The Center for Exascale-enabled Scramjet Design

University of Illinois
Urbana–Champaign

Jonathan Freund (AE)
Bill Gropp (CS/NCSA)
Predictive Science: Scramjets
Scramjets

▶ **SCRAMJET** — supersonic combustion ram jet
  - **Supersonic combustion**: avoids deceleration/compression losses
  - **Air-breathing**: avoids weight penalty of onboard oxidizer

...nominally simple, but extreme conditions are challenging

▶ **Enables**: access to space, global transport, next-generation delivery systems
Design Opportunity: Advanced Composites

- **High-**$^{T}$, low-weight composites:
  - *Dense* — strong and heat resistant
  - *Porous* — tailored thermal protection
  - *Flexible* — morphing for flight-regime robustness

- **Common features:**
  - Carbon-fiber: weave or pack
  - Coatings or matrix — ceramics, resins, phenolics, ...

- **Many-parameter design space for targeting multiple objectives**

- **Goal:** develop and demonstrate a predictive capability
Impact Design Cycle

- **Flight Tests** expensive and inflexible: NASA X-43A, Boeing X-51A, HyShot (Queensland), HIFiRE (AFRL, AFOSR, NASA, ATK-GASL, DSTG) [over last 20 years]

- **Ground Tests** conditions and their evolution is a challenge, and also expensive

  - NASA Langley DCSCTF
  - $M = 5 - 7$
  - Not shown: 70 ft diameter vacuum sphere

- **Physics-based predictive simulation will accelerate design innovation**
Preliminary Prediction Target

- **ACT-II**: on-campus AFOSR-funded supersonic combustion facility

- Arcjet driven: low cost ($\lesssim 10$), low turnaround time ($\lesssim 10$ min)

---

ACTII

Test Section

$N_2 + O_2$

$M \approx 3$

$C_2H_4$

Carbon Fiber Surrogate Material
Preliminary Prediction Target

- **ACT-II**: on-campus AFOSR-funded supersonic combustion facility
- Arcjet driven: low cost ($\lesssim 10$), low turnaround time ($\lesssim 10$ min)
Model Scramjet Flame Holder

- Design inspired by flight-test geometries

![Diagram of scramjet flame holder](image)

HIFiRE2
Jackson et al., 2015
Demo Basics

ACTII

Test Section

\[ \text{N}_2 + \text{O}_2 \]
\[ M \approx 3 \]

\[ \text{C}_2\text{H}_4 \]

Carbon Fiber Surrogate Material

Fuel: ethylene

Material:
- off-the-shelf carbon preform – a stiff carbon fiber felt
- no matrix/coating (yet): degradation over \( \sim s \) time scale of ACT-II
Preliminary Prediction Target
Preliminary Prediction Target

Spark Ignition $t \approx 0 \text{s}$

Fuel/Oxidizer Off $t \approx 1 \text{s}$

Sustained Flame $t \lesssim 1 \text{s}$

Persistent Incandescence $t \approx 2 \text{s}$

Ablation
Preliminary Prediction Target

- Degradation due to oxidation and mechanical effects
Prediction Targets

► Primary
- **Surface temperatures** — key for material state/degradation, requires accurate turbulent combustion simulation and thermal conduction into wall
- **Surface recession/degradation** — temperature dependent, requires accurate microstructural models and mechanically-coupled surface chemistry

... both are of primary engineering importance

► Secondary
- Chemical species in flames and near surface
- Post-run microstructure detail
- Flame location
- Wall pressures (locations and histories)

... adapt to target uncertainties
## Multi-scale/Multi-physics

<table>
<thead>
<tr>
<th>Physics/Scale</th>
<th>Code(s)</th>
<th>Essential Physics</th>
<th>Anticipated Physics</th>
<th>Potential Physics</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>FULL</strong></td>
<td>MIRGE-Com, Nek5000-DG, Cantera, Prometheus</td>
<td>Turbulent mixing, Shocks, Combustion, Complex geom.</td>
<td>Radiation, Flexible wall, Wall texture, Wall transpiration</td>
<td>Particle trajectories, Radicals</td>
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<tr>
<td>~ m</td>
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<tr>
<td><strong>MACRO</strong></td>
<td>WARP3D, RAPtor</td>
<td>Thermal conductivity</td>
<td>Fracture, Fragmentation, Recession, Elastic response</td>
<td>Vibration</td>
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<tr>
<td>~ m × cm</td>
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<tr>
<td><strong>MESO</strong></td>
<td>PuMA, Cedar</td>
<td>Oxidation, Transport</td>
<td>Micro-cracking, Recession, Detailed porous transport, Porous material radiation</td>
<td>Sublimation, Evaporation, Wetting</td>
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<td>~ mm</td>
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<tr>
<td><strong>MICRO</strong></td>
<td>SPARTA, WARP3D, RAPtor</td>
<td>Surface kinetics</td>
<td>Stress-coupled reaction, De-bonding</td>
<td>Grain-scale pitting</td>
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<tr>
<td><strong>NANO</strong></td>
<td>LAMMPS</td>
<td>Solid-state diff., Traction-separation, Phonon-kinetic models</td>
<td>Quantum (DFT) potentials</td>
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<td>~ nm</td>
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**Needs:** Wall conditions $T$, (maybe $Y_i$, geom.); **Provides:** Gas $T$, $Y_i$, (maybe $\sigma$)
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<td>Shock</td>
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<td>Combustion</td>
<td>Wall texture</td>
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<td>Complex geom.</td>
<td>Wall transpiration</td>
<td>Radical</td>
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| **MACRO**     | $\sim m \times cm$ | Thermal conductivity | Fracture             | Vibration          |
|               |                     |                    | Fragmentation        |                    |
|               |                     |                    | Recession            |                    |
|               |                     |                    | Elastic response     |                    |
| Needs: Local mechanical degradation, local $Y_O$, traction separation prms.; Provides: Cracking, regression, failure. |

| **MESO**      | $\sim mm$ | Oxidation Transport | Micro-cracking        | Sublimation        |
|               |           |                    | Recession             | Evaporation        |
|               |           |                    | Detailed porous transport | Wetting            |
|               |           |                    | Porous material radiation |                    |
| Provides: Thermal conductivity, convective transport, local concentrations, microstructure geometry. |

| **MICRO**     | $\sim \mu m$ | Surface kinetics | Stress-coupled reaction | Grain-scale pitting |
|               |               |                   | De-bonding            |                   |
| Provides: Local surface chemical kinetics. |

| **NANO**      | $\sim nm$ | LAMMPS            | Solid-state diff.     | Quantum (DFT) potentials |
|               |           |                   | Traction-separation   |                        |
|               |           |                   | Phonon-kinetic models |                        |
| Provides: O diffusion, O-dependent traction separation. |
Annual Predictions: Overview

- **Annual prediction goals:** unify all CEESD activities

- **Increasingly challenging (Y1→Y5):**
  - **physics:** integration & refinement targeting pacing uncertainties
  - **code:** development and analysis, all within CS framework
  - **CS:** increasing use of CS methods for platform flexible performance
  - **workflow:** monitoring and improving end-to-end workflow

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<tr>
<th>Target</th>
<th>Goals &amp; Critical Path</th>
<th>Notes &amp; Supporting Research</th>
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<tr>
<td>Y1</td>
<td>Computation, isolator &amp; unstart</td>
<td>• Key physics: unstart, critical failure mechanism&lt;br&gt;• Establish testing, verification, and code coverage for Y2-Y5&lt;br&gt;• Baseline performance modeling&lt;br&gt;• Testing at scale: resolution needs, scaling roadblocks (including 1/0)&lt;br&gt;• Workflow: use and evaluate Perl&lt;br&gt;• Provide training data for ML-alternative methods&lt;br&gt;• Assess HPC models for training and UQ&lt;br&gt;• Develop and evaluate compilers for Y2&lt;br&gt;• Initial simulation models of physics-challenged requirements&lt;br&gt;• Implement and evaluate initial traction-operation model&lt;br&gt;• Implement and evaluate physics-optimized and simulation-based analysis of component&lt;br&gt;• Implement earlier iterations: Charm++ code-design and coupling procedure</td>
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<td>Y2</td>
<td>Composite liner combuster composite combustor</td>
<td>• Key physics: unstart, critical failure mechanism&lt;br&gt;• Establish testing, verification, and code coverage for Y2-Y5&lt;br&gt;• Baseline performance modeling&lt;br&gt;• Testing at scale: resolution needs, scaling roadblocks (including 1/0)&lt;br&gt;• Workflow: use and evaluate Perl&lt;br&gt;• Provide training data for ML-alternative methods&lt;br&gt;• Assess HPC models for training and UQ&lt;br&gt;• Develop and evaluate compilers for Y2&lt;br&gt;• Initial simulation models of physics-challenged requirements&lt;br&gt;• Implement and evaluate initial traction-operation model&lt;br&gt;• Implement and evaluate physics-optimized and simulation-based analysis of component&lt;br&gt;• Implement earlier iterations: Charm++ code-design and coupling procedure</td>
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<tr>
<td>Y3</td>
<td>Flight conditions, with added flexible wall</td>
<td>• Key physics: unstart, critical failure mechanism&lt;br&gt;• Establish testing, verification, and code coverage for Y2-Y5&lt;br&gt;• Baseline performance modeling&lt;br&gt;• Testing at scale: resolution needs, scaling roadblocks (including 1/0)&lt;br&gt;• Workflow: use and evaluate Perl&lt;br&gt;• Provide training data for ML-alternative methods&lt;br&gt;• Assess HPC models for training and UQ&lt;br&gt;• Develop and evaluate compilers for Y2&lt;br&gt;• Initial simulation models of physics-challenged requirements&lt;br&gt;• Implement and evaluate initial traction-operation model&lt;br&gt;• Implement and evaluate physics-optimized and simulation-based analysis of component&lt;br&gt;• Implement earlier iterations: Charm++ code-design and coupling procedure</td>
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<td>Y4</td>
<td>Multiple configurations</td>
<td>• Key physics: unstart, critical failure mechanism&lt;br&gt;• Establish testing, verification, and code coverage for Y2-Y5&lt;br&gt;• Baseline performance modeling&lt;br&gt;• Testing at scale: resolution needs, scaling roadblocks (including 1/0)&lt;br&gt;• Workflow: use and evaluate Perl&lt;br&gt;• Provide training data for ML-alternative methods&lt;br&gt;• Assess HPC models for training and UQ&lt;br&gt;• Develop and evaluate compilers for Y2&lt;br&gt;• Initial simulation models of physics-challenged requirements&lt;br&gt;• Implement and evaluate initial traction-operation model&lt;br&gt;• Implement and evaluate physics-optimized and simulation-based analysis of component&lt;br&gt;• Implement earlier iterations: Charm++ code-design and coupling procedure</td>
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<td>Y5</td>
<td>Extrapolation: Novel design</td>
<td>• Key physics: unstart, critical failure mechanism&lt;br&gt;• Establish testing, verification, and code coverage for Y2-Y5&lt;br&gt;• Baseline performance modeling&lt;br&gt;• Testing at scale: resolution needs, scaling roadblocks (including 1/0)&lt;br&gt;• Workflow: use and evaluate Perl&lt;br&gt;• Provide training data for ML-alternative methods&lt;br&gt;• Assess HPC models for training and UQ&lt;br&gt;• Develop and evaluate compilers for Y2&lt;br&gt;• Initial simulation models of physics-challenged requirements&lt;br&gt;• Implement and evaluate initial traction-operation model&lt;br&gt;• Implement and evaluate physics-optimized and simulation-based analysis of component&lt;br&gt;• Implement earlier iterations: Charm++ code-design and coupling procedure</td>
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V/UQ
Parametric UQ: Parameters + Sensitivity

- Identify all model parameters
- Ascribe uncertainties (literature, re-calibration, ...)
- Example: ACT-II nozzle parameters and interrelations:

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value</th>
<th>Uncertainty/Status</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m_{N_2}$</td>
<td>0 g/s</td>
<td>N/A; pure $O_2$</td>
<td>$N_2$ mass flow rate</td>
</tr>
<tr>
<td>$m_{O_2}$</td>
<td>56.38 g/s</td>
<td>measured$^a$</td>
<td>$O_2$ mass flow rate</td>
</tr>
<tr>
<td>$P_0$</td>
<td>167.1 kPa</td>
<td>±0.05 psi (aleatoric)$^b$</td>
<td>Total pres.</td>
</tr>
<tr>
<td>$T_0$</td>
<td>298 K</td>
<td>isentropic gas dyn.</td>
<td>Total temp.</td>
</tr>
<tr>
<td>$U_{arc}$</td>
<td>0.0 A</td>
<td>N/A</td>
<td>Mean arc current</td>
</tr>
<tr>
<td>$V_{arc}$</td>
<td>0.0 V</td>
<td>N/A</td>
<td>Mean arc voltage</td>
</tr>
<tr>
<td>$W_{arc}$</td>
<td>0.0 kW</td>
<td>$W_{arc} = V_{arc}I_{arc}$</td>
<td>Mean arc power</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Arc heater [GyuSub Lee]</th>
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</thead>
<tbody>
<tr>
<td>$P_0$</td>
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<tr>
<td>$T_{in}$</td>
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<tr>
<td>$M_{in,k}$</td>
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<tr>
<td>$Y_{in,k}$</td>
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<td>$A_{trusted}$</td>
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<td>$P_{in,F}$</td>
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<td>$T_{in,F}$</td>
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<td>$M_{in,F}$</td>
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<tr>
<td>$A_{F}$</td>
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<tr>
<td>$\delta$</td>
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<thead>
<tr>
<th>Fuel inlet [GyuSub Lee]</th>
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<tbody>
<tr>
<td>$m_{H_2}$</td>
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<tr>
<td>$P_{0,F}$</td>
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<tr>
<td>$T_{0,F}$</td>
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</tbody>
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<tr>
<th>Air/fuel nozzle [A. Munaf` o]</th>
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<tbody>
<tr>
<td>$P_{in}$</td>
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<td>$T_{in}$</td>
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<tr>
<td>$\delta$</td>
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</tbody>
</table>

- Sensitivity analysis to reduce dimension of uncertainty ‘space’, using hierarchy of reduced-physics low-D configuration
Parametric UQ: Propagation

► Propagate pacing uncertainties
  - low-D, fast solutions: MCMC Bayesian methods
  - higher-D, higher-cost: anchored-ANOVA surrogates

► Research:
  - DGM (Deep Galerkin Method) surrogates
  - Simpler, NN-ML surrogates
Parametric UQ: Propagation

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Parametric UQ: Sample Orchestration

中国网游

Starting point:

* packages: e.g., *Dakota* evaluation tiling (mpitile -np 20 ...)

* bigger jobs, small sample sizes: scripts and machine queues

Research:

* sample automation with *Parsl* workflow manager
  
  https://github.com/Parsl/parsl

* transforms for efficient UQ sampling on ‘inner loop’
Parametric UQ: Sample Orchestration

▶ Starting point:
- packages: e.g., Dakota evaluation tiling (mpitile -np 20 ···)
- bigger jobs, small sample sizes: scripts and machine queues

▶ Research:
- sample automation with Parsl workflow manager "Katz"
  https://github.com/Parsl/parsl
- transforms for efficient UQ sampling on ‘inner loop’
Validation & Model-Form Uncertainty

- Is scarier...

- Appeal to fundamental theories/models when possible

- Leverage suite of agile physics-reduced/physics-targeted experiments
# Physics-targeted/Physics-reduced Experiments

## Focused Ion Beam (FIB)

**Measure:** products scattered from C/SiC or SiC or similar samples; **vary:** impact temperatures and species, target material, microstructure, etc.; **use:** finite-rate oxidation model closure and validation; **models:** corresponding MD simulations, 0D closure of GSI reaction kinetics; **status:** shared-use FIBs at Illinois, experience using FIB with MD simulations and continuum modeling.

## Furnace: Flow

**Measure:** interface mass spectroscopy of products, PLIF; **vary:** materials (graphite, PAN carbon fibers, C/SiC, SiC, ...), temperature, pressure, gas (O<sub>2</sub>, H<sub>2</sub>, H<sub>2</sub>O, air, CO<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, etc.); **use:** quantify passive structural degradation (SEM, EDX, XRD microscopy); **models:** 1D surface evolution transport and kinetics; **status:** furnaces and mass spectrometers on campus (MRL), experience in team with measurements and model closure.

## Furnace: Stress

**Measure:** oxidation rate, O distribution with atom-probe tomography (APT), geometric evolution, strength, stress-coupling; **vary:** materials (graphite, PAN carbon fibers, C/SiC, SiC, ...), temperature, pressure, gas (O<sub>2</sub>, H<sub>2</sub>, H<sub>2</sub>O, air, CO<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, etc.); **use:** quantify passive strength degradation; **models:** 1D surface oxidation and strength coupling; **status:** furnaces with stress-strain capabilities on campus (MRL), experience in team with measurements and model closure.

## Plasmatron Ablation

**measure:** in-situ PLIF of near-surface reactants and products; **vary:** materials, temperature, pressure, gases; **use:** quantify structural degradation under extreme aerothermal conditions simulating combustor flow conditions; **models:** 1D/2D-axi surface evolution with flow; **status:** PI with experience from NASA Ames, extensive PLIF systems available at Illinois, anticipated plasmatron ready on-site early 2020.

## Laser Ablation

**Measure:** ultrafast diagnostics of transient products; **vary:** target material, temperature, pressure, gases; **use:** transient response validation; **models:** 1D/2D-axi surface transport/kinetics models; **status:** experience with fs diagnostics and laser methods, especially laser-induced breakdown (LIB).

## Jet Mixing, Ignition and Propagation

**Measure:** mixing & evolution of ignition kernel with emission spectroscopy, PLIF; **vary:** fuels, flow conditions; **use:** validation for mixing, combustion kinetics, ignition; **models:** 2D-axi or 3D jet combustion simulations (short time for TIK); **status:** based on current LIB and transient ignition kernel (TIK) configurations and corresponding models; **variant:** add axisymmetric flame holder for predicting flame-holding limits.

## Flexible/Rough Surface Supersonic Wind Tunnel

**Measure:** wall deflection and T, PIV, FLEET, high-speed schlieren; **vary:** flow conditions, materials, material roughness; **use:** mechanical models, flow-structure interaction models; **models:** 2D analog; 3D for simple geometry turbulence studies; **status:** on-campus wind tunnels with flow and surface measurement diagnostics operated by the PIs.
### Physics-targeted/Physics-reduced Experiments

#### Focused Ion Beam (FIB)

**Measure:** products scattered from C/SiC or SiC or similar samples; **vary:** impact temperatures and species, target material, microstructure, etc.; **use:** finite-rate oxidation model closure and validation; **models:** corresponding MD simulations, 0D closure of GSI reaction kinetics; **status:** shared-use FIBs at Illinois, experience using FIB with MD simulations and continuum modeling.

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Mapping Physics of Full Application

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<td></td>
<td></td>
<td></td>
<td>1D</td>
</tr>
<tr>
<td>Flexible wall</td>
<td>×</td>
<td>×</td>
<td>×</td>
<td>×</td>
<td>×</td>
<td>×</td>
<td>×</td>
<td>×</td>
<td>s</td>
<td></td>
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<td></td>
<td>2,3D</td>
</tr>
<tr>
<td>ACT-II</td>
<td>×</td>
<td>×</td>
<td>×</td>
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<td>×</td>
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<td></td>
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<td></td>
<td>3D</td>
</tr>
<tr>
<td>Scramjet</td>
<td>×</td>
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<td></td>
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<td>3D</td>
</tr>
</tbody>
</table>

- Targeted experiments designed to ‘cover’ anticipated physics of full composite-walled scramjet
- ACT-II experiments will couple most
- Supporting experiments for stresses and long-t validation
Exascale/CS

(Gropp)
Current Performance Challenges

- Concurrency, bandwidth, latency hiding vs. chip/network/memory resources for in-flight state
- Complex memory hierarchies
- Complex and heterogeneous node architectures
- Complex communication (inter-node, intra-node)
- Power, Resilience
- System aspects: I/O

Some key CS/software challenges on the way to Exascale:

- Abundance of architectures
- Method Complexity
- Separation of Concerns (model/method/performance)
Implications

- Need to deliver fast code while application is evolving
  ⇒ Build tools into development process and ensure fall-back to supported languages and tools (baseline version or Golden Copy)

- Increasingly complex processors and innovative architectures
  ⇒ Exploit vendor compilers and (low-level) code generators
  ⇒ Enable teams of computational scientists and performance engineers, with appropriate tools for both

- Performance hard to predict a priori
  ⇒ Combine approximate performance models (compile-time) and autotuning (run-time) to get system-specific code
Lessons from XPACC

- It is not easy to extract the flow of data dependencies even in a well-modularized code.

- Code transformation tools are more fragile than expected.

- No tool generates the best code in all cases; many need guidance.

- Data management for accelerators is both in flux and remains a concern, especially in the strong scaling domain.
\[ p = \text{eos}(u) \]
\[ d = \text{diff}(u, p) \]
\[ f = \text{flux}(u, p) \]
\[ b = \text{bcs}(u, p) \]
\[ s = \text{surf}(u, p) \]
\[ r = \text{rhs}(d, f, b, s) \]
\[ u_{\text{next}} = \text{adv}(u, r) \]

**Intermediate Representation (DAG of kernels)**
- **kernel**
  - loop polyhedron
  - statements
  - dependencies
  - data: arrays
  - data layout
  - memory space

**Execution / Computation**
- **Code Generation**
- **Cache**
- **Execution**
  - PTX
  - C
  - SPIR-V
  - DAG of macrokernels

**Machine Expert Interface**
- Metadata + Machine X: transform recipe A
- Metadata + Machine Y: transform recipe B

**Transform Engines**
- Adapter
  - ROSE
- Adapter
  - PIPS
- Adapter
  - Loopy

**Computational Scientist Interface**
- **CONTROL LAYER**
  - (Python / C++)
- **Kernels**
  - (Fortran dialect)
- **while** \( t < t_{\text{final}} \):
  - \( p = \cos(u) \)
  - \( d = \text{diff}(u, p) \)
  - \( f = \text{flux}(u, p) \)
  - \( b = \text{bcs}(u, p) \)
  - \( s = \text{surf}(u, p) \)
  - \( r = \text{rhs}(d, f, b, s) \)
  - \( u_{\text{next}} = \text{adv}(u, r) \)

- **Black Box**
  - Material Models
    - WARP3D, PUMA, SPARTA

- **Volume + Flux + BCs**

- **Time Advancer**
  - \( u + \Delta t(s, u, \cdots) \)

- **Green: futures**

- **Intermediate Representation**
  - (DAG of kernels)

- **kernels + metadata**

- **Fusion**

- **DAG of macrokernels**

**Execution / Computation**
- **PTX**
- **C**
- **SPIR-V**
- **DAG of macrokernels**

**Compiler**
- **Cache**
- **Standard Compile**
  - no optimization, fallback
- **Execute**
  - PTX
  - C
  - SPIR-V

**Machine Expert Interface**
- Metadata + Machine X: transform recipe A
- Metadata + Machine Y: transform recipe B
Math · Intermediate Representation · Generation · Execution

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CS Framework (MIRGE)

**Computational Scientist Interface**

- **CONTROL LAYER** (Python / C++)
- **Kernels** (Fortran dialect)
  - $p = \text{cos}(u)$
  - $d = \text{diff}(u, p)$
  - $f = \text{flux}(u, p)$
  - $b = \text{bcs}(u, p)$
  - $s = \text{surf}(u, p)$
  - $r = \text{rhs}(d, f, b, s)$
  - $u_{\text{next}} = \text{adv}(u, r)$

**Intermediate Representation** (DAG of kernels)

**Execution / Computation**

- **Code Generation**
- **Cache**
- **CUDA**
- **OpenMP + SIMD**
- **OpenCL**
- **Fortran** (fallback)
- **DAG of macrokernels**

**Machine Expert Interface**

- **Metadata + Machine X**: transform recipe A
- **Metadata + Machine Y**: transform recipe B

**Transform Engines**

- **Adapter**
  - **ROSE**
  - **PIPS**
  - **Loopy**

**Execution / Computation**

- **PTX**
- **C**
- **SPIR-V**

**Fallback and physics dev.**: **Math** kernels + standard compile and execution

**M-Com**: portable development, but slow, CPU only, no optimization
\[ p = \text{eos}(u) \]
\[ d = \text{diff}(u \tau_p) \]
\[ \sigma = \text{flux}(u \tau_p) \]
\[ \rho = \text{bcs}(u \tau_p) \]
\[ s = \text{surf}(u \tau_p) \]
\[ r = \text{rhs}(d \tau \sigma \tau \rho \tau_s) \]
\[ u_{\text{next}} = \text{adfl}(u \tau_r) \]

Green: futures

MIRGE spans all CS faculty research (PhD-advising) sub-areas
Software & Verification

(Freund)
Software Overview

**Y1**: *PlasCom2* prediction concurrent with *MIRGE-Com* development
- C++ Control with MPI and OpenMP
- F77/F90 kernels
- HDF5 IO
- Kinetics, EoS, and transport: *Cantera*

**Y2+**: *MIRGE-Com*
- Python control layer
- DG kernels
- Couple additional codes/tools/libraries, especially for wall models
Software Development via Verification and Testing

- **LLNL-Spack**-based build system
- **Verification** is the foundation of our predictive science effort
  - Automated testing confirms correctness and monitors performance
  - Coverage assessment for key predictions
- **Parsl** Python/Jupyter-based workflow targeting dev-to-prediction adaptability, repeatability, documentation, and efficiency
Integration
Integration Is The Plan

- **CS**: *MIRGE* framework essential for exascale performance-portable predictions

- **Verification**: test-based software development for prediction confidence; including coverage & performance monitoring

- **V/UQ**: add value to predictions, guides model integration, and prioritizes physics-targeted experiments; CS tools for UQ sampling via workflow (*Parsl*) and code transforms (*Loopy*)

- **Software**: open development for our predictions, leveraging and adding to community tools for physics and exascale performance

- **Predictions**: validated, scale-resolving, exscale performance with quantified uncertainty will best impact novel scramjet designs
Integration Is The Plan

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Preliminary Integration Demonstration

- Developed new control-layer/kernel Euler-DG solver within MIRGE structure

- Leveraged Illinois *Loopy* [https://github.com/inducer/loopy](https://github.com/inducer/loopy)
  - IR of kernels
  - code transforms
  - OpenCL/CUDA generation on Nvidia GPUs using *pyopencl/pocl*

- Runs on LLNL-Lassen, ~1M tets-in-a-box mesh, $n$-nodes, 4 GPUs/node

- Much to do: performance modeling and analysis, more physics, *etc.*

- Open development: [https://github.com/illinois-ceesd/mirgecom](https://github.com/illinois-ceesd/mirgecom)
Summary: Main Challenges

▶ Balancing code development and hardware flexibility goals
  • Performance on current multi-GPU systems
  • Flexibility for performance on future platforms
  • Unconstrained development by ‘real’ computational scientists
  • Leveraging of community tools, for physics and performance

▶ Identifying, integrating, and evaluating right-fidelity models to establish predictive confidence, with quantified uncertainty

▶ Quantifying and realizing full-workflow prediction efficiency

▶ Advance design methods and options for scramjets

▶ End-to-end engagement: all students, staff, faculty, and lab partners
Questions?

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