Development of an, unstructured, three-dimensional material response model

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**Background**

### High-Temperature Gases

- **Surface Energy Balance**
- **In-depth physics**

**Radiation**

**Mass Loss**

**Convection**

**Re-radiation**

**Ablating Surface**

**Pyrolysis Gases**

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### NASA Material Response Tools

**Engineering Tools**
- STAB / CHAR *(NASA JSC)*
- FIAT / TITAN *(NASA ARC)*
- **Icarus** *(NASA ARC)*

**Research Tools**
- PATO *(NASA ARC)*

**Material Properties**
- PuMA *(NASA ARC)*

*Not an exhaustive list*
Motivation

• Why Icarus?
  ▪ Three-dimensional physics modeling and complex geometries
  ▪ Coupling to CFD simulation
  ▪ Software architecture
    ➢ Easy to add new physics, numerics, and material property models
    ➢ Linking to optimization and inverse parameter estimation methods
  ▪ Independent of other NASA material response models
    ➢ Provides verification of predictions

• Target Applications

  3D ArcJet IsoQ
  ADEPT ArcJet Test
  Orion Compression Pad
Icarus

Version 1.0

Physics Models
- Thermal Conduction
  - Decomposition
  - Pyrolysis Gas Continuity

Numerical Methods
- Time integration
  - First-order Backward Euler
  - Second-order Runge-Kutta
- Spatial integration
  - Green-Gauss reconstruction
- Mesh Motion
  - Radial-basis functions

Verification and Validation
- Analytical Heat Conduction
- Ablation Workshop Test Cases
- PICA ArcJet validation

Version 2.0

Physics Models
- Thermal Conduction
  - Pyrolysis Gas Momentum
  - Element Conservation

Numerical Methods
- Implicit Time Integration
  - Point relaxation
  - Numerical Jacobians
  - Gradient reconstruction
  - Weighted least-squares

Verification and Validation
- Orion ArcJet validation
- HEEET ArcJet validation
- MSL Flight data

Version 3.0

Physics Models
- Dust erosion / spallation
- Linear elasticity model

Numerical Methods
- AMR

Interface
- GUI
  - Design Toolbox
    - Shape optimization
    - Inverse parameter estimation
    - Uncertainty quantification
Icarus - Version 1.0 Status

Input / Output Data Formats
HDF5 / XDMF, CGNS, Tecplot

Data I/O and Initialization

Main Loop

Data I/O and Post-processing

Indicates an external binary
*Indicates a work in progress

Thermodynamics / Transport
Materials
Icarus Tables / Polynomials

Gas Mixtures
Icarus / NASA CEA Mutation++ Cantera

Numerics
Explicit Time Integration
First-order Euler
2\textsuperscript{nd}-order Runge-Kutta

Gradient Reconstruction
Green-Gauss contour integration

Physics Models
Heat Conduction
+ Decomposition
+ Pyrolysis gas production
+ Surface recession / ablation

Thermal Boundary Conditions
Isothermal
Heat Flux
- Adiabatic
- Spatial / Temporal Function
Surface Energy Balance

Utilities
Database Creation
Grid Deformation
Icarus GUI

Test Automation
Unit Testing
Integration Testing
Regression Testing
Icarus - Data Structure

• Modular data structure partitions physics, numerics, and material or gas models
  • Organization is user friendly and extensible

Blocks 1 and 2 are defined for different physics models

Blocks can contain multiple property zones:
  — Material / Gas 1
  — Material / Gas 2
  — Material / Gas 3

Unstructured index ordering
  — interior faces / cells
  — boundary faces / cells
  — processor shared faces / cells
• **Production codes require:**
  1. Sufficient documentation
     • Web-based documentation
     • Uses Sphinx, a Python tool that parses in-source code documentation to create HTML and LaTeX formatted documentation
  2. Verification
     • Automated unit and integration testing (~60% coverage currently)
     • Regression testing
  3. Validation
     • Comparison to Arc Jet data (current focus of PICA validation)
     • Shifting focus this year to AVCOAT modeling
     • MSL flight data
• **Participation in code-to-code comparisons to understand variability in modeling assumptions and prediction uncertainty**
  • Ablation Workshop
  • Relationships with research institutes and university laboratories
Outline

- **Icarus Formulation**
  - Governing equations
  - Numerical formulation

- **Verification Tests**
  - Analytical heat conduction
  - Multi-dimensional test cases

- **Current On-Going Work**
  - Mesh motion
  - Surface ablation

\[
\frac{\partial \rho_{s,n}}{\partial t} = -k_n \rho v_n \left( \frac{\rho_k - \rho_{c,n}}{\rho_{v,n}} \right) \psi_n \, e^{\left(-T_{a,n}/T\right)}
\]

\[
\frac{\partial (\phi \rho_g)}{\partial t} + \frac{\partial}{\partial x_i} \left( \phi \rho_g u_{g,i} \right) = \dot{\omega}
\]

\[
\frac{\partial (\rho e)}{\partial t} + \frac{\partial}{\partial x_i} \left( \phi \rho g h_g u_{g,i} \right) - \frac{\partial}{\partial x_i} \left( \kappa_{ij} \frac{\partial T}{\partial x_j} \right) = 0
\]
• **Pyrolysis Modeling**
  1. Solve the elemental conservation equations
     • Requires a detailed kinetic mechanism and knowledge of material composition
  2. Use empirical relationships
     • Measure quantities only at the virgin and fully-charred states
     • Use simplified kinetics

• **Three-component model**

\[
\rho_s = \Gamma (\rho_A + \rho_B) + (1 - \Gamma) \rho_C
\]

\[
\rho = \phi \rho_g + \rho_v
\]

\[
\frac{\partial \rho_s,n}{\partial t} = -k_n \rho_v,n \left( \frac{\rho_s,n - \rho_c,n}{\rho_v,n} \right)^{\psi_n} e^{(-T_{a,n}/T)}
\]

\[
\omega = \sum_{n=1}^{N} \Gamma_n \frac{\partial \rho_s,n}{\partial t}
\]

\[
\Gamma : \text{pseudo-volume fraction of pyrolyzing resin}
\]

\[
\rho : \text{total production of pyrolysis gas}
\]
• **Properties are measured for at the virgin and fully-charred states**
  - Requires linearly interpolating between two states
    \[
    \beta = \frac{\rho_v - \rho_s}{\rho_v - \rho_c} \quad \rightarrow \quad Y_v = \frac{\rho_v}{\rho_v - \rho_c} \left(1 - \frac{\rho_c}{\rho_s}\right)
    \]
  - Internal energy of the material is evaluated either as a tabular or polynomial curve-fit that is a function of temperature and pressure
    \[
    e_s(p, T) = h_s(p, T) = Y_v e_v(p, T) + (1 - Y_v) e_c(p, T)
    \]

• **Total mixture quantities are determined by weighted average using the gas mass fraction**
  \[
  e(p, T) = Y_g e_g(T) + (1 - Y_g) e_s(p, T) \quad Y_g = \frac{\phi \rho_g}{\rho} : \text{mass fraction of the gas mixture}
  \]

• **Thermal equilibrium and gas mixture in chemical equilibrium**
• **Material properties can be orthotropic**
  ▪ Principle axis of the material may not align with the Cartesian frame of reference of the simulation
    ➢ Woven TPS materials: alignment varies continuously

• **Properties defined parallel and orthogonal to the principle axis**

  Thermal conductivity tensor in material frame of reference

  \[
  \kappa_{ij} = \begin{bmatrix}
  \hat{\kappa}_\parallel & 0 & 0 \\
  0 & \hat{\kappa}_\perp & 0 \\
  0 & 0 & \hat{\kappa}_\perp \\
  \end{bmatrix}
  \]

  Project tensor onto the surface defined by the normal vector at each grid point

  \[
  \kappa = R^T \hat{\kappa} R
  \]
Decomposition of solid material

\[
\frac{\partial \rho_{s,n}}{\partial t} = -k_n \rho_{v,n} \left( \frac{\rho_{s,n} - \rho_{c,n}}{\rho_{v,n}} \right)^{\psi_n} e^{-\left(\frac{T_{a,n}}{T}\right)}, \quad n = 1, \ldots, N
\]

Pyrolysis gas continuity

\[
\frac{\partial (\phi \rho_g)}{\partial t} + \frac{\partial}{\partial x_i} \left( \phi \rho_g u_{g,i} \right) = \dot{\omega}
\]

Momentum conservation: Darcy’s Law

\[
u_{g,i} = -\frac{1}{\mu} K_{ij} \frac{\partial p}{\partial x_j}
\]

Total Energy conservation

\[
\frac{\partial (\rho e)}{\partial t} + \frac{\partial}{\partial x_i} \left( \phi \rho_g h_g u_{g,i} \right) - \frac{\partial}{\partial x_i} \left( \kappa_{ij} \frac{\partial T}{\partial x_j} \right) = 0
\]

- convection of heat by pyrolysis gases
- thermal conduction by material
Formulation: Numerics

- **Time integration**
  - Explicit first-order Euler or second-order Runge-Kutta

- **Gradient Reconstruction**
  - Gauss-Green contour integration

\[
\int_V \nabla \phi dV = \int_S \phi n \cdot dS
\]

\[
\nabla \phi_i = -\frac{1}{V_i} \sum_{j \in J_i} \phi_j \mathcal{S}_{i,j}
\]

Average the cell-centered gradients neighboring each face

\[
\nabla \phi_j = \frac{1}{2} (\nabla \phi_{i=l} + \nabla \phi_{i=r}) - \hat{d}_{lr} \left( \frac{1}{2} (\nabla \phi_{i=l} + \nabla \phi_{i=r}) \cdot \hat{d}_{lr} \right) + (\phi_{i=l} - \phi_{i=r}) \frac{\hat{d}_{lr}}{|\hat{d}_{lr}|}
\]
Outline

- Verification Tests
  - Analytical heat conduction comparisons
  - Determine scheme accuracy
- Multi-dimensional test cases
  - Qualitative verification
  - Code-to-code comparisons

- Current On-Going work
  - Mesh motion
  - Surface ablation
- Conclusions
Analytical solutions exist for the one-dimensional heat conduction equation

- Ignored pyrolysis or surface recession (constant density and volume)
- Scalar material properties (tensors are isotropic)

Conservation equations reduce to a single PDE

- Assuming linear temperature-dependent properties:

\[ \kappa(T) = \kappa_1 + \frac{\kappa_2 - \kappa_1}{T_2 - T_1} (T - T_1) \]
\[ c_v(T) = c_{v,1} + \frac{c_{v,2} - c_{v,1}}{T_2 - T_1} (T - T_1) \]

- Using the variable transformation:

\[ \theta = (T - T_1) + \frac{\kappa_2 - \kappa_1}{T_2 - T_1} \frac{1}{2\kappa_1} (T - T_1)^2 \]

- Results in:

\[ \rho c_v \frac{\partial T}{\partial t} - \kappa \frac{\partial^2 T}{\partial x^2} = 0 \]
\[ \frac{\partial \theta}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \]
Verification : 1-D Simulation Domain

- **One-dimensional computational domain of 1 m in length**
  - Resolved in the orthogonal directions by 1 grid element
  - Discretization by both triangular prisms and hexahedral elements
- **Estimate the order of accuracy the numerical scheme**
  - Scheme is expected to be second-order accurate
  - Compute the the root-mean-square error (RMS) for an increasing number of grid elements

\[
RMS = \sqrt{\frac{\sum_{i}^{N_c} (T_{\text{analytical}} - T_{\text{numerical}})_i^2}{N_c}}
\]
Verification: Analytical Solution #1

- Isothermal Boundary with constant material properties
  - Hexahedral elements: 8, 16, 32, 64, and 128

\[
\frac{T_1 - T(x, t)}{T_1 - T_0} = 2 \sum_{i=0}^{\infty} \frac{(-1)^i}{(i + \frac{1}{2})\pi} \exp \left[ -\left( i + \frac{1}{2} \right)^2 \frac{\alpha t}{L} \right] \cos \left[ \left( i + \frac{1}{2} \right) \frac{\pi x}{L} \right]
\]

\[T_0(x = 0) = 300 \text{ K}\]

\[c_v = 1 \text{ J/kg}\]
\[\kappa = 1 \text{ W/m} \cdot \text{K}\]
\[\rho = 1 \text{ kg/m}^3\]
\[\alpha = 1 \text{ m}^2/\text{s}\]

\[T_1(x = L) = 400 \text{ K}\]

Graph showing RMS (K) vs. Number of Elements.
Verification: Analytical Solution #2

- Constant heat flux boundary and constant material properties
  - Hexahedral elements: 8, 16, 32, 64, 128

\[
\frac{T(x,t) - T_0}{q_{w,1}L/\kappa} = \frac{\alpha t}{L^2} + \frac{1}{3} - \frac{x}{L} + \frac{1}{2} \left(\frac{x}{L}\right)^2 - 2 \sum_{i=0}^{\infty} \frac{1}{n^2 \pi^2} \exp \left[ -\frac{n^2 \pi^2 \alpha t}{L^2} \right] \cos \left[ \frac{n \pi x}{L} \right]
\]

\[
q_{w,0} = 0 \text{ W/m}^2
\]

\[
\alpha = 1 \text{ m}^2/\text{s}
\]

\[
q_{w,1} = 7.5 \times 10^5 \text{ W/m}^2
\]

![Graph showing RMS (K) vs. Number of Elements with Root Mean Square and Reference lines]
Verification : Analytical Solution #3

- Constant heat flux with temperature dependent (linear) material properties
  - Triangular prisms : 10, 20, 40, 80

\[
\frac{T(x, t) - T_1}{T_2 - T_1} = \left( \frac{\kappa_1}{\kappa_2 - \kappa_1} \right) \left[ \sqrt{1 + \frac{2\theta}{T_2 - T_1} \left( \frac{\kappa_2 - \kappa_1}{\kappa_1} \right)} - 1 \right]
\]
Verification: Analytical Solution #4

- **Sinusoidal varying heat flux boundary with constant material properties**
  - Solution ill-posed since analytical solution exists for semi-infinite domain

\[ T(x, t) - T_0 = \frac{q_{w,0}(t)}{\kappa} \sqrt{\frac{\alpha}{\kappa}} \exp \left[ -\frac{\omega}{2\alpha x} \right] \cos \left( \omega t - \sqrt{\frac{\omega}{2\alpha}} x - \frac{\pi}{4} \right) \]
Ablation Workshop Test Cases

- **One-dimensional domain**: $L = 5$ cm
  - Hexahedral elements: 128

- **Boundary conditions**
  - Single isothermal wall
  - All other boundaries are adiabatic
  - Initial pressure: $p = 101325$ Pa

- **Material**: PICA
  - Properties are orthotropic
  - Three-component decomposition model

Figure (above): Code-to-code comparison of Icarus and FIAT for the first ablation workshop test case. Differences are less than 3 percent.
Arc Jet Verification & Validation

- Three-dimensional iso-q geometry typical of arc jet test articles

Figure (above) : Code-to-code comparison of temperature along the x-axis between Icarus and CHAR

Figure (right) : Temperature contours for Iso-Q geometry heated along the outside radius by a constant heat flux of $q_w = 7.5 \times 10^5$ W/m² for TACOT material
Outline

• Verification Tests
  ▪ Analytical heat conduction comparisons
  ▪ Determine scheme accuracy
• Multi-dimensional test cases
  ▪ Qualitative verification
  ▪ Code-to-code comparisons
  ▪ Work in progress
    ▪ Mesh motion / Surface ablation
    ▪ Validation
    ▪ Release of Icarus v1.0
Mesh Motion

• Ablation results in surface recession
  ▪ Need a robust and efficient method to track the deformation of the computational grid during the simulation

• Radial Basis Functions
  ▪ A real-valued function whose value depends only on absolute distance
  ▪ Often use to approximate functions

\[ y(x) = \sum_{i=1}^{N} w_i \phi(|x - x_i|) \]

  ▪ Here N radial basis functions each weighted differently are used to approximate the function

• Applications to mesh motion
  ▪ Define a radial basis function for each grid point with respect to certain control points
  ▪ Compute the weights (requires solving a linear system)
Future Work and Conclusions

- Focus on the verification of one-dimensional heat conduction and pyrolysis
  - Numerical scheme
  - Thermodynamic / Transport Properties
  - Grid deformation

- Future Work
  - Validation to arc-jet data and continuation of code-to-code comparisons
  - Addition of surface recession / ablation modeling using radial basis function methodology
  - Integration of inverse estimation and Monte-Carlo analysis tools