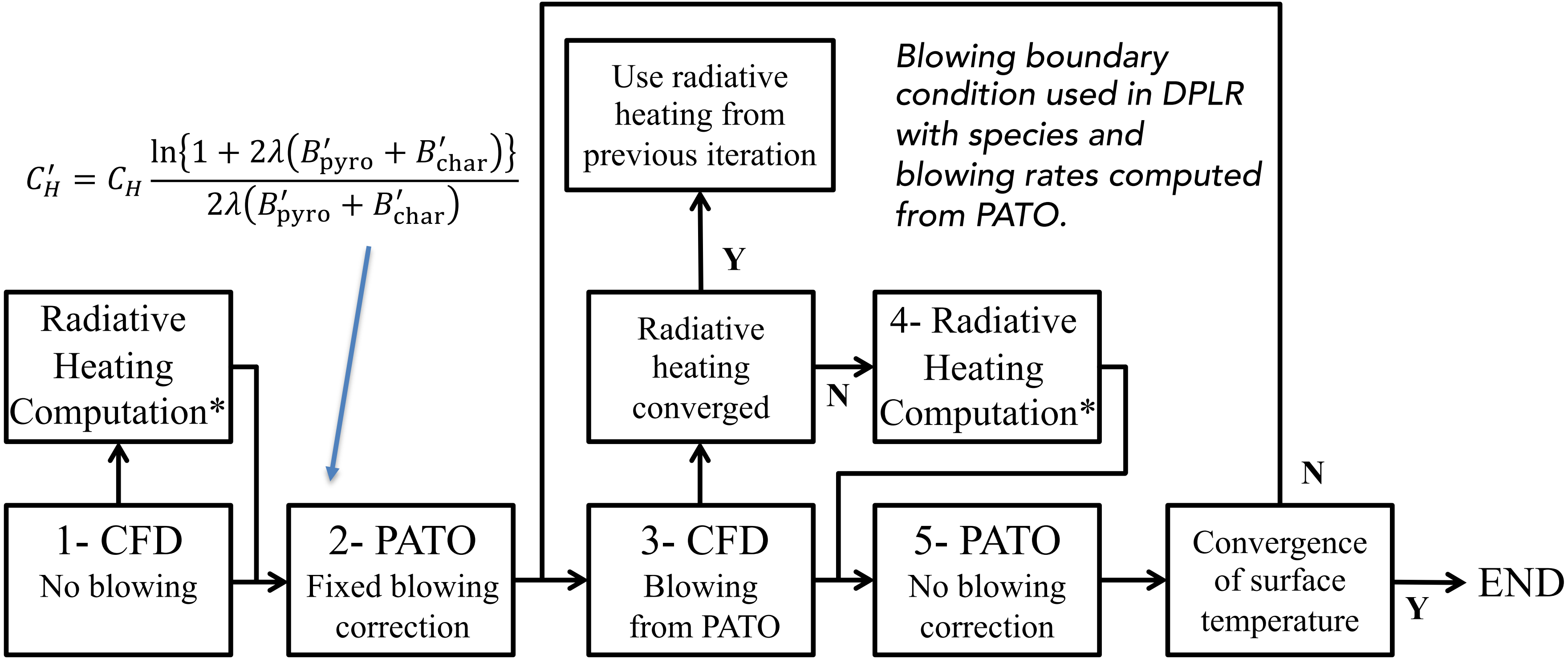
Coupling via pyrolysis gas blowing at the heatshield surface:

- Blowing gases computed in PATO and given to DPLR for use in a blowing boundary condition.
- Pressure, heat transfer coefficient and boundary layer edge enthalpy computed in DPLR and given to PATO.



***Objective is to utilize this coupling in computing MSL and Mars 2020 material responses.***

# Coupling Methodology



$$C_H' = C_H \frac{\ln\{1 + 2\lambda(B'_{\mathrm{pyro}} + B'_{\mathrm{char}})\}}{2\lambda(B'_{\mathrm{pyro}} + B'_{\mathrm{char}})}$$

Radiative Heating Computation*

1- CFD
No blowing

2- PATO
Fixed blowing correction

3- CFD
Blowing from PATO

Radiative heating converged

Y

Use radiative heating from previous iteration

N

4- Radiative Heating Computation*

5- PATO
No blowing correction

Convergence of surface temperature

N

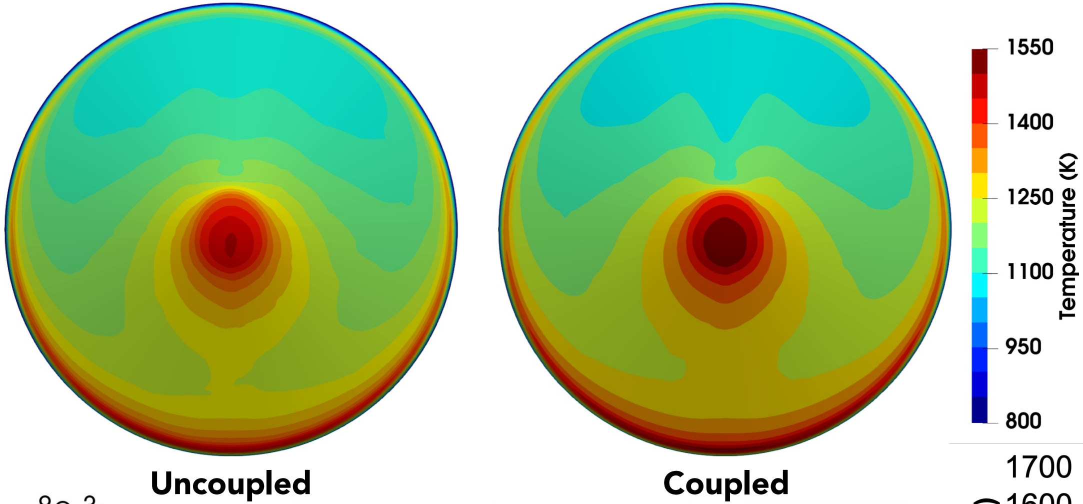
Y

END

*Blowing boundary condition used in DPLR with species and blowing rates computed from PATO.*

*Using NEQAIR: E. Whiting et al. (1996) *NASA RP-1389*.

# Heatshield Surface at 65s

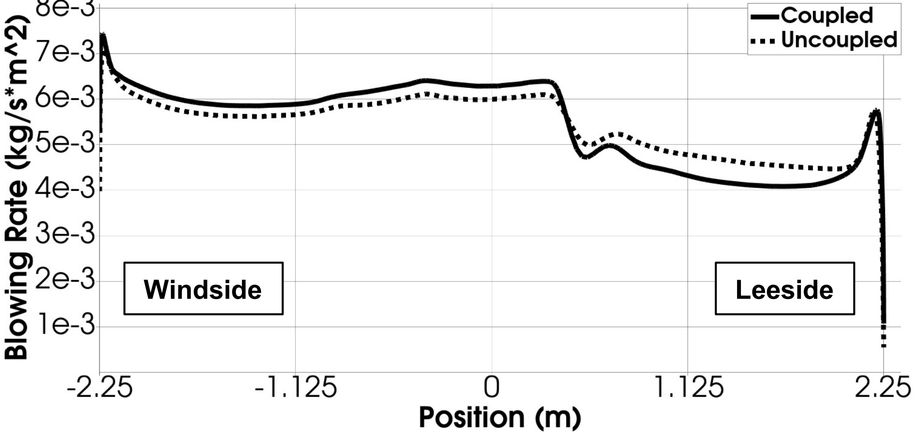


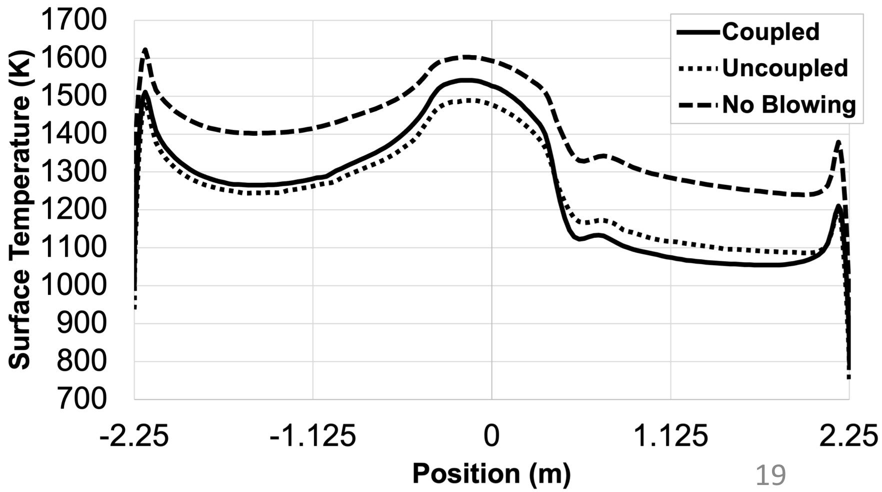
**Uncoupled**

**Coupled**

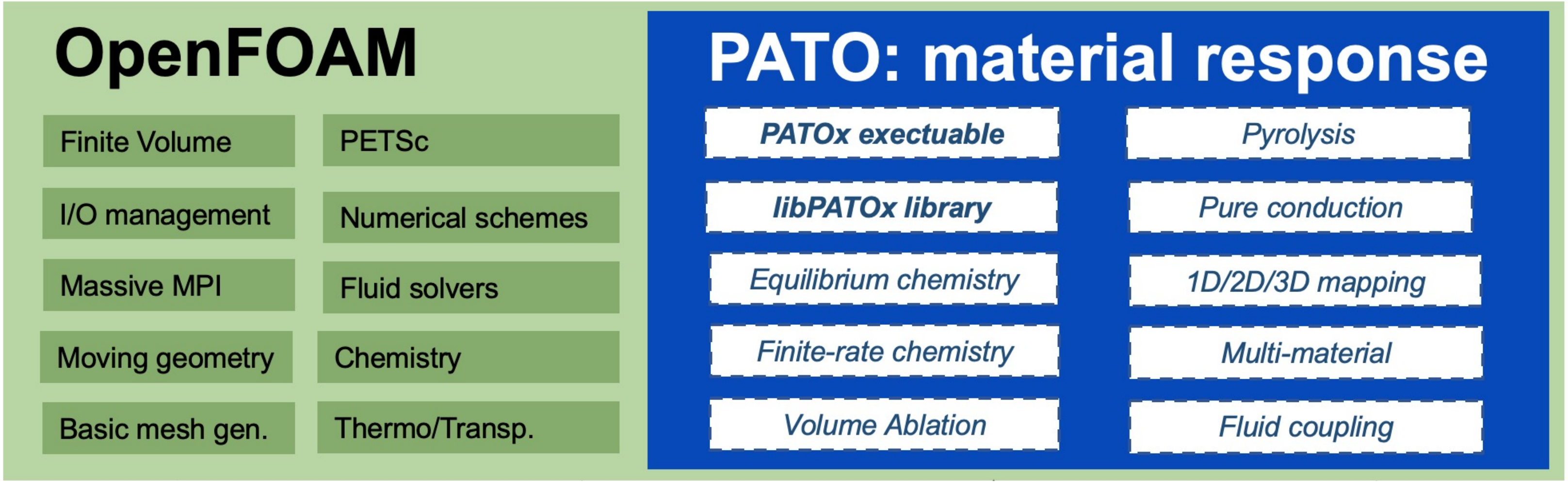
**Contour plots of surface temperature for the coupled and uncoupled simulations at 65s**

**(Below) Centerline plots of pyrolysis mass flux at the surface (left) and temperature (right). The surface temperature without blowing was computed directly by DPLR.**





# Summary



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PATO release: https://www.pato.ac/

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*john.m.thornton@nasa.gov*

**Current Efforts:**

- Surface Phenomena Modeling with NuSil Coating
- Mechanical Erosion Modeling
- Loose Coupling with CFD