Integrated Simulations using Exascale Multiphysics Ensembles

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Caetano Melone: Verifying Functionality and Performance of HPC Applications with Continuous Integration

Shahab Mirjalili & Henry Collis: Multi-physics Modeling of Laser-induced Ignition in a Multiphase Rocket-module Combustor

Donatella Passiatore: Laser-induced Ignition of a Non-premixed CH_4/O_2 Mixture in a Rocket-module Combustor

Verifying Functionality and Performance of HPC Applications with Continuous Integration

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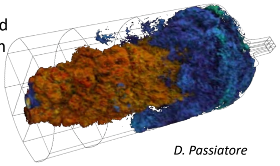
PSAAP III - INTEGRATED SIMULATIONS USING EXASCALE MULTIPHYSICS ENSEMBLES

1. Motivation and Significance

- HTR-solver: hypersonic aerothermodynamics code and primary software project of the PSAAP-III program at Stanford
- Targeting compatibility on multiple supercomputers; depends on architecture, software dependencies, and other factors
- Our role: improving developer productivity and enabling concurrent developments by automating the verification of changes and identifying performance regressions in real-time

2. Background



D. Passiatore

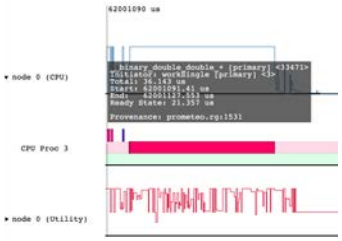
- Center Objective: Physics simulations of a laser-induced ignition in a rocket combustor, including representation of high-speed flow, turbulence, multiphase flow, combustion, and laser energy deposition
- HTR should be portable, bug-free software; helps our center achieve scientific goals
- Continuous Integration (CI) infrastructure has become commonplace in HPC environments and is leveraged to support this automated framework
- HTR dependencies: Legion, Regent, GASNet, LLVM, and CUDA/HIP

3. Implementation

GitLab

- Utilizing CI tools supported by DOE initiatives: Jacamar Runners through GitLab
- In addition to a commit-level CI, we crafted a suite of jobs that test scale, inter-node communications, and correctness on a scheduled basis
- Automated processes collect performance and functionality data during execution
- Ability to instantly reproduce the environment where a bug occurs helps to resolve issues quickly

4. Measuring Computational Performance



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Ready State: 21.357 us

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Legion Profiler

Evaluating performance is a long-term priority of our center

Resource Utilization and Code Optimization

- Setting a standard for how long it should take to execute certain problems
- This can be done by comparing HTR's results to those of another solver (e.g. S3D)
- Use profiling tools (Legion, NVIDIA Nsight) to identify bottlenecks, areas ripe for optimization, and other aspects where the code can be improved

Scaling

- When the scalability of an execution is in question, being able to point to data that disproves the influence of certain factors is consequential
    - Ex: thinking a dependency has degraded performance when it is due to other inefficiencies
- We are currently developing tooling that will collect scaling metrics along with covariates
- Can plot trends over time and notify developers when efficiency has suffered

5. Testing and Verification

Regression and Correctness Tests

- Testing the merging of features into HTR
- Solver's output vs. analytical solution
- Combination of tests complement each other (problem, numerical scheme, etc.)
- Catch issues early on by scaling to production environment
- Channel Flow, Shock Tube, Taylor-Green, etc.

Unit Tests

- Small checks for individual modules
- Isolated from the rest of the solver

Principles

- Changes to code, dependencies, and platforms can have adverse effects on functionality and correctness
- Automated testing can find issues early on with the right amount of code coverage
- Tradeoffs must be made to ensure the verification process is efficient for developers and the CI system

6. Conclusions

- CI is an integral aspect of our verification strategy
- We identify issues early so developers can focus their efforts elsewhere
- Addition of performance measurement metrics will allow us to optimize the code and determine regressions before they negatively affect users

Next steps:

- Supporting the transition to the next version of HTR by improving packaging, technical documentation, and development utilities
- Increasing the robustness of our testing strategy
- Compare HTR's performance to a state-of-the-art solver

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Multi-physics modeling of laser-induced ignition in a multiphase rocket-module combustor

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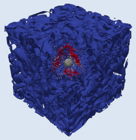
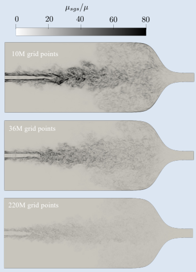
Sub-grid turbulence

- **Large Eddy Simulation** (LES) of compressible, reactive, multi-component flow
- Unresolved sub-grid scale (SGS) terms modeled with Smagorinsky model and constant turbulent Prandtl and Schmidt numbers
- Spatial discretization with **hybrid SS/ENO** type schemes



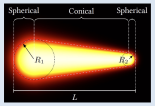
Laser ignition in HIT used as a unit test for SGS model and turbulent combustion model assessment and verification



SGS model performs correctly: contribution of eddy viscosity decreases with increased resolution

Combustion modeling

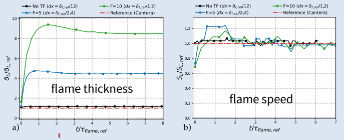
Finite-rate chemistry (12 species, FFCM[1])

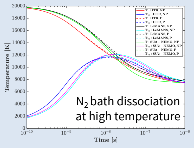


Simplified kernel representation as a **laser-equivalent heat source**[2]

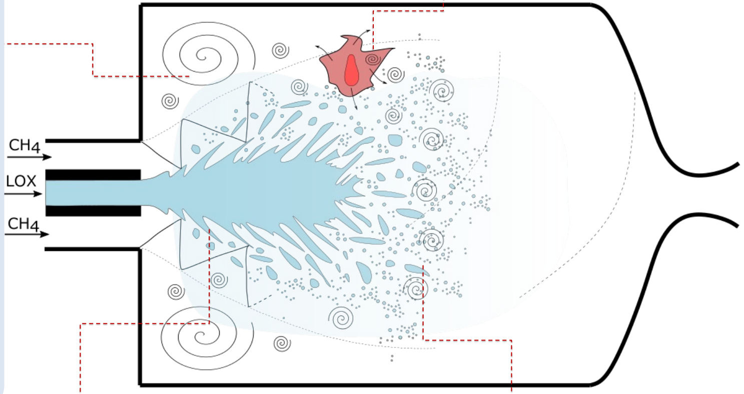
Turbulent combustion effects captured via the **thickened flame** treatment→ laminar flame speed preserved

$$D \longrightarrow \varepsilon F D$$
$$\dot{\omega}_k \longrightarrow \frac{\varepsilon}{F}\dot{\omega}_k$$



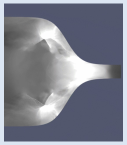


Non-equilibrium thermodynamics modeled using **two-temperature** models

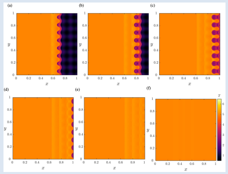


Outflow BC

- NSCBC extended to multi-physics problems (e.g. non-equilibrium thermodynamics)
- Substantially reduce reflections into the domain



Shock/entropy-wave interaction



Diffuse interface modeling for two-phase flow

- 4eqn model[3] enforces **mechanical + thermal equilibrium** → direct integration into a multi-physics setting
- Regularizing terms in diffuse interface models maintain an interface thickness on the order of the grid-size

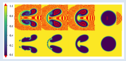
$$\frac{\partial m_l}{\partial t} + \vec{\nabla}\cdot(\vec{u}m_l) = \vec{\nabla}\cdot\vec{R}_l, \quad l = 1,2$$
$$\frac{\partial \rho\vec{u}}{\partial t} + \vec{\nabla}\cdot(\rho\vec{u}\otimes\vec{u} + p\mathbb{1}) = \vec{\nabla}\cdot(\vec{f}\otimes\vec{u})$$
$$\frac{\partial E}{\partial t} + \vec{\nabla}\cdot(\vec{u}E) + \vec{\nabla}\cdot(p\vec{u}) = \vec{\nabla}\cdot(\tau\cdot\vec{u}) + \vec{\nabla}\cdot(\lambda\nabla T) + \vec{\nabla}\cdot(\vec{f}k) + \sum_l \vec{\nabla}\cdot(\rho_l h_l \vec{a}_l)$$
$$\vec{R}_l = \rho\Gamma\left(\epsilon\vec{\nabla}\phi_l - \phi_l(1-\phi_l)\frac{\vec{\nabla}\phi_l}{|\vec{\nabla}\phi_l|}\right) \qquad \vec{f} = \sum_{l=1}^{2}\vec{R}_l \qquad \vec{a}_l = \vec{R}_l/\rho$$

diffusion + sharpening

Regularizing terms (1) are in **conservative** form (2) provide an analytical avenue for guaranteeing **bounded volume fractions** and **finite-thickness interfaces**

Shock capturing schemes + regularization → **immiscible phases** and better **boundedness**

Helium-Air, Mach 1.22



WENO5

WENO5+DI

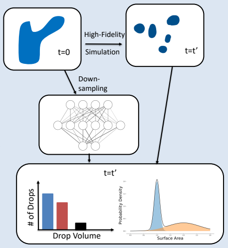
Positivity-preserving treatment extends the framework to handle **high-density ratios** and **strong shocks**

Water-Air, Mach 1.9

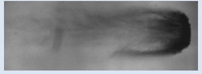
TENO6+DI

Secondary atomization and spray

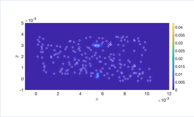
- Breakup of under-resolved drops can be modeled using **machine learning (ML)**
- Training on high-fidelity simulations of single-drop aero-breakup events
- Proof of concept studies on Taylor-Green vortices and HIT: ML model performs well in predicting (1) breakup probability (2) histogram of daughter drops (3) surface area



aero-breakup at high slip velocities leads to a very fine spray [4]



Very high velocities → violent breakup events → smaller daughter drops → more surface area → rapid evaporation → **particle tracking after breakup may be bypassed by assuming direct evaporation**



small errors in predicting vapor mass fraction in a simplified model problem

Contributors

Zoe Barbeau, Chris Cundy, Mario Di Renzo, Suhas Jain, Charlélie Laurent, Donatella Passiatore, Jonathan Wang, Christopher Williams

References

[1] Tao, Y., Smith, G. P., & Wang, H. (2018). Critical kinetic uncertainties in modeling hydrogen/carbon monoxide, methane, methanol, formaldehyde, and ethylene combustion. *Combustion and Flame*, *195*, 18-29.
[2] Wang, J. M., Panesi, M., & Freund, J. B. (2021). Thermal effects mediating the flow induced by laser-induced optical breakdown. Physical Review Fluids, 6(6), 063403.
[3] Jain, S. S., Adler, M. C., West, J. R., Mani, A., Moin, P., & Lele, S. K. (2023). Assessment of diffuse-interface methods for compressible multiphase fluid flows and elastic-plastic deformation in solids. Journal of Computational Physics, 475, 111866.
[4] Theofanous, T. G., & Li, G. J. (2008). On the physics of aerobreakup. Physics of fluids, 20(5), 052103.

PSAAP III -INTEGRATED SIMULATIONS USING EXASCALE MULTIPHYSICS ENSEMBLES

Laser-induced ignition of a non-premixed CH4/O2 mixture in a rocket-module combustor

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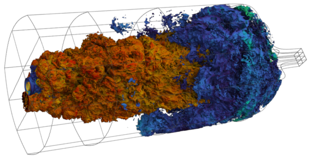
Motivation

- This work investigates the laser-ignition process and the effect of the laser target location in a rocket-module combustor
- The project goal is to build probability maps of ignition success/failure using computations and validated by experiments
- **Why probability?** Laser-induced breakdown is a stochastic process that depends on multiple parameters, including instantaneous flow-field at the time of energy deposition

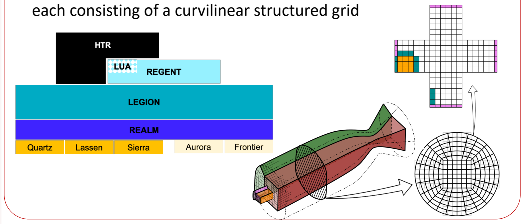


Method

- The governing equations are the compressible, multicomponent Navier-Stokes with finite rate chemistry; the laser energy deposition is modeled as a source term in the energy equation
- The numerical discretization is based on a 6th order Skew-Symmetric hybridized with ENO-type scheme
- Chemical mechanism based on [1] and the energy-deposition model based on [2]

Hypersonic Task-based Research solver

- Simulations are performed with **HTR** [3]
- HTR is a task-based parallel solver built using the Legion programming model and runtime
- Targets distributed systems w/ CPUs and GPUs
- It can handle computational domains composed of multiple blocks each consisting of a curvilinear structured grid

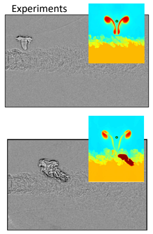


Results

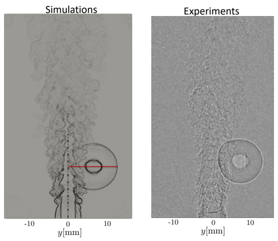
Verifications/Validation

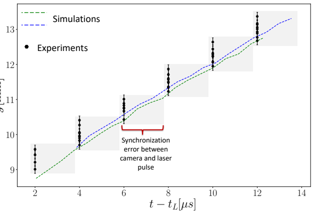
- Verification studies (not reported) have been carried out using multiple test problems
- Validation studies (right) focused on experimental data generated at Purdue propulsion lab
- Simulations (confirmed by experiments) indicate that laser-induced ejection of hot gases is critical for ignition success
- The velocity of the laser-induced shock is also validation against experiments

Laser induced ejection



Laser generated shock



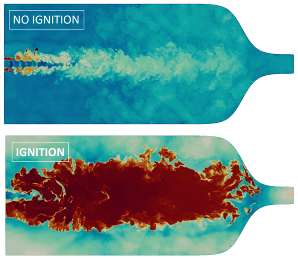


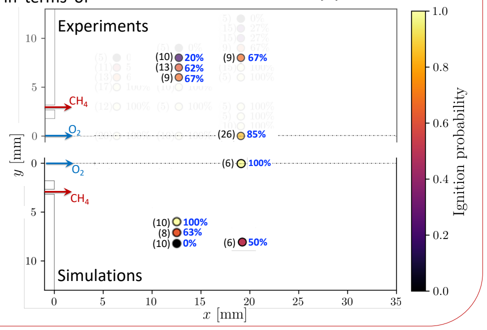
Ignition Probability Map

For each laser target location, an ensemble simulations are performed, by varying:

- laser geometrical parameters
- instantaneous turbulent flow field.

The output of the simulations is reported in terms of fraction of successful ignition





Conclusions & ongoing work

- Simulations show good agreement in selected locations of laser target, but some differences remain
- Detailed validation of the energy deposition and uncertainty quantification studies are currently ongoing
- Additionally, we are investigating the effect of refining numerical and physical modeling
- Next year's plan is to initiate simulations of a configuration with liquid oxygen

[1] Smith, G. P., Tao, Y., & Wang, H. (2018). Critical kinetic uncertainties in modeling hydrogen/carbon monoxide, methane, methanol, formaldehyde, and ethylene combustion. *Combustion and Flame*
[2] Wang, Buchta, & Freund (2020). Hydrodynamic ejection caused by laser-induced optical breakdown. *Journal of Fluid Mechanics*
[3] Di Renzo, Fu & Urzay (2020). HTR solver: An open-source exascale-oriented task-based multi-GPU high-order code for hypersonic aerothermodynamics. *Computer Physics communications*