The Porous Microstructure Analysis (PuMA) software for high-temperature microscale modeling

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Overview

• Quick Description
• Motivation
• Capabilities
• Conclusions and Outlook
What is PuMA?
A collection of tools for the analysis of porous materials and generation of material microstructures
Porous Microstructure Analysis (PuMA)

Technical Specifications

- Written in C++
- GUI built on QT
- Visualization module based on OpenGL
- Parallelized using OpenMP for shared memory systems

Motivation
Thermal Protection Systems (TPS)

NASA TM 101055, 1989
Ablative Thermal Protection Systems

Carbon preform + Resin = PICA

Stackpoole et al., AIAA 2008-1202

Stardust Capsule

www.apl-ucla.com

Dragon V1 & V2

Mars Science Laboratory
Material Design and Modeling
Material Design and Modeling

Bow Shock

Boundary Layer

Char Layer

Pyrolysis Zone

Virgin Material

Substructure

Lawson et al. 2010

Lachaud and Mansour, JHT 2013
Material Design and Modeling

P. Agrawal et. al. 2016.

Virgin PICA Sample

Charred PICA Sample

Arcjet Testing
1. Material Properties
   1. Phenomenological Properties
   2. Thermal transport
   3. Mass transport

2. Material Decomposition
   1. Oxidation
   2. Sublimation
   3. Spallation
High fidelity characterization of heat shield materials in extreme environments is needed

Cannot be achieved with experiments alone
Other applications

- Main impact derives from the ubiquity of the underlying physics.

Plastic/Copper Composites

Parachute Materials

Meteorite Samples
Capabilities
Porous Microstructure Analysis (PuMA)

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X-ray micro-tomography

- Advanced Light Source (ALS) at the Lawrence Berkeley Natl. Laboratory
- Synchrotron electron accelerator used to produce 14Kev X-rays
- Used for many research areas, including optics, chemical reaction dynamics, biological imaging, and X-ray micro-tomography.


http://www2.lbl.gov/MicroWorlds/ALSTool
X-ray micro-tomography

Collect X-ray images of the sample as you rotate it through 180°

Use this series of images to “reconstruct” the 3D object

Penetrating power

Multiple angles

Courtesy of D. Parkinson (ALS)
Complex Fiber Generation

- Under Development for PuMA V3
- Capable of generating:
  - Curved fibers
  - Hollow fibers
  - Fibers with complex cross sections
- Degree of randomness can be specified to each of these parameters
Weave Generation

- Under Development for PuMA V3
- TexGen library fully integrated
Effective Material Properties

Porosity

- Based on the grayscale threshold
- Sum of all void voxels over the total volume

Specific Surface Area

- Based on the Marching Cubes algorithm
- Overall surface area computed as a sum of individual triangle areas
Effective Thermal Conductivity

- Computes effective thermal conductivity using a finite difference method [Weigmann, 2006]
- BicGStab iterative method and FFTW used to solve linear system of equations [Sleijpen, 1993]
- Parallelized based on OpenMP
- Verified against complex analytical solutions
Effective Electrical Conductivity

- Computes effective electrical conductivity using a finite difference method [Weigmann, 2006]
- 1V voltage differential applied; solved with periodic boundary conditions
- BicGStab iterative method and FFTW used to solve linear system of equations [Sleijpen, 1993]
- Parallelized based on OpenMP
- Verified against complex analytical solutions
- Steady state current flow through a material can be determined

Steady state current flow through a carbon fiber material with an imposed voltage differential
Anisotropic Thermal/Electrical Conductivity

- Allows for constituents with anisotropic thermal conductivities
- Method uses Multi-Point Flux Approximation (MPFA) which involves integrating over a control volume and enforcing continuity across separate interaction volume
- Solved with periodic boundary conditions
- Parallelized based on OpenMP
- Verified against complex analytical solutions

Steady state current flow through a carbon fiber material with an imposed voltage differential
Diffusivity / Tortuosity

Continuum

- Quantifies a material's resistance to a diffusive flux
- Solves for effective diffusivity using a finite difference method
- Valid for Kn << 1
- Solves diffusion equation using periodic boundary conditions

Ferguson et al., Particle methods for tortuosity factors in porous media, 9th Ablation Workshop, Bozeman MT. (2017).
Diffusivity / Tortuosity – Random Walk

Transitional/Rarified

- Random walk method to simulate diffusion
- Mean square displacement method used to solve effective diffusion
- Valid for all Knudsen numbers.
- Knudsen number is varied by changing the molecular mean free path

\[ Kn = \frac{\bar{\lambda}}{d} = \frac{\text{mean free path}}{\text{characteristic length}} \]

- Surface collisions based on marching cubes triangles with diffuse reflections used

Ferguson et. al, Particle methods for tortuosity factors in porous media, 9th Ablation Workshop, Bozeman MT. (2017).
Representative Elementary Volume

- Defined in PuMA V2.1 as the size for which the std. dev. in a given property falls below a given threshold, usually 2%
- Power law used to interpolate/extrapolate REV
- Provides std. dev. of a given property as a function of sample size, helping to quantify the uncertainty in a calculation

Surface rendering of FiberForm tomography in PuMA V2.1. Visualization contains ≈ 500 million triangles.
Domain Generation
- Artificial Material Generator
- Micro-tomography Import, Processing, and Thresholding

Visualization
- Marching Cubes
- OpenGL Surface Rendering

Material Properties
- Porosity
- Specific Surface Area
- Effective Thermal Conductivity
- Effective Electrical Conductivity
- Diffusivity / Tortuosity (Bulk and Knudsen)
- Representative Elementary Volume

Material Response
- Oxidation Simulations
- Hyperthermal Beam
Micro-Scale Oxidation Simulations

- Particle-based oxidation method
- Diffusion simulated through random walks
- Collision detection with linear interpolation method
- Sticking probability method for material recession
- Verified against analytical solutions for single fiber

Micro-Scale Oxidation Simulations

Molecular Beam Simulations

- Used in conjunction with molecular beam experiments [1] to calibrate finite rate chemistry models
- Particle-based method to solve transport of gas reactants and products
- Simulation of gas-surface collisions with complex, customizable reaction models
- Since particle-particle collisions are negligible, it provides a significant speed increase over DSMC simulations [2].

Conclusion and Outlook

- Future work will expand the material properties to include permeability and structural analysis.

- Material generation will be expanded to allow realistic materials to be computationally designed, optimized over a set of characteristics.

- **Need for good quality experimental data for model verification**
Microscale Modeling Research Group

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DSMC Development: A Borner

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Questions?

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