UPDATES TO THE PREDICTIVE MATERIAL MODELING SOFTWARE TOOLS

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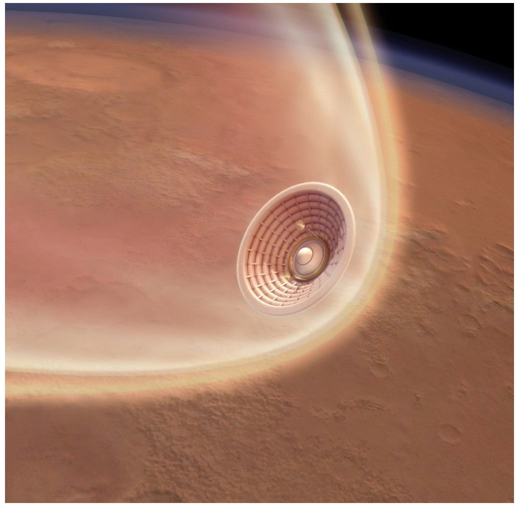
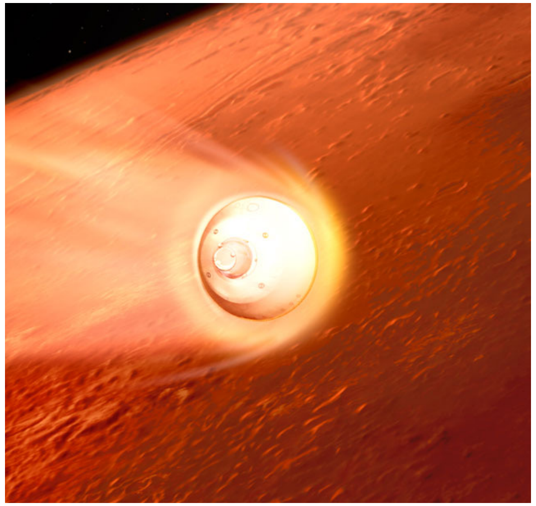
ANALYTICAL MECHANICS ASSOCIATES

FAR 2022 conference| June 21st, 2022

Thermal Protection Systems (TPS)

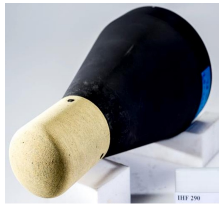
Need for Thermal Protection Systems





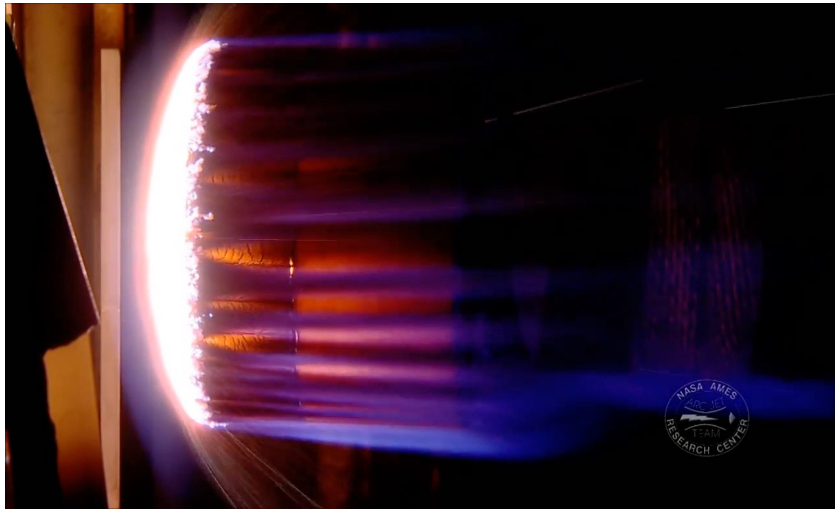
Ground-based Testing

P. Agrawal et. al. 2016.



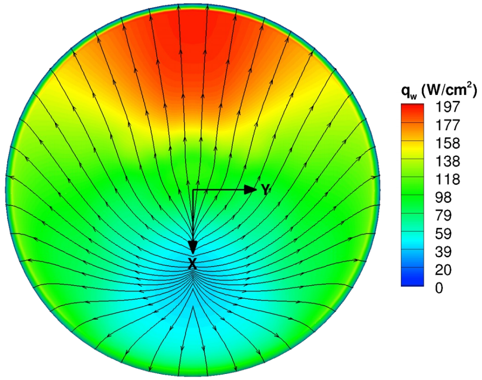
Virgin PICA Sample

Charred PICA Sample

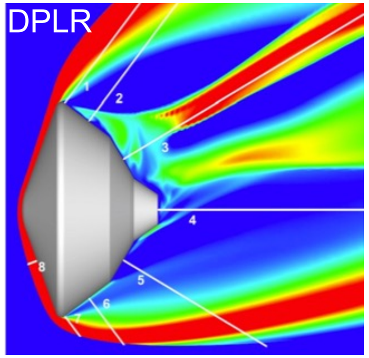


Arc Jet Testing of TPS

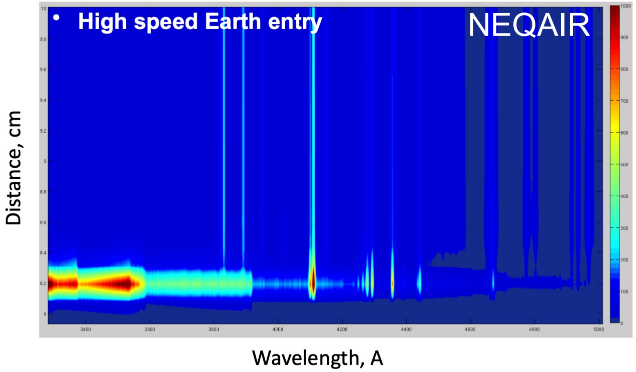
Computational Modeling



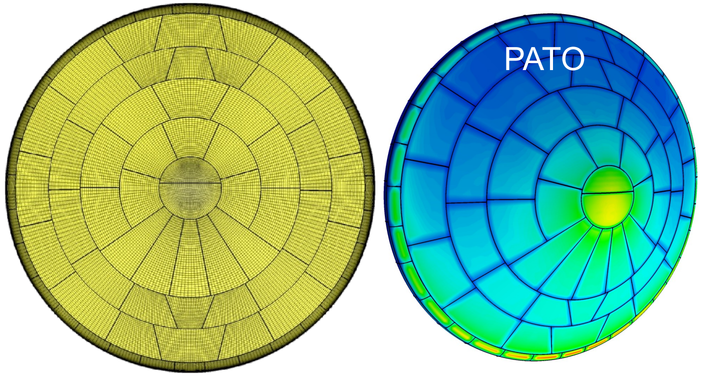
Hypersonic CFD



Radiation Analysis



Material Response

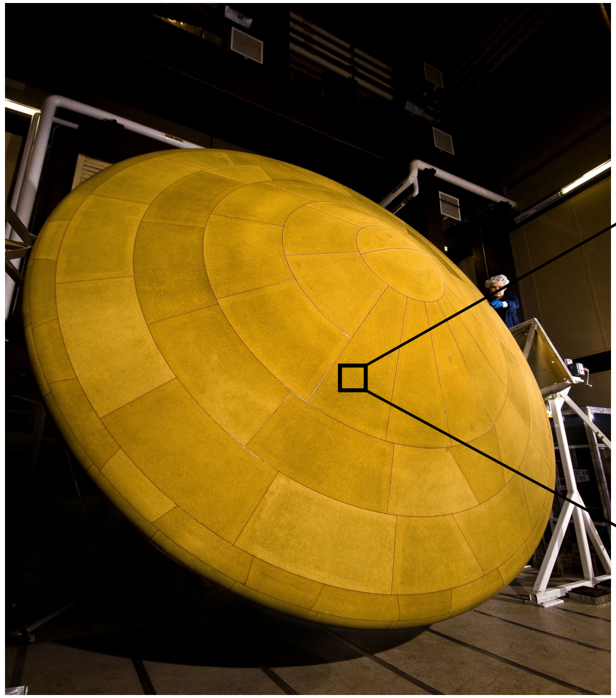


Computational modeling is critical for entry systems

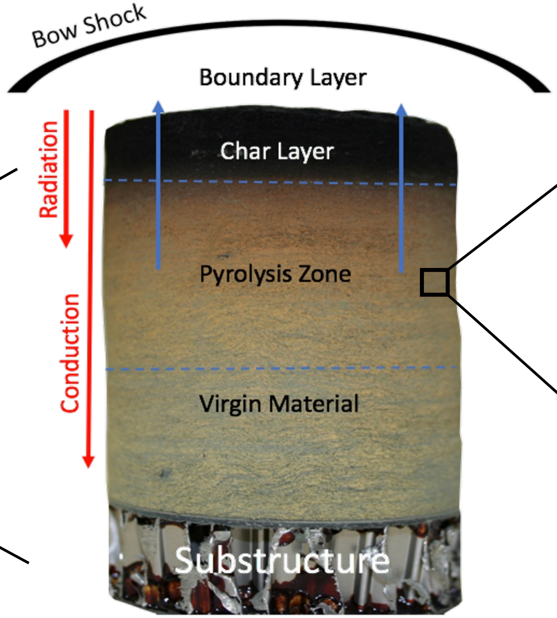
NASA Modeling Capabilities

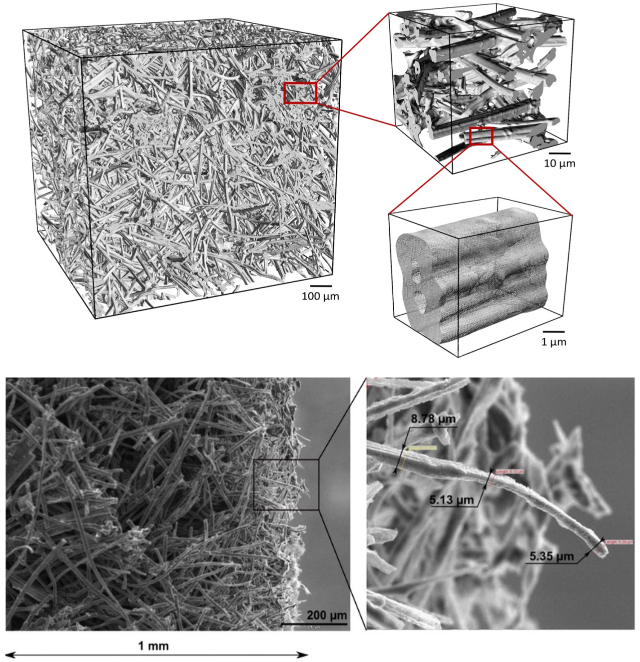
FIAT | CHAR | Icarus | PATO → **Full scale**

PuMA → **Microscale**



Mars Science Laboratory (MSL) heat shield

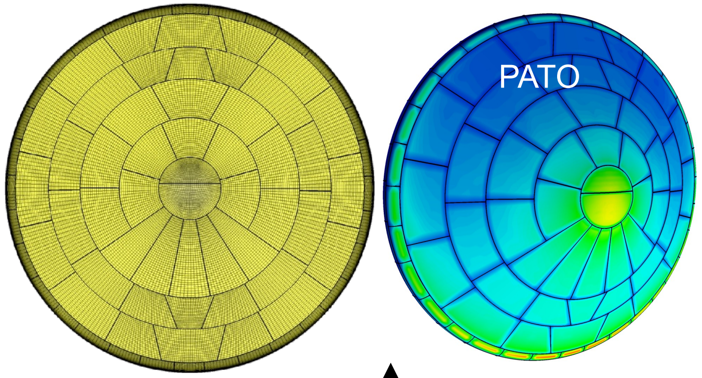




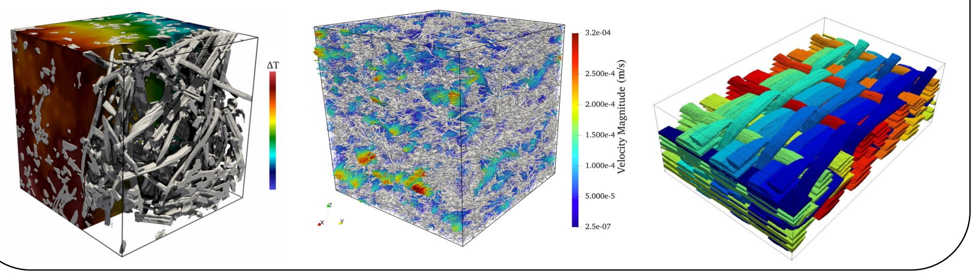
Carbon-fiber microstructure

Importance of Microstructure Analysis

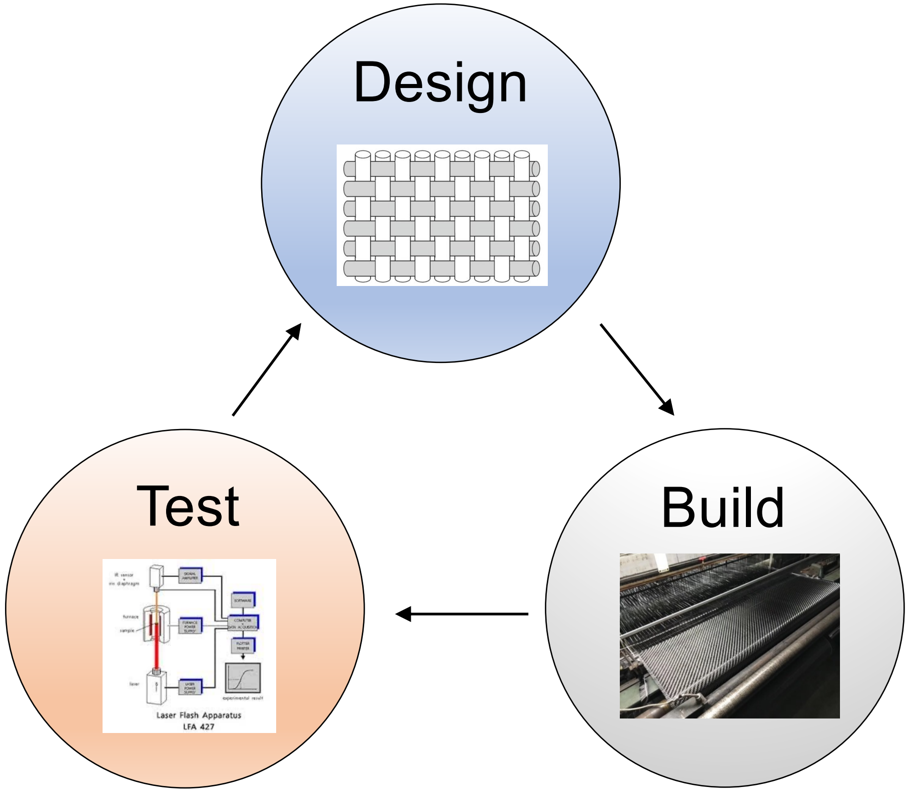
Improved Material Response



Microscale materials modeling



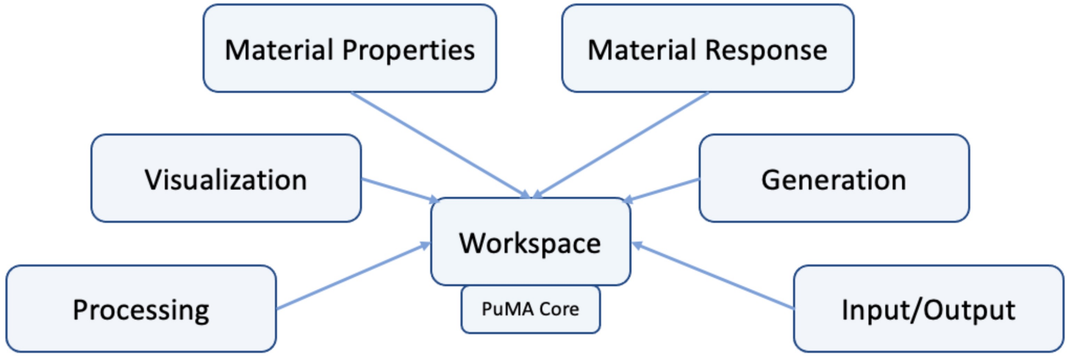
Improved Material Design

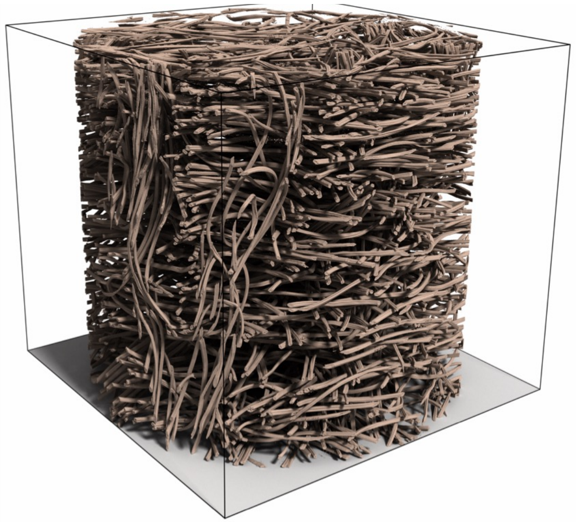


Current material design processes are costly and slow

Microscale modeling improves NASA's predictive modeling and can improve material design

The PuMA software





Installation: conda install -c conda-forge puma
Open-source repository: https://github.com/nasa/puma
Documentation: https://puma-nasa.readthedocs.io
Video tutorials: PuMA YouTube channel
Main developers: federico.semeraro@nasa.gov, joseph.c.ferguson@nasa.gov

Porous Microstructure Analysis (PuMA)

Domain Generation
- ● X-ray Microtomography import / filtering
- ● Woven Material Generation (TexGen)
- ● Simplified Geometry Generation
  - ● Analytical shapes
  - ● Fibrous Materials
  - ● Sphere Beds
  - ● Triply Periodic Materials

Material Properties
- ● Porosity / Volume Fractions
- ● Specific Surface Area
- ● Pore Diameter
- ● Effective Thermal & Electrical Conductivity
- ● Anisotropic Thermal & Electrical Conductivity
- ● Anisotropic Elasticity
- ● Material Orientation
- ● Continuum Tortuosity
- ● Rarefied Tortuosity
- ● Permeability

Shared Utilities
- ● Matrix & Vector data structures / operations
- ● Linear Solvers
- ● Iso-surface extraction
- ● Input/output utilities

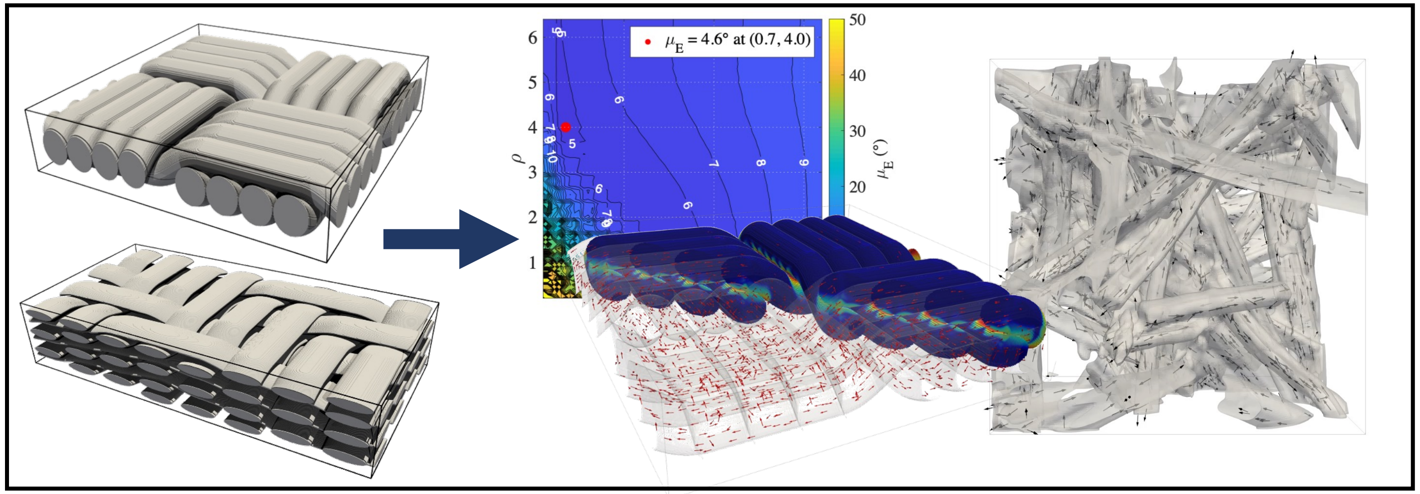
Material Response
- ○ Microscale Oxidation
- ○ Hyperthermal Beam Simulations

● Included in open-source release
○ Not included in open-source release

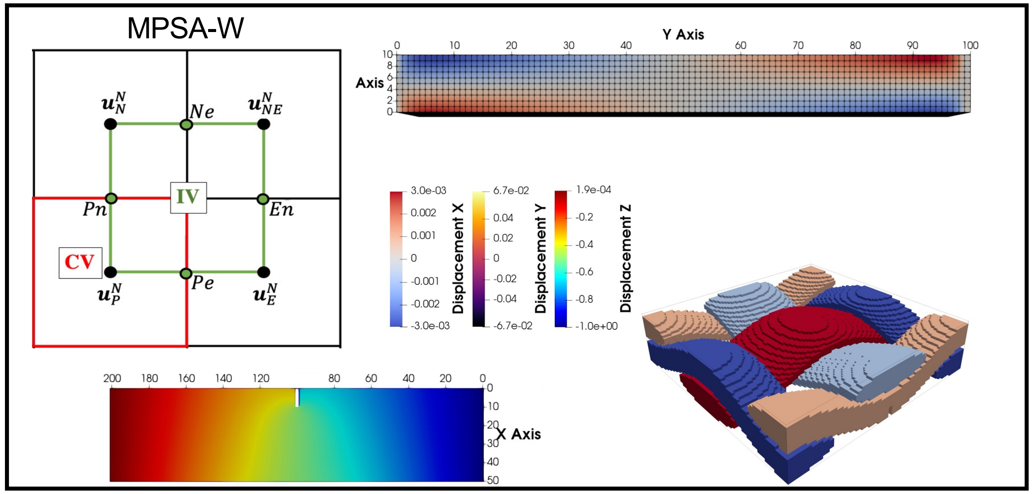
PuMA is an all-in-one toolbox for microstructure analysis and design

Overview of Material Properties Computations

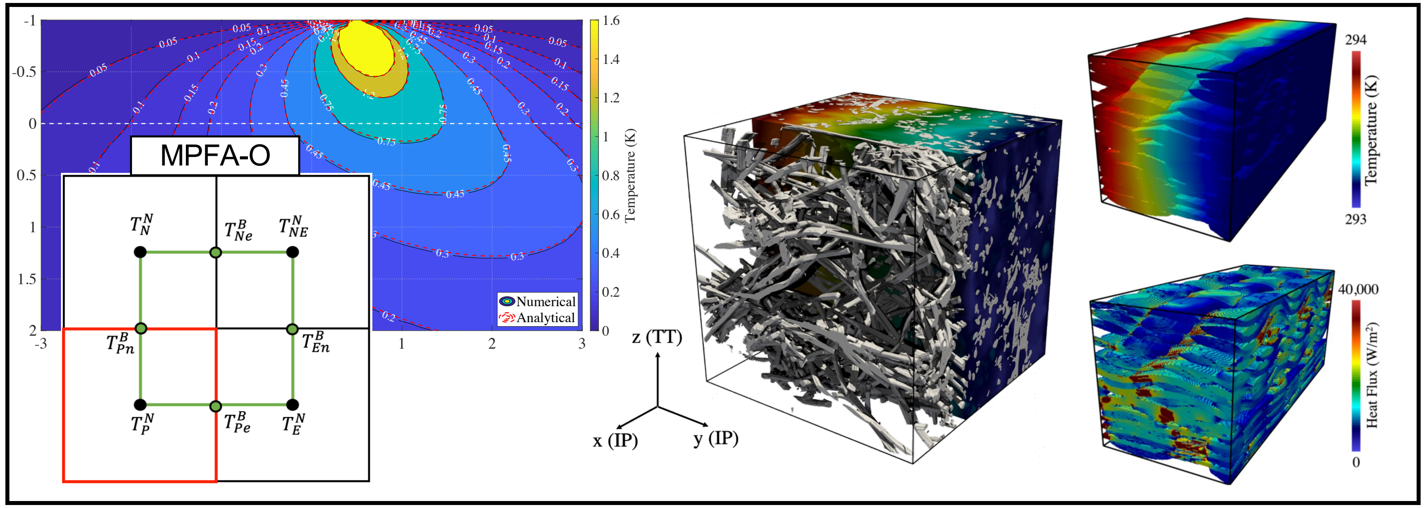
Part 1: Estimation of local orientation. *Computational Materials Science* (2020)



Computation of effective elasticity

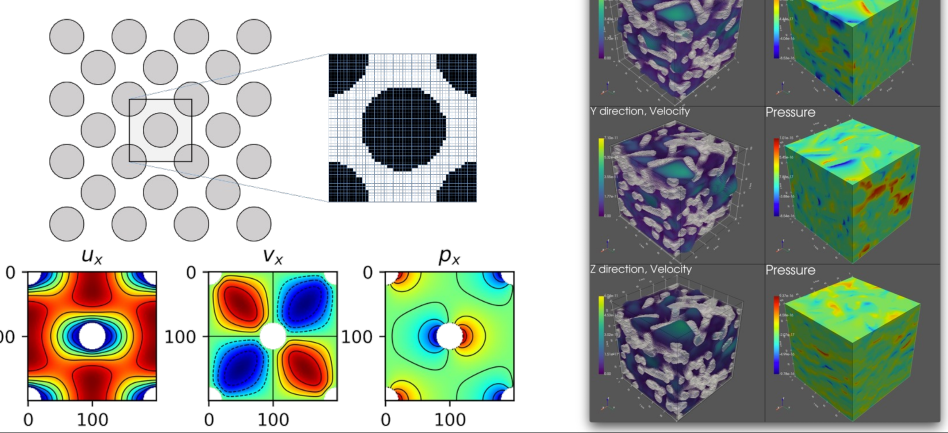


Part 2: Computation of effective conductivity. *Computational Materials Science* (2021)



Computation of effective permeability

$$-\mu\nabla^2\boldsymbol{u} + \nabla p = \boldsymbol{f}$$



PATO

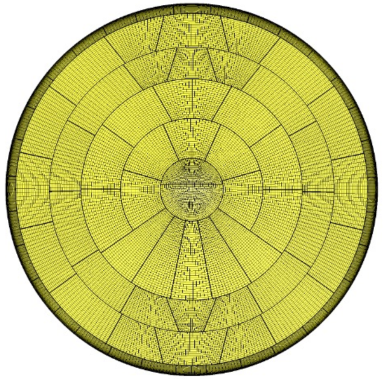
OpenFOAM

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

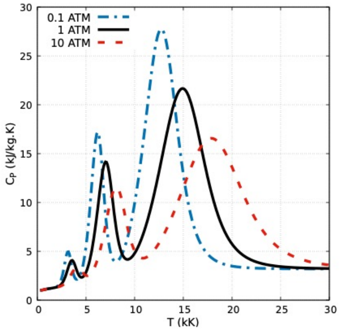
PATO: material response

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

Complex mesh generation	Thermo/Transport/ Chemistry	Optimization/ UQ/SA/PE	Post-processing 1D/2D/3D

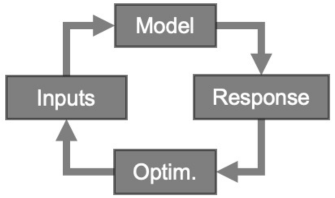


POINTWISE/GMSH

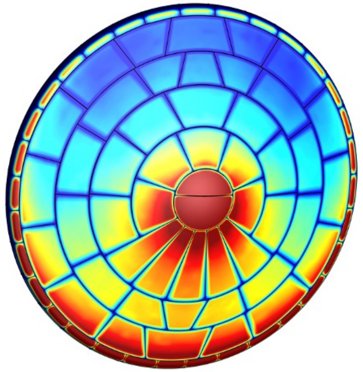


MUTATION++

DAKOTA
Explore and predict with confidence.



DAKOTA



FV/TEC

PATO
Porous Material Analysis
NASA ARC

More info on PATO

Open-source installation

conda config --add channels conda-forge
conda config --add channels pato.devel
conda config --set channel_priority strict
conda create -y --name pato pato

PATO website

http://pato.ac

Documentation

https://pato.ac/index.php/documentation

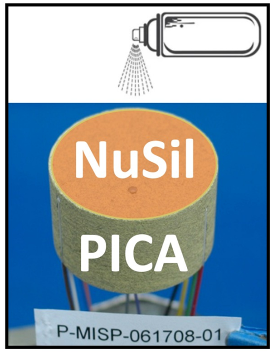
Main developer

jeremie.b.meurisse@nasa.gov

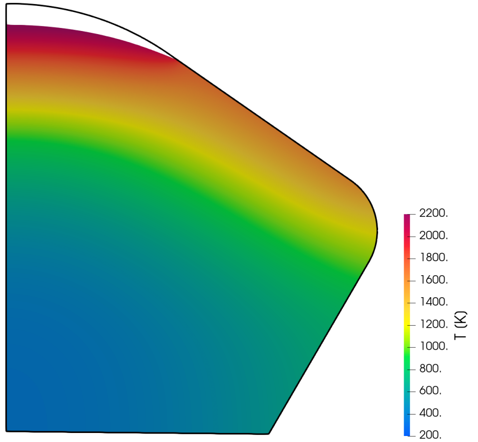
PICA-NuSil Material Response

NuSIL CV-1144-0

Controlled volatility RTV silicone oxygen protective overcoat
https://www.avantorsciences.com/assetsvc/asset/en_US/id/29017290/contents



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**. A novel material response model for **PICA-NuSil** was implemented in **PATO** using results from **dedicated experiments**.



Temperature and shape change at 30 sec

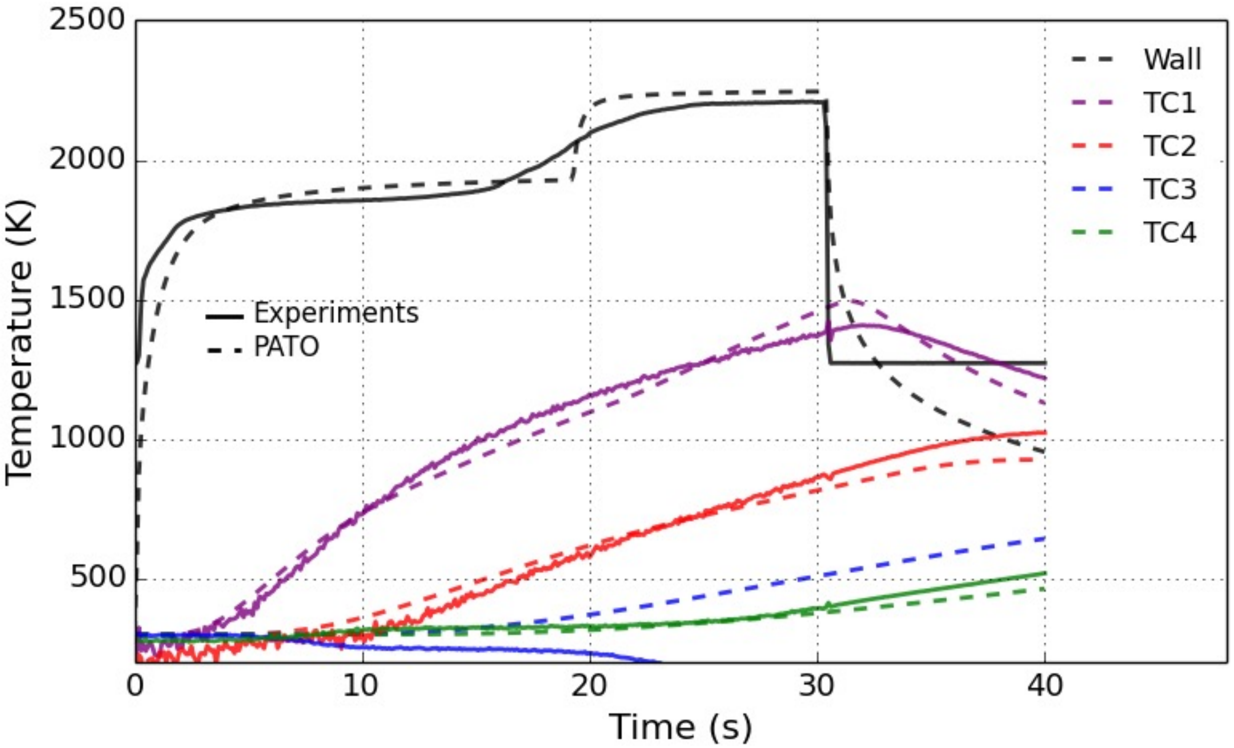
HYMETS PS02 at 28 sec

B. Bessire *et. al.* 2019

HyMETS Test Campaign from March 2019

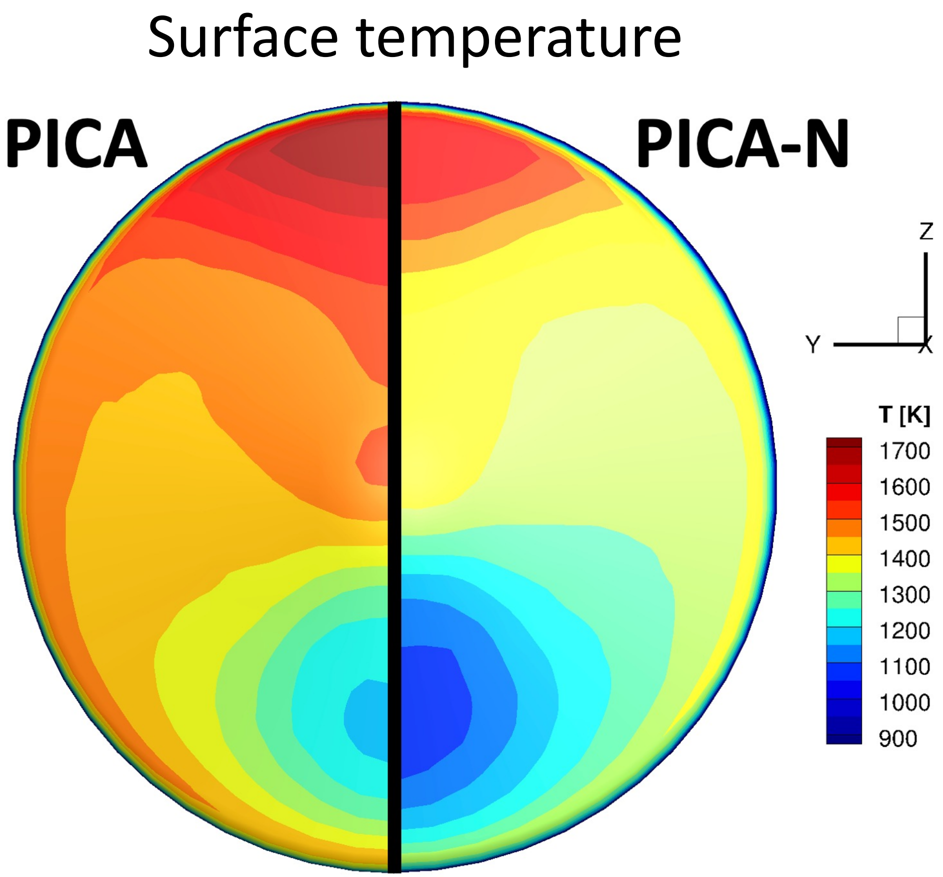
B. Bessire *et. al.* 2019

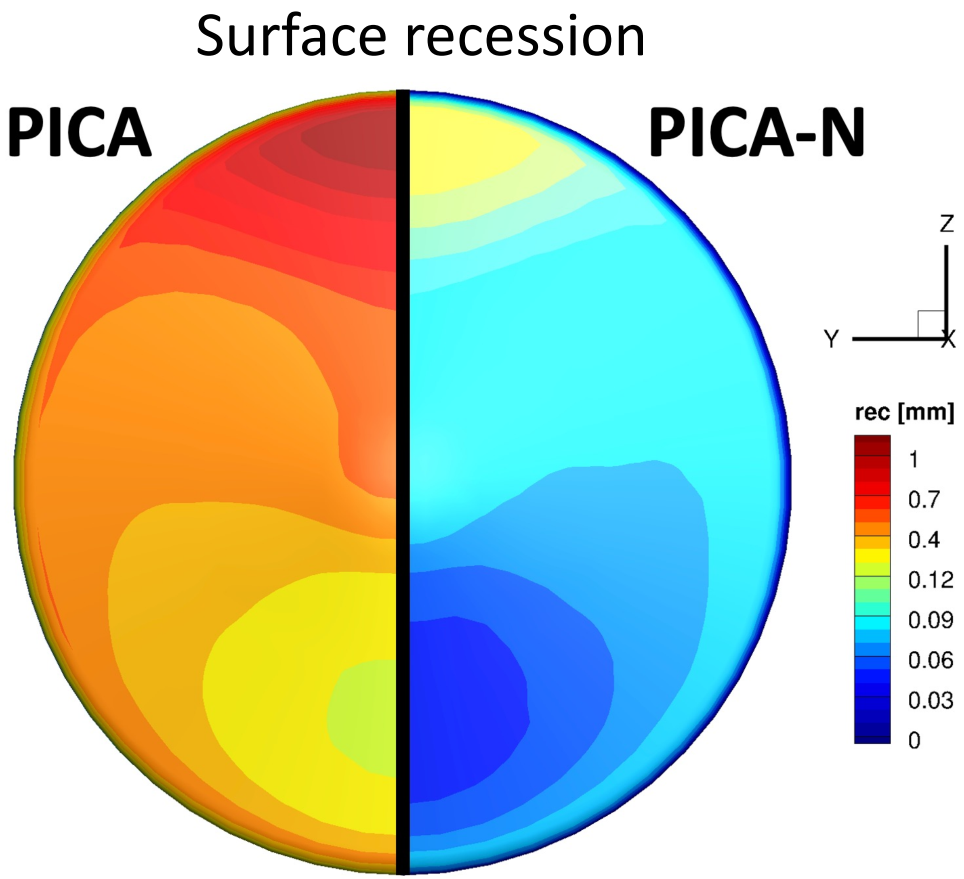
Material	Model	Atmosphere	Heat flux [W/cm^2]	Pressure [kPa]
PICA-NuSil	PS02	Air	140	5.6



Evolution in time of the temperature

Comparison of PICA and PICA-N Models





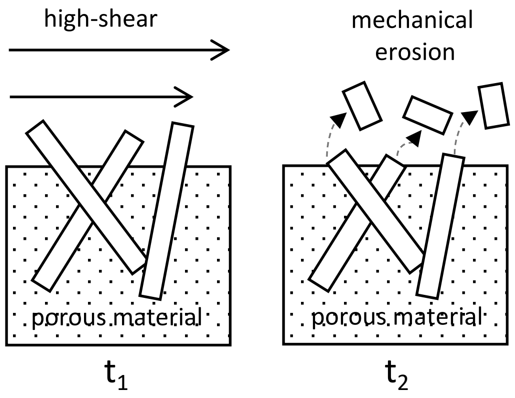
3D material response of the MSL heatshield using PICA and PICA-NuSil as silica at 80 sec after EI for a fully turbulent environment computed in DPLR. The estimation of the **NuSil layer thickness** on top of PICA was **200** μm. The PICA-N model gave lower surface temperature and recession results than the PICA model. According to the PICA-N model, the NuSil coating **still fully covered** the MSL heatshield.

Mechanical Erosion Model in PATO

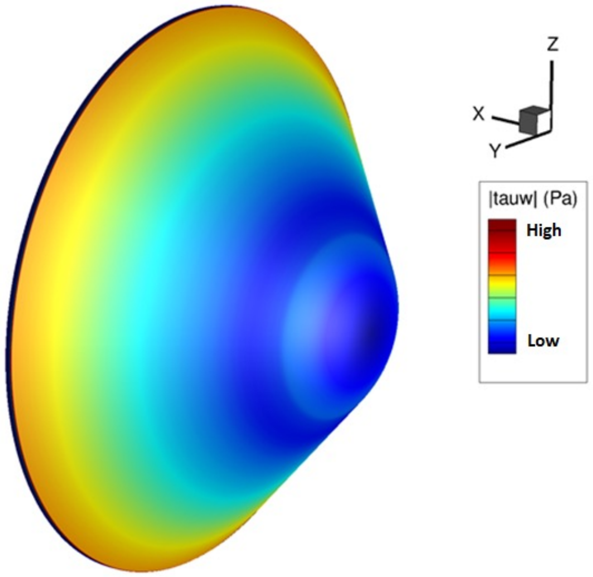
Mechanical erosion may lead to additional mass removal of TPS material during atmospheric entry, increasing the total surface recession.

Main mechanisms identified:

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



Schematic of the shear induced mass removal



Shear stress for MSR-EEV entry

DPLR

Aerothermal environment Hypersonic CFD

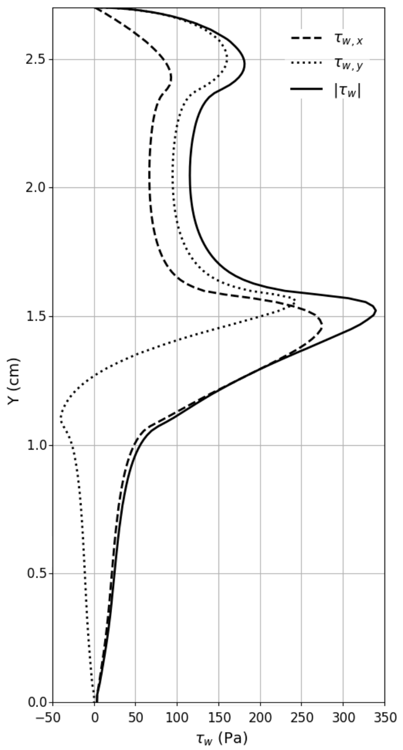
p_w h_r C_H $\overline{\overline{\tau_w}}$ →

PATO

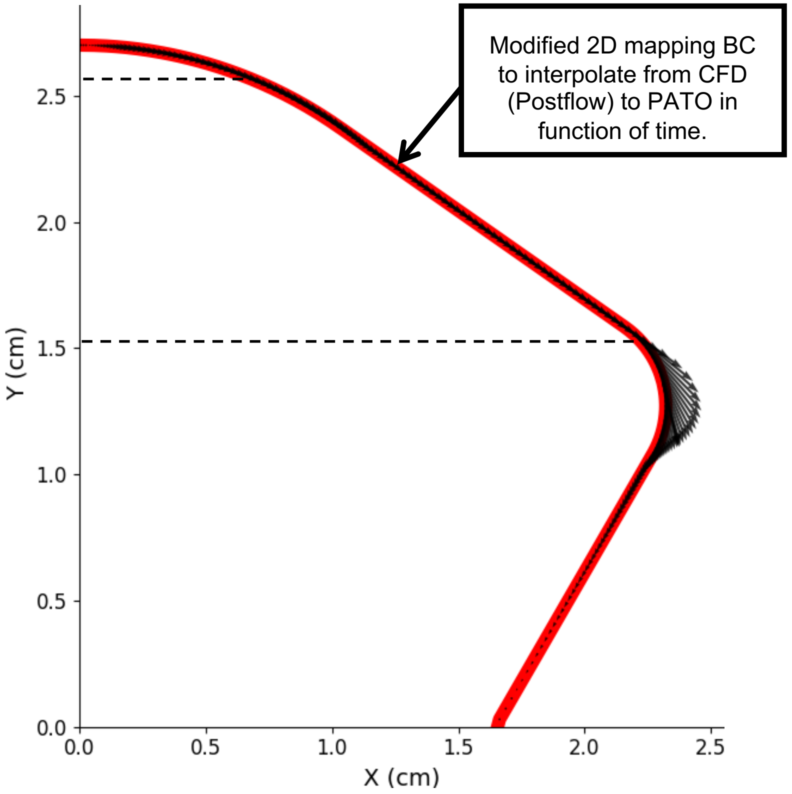
Material response solver → Update Mechanical properties → Stress analysis solver → Failure criteria model → Mass removal model

T $\dot{s}$ →

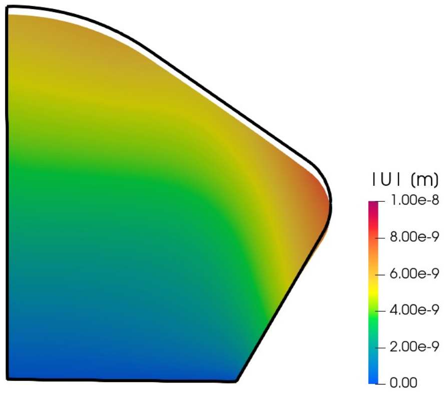
Mechanical Erosion Model in PATO



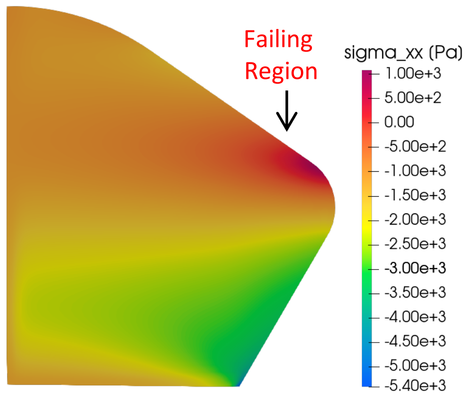
Components of the wall shear stress in function of the Y axis



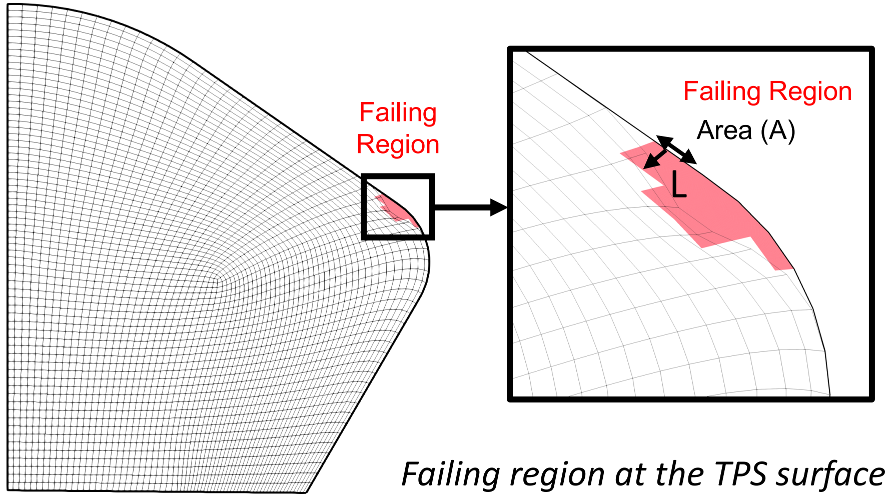
Direction and magnitude of the wall shear stress



Displacement due to shear stress with a scale factor (x10^5)



Component X of the stress tensor and theoretical failure criteria



Failing region at the TPS surface

Theoretical failure criteria

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

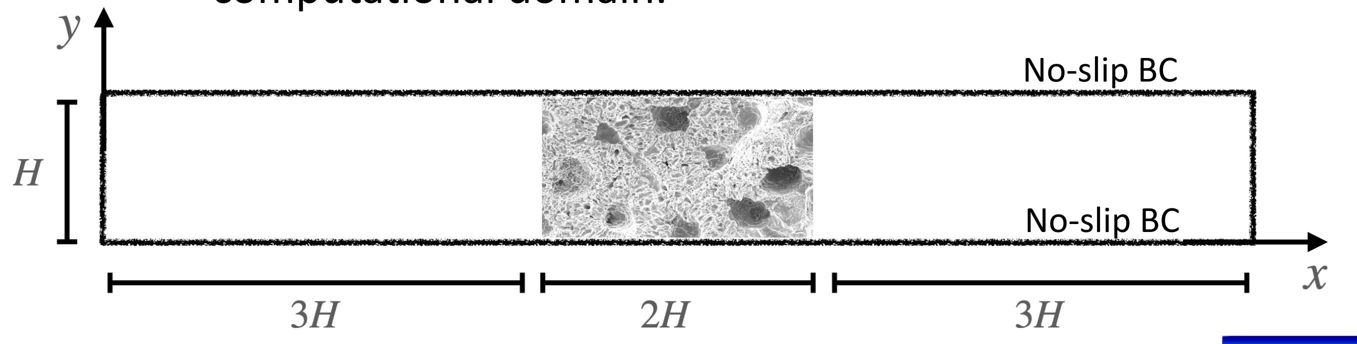
The recession rate and the mass loss are computed as follows:

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

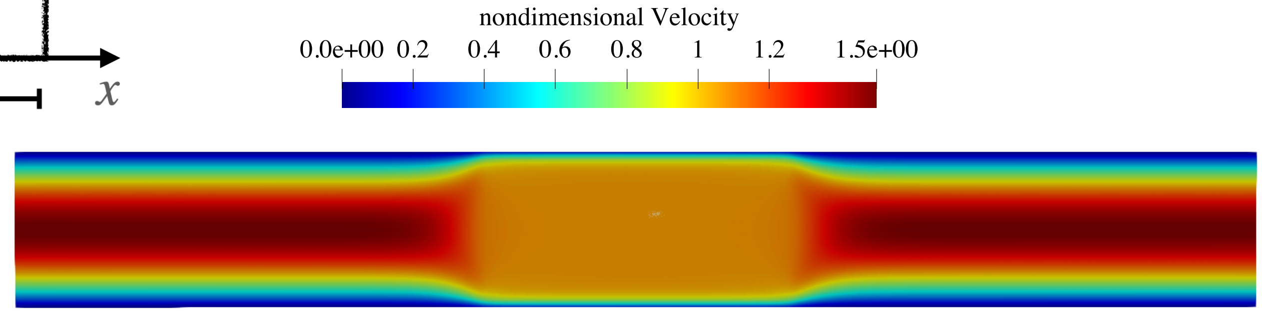
Ultimate Strength
tu: Traction
cu: Compression
su: Shear

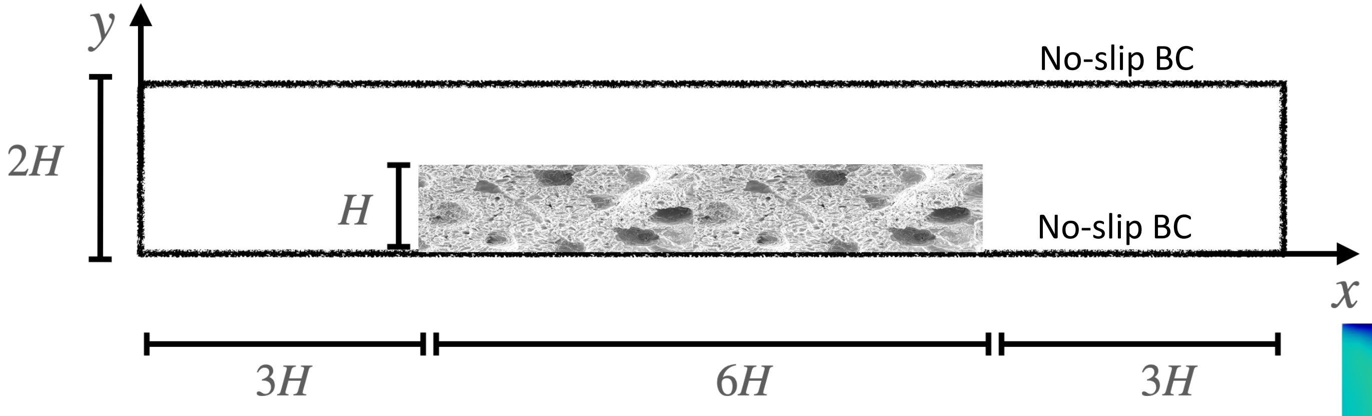
On-going Effort on the Universal Solver Development

- The governing equations for the pure fluid and porous medium are coupled and solved in the same computational domain.

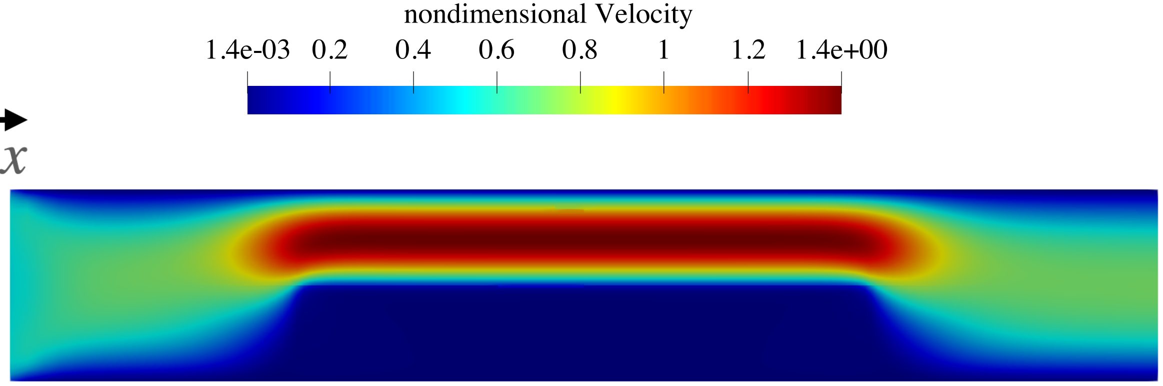


Porous Plug Flow from Betchen





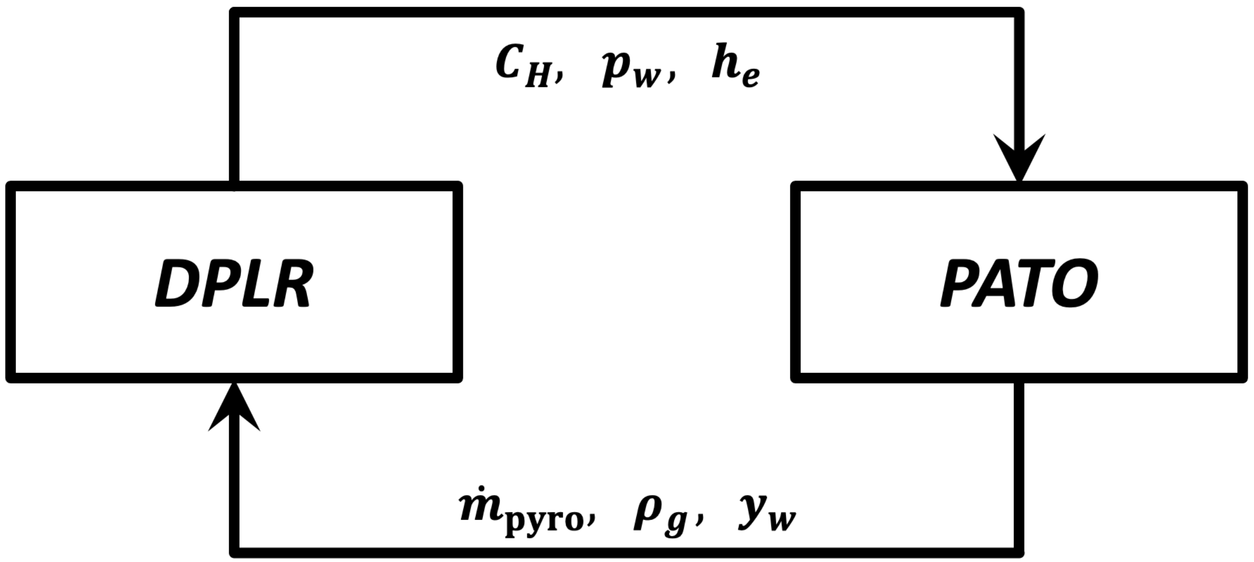
Beavers & Joseph problem



Loose Coupling Between Environment and Material Response

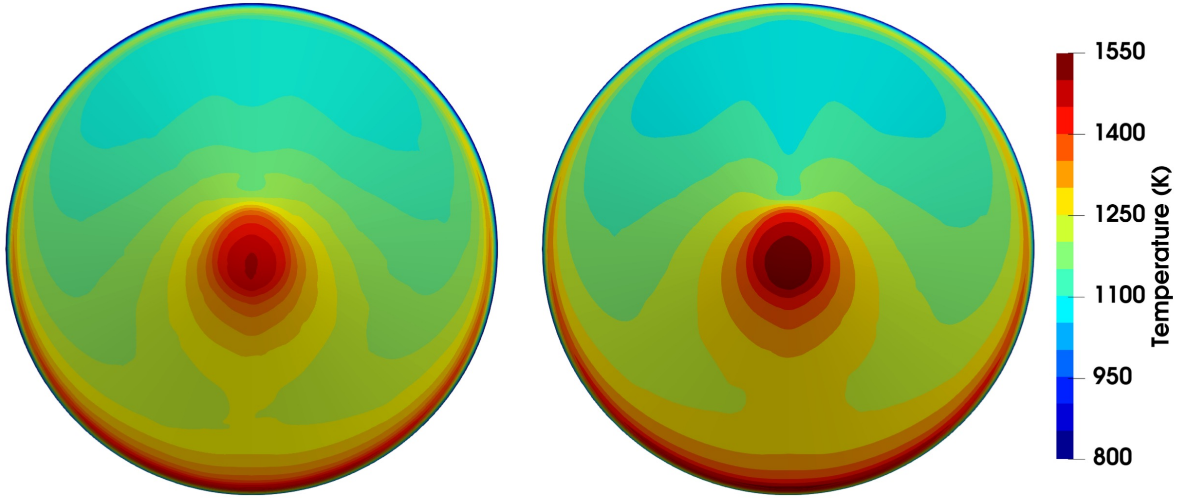
Coupling via pyrolysis gas blowing at the heatshield surface:

- 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

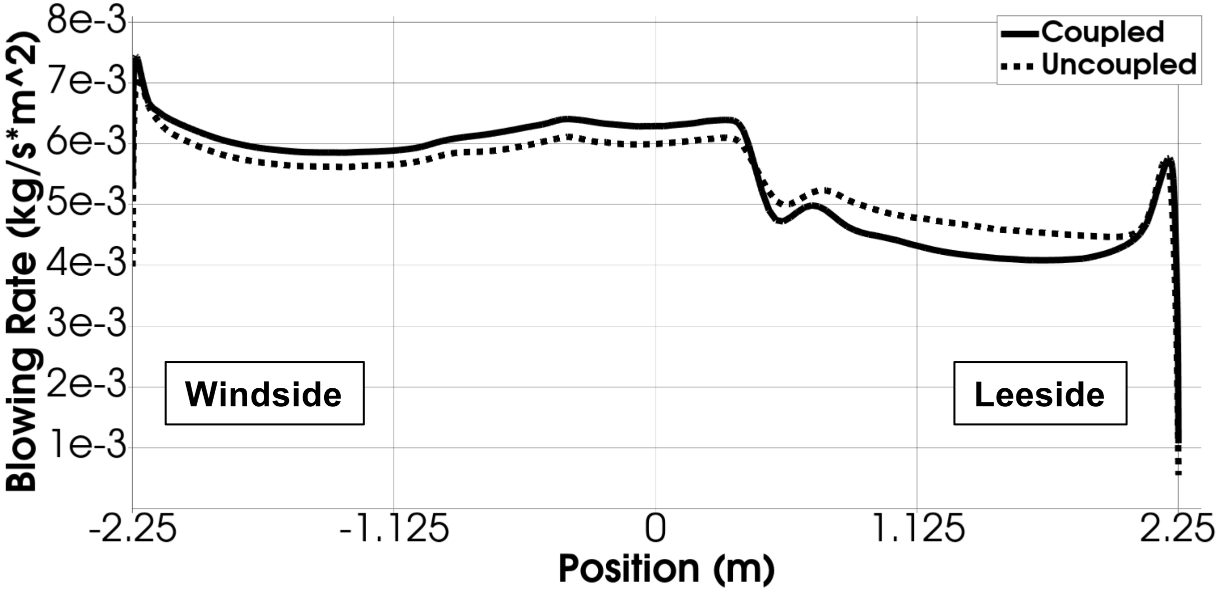
Heatshield Surface at 65s

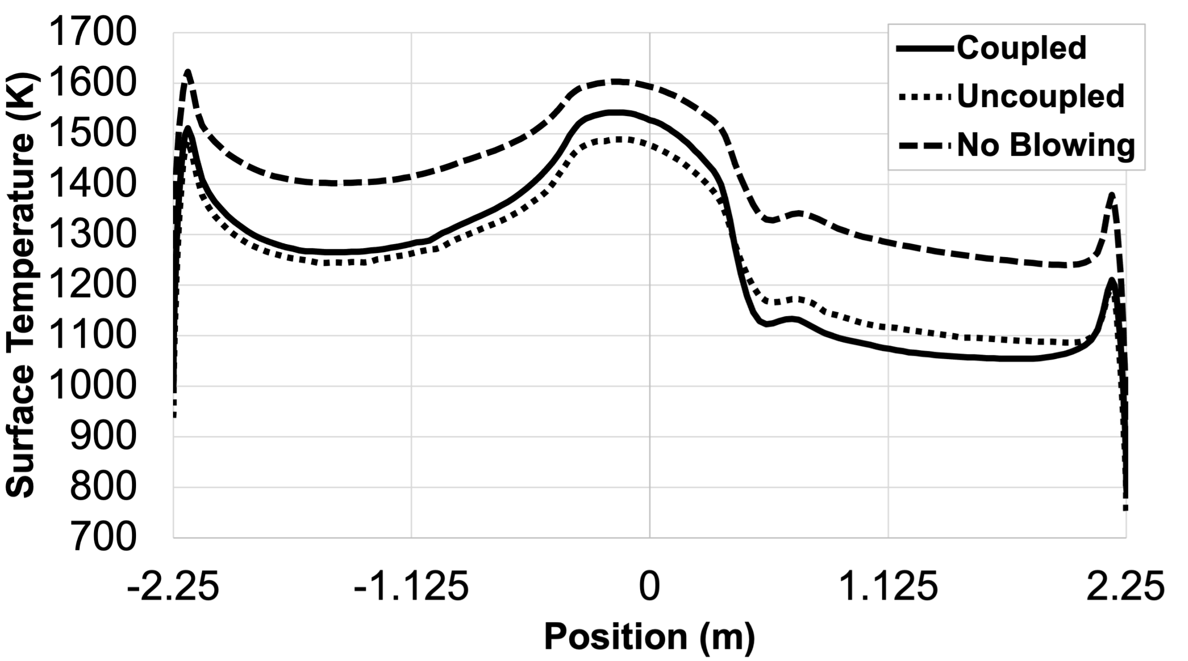


Uncoupled | Coupled

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.

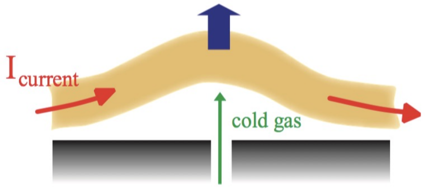




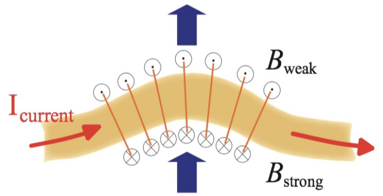
3D Unsteady Simulations of Arc Heater Plasma Flow

ARCHeS = ARC Heater Simulator
3D unsteady plasma flow analysis tool
Coupled MHD and radiation models using OpenFOAM

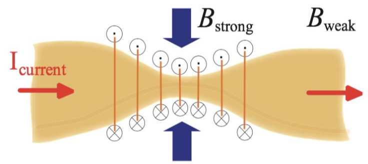
Main developer
jeremie.b.meurisse@nasa.gov



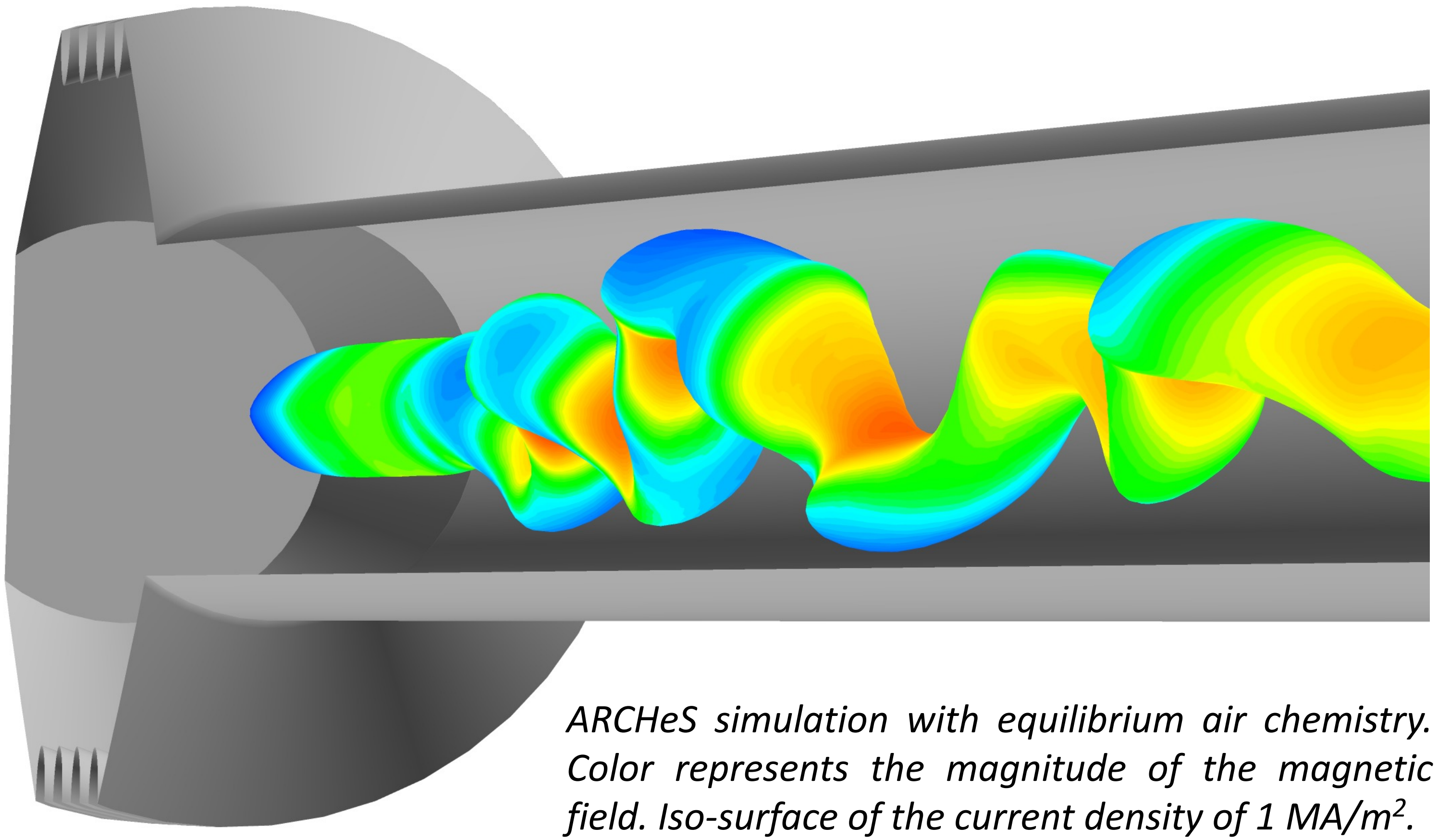
Thermal instability



Kink instability



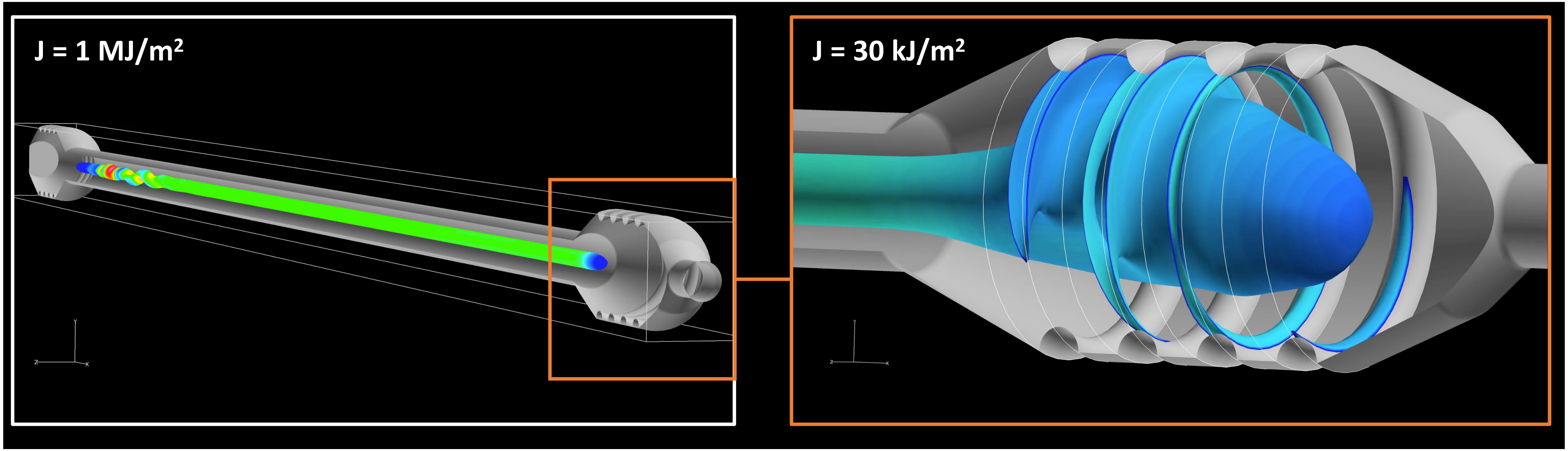
Sausage instability



ARCHeS simulation with equilibrium air chemistry. Color represents the magnitude of the magnetic field. Iso-surface of the current density of 1 MA/m^2.

Stable arc next to the electrode chambers
Instablilities arise in the constrictor

3D Unsteady Simulations of Arc Heater Plasma Flow

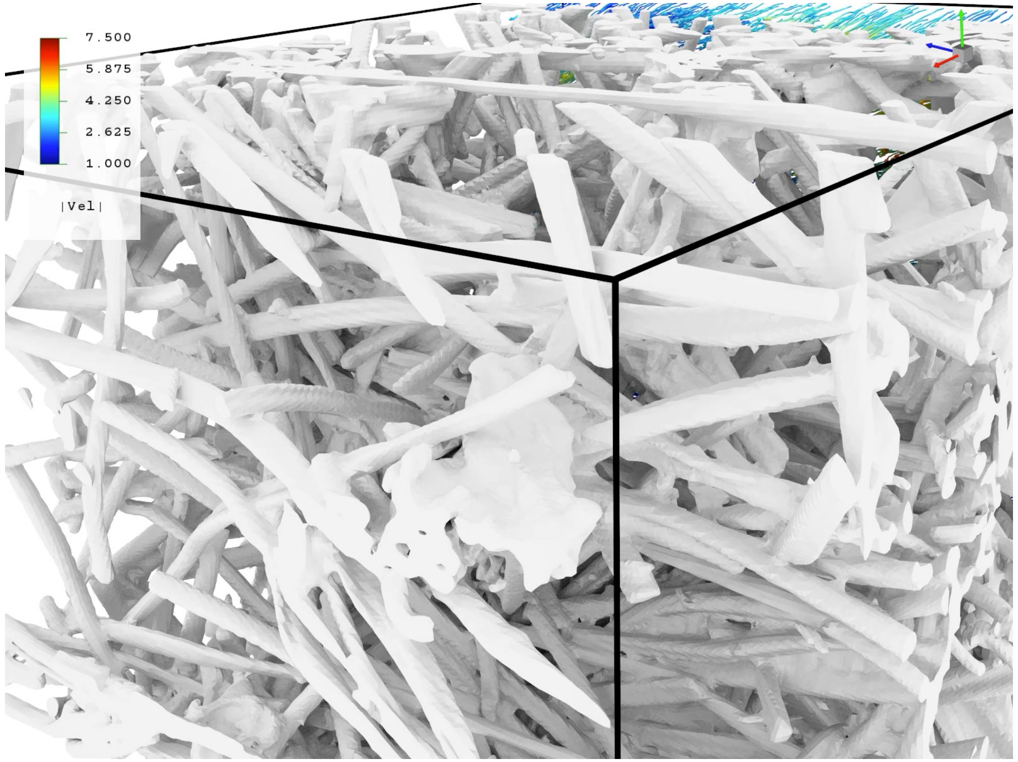


The location and frequency of the arc attachment at the cathodes are found to be mainly driven by the upstream arc instabilities

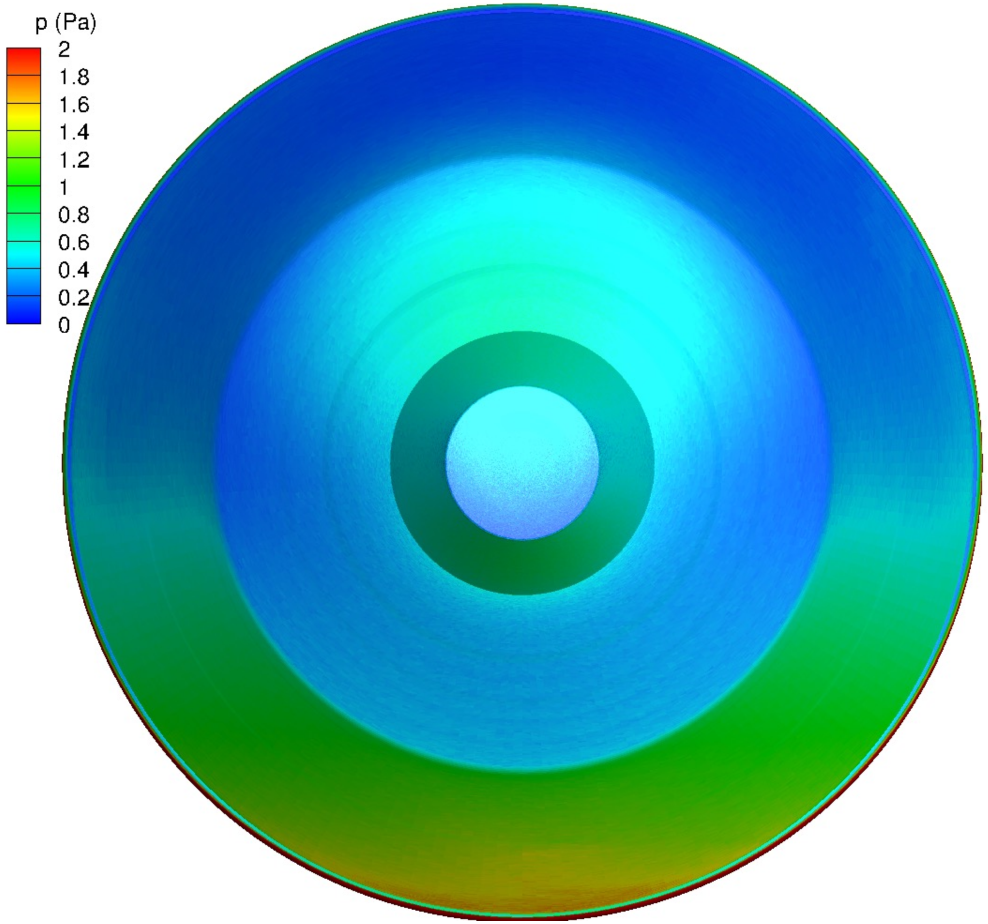
SPARTA: an Exascale DSMC Code

SPARTA = **S**tochastic **PA**rallel **R**arefied-gas **T**ime-accurate **A**nalyzer

- Open-source DSMC solver initiated at SNL, currently co-developed by Sandia and NASA with multiple users internationally and domestically: https://sparta.sandia.gov/
- Can be run from single processor to petascale.
- Has been used to run the largest (we think!) DSMC models up-to-date, with up to **100 billion particles and billions of grid cells. Can also handle billions of surface elements**

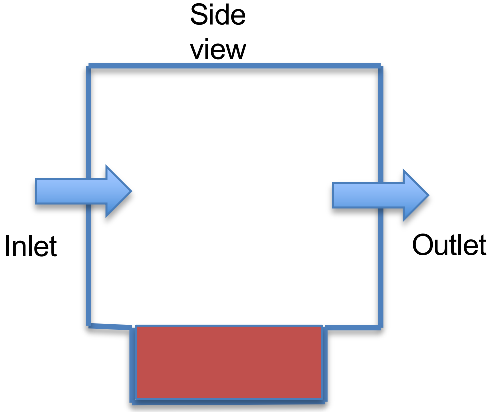


Flow through a FiberForm sample

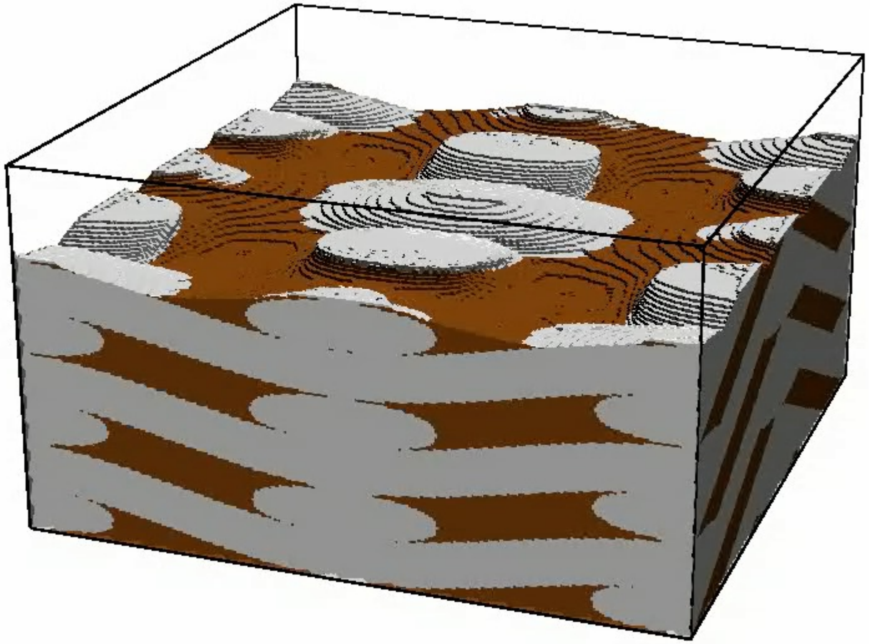


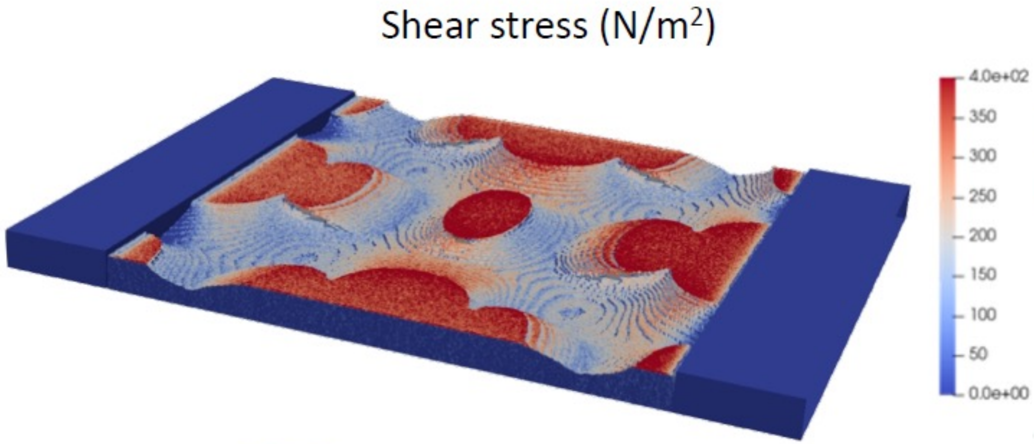
Mars2020 backshell pressure at t = 39s after EI

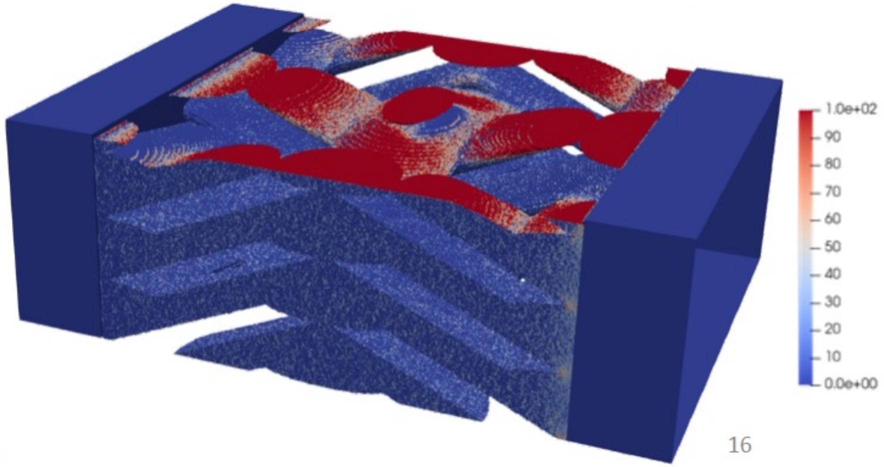
Computation of Shear Stress on Woven TPS

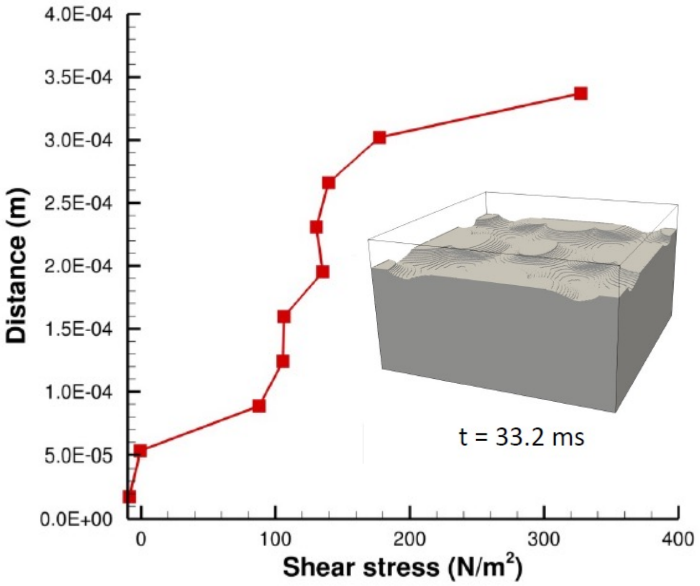


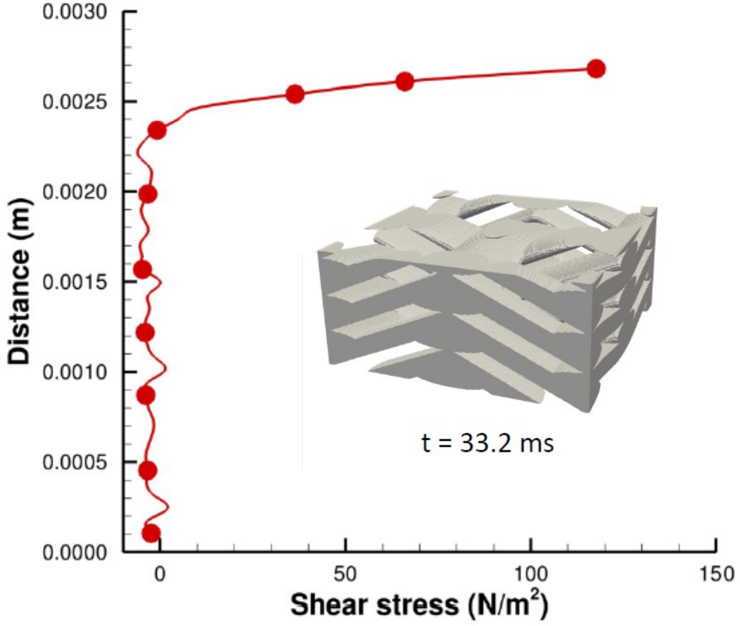
Woven TPS







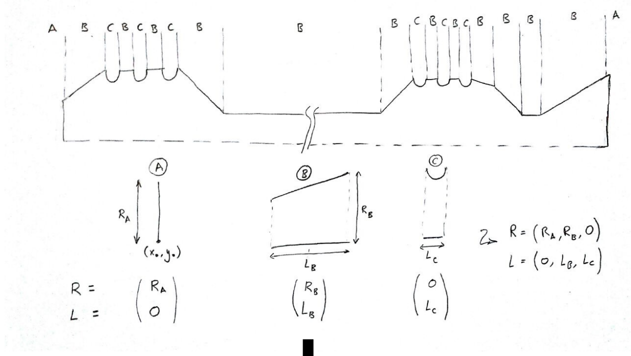




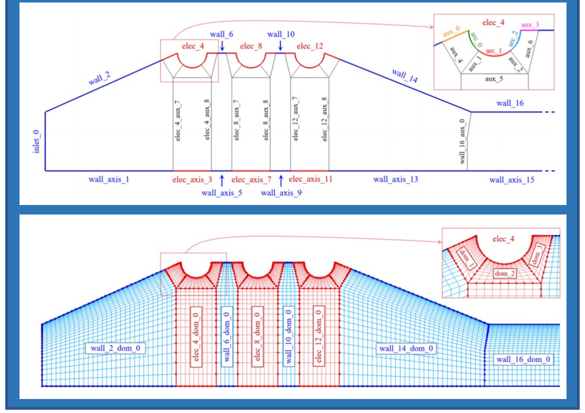
Questions?

ARCHeS

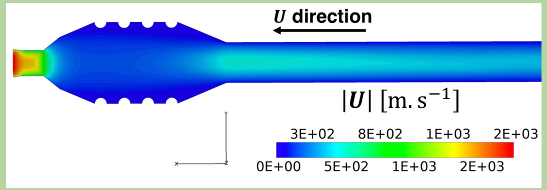
Geometry concept



Lynx
Automatic mesh inputs



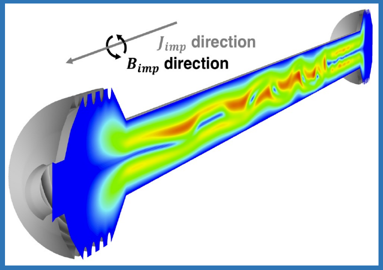
OpenFOAM



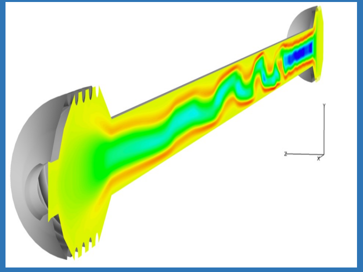
- Finite Volume
- I/O management
- Massive MPI
- Mixture tables
- Turbulence
- Moving geometry
- Chemistry
- Compressible flow
- Basic mesh gen.
- Thermo/Transp.
- Radiation

ARCHeS

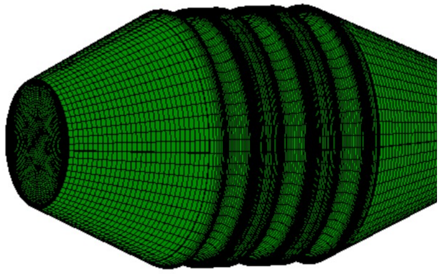
MHD + ballast BC



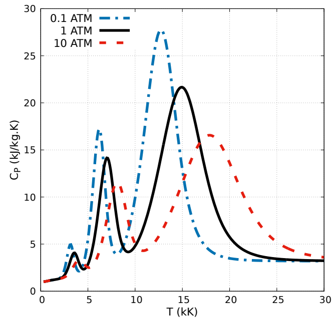
3D radiative transfer



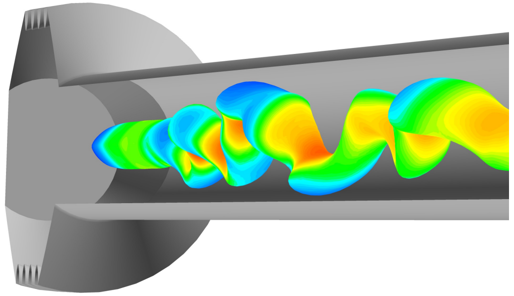
Complex mesh generation



Thermo/Transport/Chemistry

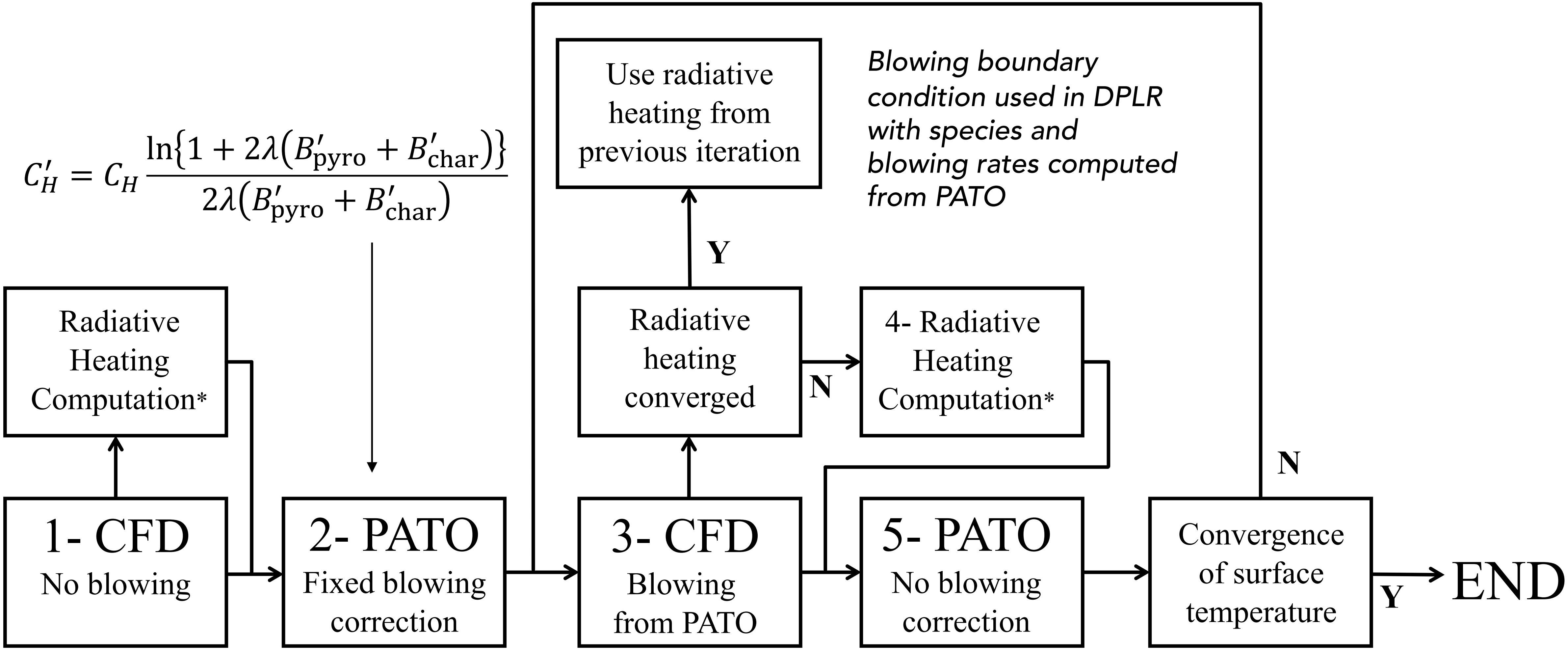


Post-processing 1D/2D/3D



Coupling Methodology

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



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