CHyPS: An MFEM-Based Material Response Solver for Hypersonic Thermal Protection Systems

April 26, 2022
FEM@LLNL Seminar Series

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Challenges of Hypersonic Flight

Hypersonic flight leads to a wealth of technical challenges
• Speeds exceeding 4,000 miles per hour
• Surface temperatures exceeding that of the sun
• Communication blackout due to gas ionization
• Vehicle guidance and control
• … and many more
Center for Hypersonics and Entry-Systems Studies

High-Temperature Materials

Aerosciences

High-Enthalpy Wind Tunnels

Machine Learning & UQ

Guidance, Navigation & Control

High-Temperature Materials

Optical Diagnostics

Detection & Tracking

Large Scale Computing

Propulsion

Large Scale Computing
Material Response during Hypersonic Flight
CHESS Experimental Capabilities

Newly completed Plasmatron-X
CHESS Computational Capabilities

DOE SPARTA DSMC

Solution for electric field in torch

Time: 0.000000 ms

Time-accurate simulation of a Plasmatron facility
My Background is not in FEM…
Requirements for a New Material Response Tool

Goal: A state of the art material response solver that can perform full-vehicle simulations and readily couple to external solvers to add additional physics

Tool features required for full-vehicle simulation
- Scalability to large problems and core counts
- Faithful representation of vehicle geometry features
- Robustness to low quality meshes
- Correct level of abstraction and flexibility for physical model

Targeting cases where coupled response is important
- Material response of control surfaces and thin-ablators
- Boundary layer stability and transition on ablating surfaces
- Development of small-dimension models for guidance and control
Macroscopic phenomenology

- Long distance effects
  - Radiation
- Material-flow coupling
  - Boundary layer transfers (heat and mass)
  - Recombination/catalicity
  - Ablation (oxidation, sublimation, spallation)

Interface phenomena: Heat and mass balance (1), Subsurface phenomena
- In-depth ablation (3)
- Penetration of radiation (3)
- Gas flow entering into the material (3)
- Conduction heat transfer (1)
- Radiation heat transfer (empirical: 1, modeled: 3)
- Finite rate chemistry of the pyrolysis gases (3)
- Coking (3)
- Multicomponent diffusion (3)
- Convective transport (Darcy: 2, Klinkenberg: 3)
- Charring process (evolution of the density: 1, porosity: 2, tortuosity: 3, permeability: 2, effective conductivity: 1, effective surface area: 3)
- Phenolic-decomposition product (3)
- Phenolic-decomposition rate (1)

1: in all material response models (type 1)
2: in some material response models (type 2)
3: in analysis material response models (type 3)

Macroscopic illustration

Nonviscous flow
\[ \approx 6000 \text{ K} \]

Boundary layer
\[ \approx 3000 \text{ K} \]

Ablation zone
\[ \approx 1400 \text{ K} \]

Coking zone
\[ \approx 1200 \text{ K} \]

Pyrolysis zone
\[ \approx 400 \text{ K} \]

Chemistry mechanisms (simplified illustration)

3-D simulation of the ablation of a carbon/phenolic composite [Lachaud [6]]

Microscopic illustration

Gas/surface interactions in porous fibrous media (3):
- In-depth ablation
- Erosion
- In-depth recombination
- Coupled heat transport (diffusion, convection, radiation)

Scanning electron microscopy (SEM): Carbon preform

3-D reconstitution of a carbon/phenolic composite

SEM: carbon/phenolic (virgin) [Stackpoole, 2008]

Governing Physics

SEM of carbon preform prior to phenolic impregnation [1]

[1] Lachaud et al. IJHMT. 2015
Gas properties
Volume fraction $\epsilon_g$
Pressure $P_g$
Enthalpy $h_g$
Density $\rho_g$
Viscosity $\mu_g$

Material properties ($i \in [1,N_p]$)
Volume fraction $\epsilon_i$
Density $\rho_i$
Specific heat $c_{p,i}$
Enthalpy $h_i$
Pyrolysis specie production $\pi_{i,k}$

Bulk properties
Temperature $T$ (thermal equilibrium)
Conductivity $\kappa$
Permeability $K$

[1] Lachaud et al. IJHMT. 2015
Volume-Averaging over a Representative Elementary Volume

Smallest volume that is representative of the bulk properties of the whole

Phase indicator functions:

\[ H(\vec{x}) = \begin{cases} 
1, & \vec{x} \in \text{phase} \\
0, & \vec{x} \notin \text{phase} 
\end{cases} \]

For a fiber/matrix composite, three total phases

Volume fraction:

\[ \epsilon_i = \frac{\int_{\Omega_i} H_i(\vec{x}) \, d\vec{x}}{\int_{\Omega} d\vec{x}} \quad \text{or} \quad \epsilon_i = \frac{\int_{\Omega_i} d\vec{x}}{\int_{\Omega} d\vec{x}} \]

Average solid density:

\[ \rho_s = \frac{\sum_{i \in N_p} \int_{\Omega_i} \rho_i \, d\vec{x}}{\int_{\Omega} d\vec{x}} = \sum_{i \in N_p} \epsilon_i \rho_i \]
Governing Equations

Solid mass conservation:
\[
\frac{\partial \varepsilon_i \rho_i}{\partial t} = - \sum_{k \in [1, N_{sp}]} \pi_{i,k}
\]

Gas mass/momentum conservation:
\[
\frac{\partial}{\partial t} \left( \frac{\varepsilon_g M P_g}{RT} \right) - \nabla \cdot \left( \frac{P_g M}{RT \mu} K \nabla P_g \right) = \sum_{i \in [1, N_p], k \in [1, N_{sp}]} \pi_{i,k}, \quad \vec{u}_g = - \frac{K}{\varepsilon_g \mu} \nabla P_g
\]

Energy conservation:
\[
\left( \sum_{i \in [1, N_p]} \varepsilon_i \rho_i c_{p,i} \right) \frac{\partial T}{\partial t} - \nabla \cdot \kappa \nabla T = - \sum_{i \in [1, N_p]} h_i \frac{\partial \varepsilon_i \rho_i}{\partial t} - \frac{\partial \left( \varepsilon_g \rho_g h_g - \varepsilon_g P_g \right)}{\partial t} - \nabla \cdot \left( \varepsilon_g \rho_g h_g \vec{u}_g \right)
\]

Pyrolysis chemistry:
\[
\frac{\partial X_{i,j}}{\partial t} = \left( \frac{1 - X_{i,j}}{m_{i,j}} T^{n_{i,j}} A_{i,j} \exp \left( - \frac{E_{i,j}}{RT} \right) \right), \quad \pi_{i,k} = \sum_{j \in [1, P_i]} \zeta_{i,j,k} \epsilon_{i,0} \rho_{i,0} F_{i,j} \frac{\partial X_{i,j}}{\partial t}
\]

[1] Lachaud et al. IJHMT. 2017
Ablative Boundary Condition
Ablative Boundary Condition
Ablative Boundary Condition

Ablative surface boundary condition from local equilibrium assumption

Provides Neumann boundary condition (heat flux) for energy equation

\[ q_{\text{cond}} = q_{\text{conv}} - \rho V H_w + q_{\text{rad, in}} - q_{\text{rad, out}} + \dot{m}_{pg} H_{pg} + \dot{m}_{ca} H_{ca} \]

\( B' \) table is used to compute \( \dot{m}_{ca} \) and \( H_w \) as a function of \( f(P, T, \dot{m}_{pg}) \)

\( \dot{m}_{ca} \) directly controls the ablative surface recession

[1] Lachaud et al. IJHMT. 2017
Governing Equations - ALE

An Arbitrary Lagrangian Eulerian (ALE) used to allow moving mesh

Employ the conservative direct ALE method of Ivančić et al. 2019

Consider the heat equation \( \frac{\partial u}{\partial t} \bigg|_{\hat{x}} - \alpha \nabla^2 u - \vec{w} \cdot \nabla u = f \) in weak form with backward Euler time-integration

\[
\int_{\Omega} \hat{\psi} \hat{u}_{n+1} \hat{J}_{n+1} d\hat{x} - \int_{\Omega} \hat{\psi} \hat{u}_n \hat{J}_n d\hat{x} + d_{n,n+1}(\hat{u}_{n+1}, \hat{\psi}) - b_{n,n+1}(\hat{u}_{n+1}, \hat{\psi}) - M_{n,n+1}(\hat{u}_{n+1}, \hat{\psi}) = 0
\]

\[
d_{n,n+1}(\hat{u}_k, \hat{\psi}) = \Delta t \int_{\Omega} \alpha \frac{1}{\hat{J}_{n,n+1}(\Delta t)} \hat{F}_{n,n+1}(\Delta t) \hat{F}_{n,n+1}^T (\Delta t) \hat{\psi} \cdot \hat{\nabla} \hat{u}_k d\hat{x}
\]

\[
b_{n,n+1}(\hat{f}_k, \hat{\psi}) = \Delta t \int_{\Omega} \hat{\psi} \hat{f}_k \hat{J}_{n,n+1}(\Delta t) d\hat{x}
\]

\[
M_{n,n+1}(\hat{u}_k, \hat{\psi}) = \int_{\Omega} \hat{\psi} \left[ \int_0^{\Delta t} \hat{F}_{n,n+1}(t) \hat{w}_{n,n+1}(t) dt \right] \hat{\nabla} \hat{u}_k d\hat{x} + \int_{\Omega} \hat{\psi} \hat{u}_k \hat{\nabla} \left[ \int_0^{\Delta t} \hat{F}_{n,n+1}(t) \hat{w}_{n,n+1}(t) dt \right] d\hat{x}
\]

Multi-Stage BilinearForm

Created a Multi-Stage BilinearForm to implement the direct ALE method

- Assumes integrating over $t \in [t_0, t_0 + \Delta t]$ and known nodal displacement

Integrators are added to specific time-stages of the BilinearForm

- Added independently for each time stage
- Can include both domain and boundary integrators

Each time-stage has an associated GridFunction denoting nodal locations

- Nodes set on Mesh before building of each time-stage
- References to nodes stored, allowing external update of locations
Governing Equations - ALE

\[ \partial_t u - 0.1 \Delta u = f \text{ in } \Omega(t) \times (0, T), \]
\[ u = 0 \text{ on } \partial \Omega(t) \times (0, T), \]
\[ u(0) = 16 x(1 - x)y(1 - y) \text{ in } \Omega(0) \]
\[ u(x, t) = 16 \left( 1 + \frac{1}{2} \sin(\pi t) \right) x(1 - x)y(1 - y) \]

Deformation results coincident with fixed mesh
Implementation

Implemented in the Coupled Hypersonic Protection System (CHyPS) Simulator

Discontinuous Galerkin spatial discretization via MFEM library [1]

Crank-Nicolson, Forward Euler, and Backward Euler time integration available
  • Custom time-integration currently used, would like to return to MFEM ODE solvers

Tensor properties for conductivity and permeability

Coupling to external solvers using the preCICE library

[1] mfem.org
[2] precice.org
Ablation Test Case Series

Series of test cases developed over the last decade for code comparison

- Makes available open-results for a field dominated by national defense
- Feature Theoretical Ablative Composite for Open Testing (TACOT)
- Provide gradual increase in physical and computational complexity

Ablation Test Case 2

- Mimics the 1D heating of a sample in an arc jet facility
- Will compare against the Porous-Material Analysis Toolbox Based on OpenFOAM (PATO)

Ablative BC, Temperature computed via energy balance

<table>
<thead>
<tr>
<th>Heat for 60 s</th>
<th>Radiative cooling for 60 s</th>
<th>Material: TACOT</th>
<th>Insulated</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Length: 50 mm</td>
<td>Impermeable</td>
</tr>
</tbody>
</table>

Ablation Test Case 2.3

Ablative BC, Temperature computed via energy balance

<table>
<thead>
<tr>
<th>Heat for 60 s</th>
<th>Material: TACOT</th>
<th>Insulated</th>
</tr>
</thead>
<tbody>
<tr>
<td>Radiative cooling for 60 s</td>
<td>Length: 50 mm</td>
<td>Impermeable</td>
</tr>
</tbody>
</table>

Ablation Test Case 2.3

Ablative BC, Temperature computed via energy balance

Heat for 60 s
Radiative cooling for 60 s
Material: TACOT
Length: 50 mm
Insulated
Impermeable

Temperature

320 K
3000 K

Ablation Test Case 2.3

Ablative BC, Temperature computed via energy balance

Heat for 60 s
Radiative cooling for 60 s

Material: TACOT
Length: 50 mm
Insulated
Impermeable

<table>
<thead>
<tr>
<th>Probe</th>
<th>x (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Surface</td>
<td>0.0</td>
</tr>
<tr>
<td>1</td>
<td>1.0</td>
</tr>
<tr>
<td>2</td>
<td>2.0</td>
</tr>
<tr>
<td>3</td>
<td>4.0</td>
</tr>
<tr>
<td>4</td>
<td>8.0</td>
</tr>
<tr>
<td>5</td>
<td>12.0</td>
</tr>
<tr>
<td>6</td>
<td>16.0</td>
</tr>
<tr>
<td>7</td>
<td>24.0</td>
</tr>
</tbody>
</table>

Ablation Test Case 2.3

Ablative BC, Temperature computed via energy balance

Heat for 60 s
Radiative cooling for 60 s

Material: TACOT
Length: 50 mm
Insulated
Impermeable

Probe | x (mm)
--- | ---
Surface | 0.0
1 | 1.0
2 | 2.0
3 | 4.0
4 | 8.0
5 | 12.0
6 | 16.0
7 | 24.0

Surface Recession (m) vs. Time (s)

Ablation Test Case 2.3

Material: TACOT
Length: 50 mm

Heat for 60 s
Radiative cooling for 60 s

Ablative BC, Temperature computed via energy balance

Axysymmetric Mini Arc Jet Case

Ablative Boundary Condition
\[ P(\vec{x}, t) = 101325 \text{ Pa} \]

TACOT
\[ T_0 = 300 \text{ K} \]
\[ P_0 = 101325 \text{ Pa} \]

Insulated, Impermeable

Mapping of stagnation value

\[ \rho_e u_e C_H \]
kg / (m\(^2\) s)

Axis

25.4 mm

31.75 mm

CHyPS
20 elements along radius
50 elements along height
DG, \( p = 1 \) polynomials

PATO
40 elements along radius
100 elements along height
Finite-volume method

\[ h_e \]
MJ / kg

\[ r \text{ (mm)} \times \]
\[ \text{Time (s)} \]
\[ 0 \quad 5 \quad 10 \quad 15 \quad 20 \quad 25 \quad 30 \]
\[ 0 \quad 0.3 \quad 0.2 \quad 0.1 \quad 0.0 \]

\[ 0 \quad 1 \quad 0.75 \quad 0.5 \quad 0.25 \quad 0 \]

\[ 0 \quad 10 \quad 20 \quad 30 \quad 40 \quad 50 \]

\[ 0 \quad 10 \quad 7.5 \quad 5 \quad 2.5 \quad 0 \]
Axisymmetric Mini Arc Jet Case

Temperature
- 300 K
- 1400 K
- 2500 K

Gas Pressure
- 101325 Pa
- 102350 Pa
Axisymmetric Mini Arc Jet Case

Pyrolysis State

Gas Pressure and Velocity

\[ t = 20 \text{ s} \]

Virgin

Char

101325 Pa

102350 Pa
Axisymmetric Mini Arc Jet Case

Probe Locations

<table>
<thead>
<tr>
<th>Probe</th>
<th>r (mm)</th>
<th>y (mm)</th>
<th>Probe</th>
<th>r (mm)</th>
<th>y (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>1.4</td>
<td>7</td>
<td>20</td>
<td>1.4</td>
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<tr>
<td>2</td>
<td>0</td>
<td>2.4</td>
<td>8</td>
<td>20</td>
<td>2.4</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>3.4</td>
<td>9</td>
<td>20</td>
<td>3.4</td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td>4.4</td>
<td>10</td>
<td>20</td>
<td>4.4</td>
</tr>
<tr>
<td>5</td>
<td>0</td>
<td>5.4</td>
<td>11</td>
<td>20</td>
<td>5.4</td>
</tr>
<tr>
<td>6</td>
<td>0</td>
<td>10.4</td>
<td>12</td>
<td>20</td>
<td>10.4</td>
</tr>
</tbody>
</table>

Time (s)

Increasing Depth

Increasing Depth
Ablative Boundary Condition

\[ P(\vec{x}, t) = 101325 \text{ Pa} \]

TACOT

\[ T_0 = 300 \text{ K} \]
\[ P_0 = 101325 \text{ Pa} \]

Insulated, Impermeable

25.4 mm

Axis

31.75 mm

NASA MSL Heat Shield
High-Order Solutions

10 element $p = 3$ solution compared to 100 element $p = 1$
3.67x faster time to solution

$p = 3$
$p = 1$

$T$ (K)

Temperature

Time (s)
High-Order Meshes

Boundary Condition:

\[ \rho U e C_H = \frac{0.3(R - x)}{2R} \]

\[ h_e = 1.5 \text{ MJ/kg} \]

\[ P = 101325 \text{ Pa} \]

TACOT

\[ T_0 = 300 \text{ K} \]

\[ P_0 = 101325 \text{ Pa} \]

\[ R = 20 \text{ mm} \]
High-Order Meshes

Refined Linear Mesh
2100 Elements

Coarse Mesh (Linear)
176 Elements
High-Order Meshes

Radial Sweep

Side Sweep

Not to scale

<table>
<thead>
<tr>
<th>Probe</th>
<th>x (mm)</th>
<th>y (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-9.50</td>
<td>0.0</td>
</tr>
<tr>
<td>2</td>
<td>-9.25</td>
<td>0.0</td>
</tr>
<tr>
<td>3</td>
<td>-9.00</td>
<td>0.0</td>
</tr>
<tr>
<td>4</td>
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<td>0.0</td>
</tr>
<tr>
<td>5</td>
<td>-8.50</td>
<td>0.0</td>
</tr>
<tr>
<td>6</td>
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</tr>
<tr>
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<tr>
<td>9</td>
<td>-7.07</td>
<td>6.32</td>
</tr>
</tbody>
</table>
High-Order Meshes

Radial Sweep

Side Sweep

Both use $p = 2$ for internal solution
High-Order Meshes

Refined Linear Mesh
2100 Elements

Coarse Mesh (Quadratic)
176 Elements
High-Order Meshes

Radial Sweep

Side Sweep

Same result achieved 8.2x quicker

Coarse Quadratic Mesh
Refined Linear Mesh

Both use $p = 2$ for internal solution
Future Work

Coupling with External Flow Solvers

Mini-Arc Jet Case
Future Work

Coupling with External Flow Solvers

Use PlasCom2 to generate the external flow solution
Future Work

Coupling with External Flow Solvers

Material Response after 10 Seconds
Future Work

Internal Radiation using P1 Approximation

\[
\frac{1}{3\kappa} \nabla \cdot \left( \frac{1}{\beta - \frac{A_1\sigma_s}{3}} \nabla G \right) - G = -4\pi I_b,
\]

\[
- \frac{2 - \epsilon}{\epsilon} \frac{2}{3\beta - A_1\sigma_s} \hat{n} \cdot \nabla G + G = 4\pi I_{bw}
\]

\[
q = - \frac{1}{3\beta - A_1\sigma_s} \nabla G
\]

Future Work

Insulation Estimation for Experimental Samples

Cross-section after 10 s of heating
Conclusions

• Design of next-generation thermal protection systems and hypersonic vehicles will benefit greatly from computational studies
• Macroscopic volume averaged approach to simulating reactive porous materials aimed at enabling full-vehicle simulations
• Code-to-code comparison has been performed against NASA’s PATO code
• Continued work will be done to leverage use of high-order solutions

Temperature

320 K  2500 K

Simulation of micro arc jet