Recent developments to the Porous Microstructure Analysis (PuMA) software

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Overview of the Effort

The Porous Microstructure Analysis (PuMA) software is a suite of tools for the analysis of porous materials and generation of material microstructures. From microstructural data, often obtained through X-ray microtomography, PuMA can determine a number of effective material properties and perform material response simulations. Version 2.2 includes capabilities for computing volume fractions, porosity, specific surface area, effective thermal and electrical conductivities, and continuum and rarefied diffusive tortuosity. PuMA can also simulate competitive diffusion/reaction processes at the micro-scale, such as surface oxidation. In this poster, recent advancements to the PuMA software are detailed, including the full refactoring of PuMA into v3.0, a new module to compute heat conduction in anisotropic materials, a particle method for simulating molecular beam experiments, a new finite-volume Laplace solver, complex fibrous material generation, woven material generation, and a coupling of PuMA with the DAKOTA software for advanced statistics.

Computationally Generated Woven Materials

Weave generation capabilities were implemented into the Porous Microstructure Analysis (PuMA) software [1]. The effort involved a coupling and encapsulation of the TexGen software [2] for weave generation with the PuMA software for material properties and response.

A custom weave diagram format was designed to allow for complex 2D and 3D woven materials to be generated in PuMA. The implementation was parallelized using OpenMP.

Rendering of 3D weave generated in PuMA

Example replication of nylon parachute fabric weave
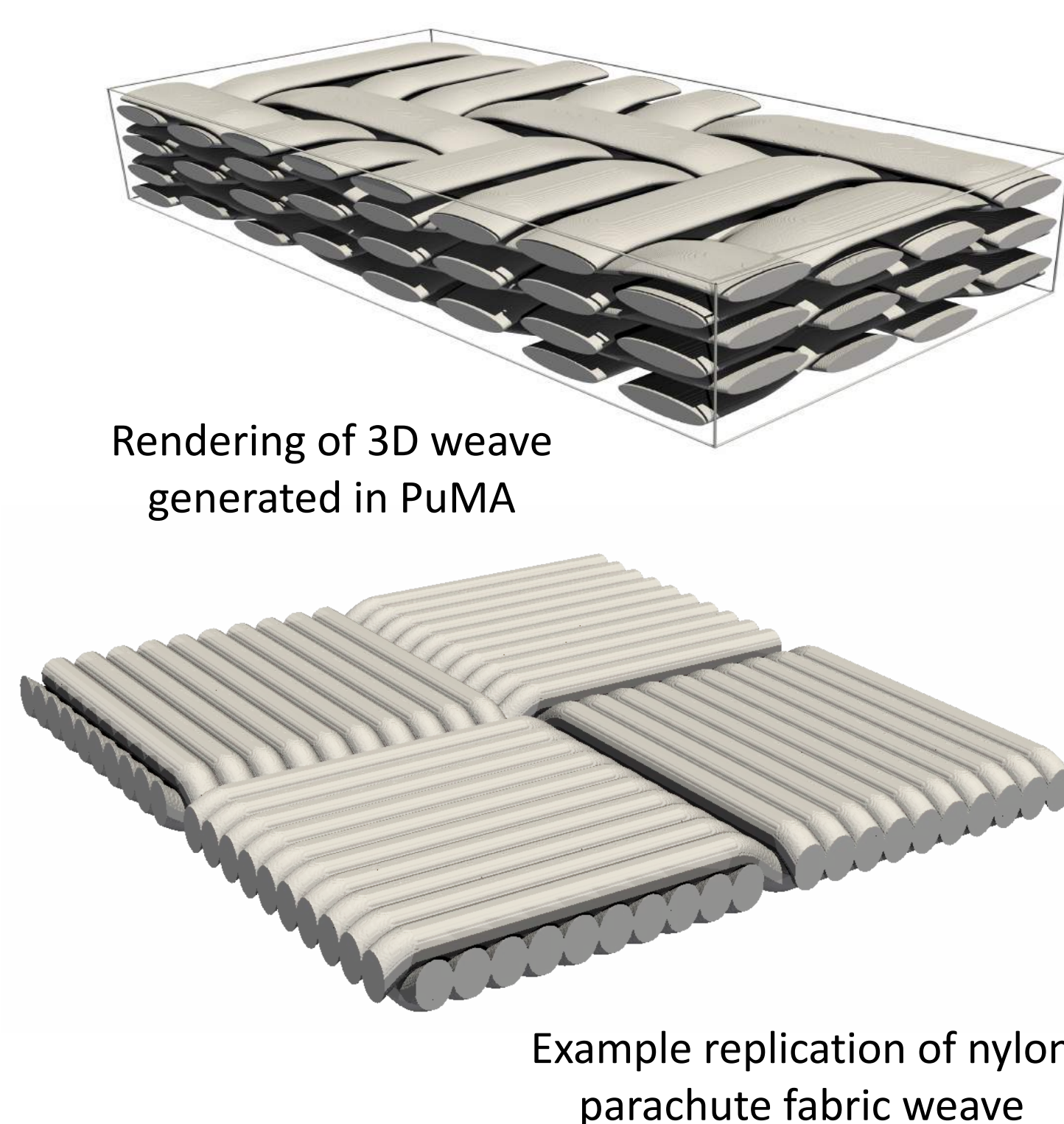
Complex Fibrous Materials Generation

Complex fibrous material generation capabilities were added to the PuMA v3.0 software. In the new module, fibrous materials can be computationally generated with complex fiber cross sections, hollow fibers, curved fibers, and non-uniform fiber clustering. These capabilities allow the computationally generated material to more closely resemble true microstructures [3].

Fibrous material with curved fibers

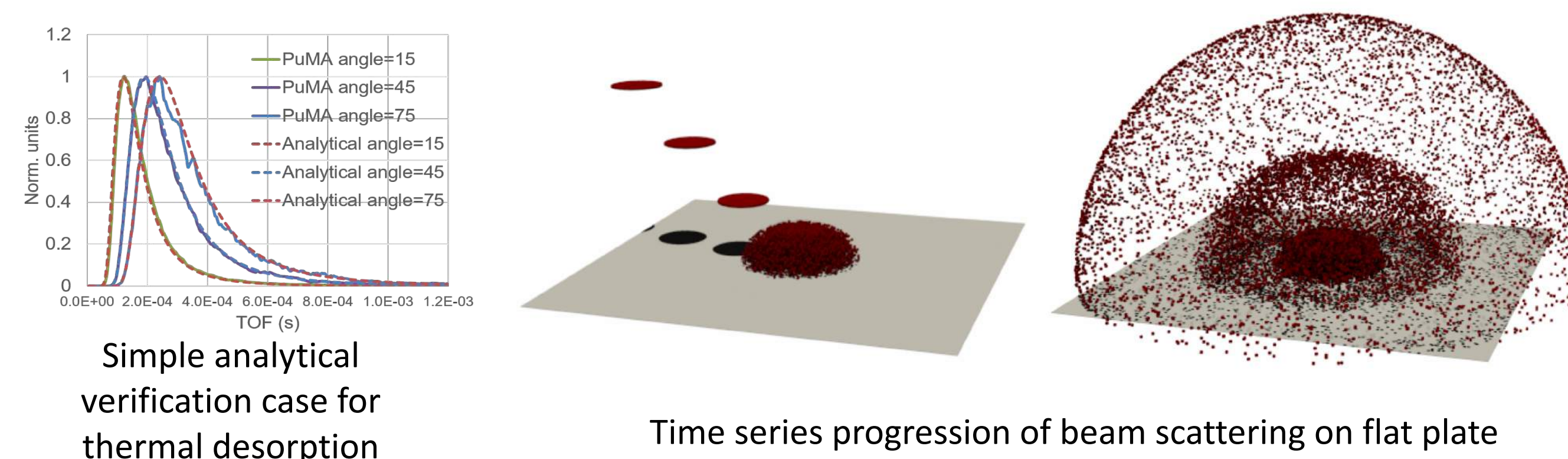Fibrous material with irregular cross sections
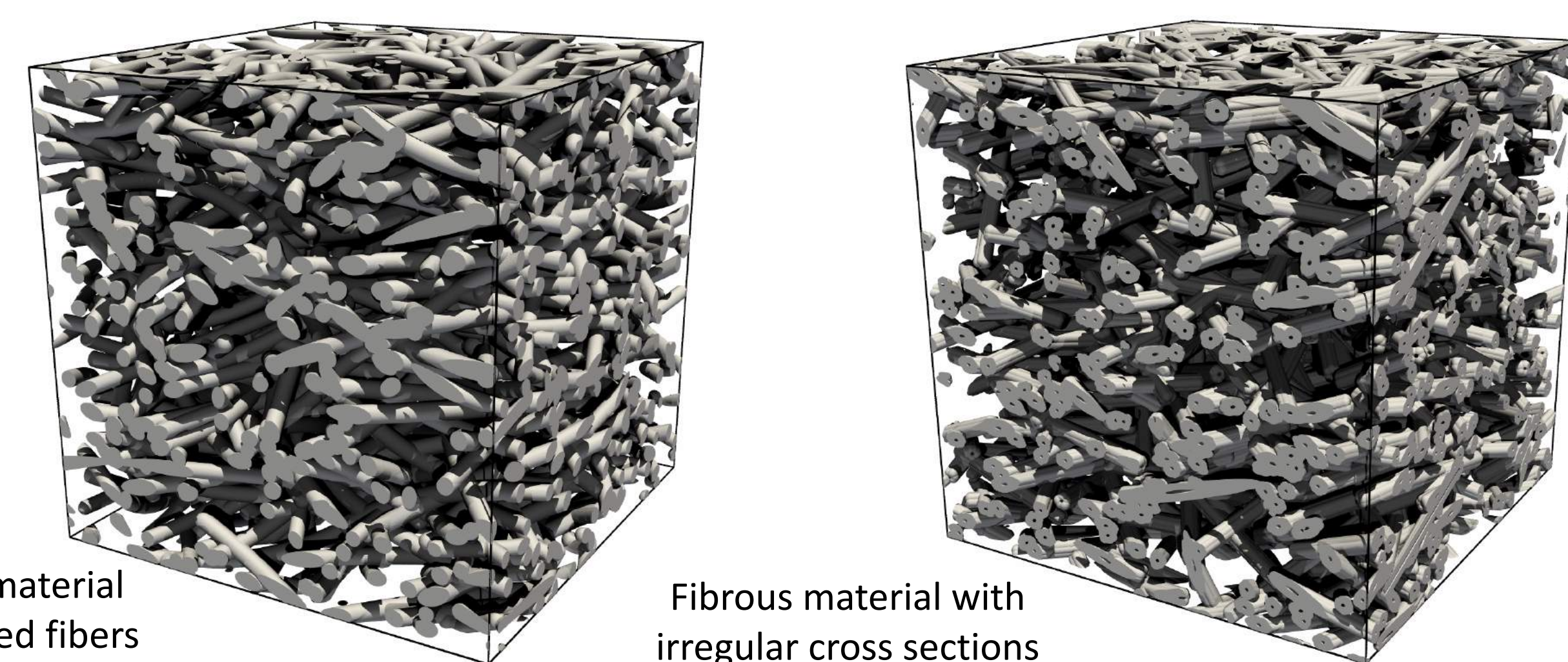
Anisotropic thermal conductivity

Modeling heat transfer in woven materials presents unique challenges. For micro-scale modeling, woven materials become a multi-scale problem, as a single domain size cannot resolve both a weave unit-cell and the individual fibers contained within each yarn. As such, at the unit-cell scale, heat transfer must be modeled assuming anisotropic constituents, since the yarns have a preferential direction for heat conduction. A multi-point-flux-approximation finite-volume method [4] was implemented in the PuMA software to solve the anisotropic heat conduction.

Steady state temperature profiles of PuMA and analytical solutions [5]
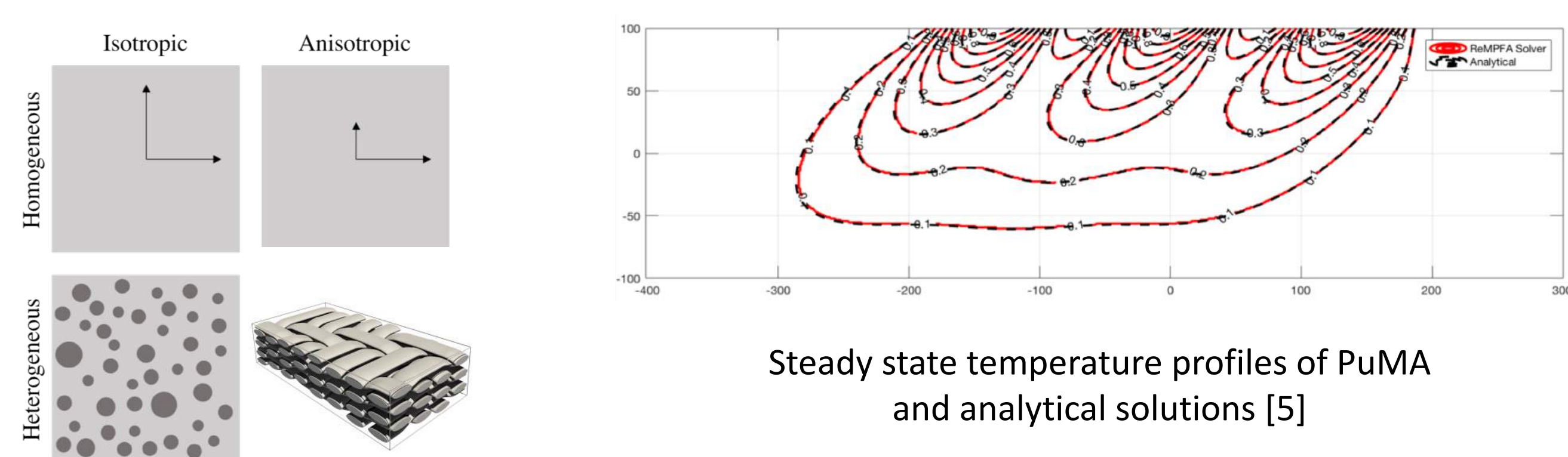
Molecular Beam Simulations

A particle based method for simulating molecular beam experiments [6] was implemented into the PuMA software. The module can simulate transport of gas reactants and products, gas-surface collisions, complex reaction models, and complex gas scattering models. The implementation was fully parallelized using OpenMP for shared memory systems, and has a significant speed increase over similar DSMC simulations [7]. The simulations can be run on any microstructural configuration, and can simulate hundreds of millions of particles and surfaces containing hundreds of millions of triangles.

Simple analytical verification case for thermal desorption

Time series progression of beam scattering on flat plate

Refactoring of PuMA into v3.0

A full refactoring of the PuMA software is ongoing. The new software architecture utilizes a highly modular structure, such that development from outside collaborators is simplified.

As a part of the software refactoring, a testing framework, PuMA_Test was designed and developed in order to allow for more robust unit, system, and regression testing in the PuMA software.

The new architecture also allows for seamless coupling of PuMA with external libraries and softwares. As a proof-of-concept, PuMA v3.0 was coupled with the DAKOTA software, developed at Sandia NL in order to perform uncertainty quantification, sensitivity analysis, and calibration of PuMA simulations.

Porous Microstructure Analysis (PuMA)
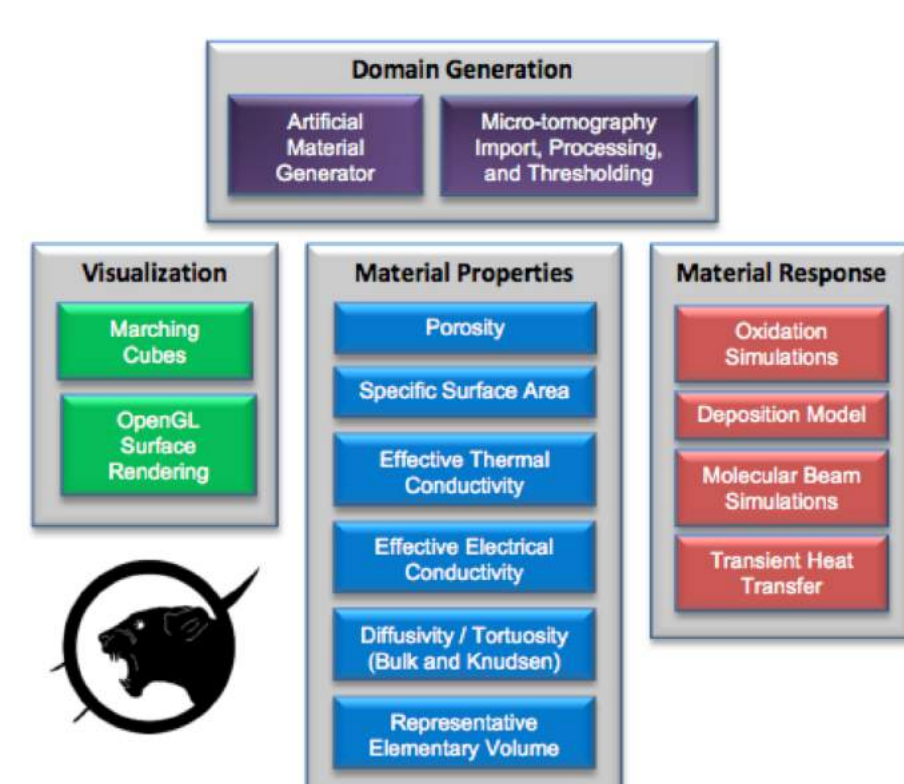
Acknowledgements

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