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

Conduction

Decomposition Zone

Virgin Composite

Sub-structure

NASA Material Response Tools

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

Inform engineering models

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 Development Roadmap

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

**Data I/O and Initialization**

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

**Main Loop**

- **Numerics**
  - Explicit Time Integration
    - First-order Euler
    - 2nd-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

**Indicates an external binary**

*Indicates a work in progress*
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
Icarus - Production Code

**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

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

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

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

- **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**

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

\[
\rho = \phi \rho_g + \rho_s \quad ; \quad \phi \text{ is the material porosity}
\]

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

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

: total production of pyrolysis gas

\[\text{Decomposition Zone}\]

\[\text{Pyrolysis Gases}\]

\[\text{Virgin Composite}\]

\[\text{Sub-structure}\]
Formulation: Material Properties

• Properties are measured for at the virgin and fully-charred states
  ▪ Requires linearly interpolating between two states

\[
\beta = \frac{\rho_v - \rho_s}{\rho_v - \rho_c} \quad Y_v = \frac{\rho_v}{\rho_v - \rho_c} \left(1 - \frac{\rho_c}{\rho_s}\right)
\]

  ▪ 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

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

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

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

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

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

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

\[ \nabla \phi_i = -\frac{1}{V_i} \sum_{j \in J_i} \hat{n}_j s_{i,j} \]

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:
    \[
    \kappa(T) = \kappa_1 + \frac{\kappa_2 - \kappa_1}{T_2 - T_1} (T - T_1) \quad \quad c_v(T) = c_{v,1} + \frac{c_{v,2} - c_{v,1}}{T_2 - T_1} (T - T_1)
    \]
  ▪ 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:
    \[
    \rho c_v \frac{\partial T}{\partial t} - \kappa \frac{\partial^2 T}{\partial x^2} = 0 \quad \rightarrow \quad \frac{\partial \theta}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}
    \]
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

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

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

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

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

- \(c_v = 1 \text{ J/kg}\)
- \(\kappa = 1 \text{ W/m} \cdot \text{K}\)
- \(\rho = 1 \text{ kg/m}^3\)

\(\alpha = 1 \text{ m}^2/\text{s}\)

\[T_1(x = L) = 400 \text{ K}\]
Verification: Analytical Solution #2

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

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

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

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

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

\[\text{RMS (K)}\]

\[\text{Number of Elements}\]
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

\[ T(x, t) - T_0 = \frac{q_{w,0}(t)}{\kappa} \sqrt{\frac{\kappa}{\alpha}} \exp\left(-\frac{\omega}{2\alpha x}\right) \cos\left(\omega t - \sqrt{\frac{\omega}{2\alpha}} x - \frac{\pi}{4}\right) \]
• **One-dimensional domain** : \( L = 5 \) cm
  - Hexahedral elements : 128

• **Boundary conditions**
  - Single isothermal wall
    \[ T_{x=0} = \begin{cases} 
    298 \text{ K} : & t \leq 0.1 \text{ sec} \\
    1644 \text{ K} : & t > 0.1 \text{ sec} 
    \end{cases} \]
  - All other boundaries are adiabatic
  - Initial pressure : \( p = 101325 \) Pa

• **Material** : PICA
  - Properties are othrotropic
  - 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
• 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
• 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)
Mesh Motion
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