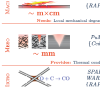
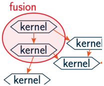
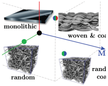
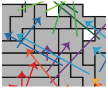
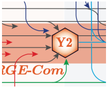
Parsl and funcX Driven Scientific Workflows in HPC

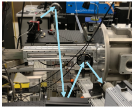


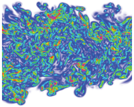








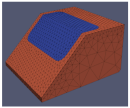




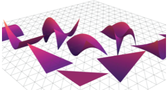
100×10^{-6} s

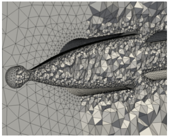
10×10^{-9} s

0.1×10^{-9} s

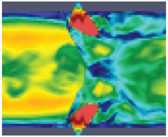


MIRGE-Com	Main sin
Python	Base lan
MPI	Underlyi
mpi4py	MPI sup
pyopencl	OpenCL
pocl	OpenCL
conda	Environr





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%



Michael Anderson

The Center for
Exascale-enabled Scramjet Design

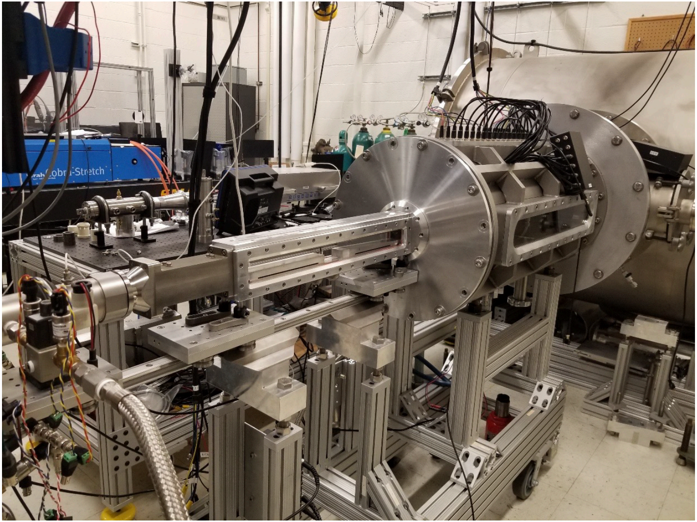
CEESD

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

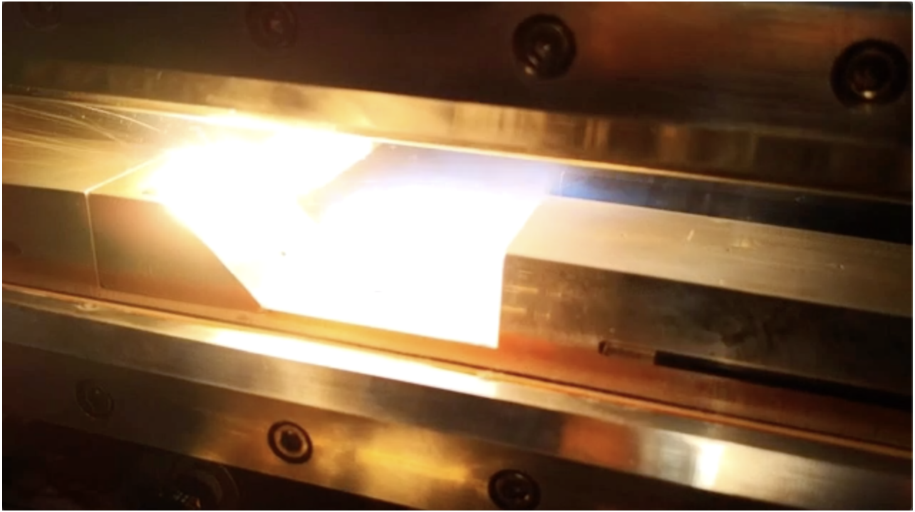
CEESD Prediction Target

ACT-II Experimental Facility



*Experimental images from 2021 CEESD review slides

Preliminary Prediction Target



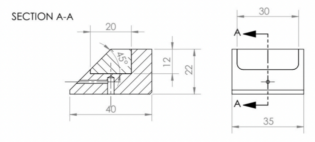
Y2 Simulation Inputs

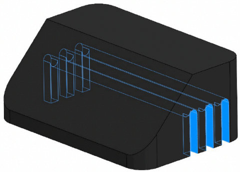
- Geometry (CAD)
- Facility stagnation conditions measured upstream of nozzle
- Fuel flow conditions (mass flow rate and composition)

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

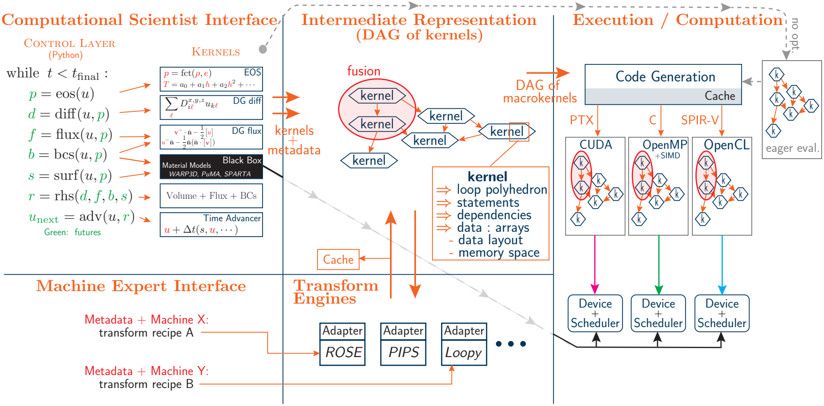
- Primary QoI
  - Material temperature history
  - Mass loss
- Secondary QoI
  - Material structure
  - Flame characteristics
  - Tunnel wall pressures
  - Surface temperature history
  - Gas dynamics (shocks and angles)





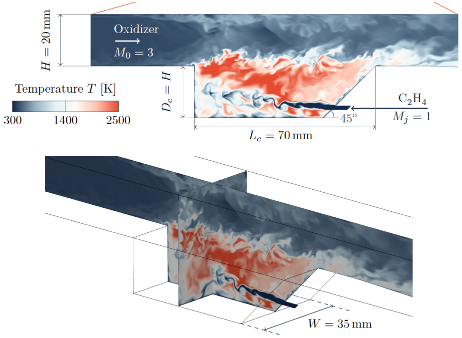
Simulation Tool: MIRGE-Com

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



Simulation Strategy

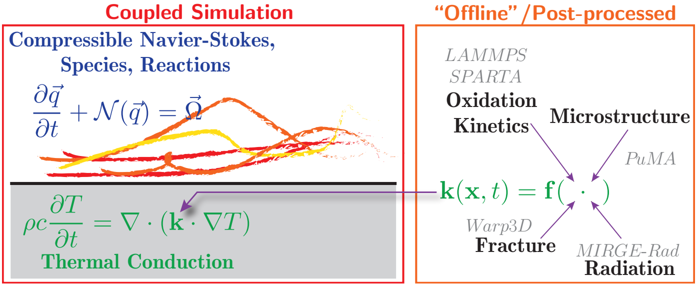
- Coupled (2-way) *MIRGE-Com*/*MIRGE-Heat* simulations
- Surface state (T, Y_i, σ) passed to mircoscale physics models to assess surface degradation, material properties
- Post-process results to assess QoI
- Suite of simulations for Uncertainty Quantification



Additional Simulation Tools

Future simulation tools coupled across length and time scales

- Oxidation kinetics
- Radiation
- Fracture
- Microstructure/conduction

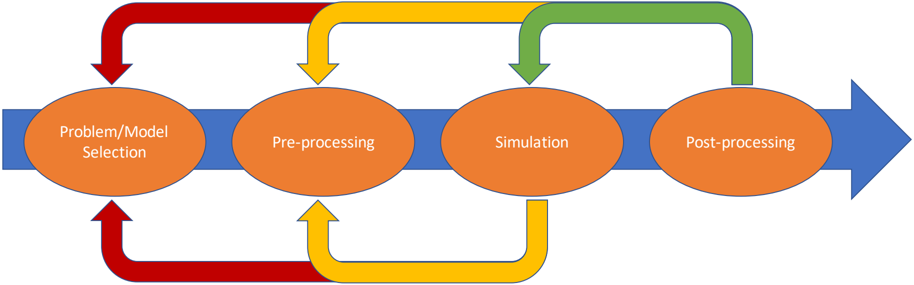


Workflow Streamlining with `Parsl`

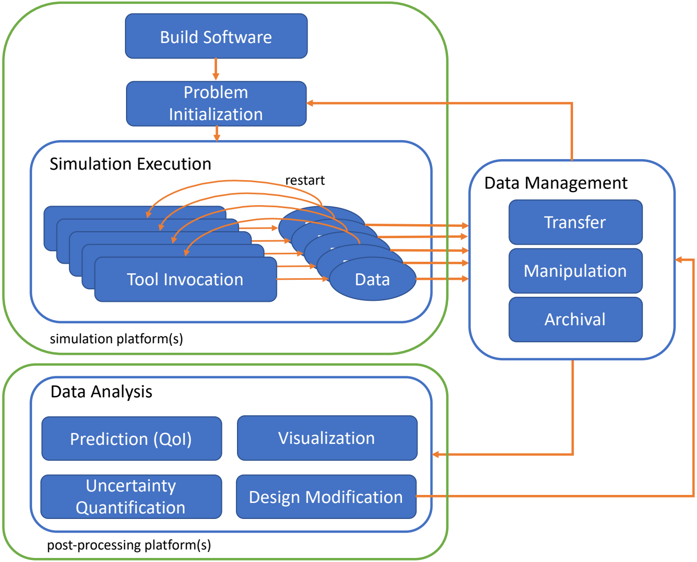
Workflow Management

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

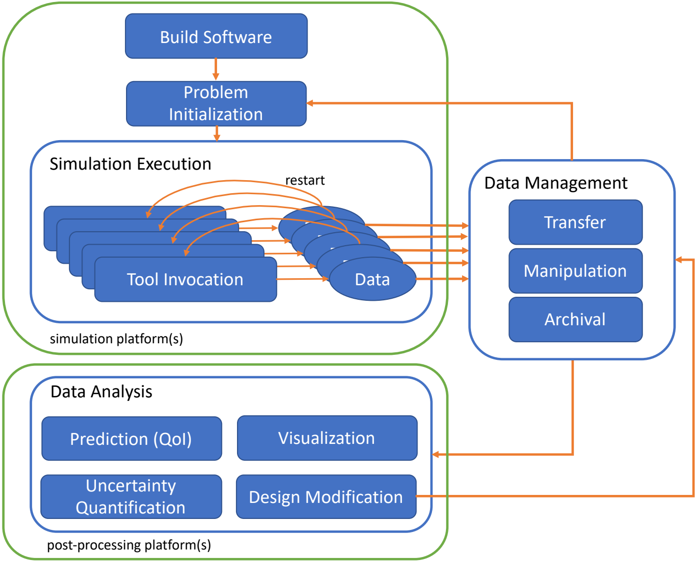
FuncX

- 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 with Parsl/FuncX



Questions?

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