ENTRY SYSTEMS MODELING

Advancements in Coupled Flow and Material Modeling for Entry Systems

14th Ablation Workshop

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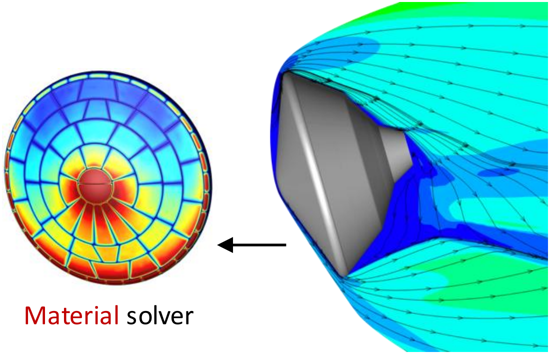
Nov 5th, 2024

ANALYTICAL MECHANICS ASSOCIATES

Main Strategies to Couple Flow and Material

One-Way Coupling

Exchange of boundary conditions
from flow solver to material solver



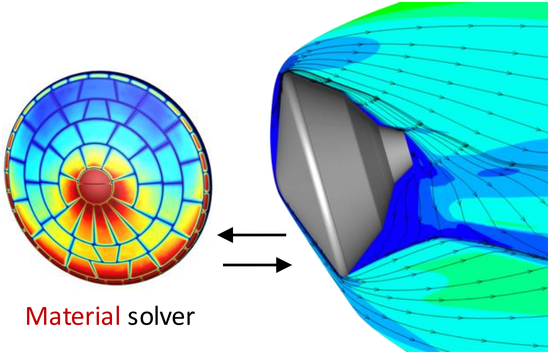
Material solver

Flow field solver

- decouples the flow field entirely from the material response;
- assumes that the flow field reaches steady state;
- assumes that the material ablation is in chemical equilibrium.

Two-Way Coupling

Exchange of boundary conditions
between flow and material solvers



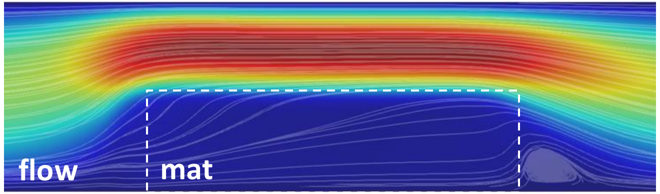
Material solver

Flow field solver

- is based on a iterative procedure to couple the flow field and material;
- assumes that the flow field adapts instantaneously to the material shape change.

Unified Coupling

No exchange of boundary conditions
between flow and material



Combined flow field and material solver

- 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.

Multi-Physics One-Way Coupling for Venus Mission Concept

Aerosol Capture
AERACEPT[1-3]

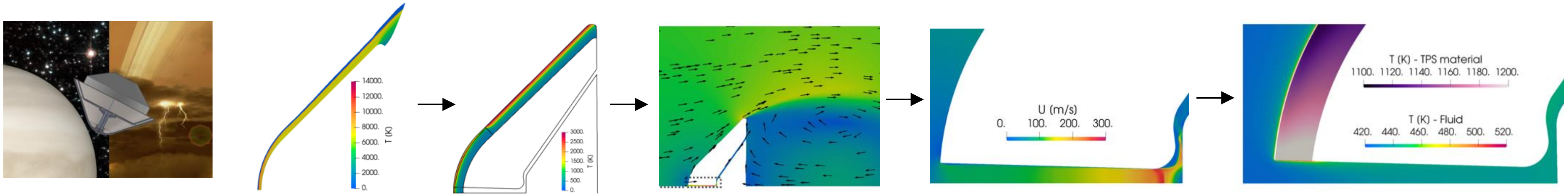
Hypersonic CFD
DPLR[4]

Material Response
PATO[5]

Subsonic CFD
OpenFOAM[6]

Particle Tracking
OpenFOAM

Thermal Analysis
OpenFOAM



Hypersonic CFD to Material

- Heat transfer coefficient C_H [kg/m^2/s]
- Recovery enthalpy h_r [J/kg]
- Wall pressure p_w [Pa]

Surface Mass & Energy Balance

$$B'_c = \frac{B'_g(z_{C,g} - z_{C,w}) + z_{C,e} - z_{C,w}}{z_{C,w} - 1}$$

$$-\left(\bar{\bar{\boldsymbol{k}}}_w \cdot \frac{\partial T_w}{\partial \boldsymbol{n}}\right) = C'_H(h_r - h_w) \cdot \\ + \dot{m}_g(h_g - h_w) + \dot{m}_c(h_c - h_w) \\ - \varepsilon_w \sigma (T_w^4 - T_\infty^4) + \alpha_w q_{rad}$$

Trajectory/TPS to CFD/Particle

- Freestream conditions:
  U_∞ [m/s], p_∞ [Pa], T_∞ [K]
- TPS wall temperature: T_w [K]

Particle Motion & Heat Transfer

$$m_p \partial_t \boldsymbol{v}_p = \sum_i \boldsymbol{F}_i$$

$$\boldsymbol{F}_D = \frac{3}{4} C_D \frac{m_p \mu_g \epsilon_g^{-1.65}}{\rho_p (d_p)^2} (\boldsymbol{v}_g - \boldsymbol{v}_p)$$

$$\partial_t T_p = \frac{S_p}{m_p c_{p,p}} \left(\mathcal{H}_g (T_g - T_p) \\ + F \sigma \varepsilon_w (T_w^4 - T_p^4)\right)$$

Aerosol Capture Predictions

Sample Quantification

- 623 million droplets, mostly 2 μm in diameter
- Total volume of 24.95 μL, mostly 8 μm in diameter
- Capture efficiency below 1% for small particles (0.4 μm and less)

Sample Integrity

- Limited effect from convection: maximum increase of 13 K
- Significant effect from radiation: 10% reduction in total volume

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[4] Wright, M.J., et al. "Data Parallel Line Relaxation (DPLR) Code User Manual: Acadia-Version 4.01.1." 2009.
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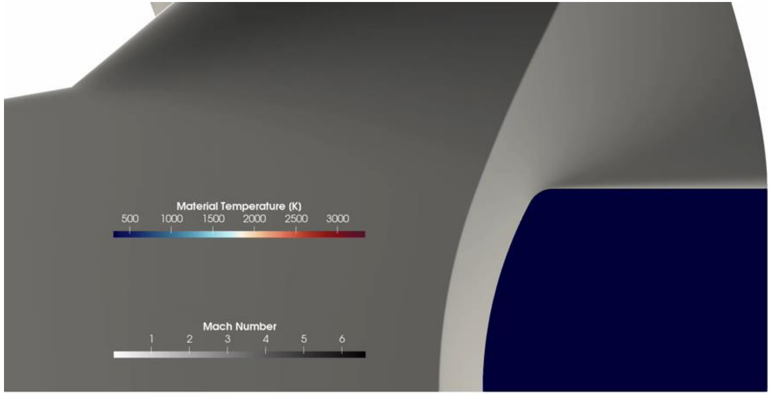
[6] Weller, H.G., et al. "A tensorial approach to computational continuum mechanics using object-oriented techniques." 1998.

Two-Way Coupling with Mesh Motion for 3MDCP Model Validation

Hypersonic CFD
US3D[7]

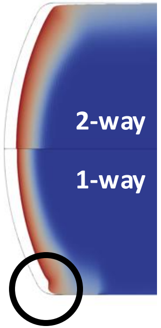
Coupler
Ares[8]

Material Response
Icarus[9]



Arc-Jet Test for Model Validation

- IHF-385 IsoQ sample with 3MDCP thermal protection material
- Exposure times = 38 - 39 sec
- Recession measured= 4.3 - 4.8 mm
- Recession computed = 4.9 mm
- Validate 3MDCP material model



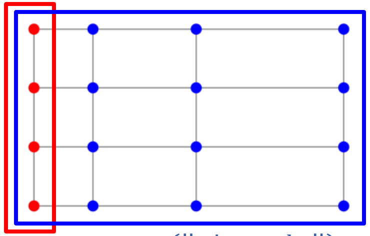
Two-way Coupling with Mesh Motion

algo

```
Load MR data into CFD code
Set coupling BC, frequency and algorithm type
Solve CFD to quasi-steady state
While MR is running:
  Solve MR + Update MR mesh
  If coupling frequency reached:
    Move CFD mesh based on MR mesh boundary
    Solve CFD to quasi-steady state + Update MR BC
```

Mesh Motion Approach

$$\mathbf{M}^{\mathrm{bc}} = \phi\left(\left\|\mathbf{x}_{\mathrm{i}}^{\mathrm{bc}} - \mathbf{x}_{\mathrm{j}}^{\mathrm{bc}}\right\|\right)$$



$$\mathbf{A}^{\mathrm{in}} = \phi\left(\left\|\mathbf{x}_{\mathrm{i}}^{\mathrm{in}} - \mathbf{x}_{\mathrm{j}}^{\mathrm{bc}}\right\|\right)$$

$\mathbf{M}^{\mathrm{bc}}$ and $\mathbf{A}^{\mathrm{in}}$ are built using Wendland[10]
Radial Basis Function: $\phi(\|x\|) = (1 - \|x\|)^2$

$$\mathbf{r}_{\mathrm{MR}}^{\mathrm{bc}} = \mathbf{M}_{\mathrm{MR}}^{\mathrm{bc}} \boldsymbol{\alpha}$$

$$\boldsymbol{\alpha} = \left(\mathbf{M}_{\mathrm{MR}}^{\mathrm{bc}}\right)^{-1} \mathbf{r}_{\mathrm{MR}}^{\mathrm{bc}}$$

$$\mathbf{r}_{\mathrm{MR}}^{\mathrm{in}} = \mathbf{A}_{\mathrm{MR}}^{\mathrm{in}} \boldsymbol{\alpha}$$

$$\mathbf{r}_{\mathrm{CFD}}^{\mathrm{in}} = \mathbf{A}_{\mathrm{CFD}}^{\mathrm{in}} \boldsymbol{\alpha}$$

α is computed once on MR grid, then re-used on CFD grid, significantly reducing computational cost.

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[10] Rendall, T., et al. "Efficient mesh motion using radial basis functions with data reduction algorithms." 2009.

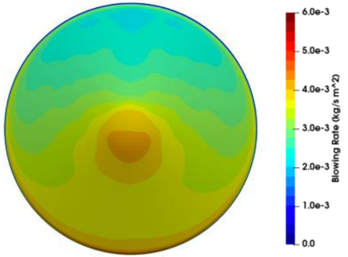
Approaches for Two-Way Coupling with Pyrolysis Gas Blowing

Hypersonic CFD
DPLR & US3D

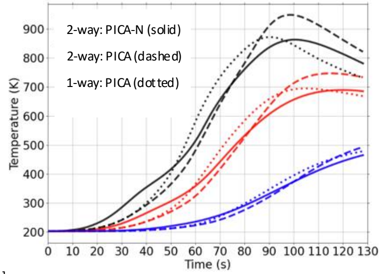
Coupler
Ares

Radiation
NEQAIR[11] & NERO[12]

Material Response
PATO & Icarus



PICA-NuSil
$\gamma = 0.05$
80.2 sec



credit: John M. Thornton (2024 ARC-TSM contractor)[13]

Two-way Coupling with Pyrolysis Gas Blowing

algo

```
For all trajectory points:
    Solve CFD without blowing BC + solve Radiation
    Update MR BC using CFD results [$q_w$, $p_w$]
    Solve MR with blowing correction
    While $|T_{w,CFD} - T_{w,MR}| >$ threshold:
        Update CFD BC using MR/GSI [$\dot{m}_g$, $y_w$, $\dot{m}_c$, $\rho_g$]
        Solve CFD with blowing BC + solve Radiation
        Update MR BC using CFD results [$q_w$, $p_w$]
        Solve MR without blowing correction
```

Surface Mass & Energy Balance Approach

Wall Composition using B'

$$z_{w,k} = \frac{z_{e,k} + B'_g \; z_{g,k}}{\sum_k^{N_e} \; z_{wsg,k}}$$

$$z_{w,C} = \frac{L + z_{e,C} + B'_g \; z_{g,C}}{\sum_k^{N_e} \; z_{wsg,k}}$$

$$L = \max(100 B'_g, \; 200)$$

$$\text{Equilibrium } (p_w, T_w, z_{w,k}) \rightarrow x_{wg,k}$$

$$h_w = \sum_i^{N_s} x_{wg,i} \; h_{wg,i}$$

Blowing Correction

$$C_H = \frac{q_w}{h_e - h_w}$$

$$\frac{C'_H}{C_H} = \frac{\ln\left(1 + 2\lambda(B'_g + B'_c)\right)}{2\lambda(B'_g + B'_c)}$$

Limitations

After the peak heating,
$h_w - h_e < 0$

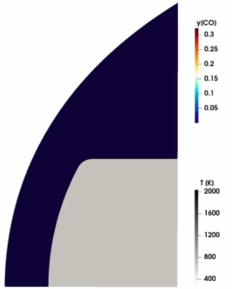
$$q_w = q_{conv} + q_{diff} + q_{adv}$$

Diffusive Flux Approach[14-16]

Wall Composition using J_k

$$J_k + (\dot{m}_g + \dot{m}_c) z_{w,k} = \dot{m}_g z_{g,k} + \dot{m}_c z_{c,k}$$

Computing the mass balance using diffusive flux from CFD allows the computation of $\dot{m}_c$ without B' assumption



Two-way coupling with pyrolysis gas blowing (19 species) and mesh motion for simulating a PICA arc-jet case based on Milos[17]

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[17] Milos, F.S. and Chen, Y-K. "Ablation and thermal response property model validation for phenolic impregnated carbon ablator." 2010.

Unified Coupling for Oxidation Model Validation using Flow Tube Data

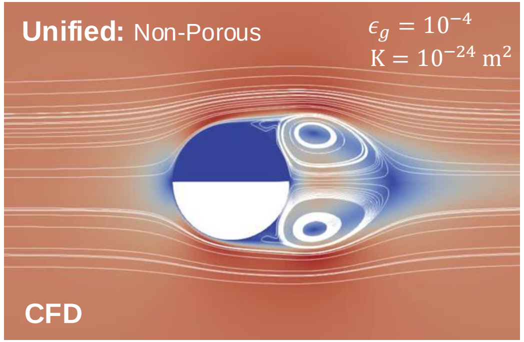
Unified Solver: Governing Equations[18]

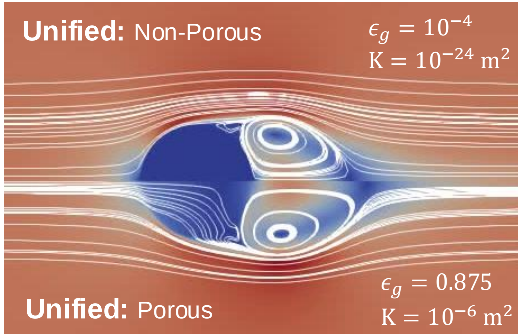
$$\partial_t\left(\epsilon_g \boldsymbol{U}\right) + \boldsymbol{\partial_x} \cdot \left[\epsilon_g\left(\boldsymbol{F}^{inv} + \boldsymbol{F}^{vis}\right)\right] = \boldsymbol{S}$$

$$\partial_t \epsilon_s = \frac{-\dot{\omega}^{het}}{\rho_s}$$

$$\boldsymbol{S} = \begin{bmatrix} \epsilon_g \dot{\omega}^{chem} + \dot{\omega}^{het} \\ -\boldsymbol{F}^{drag} \\ -\boldsymbol{F}^{drag} \cdot \boldsymbol{u} \end{bmatrix}$$

$$\boldsymbol{F}^{drag} = -\mu \bar{\bar{\boldsymbol{K}}}^{-1}\left(\bar{\bar{\boldsymbol{I}}} + \bar{\bar{\boldsymbol{F}}}\right)\epsilon_g^2 \boldsymbol{u}$$



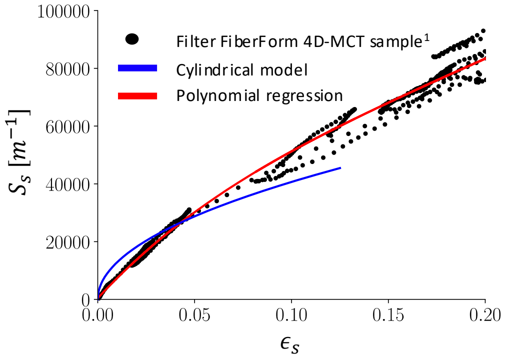


Unified Solver: Oxidation Model[19]

$$C(s) + O_2(g) \rightarrow CO_2(g)$$
$$2C(s) + O_2(g) \rightarrow 2CO(g)$$

$$\dot{\omega}_i^{het} = -S_f\ k_i\ \rho_{O_2}\ \frac{M_i}{M_{O_2}}$$
$$\dot{\omega}^{het} = \sum_i \dot{\omega}_i^{het} \qquad i \in [O_2, CO, CO_2]$$

4D-MCT sample courtesy of Ringel[20]



FiberForm surface area using filtering

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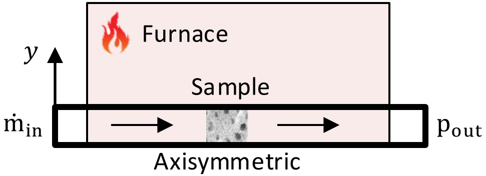
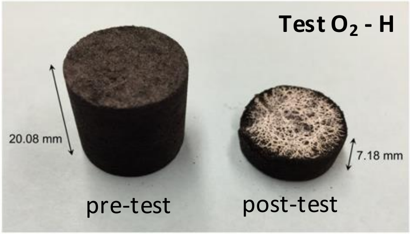
[18] Dias, B., et al. "Numerical Simulation of FiberForm Using a Unified Flow-Material Approach: A Comparison With Flow-Tube Reactor Experiments." 2024.
[19] Panerai, Francesco, et al. "Experimental and numerical study of carbon fiber oxidation." 2014.
[20] Ringel et al. "Carbon Fiber Oxidation" in 4D, In preparation.

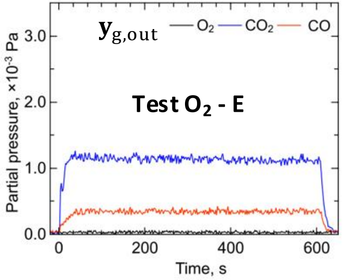
Unified Coupling for Oxidation Model Validation using Flow Tube Data

High-Temperature FiberForm Oxidation

Flow Tube Reactor[21]

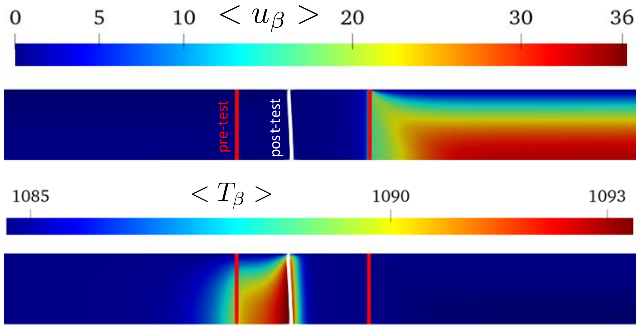




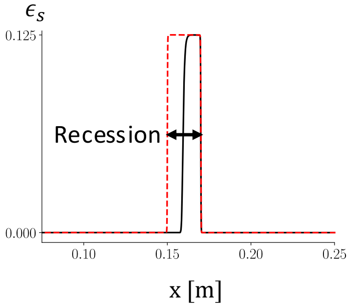


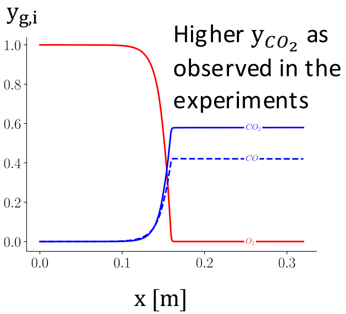
Combined CFD and Material Response

PATO unified solver[18]



Test O_2 - E

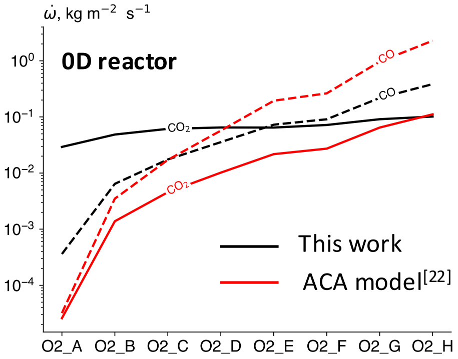


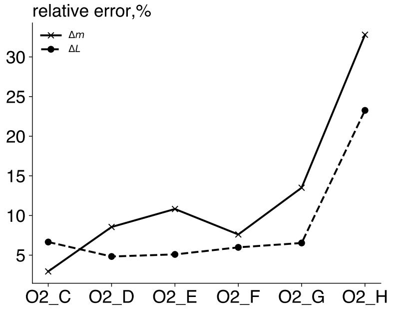


Higher y_{CO_2} as observed in the experiments

Oxidation Rates and Mass Loss

Comparison to experiments





[18] Dias, Bruno, et al. "Numerical Simulation of FiberForm Using a Unified Flow-Material Approach: A Comparison With Flow-Tube Reactor Experiments." 2024.

[21] Panerai, Francesco, et al. "Experimental measurements of the high-temperature oxidation of carbon fibers." 2019.

[22] Prata, Krishna Sandeep, et al. "Air–carbon ablation model for hypersonic flight from molecular-beam data." 2022.

Conclusion

Flow and Material Coupling Strategies for Entry Systems

Coupling strategies play a crucial role in capturing multiphysics interactions between flow and material, providing varying levels of accuracy and computational efficiency depending on the application.

1. **One-Way Coupling** offers a computationally efficient approach for providing initial estimates in multiphysics problems. It is ideal for mission concept studies and the development of novel physics-based models (e.g., AERACEPT).
2. **Two-Way Coupling** ensures accurate modeling by capturing interactions between material mesh motion and flow fields through iterative exchanges. This approach is essential for arc-jet simulations (e.g., 3MDCP validation) and flight mission predictions involving trajectory and radiation (e.g., Dragonfly). Fidelity can also be enhanced through pyrolysis gas coupling.
3. **Unified Coupling** offers a combined flow and material solution within a single solver, eliminating the need for mesh motion and iterative steps. The oxidation model has been validated using flow tube experiments. It relies on a pressure-based solver, restricted to subsonic regimes. Future work will involve a coupling between the unified solver and hypersonic CFD.

Achieving the right balance between computational cost and fidelity is essential, as different applications demand different levels of precision to meet their specific goals.

References

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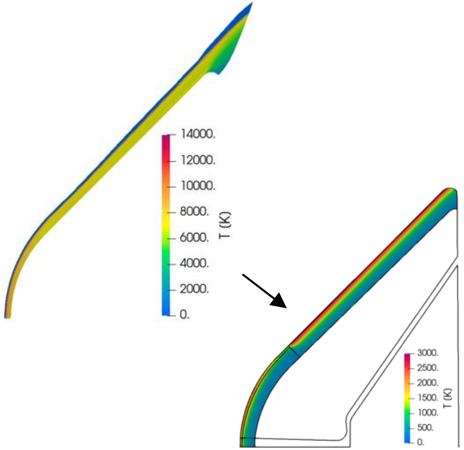
Thank you for your attention! Any questions?

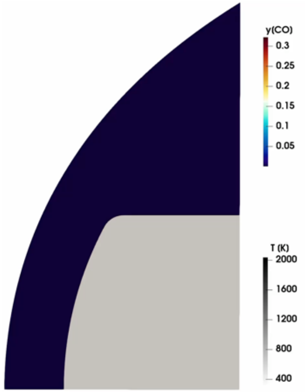
One-Way Coupling

Computationally efficient,
ideal for initial estimates



Two-Way Coupling

Accurate CFD-MR modeling with mesh motion,
computationally expensive due to iterations



Unified Coupling

Accurate flow-mat. modeling without mesh motion,
computationally efficient, under development