Multiphysics Coupling: Hypersonic Flow with Radiation and Ablation
Current Results and Future Strategies

Paul T. Bauman, Roy H. Stogner

The University of Texas at Austin

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Outline

Current Progress

- Combined 1-D radiation code, 1-D Charring Material Ablation code, 2-D + 3-D hypersonic flow code
  - Mach 11-31 Cylinder Tests
  - Mach 31 Axisymmetric Capsule at high AoA
- Pseudo-timestepping flow to quasi-steady state
- Loose coupling

Future Goals

- Tight coupling, full Jacobians
- Optional 2-D/3-D radiation/ablation
## Outline

### Past Coupling Challenges

- **Algorithmic and Software Issues:**
  - Loose Coupling strategies

- **Modeling Issues:**
  - Radiation (Overlapping Domains)
  - Ablation (Interface Domains)

### Current Progress

- DPLR-internal loose coupling with Radiation Model Discrete Transfer from Andre
- DPLR-external loose coupling with Charring Material Ablation from Rochan
Initial Coupling Challenges
Loose Coupling Strategy

“Loose” Two-way Coupling

- Radiation, Ablation each add terms to flow equations
  - $\frac{d\rho e}{dt} = F(U) + \nabla \cdot \vec{q}_{\text{rad}}$
  - $\nabla \cdot \vec{q}_{\text{rad}} = R(U)$
  - $\frac{d\rho e}{dt} = F(U) + R(U)$
  - $U|_{\Gamma} = A(U|_{\Gamma}, \frac{\partial U}{\partial n}|_{\Gamma})$

- Operator splitting with implicit-explicit solves
  - $M(U^{(new)}, U^{(old)}, \Delta t) = F(U^{(new)}) + R(U^{(old)})$
  - $U^{(new)}|_{\Gamma} = A(U^{(old)}|_{\Gamma}, \frac{\partial U^{(old)}}{\partial n}|_{\Gamma})$

- Iterate between coupled models
  - Timestep size $\Delta t$ - critical
  - Few intrusive DPLR modifications
Radiative Coupling: Overlapping Domains

- Radiation active on sub-domain of flow
- Currently modeled on entire flow, with $k_{abs}$ cutoff at low $T$, $P$
# Radiative Coupling

## Pre-existing capabilities in DPLR
- One-way coupling: read file for heat flux
- Tight coupling for limited models

## Current Implementation
- Determine line of cells approximately normal to surface
- Select radiation subroutine based on DPLR input config
- Pass cell line data to radiation subroutine e.g. `RMDT()`
  - Currently: line mesh, temperature, pressure
  - Future: chemical species
- `RMDT` returns $k_{\text{abs}}$, $\nabla \cdot q_{\text{rad}}$ along each line
- Add cell-integrated $\nabla \cdot q_{\text{rad}}$ to energy equation
- Continue to next timestep
Radiation Coupling Issues:

Convergence Failure Modes

- Receding shock: freestream radiation
  - Shock passes radiation, $T$ and $P$ fall, $\nabla \cdot q_{\text{rad}}$ fixed
  - Non-physical freestream cooling
  - Sudden failure in one timestep
- Advancing shock: oscillation
  - Excessive $\nabla \cdot \left( q_{\text{rad}}^{(\text{old})} - q_{\text{rad}}^{(\text{older})} \right) \Delta t$
  - Cells overshoot equilibrium $T$
  - Gradual growth of instability over many timesteps
  - Sudden failure when $T$ drops to non-physical values

Convergence Control

- Convergence achieved by limiting $\Delta t$
- Effect on time stepping depends on $Ma$. 
Cylinder Test Problems

Flow Conditions

- 1 mm cylinder, perfect gas air at Mach 31
- Discrete Transfer radiation, curve-fit absorptivity

No Radiation: peak 46000K

With Radiation: peak 31600K
Cylinder Test Problems

Flow Conditions

- 5 species air (N$_2$, O$_2$, N, O, NO) at Mach 31
- More moderate radiation results

No Radiation: peak 30500K

With Radiation: peak 29000K
Cylinder Test Problems

Flow Conditions

- 5 species air (N₂, O₂, N, O, NO) at Mach 21
- Scaled up cylinder ( [m] in diameter)

No Radiation: peak 12800K

With Radiation: peak 12100K
Cylinder Test Problems

Radiation Sensitivity

- Highly nonlinear absorptivity coefficient $k_{abs}(T, P)$ model
Cylinder Test Problems

Temperature, Pressure, Absorptivity

Radiation Sensitivity

- Absorptivity model greatly influences heat flux
Capsule Reentry Convergence

The Bad News

- Problem sizes exceed local PECOS resources
- Unsteady wake makes convergence, detection difficult

The Good News

- Continuation is effective for near-benchmark problems
- Downstream error has negligible upstream effect
Capsule Reentry Results

Shock Effects

- Chemistry, Radiation greatly reduce shock size, temperature
Capsule Reentry Results

Mesh Alignment

- Critical shock distance, slope changes
- Mesh realignment necessary for accurate heat transfer
Capsule Reentry Results

Forebody Heating

- Chemistry greatly reduces heat transfer
- Radiation reduces integrated transfer, increases peak
Ablation Discussion
Ablation Coupling

Existing work

- Failed fully-implicit coupling attempt with CHALEUR at NASA
- Heath Johnson at Minnesota worked with blowing only in “loose” coupling with a “DPLR like” 2-D code and had success. [1]
- Amar open to providing support/collaboration.

Preliminary Studies

- Preliminary studies with DPLR “material boundary conditions” encouraging - reasonably robust convergence given converged flow initially (2-D cylinder, 13 species Park model, $Ma = 21$)
- Initially fully converged flow a MUST
Ablation Coupling

Ablation Interface

- Ablation model is 1-D: treat each surface cell as a 1-D ablator
- Set of interface equations couple flow and ablation:

\[
k \frac{\partial T}{\partial y} |_{gas,w} + \sum_{i=1}^{N_s} h_i(T_w) \rho D_i \frac{\partial C_i}{\partial y} |_{gas,w} + \dot{m}_c h_c(T_w) \\
- \rho v_{cs,w} h_w(T_w) + \alpha \dot{q}_r - \sigma \epsilon T_w^4 = k \frac{\partial T}{\partial y} |_{solid,w}
\]

\[
\rho D_i \frac{\partial C_i}{\partial y} |_{gas,w} + \rho v_w C_{i,w} = \tilde{N}_i(C_{i,w}, T_w); (i : 1..N_s)
\]

- These equations must be satisfied across the interface of the heat shield and the flow. May require subiteration within timestep.
Ablation Coupling

Coupling strategy

- Nonoverlapping Schwarz Method
- DPLR computes flow quantities, using species concentration, mass flux, and temperature at the wall as Dirichlet data, supplied by ablation model.
- Wall quantities extracted and used as Neumann data for the ablation model.

\[
\begin{align*}
\frac{k}{\partial y} |_{gas,w} + \sum_{i=1}^{N_s} h_i(T_w) \rho D_i \frac{\partial C_i}{\partial y} |_{gas,w} + \dot{m}_c h_c(T_w) \\
- \rho v_{cs,w} h_w(T_w) + \alpha \dot{q}_r - \sigma \epsilon T_w^4 = k \frac{\partial T}{\partial y} |_{solid,w} \\
\rho D_i \frac{\partial C_i}{\partial y} |_{gas,w} + \rho v w C_{i,w} = \tilde{N}_i(C_{i,w}, T_w); (i : 1 .. N_s)
\end{align*}
\]
Ablation Coupling

Preliminary Results with Material Coupling BC in DPLR

- 13 species Park model - flow converged than boundary condition enabled
- non-physical, extreme values used for testing
Ablation Coupling

Current implementation

- Current coupling through Python script that exchanges input files between DPLR and ablation code.
- Verification testing under way of ablation code with data from DPLR.
- Current tests suggest diffusion coefficients particularly sensitive parameter related to convergence of ablation model.
- No converged results as yet.
- Working with ablation team to solidify interface for thermodynamic quantities. Particularly tricky with DPLR - thermodynamic data not well exposed in code.
- Explicit DPLR/ablation interface being constructed while verifying initial simulations.
## Software Issues: Tight Coupling in DPLR

### Overlapping Domain Coupling
- Requires fluxes from (linearization of) all coupled models
- No built-in interfaces; highly intrusive
- No sparse matrix access

### Non-overlapping Interfacial Coupling
- Built-in interface exists for fully implicit nonlinear boundary conditions
- The interface is broken
- No capability for per-domain variables, full global Jacobian
Software Issues: Tight Coupling in FINS, libMesh

Overlapping Domain Coupling

- Easy to add new variables, equations without modifying existing code
- Requires residuals, and preferably local Jacobians, from external coupled models
- Or can directly evaluate weak formulation residuals/Jacobians
- Direct access to PETSc/LASPACK/Trilinos sparse matrix Jacobian

Non-overlapping Interfacial Coupling

- SVN libMesh now supports per-domain variables
- Independent discretizations possible
- Support for coupled solid body heat conduction being added to FINS
- Would require physics models compatible with adaptive meshes
  - (or models solveable on coarse mesh alone)
Radiation Coupling Interface

Module structures

- **radiation_flags**: all input flags stored here. Exposes input flags for use at input time by different parts of code.

- **radiation_proxy**: direct interface to DPLR. Encapsulates the interfaces to the different models. Minimizes changes when interface to DPLR changes.

- **one,two,three_dimensional_models**: Each dimensional model is encapsulated within these modules. This way however we decide to project/interpolate the data, we only have to change it in one place. The calling sequence is through the proxy, i.e. based upon the model set in the input at runtime, the correct model is called (polymorphism). It is within each of these modules that each of the radiation models are called.
Module structures, cont’d

- **discrete_transfer_model**: Implementation of the discrete transfer method radiation model (Andre). Notice that this does **not** depend on DPLR at all - it accepts a 1-D radiation line with the necessary values and works on that line. All mesh transformation has already taken place. This is encapsulation - allows Andre to develop model independently.

- **absorption_coefficients**: Utility module to store the various models of the absorption coefficients. Andre’s code will call the correct one based upon the model set in input at run time.
Ablation Interface

- Similar structure to radiation: proxy to call the correct dimensional model (leaves place holders for future work), mesh mappings for each dimension, call to actual solver, any supporting utility modules for the model.

- An addition here not present in the radiation case is that there may be subiteration for interface between flow and ablation. Need a module to iterate on the interface residual and control number of subiterations and convergence criterion of the interface.

UQ Interface

- Expose the uncertain parameters through modules in each of the model codes.

- This will allow easy access to QUESO, DAKOTA, etc. to vary these parameters as needed by the UQ algorithm.
Validation process for blowing and transpiration-cooling in DPLR.
Thank you!
Questions?