A parallelized oxidation-driven surface recession framework in DSMC code, SPARTA

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Spacecrafts rely on ablative thermal protection systems (TPS) made of composites consisting of a carbon-based reinforcement and a polymeric matrix. These materials are designed to withstand high-temperature oxidation and surface recession during re-entry into the Earth's atmosphere. However, ablation occurs due to a complex interplay of thermal, mechanical, and chemical factors, making it challenging to determine the individual impact of each on the TPS's overall degradation. In this study, we have developed an ablation model that can leverage a finite rate carbon oxidation model to predict material recession and surface states more accurately.

Stochastic PArallel Rarified-gas Time-accurate Analyzer (SPARTA) [1], a direct-simulation Monte Carlo (DSMC) code, is modified to allow oxidation-driven ablation of implicitly defined carbon surfaces. In SPARTA, implicit surfaces are generated from the grid corner point values via a marching cubes algorithm, therefore creating a new set of surface elements every time ablation is performed. The finite-rate oxidation model developed by Gopalan et. al [2] can perform both gas-surface and pure-surface reactions and is now adapted to tally surface data on a per-grid cell basis. The ablation functionality was also adjusted so once the reactions have occurred, the number of reactions leading to CO formation can be converted to corner point reduction values; therefore, carbon removal is directly proportional to surface recession. We also briefly discuss some unique challenges associated with parallelizing this dynamic surface state and geometry. Finally, we analyze the performance of this parallelized implicit chemistry model with simple 2D and 3D benchmark cases by producing surface state statistics, area changes over time, and visualization across a range of surface temperatures and processors with and without load-balancing.

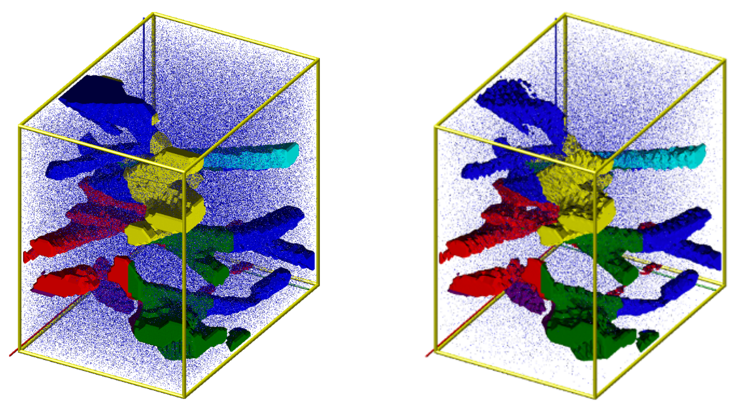

Fig. 1. Snapshots of a realistic carbon fiber implicit surface (converted from microCT TIFF file) that are receding from t = 0 ms (left) to t = 100 ms (right); each triangulated surface element is colored by processor.

[1] Plimpton, S. J., et al. "Direct simulation Monte Carlo on petaflop supercomputers and beyond." *Physics of Fluids* 31.8 (2019): 086101.
[2] Swaminathan-Gopalan, Krishnan, et al. "Development and validation of a finite-rate model for carbon oxidation by atomic oxygen." *Carbon* 137 (2018): 313-332.

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