Integrated Simulations using Exascale Multiphysics Ensemble (INSIEME)

Stanford University - PSAAP III Kick-Off Meeting – 8/18/2020

INSIEME

ITALIAN: 1) TOGETHER, 2) AT THE SAME TIME

INTEGRATION & CONCURRENCY

Integrated Simulations using Exascale Multiphysics Ensemble (INSIEME)

Stanford University - PSAAP III Kick-Off Meeting - 8/18/2020

Overarching Application

Integrated Simulations using Exascale Multiphysics Ensemble (INSIEME)

Stanford University - PSAAP III Site Visit - 10/21 & 22/2019

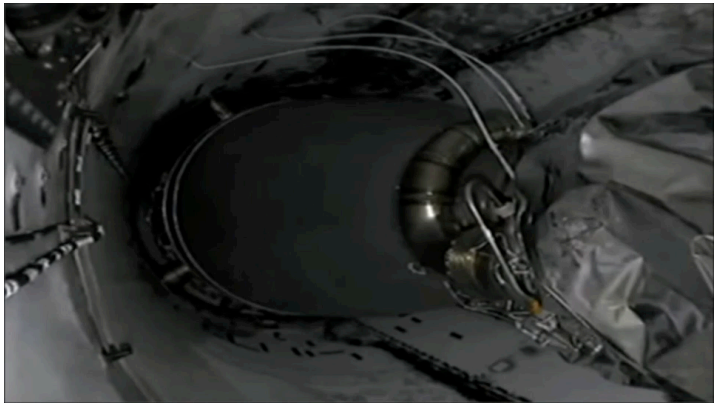
Overarching Application

Predicting Reliability of In-Space Laser Ignition of Cryogenic Propellants

Ignition of upper stages occurs in harsh environment AND is fundamental to space missions :

- 80-120 km of altitude (near the edge of space or in space) and very low pressures and temperatures (nearing vacuum)
- Low Earth Orbit and missions to Moon/Mars and Translunar/Transmartian injection

→ The ignition system must be nearly 100% reliable!



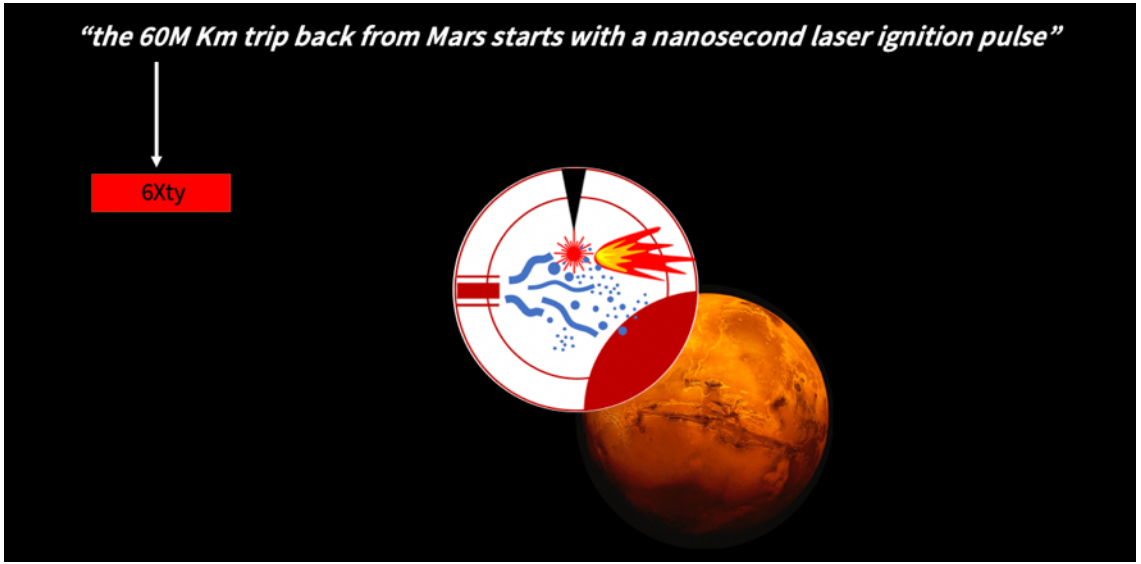
SpaceX Starlink-7 Main Engine Cutoff & Second Stage Burn (Onboard View)

Overarching Application

Predicting Reliability of in-Space Laser Ignition of Cryogenic Propellants

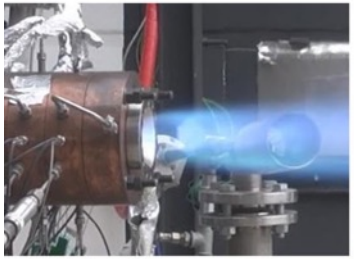
This project: Ignition using nano-second high-energy laser pulses

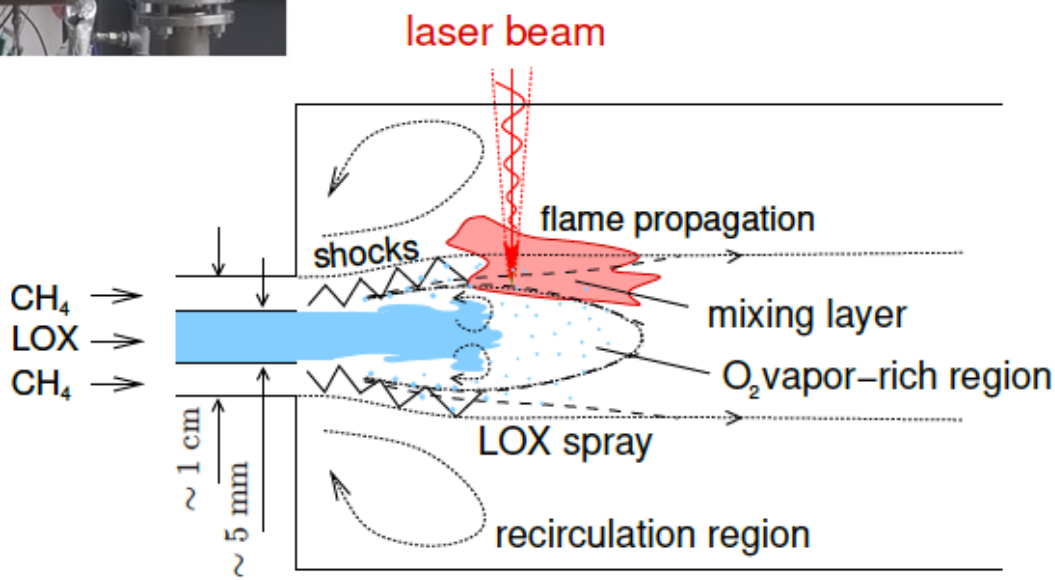
- Technology under active technological development
- Complex multi-scale multi-physics problem
- Current reliability assessment heavily experimental-based



Overarching Application

Predicting Reliability of in-Space Laser Ignition of Cryogenic Propellants





compressible fluid dynamics
low-p, low-T thermodynamics
turbulence
mixing
multiphase flow
atomization
laser energy deposition
combustion

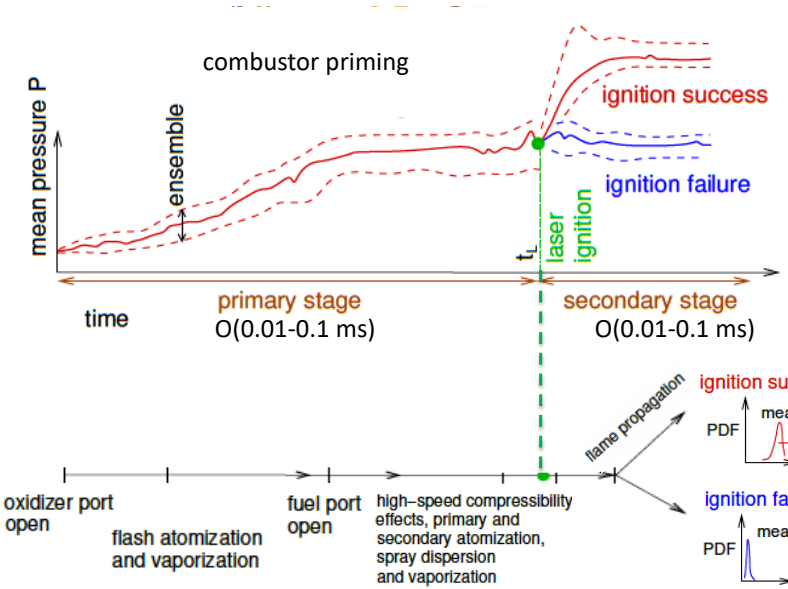
physical phenomena

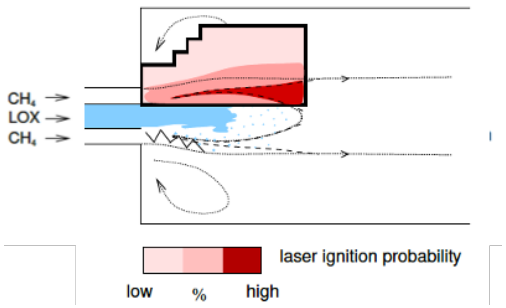
Overarching Application

Predicting Reliability of in-Space Laser Ignition of Cryogenic Propellants

construct spatial probability maps obtained from O(10^5-10^6) concurrent multifidelity samples on exascale machine

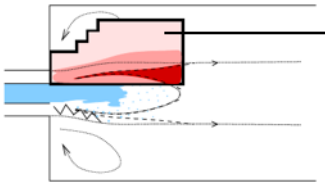
prediction goal





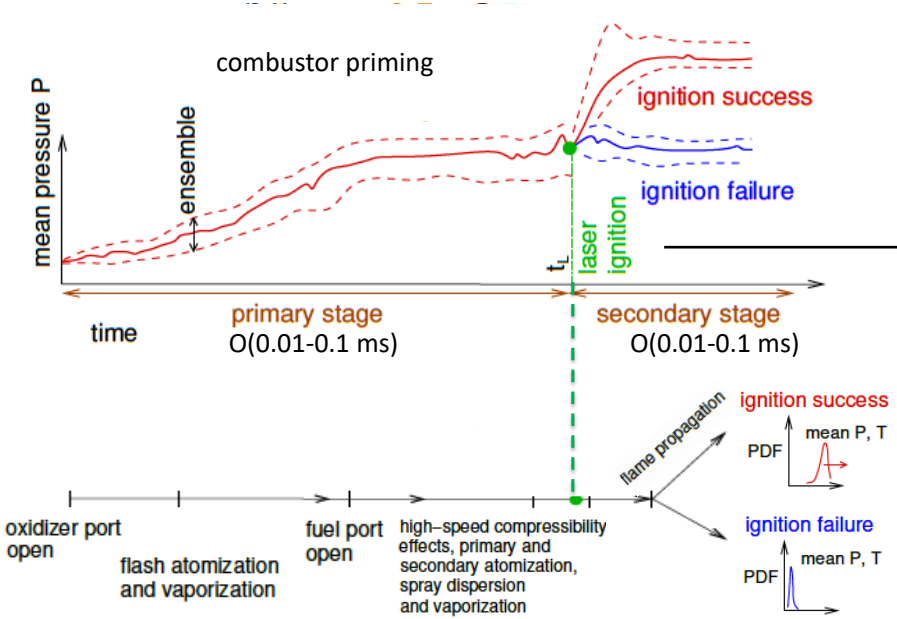
$$\int_{\rho \in U} \mathbb{I}\left[\Phi(\vec{x}, t \gg T_{ignition}) > \Phi_{critical}\right] d\rho$$

Metrics, Quantity of Interest

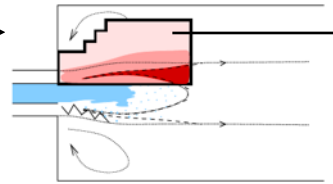


$$\int_{\rho \in U} \mathbb{I}\left[\Phi(\vec{x}, t \gg T_{ignition}) > \Phi_{critical}\right] d\rho$$

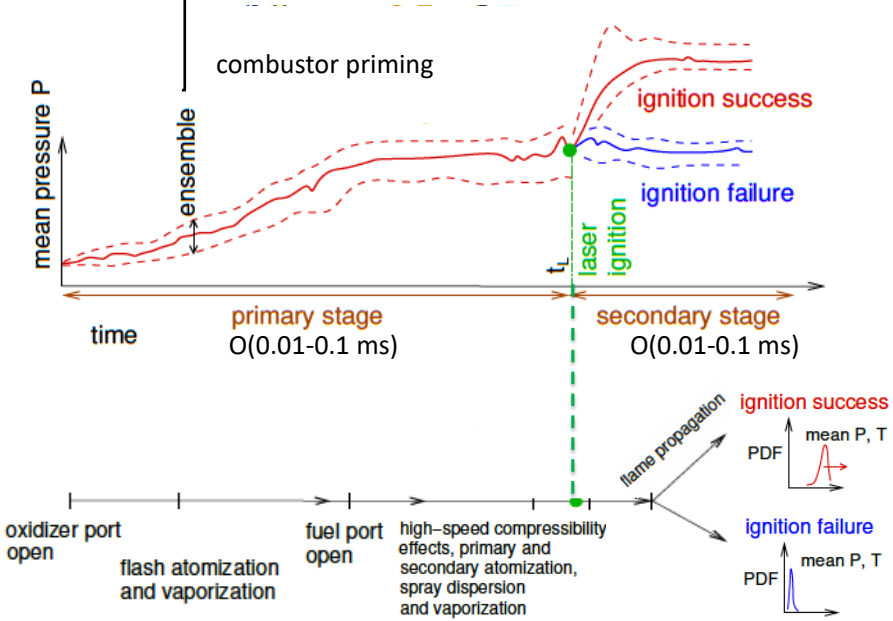
chamber pressure, temperature, etc



Uncertainties



$$\int_{\rho \in U} \mathbb{I}\left[\Phi(\vec{x}, t \gg T_{ignition}) > \Phi_{critical}\right] d\rho$$



System level (informed by experiments)

- propellant properties and conditions
- time-scale of the injection valve actuation
- timing of the ignition laser pulse
- pulse energy and spatial mode
- …

Simulation level (assumptions)

- inherent stochasticity – turbulence, mixing
- chemical modeling of energy deposition
- liquid fuel atomization, drop distribution
- ….

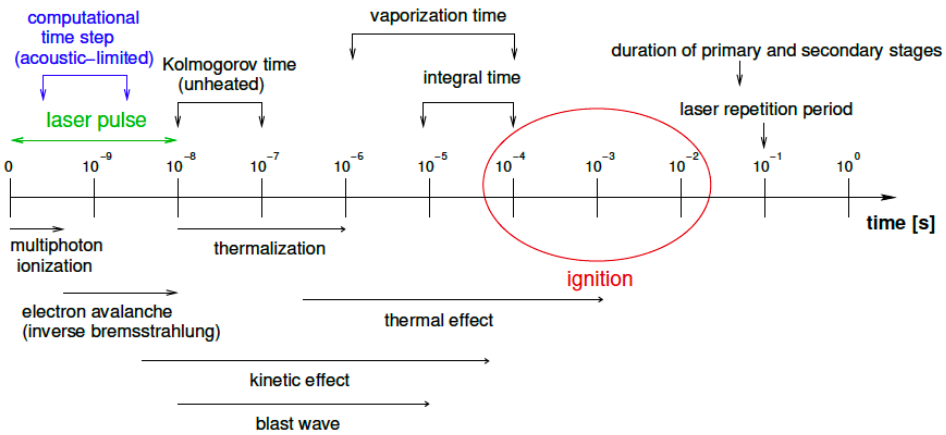
Scientific Questions

- Can we Build Reliability Maps of a Realistic Laser Ignition System in Conditions Relevant to Space Missions?

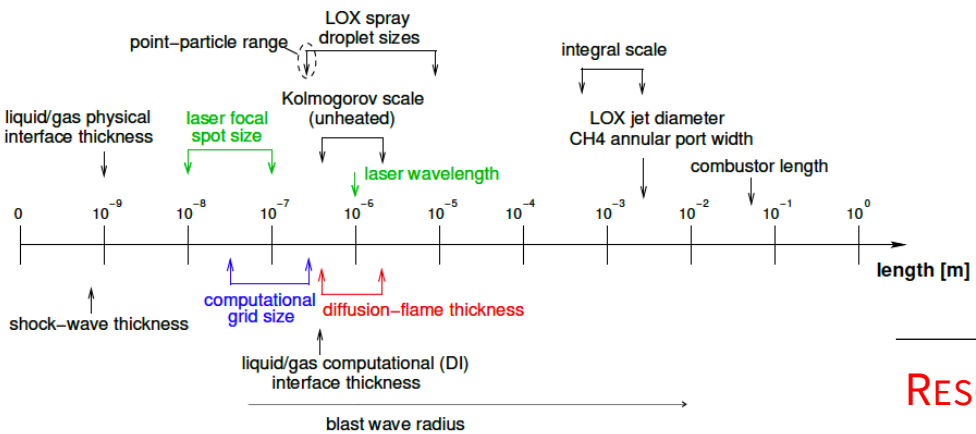
- Can we Reproduce the Failure/Success Frequency Observed in Experiments?

- Why do we observe Failure? And what are the Physics Pathways and the Driving Uncertainties?
  - Mixture is outside flammability limits (composition and temperature bounds)
  - Laser does not provide minimum ignition energy
  - Turbulence is too intense (too large strain rate)
  - Laser beam energy is scattered by interfaces and spray droplets
  - Ignition kernel develops but flame extinguishes before stabilization
  - …

Exascale-Level Computing



TIME SCALES +



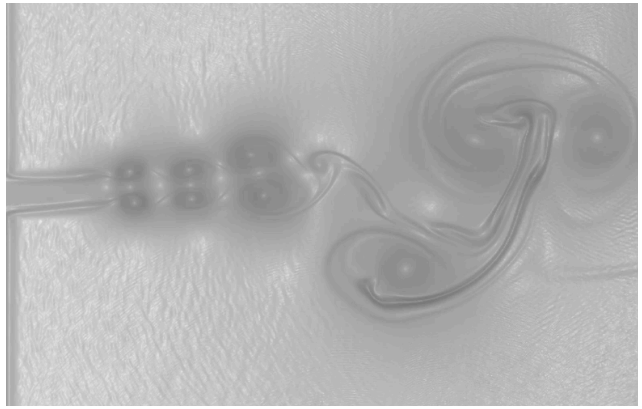
LENGTH SCALES =

RESOLUTION REQUIREMENTS....

Exascale-Level Computing

pre-6Xty

a task-based solver prototype



- Preliminary information: pre-6Xty data from 2D jet calculation
  - Momentum, energy, 4 species (reacting)
  - Total of 37×10^6 (million) degrees-of-freedom (DoF)
  - Time-step iteration requires approx. 0.3 node-seconds (Lassen machine)
  - This corresponds to a throughput of **450×10^9 (billion) (DoF x time-step)/(node x hour)**

- **Year 5 milestone: will require**
  - **complex thermophysical models**
  - **interface-capturing with mass and energy transport + Lagrangian tracking and SGS**
  - **high-fidelity ignition and reaction models**
  - **on-the-fly analysis, post-processing and data compression at scale**
  - **We assume throughput will reduce to 100×10^9 (billion) (DoF x time-step)/(node x hour),**

Exascale-Ensembles

- **Ensemble of Multi-fidelity Computations:** Efficient to perform UQ and reliability analysis
  - ensemble adaptivity and stirring
  - automatic search for low-fidelity
  - optimal scheduling on heterogenous hardware

- **Ensemble cost estimation:** multi-fidelity concurrent & coupled samples
  - A HF sample will consist of 10×10^9 (billion) DoF and 10^6 (million) time-steps
  - Assume MF ensemble composed of HFs and LFs with total cost of ~10 equivalent HFs

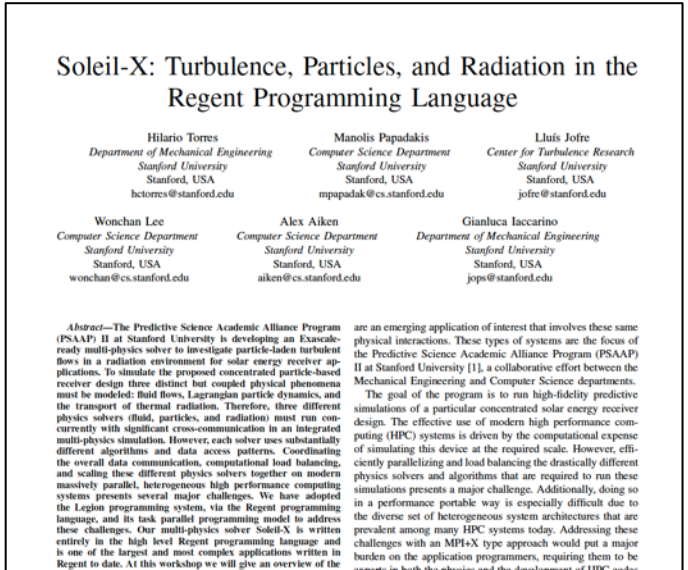
- **Y5 Calculations on an Exascale system: e.g., the upcoming Frontier-ORNL machine**
  - **Throughput calculated based on Lassen node (similar to Summit node)**
  - **Summit has 4608 nodes (GPU-accelerated)**
  - **Frontier is expected to be ~5-10x larger, resulting in ~45000 "Summit-nodes"**

  - **Using an Exascale machine (Frontier), ensemble calculation performed in ~1 day**

Our Track Record: PSAAP II Simulations

Soleil-X exposes multiple parallel levels

- Across physics modules: particle/flow/radiation
- In each physics module: i.e. domain decomposition
- Inside a subdomain: i.e. data parallelism within a tile
- Within specific algorithms: i.e. independent sweeps
- At the hardware level: GPU, CPU



Soleil-X: Turbulence, Particles, and Radiation in the Regent Programming Language

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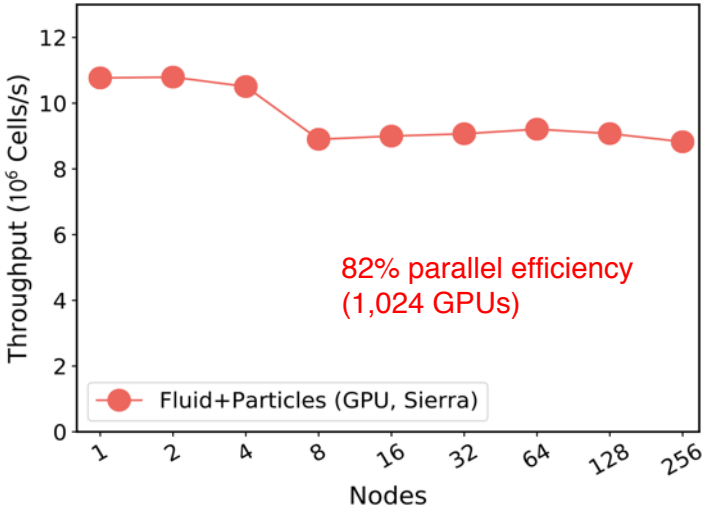
***Abstract*—The Predictive Science Academic Alliance Program (PSAAP) II at Stanford University is developing an Exascale-ready multi-physics solver to investigate particle-laden turbulent flows in a radiation environment for solar energy receiver applications. To simulate the proposed concentrated particle-based receiver design three distinct but coupled physical phenomena must be modeled: fluid flows, Lagrangian particle dynamics, and the transport of thermal radiation. Therefore, three different physics solvers (fluid, particles, and radiation) must run concurrently with significant cross-communication in an integrated multi-physics simulation. However, each solver uses substantially different algorithms and data access patterns. Coordinating the overall data communication, computational load balancing, and scaling these different physics solvers together on modern massively parallel, heterogeneous high performance computing systems presents several major challenges. We have adopted the Legion programming system, via the Regent programming language, and its task parallel programming model to address these challenges. Our multi-physics solver Soleil-X is written entirely in the high level Regent programming language and is one of the largest and most complex applications written in Regent to date. At this workshop we will give an overview of the**

are an emerging application of interest that involves these same physical interactions. These types of systems are the focus of the Predictive Science Academic Alliance Program (PSAAP) II at Stanford University [1], a collaborative effort between the Mechanical Engineering and Computer Science departments.

The goal of the program is to run high-fidelity predictive simulations of a particular concentrated solar energy receiver design. The effective use of modern high performance computing (HPC) systems is driven by the computational expense of simulating this device at the required scale. However, efficiently parallelizing and load balancing the drastically different physics solvers and algorithms that are required to run these simulations presents a major challenge. Additionally, doing so in a performance portable way is especially difficult due to the diverse set of heterogeneous system architectures that are prevalent among many HPC systems today. Addressing these challenges with an MPI+X type approach would put a major burden on the application programmers, requiring them to be

Weak Scaling (67M Cells/Node, 32M Particles/Node)



SC19
Denver, CO | hpc is now.

Stanford University

Physics, Exascale & VVUQ Integration

Integrated Simulations using Exascale Multiphysics Ensemble (INSIEME)

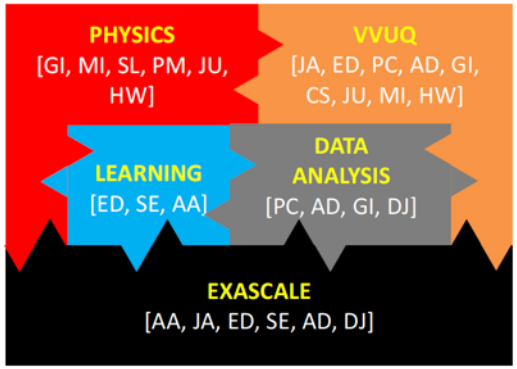
Stanford University - PSAAP III Site Visit - 10/21 & 22/2019

Integration

Predicting Reliability of in-Space Laser Ignition of Cryogenic Propellants

Heterogeneous Simulations on Exascale Architectures (INSIEME)

Multiphysics Integration
Multifidelity Ensemble
Data Management
Machine Learning
Simulation Browsing



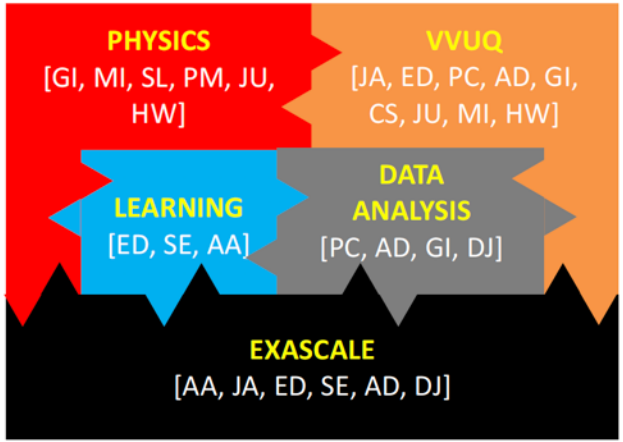
Legion Task-based Programs
Software/Hardware Mapping
Software Integration
Resilience
Portability & Performance

Integration

Heterogeneous Simulations on Exascale Architectures (INSIEME)

Development & Integration Roadmap

- Physics Fidelity: Modeling at Different (increasing) Fidelity for Critical Processes to Assess Sensitivity and Gains
- Adaptivity: consider both Physics & Numerical Modeling Adaptivity to Enable a Flexible Simulation Framework



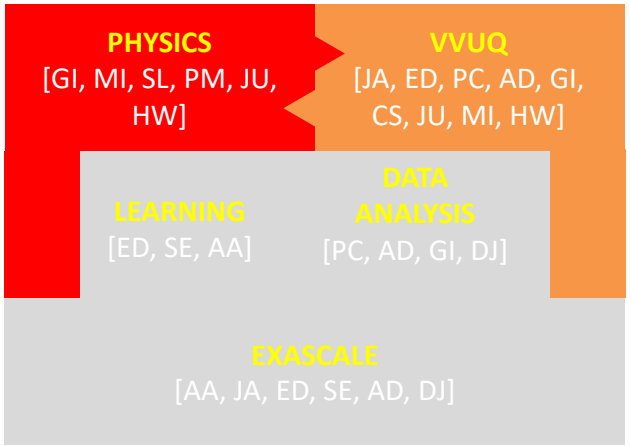
- Ensemble: Develop all the components within the Legion Tasking Environment to Ensure Interoperability
- Experimental Milestones: Designed a Logical Sequence of Experiments but Retaining Agility to Adjust Schedule based on Simulation Shortcomings

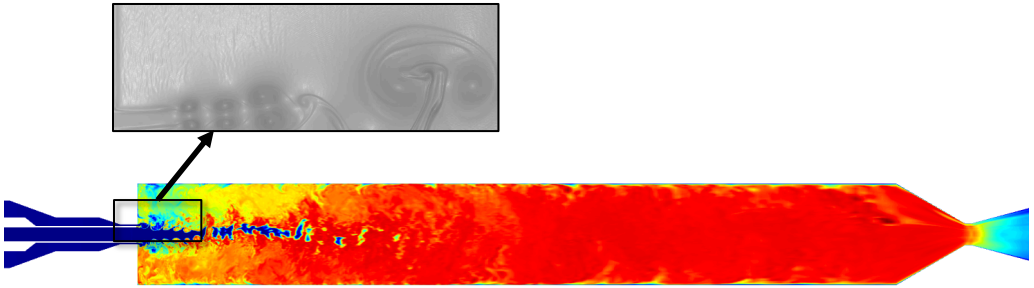
Integration

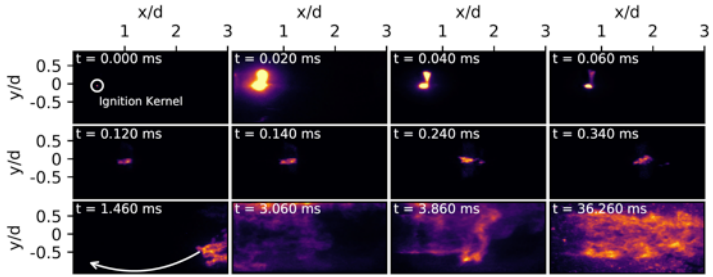
Heterogeneous Simulations on Exascale Architectures (INSIEME)

Multiphysics

- Coupled Processes
- Hierarchical Modeling
- Detailed Validation
- UQ-based Prioritization







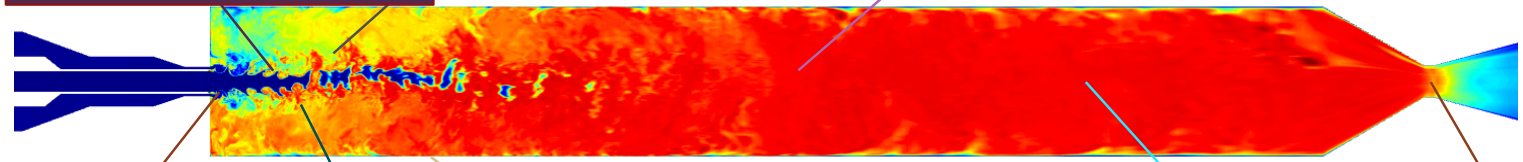
MultiPhysics

Rich & Coupled Multiphysics Environment

Multiphase flows
- Flash evaporation
- Droplet and atomization
- Subcritical and supercritical LOX injection
- Regenerative heating of LCH4 → GCH4

Ignition
- Spark ignition
- Plasma Ignition
- Pyrophoric, Hypergolic, Solid powder charges
- Ignition pop

Numerical and Modeling
- SGS and TCI for supercritical flows
- Strong density gradients
- Stabilization and solution regularization
- Properties of numerical scheme: adiabatic mixing vs. isothermal mixing
- Fully vs. quasi conservative schemes



Underexpanded Jet LOX/CH4
- Injector geometry
- Mixing of O2/CH4
- Shocks, turbulence

Thermodynamics
- Supercritical mixtures
- Mixing rules
- Response functions
- Molecular structure

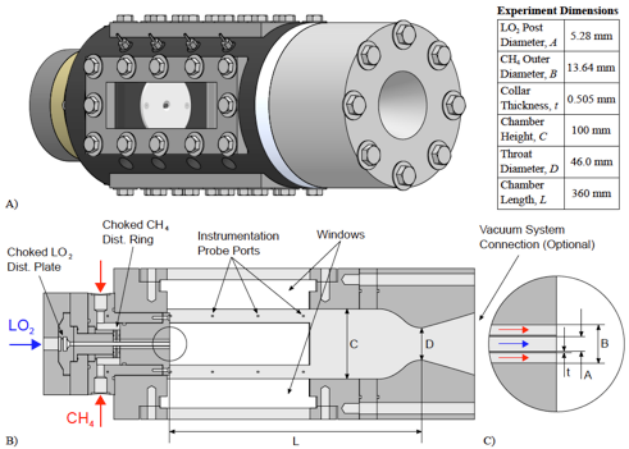
Heat transfer
- Convective heat transfer
- Flame wall/coupling
- Radiation
- Ablative heating

UQ
- **Everywhere**, but biggest factors are
- Heat-transfer
- State-equation
- Mixing rules
- Ignition probability
- Successful ignition

Nozzle exhaust
- Chocked flow
- Nozzle exhansion

Tailored Experiments for Validation

1) Develop a purpose-built experiment to enable cross-platform 'apples-to-apples' comparison with companion simulations in this PSAAP III program,



Experiment Dimensions	
LO_2 Post Diameter, A	5.28 mm
CH_4 Outer Diameter, B	13.64 mm
Collar Thickness, t	0.505 mm
Chamber Height, C	100 mm
Throat Diameter, D	46.0 mm
Chamber Length, L	360 mm

2) Complete a parametric survey of ignition probability (100s repetitions)
   - Vary key parameters: spatial location, laser pulse energy, pulse timing, and flow conditions.

3) Perform high-fidelity, measurements of the flow, flame, and plasma properties
   - Simultaneous Mie Scattering and Planar Laser-Induced Fluorescence (PLIF)
   - Simultaneous Dual-Pump Coherent anti-Stokes Raman Scattering (DP-CARS), Laser-Induced Breakdown Spectroscopy (LIBS), and Chemiluminescence Imaging.

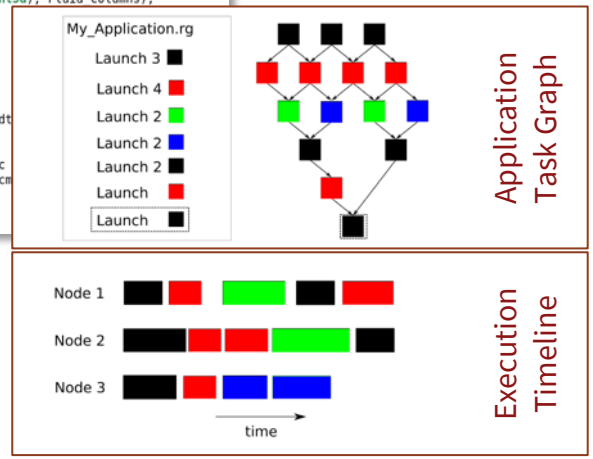
Integration

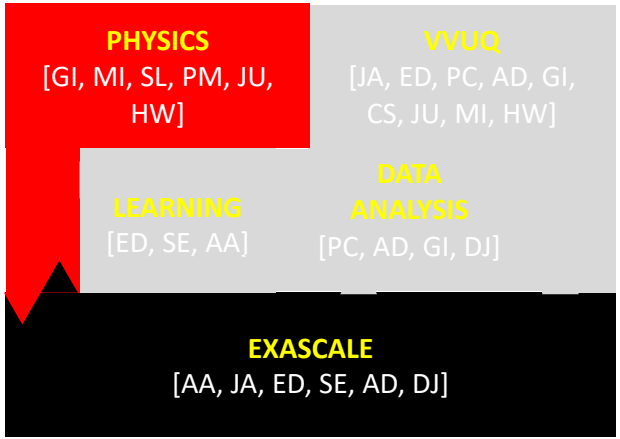
Heterogeneous Simulations on Exascale Architectures (INSIEME)

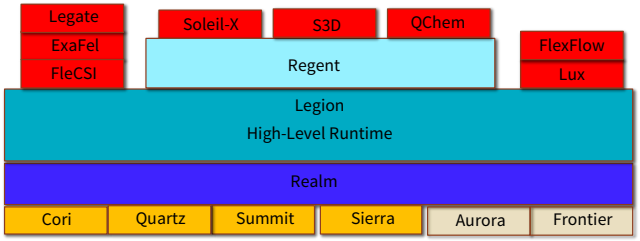
Task-Based Environment

- Legion Runtime
- Regent Programming Model
- Back-ends for Diverse Architectures

```
__demand(__parallel, __cuda, __leaf)
task UpdateUsingFluxX(Fluid : region(ispace(int3d), Fluid_columns),
                      Fluid_bounds : rect3d)
where
   reads(Fluid.{cellWidth, FluxX}),
   reads writes atomic(Fluid.Conserved_t)
do
   __demand(__openmp)
   for c in Fluid do
      var xCellWidthInv = 1.0/Fluid[c].cellWidt
      var cm1 = (c+{-1, 0, 0})%Fluid_bounds
      for i=0, nEq do
         Fluid[c].Conserved_t[i] += (((Fluid[c
                                        Fluid[cm
      end
   end
end
```







Physics solvers in Regent/Legion: how

Asks the compiler to generate a CUDA kernel

A task in pre-6Xty

Data Declaration & Permission

Tells the compiler to optimize the loop with OpenMP

Triggers the auto-parallelization (decomposition) algorithm of Regent

```
__demand(__parallel, __cuda, __leaf)
task UpdateUsingFluxX(Fluid : region(ispace(int3d), Fluid_columns),
                      Fluid_bounds : rect3d)
where
  reads(Fluid.{cellWidth, FluxX}),
  reads writes atomic(Fluid.Conserved_t)
do
  __demand(__openmp)
  for c in Fluid do
     var xCellWidthInv = 1.0/Fluid[c].cellWidth[0]
     var cm1 = (c+{-1, 0, 0})%Fluid_bounds
     for i=0, nEq do
        Fluid[c].Conserved_t[i] += (((Fluid[c  ].FluxX[i] -
                                     Fluid[cm1].FluxX[i]))*xCellWidthInv)
     end
  end
end
```

Physics solvers in Regent/Legion: why

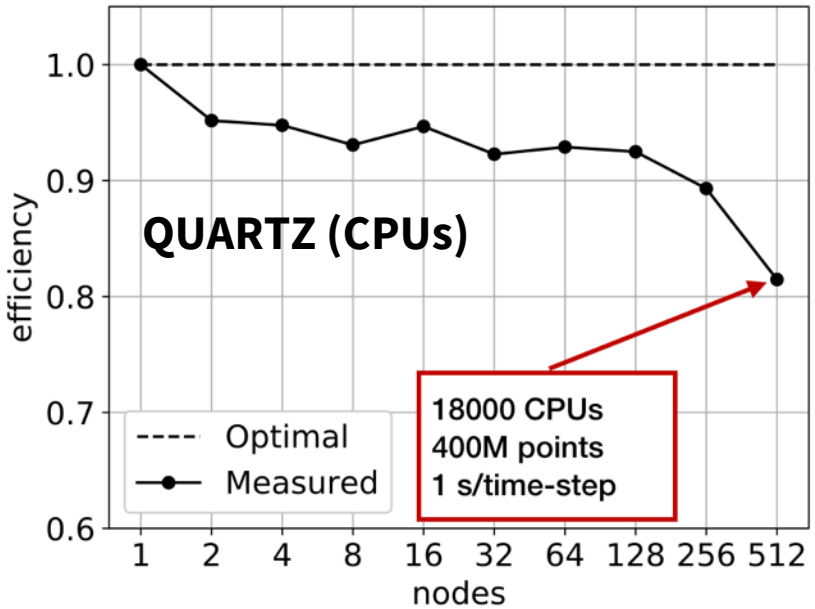
1. Mathematical and numerical formulations are separate from the execution model of the solver
   the user can optimize the performance of each task without changing the source code that define its functionality

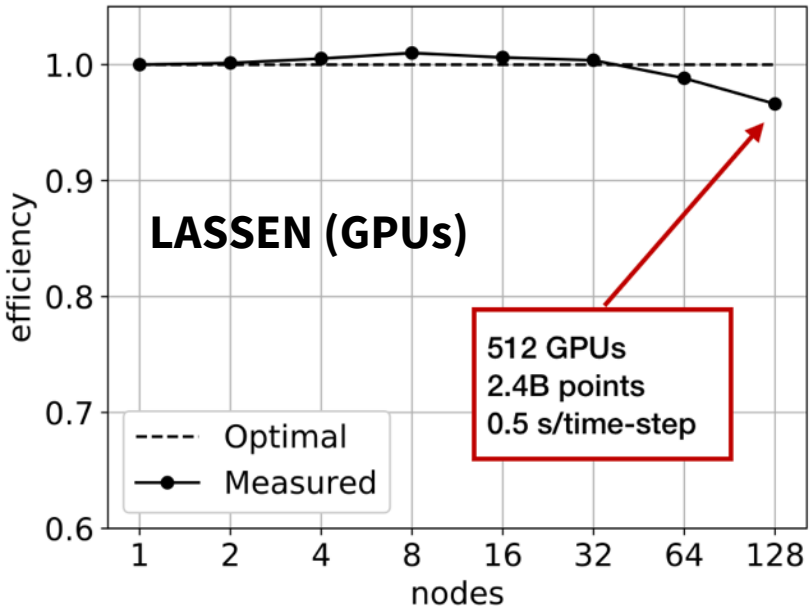
2. A single source file produces executables for completely different architectures
   avoids duplication

3. The compiler distributes the work among different nodes of the machine scheduling the required communications in order to preserve correctness:
   Multiple parallelization strategies can be easily implemented without programming the explicit communications strategy

Physics solvers in Regent/Legion: what

Pre-6Xty Weak Scaling Tests





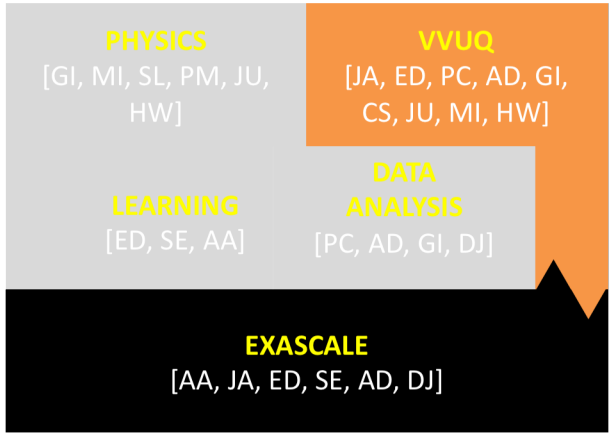
porting the solver on the two systems did not require source code changes

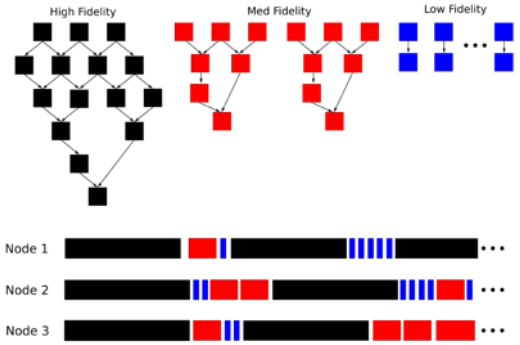
Integration

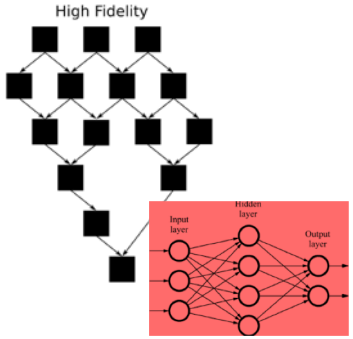
Heterogeneous Simulations on Exascale Architectures (INSIEME)

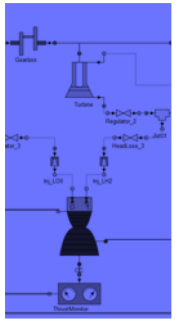
Multifidelity Ensemble in Legion

- Different Fidelity in Numerics, Physics, ML, Etc.
- Dynamic Scheduling
- Decision Making, Steering
- Start/End/Restart Samples







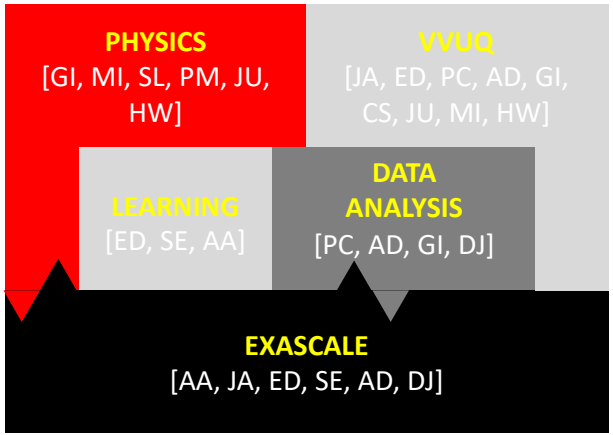


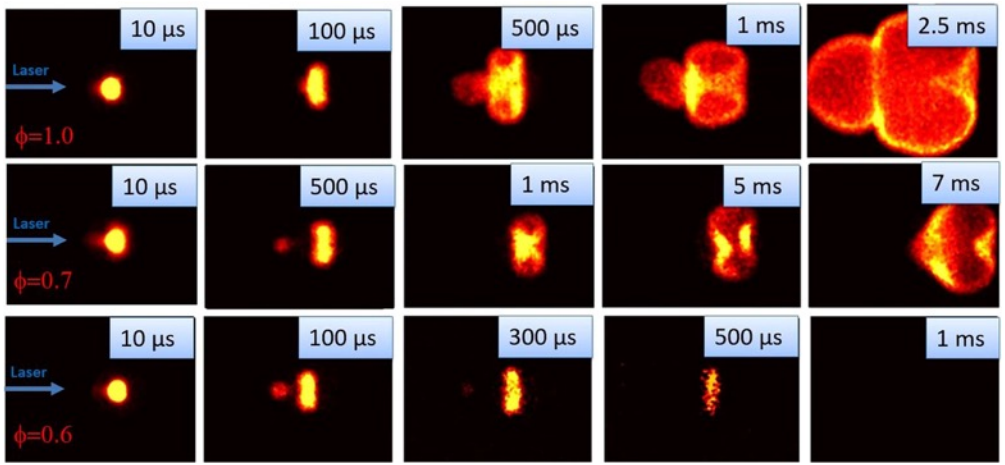
Integration

Heterogeneous Simulations on Exascale Architectures (INSIEME)

Many-World Simulation Browsing

- Exascale Exploratory Data Analysis (EDA)
- Queries for Spatial/Temporal and Parametric Analysis
- Investigate Pathways to Failure
- ….





Dumitrace et al, Scientific Reports 2017

Relevance to NNSA and the Broader Community

Physics

- Detonations
- inertial confinement
- Propulsion Technologies
- Mixing and Combustion
- Directed Energy Deposition
- Low-Pressure, Low-Temperature EOS
- Instabilities of material interfaces
- Multiphase flow and phase transition
- ….

System Engineering

- Reliability Prediction
- Multifidelity Strategies for UQ
- Exascale Exploratory Data Analysis
- …

Computer Science

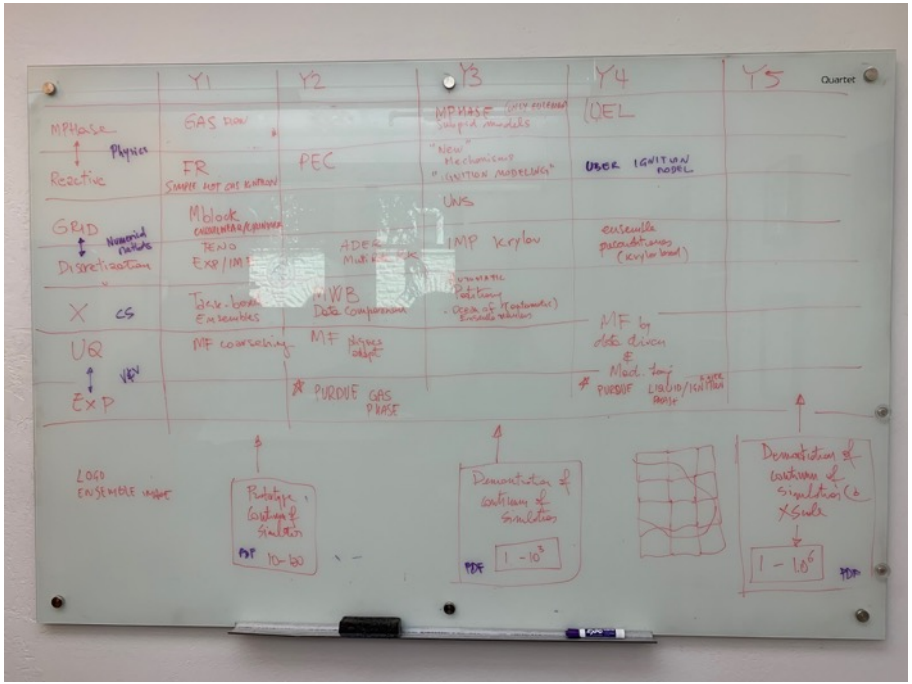
- Runtime and Programming Models for Heterogeneous Architectures
- Ensemble Simulations Management and Acceleration
- …

Roadmap & Team

Integrated Simulations using Exascale Multiphysics Ensemble (INSIEME)

Stanford University - PSAAP III Site Visit - 10/21 & 22/2019

Development and Integration Roadmap



Year 1. Involves the determination of the ignition probability under purely gaseous injection conditions for both propellants. The research effort will centered around the development and deployment of 6Xty. Finite-rate chemistry, compressibility, and a simple representation of the ignition kernel will be considered. Coarsening will be used with the goal of constructing multifidelity estimates of the ignition probability. The first prototype of task-based ensembles will manage O(10 - 100) simulations.

Year 2. Flexible time-integration strategies and adaptive combustion models will be finalized. Focus will shift to extending the liquid/gas diffuse-interface approach to include species transport and vaporization. A more comprehensive uncertainty analysis will be carried out by considering both inflow and laser characterization informed by experiments. The ensemble simulation environment in Legion will be complemented by data compression/retrieval and browser-analysis capabilities to enable the identification of system pathways to successful ignition. Experiments of the full configuration under purely gaseous injection will be completed.

Year 3. Incorporate multi-phase effects in the full-system simulations and to increase the fidelity of the ignition model. The diffuse-interface method and the subgrid-scale model for primary atomization will be deployed in 6Xty together with an updated kinetic mechanism for plasma-assisted CH4/O2 ignition at low pressures. Validation of the spray droplet size and velocity distribution will be carried out by comparing to SLIPI LIF/Mie scattering measurements. The multifidelity ensemble will be enriched by physics-based coarsening based on the adaptive combustion model and will target O(10^3 – 10^4) coordinated simulations.

Year 4. Refinements of the multi-phase model via Euler-to-Lagrange treatment of the atomization process and a detailed representation of the ignition kernel will be completed. Validation will involve OH=chemiluminescence and OH-PLIF images to detail the global and local flame kernel evolution. High-order discretization stencils, implicit time integrators, and ensemble preconditioners will be completed. Data-driven model and machine-learning strategies will be explored as elements of the multifidelity ensemble to accelerate the estimation of the ignition probability. Automatic data-partition in Regent

Year 5. The multidelity ensemble environment with O(10^5 – 10^6) members will be deployed on Frontier (or equivalent Exascale system). Detailed experimental validations of the simulations of the ignition kernel and flame propagation will be performed using simultaneous CARS and LIBS to measure the temperature and equivalence ratio at the point of initiation immediately before and after the laser ignition pulse. The laser-induced ignition probability map will be constructed from the vsimulation ensemble for a relevant spatial region of the combustor. Exascale simulations browsing and querying will be exercised to elucidate successful ignition pathways. will be deployed and demonstrated at large scale.

Roadmap and Principal Milestones

	Y1	Y2	Y3	Y4	Y5
PHYSICS/MODELING	gas-only, high-T laser kernel	adaptive combustion models	multiphase off-line ignition model	high-fidelity ignition model, tailored kinetics	-
NUMERICAL METHODS	3D, TENO schemes	adaptive time integration	unstructured grids	dynamic grid adaptivity	-
COMPUTER SCIENCE	task-based ensembles	off-line browsing, data compression extended automatic parallelization	automatic mapping, dynamic ensemble	on-line browsing, search-based parallelization	-
UQ	MF by coarsening	MF by physics adaption	MF by data-driven surrogates	MF by machine learning , autoencoders	-
EXPERIMENTS	apparatus & diagnostics setup	gas-fuel experiment	spray characterization	liquid-fuel experiment	-

gas-phase ensemble dry-run

ignition probability at selected locations
O(10-100) ensemble members

multiphase-phase ensemble dry-run

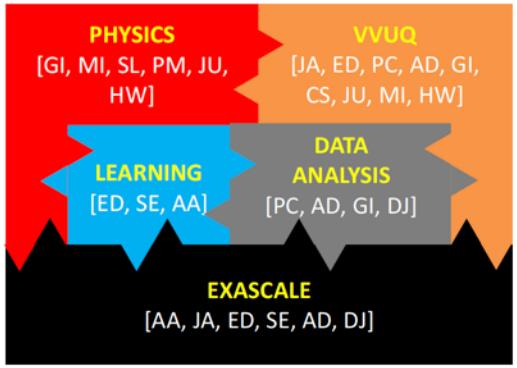
ignition probability map
$O(10^3\text{-}10^4)$ ensemble members

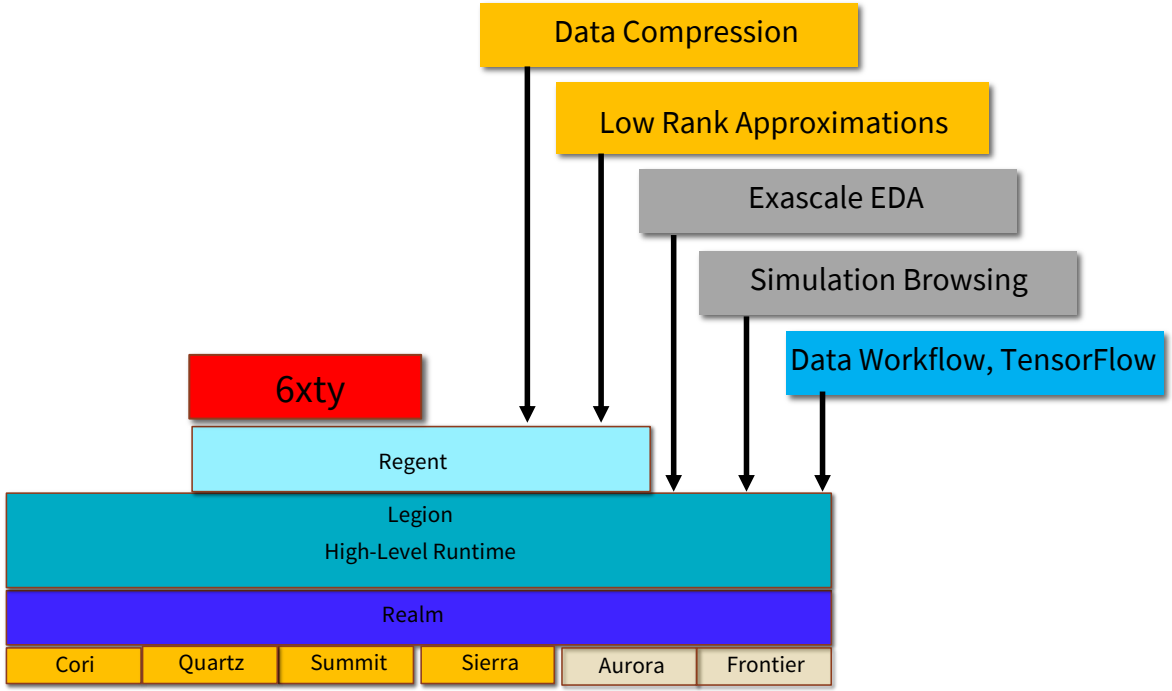
ignition probability map
$O(10^5\text{-}10^6)$ ensemble members
on full-size Frontier

Development and Integration Roadmap

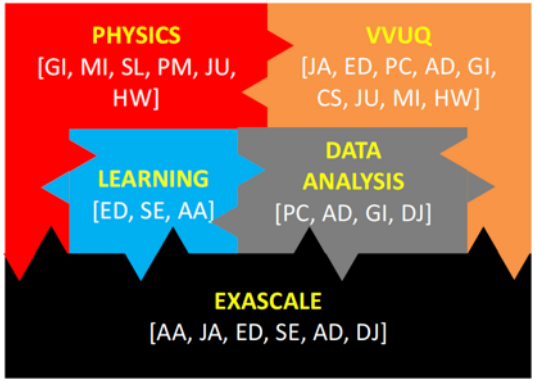
Integration Principles

- Focus Software Development on Legion/Regent from Day 1





Team



G. Iaccarino (GI): Fluid Mechanics, UQ, HPC, Numerical Methods
A. Aiken (AA): Programming Models, Resiliency, HPC
J. Alonso (JA): Compressible Flows, UQ, ROMs
E. Darve (ED): Numerical Analysis, HPC, Machine Learning,
S. Ermon (SE): Machine Learning, Stochastic Modeling
M. Ihme (MI): Combustion Modeling, HPC, Numerical Methods
D. James (DJ): Computer graphics, Reduced Order Models, Data Compression
S. Lele (SL): Compressible Multiphase Flows, Turbulence, Numerical Methods
P. Moin (PM): Turbulence, Subgrid Scale Modeling, Multiphase Flows, Numerical Analysis, HPC
J. Urzay (JU): Combustion Modeling, Multiphase Flows, Turbulence
H. Wang (HW): Chemical Kinetics Modeling, Thermodynamics, Experimental Combustion

P. Constantine (PC) UC Boulder: UQ, Statistical Analysis, Reduced Order Models
A. Doostan (AD) UC Boulder : UQ, ROMs, Data Compression

C. Slabaugh (CS) Purdue: Experiments in Reactive Flows, Diagnostics
R. Lucht (RL) Purdue: Experiments in Compressible, Reactive Flows, Diagnostics

Thank You for Your Attention

Questions?

Integrated Simulations using Exascale Multiphysics Ensemble (INSIEME)

Stanford University - PSAAP III Kick-Off Meeting – 8/18/2020