# Development of new physics-based models in PATO

## 13th Ablation Workshop

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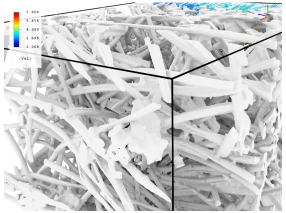
Nov 7th, 2023

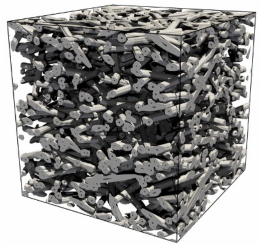
# ESM: Predictive Material Modeling[1]

## MICRO-SCALE MODELING

SPARTA

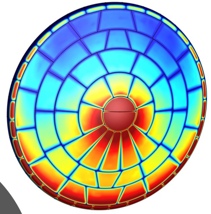


PuMA



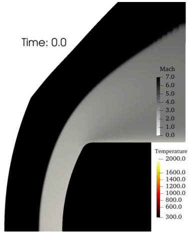
## MACRO-SCALE MODELING

PATO



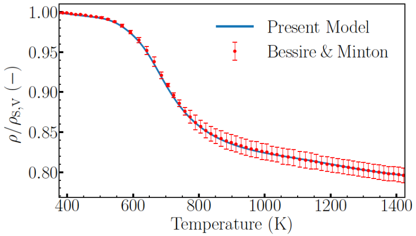
*Transfer of relevant physics-based models*

Icarus/Ares



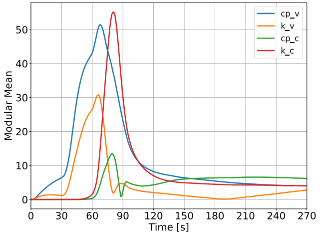

## EXPERIMENTS

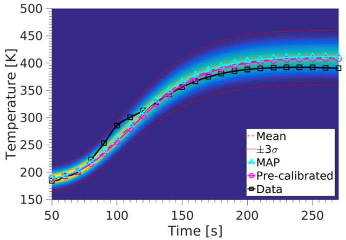
Verification & Validation



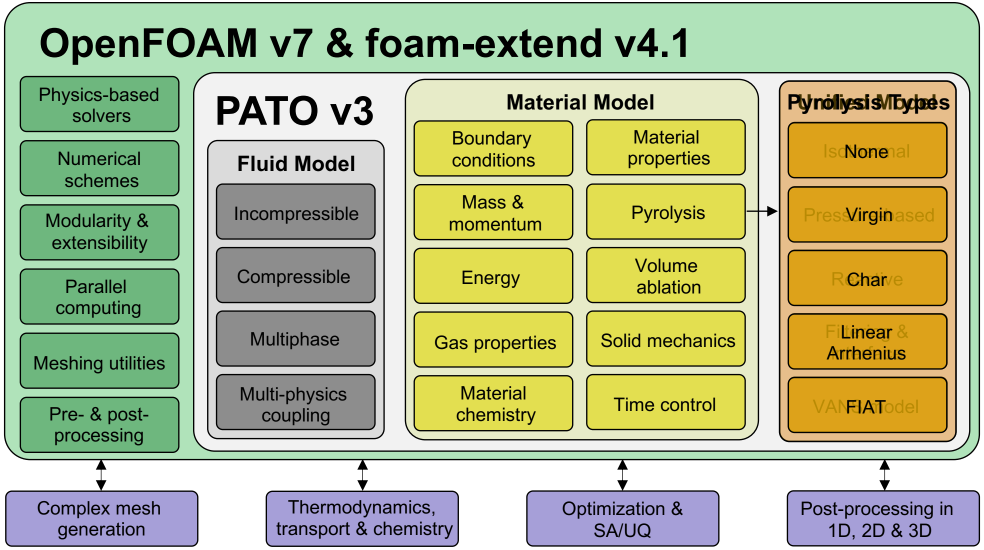

## OPTIMIZATION & SA/UQ

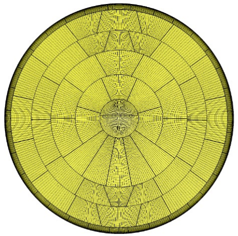
Dakota



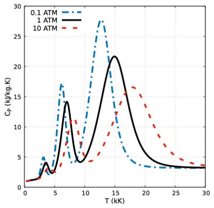



# PATO: Platform to Design New Physics-based Models[2]

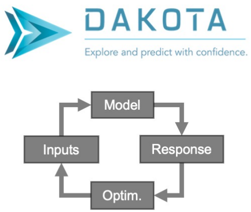


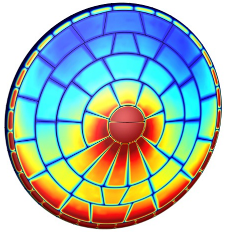
**POINTWISE/GMSH**




**MUTATION++**




**DAKOTA**



**FV/TEC**

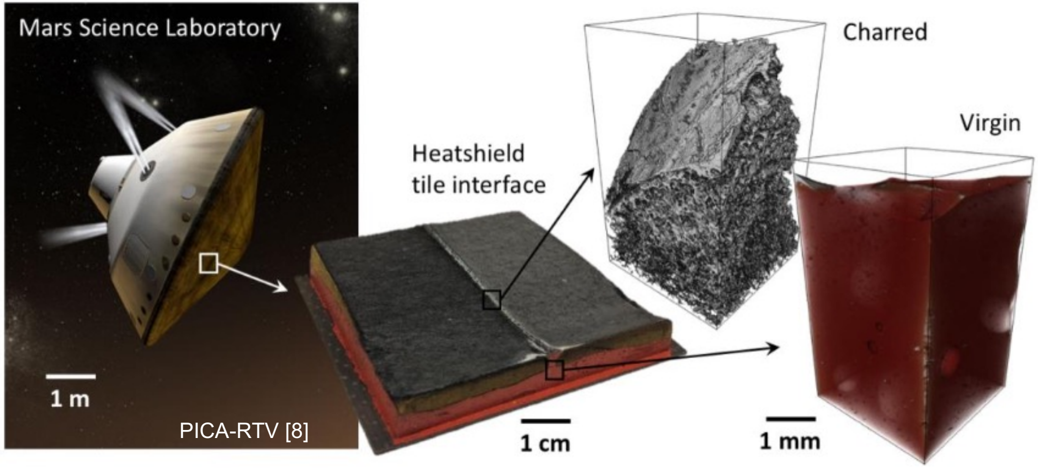
## PATO overview

- **Created in 2010** by Jean Lachaud and Nagi Mansour.
- Estimated **200+ active users** as of 2023. Membership on the developer Gitlab reached **100 members** last month.
- Comprehensive details and updates about PATO: https://www.pato.ac
- PATO v3.1 was released in September 2023 on: https://github.com/nasa/pato
- Installation of PATO and its dependencies, such as OpenFOAM and foam-extend, is streamlined via conda:

```
conda create --name pato-3.1 -c conda-forge -c pato.devel pato=3.1
conda create --name pato-dev -c conda-forge -c pato.devel pato=dev
```

- Over **60 tutorials** and a 100-page **User Manual.**
- **Core team of PATO developers** at NASA Ames includes Jeremie Meurisse, Bruno Dias, John M. Thornton, Georgios Bellas Chatzigeorgis, and Sergio Fraile Izquierdo.

# PICA-RTV: Fencing Effect

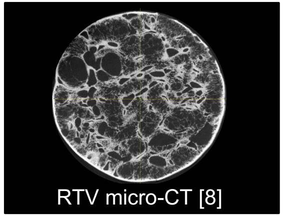


PICA-RTV [8]


Virgin Avcoat-RTV [NASA]


Charred Avcoat-RTV [NASA]


PICA-RTV [7]


RTV micro-CT [8]

Current tiled ablative heatshields use Room Temperature Vulcanizing (RTV) silicone as a gap filler between tiles. Fences are formed between tiles during ablation impacting the environment.

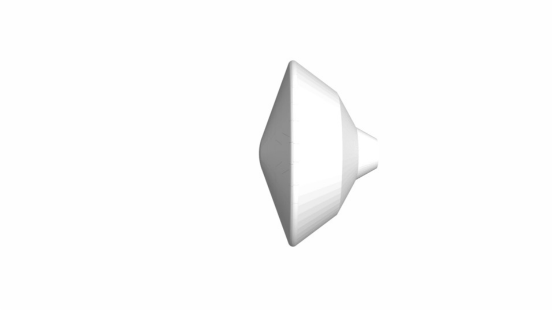
**How much impact RTV fencing effect has on the thermal response of a tiled heatshield?**

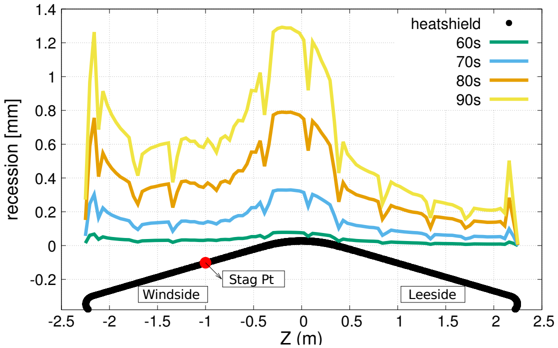


P.O.C. Sergio Fraile Izquierdo, AMA Inc. at NASA ARC TSM.

# PICA-RTV: Intumescence Model

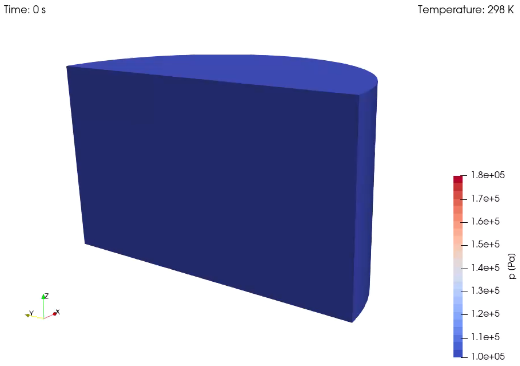
## 3D simulations of a full-scale tiled ablative heatshield[3]






## Macro-scale intumescence model to predict the RTV expansion and shrinkage[4]

*Check out Vishnu Oruganti's poster!*




**Stress analysis module**:

- Mechanical properties as function of temperature.
- Thermal expansion & shrinking.
- Stress due to the pressure build-up from pyrolysis.

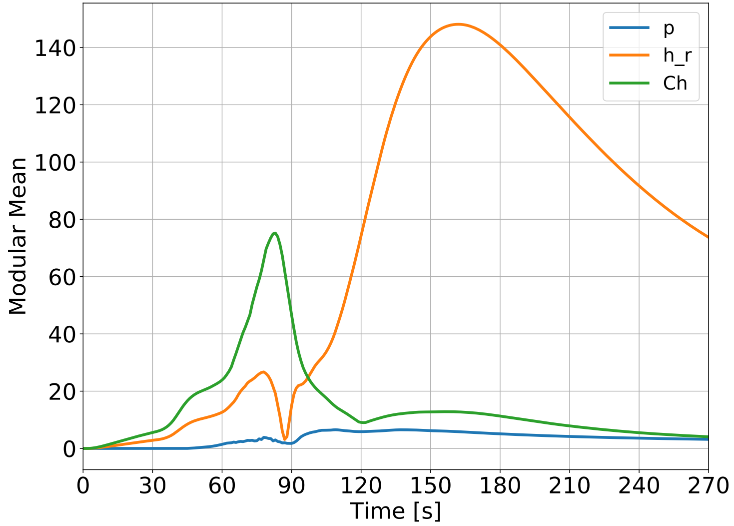
$$\frac{\partial}{\partial t}\int_{\Omega_0}\rho\,\frac{\partial u}{\partial t}\,\mathrm{d}\Omega_0 = \overbrace{\oint_{\Gamma_0} n_0\cdot(K\cdot\nabla u)\,\mathrm{d}\Gamma_0}^{\text{Implicit Term}}$$

$$+\overbrace{\oint_{\Gamma_0} n_0\cdot\sigma\,\mathrm{d}\Gamma_0 - \oint_{\Gamma_0} n_0\cdot(K\cdot\nabla u)\,\mathrm{d}\Gamma_0 - \int_{\Omega_0}\nabla P\,\mathrm{d}\Omega_0}^{\text{Explicit Terms}}$$

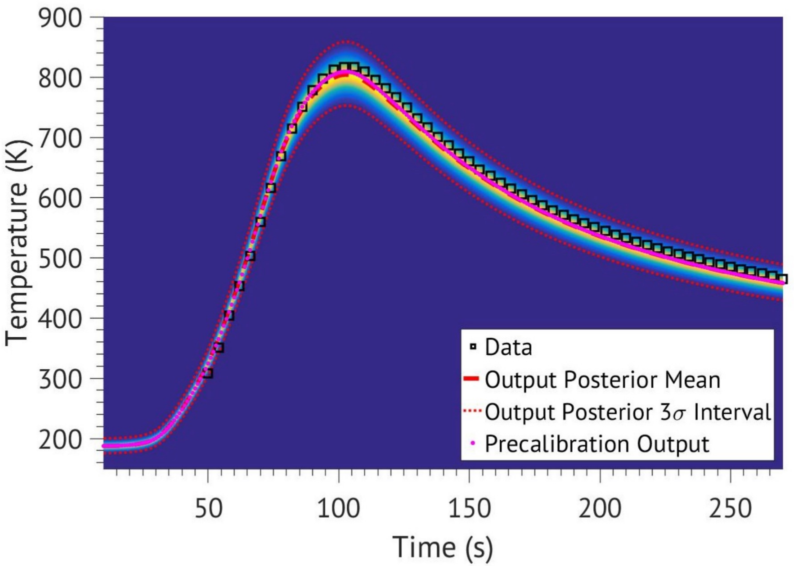
P.O.C. Sergio Fraile Izquierdo, AMA Inc. at NASA ARC TSM.

# PICA: Sensitivity & Uncertainty Analysis

**Sensitivity Analysis:** aerothermal environment




**Uncertainty Quantification:** MSL flight data[5]

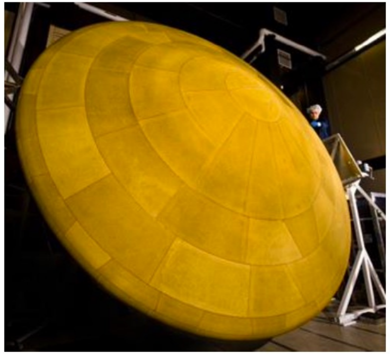



**How much uncertainty exists in the thermal prediction of PICA for future flight missions?**

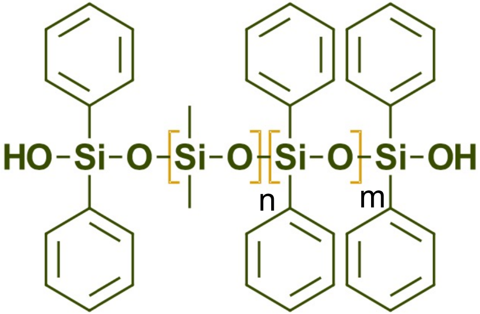
P.O.C. John M. Thornton, AMA Inc. at NASA ARC TSM.

# PICA-NuSil: Particle Shedding Mitigation[6]

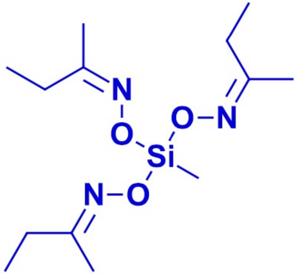
**PICA**



**Siloxane Copolymer Backbone**




**Oxime Crosslinking Agent**




**Credit: Bessire**

The phenolic phase of PICA is friable. A thin coating of NuSil (CV-1144-0) is applied to the surface of flight hardware to mitigate particle shedding during pre-flight activities.

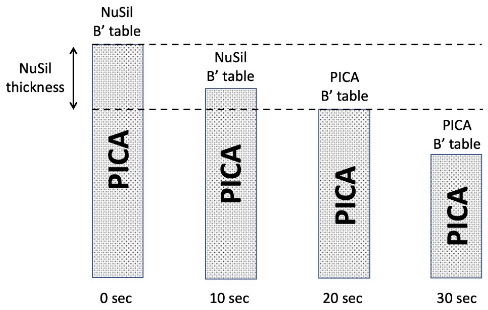
**What is the impact of NuSil on the performance of PICA during arc-jet testing and in flight?**

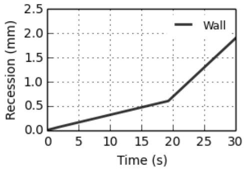
P.O.C. Brody Bessire, NASA ARC TSM.

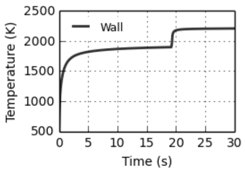
# PICA-NuSil: Coating Model

## Thin coating assumption

Only the surface is modeled, the material and pyrolysis gas properties are ignored for NuSil.



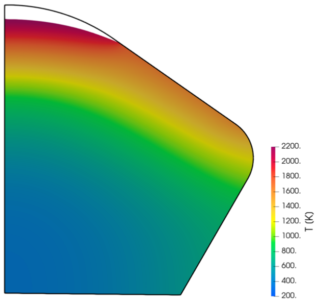



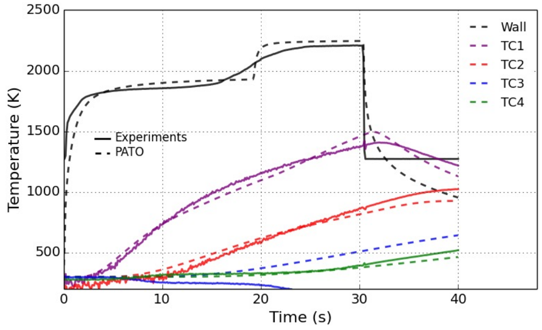

$$B'_{c} = \frac{\sum_{l=1}^{N_{el}^{s}} \left[B'_{g}\left(z_{l,pg} - z_{l,w}\right) + z_{l,e} - z_{l,w}\right]}{\sum_{l=1}^{N_{el}^{s}} \left(z_{l,w} - z_{l,ca}\right)}$$

## Ground facility model[7]

Pure $SiO_2$ model was modified to match the experiments (mostly air).

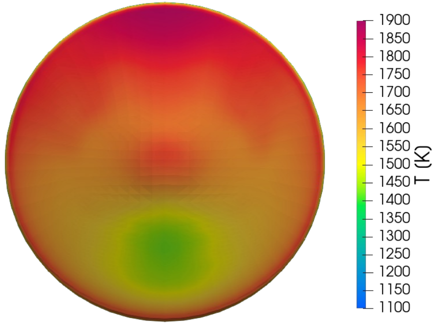


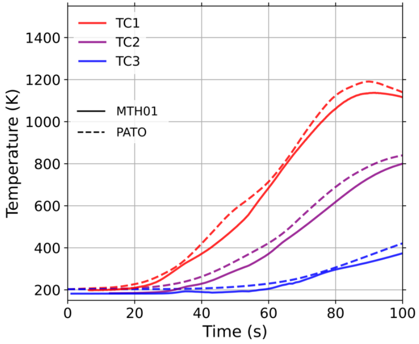





## Flight model[8]

Good agreement was found between pure $SiO_2$ model and flight data (MTH).



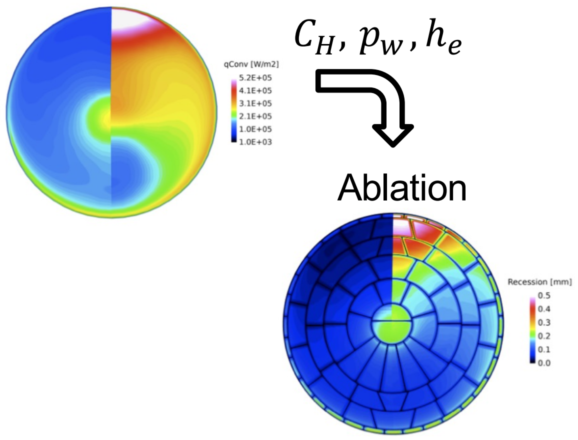



# PICA: Coupled CFD and Ablation via Pyro Gas[9]



## Uncoupled approach

CFD

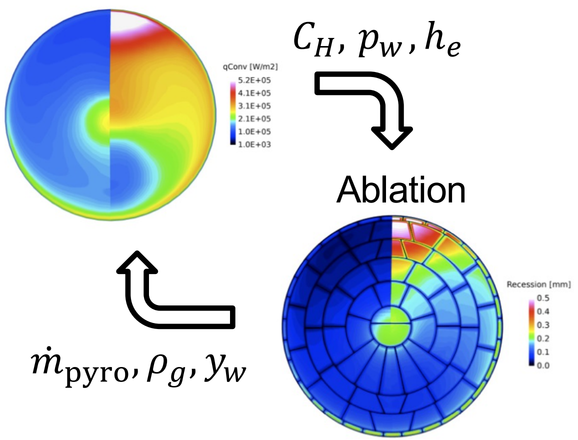



$C_H, p_w, h_e$

Ablation

## Coupled approach

CFD




$C_H, p_w, h_e$

Ablation

$\dot{m}_{\text{pyro}}, \rho_g, y_w$

## Coupling Methodology

1. **DPLR** No blowing
2. **NEQAIR** Radiation
3. **PATO** Fixed blowing correction
4. **DPLR** Blowing from PATO
5. **NEQAIR** Radiation
6. **PATO** No blowing correction

Loop up to convergence of surface temperature

Blowing correction

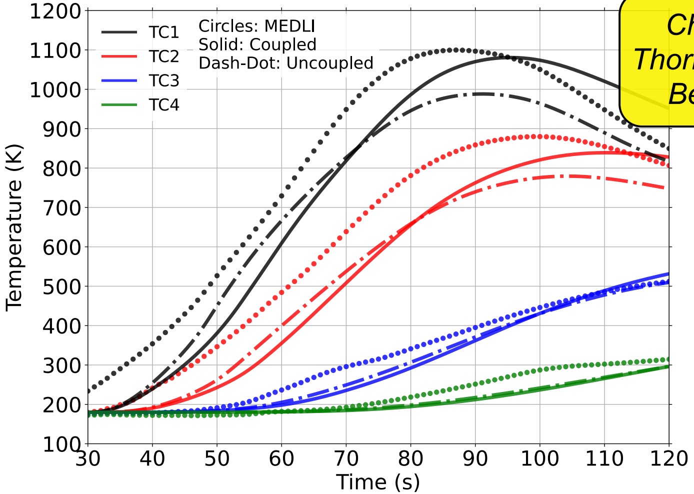
$$C'_H = C_H \frac{\ln\{1 + 2\lambda(B'_{\text{pyro}} + B'_{\text{char}})\}}{2\lambda(B'_{\text{pyro}} + B'_{\text{char}})}$$

**How does enhancing the accuracy of CFD/MR coupling affect thermal predictions for PICA?**

P.O.C. John M. Thornton, AMA Inc. at NASA ARC TSM.

# PICA: Coupled CFD and Ablation via Pyro Gas[9]

## Sphere Case for MSL MISP1




*Check out John Thornton's & George Bellas' posters!*

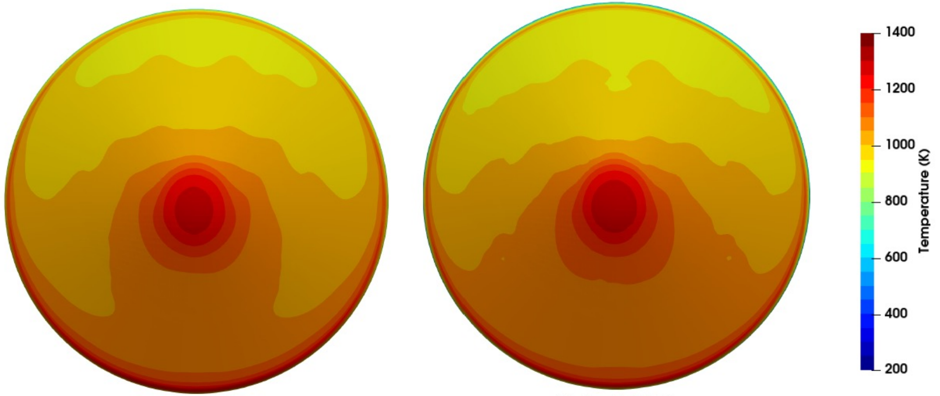
- 2D axisymmetric sphere case.
- Environments from MSL MISP1.
- Includes radiative heating.
- No early trajectory (DSMC) or recession.
- Good agreement with MISP flight data.

## Massive Mars 2020 Coupled Simulations

| | |
|---|---|
| *Resources:* | 600 processors (Haswell) |
| *Runtime:* | 14 days |
| *3D Refined Grid:* | 9M (DPLR) & 1M (PATO) |

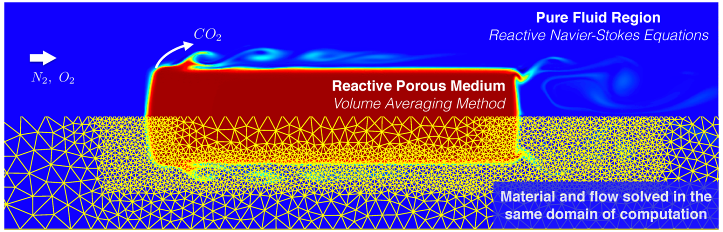
## PICA Surface Temperature at 80 sec

Uncoupled Coupled



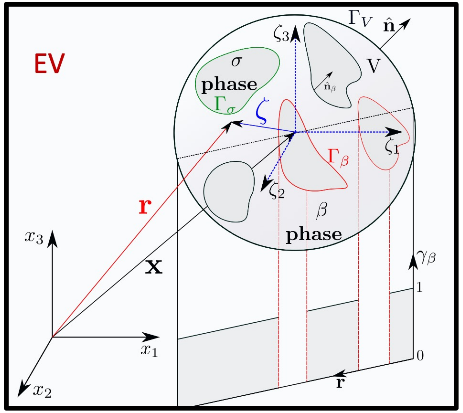

P.O.C. John M. Thornton, AMA Inc. at NASA ARC TSM.

# FiberForm: Unified Flow-Material Coupling[10]




**Credit: Schrooyen et al.[11]**

- Solves the flow field and the material in the same computational domain.
- Models the interface progression as a cause of the material degradation.
- Requires effective properties at the interface region.




To consider both phases in the same computational domain, one must account for the multi-scale aspects of porous media structures. **One must locally average the governing equations using Volume Average Navier-Stokes (VANS) equations[10]** over a volume that might contain n-phases.

$$\partial_t \boldsymbol{U}_\beta + \boldsymbol{\nabla} \cdot \boldsymbol{F}_\beta^{\text{inv}} + \boldsymbol{\nabla} \cdot \boldsymbol{F}_\beta^{\text{vis}} = \boldsymbol{S}_\beta$$

$$\partial_t \varepsilon_\beta \left\langle \boldsymbol{U}_\beta \right\rangle + \boldsymbol{\nabla} \cdot \varepsilon_\beta \left\langle \boldsymbol{F}_\beta^{\text{inv}} \right\rangle + \boldsymbol{\nabla} \cdot \varepsilon_\beta \left\langle \boldsymbol{F}_\beta^{\text{vis}} \right\rangle + \oint_{\Gamma_\beta} m \boldsymbol{S}_\beta^{\text{surf}} \cdot \hat{\boldsymbol{n}}_\beta \mathrm{d}\Gamma_\beta = 0$$

**What is the impact of removing heritage boundary assumptions using a unified coupling?**

P.O.C. Bruno Dias, ORAU at NASA ARC TSM.

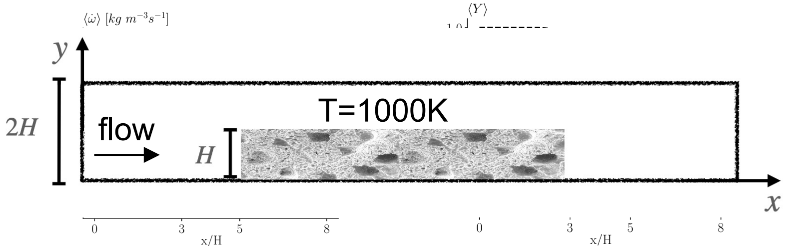
# FiberForm: Flow Tube Modeling using Unified Coupling

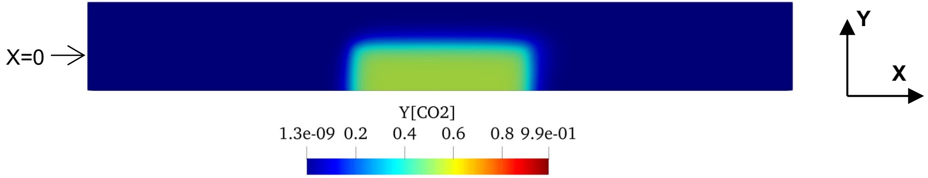
*Check out Bruno Dias' poster!*

## $CO_2$ production

The initial temperature is 1000 K in the pure fluid and porous material. These conditions represent the flow tube experiment carried out by Panerai et al.[12]

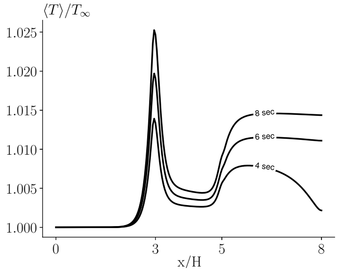
The molecular oxygen reacts with the carbon fibers, leading to the production of $CO_2$. The production of $CO_2$ is higher at x/H = 3 due to a high concentration of $O_2$, causing a higher reaction rate of the fibers.

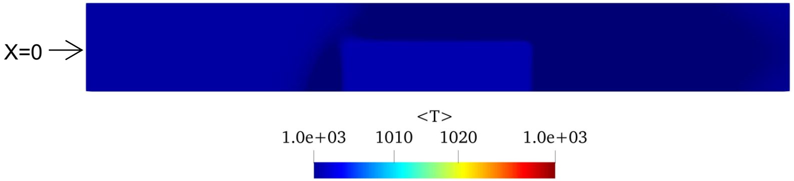



## Temperature Increase

The temperature increase at the porous material surface is due to the chemical source term and the increase of the diffusive heat flux. This chemical source is caused by the formation of $CO_2$ due to the heterogeneous reactions, while the concentration gradient drives the diffusive heat flux. A similar trend was observed by Panerai et al.[13]




P.O.C. Bruno Dias, ORAU at NASA ARC TSM.

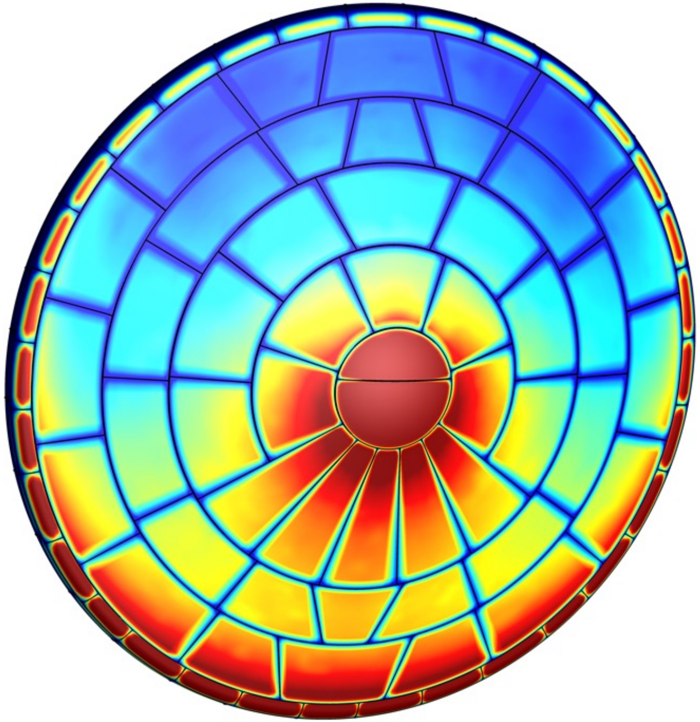
# Conclusion

## New physics-based models implemented in PATO:

- **Solid mechanics models** for solving stress analysis problems, incorporating temperature-dependent material properties.
- **Intumescence model** for simulating RTV-like materials under heat, considering their thermal and pyrolysis-induced volume changes.
- **Tiled heatshield simulations** to analyze fencing effects resulting from disparate recession rates between PICA and RTV materials.
- **Sensitivity and uncertainty analysis** to establish predicted temperature uncertainty bounds compared to MEDLI flight data.
- **Coating model** to evaluate NuSil's effect on PICA showing lower recession and temperature, aligning well with MEDLI2 flight data.
- **Pyrolysis gas coupling** enhances blowing correction fidelity, yielding a higher peak heating than in the uncoupled scenario.
- **Unified material-flow coupling** allows modeling oxidation of porous materials without using heat transfer coefficient approach.

**PATO is a modular research & development platform designed to test innovative physics-based models for porous materials submitted to high-temperature environments at the macro-scale.**

# Thank you for your attention! Any questions?



## PATO version 3

https://www.pato.ac

**P**orous-material
**A**nalysis
**T**oolbox based on
**O**penFOAM

# References

[1] Brandis, Aaron M., et al. "New Developments in NASA's Entry Systems Modeling Project." AIAA SCITECH 2023 Forum. 2023.
[2] Lachaud, Jean, et al. "A generic local thermal equilibrium model for porous reactive materials submitted to high temperatures." International Journal of Heat and Mass Transfer 108 (2017): 1406-1417.
[3] Meurisse, Jeremie BE, et al. "Multidimensional material response simulations of a full-scale tiled ablative heatshield." Aerospace Science and Technology 76 (2018): 497-511.
[4] Oruganti, Sreevishnu, et al. "Microstructure of pyrolyzing RTV silicone." Polymer Degradation and Stability 207 (2023): 110237.
[5] Rostkowski, Przemyslaw. Construction of predictive uncertainty quantification framework to the extension of TPS plasma wind tunnel experiment data to flight conditions. Diss. 2022.
[6] Bessire, Brody K., et al. "Material Response Analysis of PICA-NuSil at the Hypersonic Materials Environmental Test System." AIAA AVIATION 2023 Forum. 2023.
[7] Meurisse, Jeremie BE, et al. "Equilibrium model for the ablation response of silicone-coated PICA." International Journal of Heat and Mass Transfer 201 (2023): 123523.
[8] Meurisse, Jeremie B., et al. "3D ablation modeling of silicone-coated heatshield compared to MEDLI2 in-flight data." AIAA SCITECH 2023 Forum. 2023.
[9] Thornton, John M., et al. "Coupling Heatshield Response and Aerothermal Environment for Mars Entry via Surface Gas Blowing." AIAA SCITECH 2023 Forum. 2023.
[10] Dias, Bruno, et al. "Towards a flow-material unified solver for heatshield modeling." AIAA SCITECH 2023 Forum. 2023.
[11] Schrooyen, Pierre, et al. "Fully implicit Discontinuous Galerkin solver to study surface and volume ablation competition in atmospheric entry flows." *International Journal of Heat and Mass Transfer* 103 (2016): 108-124.
[12] Panerai, Francesco, et al. "Flow-tube oxidation experiments on the carbon preform of a phenolic-impregnated carbon ablator." Journal of Thermophysics and Heat Transfer 28.2 (2014): 181-190.
[13] Panerai, Francesco, et al. "Experimental and numerical study of carbon fiber oxidation." Proc. 52nd Aerospace Sciences Meeting, AIAA paper. No. 2014-1208. 2014.