This presentation is dedicated to the memory of Homer Carhart, 1914-2011

US Naval Research Laboratory
1942-1994

Director,
Navy Technology Center for Safety and Survivability

“The world is divided into two states: Fire and Nonfire.”
Some Background Terminology

- **Laminar Flame**
  - $M << 1$
  - Energy Release
  - Expansion
  - Thermal Conduction
  - Molecular Diffusion
  - Radiation ...
  
  Products of Reactions  
  $$x_l$$

- **Turbulent Flame**
  - $M < 1$
  - Wide Range of Conditions:
    - Flamelets
    - Distributed Flames
    - Shocks ...
    - Deflagration ...
    - “Vigorous burning with subsonic flame propagation”

- **Detonation**
  - $M > 1$
  - Energy Release
  - Compressible Flow
  - Shocks, and
  - Complex Shock Structures ...

These are basic elements of combustion.
Some Background Terminology

**Laminar Flame**

- \( M << 1 \)
- Energy Release
- Expansion
- Thermal Conduction
- Molecular Diffusion
- Radiation ....

**Turbulent Flame**

- \( M < 1 \)
- Wide Range of Conditions:
  - Flamelets
  - Distributed Flames
  - Shocks ...
  - **Deflagration** ...
    - “Vigorous burning with subsonic flame propagation”

**Detonation**

- \( M > 1 \)
- Energy Release
- Compressible Flow
- Shocks, and
- Complex Shock Structures ...

---

Turbulent flames are not as well understood. Transitions among these states are not well understood.
Structural Damage Caused by Explosions

Deflagration
- Damage to window glass

\[ \Delta p \approx 2 \text{ kPa} \]

Detonation
- Damage to building structure, eardrum

\[ \Delta p \approx 200 \text{ kPa} \]
Structural Damage Caused by Explosions

Deflagration
- Damage to window glass

\[ \Delta p \sim 2 \text{ kPa} \]

Detonation
-Damage to building structure, eardrum

\[ \Delta p \sim 200 \text{ kPa} \]

Deflagrations are bad; Detonations are terrible. DDT (deflagration-to-detonation) is catastrophic.
Outline of Today’s Presentations

Discuss a particularly challenging combustion project that is almost as difficult (multiphysics, multiscale, ...) as bushfires.

Explain how we identified fundamental, generic issues and approached solving them.

Summarize and discuss the outcome, relating it to what we learned about deflagrations and transitions.

Discuss finding on structure and dynamics of turbulent flames.

Discuss (ask about, actually) transitions in bushfires.

Describe fire whirls and fire whirl calculations.
Galaxy NGC4536

Type Ia Supernova, ..... 1981B
Released \( \sim 10^{51} \) ergs in 2s
Explosion from an Experimental Coal Mine
Pittsburgh, PA
These three “turbulent combustion” and “explosion” scenarios are very different in terms of scales, fuels, and levels of confinement (boundary conditions).

Yet critical questions for each scenario were really the same:

**Buncefield:** What were the flame acceleration mechanisms, and did it detonate?

**Type IA Supernovae:** What is the nature of the turbulent flame? Does it detonate? If so, how? (How could shocks form in unconfined media?)

**Coal Mines:** Given a small spark in a mixture of natural gas and air, can it detonate?
Background Information
(Based on Theory and Observations)

- White dwarf star exists $10^8$-$10^{10}$ yrs. Explosion time: $\sim 2$ s.
- Bright as an entire galaxy .... Releases $10^{51}$ ergs ($10^{27}$ Mton)
- All SNIa have similar spectra, light curves, ejecta velocity, density, composition profiles, isotopic abundances ...
- Form heavy elements ... $^{12}\text{C} + ^{16}\text{O} \Rightarrow$ heavier elements.
  Produce elements from Mg, Si ... to Ni
- In the pre-explosion state,
  Radius is $2\times10^8$ cm ( ~ earth), $M \sim M_{\text{sun}}$
  Density is $10^9$ g/cm$^3$ (center), decreases to $\sim 10^6$ g/cm$^3$
- Explode by a thermonuclear process
  Carbon-oxygen reactions support flames and detonations
  Reaction temperature $10^9$ - $10^{10}$ K
  Major energy-releasing reaction: $^{12}\text{C} + ^{12}\text{C} (\rightarrow \text{He, \(\alpha\), Ni, Mg})$
  Reaction proceeds to produce Mg, Si .... Ni (50%)
  Equation of state: $P = (\gamma - 1) E$, $\gamma = 1.3$ - 1.5
Almost 20 years ago, we were challenged to address a series of fundamental questions in Combustion Science related to transitions.

If we understand transitions, we can predict, control design, ....

How does a deflagration form?
What causes it to accelerate?
How fast can it go?
How and when does a detonation form?
How does a flame or detonation extinguish?

Unless we can answer these question, we will never really be able to explain Buncefield, SN1a, etc.
**What Controls Combustion?**

Chemical reactions  
Convective transport (fluid dynamics)  
Phase change (including particle growth)  
Diffusive transport (diffusion, thermal conduction)  
Radiation  
Gravity (body forces leading to buoyancy)

Background Conditions, \( f(x,y,z,t) \):  
Initial temperature, pressure, composition  
Geometry (containment, topography)

*These result in:*

*Reactive Fronts* -- Flames, Detonations, Other Waves  
-- Ignition, Front Propagation, Extinction  

*Turbulence* -- Reactive & Nonreactive  
-- Unsteady, Nonequilibrium
What Controls Combustion?

Chemical reactions
Convective transport (fluid dynamics)
Phase change (including particle growth)
Diffusive transport (diffusion, thermal conduction)
Radiation
Gravity (body forces leading to buoyancy)

Background Conditions, $f(x,y,z,t)$:
Initial temperature, pressure, composition
Geometry (confinement, obstructions, etc.)

These result in:

*Reactive Fronts* -- Flames, Detonations, Other Waves
-- Ignition, Front Propagation, Extinction

*Turbulence* -- Reactive & Nonreactive
-- Unsteady, Nonequilibrium
Fundamental Assumption: The physics of combustion is contained in the reactive Navier-Stokes Equations

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0 , \]
\[ \frac{\partial (\rho \mathbf{U})}{\partial t} + \nabla \cdot (\rho \mathbf{UU}) + \nabla P + \nabla \cdot \hat{\mathbf{r}} = 0 , \]
\[ \frac{\partial E}{\partial t} + \nabla \cdot ((E + P) \mathbf{U}) + \nabla \cdot (\mathbf{U} \cdot \hat{\mathbf{r}}) + \nabla \cdot (K \nabla T) = 0 , \]
\[ \frac{\partial (\rho Y)}{\partial t} + \nabla \cdot (\rho Y \mathbf{U}) + \nabla \cdot (\rho D \nabla Y) - \rho \dot{\omega} = 0 , \]

\[ \hat{\mathbf{r}} = \rho \nu \left( \frac{2}{3} (\nabla \cdot \mathbf{U}) \hat{\mathbf{I}} - (\nabla \mathbf{U}) - \nabla \mathbf{U} \right) \]

\[ P = \frac{\rho RT}{M} , \quad E = \frac{P}{(\gamma - 1)} + \frac{\rho U^2}{2} , \]

\[ \frac{dY}{dt} \equiv \dot{\omega} = -A \rho Y \exp \left( -\frac{Q}{RT} \right) \]

\[ \nu = \nu_0 \frac{T^n}{\rho} , \quad D = D_0 \frac{T^n}{\rho} , \quad \frac{K}{\rho C_p} = \kappa_0 \frac{T^n}{\rho} \]

\[ Le = \frac{K}{\rho C_p D} = \frac{\kappa_0}{D_0} , \quad Pr = \frac{\rho C_p \nu}{K} = \frac{\nu_0}{\kappa_0} , \quad Sc = \frac{\nu}{D} = \frac{\nu_0}{D_0} \]
After an considerable amount of preliminary work on fundamental interactions .... e.g.,

Chemical model development; Algorithm and code development.

Propagation of detonations and laminar flames
Flame instabilities

Multidimensional shock-flame interactions and comparisons to laboratory experiments

Multidimensional transition from laminar to turbulent flames

Flame, shock, boundary-layer interactions

We found ...
the right experiments for comparisons and study that would allow us to synthesize what we learned, and, more important, ask the right questions.
Start with a small flame in a channel containing a combustible mixture, and study how it evolves.

( Simulations done as part of a NEDO-sponsored program in hydrogen fuel safety, collaboration with Shimizu Corporation and Seikei University, Tokyo.)
Starting with a small flame in a channel containing a combustible mixture, a turbulent flame develops and produces shock waves. This leads to the formation of unsteady shock-flame complexes and detonations.
The initially laminar flame moves slowly into the unreacted material (to the right).

This is when fluid-diffusive-chemical instabilities may become important. They can wrinkle the flame front and so increase the energy-release rate.

On the time scales of this simulation, these instabilities might not have a major effect on the dynamics before other, stronger interactions come into play.
The initially laminar flame moves slowly into the unreacted material (to the right).

Obstacles perturb the flow, which then interacts with and distorts the flame, so that the flame becomes turbulent.

Flow interactions with obstacles create perturbations that distort the flame. These increase the surface area of the flame, enhance energy the energy-release rate, and thus accelerate the flame and background flow.
Shock Wave Formation

The turbulent flame generates compression waves, which eventually coalesce to form a shock in front of the flame.

The shock is continuously strengthened by compression waves coming from behind.

Shock-flame interactions are important - increase flame area and generate vorticity.
Transition to Detonation

The shock reflects from an obstacle ... creates a hot spot, or ignition center, which can become a spontaneous wave ... 

- A detonation wave results that may or may not survive.
The detonation diffracts from the obstacle, and the shock and flame separate.

Detonation decays to deflagration.

This phenomenon repeats.

Detonation occurs again.

The detonation diffracts from the obstacle, and the shock and flame separate.

**Quasi-detonation for smaller channels**

Detonation Wave Propagation
For large enough channels, the detonation successfully propagates over the obstacle.

The detonation is partially extinguished, but quickly recovers.
Solve the unsteady, compressible Navier-Stokes equations in one-, two-, and and three-dimensions by four different numerical methods: a low-order Gudonov method (Gamezo), a high-order FCT method (Ogawa), a high-order PPM-type method (Poludnenko), (and recently) a high-order Gudonov method (Ogawa).

Include models for chemical reactions, energy release, thermal conduction, and molecular diffusion, and *calibrate them to reproduce basic flame and detonation properties*.

Resolve the flow down to necessary microscale (viscous, other?)

- direct numerical simulation (DNS), or
- AMR (adaptive mesh refinement) by fully *threaded tree* (FTT) or *block refinement* *(PARAMESH)* algorithms.

Simulate specific laboratory experiments, some specifically designed to test the model. Experiments on DDT (Thomas et al.), on hydrogen flame acceleration (Teordorczyk et al.), and natural gas, (Kuznetzov et al., and Zipf et al.).
THE PHYSICAL MODEL

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0, \\
\frac{\partial (\rho \mathbf{U})}{\partial t} + \nabla \cdot (\rho \mathbf{U} \mathbf{U}) + \nabla P + \nabla \cdot \hat{\tau} = 0, \\
\frac{\partial E}{\partial t} + \nabla \cdot ((E + P) \mathbf{U}) + \nabla \cdot (\mathbf{U} \cdot \hat{\tau}) + \nabla \cdot (K \nabla T) = 0, \\
\frac{\partial (\rho Y)}{\partial t} + \nabla \cdot (\rho Y \mathbf{U}) + \nabla \cdot (\rho D \nabla Y) - \rho \dot{w} = 0,
\]

\[
\hat{\tau} = \rho \nu \left( \frac{2}{3} (\nabla \cdot \mathbf{U}) \hat{I} - (\nabla \mathbf{U}) - \nabla \mathbf{U} \right)^{\dagger}
\]

\[
P = \frac{\rho RT}{M}, \quad E = \frac{P}{(\gamma - 1)} + \frac{\rho U^2}{2},
\]

\[
\frac{dY}{dt} \equiv \dot{w} = -A \rho Y \exp \left( -\frac{Q}{RT} \right)
\]

\[
\nu = \nu_0 \frac{T^n}{\rho}, \quad D = D_0 \frac{T^n}{\rho}, \quad \frac{K}{\rho C_p} = \kappa_0 \frac{T^n}{\rho}
\]

\[
Le = \frac{K}{\rho C_p D} = \frac{\kappa_0}{D_0}, \quad Pr = \frac{\rho C_p \nu}{K} = \frac{\nu_0}{\kappa_0}, \quad Sc = \frac{\nu}{D} = \frac{\nu_0}{D_0}
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\]
# Material, Chemistry, and Reaction Wave Parameters

## Stoichiometric Hydrogen-Air

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<tr>
<th>Quantity</th>
<th>Value</th>
<th>Definition</th>
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</thead>
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<tr>
<td>$T_0$</td>
<td>293 K</td>
<td>Initial temperature</td>
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<tr>
<td>$P_0$</td>
<td>1 atm</td>
<td>Initial pressure</td>
</tr>
<tr>
<td>$\rho_0$</td>
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<td>Initial density</td>
</tr>
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<td>$\gamma$</td>
<td>1.17</td>
<td>Adiabatic index</td>
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<tr>
<td>$M$</td>
<td>21 g/mol</td>
<td>Molecular weight</td>
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<td>Pre-exponential factor</td>
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<td>$E_a (= Q)$</td>
<td>$46.37 R T_0$</td>
<td>Activation energy</td>
</tr>
<tr>
<td>$q$</td>
<td>$43.28 R T_0 / M$</td>
<td>Chemical energy release</td>
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<td>$\nu_0 = \kappa_0 = D_0$</td>
<td>$2.9 \times 10^{-5}$ g/s-cm-K$^{0.7}$</td>
<td>Transport constants</td>
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<table>
<thead>
<tr>
<th>Quantity</th>
<th>Value</th>
<th>Definition</th>
</tr>
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<tbody>
<tr>
<td>$S_l$</td>
<td>298 cm/s</td>
<td>Laminar flame speed</td>
</tr>
<tr>
<td>$T_b$</td>
<td>7.289 $T_0$</td>
<td>Post-flame temperature</td>
</tr>
<tr>
<td>$\rho_b$</td>
<td>0.1372 $\rho_0$</td>
<td>Post-flame density</td>
</tr>
<tr>
<td>$x_l$</td>
<td>0.035 cm</td>
<td>Laminar flame thickness</td>
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</table>

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<thead>
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<th>Quantity</th>
<th>Value</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_{CJ}$</td>
<td>$1.993 \times 10^5$ cm/s</td>
<td>CJ detonation velocity</td>
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<td>$P_{ZND}$</td>
<td>31.47 $P_0$</td>
<td>Post-shock pressure</td>
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<tr>
<td>$P_{CJ}$</td>
<td>16.24 $P_0$</td>
<td>Pressure at CJ point</td>
</tr>
<tr>
<td>$T_{ZND}$</td>
<td>3.457 $T_0$</td>
<td>Post-shock temperature</td>
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<tr>
<td>$T_{CJ}$</td>
<td>9.010 $T_0$</td>
<td>Temperature at CJ point</td>
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<tr>
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<td>9.104 $\rho_0$</td>
<td>Post-shock density</td>
</tr>
<tr>
<td>$\rho_{CJ}$</td>
<td>1.802 $\rho_0$</td>
<td>Density at CJ point</td>
</tr>
<tr>
<td>$x_d$</td>
<td>0.01927 cm</td>
<td>1D half-reaction thickness</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>1–2 cm</td>
<td>Detonation cell size</td>
</tr>
</tbody>
</table>
Cell-by-cell AMR based on Fully-Threaded Tree (FTT)

Dynamically controlled by gradients of flow variables

Enhances resolution of important flow features
Experimental Tests
Effect of Channel Height on DDT Distance

(Teodorczyk, 2007)

Distance to DDT $\propto d^2$

---

Test channel

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Distance to DDT (cm)

(d/2)$^2$ (cm)
**Stochasticity**

The ability of a process to deviate randomly from its path.

Turbulence is a stochastic process.

Experimentally, DDT occurs with some uncertainty in time and location. (Different physical regimes often have different levels of dispersion in the experimental result.)

This is the natural behavior of complex systems with multiple stochastic phenomena: turbulence and hot-spot formation.

We tested this ....

Imposed random perturbations in background initial conditions of $\Delta T = 0.01K$.

Result: Level of fluctuation we find depends on the controlling physical mechanism. Sometimes an result is very well predicted, sometimes in is completely unpredictable.
In Summary ...

* Dynamic, chemically reacting flows are not in steady states, but continually change and undergoing transitions, due both to a natural evolution and in response to local changes.

* Both turbulence and shocks interact with the flame to create more turbulence in the flow, and this prepares the system for transitions.

* Turbulence is generated on many scales as the flow interacts with the geometry and flame.

* Shocks and shock-interations are extremely important in this flow. The most obvious are shock-flame interactions, which generate vorticity, stretch the flame, and completely change the dynamics of the flow.
Chemically Reactive Flow Transitions

The chemically reacting flow system described is not in equilibrium. System changes by going through a series of transitional states.

For example, consider the **flame-shock complex**, in which the leading shock and turbulent flame appear coupled for varying time spans. A shock-flame complex may persist until there is no more fuel or a detonation appears.
Shocks and turbulence are critically important in this flow.

**Shock-flame interactions and turbulence-flame interactions** generate vorticity, stretch the flame, and this changes the flow dynamics and how the system evolves.

The result is that turbulence is driven over a wide range of scales in the system, so that the turbulence is broadband, and not Kolmogorov (driven at a single, system-sized scale).
Another Application: Natural Gas Explosions in Coal Mines

This illustration is a conceptual representation of a mine. It is not complete in every detail, it is intentioned to illustrate the general layout of a modern mine, the methods of mining used and the technology employed.

**UNDERGROUND MINE:**
A. PORTAL FACILITIES
B. EXHAUST FAN
C. VENTILATION SHAFT
D. LONGWALL MINING SECTION
E. JOB
F. ROOF DRILL
G. SHEILD
H. CONVEYOR
I. CONTINUOUS MINING SECTION
J. CONTINUOUS MINER
K. INTEGRATED ROOF BOLTERS
L. LOADING MACHINE
M. SHUTTLE CAR
N. SECTION FAN
O. SECTION CONVEYOR BELT
P. TRACK
Q. SLOPE BELT
R. STOPPING
S. OVERCAST

**SURFACE FACILITIES:**
1. TRANSFER BUILDING
2. RAW COAL CONVEYOR
3. WASHED COAL SLUG
4. BRIQUETTE BUILDING
5. REFINERY PLANT
6. THERMAL DRYER
7. PLANT SAMPLE BUILDING
8. CLEAN COAL SLUG
9. RAILROAD TIEOUT
10. RAILROAD
11. REFUSE CONVEYOR
12. FRESH WATER IMPOUNDMENT

**KEY**
- Indicates Return Air
- Indicates Intake Air

**PORTION OF MINE MAP**

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**Diagram Notes:**
- Longwall Mining Section
- Continuous Mining Section
- Surface Facilities
- Underground Mine
- Key indicators for air flow

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**Conclusion:**
This diagram highlights the integration of natural gas explosions in modern coal mine operations, emphasizing the critical infrastructure and safety mechanisms in place.
Experiments at Lake Lynn Experimental Mine

Lake Lynn Laboratory
Lake Lynn PA. Experiments designed to benchmark and test the computations.
# Parameters for Stochiometric Methane-Air

## Input

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_0$</td>
<td>1 atm</td>
<td>Initial pressure</td>
</tr>
<tr>
<td>$T_0$</td>
<td>298 K</td>
<td>Initial temperature</td>
</tr>
<tr>
<td>$\rho_0$</td>
<td>$1.1042 \times 10^{-3}$ g/cm$^3$</td>
<td>Initial density</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>1.197</td>
<td>Adiabatic index</td>
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<tr>
<td>$M$</td>
<td>27 g/mol</td>
<td>Molecular weight</td>
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<td>$A^*$</td>
<td>$1.0-1.64 \times 10^{13}$ cm$^3$/g-s</td>
<td>Pre-exponential factor</td>
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<tr>
<td>$E_a$</td>
<td>$67.55 \frac{RT_0}{M}$</td>
<td>Activation energy</td>
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<td>$q$</td>
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<td>Chemical energy release</td>
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<td>$\nu_0$</td>
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<td>Viscosity</td>
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<td>$\kappa_0 = D_0$</td>
<td>$6.25 \times 10^{-6}$ g/s-cm-K$^{0.7}$</td>
<td>Transport constants</td>
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</table>

## Output †

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_l$</td>
<td>32.53 cm/s</td>
<td>Laminar flame speed</td>
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<tr>
<td>$T_b$</td>
<td>$7.419 T_0$</td>
<td>Post-flame temperature</td>
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<tr>
<td>$\rho_b$</td>
<td>$0.1348 \rho_0$</td>
<td>Post-flame density</td>
</tr>
<tr>
<td>$x_l$</td>
<td>0.049 cm</td>
<td>Laminar flame thickness</td>
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<tr>
<td>$D_{CJ}$</td>
<td>$1.820 \times 10^5$ cm/s</td>
<td>CJ detonation velocity</td>
</tr>
<tr>
<td>$P_{ZND}$</td>
<td>$32.79 P_0$</td>
<td>Post-shock pressure</td>
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<tr>
<td>$P_{CJ}$</td>
<td>$16.89 P_0$</td>
<td>Pressure at CJ point</td>
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<tr>
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<td>Post-shock temperature</td>
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<tr>
<td>$T_{CJ}$</td>
<td>$9.460 T_0$</td>
<td>Temperature at CJ point</td>
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<tr>
<td>$\rho_{ZND}$</td>
<td>$8.344 \rho_0$</td>
<td>Post-shock density</td>
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<td>$\rho_{CJ}$</td>
<td>$1.785 \rho_0$</td>
<td>Density at CJ point</td>
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<tr>
<td>$x_d$</td>
<td>0.3131 cm</td>
<td>Half-reaction thickness</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>16–31 cm</td>
<td>Detonation cell size</td>
</tr>
</tbody>
</table>

* Final recommended value $A = 1.2 \times 10^{13}$ cm$^3$/g-s

† Output values based on $A = 1.2 \times 10^{13}$ cm$^3$/g-s
Simulations of Experiments by Kuznetsov et al.
Stoichiometric CH₄ + Air

Spark ignition

Evenly spaced obstacles

Movie shows the evolution of the spark, formation of a flame, transition to a turbulent flame, and hot-spot ignition of a detonation

$d = 17.4, 52 \text{ cm}$
Blockage ratios $BR = h/d = 0.3, 0.6$
Experiments in a cylindrical tube
Lake Lynn PA. Experiments designed to benchmark and test the computations.
These three “turbulent combustion” and “explosion” scenarios are very different in terms of scales, fuels, and levels of confinement (boundary conditions).

Yet critical questions for each scenario were really the same:

**Buncefield:** What were the flame acceleration mechanisms, and did it detonate?

**Type IA Supernovae:** What is the nature of the turbulent flame? Does it detonate? If so, how? (How could shocks form in unconfined media?)

**Coal Mines:** Given a small spark in a mixture of natural gas and air, can it detonate?

Yes!
Some Properties of Randomly Forced, Broad-Band Turbulence

Energy spectrum can have a number of envelopes, including $k^{-5/3}$ typical of Kolmogorov spectra.

Higher moments, such as vorticity or enstropy can behave differently. *Intermittency is suppressed.*
Turbulence in the simulations is not equilibrium Kolmogorov turbulence. It is generated at the same time on many scales.

In chemically reacting flow systems, is the turbulence ever the pure Kolmogorov turbulence of standard fluid dynamics theory?

What Does Turbulence Do to a Flame?

What Does a Flame Do to Turbulence?
We Have Isolated and Studied Properties of Flame-Turbulence Interactions

* Developed, implemented a method for driving turbulence in NS flows. 
  * Goes to statistical quilibrium quickly; Takes an arbitrary input spectra.

* Computed properties of nonreactive driven turbulence that results from forced spectra. Driving ranges from Kolmogorov (only drive largest scale) to Richtmyer-Meshkov (flat) spectra driven on many scales.

* Computed behavior of a flame immersed in either RM or Kolmoogorov turbulence. Results of comparisons were inconclusive.

To make sense of what we were seeing, we required

* Data from Kolmogorov-driven DNS in comparable reacting and nonreacting flows compressible flows, covering a range of intensities;
* Additional flow and combustions diagnostics

* Created data base of simulations of H₂-air and CH₄-air flames in Kolmogorov turbulence, as a function of a range of \( I_T \) and \( L \).

* Studied flame structure in turbulent flame brush. Considered:

  Effects of the turbulence on the flame, and
  Effects of the flame on the turbulence.
Kolmogorov and Broadband Turbulence Spectra

512 x 512 x 512 Simulation

Energy Injection rate

$2.4 \times 10^8 \text{ erg/cm}^3/\text{s}$
Some Preliminary Results

Vorticity and intermittency suppressed in broadband turbulence:

Broadband turbulence
(driven at all scales)

Kolmogorov turbulence
(driven at largest scale)

(Poludnenko, Hamlington, Oran, 2010)
High-Intensity H₂-Air Simulation

Fuel Isosurfaces

Pressure

Fuel Mass Fraction

Temperature
Turbulence is most influenced by the flame for low turbulence intensities and least affected for high intensities.

**Turbulent Flame Structure**

<table>
<thead>
<tr>
<th>Facing</th>
<th>$Y = 0.95$</th>
<th>$0.05$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$U_L / S_L$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td></td>
<td></td>
</tr>
<tr>
<td>30</td>
<td></td>
<td></td>
</tr>
<tr>
<td>50</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Isocontours of concentration (Y) Isocontours of $|\omega|$*

(Hamlington, Poludnenko, & Oran 2010-11)
Reactive turbulence itself is never Kolmogorov, even when the large-scale driving is Kolmogorov. Energy is injected on a range of scales in the flame brush.

Turbulence “moves energy around” in the scales of the flame brush. It suppresses small scales, enhances large scales.

(Hamlington, Poludnenko, Oran, 2010-11)
For H₂-air flames, the flame structure inside the brush is very robust, even in extremely intense turbulence.

The preheat zone of the flamelet is extremely important in the flame-turbulence interaction. Whereas the turbulence does not seem to penetrate or affect the reaction zone very much, it does penetrate and alter the structure of the preheat zone.

*(Poludnenko & Oran, CNF, 2010)*
Turbulence Also affects Flamelet Structure

Weak turbulence affects preheat zone. Stronger turbulence also affects energy-release zone.

(Statistical variations about the mean increase with turbulence intensity.)

(Hamlington, Poludnenko, & Oran 2010-11)
Observations and Conclusions

As the turbulent intensity increases, and the flame is packed tighter, there are more regions of high flame curvature (cusps), and there are more frequent flame collisions.

The local flame speed in cusps substantially exceeds its laminar value. This result increases the turbulent velocity beyond what is possible from burning at the existing flame surface area.

(Poludnenko & Oran, CNF, 2011)
Observations and Conclusions

For higher-intensity turbulent-flame interactions, detonations can arise “spontaneously.”

A detailed analysis of one H$_2$-flame simulation showed that the transition was preceded by a large increase in the flame-brush pressure resulting from intense turbulent-flame interactions. At that point, the entire flame brush accelerated to the CJ flame speed, shocks began to form locally inside the flame brush, and a DDT occurred inside the flame brush.

(Poludnenko, Gardiner, Oran, PRL, 2011, Science (Editors’ Choice))
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\[ S_T = \frac{c_s}{(\rho_f/\rho_p)} \]

(Poludnenko, Gardiner, Oran, PRL, 2011, Science (Editor’s Choice))
Three “turbulent combustion” and “explosion” scenarios -- very different in terms of scales, fuels, and levels of confinement (boundary conditions).

Yet critical questions for each scenario were really the same:

Buncefield: What were the flame acceleration mechanisms, and did it detonate?  

Type Ia Supernovae: What is the nature of the turbulent flame? Does it detonate? If so, how? (How could shocks form in unconfined media?)

Coal Mines: Given a small spark in a mixture of natural gas and air, can it detonate?

Could have detonated, but it’s not clear that it’s needed to explain observations.  

SNIIa will detonate. Shocks formed by turbulence-flame interactions.  

Yes!
DNS Data Bases

Each symbol represents a set of simulations that include tests of resolution, boundary effects, etc. Most H₂-air, some CH₄-air.

(Poludnenko et al., PRL, submitted)

(Hamlington et al., Phys. Fluids, submitted)
The combustion diagram is the key
The combustion diagram is the key:

What is the shape of the DDT region?

How does the diagram change with stoichiometry?

How do statistics and scale interplay?
Observations and Conclusions

Depending on the fuel, the structure of the laminar flamelet is more or less robust to turbulence.  
  e.g., Stoichiometric H2-air is robust. (The results we have are already predictive.  
  We don’t know how CH4 behaves yet -- we have one or two points on the combustion diagram.

Larger scale correlates with higher probably of an event.  
Length scale can be interchanged with pressure.

The important intensity is related to fluctuations on the scale of the flame thickness. How the driving occurs on larger scale does not seem as important (e.g., broad band vs Kolmogorov).

Hydrocarbon fuels, and biofuels, behave a little differently:  
They must pyrolyze first to produce smaller species (H, CH4, C2...) and the smaller species burn first to raise the temperature for larger species. There is a feedback here to the change the amount of H, CH4, etc that form, etc.
For H₂-air flames, the flame structure inside the brush is very robust, even in extremely intense turbulence.

The preheat zone of the flamelet is extremely important in the flame-turbulence interaction. Whereas the turbulence does not seem to penetrate or affect the reaction zone very much, it does penetrate and alter the structure of the preheat zone.

*(Poludnenko & Oran, CNF, 2010)*
Outcomes of These Studies

Numerical Methods, AMR, CHEMEQ2, and several new codes.

Understanding of the level of physical complexity required to solve the problem.

Some understanding of what is causes transitions, even DDT.

Proof for NIOSH that, in a coal mine, a small spark can evolve into a very turbulent flame, and even a detonation for very lean methane concentrations.

Evidence that flame-tubulence effects are extremely important: nonlinear feedback changes the properties of both.

A mechanism for unconfined DDT: How does a supernova explode? We probably know the answer now. *(Let me show you ... .)*

Fundamental issues for using detailed chemical mechanisms for the high-pressure, high-temperatures conditions that often occur in nonequilibrium flows.

Questions about the nature of tubulence for high Re flow.
Summary of Flame and Turbulence Studies

Many of our usual ideas of turbulence and chemical reaction mechanisms have come into question.

Chemical reaction mechanisms are not valid in high-pressure, high-temperature regimes.

In real problems, the turbulence is not steady-state Kolmogorov turbulence.

The presence of the flame changes the turbulence, and the turbulence changes the flame.

There is no such thing as an overall steady state, except perhaps the pre- and post-ignition states.

There could be some intermediate states that last a relatively long time (“metastable states”).
Observations and Conclusions

Resolutions tests show:

It is not necessary to resolve the turbulent cascade down to the cold-flow viscous scale, but only to ensure that the inertial range extends well through the scale of the laminar flame thickness. (Consistent with a MILES approach.)

Poludnenko & Oran, Combustion and Flame, 2010.
Talk 2
Flame Acceleration Studies .... Procedure

Scale analysis: The problem is dominated by the interaction of turbulence and energy release, all occurring over space and time scales varying by many orders of magnitude.

First objective of simulations: to include the minimum relevant physics and enough of the relevant time and space.

The question is what and how much to simply

Assumed that to resolve combustion system adequately:
* $\Delta x$ must resolve the laminar flame thickness, $\delta_f$, and
* $\Delta t$ must be small enough to resolve $\delta_f$ and capture important short time-scale phenomena.

This required that we:
* develop special simplified chemical (energy-release) models
* develop special grid refinement algorithms
* find or design experiments for comparison

Extracted and checked basic chemical-fluid interactions (such as shock-vortex and flame-vortex, etc.) and instabilities. Some comparisons to theory were possible and these tested simulations in limits.

Attempt simulations of real scenarios: Laboratory experiments, Coal mines, Refueling facilities, SNIa, ... .
Delflagrations alone generate turbulent flows. Turbulent flows interacts with flames and accelerate them. Accelerating flam can drive shocks.

Shocks can have important local or global effects on the flow.

Shock-flame interactions, on any scale, affect the nature (structure) of the turbulence.

Changes in conditions in the background flow (e.g., conditions that generate turbulence or shocks) can create conditions that accelerate flames (e.g., bushes in Buncefield)

Turbulent and accelerating flames can lead to fluctuations or hot spots in unreacted (gas) fuel, and these hot spots can create gradients of reactivity strong enough to cause further ignitions, and even detonation (Zeldovich or modified Zeldovich mechanism).

For reacting flows in more complicated geometries, or with additional important physical processes, the evolution of the system prior to transitions can be modified, and so the transition itself can be modified, quantitatively or even qualitatively.
Tour de Force

This problem shows: ignition from a spark, evolution to a turbulent flame, effects of particular geometry, flame-flame interactions, flame-shock interactions, flame-brush acceleration, eventually ... DDT.

Hydrogen-air, 1 atm, 298K

3D simulation, but show 2D slice through z=0 plane.

Mirror boundaries (left and bottom), Open boundaries (top and right).

Solid wall or stretched outflow boundary on “top.”
An Array of Obstacles

1. Initial flame

2. Flame becomes turbulent

3. Shock-flame complex forms
An Array of Obstacles

1. Initial flame

2. The flame becomes turbulent.

3. Shock wave formation

4. DDT: shock reflection from obstacles
Outline of Today’s Presentations

Discuss a particularly challenging combustion project that is almost as difficult (multiphysics, multiscale, ...) as bushfires.

Explain how we identified fundamental, generic issues and approached solving them.

Summarize and discuss the outcome, relating it to what we learned about deflagrations and transitions.

Discuss finding on structure and dynamics of turbulent flames.

Discuss (ask about, actually) transitions in bushfires.

Describe fire whirls and fire whirl calculations.
“Fire behavior is not a one-dimensional steady state process* but ... the result of combustion of ... fueled elements arranged non-uniformly on a landscape.”

“... We must improve our modeling framework and underlying basic knowledge to reflect the complexity ..., ... heat transfer within the fuel and across gaps in the fuels, the role of ... moisture ..., and the residence time of combustion in all stages.”

“Current operational fire models do not accurately reflect the complexity of combustion processes, the temporally and spatially variable physical environment in which they occur or, or fire-atmosphere interactions.”

This is a rather tall order ...
Critical questions for bushfires:
What causes transitions among states of the fire?
What are the signals that a transition could occur?

Interested in transitions among stages; transitions to extreme events; evolution of extreme events;

Point of view: All governed by the set of reactive Navier-Stokes equations.
Transitions and Dynamics in Wildfires

Transitions ...
   From ignition to large-scale conflagration proceeds through stages:
      ignition, surface propagation, crown fires (firebrands), smoldering, extinction, etc.

   ... are caused by dynamic interactions:
      Feedback between fire dynamics and atmospheric flow and turbulence
      Effects of local topography and fuel structure on fire through effects on wind fields
      Effects of fire-induced winds on heat transfer to fuel

      *All Involve buoyancy, turbulence, background flow, properties of fuel distribution, and fuel and terrain geometry.*

      *This is too much to handle at once, and too much to consider at once if we are to extract fundamental principles*
Chemical reactions
Convective transport (fluid dynamics)
Phase change (including particle growth)
Diffusive transport (diffusion and conduction)
Radiation
Gravity (body forces leading to buoyancy)

**Basic Physical Processes of Combustion Science**

These result in:
Reactive Fronts (Flame, Detonation, Other Waves)
Ignition, Front Propagation, Extinction
Turbulence (Reactive & Nonreactive)
(nonsteady, nonequilibrium)

*How do we use this to create minimal, but relevant models that show transitions?*

Background Conditions, $f(x,y,z,t)$:
Initial temperature, pressure, composition
Geometry (containment, topography)
Spinning vortex columns of hot air and gases rising from a fire...

They carry smoke, debris, and flames.

Range in size from less than 10 cm to more than 200 m in diameter.

Can equal the intensity of a small tornado.

http://www.forestsandrangelands.gov/resources/glossary/

Three-Dimensional Simulations of Firewhirls

(Liu, Oran, and Williams, 2008)
Fire whirls may be disastrous in urban areas, farmland, and forests. They are capable of destroying ... everything in their paths!

Fire whirls appear “spontaneously” and frequently in large forest fires.

The Great Kanto Earthquake (Tokyo) led to small fires, which, combined with winds, generated a fire whirl that killed 40,000 people huddled in an open area outside away from the fires.
Some Questions about Fire Whirls

How do fires interact with a vortices?

How are fire whirls generated?

Can we predict their occurrence?

Are there geometries that are more or less susceptible to forming fire whirls?

Do scaling laws work?

Home Movie
Area of the Hifukusho-ato Fire Whirl
Great Kanto Earthquake, September 1, 1923
The Hifukusho-ato Fire Whirl
Great Kanto Earthquake, September 1, 1923
Classification of Fire Whirls

Type 1: Steady and centered over burning area. Studied by Emmons and Ying, 

Type 2: Steady or transient downwind of burning area. Often seen in wildland fires 
(E.g., Brown and Davis, McGraw Hill, 1973 Forest Fire: Control and Use)

Type 3: Steady or transient and centered over an open area adjacent to an asymmetric burning with wind area. Could be the most severe.
Diagram of Types of Fire Whirls

Type 3 Fire Whirl

Type 3 fire whirls are generated when the fire and plume in the burning area obstruct the lateral wind, preventing flow across the burning area and causing air entrainment and creating a circulation region for fuel.

From scale-model experimental results, and considering overall balance equations, an estimate for the scaling of the critical wind velocity for generating the most severe whirls is:

\[ U_c \sim L^{3/8} m^{1/4} \]
Experiments and Theory

Experiments on smaller-scale prototypes:

Experiments based on geometry of Tokyo fire whirl.
- Somo and Saito (1991) (scale: 1/100th, 1/2500th)
- Kuwana et al. (2006) (scale: 1/1000th)

Fire whirls occur only in a certain range of wind velocities and topologies of the burning area.

Theoretical analysis:

Somo and Saito (1991): proposed a scaling law predicting critical wind velocity based on the Froude number
- Kuwana et al. (2006) expanded this to include effect of a burning rate,

\[ U_c \sim L^{3/8} m^{1/4}, \]

where \( U_c \) is critical wind velocity,
\( m \) is burning rate, and
\( L \) is the scale of the burning area.
Scale Modeling of Type 3 Fire Whirls

- $1/100^{th}$ scale field experiment: Soma and Saito, (Combustion and Flame, 1991).

- $1/1000^{th}$ scale wind-tunnel experiments: Hayashi, Ohmiya, & Saga (Int. J. Fire Science and Technology, 2003).

- $1/2500^{th}$ scale laboratory experiment: Saito (Kozo), personal communication, 2006.
Experiment at 1/1000th Scale
Building Research Institute, Tsukuba, Japan

14 rectangular pans, 0.3m by 0.4 m, n-heptane fuel, ignited simultaneously, wind velocity: 0.5 m/s - 2.0 m/s, burning for 2 min

Weak whirls
at 0.5 m/s;

Fire plumes
strongly tilted
downstream at
1.0 m/s;

Intense type 3 fire whirls at 2.0 m/s
Computations of Type 3 Fire Whirls

- Roughly 1/1000th scale: Liu, Oran, Williams (2008, unpublished)

  Length: \( L = 2.4 \, m \)

  Fire modeled by energy release rate:
  \[ q = 125-2000 \, kW/m^2 \]

  Wind velocity \( U = 0.25 - 1.5 \, m/s \)

- Results similar to experiments, even though not fully resolved (i.e., MILES)

- Compared to predictions of scaling law, with
  \[ U_c = 4 \, m/s \] for Kanto, gives
  \[ U_c = 0.7 \, m/s \] for \( q = 500 \, kW/m^2 \)

- Computations show most intense whirls at 0.5 m/s for this case, which is close.
Create vortices by flowing wind over a burning area, which might model a building, and stand of trees, etc.

Height of burning region (H) = 0.3 m

This size and shape models experiments by Kuwana et al.

Vary:
- Amount of energy release, from $Q = 125 - 2000$ KJ/m$^2$
- Wind velocity, $U_c$ from 0.25 - 1.5 m/s
- Direction of inflow
- Topology of burning area (to a limited extent)
Summary of Solution Method

Solve the 3D fully compressible Euler equations

Source terms for gravity and energy release

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0
\]

\[
\frac{\partial (\rho \mathbf{U})}{\partial t} + \nabla \cdot (\rho \mathbf{UU}) + \nabla P = (\rho - \rho_\infty)g
\]

\[
\frac{\partial E}{\partial t} + \nabla \cdot ((E + P)\mathbf{U}) + \dot{q} = 0
\]

\[P = \frac{\rho RT}{M} \quad E = \frac{P}{\gamma - 1} + \frac{1}{2} \rho U^2 \quad \text{where here} \quad \dot{q} = \frac{Q}{H}\]
Numerical Method

Numerical solution
Based on direction-split FCT.
Tested splitting and its effects on solution.
Use MILES to handle subgrid dissipation.

Resolution
Varied grid cells from 0.1 m to 0.05 m.
Cluster cells around burning area.
Results shown with finest resolution.
Large-scale vortices in solutions converged.

Energy-release model
Constant volumetric energy-release rate $Q$ added to burning area.
More complex burning model under development.
Typical Simulations Results

Instantaneous Profiles

\( Q = 500 \text{ KJ/m}^2, \ U = 0.5 \text{ m/s} \)
Time-averaged Temperature, Streamlines, and Velocity

1. Fix $Q$ (2000 KJ/m$^2$), Vary $U$ (m/s)

   $U = 0.5$

   | 0.5 | 0.75 | 1.0 | 1.5 |

2. Fix $Q$ (500), Vary $U$

   $U = 0.25$

   | 0.5 | 0.75 | 1.0 |

3. Fix $U$ (0.5), Vary $Q$

   | Q = 125 | 500 | 125 |
With certain combinations of shape of burning area and $U$, vortices are always present and fire whirls can develop.

Can we say something about the combinations?

The balance between $U$ momentum and buoyancy-induced upward momentum determines location of the vortex.
Three Types of Vorticies Form

(1) A large vortex in the open area, surrounded by the burning. This can form the fire whirl.

(2) A smaller, counter-rotating vortex above (1) and downstream from the burning area.

(3) Another smaller, counter-rotating vortex over the burning area.
The position of the larger vortex, in open area (1), depends on the wind velocity. 

As $U$ increases, the large vortex moves out of the burning area, into the open area, and then downstream.

As $Q$ increases, higher $U$ is needed to move the vortex from the burning to the open area.

The simulations are in qualitative agreement with observed vortex structures.
Flow of Smoke through Cities and Buildings

General Information:
Duration: 30 min
Domain: 1.7 x 1.7 x 0.4 km³
Wind: from NW, 1 m/s
Release lasts 30 s
Tree model
Terrain model

Boris & Young, 1996
Contaminant Transport through Cities ... Current Status

**Houston**

**New York 1**

ROCKEFELLER CENTER

**Chicago**

**New York 2**

0 Minutes

0 Minutes

0 Minutes

0 Minutes

Boris, Doyle, Patnaik, Young, Obenschain, 2004-present
Thank you for your kind attention!