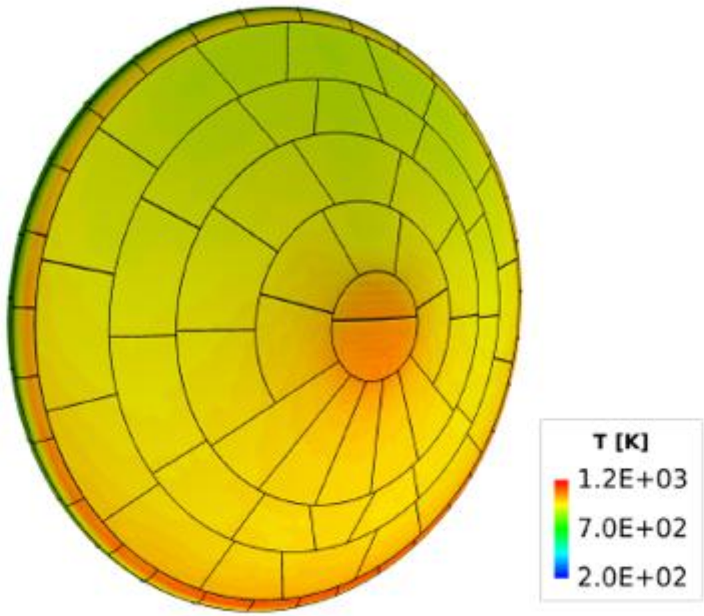
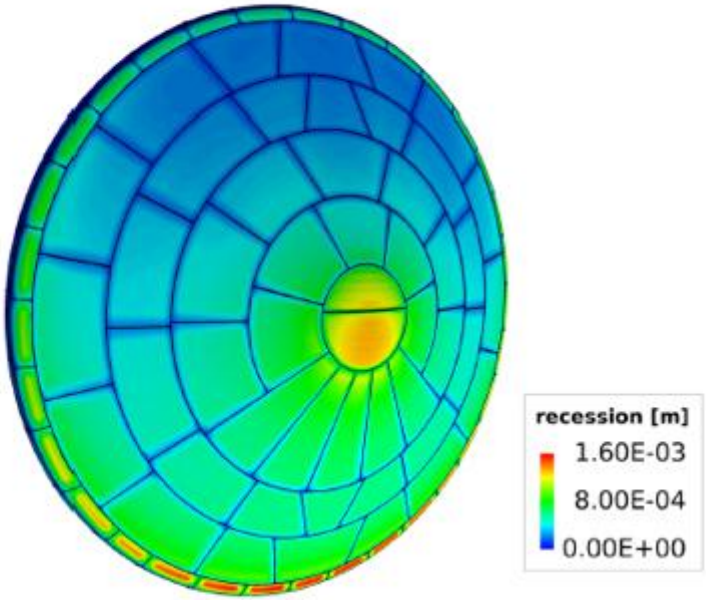
PATO

POROUS MATERIAL ANALYSIS TOOLBOX BASED ON OPENFOAM

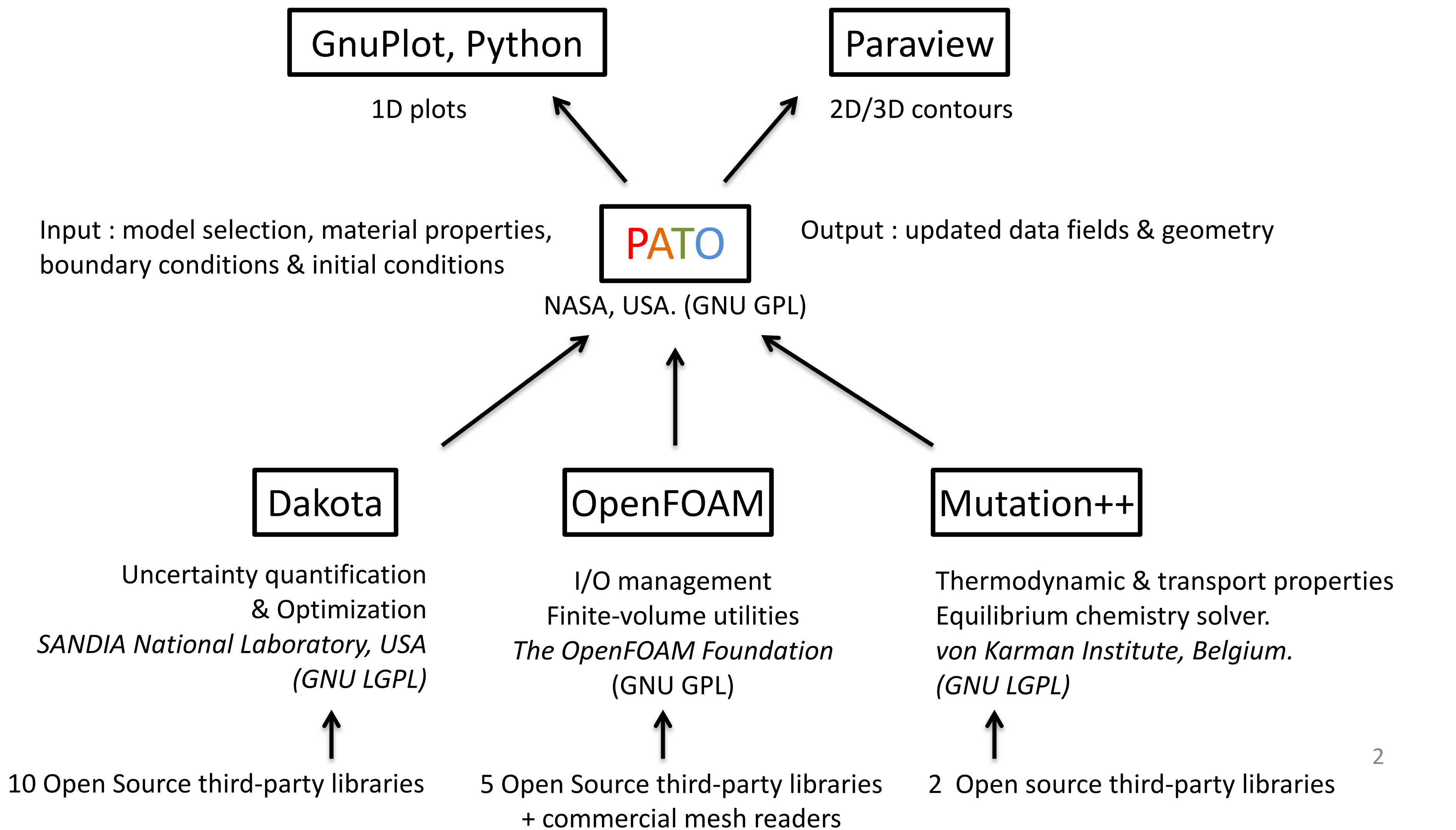
About	Notices	Download	Documentation	Projects	Team & contacts





About

A flexible toolbox for Multiphase Porous Reactive Materials & Less



Notices

❑ PATO is distributed Open Source by NASA.

https://software.nasa.gov/software/ARC-16680-1A redirects to www.pato.ac

❑ Two types of agreements

- For users : NASA Open Source Agreement version 1.3
- For contributors : Contributor License Agreements (signature required)

Both follow usual “good practice terms” of standard Open Source agreements.

❑ In short :

- PATO is free to use, modify, redistribute (no signature required)
- NASA will continue integrating contributions in the official release (signature required)

Download

- ❑ Two options (online)

- For users
  - “Stable” NASA releases
  - Zip file on www.pato.ac, about 200 Mo
  - Updated in April and September

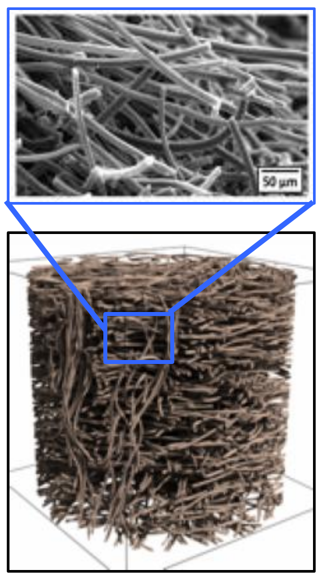
- For developers
  - “Live” development version
  - Repository on www.gitlab.com/PATO-dev
  - 28 members

- ❑ Ask me a bootable USB 3 with Linux OS

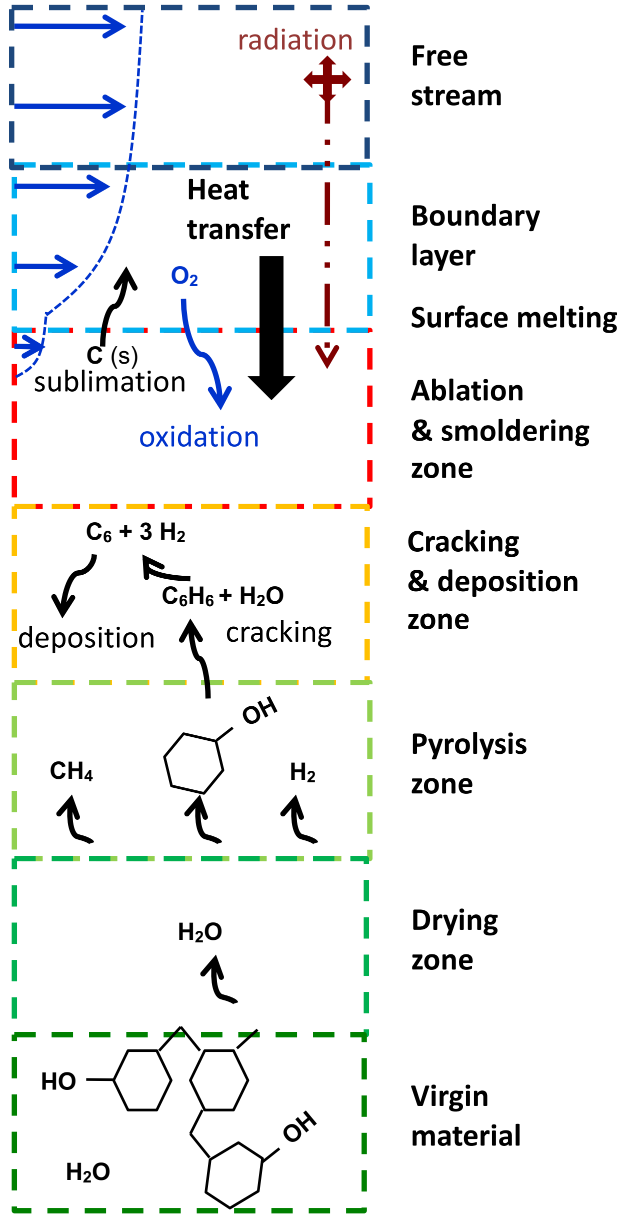
Documentation

A pragmatic generic model for porous reactive materials

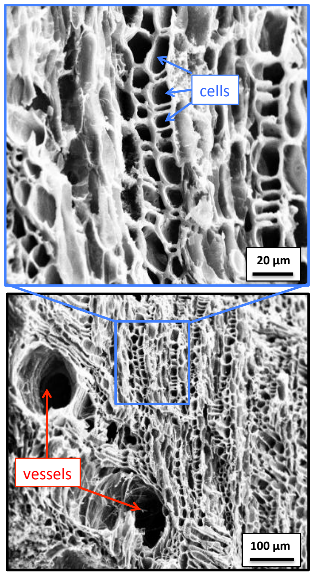
Thermal protection systems



Carbon fiber preform
(NASA/UC Berkeley)



Biomass pyrolysis

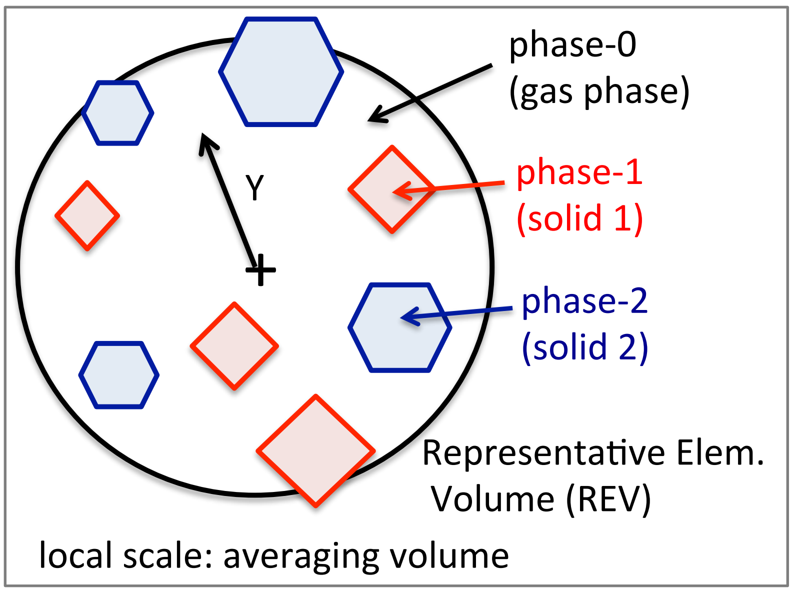


Charred wood
(University of New Caledonia)

A pragmatic generic model for porous reactive materials

Hypotheses

- multi-phase reactive material (Np solid phase)
- multi-species reactive gas mixture (Ng gaseous species)
- local thermal equilibrium : all the phases are locally at the same temperature
- each solid phase can pyrolyze, vaporize, sublimate, and release species in the gas phase
- each solid phase can react with the gas phase (e.g. oxidation of a carbon phase)
- gas phase chemistry can be in equilibrium, follow a finite-rate mechanism, or be frozen



Averaged effective properties, e.g. density :

$$\rho = \epsilon_g \, \rho_g + \sum_{i \in [1, N_p]} \epsilon_i \rho_i = \sum_{i \in [0, N_p]} \epsilon_i \rho_i$$

volume fraction (ϵ_i), intrinsic density (ρ_i)

Rule also applies for porosity, heat capacity, and enthalpy. Unfortunately does not apply for permeability, tortuosity, conductivity. We use linear interpolation between measured values.

Continuity equations : mass

- For each solid phase i

$$-\partial_t(\epsilon_i \rho_i) = \sum_{j \in [1, P_i]} \epsilon_{i,0} \rho_{i,0} F_{i,j} \partial_t \chi_{ij} + \omega_i^h$$

evolution of density — pyrolysis — heterogeneous reactions

- Gas phase (sum of all the species)

$$\partial_t(\epsilon_g \rho_g) + \partial_{\mathbf{x}} \cdot (\epsilon_g \rho_g \mathbf{v_g}) = -\sum_i \partial_t(\epsilon_i \rho_i)$$

evolution of density — convection — exchange with solid phases

- Momentum conservation (Darcy-Klinkenberg)

$$\mathbf{v_g} = -\frac{1}{\epsilon_g} \left(\frac{1}{\mu} \underline{\underline{\mathbf{K}}} + \frac{1}{p} \underline{\underline{\beta}} \right) \cdot \partial_{\mathbf{x}} p$$

gas velocity — Darcian permeability — Klinkenberg slippage — pressure gradient

Re < 1
Kn < 1

Continuity equations : species & elements

One of the following models can be used

- Constant elemental composition of the pyrolysis gases

  Standard approximation in NASA design codes.
  Thermodynamic properties from tables or computed with Mutation ++.

- Element conservation, for detailed equilibrium chemistry modeling

$$\partial_t(\epsilon_g \rho_g z_k) + \partial_{\mathbf{x}} \cdot (\epsilon_g \rho_g z_k \mathbf{v}_\mathbf{g}) + \partial_{\mathbf{x}} \cdot \mathcal{F}_k = \pi_k, \ \forall\, k \in N_g^e$$

evolution of elements mass-fraction — convection — diffusion — pyrolysis elements — gaseous elements

- Species conservation, for finite-rate chemistry

$$\partial_t(\epsilon_g \rho_g y_i) + \partial_{\mathbf{x}} \cdot (\epsilon_g \rho_g y_i \mathbf{v}_\mathbf{g}) + \partial_{\mathbf{x}} \cdot \mathcal{F}_i = \pi_i + \epsilon_g \omega_i \mathcal{M}_i, \ \forall\, i \in N_g^s$$

evolution of species mass-fraction — convection — diffusion — pyrolysis species — chemistry source terms — gaseous species

Continuity equations : energy

- Total local energy : sum of the energies of all the phases

$$\rho_t e_t = \epsilon_g \rho_g e_g + \sum_{i\in[1,N_p]} \epsilon_i \rho_i h_i$$

total energy — gas phase energy — energy of the solid phases

- Energy conservation under local thermal equilibrium = "T can be defined"

$$\partial_t(\rho_t e_t) + \partial_{\mathbf{x}}\cdot(\epsilon_g \rho_g h_g \mathbf{v_g}) + \partial_{\mathbf{x}}\cdot\sum_{k=1}^{N_g}(\mathcal{Q}_k) = \partial_{\mathbf{x}}\cdot(\underline{\underline{\mathbf{k}}}\cdot\partial_{\mathbf{x}} T) + \mu\epsilon_g^2(\underline{\underline{\mathbf{K}}}^{-1}\cdot\mathbf{v_g})\cdot\mathbf{v_g}$$

total energy — convection — effective diffusion (species or elements) — effective heat transfer — effective viscous dissipation

Implicit resolution in T in PATO

$$\sum_{i\in[1,N_p]}[(\epsilon_i\rho_i c_{p,i})\,\partial_t T] - \partial_{\mathbf{x}}\cdot(\underline{\underline{\mathbf{k}}}\cdot\partial_{\mathbf{x}} T) = \left| \begin{array}{l} -\sum_{i\in[1,N_p]} h_i \partial_t(\epsilon_i\rho_i) \\ -\partial_t(\epsilon_g\rho_g h_g - \epsilon_g p) + \partial_{\mathbf{x}}\cdot(\epsilon_g\rho_g h_g \mathbf{v_g}) \\ +\partial_{\mathbf{x}}\cdot\sum_{k\in[1,N_g]}(\mathcal{Q}_k) + \mu\epsilon_g^2(\underline{\underline{\mathbf{K}}}^{-1}\cdot\mathbf{v_g})\cdot\mathbf{v_g} \end{array} \right.$$

energy stored in the solid phases — effective heat transfer — explicit source terms (pyrolysis, chemistry, convection, diffusion, dissipation)

Projects

Fundamental research – e.g. # Thermal equilibrium assumption

Validity of the local thermal equilibrium assumption : Tg = Ts ?

-> why wondering : Tg (gas) not well predicted → inaccurate finite-rate chemistry

-> how can we verify : explicit verification of local thermal equilibrium

$$\partial_t(\epsilon_g \rho_g e_g) + \partial_{\mathbf{x}} \cdot (\epsilon_g \rho_g h_g \mathbf{v_g}) + \partial_{\mathbf{x}} \cdot \sum_{k=1}^{N_g} (\mathcal{Q}_k) = H_v \, (T_s - T_g)$$

gas energy | convection | diffusion | heat exchange

$$T_g = T_s - \frac{1}{H_v} \left(\partial_t(\epsilon_g \rho_g e_g) + \partial_{\mathbf{x}} \cdot (\epsilon_g \rho_g h_g \mathbf{v_g}) + \partial_{\mathbf{x}} \cdot \sum_{k=1}^{N_g} (\mathcal{Q}_k) \right)$$

The idea is to estimate H_v and explicitly compute T_g at each time step and in each cell.

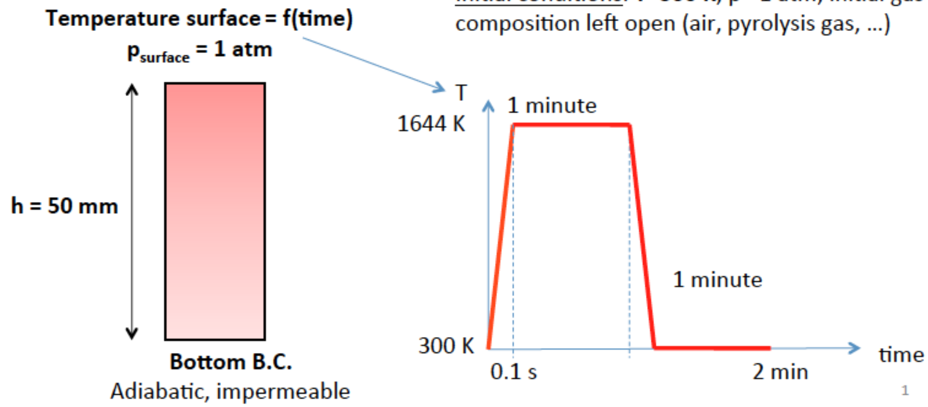
If $T_g \neq T_s$ then we know that the model becomes wrong.

Projects

Fundamental research – e.g. # Thermal equilibrium assumption

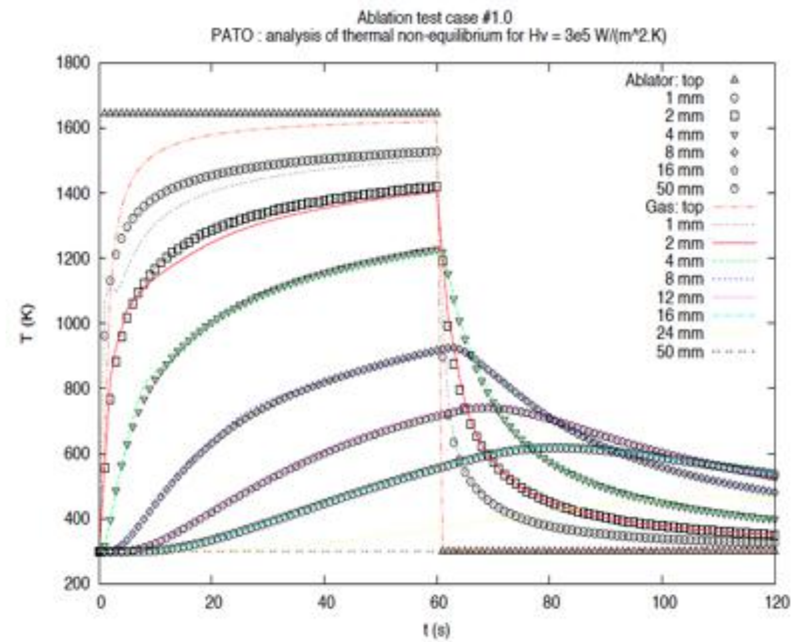
Example : ablation test-case 1.0

Initial conditions: **T=300 K**, p= 1 atm, initial gas composition left open (air, pyrolysis gas, …)



Estimated $H_v = 3\ 10^5$ W/(m^2.K)

→ Thermal disequilibrium : Tg < Ts



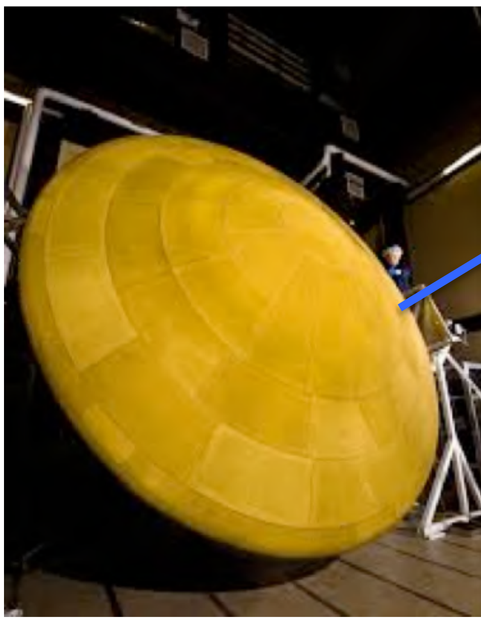
In these conditions, local thermal equilibrium is obtained for $H_v > 10^6$ W/(m^2.K)

Projects

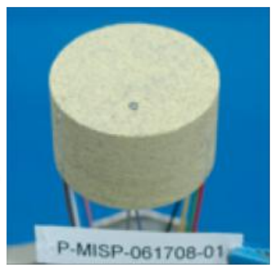
Engineering & design– e.g. # MSL heatshield

Objectives of TPS design
1- choose suitable material
2- compute TPS thickness

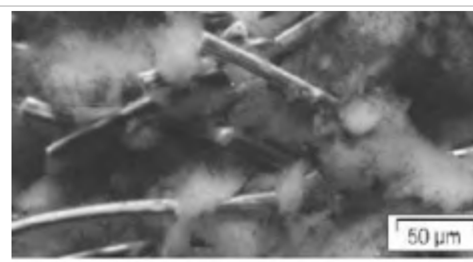
Mars Science Laboratory (MSL)
Thermal Protection System



Credits: NASA

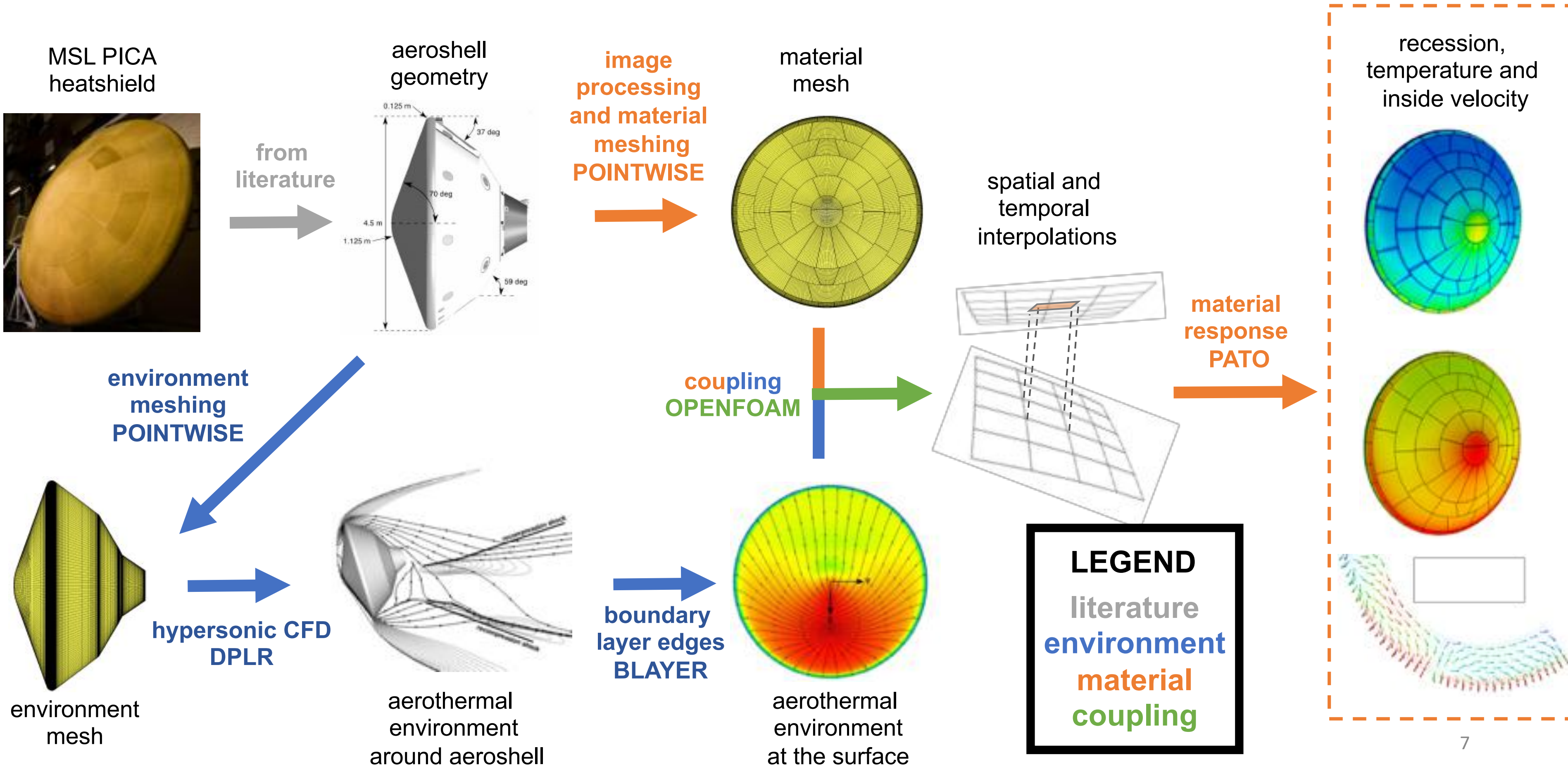


tile material : PICA
porous carbon/phenolic



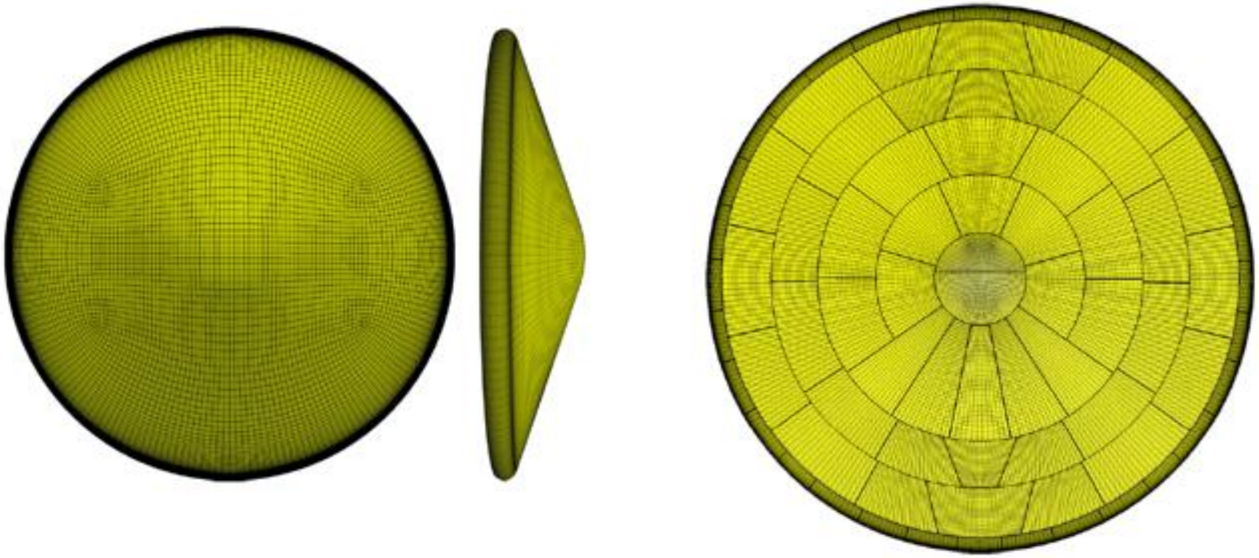
Projects

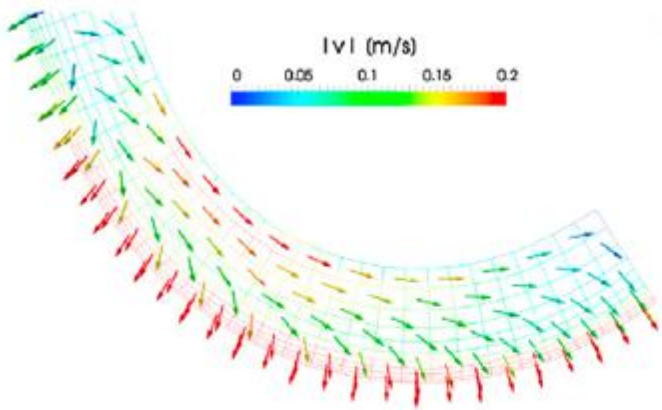
Engineering & design– e.g. # MSL heatshield



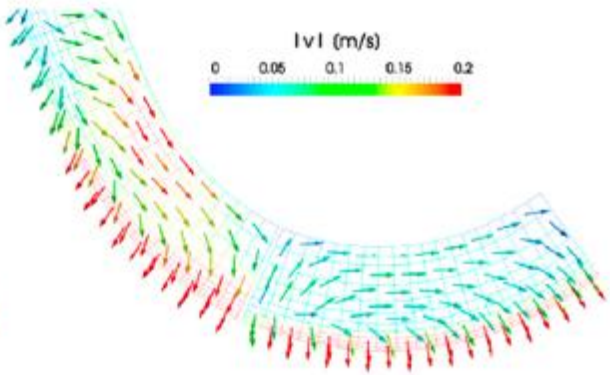
Projects

Engineering & design– e.g. # MSL heatshield





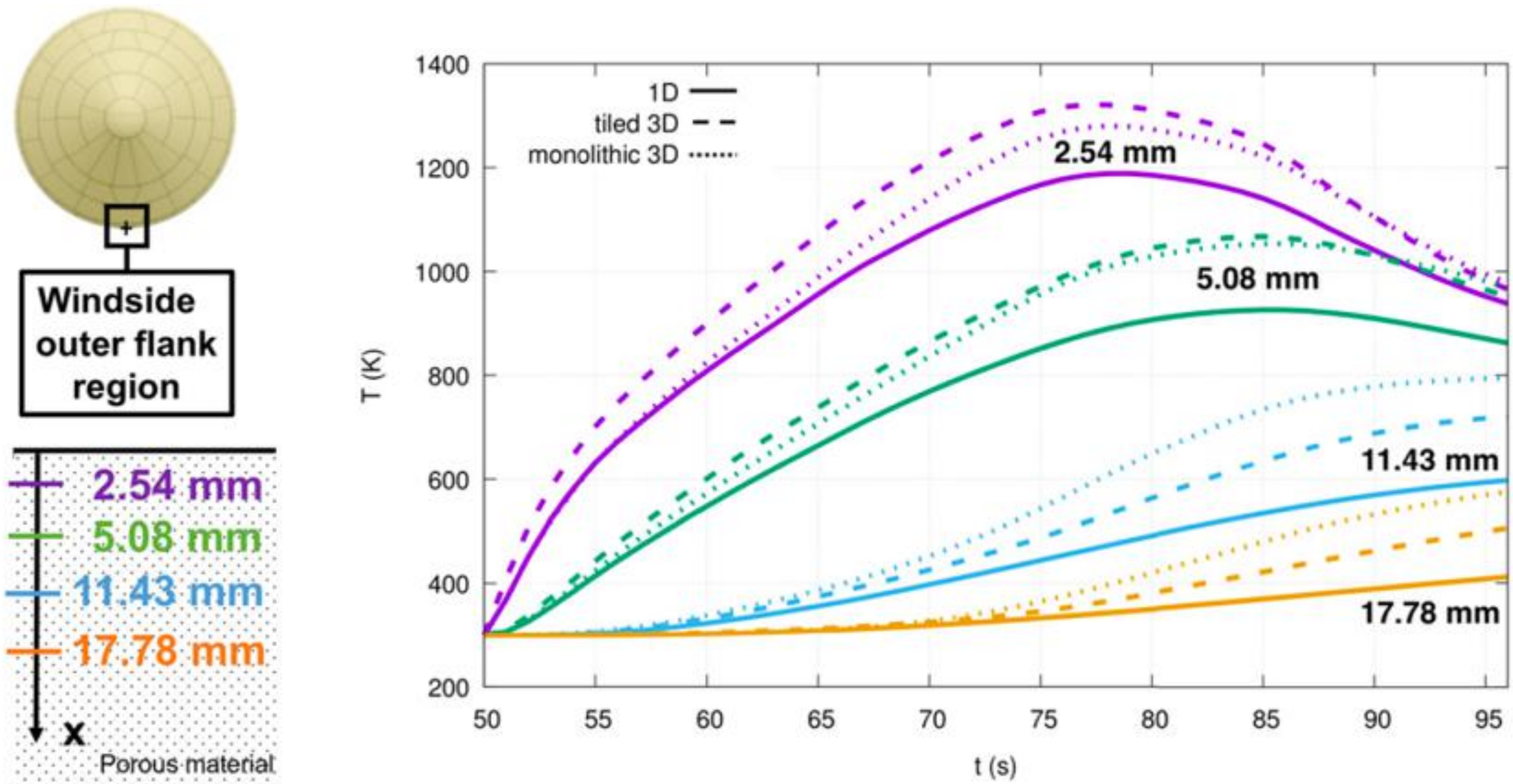
(a) Monolithic configuration.



(b) Tiled configuration.

Multi-dimensional effects reduced by the tile joints.

Engineering & design– e.g. # MSL heatshield

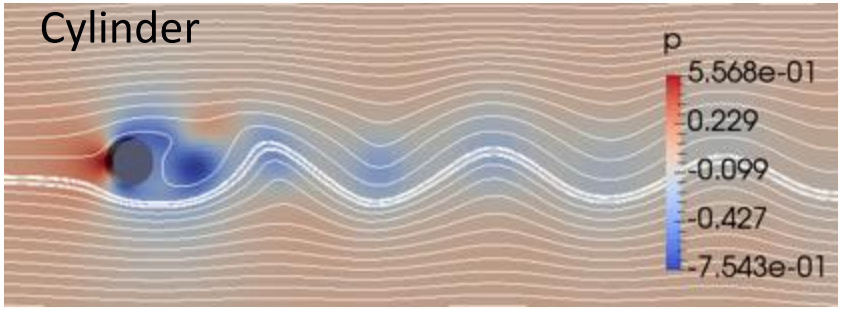


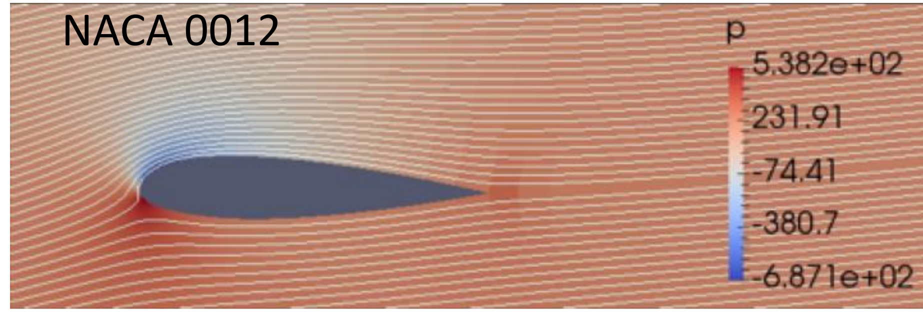
Quantitative analysis of multi-dimensional effects

Projects

Code development – e.g. # material-flow coupling

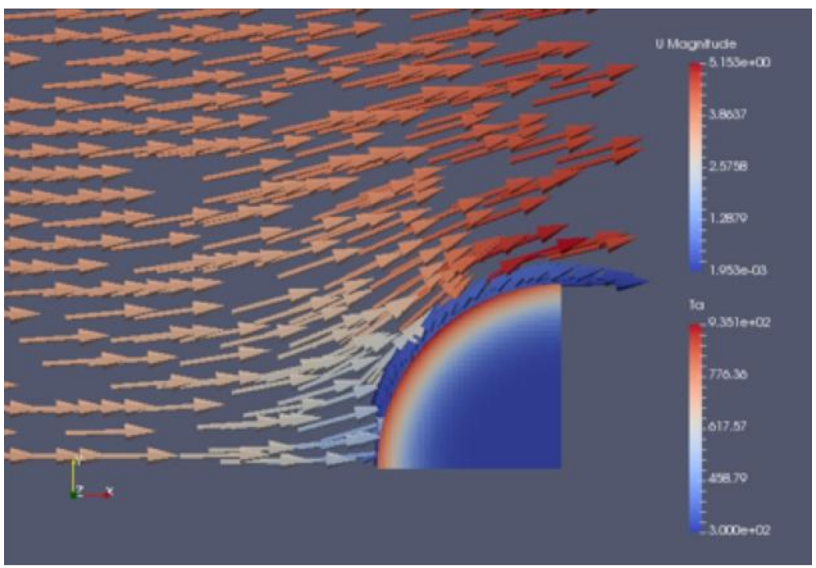
Native OpenFoam solvers



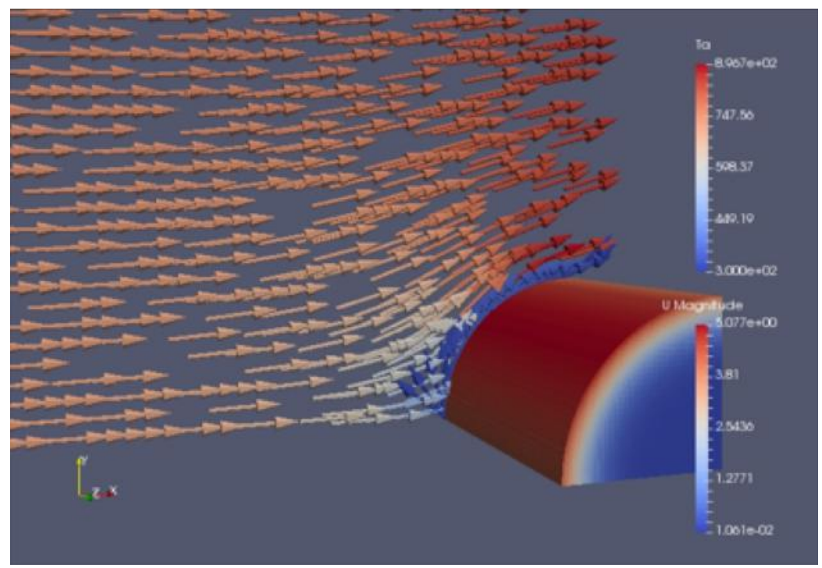


New coupled capability

Ex: Incompressible hot flow (1000 K) around a cold cylinder (300 K) of TACOT (low density C/P) that pyrolyzes



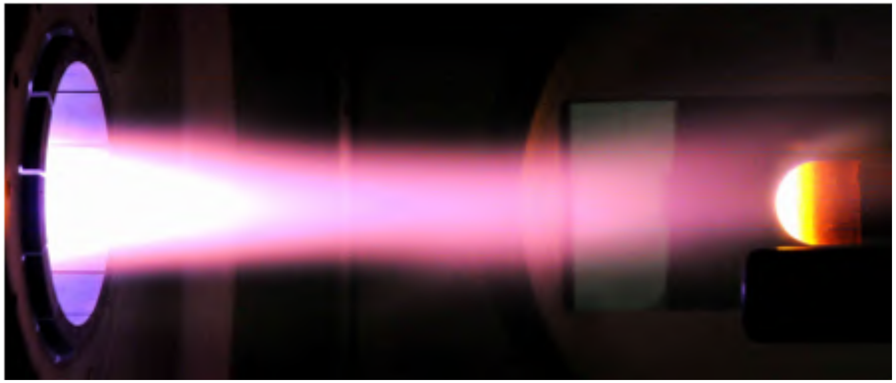
Energy coupled, flow uncoupled



Fully coupled

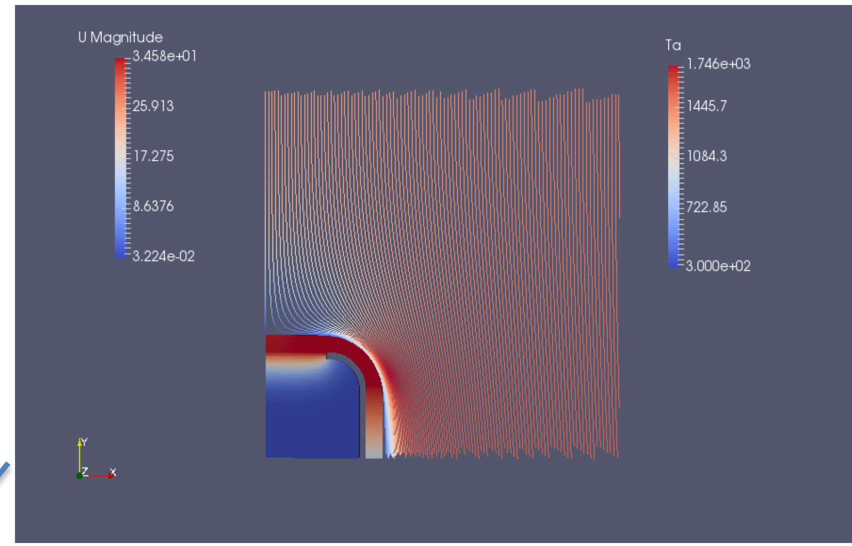
Projects

Code development – e.g. # material-flow coupling

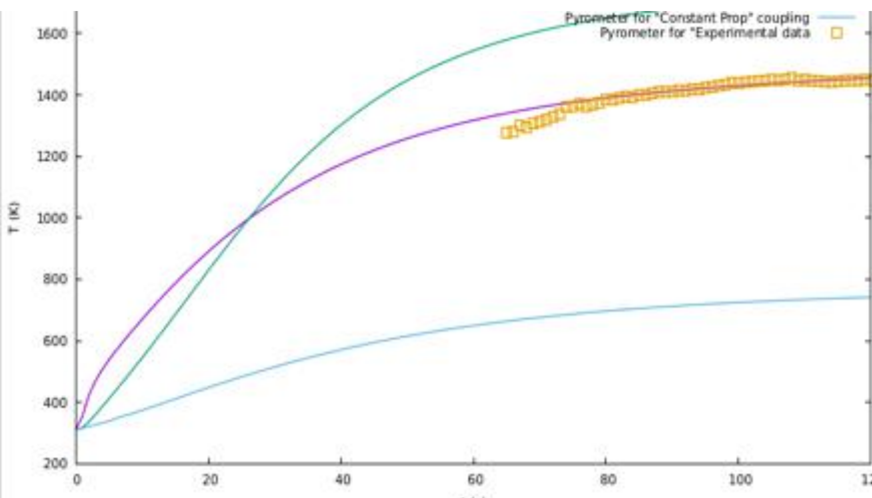


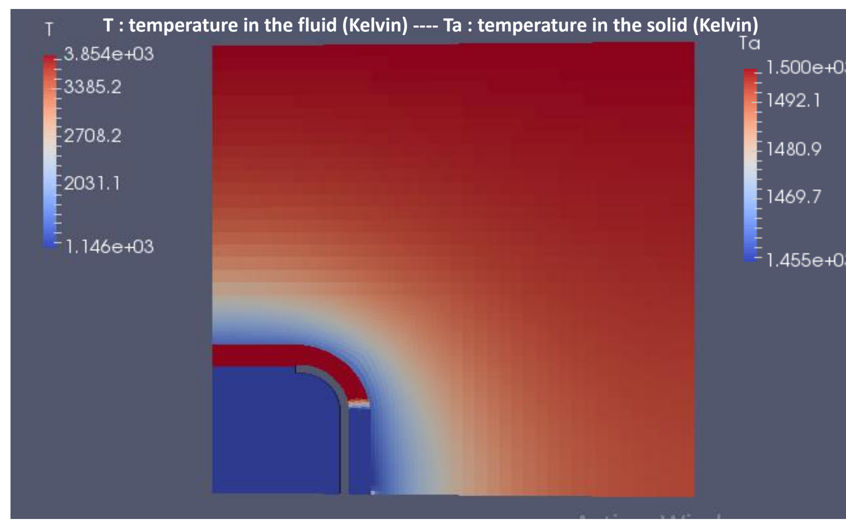
Picture taken during ablation testing of carbon-phenolic ablator
(1 MW/m2, 15 hPa)

U : velocity in the fluid (m/s) **Ta : temperature in the solid (Kelvin)**



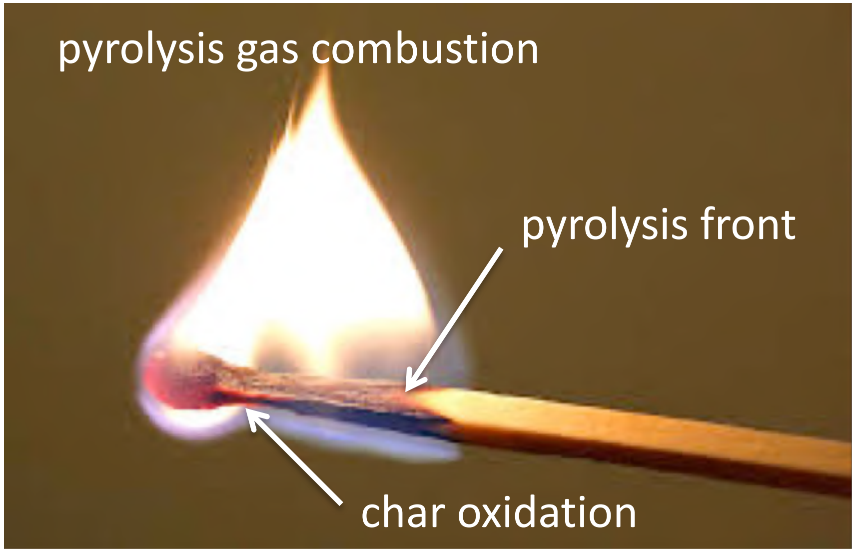
Test of Iron in the frame of ESA ATD3 debris demise project

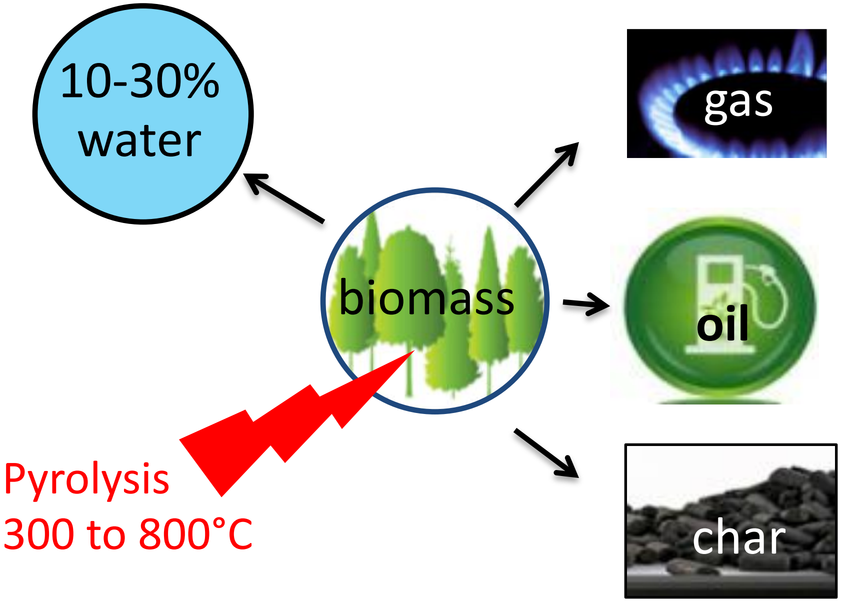




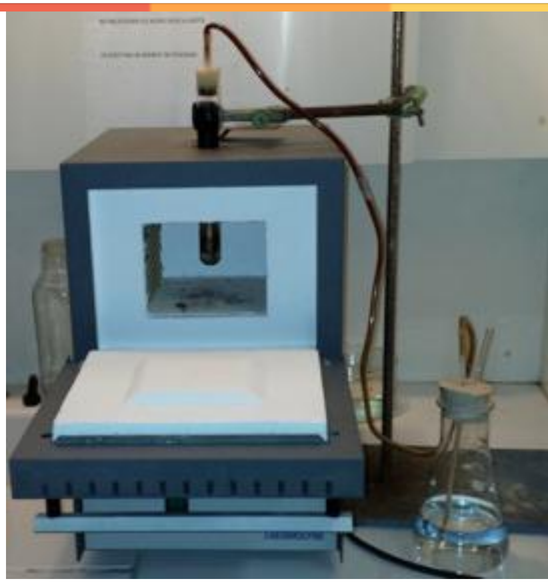
Projects

R & D analyses – e.g. # Wood pyrolysis

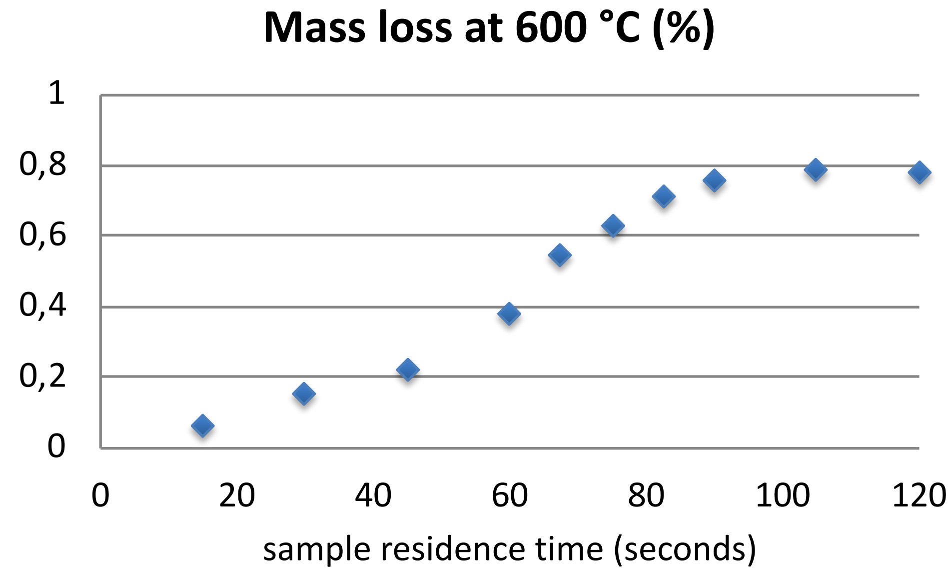


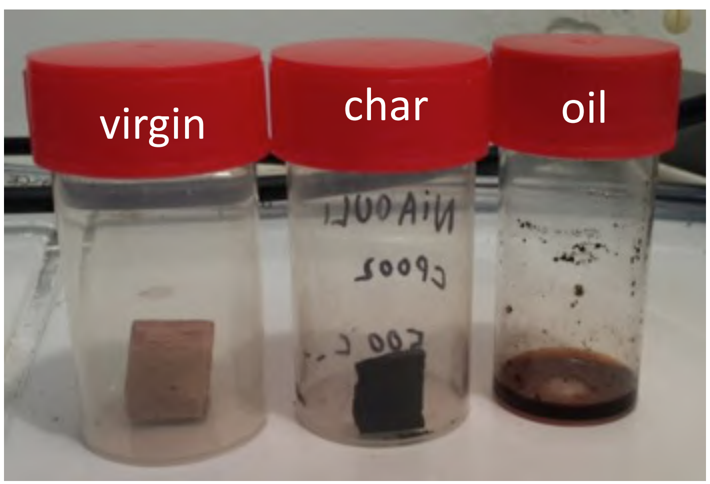


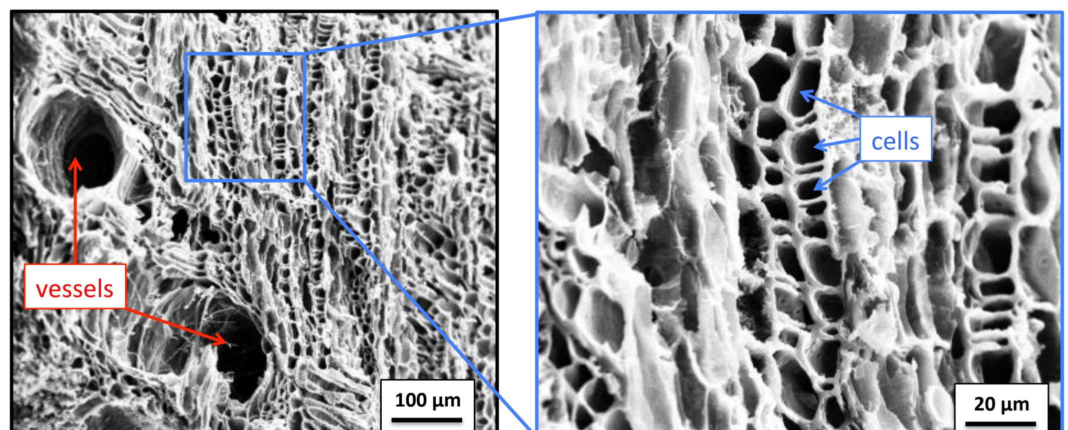
R & D analyses – e.g. # Wood pyrolysis



1000 °C laboratory oven



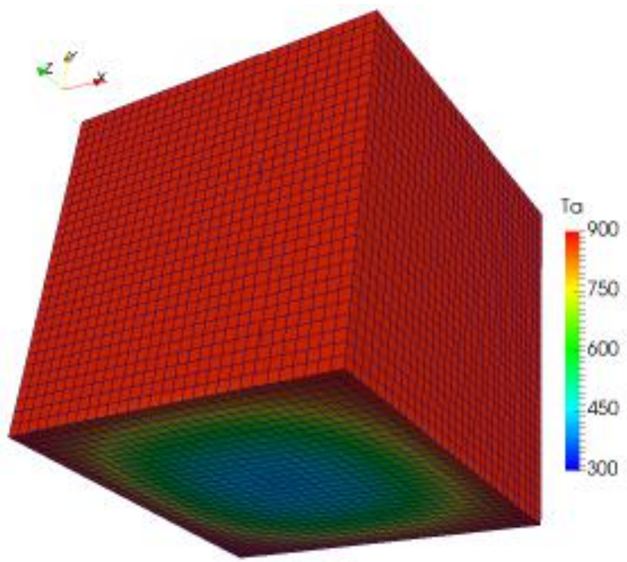


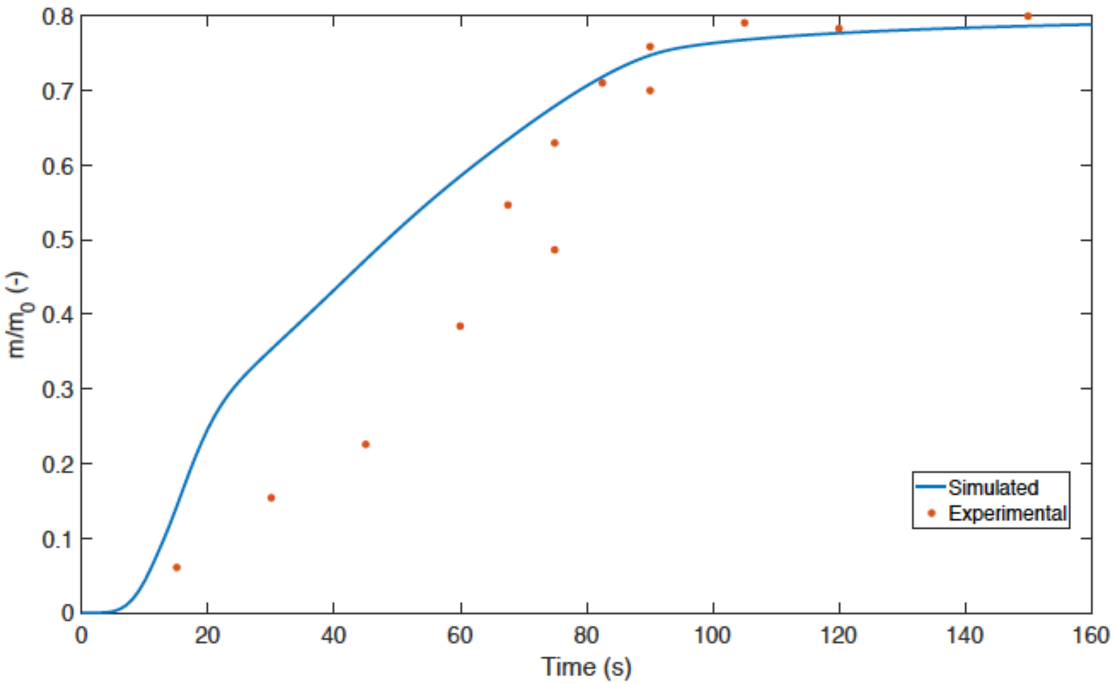


SEM of Niaouli wood, after pyrolysis at 600°C
(University of New Caledonia, France)

R & D analyses – e.g. # Wood pyrolysis

Wood counts 4 “solid” phases : trapped water, cellulose, hemi-cellulose, lignin.

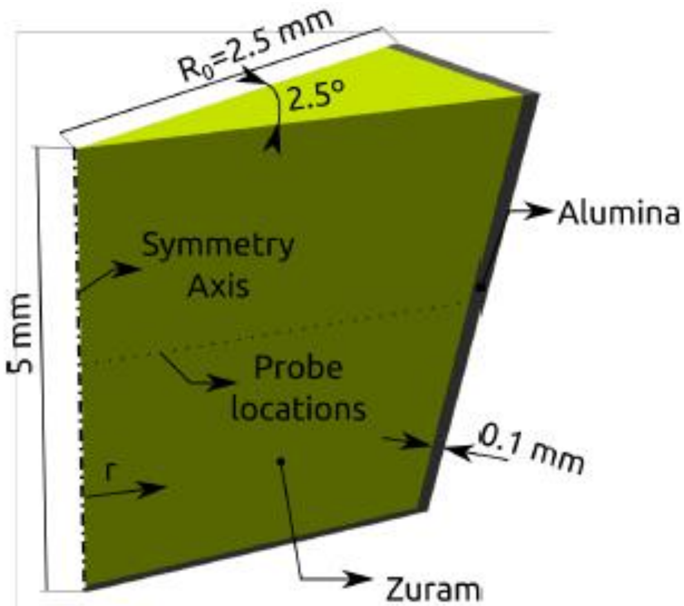




Efforts in progress to improve the wood database and drying model.

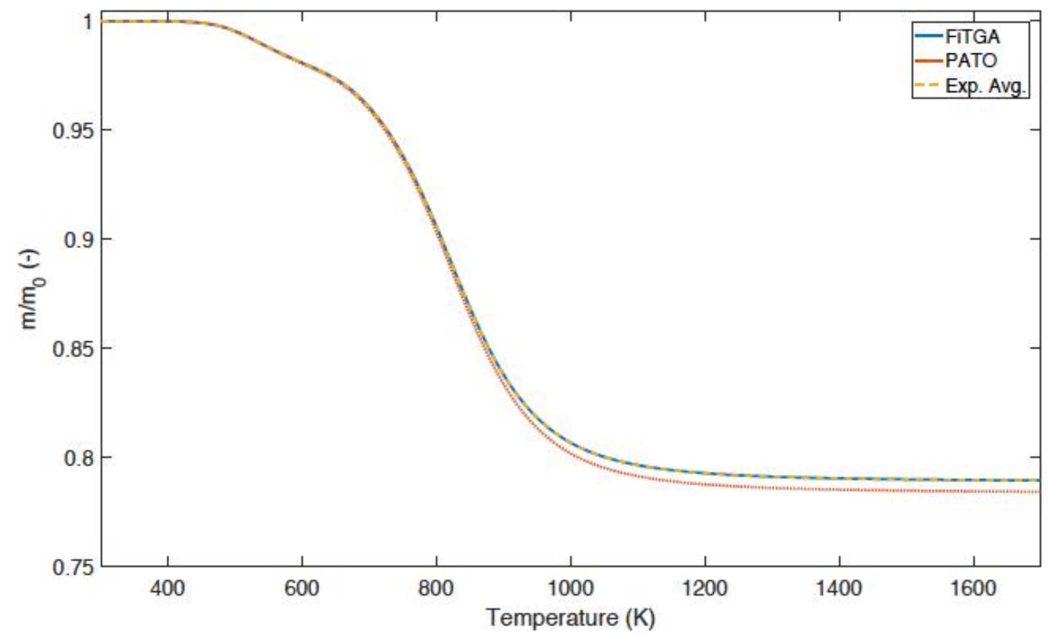
Projects

R & D analyses – e.g. # TGA – DSC



No temperature gradients observed up to very high heating rates.

Reproduction of TGA mass loss



In progress : modeling of DSC with the objective of understanding differences observed with heating rates, presence of lid, pressure, etc.

Team & contacts

Join the team ! We are committed to provide support and integrate contributions.

PATO was originally developed by a team of researchers at the NASA Ames Research Center (California) in collaboration with colleagues from the von Karman Institute for Fluid Dynamics (Belgium).

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