| | Target | Goals & Critical Path | Notes & Supporting Research |
|------------|--|---|--|
| Y 1 | • Existing data from recent ACT-II-based dissertation? • Post-diction: unstart and underlying mechanisms | Key physics: unstart, critical failure mechanism Establish testing, verification, and code coverage for Y2-Y5 Baseline performance modeling Testing at scale: resolution needs, scaling roadblocks (including I/O) Workflow: use and evaluate Parsl | Provide training data for ML-anticipation of unstart Assess 1D/2D models for training and UQ Develop and evaluate composites for Y2 Initial simulation models of physics-targeted experiments Implement and evaluate initial traction-separation model Initial surface/volume tomography and FIB-based analysis of composites Implement surface kinetics, GSI/DSMC code design and coupling procedure |
| Y2 | Direct-connect composite combustor • Composite-lined combustor • Predict: material <i>T</i> and recession, flame characteristics, combustion completeness | Packaged DG kernels in control layer + kernels Transform to Loo.py IR, execute Evaluate performance model for prediction; identify opportunities Evaluate workflow and suitability of workflow metrics; identify opportunities Identify pacing uncertainties; plan/refine models & targeted experiments | Carbon fiber preform prediction Runs with coupled WARP3D solver Train ML for local material model selection Evaluate ML for operator-trained surrogate MD for T and O coupled traction separation curves Evaluate performance models in new run scenarios, with local detailed materials models First predictions and measurements of radiation contributions Evaluate and refine IR strategy for facilitating transforms and generation Courses: ML for Science; updated exascale; updated UQ; experiments for predictive science |
| Y3 | Flight conditions, with added flexible wall Flexible Composite University • Composite combustor; flexible composite in intake/isolator • Predict: material T and degradation, deformations, unstart, combustion completeness | Simulation analysis of flexible materials Coupled material degradation model codes Use full-scale + low-D models with ML to propose designs Full CS MIRGE infrastructure, evaluation of transform options Quantify/analyze Δ performance: baseline code vs. CS optimized vs. predictions | Identify and reduce pacing uncertainties Physics-targeted experiments on coated materials and weaves Beta-release MIRGE-Com under MIT licence Complete fusion of kernels using select CS tools Head-to-head comparison of available transform tools ROSE, PIPs, Polly, etc. Bridge time scales: predict long-time temperature and degradation, bringing in furnace tests Coupled solver to long-time thermal conduction, implicit time advancement, and (if needed) radiation models Evaluate WENO-DG coupling |
| Y4 | • Predict: improved design, geometry and materials • Morphed geometries: including unstart-prone and stable | Assess prediction fidelity for design extrapolation Evaluate workflow and suitability of metrics for improvement Evaluate Δ performance, compare with models for strong and weak scaling Evaluate hardware portability of MIRGE framework | Adapt physics-targeted experiment to pacing uncertainties and needed model refinements Refine performance model, accounting for multi-physics (MD, DSMC, DG) experience from actual predictions Head-to-head workflow evaluation of CS tool options Critical evaluation of ML: switching models, anticipating unstart, providing UQ/design surrogates Assess and quantify fidelity of reduced models for full system to inform use (with uncertainty) in design strategies |
| Y5 | • Predict: Simulation-based composite scramjet design • Test proposed design in ACT-II • Test variants (geometry, operation) to assess design optimality | Multi-platform demonstration and analysis of achievable performance; identify pacing/limiting items Testing at scale: resolution needs, scaling roadblocks (including I/O) Document conception-to-decision workflow improvements with metrics | Report scientific outcomes in open literature, especially successes in demonstrating scramjet design Document workflow strengths and weaknesses, including strength and weaknesses of workflow monitoring metrics Release/document: workflow, final code, end-to-end strategies Pursue translation, CS & Phys.: NNSA, Charm++, Charmworks, NASA, AFRL, etc. Refined ML course, covering strengths and limitations for scientific impact Refined exascale course, based on evolving hardware |