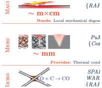
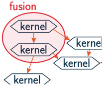
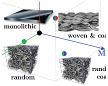
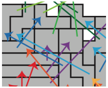
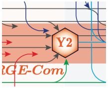
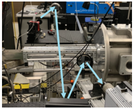
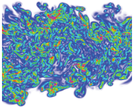
Remote Workflows using

Parsl and funcX

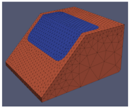





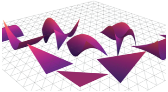
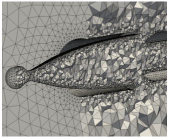



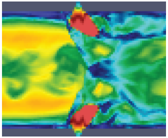
100×10^{-6} s
10×10^{-9} s
0.1×10^{-9} s



MIRGE-Com	Main sin
Python	Base lan
MPI	Underlyi
mpi4py	MPI sup
pyopencl	OpenCL
pocl	OpenCL
conda	Environr

Tested	NotTested	Coverage
74	7	91%
291	66	77%
87	6	93%
154	54	65%
26	9	65%
40	1	98%
85	6	93%
22	1	95%



The Center for
Exascale-enabled Scramjet Design

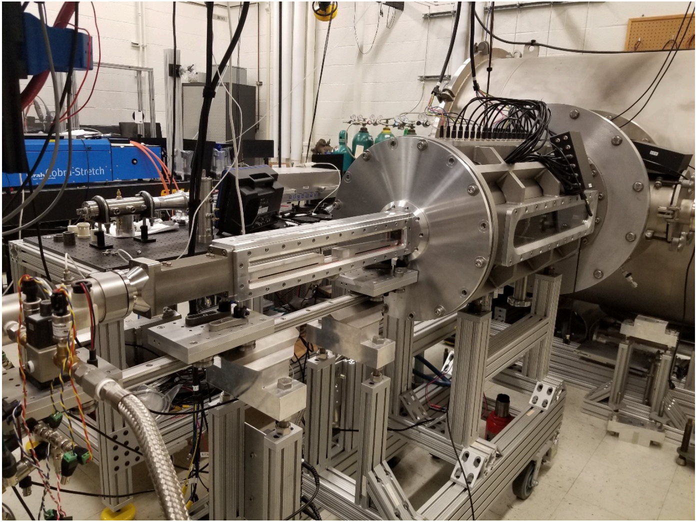
Michael Anderson
CEESD

CEESD Introduction

- CEESD is a DOE-funded, integrated center hosted at the University of Illinois, with computer scientists, computational scientists, and experimentalists working in concert
- Established a suite of physics-targeted experiments for model development, validation, integration, and UQ
- Principal code (*MIRGE-Com*: DG NS + combustion) being developed within our CS approach
- Experimental target case set, with data acquired; corresponding computational prediction underway

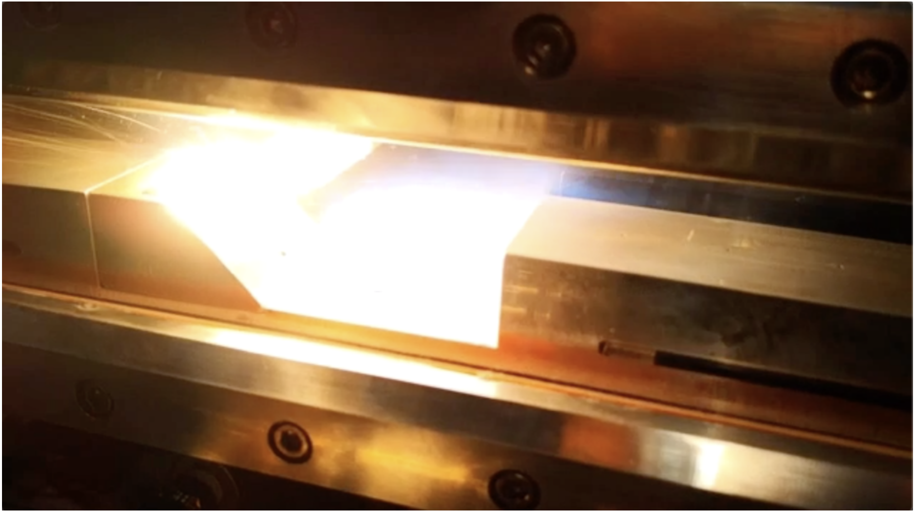
CEESD Prediction Target

ACT-II Experimental Facility



*Experimental images from 2021 CEESD review slides

Preliminary Prediction Target



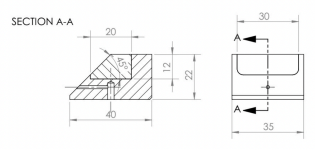
Y2 Simulation Inputs

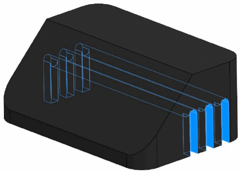
- Geometry (CAD)
- Facility stagnation conditions measured upstream of nozzle
- Fuel flow conditions (mass flow rate and composition)

Y2 flow conditions	
tunnel flow conditions	
Total Pressure (bar)	2.74
Total Temperature (K)	2076.43
Mass flow rate (g/s)	30.18
O_2 mass fraction	0.273
fuel flow conditions	
Mass flow rate (g/s)	0.1747
Composition	50:50 H_2/C_2H_4
Equivalence ratio	0.079

Y2 Prediction: Quantities of Interest

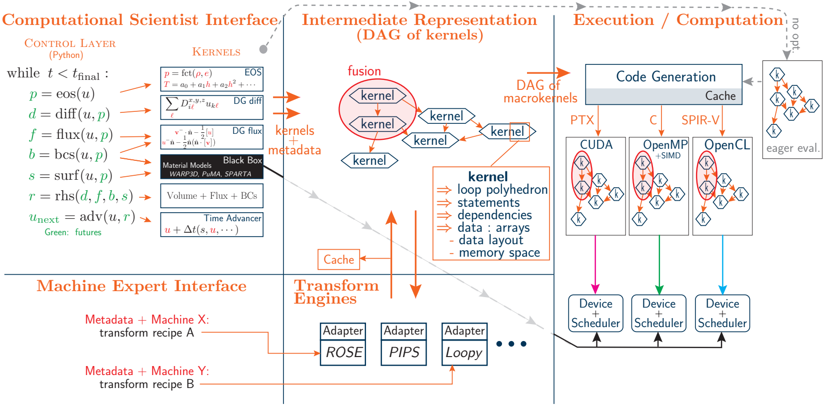
- Primary QoI
  - Material temperature history
  - Mass loss
- Secondary QoI
  - Material structure
  - Flame characteristics
  - Tunnel wall pressures
  - Surface temperature history
  - Gas dynamics (shocks and angles)





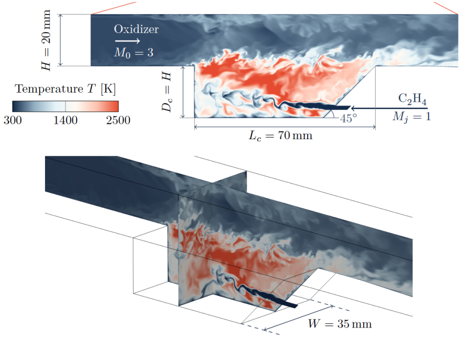
Simulation Tool: MIRGE-Com

- Discontinuous Galerkin
- Compressible Navier-Stokes and combustion
- CS-targeted approach



Simulation Strategy

- Coupled (2-way) *MIRGE-Com*/*MIRGE-Heat* simulations
- Surface state (T, Y_i, σ) passed to mircoscale physics models to assess surface degradation, material properties
- Post-process results to assess QoI
- Suite of simulations for Uncertainty Quantification



Workflow Streamlining with `Parsl`

Workflow

Anticipated Basic Workflow

- Generate mesh
- Simulation initialization
- Baseline simulations (coarse resolution/simplified physics)
- Increase simulation fidelity
- Ignition and combustion
- Post-processing QoI
- Cycle can be month^{+} sized

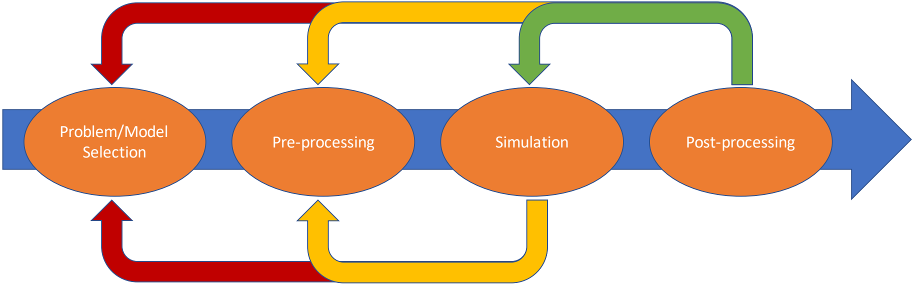
Several iterations for Uncertainty Quantification

- Simulation parameter modification and restart
- Day to week size runs

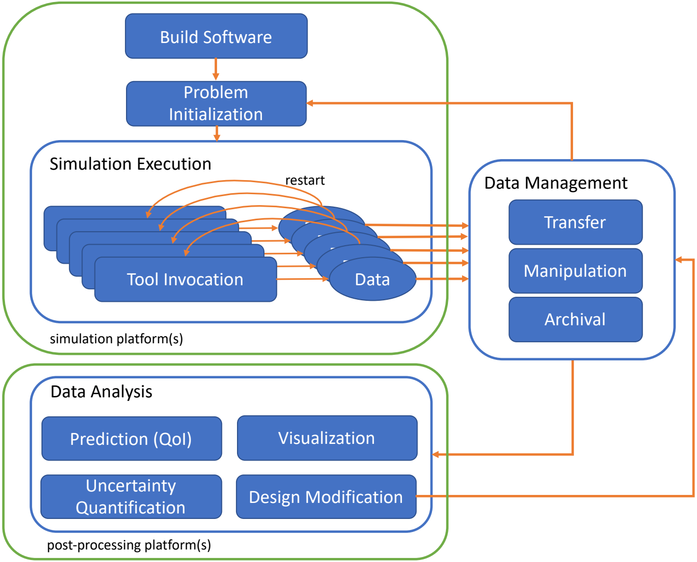
Generalized Workflow Management

Goal: Reduce overall simulation time by streamlining inter-connected simulation tasks

- Expected iterations
  - multiple submissions
- Unexpected, but anticipated iterations
  - mesh issues (instability)
  - software bugs
- Unexpected iterations
  - mistakes



Workflow Management Realized



Workflow Management with Parsl/FuncX

Parsl

- Workflow management tool
- Use Python to piece together external components or functions
- Automate data flow between computations
- Support for execution on a wide-variety of compute resources
- Execute workflows in parallel

FuncX

- Function as a service
- Built on *Parsl*
- Facilitate distributed processing (across platforms) using *Globus*

Target workflow

- Automate pre-process, compute, and post-process workflow
- Distributed across platforms
- Bring results back to a centralized location for easy access/display

Workflow Management Progress

Progress to date

- *Parsl*-enhanced *MIRGE-Com* driver (Doug Friedel)
- Kickoff from local server using *Parsl*
- Batch submit on remote host (LLNL Quartz) using *FuncX*
- Transfer of simulation data back to local server through *Globus*

Next steps

- Transfer of in-progress simulation data
- Enhance driver to handle fault control, post-mortem analysis

Questions?

This material is based in part upon work supported by the Department of Energy, National Nuclear Security Administration, under Award Number DE-NA0003963.