DIRECT NUMERICAL SIMULATION OF TURBULENCE-CHEMISTRY INTERACTIONS: FUNDAMENTAL SCIENCE TOWARDS PREDICTIVE MODELS

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Accelerating Computational Science Symposium 2012
March 29-30, 2012
Washington D.C.

Computing allocations from DOE INCITE and ALCC grants at NCCS/ORNL and NERSC

Office of Science
U.S. Department of Energy

Acknowledgments

Contributions from:

Ray Grout, Hemanth Kolla, Edward Richardson, Andrea Gruber, Chun Sang Yoo, Ramanan Sankaran, Tianfeng Lu

Sponsors:

DOE Basic Energy Sciences Division of Chemical Sciences, Geosciences and Biosciences, Combustion Energy Frontier Research Center, Advanced Scientific Computing Research Office

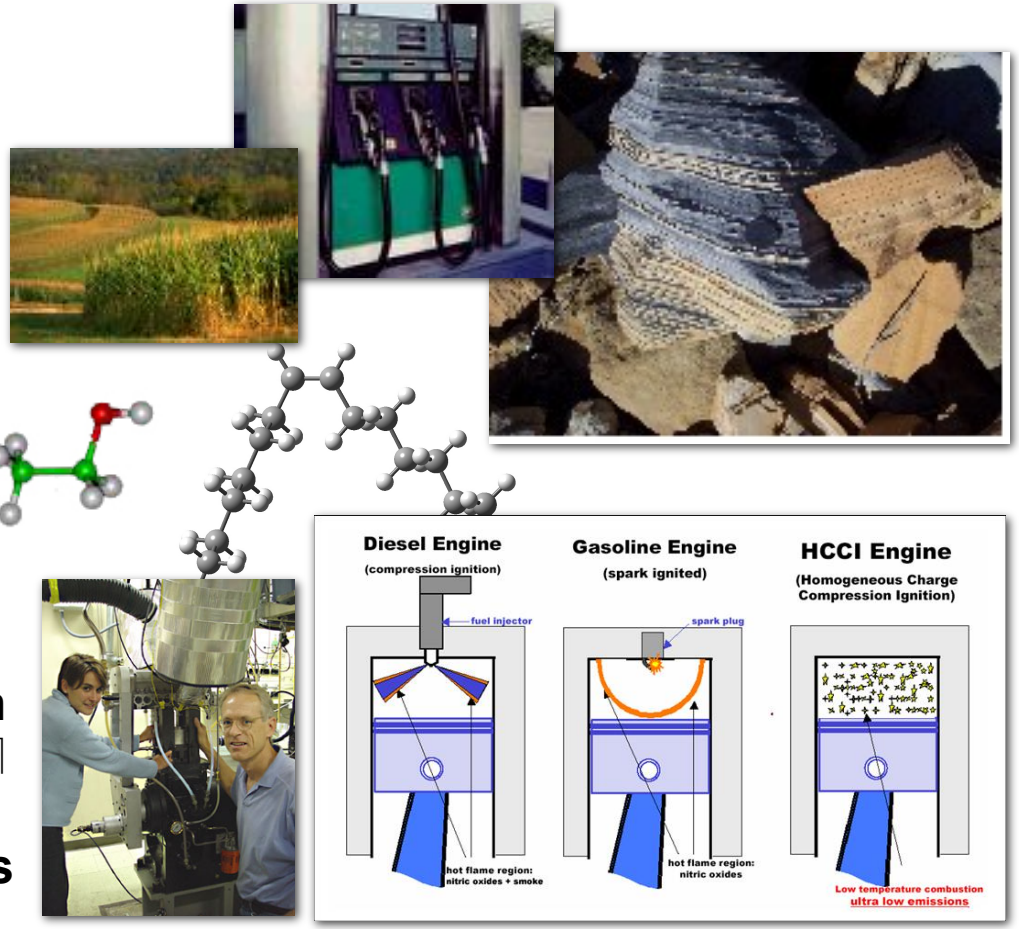
Why combustion? Energy security, climate change, economic competetiveness

- Combustion of fossil fuels accounts for 83% of energy used in U.S.
- Transportation alone accounts for 2/3 of petroleum usage and ¼ of CO_2 emissions
- National goals to reduce petroleum usage by 25% by 2020 and greenhouse gas emissions by 80% by 2050
- Concurrently new fuels are evolving
- Meeting these goals requires new generation of high efficiency, low emissions combustion systems using diverse future fuel sources
- New scientific understanding to develop predictive, validated multi-scale models to shorten product design cycle

Potential for improvement in thermal efficiency by 25%→50%

Motivation: Changing World of Fuels and Engines

- **Fuel streams are rapidly evolving**
  - **Heavy hydrocarbons**
    - ✓ **Oil sands**
    - ✓ **Oil shale**
    - ✓ **Coal**
  - **New renewable fuel sources**
    - ✓ **Ethanol**
    - ✓ **Biodiesel**
- **New engine technologies**
  - **Direct Injection (DI**
  - **Homogeneous Charge Compression Ignition (HCCI**
  - **Low-temperature combustion**
- **New mixed modes of combustion (dilute, high-pressure, low-temp.)**
- **Sound scientific understanding is necessary to develop predictive, validated multi-scale models!**

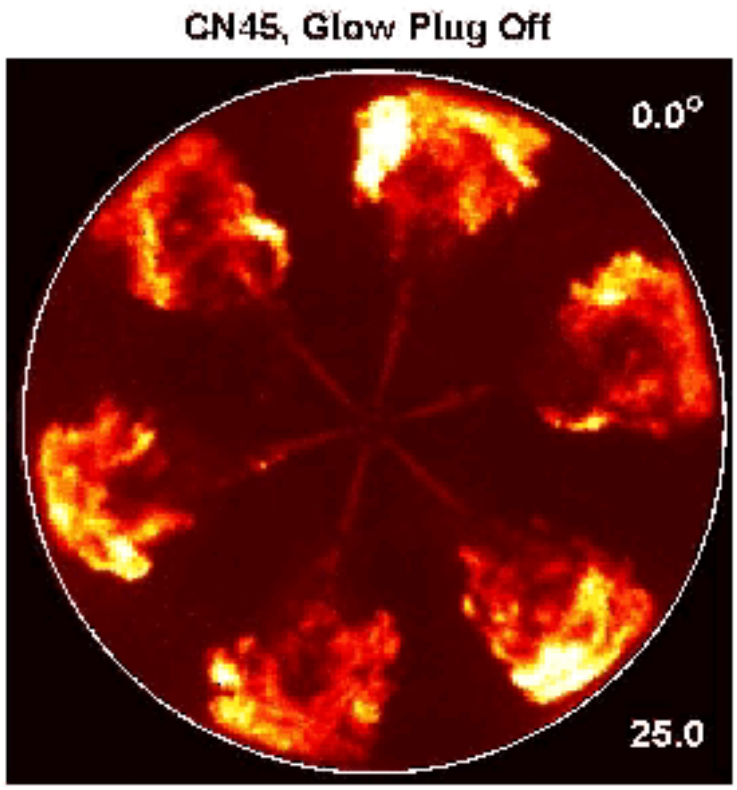


Tailoring fuels to engine design

- *Hundreds* of molecules have been proposed as alternative fuels many from biology.
  - How to assess which are worth pursuing? Not practical to run them all in comprehensive engine tests
  - Full engine experimental campaigns would require manufacturing large amount of each proposed new fuel and fuel blend…
- Many new engine designs in development, not clear which engine to use to test future fuels.
  - Experimentally building/testing each new engine is expensive and slow; fuel-in-engine experiments are relativey expensive and unreliable
  - Fuel needs to work over broad range (T, P, Composition)
  - Hard to experimentally test over the whole range of conditions
- Ability to *predict* behavior of new fuels at many conditions, and in proposed engine designs, would be extremely valuable!

Anecdote from Professor Bill Green, MIT

IC Engine Combustion Is A Complex, Multi-physics, Multi-scale Problem



Diesel Engine Autoignition, Soot Incandescence
Chuck Mueller, Sandia National Laboratories

Stiffness : wide range of length and time scales

- In-cylinder geometry (cm)
- Turbulence-chemistry (mm)
- Soot inception (nanometer)

Chemical complexity

- large number of species and reactions (100's of species, thousands of reactions)

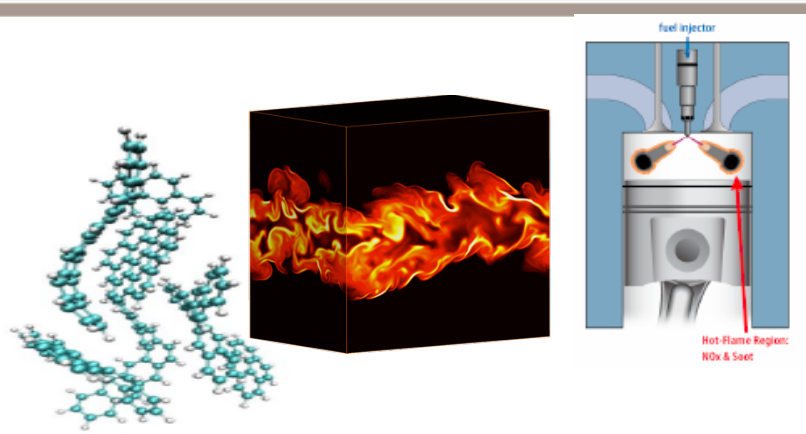
Multi-Physics complexity

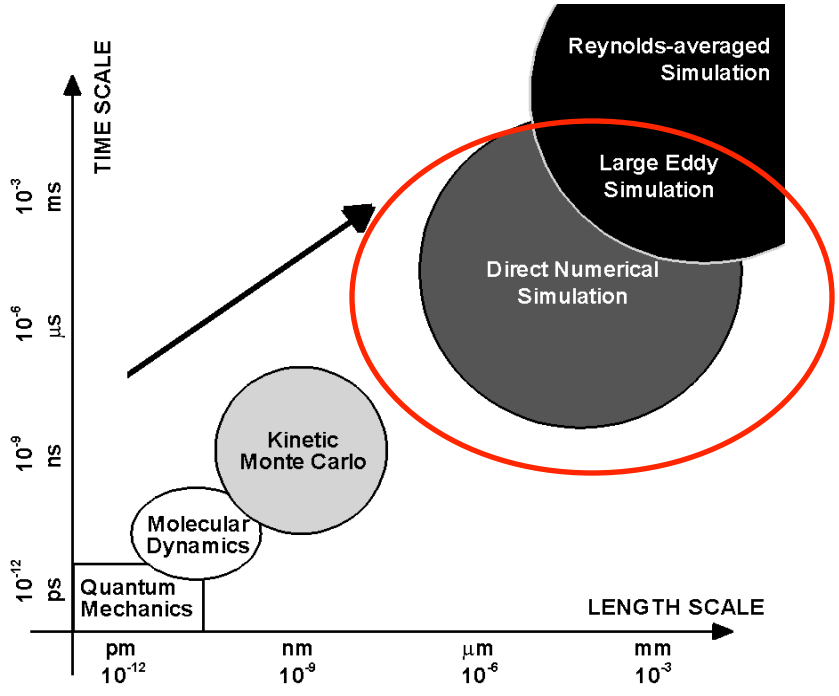
- multiphase (liquid spray, gas phase, soot, surface)
- thermal radiation
- acoustics ...

- All these are tightly coupled

Multi-scale Modeling of Combustion Processes

- Multi-scale modeling describes combustion processes, from quantum scales up to device-level, continuum scales
- Multi-scale Strategy:
  - Use petascale computing power to perform direct simulation at the atomistic and fine-continuum scales (~4 decades), and develop new parameterizations that will enable bootstrapping information upscale

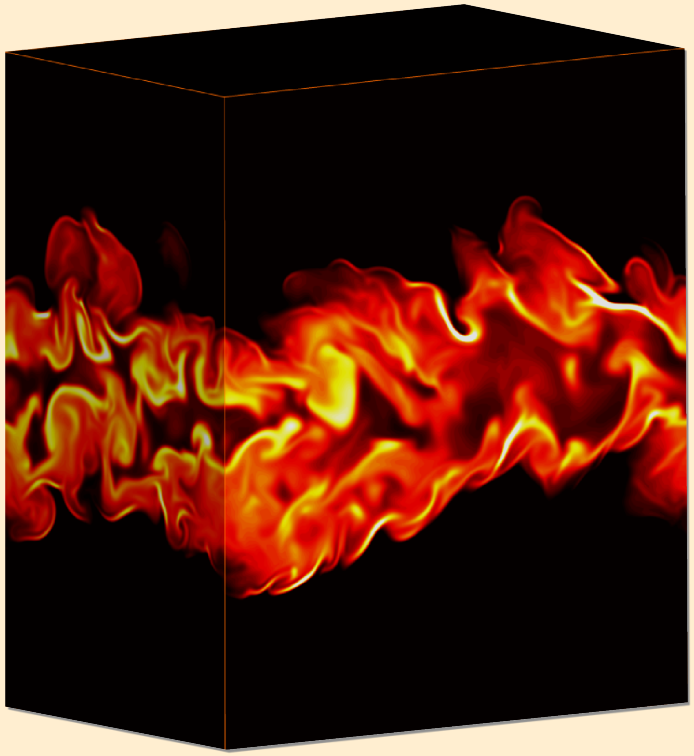




Direct Numerical Simulation (DNS) – Sandia S3D

- Used to perform first-principles-based DNS of reacting flows
- Solves compressible reacting Navier-Stokes equations
- High-fidelity numerical methods
- Detailed reaction kinetics and molecular transport models
- Multi-physics: sprays, radiation and soot
- Ported to all major platforms, scales well on petascale machines
- Particle tracking cabability

DNS ⟷ *Physical models* ⟷ *Engineering CFD codes (RANS, LES)*



DNS provides unique fundamental insight into the chemistry-turbulence interaction

Chemistry-Turbulence Interactions

- Turbulence entrains, advects, strains and wrinkles a flame creating more area for burning
- Through turbulence cascade eventually reactants are molecularly mixed
- Chemical reactions are enhanced with mixing to a limit – extinction - and create heat release
- Heat release, dilatation reduce turbulence intensity through density, and property changes
- Need Capability computing: $N_{grids} = Re^{9/4}$

Role of DNS

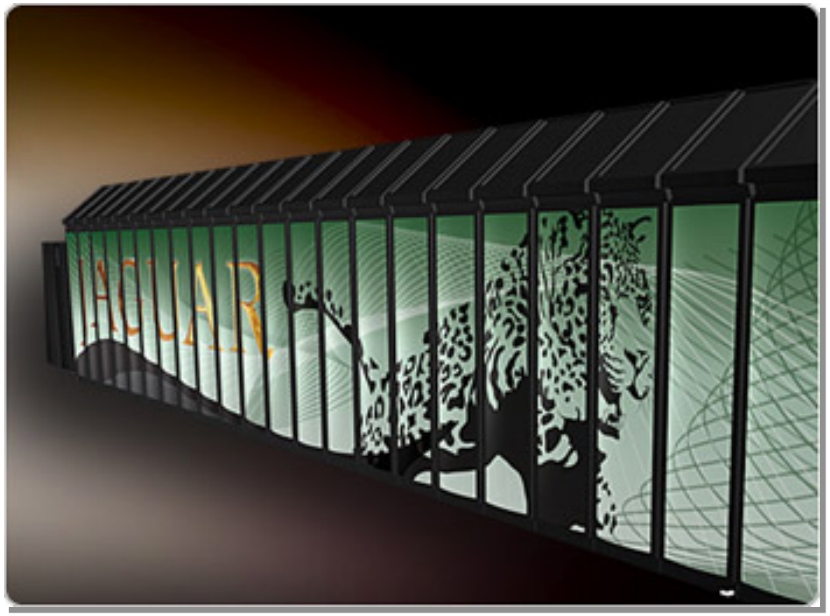
- Glean fundamental insight into ‘turbulence-chemistry’ interactions in canonical configurations relevant to transportation and power generation
- Validation data for development of RANS and LES subgrid mixing and combustion models used in engineering CFD
- Validation of chemical mechanisms over relevant aero thermochemical conditions (wide range of T, P, compositions)

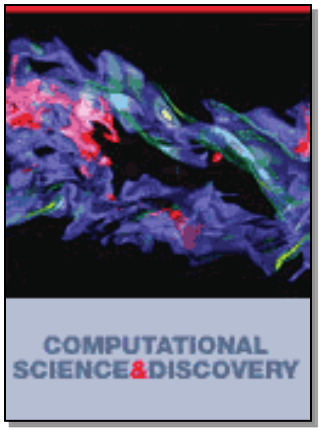
Combustion DNS Enabled by Large Computer Allocations

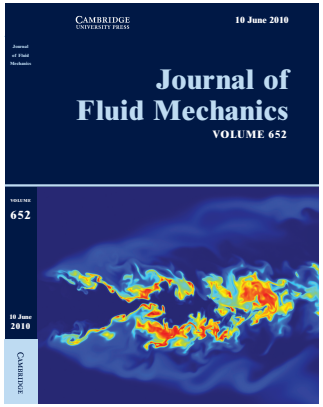
Office of Science U.S. DEPARTMENT OF ENERGY

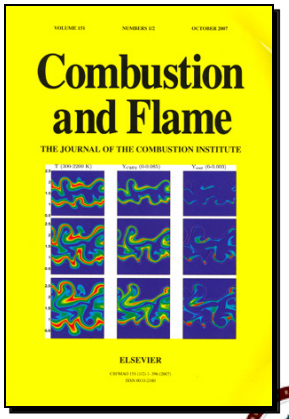
INCITE

Advancing America's Science and Industrial Competitiveness









Preparing for the Future: Hybrid Multi-Core Architectures (Titan 10-20 Pflop)

OLCF-3 Application Readiness:
Ray Grout (NREL), John Levesque (Cray), Ramanan Sankaran (ORNL), Cliff Woolley and Stan Posey (nVidia) refactored S3D in preparation for 10-20 Pflop multi-core hybrid architectures like Titan

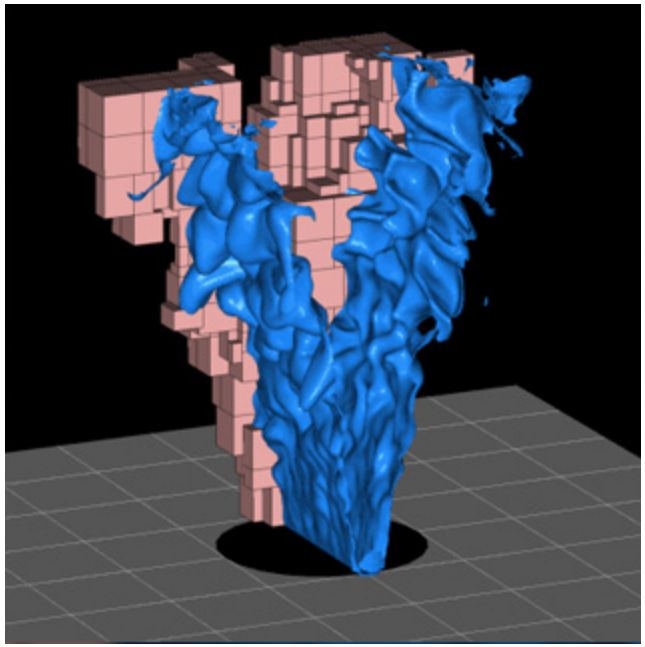
Stay tuned for Ray's talk!

Exascale Combustion Co-Design Center

CENTER FOR EXASCALE SIMULATION
ExaCT
OF COMBUSTION IN TURBULENCE

Through co-design combustion science requirements influence computer architecture design and technology constraints inform design of algorithms and software

- Compressible and low-Mach high-order adaptive mesh refinement
- In situ uncertainty quantification (adjoint sensitivities and polynomial chaos expansion)
- In situ topological analytics and visualization



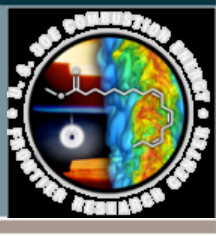
Role of DNS – Case Studies

- Homogeneous Charge Compression Ignition (HCCI) Combustion
- Turbulent Jet Flames in Heated Co-Flow
- Turbulent Jet Flames in Cross-Flow

Role of DNS – Case Studies

- **Homogeneous Charge Compression Ignition (HCCI) Combustion**
- Turbulent Jet Flames in Heated Co-Flow
- Turbulent Jet Flames in Cross-Flow

DNS of Autoignition in Stratified Di-Methyl Ether (DME)/Air Turbulent Mixtures

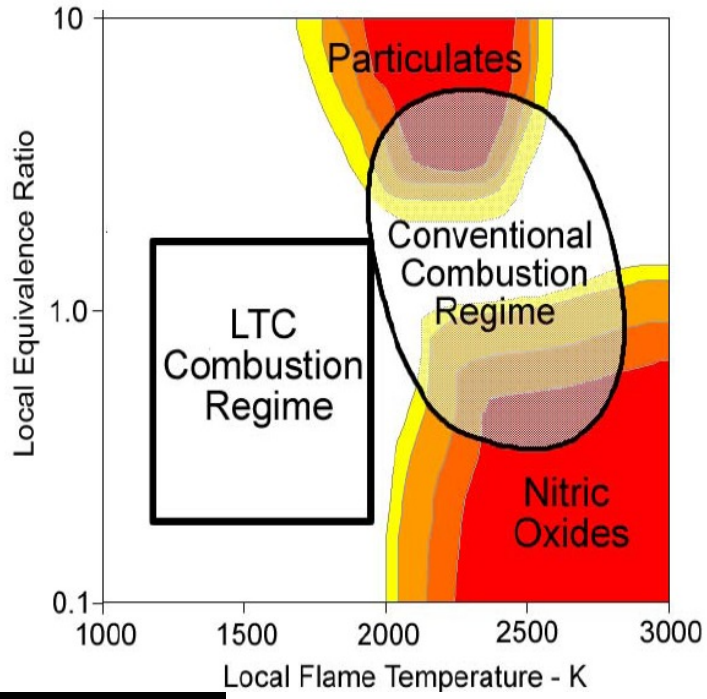


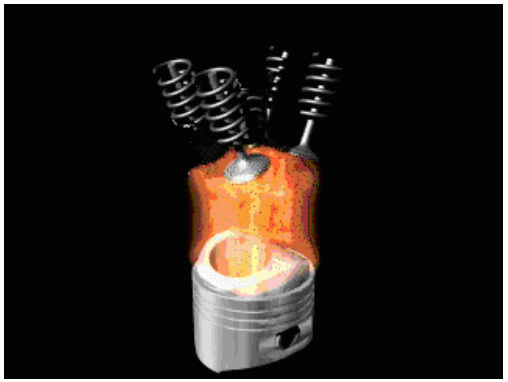
Gaurav Bansal and Jackie Chen
Combustion Research Facility
Sandia National Laboratories, USA

Tianfeng Lu & Zhaoyu Luo
University of Connecticut, USA

Numerical Combustion Meeting, Corfu Greece, 2011
In prep. for Combust. Flame, 2012

Homogeneous Charge Compression Ignition (HCCI) Engines

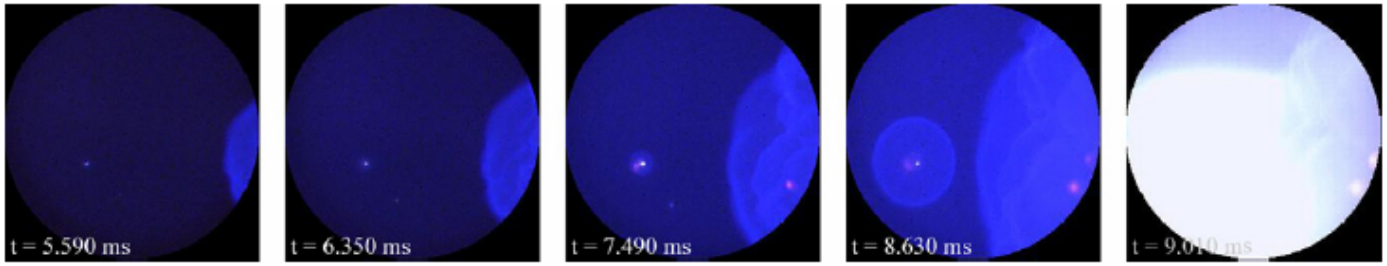




- Potential for high diesel-like efficiencies but low soot and NO_x emissions
- Fuel-lean and at low temperatures – no flame, spontaneous autoignition
- Hard to control ignition timing, sensitive to fuel chemistry, need to moderate burn rate (high load)
- Better understand ignition chemistry of fuel blends and oxygenated hydrocarbon molecules in biomass derived fuels

Optimum combined fuel chemistry and mixing to moderate the rate of combustion in HCCI engines

- Inhomogeneities (thermal or composition) lead to sequential ignition front propagation down a temperature gradient - combustion modes ranging from homogeneous explosion to propagating flames
- New modes operate far from equilibrium with highly transient intermittent ignition occurring at multiple sites
- Low pre-ignition temperatures, strong finite-rate kinetic effects due to competition between mixing and chemistry
- Strong sensitivities to fuel chemistry and mixing provide multiple control options (e.g. combustion retard, multiple fuel injection)
- Better understand and predict behavior of alternative fuels in HCCI engines



Optical engine experiments by Walton et al. show front-like propagation

Mixture inhomogeneities reduce peak heat release rates and pressure rise rates – hot spots preferred ignition spots – deflagration waves or spontaneous ignition?

DNS of DME HCCI Autoignition

Turbulence and scalars initialized using an energy spectrum

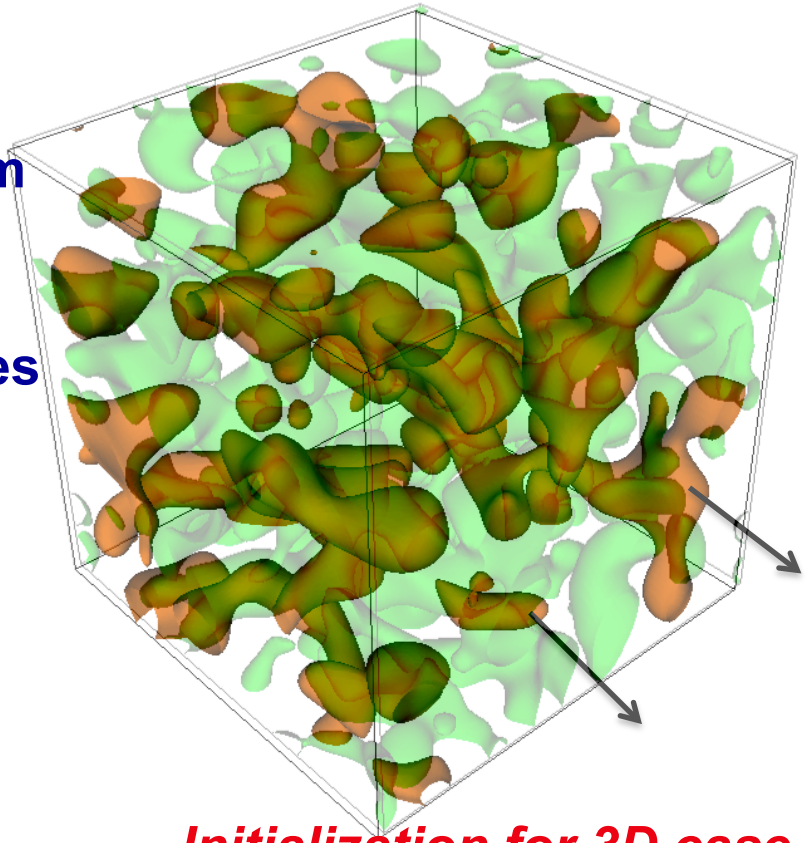
Initial turbulence integral time-scale and scalar RMS values – guided from practical engine experiments

Reduced DME chemistry – 30 species

Initially homogeneous composiion (ϕ = 0.3) with Gaussian temperature distribution, T' = 25K

Mixture averaged transport

Isentropic compression simulates HCCI engine operation from 36 CAD to TDC

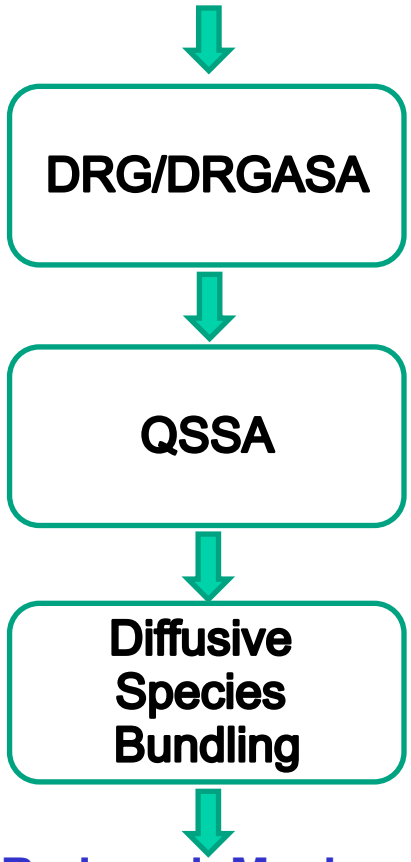


Initialization for 3D case

DME Chemistry Reduction Procedure

Detailed Mechanism (Zhao et al, 2008)
55 species, 290 reactions

Reduction by
T. Lu and Z. Luo, U. Conn.



Skeletal Mechanism
39 species, 175 reactions

Reduced Mechanism
30 species

Parameter range:
p = 1-30 atm;
T=600-1800K;
φ= 0.3-2

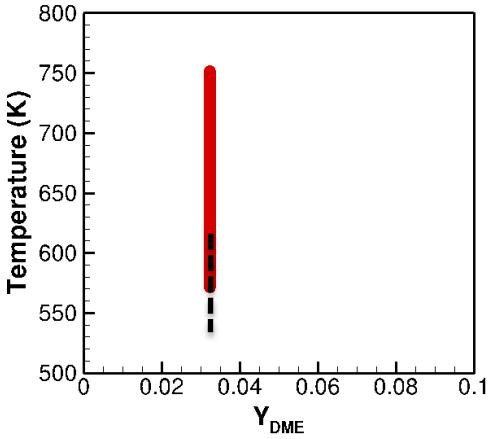
Worst case error: ~20%

Reduced Mechanism
30 species, 14 diffusive species

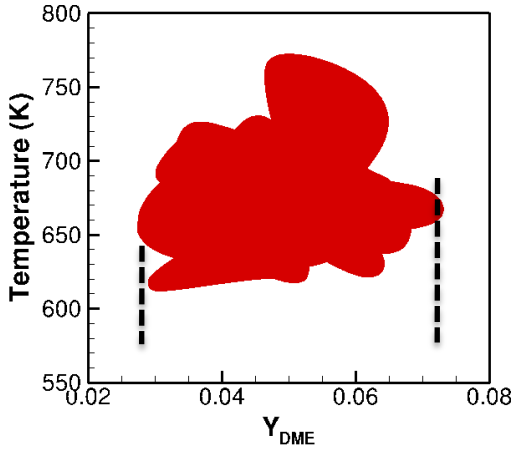
→ **Chemical Stiffness Removed On-the-fly**
explicit integration time step up to 10 ns

Three-stage Ignition in DME/Air Mixtures with Thermal and Composition Stratification

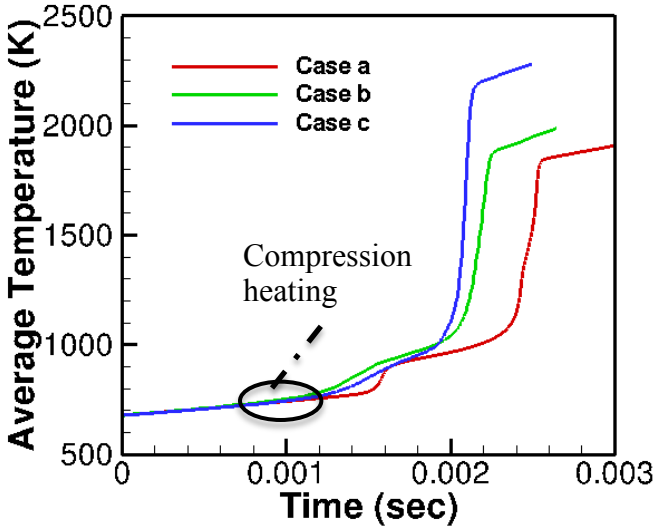
Initial Conditions



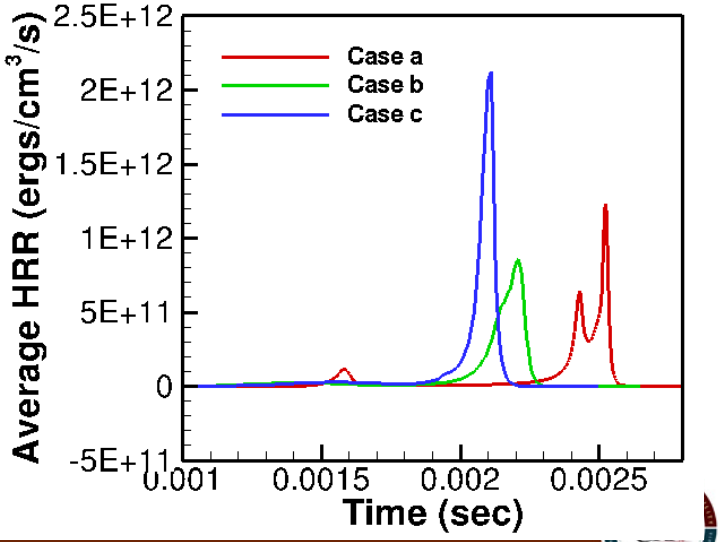
Case b



Case c
(with 70% EGR)



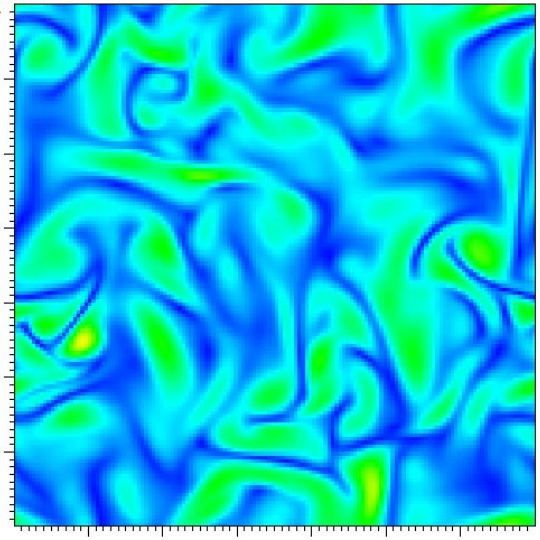
Initial mean temperature 678K, pressure = 10.8 atm
Compression ratio of 18:1, rpm=1200

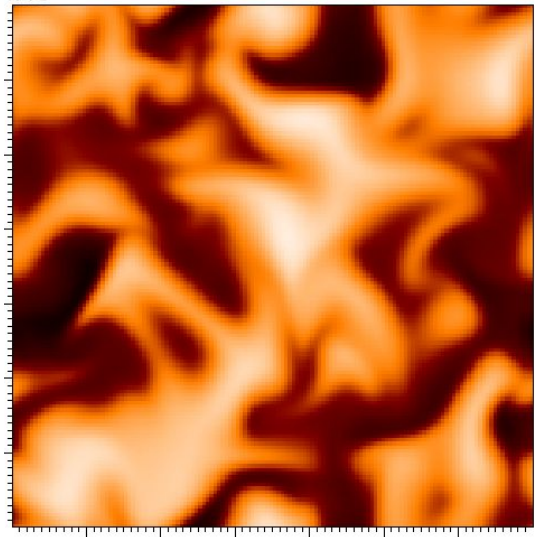


I. **LTC ignition, CH3OCH2O2 (low T)**
II. **H2O2 dissociation (intermediate T)**
III. **H+O2 = OH + O (high T)**

Existence of highly wrinkled thin "cool flame" fronts – first ignition stage

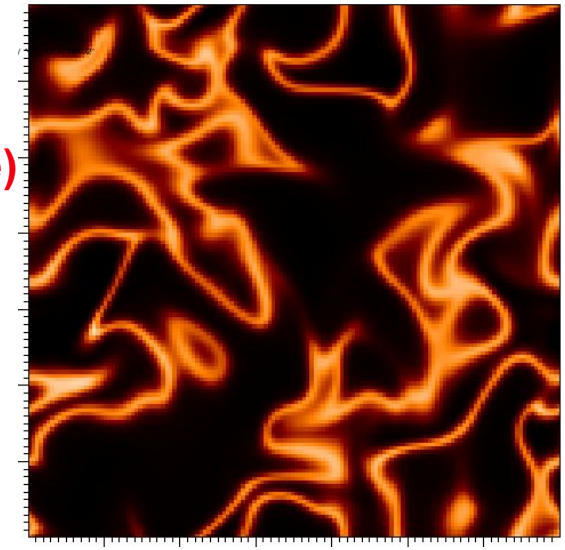
Vorticity

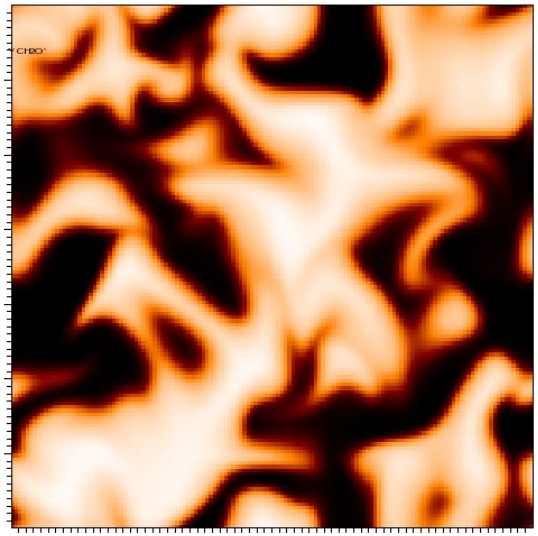




Temp

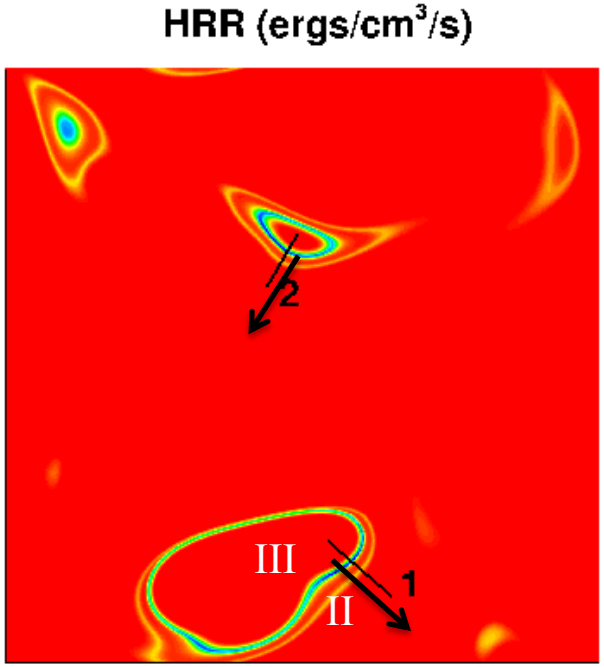
$Y_{CH3OCH2O2}$ (Key intermediate)



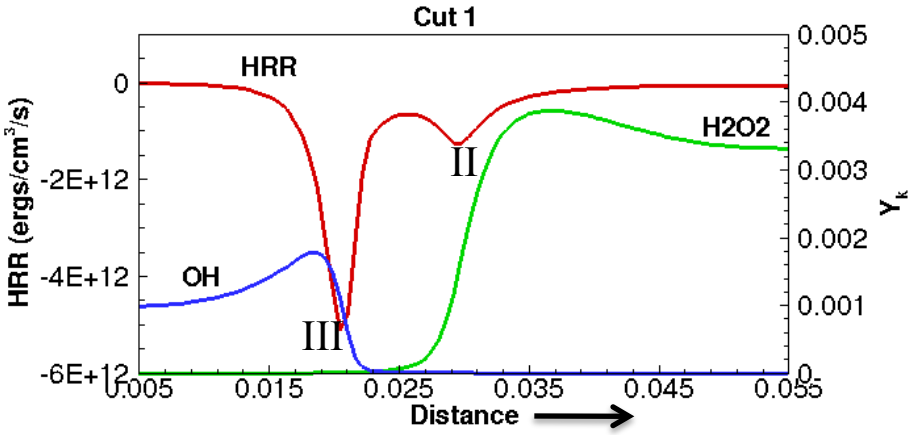


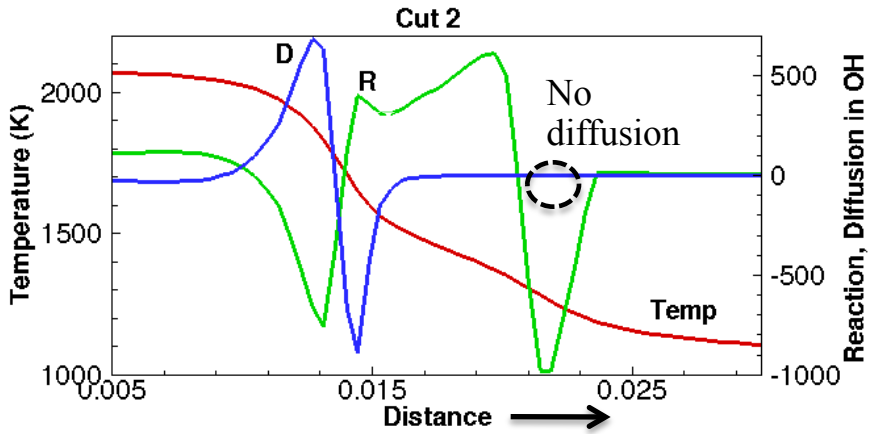
Y_{CH2O}

Simultaneous Existence of Flames and Spontaneous Ignition



A *twin-ring* structure of heat release





Close proximity of IInd and IIIrd stage waves – inter-diffusion of heat and radicals
IInd stage is chemistry driven spontaneous front; IIIrd stage is a deflagration wave

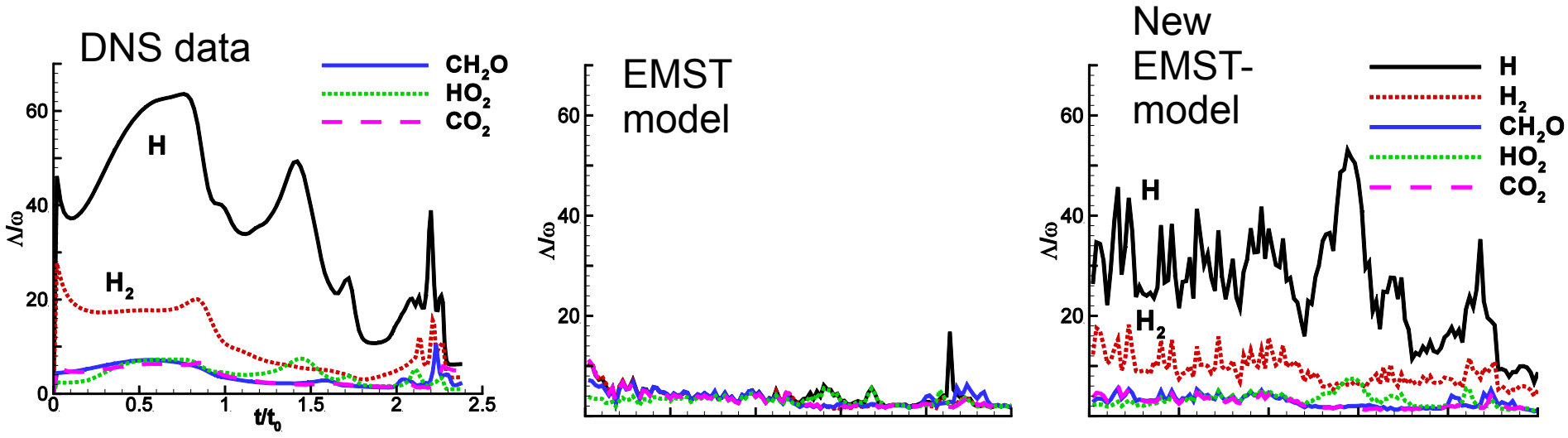
Transported PDF Modeling of Molecular Mixing in Flames With Differential Diffusion

- Differential diffusion of species provides a mechanism for different molecules to diffuse at different speeds – strongly influencing flame dynamics, pollution, and radiation.
- DNS is currently the ONLY tool that gives resolved 3D information on differential diffusion physics in turbulent flow.
- DNS data are providing unprecedented opportunities to validate and refine predictive models.
- Transported PDF methods handle mixed mode combustion – provides exact closure for chemical source terms, but multi-scalar molecular mixing requires modeling in both RANS and as a subgrid LES model
- Can we model differential diffusion in a PDF mixing model that satisfies conservation of means, localness, and realizability?

PDF modeling of molecular mixing in flames with differential diffusion

- The DNS data reveal individual species mixing at vastly different rates – due to species diffusivities **and** flame structure.
- Predictions of the state-of-the-art EMST model: Accounts for flame structure but unable to account for differential diffusion.
- New PDF modelling developed by Richardson and Chen (*Combustion and Flame 2012*) includes species diffusivities in a rigorous manner and correctly predicts the physics observed in the DNS.

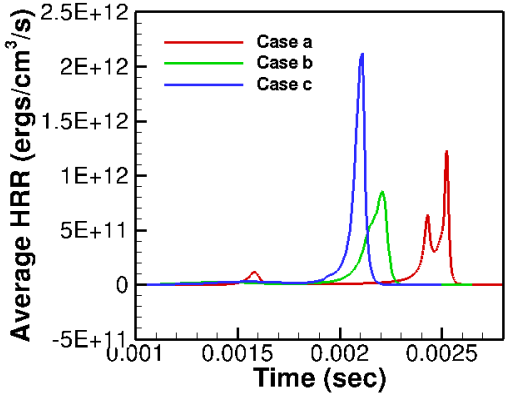
Variation of normalised species mixing rates versus time:

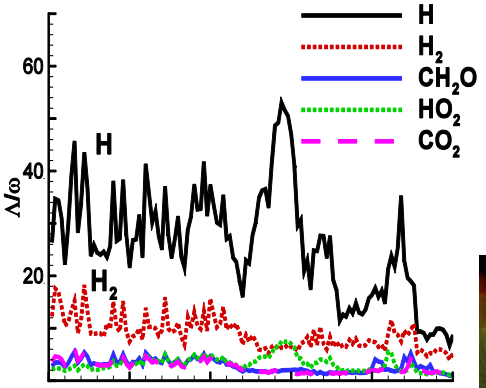


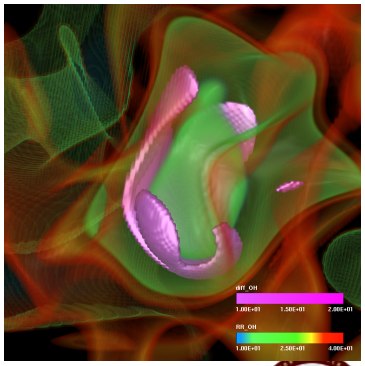
Richardson, Bansal and Chen in prep 2012

Summary of DME HCCI DNS and Modeling

- **DME autoignition occurs in three distinct chemical stages**
- **2nd and 3rd stage can occur in close physical proximity**
- **Due to strong reaction generated gradients –scalar dissipation due to reaction**
- **Multi-scalar mixing models treating localness and differential diffusion (EMST-DD)**
- **2nd stage is predominantly spontaneous ignition front; 3rd stage is predominantly premixed deflagration**



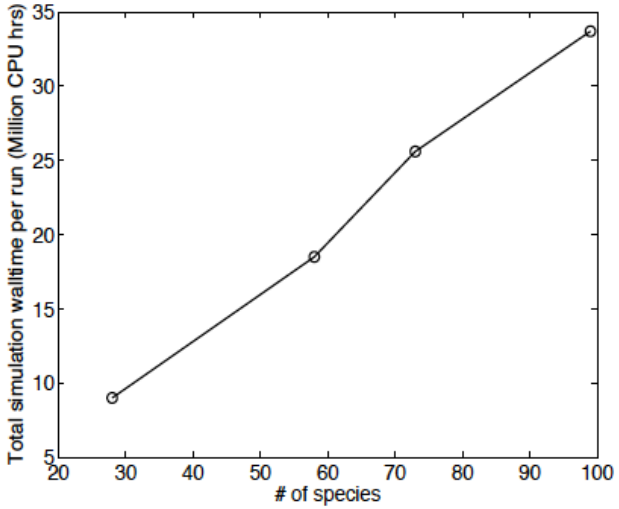




Combustion Science on a 10-20 Pflop Hybrid Many-Core Machine (Titan) – 1. More Chemistry

Increased Chemical Kinetic Complexity for low temperature, high pressure:

- 9-22 species Jaguar (H_2, syngas, methane, ethylene)
- 60-100 species Titan (nheptane, iso-octane, biofuels)



Fuel	Species	Unit Cost (us)	Total cost (million CPU hrs)
Ethanol	28	370	9.0
N-Heptane	58	760	18.5
Biodiesel	73	1050	25.6
Iso-octane	99	1380	33.7

Combustion Science on a 10-20 Pflop Hybrid machine (Titan) – 2. Higher Reynolds number

Maintaining simple chemistry, increase dynamic range of fluid scales by increasing mesh size (Reynolds number)

- 9-22 species Jaguar (H_2, syngas, methane, ethylene) increase the turbulent Reynolds number in a laboratory scale jet flame – better validation data for model assessment