DNS of Turbulent Combustion in Complex Flows

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DNS of Flame Propagation and Structure Behind a Backwards Facing Step

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Motivation

Gain insights into:
- Flame stabilization mechanism
- Effect of heat release
- Turbulence-chemistry interactions

Experiments PIV, PLIF (UVa, GWU, NASA)
S3D - multiblock

Multiblock construction

Weak scaling on Titan

48³ grid points per core

Sample from 2D simulation

With IBM

Immersed boundary
Backward-facing step

**Mechanism:** 22 species non-stiff reduced ethylene-air (Lu et al. 2012)

**Transport model:** mixture averaged

**Turbulent inflow profile:** feed data generated from a separate 3D DNS of channel

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**Inflow**

Ethylene-air  
$\Phi = 0.42$  
$U = 200$ m/s  
$u' = 10\%$  
$T = 1125$ K

**Isothermal wall**  
$T_{\text{wall}} = 600$ K

**Outflow**

<table>
<thead>
<tr>
<th><strong>Parameter</strong></th>
<th><strong>Value</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>$H$</td>
<td>1.47 cm</td>
</tr>
<tr>
<td>$D$</td>
<td>0.3048 cm</td>
</tr>
<tr>
<td>$Re_H$</td>
<td>35000</td>
</tr>
<tr>
<td>$Re_T$</td>
<td>788</td>
</tr>
<tr>
<td>Grid count</td>
<td>2.6 billion</td>
</tr>
<tr>
<td>CPU hrs</td>
<td>25 million</td>
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</tbody>
</table>

**Periodic channel**

**Inflow profile sampling**
Results

Vorticity magnitude

Heat release rate
Vorticity dynamics

- Enstrophy present dominantly on product side

Iso-line of Heat release rate
Vorticity dynamics
Flame stabilization

Reaction rate OH

Significant consumption

Flux OH - x

Flux OH - y
- Flame structure varies with distance from the step
- Flame-flame interaction present due to the shear
- Incomplete oxidation
Flame structure

Temperature (K)

Heat release rate

Enstrophy

Y CO
Summary

- DNS of C2H4/air flame stabilization behind a backwards facing step
- Strong interaction between recirculation zone, shear layer, and flame brush
- Radicals from the recirculation zone assist in anchoring the flame
- Turbulence generation migrates towards products downstream of the stabilization point
- Implications for modifications to flame structure and heat losses to the wall
Direct Numerical Simulation of flame stabilization assisted by auto-ignition at reheat conditions

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Staged gas turbine combustion

- Originally developed by ABB for high efficiency, load flexibility and low emissions
- Recently improved and simplified (reduced cost) for the H-class GT36
- First (premix) combustion stage based on flame propagation
- Second (sequential) combustion stage based on auto-ignition
• Adjusting firing temperature of 1st stage allows control of $t_{\text{ign}}$ in 2nd stage
Staged gas turbine combustion

Hydrogen fuel
- Flashback in 1st stage
- Early auto-ignition in 2nd stage

- 2nd stage is mainly auto-ignition stabilized
- 2nd stage inlet temperature needs to be decreased and not 2nd stage flame temperature
Hydrogen fuel

- Flashback in 1st stage
- Early auto-ignition in 2nd stage

- 2nd stage is mainly auto-ignition stabilized
- 2nd stage inlet temperature needs to be decreased and not 2nd stage flame temperature
- 1st stage de-rating is compensated by shifting fuel to 2nd stage
Reheat burner

DNS of idealized reheat burner configuration from Ansaldo Energia

Operating conditions:
- Inlet temperature: $\sim 1100 \text{ K}$
- Pressure: $\sim 20 \text{ atm}$

Scaled conditions:
- Mean inlet temperature:
- Pressure: 1 atm
- Fuel: hydrogen

Objective:
- Understand the flame stabilization
- Identify the modes of combustion
- Quantify the role of auto ignition
S3D - Multiblock

- Mildly complex geometry enabled by multi-block DNS capability
- Construct geometries by assembling several cuboidal blocks (like Lego)
- Compressible formulation (J. H. Chen et al., CSD 2009)
- Spatial derivatives: 8th order CD schemes & 10th order filter
- Time integration: 4th order Runge-Kutta
- Mixture averaged transport model

Weak scaling on Titan

![Graph showing weak scaling on Titan](image)

- Code scales well on hundreds of thousands of processors
Simulation details

- **Chemical mechanism**: 9 species hydrogen-air (Li et al., 2004)
- **Inflow composition**: premixed H$_2$ + O$_2$ + N$_2$ + H$_2$O ($\phi = 0.35$)
- **$U_{bulk}$**: 200m/s, $u' = 20$ m/s, $T_{inlet} = 1100$K, $T_{wall} = 750$K
- **Inflow profile**: feed from DNS of a fully developed channel flow

1.25 billion grid points
20 million CPU hours
$Re_b = 13000$
Two combustion configurations are observed:

- Design state: mainly auto-ignition in the combustion chamber
- Intermittent auto-ignition state: ignition in mixing section
Design combustion state

Heat release rate

Combustion modes:
- Autoignition along centerline
- Flame propagation near corners
- $\text{HO}_2$: indicative of chain branching
Transport budget analysis

\[
\frac{\partial (\rho Y_{OH})}{\partial t} = -\nabla_\beta \cdot (\rho Y_{OH} \mathbf{u}_\beta) - \nabla_\beta \cdot (\rho Y_{OH} \mathbf{v}_{\beta,OH}) + W_{OH} \dot{\omega}_{OH}
\]

Advection  Diffusion  Reaction

- Auto-ignition: balance between advection and reaction
- Flame propagation: balance between diffusion and reaction

![Graphs showing auto-ignition and flame propagation]
Chemical Explosive Mode Analysis

- $\alpha = \phi_s / \phi_\omega$: ratio of the projected non-chemical source term and the projected chemical source term (C. Xu et al., PROCI 2018)

Three modes are identified:
- **Assisted-ignition ($\alpha > 1$)**: diffusion significantly promotes reaction
- **Auto-ignition ($-1 < \alpha < 1$)**: chemistry plays a dominant role
- **Extinction zone ($\alpha < -1$)**: diffusion dominates chemistry and suppresses ignition
Intermittent auto-ignition state

Heat release rate

- Early auto-ignition in the mixing section

Temperature

- Ignition kernel advects downstream

Mass fraction of $HO_2$

- Occurs intermittently
Intermittent auto-ignition state

- Local rise in pressure
- Increases local temperature by 20-30 K
- High reactivity of hydrogen
- Decrease in ignition delay time (30%)
Conclusions

• Performed DNS of a reheat burner at scaled conditions
• Two states of hydrogen/air combustion have been observed:
  • design state: flame propagation and auto-ignition in the combustor
  • intermittent auto-ignition in mixing section
• Premature auto-ignition arises due to pressure (and following temperature) rise in mixing section
• Quantified the contribution of different modes towards heat release using chemically explosive mode analysis (CEMA)
• Future work:
  • characterize the unstable flame behavior and the conditions leading to it
  • find the inlet conditions for statistically stationary reheat flame
  • perform 2D and 3D simulations with varying fuel composition and its stratification
ECP has formulated a holistic approach that uses co-design and integration to achieve capable exascale

<table>
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<tr>
<th>Application Development</th>
<th>Software Technology</th>
<th>Hardware Technology</th>
<th>Exascale Systems</th>
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<tr>
<td>Science and mission applications</td>
<td>Scalable and productive software stack</td>
<td>Hardware technology elements</td>
<td>Integrated exascale supercomputers</td>
</tr>
</tbody>
</table>

ECP’s work encompasses applications, system software, hardware technologies and architectures, and workforce development

From Paul Messina’s ASCAC talk April 19, 2017

30 Exascale Computing Project, www.exascaleproject.org
ECP application: Transforming Combustion Science and Technology Through Exascale Simulation (Pele)

Effects of reactivity stratification at:
- high pressure
- high turbulence
- fuel blends

on:
- ignition delay
- combustion rates
- emissions

Pele: Block-structured adaptive mesh refinement, multi-physics: spray, soot, and radiation, real gas, complex geometry

Automated Mechanism Generation

S3D: multi-block compressible reacting DNS multi-physics validation: spray, soot, radiation
The Pele Project

Transforming Combustion Science and Technology with Exascale Simulations

- Use exascale platforms to solve first of exascale-era combustion problems
- Anchored in basic research needs: requirements driven by gas phase chemical kinetics research questions
  - turbulence chemistry interaction in conditions motivated by IC engine research
  - provide a path for development of scalable design codes suitable for exascale hardware
Challenge Problem - Motivation

Advanced combustion regimes (LTC)

PCCI/HCCI – load limitations
Requires precise charge preparation and combustion control mechanisms
(for auto-ignition and combustion timing)
## High Fidelity DNS and Hybrid DNS/LES of RCCI Diesel Combustion

### Characteristic / Need

<table>
<thead>
<tr>
<th>Characteristic / Need</th>
<th>Approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>Impulsively started jets with disparate scales between fronts and turbulence.</td>
<td>Dynamic adaptive mesh refinement</td>
</tr>
<tr>
<td>(Outer scales: 10cm, ms</td>
<td></td>
</tr>
<tr>
<td>Inner timescales: microns, ns)</td>
<td></td>
</tr>
<tr>
<td>High speed injection followed by subsonic conditions downstream</td>
<td>Compressible and low-Mach capabilities</td>
</tr>
<tr>
<td>Long time horizons to set up turbulence for studying fundamental TCI</td>
<td>Hybrid DNS/LES [Non-reacting LES, DNS for flame]</td>
</tr>
<tr>
<td>Lean, rich, and low temperature chemistry critical in multi-stage ignition and</td>
<td>Accurate and detailed thermochemistry.</td>
</tr>
<tr>
<td>formation of soot precursors.</td>
<td></td>
</tr>
<tr>
<td>Liquid fuel injection</td>
<td>Lagrangian spray model</td>
</tr>
<tr>
<td>Coupling between mixture preparation and emissions</td>
<td>Detailed kinetics including emissions, sectional model for soot with</td>
</tr>
<tr>
<td></td>
<td>radiation</td>
</tr>
<tr>
<td>Mixture preparation dependent on re-entrainment of combustion products</td>
<td>Realistic piston dish and cylinder wall geometry</td>
</tr>
</tbody>
</table>

**Performant on exascale architecture**
Design Philosophy, Strategy

• The Pele suite:
  – Compressible (PeleC) and low Mach number (PeleLM) integrators, compatible design, data, I/O, etc
  – Shared physics (ideal/real gas kinetics, thermodynamics, transport, sprays, etc) - PelePhysics
  – Block-structured adaptive mesh refinement, built on AMReX framework
  – Robust, accurate, extensible finite-volume (conservative) discretizations
  – Embedded boundary treatment of arbitrary geometries
    • Enables CAD-to-compute, avoids expensive, time-consuming difficult mesh generation step
  – AMReX-supported X+Y parallelism (inter-node X and intra-node Y)
  – Parallel mesh and particle data, specialized to needs of AMR (temporal subcycling, etc), plus Fork-Join type temporary redistribution strategies, high-performance I/O and in-situ/in-transit analysis support
  – Combustion-specific agile code generation: Fuego+SINGE for GPU-optimized CUDA kinetics evaluation, Kokkos-based kernels for particle/fluid coupling terms
• Agile development framework, open source modular design, continuous integration/testing
• Close interaction with AMReX for new capabilities in development
  – App-relevant GPU/A21 implementation of AMReX structures/algorithms
  – Leverage AMReX multi-app development
Pele Code Design Overview

• Baseline algorithm design for multicomponent flow with stiff reactions, AMR
  – **PeleC**: Comparable advection, diffusion time scales, motivates IMEX-type scheme based on Spectral Deferred Corrections (SDC) with *time-implicit* chemistry
    • Robust highly efficient time-explicit Godunov-type upwind advection, simple centered diffusion
    • BDF-style implicit chemistry ODE integration, with sources that approximate the other processes
  – **PeleLM**: acoustics filtered away analytically, but still want robust, time-explicit advection
    • Chemistry *and* diffusion are now *time-implicit* – *iterative timestep* simultaneously incorporates flow constraint (constant pressure), mutually coupled species/energy diffusion and chemistry. Entire system evolved stably on slower advection time scales across AMR grid hierarchy
• SDC-based iterative timestep – treats each process essentially independently, with accelerated iteration to couple everything nicely together
• Robust baseline allows stable, well-behaved *extensible* time step
  – Switch 2nd order advection scheme with more accurate 4th order algorithm
  – Option for “destiffened” chemistry model that allows highly efficient time-explicit advance
  – Robust to other, potentially stiff, tightly coupled processes, such as sprays, radiation, soot, etc
## Project Roadmap

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<tr>
<th></th>
<th>2017</th>
<th>2018</th>
<th>2019</th>
<th>2020</th>
<th>2021</th>
<th>2022</th>
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</thead>
<tbody>
<tr>
<td><strong>Model Development</strong></td>
<td>Hybrid LES/DNS</td>
<td>Deep learning SGS model training methodology</td>
<td>Rare event detection</td>
<td>In situ training</td>
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<tr>
<td><strong>Compressible Capabilities</strong></td>
<td>Non-ideal, single level sprays, static EB geometry</td>
<td>Non-reacting LES, AMR sprays</td>
<td>Hybrid LES/DNS</td>
<td>Soot</td>
<td>Radiation</td>
<td>Moving EB geometry</td>
</tr>
<tr>
<td><strong>Capability Towards Challenge Problem</strong></td>
<td><img src="image1.png" alt="Image" /></td>
<td><img src="image2.png" alt="Image" /></td>
<td><img src="image3.png" alt="Image" /></td>
<td><img src="image4.png" alt="Image" /></td>
<td><img src="image5.png" alt="Image" /></td>
<td><img src="image6.png" alt="Image" /></td>
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<td></td>
<td>60 Bar open, gas phase dodecane low mach jet</td>
<td>Atmospheric pressure, compressible static geometry flows</td>
<td>60 Bar open, ideal gas dodecane low mach jet wall impingement</td>
<td>60 Bar open, dodecane jet with hybrid multi-physics</td>
<td>60 Bar compressible + low Mach, re-entrainment</td>
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<tr>
<td><strong>Low Mach Capabilities</strong></td>
<td></td>
<td>Static EB geometry</td>
<td>Sprays, Hybrid LES/DNS</td>
<td>Hybrid compressible / LM</td>
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<tr>
<td><strong>Automated Thermochem</strong></td>
<td>Initial demonstration</td>
<td>Pressure independent kinetics</td>
<td>Mechanism generation</td>
<td>Reduced dual-fuel mechanism</td>
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</tr>
<tr>
<td><strong>Performance and software</strong></td>
<td>PeleC Exists</td>
<td>PeleLM tiling</td>
<td>GPU performance Multi-physics load balancing</td>
<td>Performance portability</td>
<td></td>
<td>A21 / Frontier Performance Enhancements</td>
</tr>
</tbody>
</table>

*Non-ideal EOS*
DNS of Ndodecane Multi-injection Jet at diesel conditions - Parameters

- N-dodecane/air injection with $Y_{NC12H26} = 0.45$, 446K
- Jet: $D=0.17\text{mm}$, $U=30\text{m/s}$, $Re=15,000$
- Environment: 60 bar, 900K, 15/85% O2/N2 (‘spray A’)
- 10 micron resolution
- 53 species mechanism
  - Age variable tracks the fluid age/residence time

Diffusion coefficient based on $Le=1$ for all add. scalars

$$\frac{\partial \rho a}{\partial t} + \frac{\partial \rho u_j a}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial a}{\partial x_j} \right) + \rho$$
Reactor studies – standard conditions (‘spray A’)

Fuel side: NC12H26/air @Z=0.45 & 446K, oxidizer: 15%O2 900K, 60atm

Low T ign.: 0.05ms, Z<0.02

High T ign.: 0.25ms, Z=0.057 (~1.24 Zst)

ΔτHT,LT=0.2ms
Reactor studies – oxidizer consists of lean products (Z=0.01)

Fuel side: NC12H26/air @Z=0.45, oxidizer: equilibrated NC12H26/air @Z=0.01, 60atm

Low T ign.: 0.05ms, Z=0.12
High T ign.: 0.2ms, Z=0.042 (~0.91 Z_{st})

\[ \Delta t_{HT,LT} = 0.15 \text{ms} \]
Reactor studies – oxidizer consists of lean products (Z=0.025)

Fuel side: NC12H26/air @Z=0.45, oxidizer: equilibrated NC12H26/air @Z=0.025, 60 atm

- Low T ign.: 0.03ms, Z=0.2
- High T ign.: <0.01ms, Z<0.02 (<~0.44 Z_{\text{st}})

\[ \Delta T_{HT,LT} < 0 \text{ ms} \]
Comparison at 0.4ms after pilot/main injection start

\[ Z_{\text{pilot}}, Z_{\text{main}} \]

0.4ms after pilot start
0.4ms after main start

Pilot: 0.26ms, dwell: 0.17ms, main: 0.74ms
left: times w.r.t pilot start (0.4ms total time), right: times w.r.t. main start (0.83ms total time)
Comparison at 0.4ms after pilot/main injection start

$Z_{pilot}, Z_{main}$

$Y_{H_2O_2}$
Comparison at 0.4ms after pilot/main injection start

\[ Z_{\text{pilot}}, Z_{\text{main}} \]

\[ Y_{\text{OH}} \]
Difference in pilot and main ignition - temperature

Pilot: 0.26ms, dwell: 0.17ms, main: 0.74ms; left: times w.r.t. pilot start, right: times w.r.t. main start

- Stoich. conditions close to homogeneous ign.
- Difference for rich cond.

Main:
- Significant differences on rich side
Difference in pilot and main ignition – OC12H23OOH

Pilot: 0.26ms, dwell: 0.17ms, main: 0.74ms; left: times w.r.t pilot start, right: times w.r.t. main start