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TEXAS A&M UNIVERSITY

Modeling of Terrestrial and Astrophysical Reacting Flows with Athena and Athena++

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Texas A&M University

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Sandia National Laboratories

NASA

DoD HPC Modernization Program
SOLVING THE HARD PROBLEMS

DAAC
Data Analysis and Assessment Center

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH
UNITED STATES AIR FORCE

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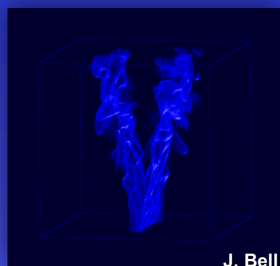
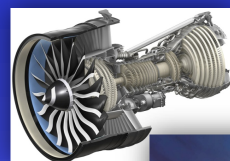
Many facets of reacting flows

… from a laboratory scale to cosmological scales

1 mm | 1 cm | 10 cm | 1 m | 10 m | 100 m | 1 km



Laboratory flames

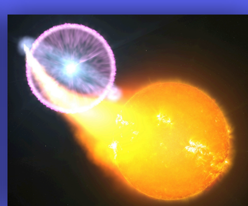


Propulsion and power generation

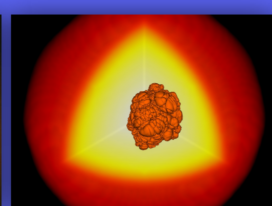
Industrial accidents

10^5 cm 1km | 10^6 cm 10 km | 10^7 cm 100 km | 10^8 cm 1000 km | … | 10^{11} cm 1 solar radius | … | 10^{14} cm 10 au | … | 10^{19} cm 10 ly | …

Neutron star X-ray bursts

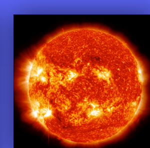


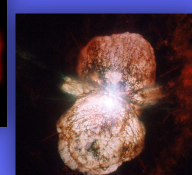
Classical novae

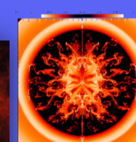


Type Ia supernovae

Explosive burning





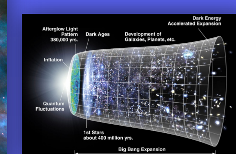


Normal and massive stars
Core-collapse supernovae

Hydrostatic and explosive burning

Star-forming regions

Dust formation



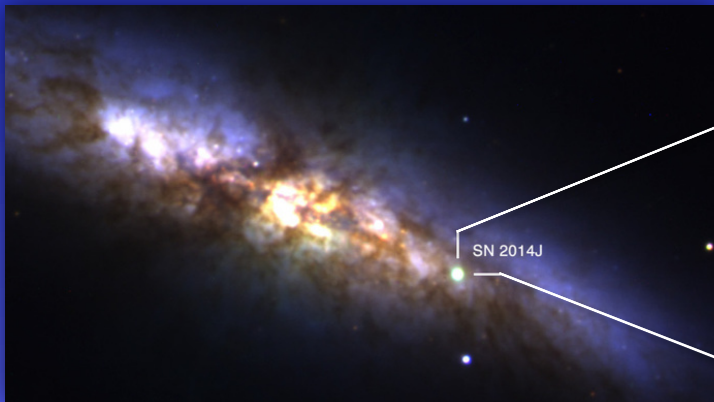
Big Bang

Electroweak phase transition

Thermonuclear Type Ia supernovae

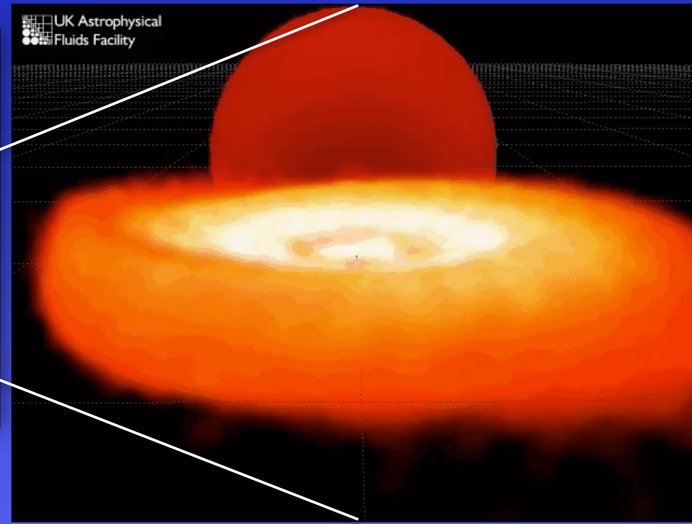
Combustion on an extreme scale

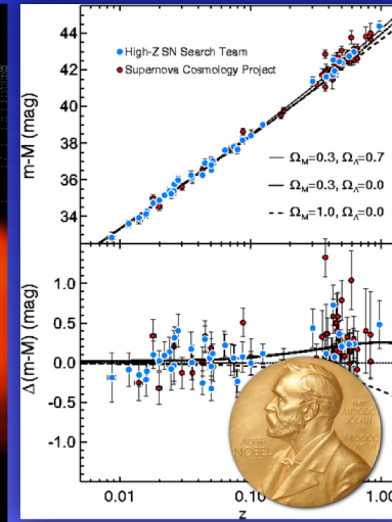
Thermonuclear explosion of compact white dwarf stars in stellar binary systems



SN 2014J in M82

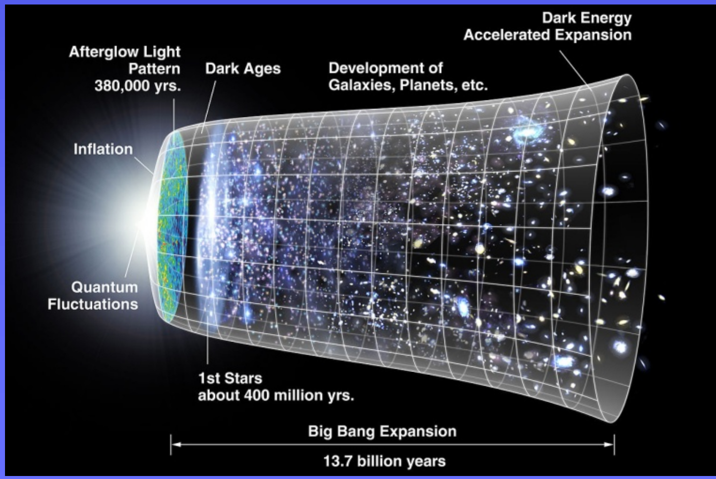
Image: Nordic Optical Telescope, J. Johansson



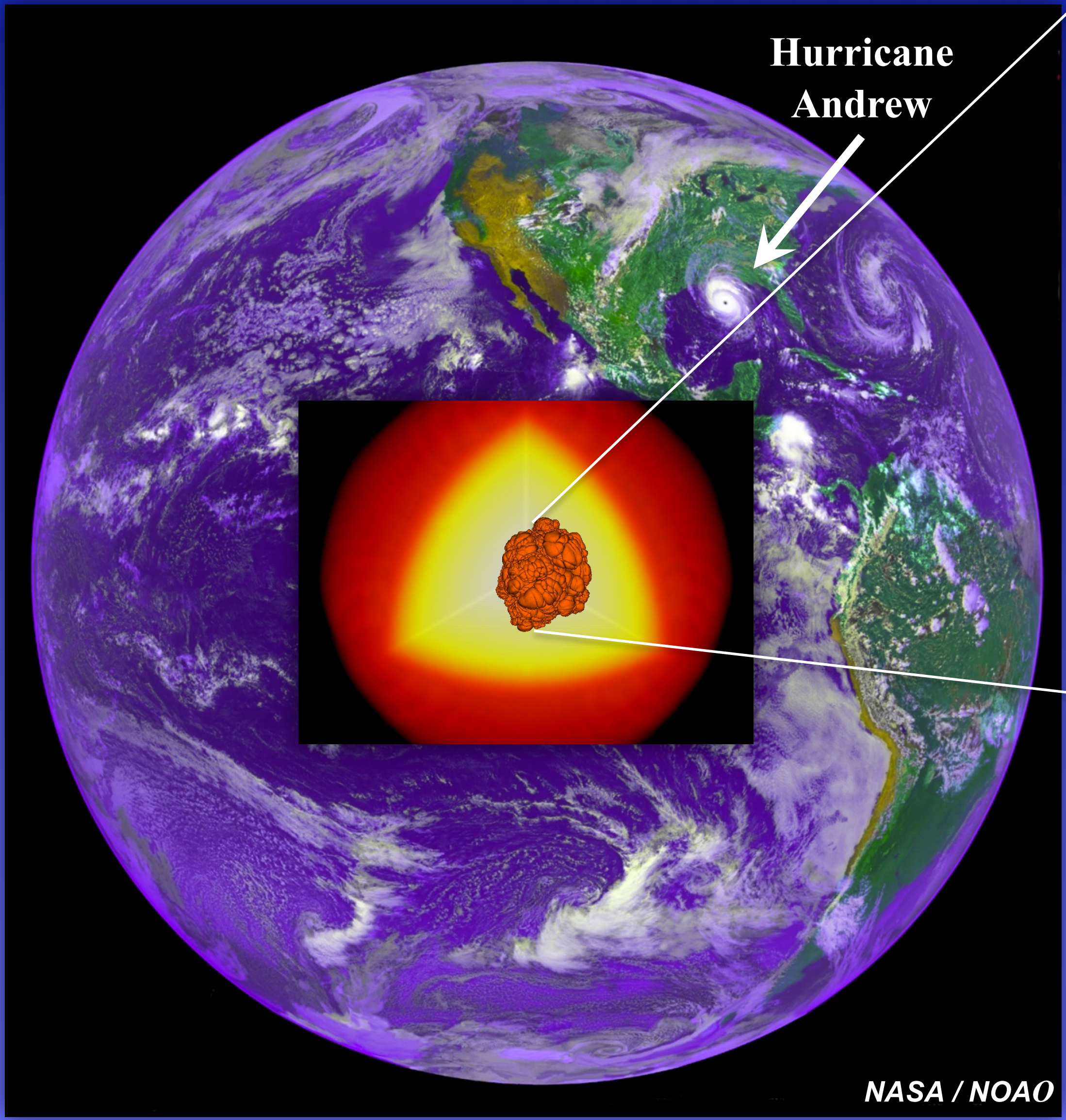


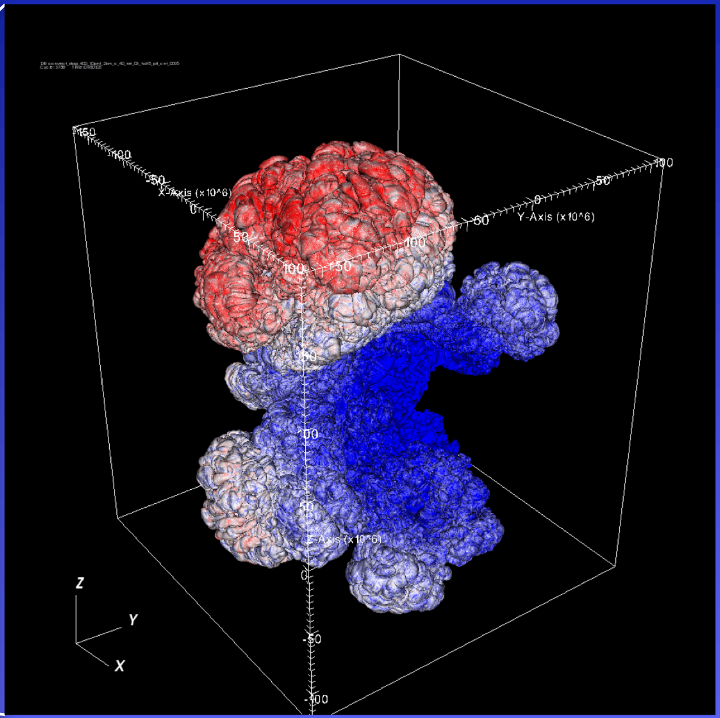
- Some of the brightest and most powerful explosions
- ***Standardizable*** cosmological distance indicators
- Probe the structure of the Universe and led to the discovery of dark energy (Nobel Prize in physics, 2011)
- Form most of the elements around us from O to Fe
- Currently no first-principles understanding, ***but…***

Powered by turbulent thermonuclear flames



Thermonuclear Type Ia supernovae
Combustion on an extreme scale



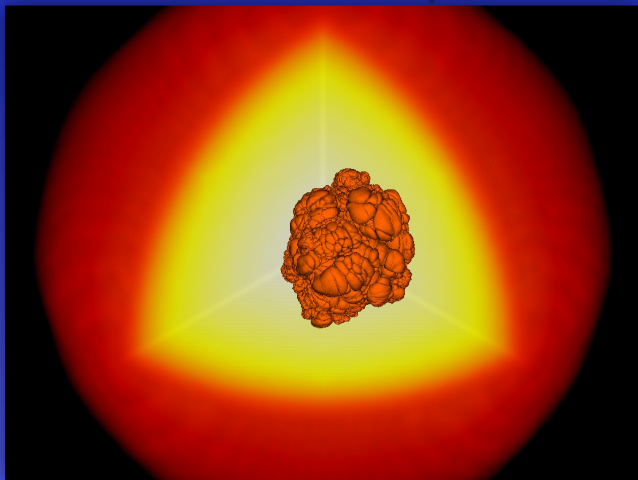


Aaron Jackson (calculation performed at ALCF/ANL under INCITE program)

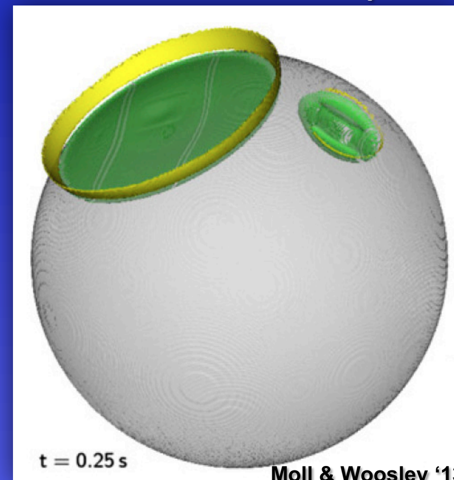
Spatial scales:	$10^{-4} - 10^{15}$ cm
Temporal scales:	$10^{-10} - 10^{6}$ s
Temperature:	$10^{10} - 10$ K
Density:	$10^{9} - 10^{-20}$ g/cc

Thermonuclear Type Ia supernovae
Modern explosion models

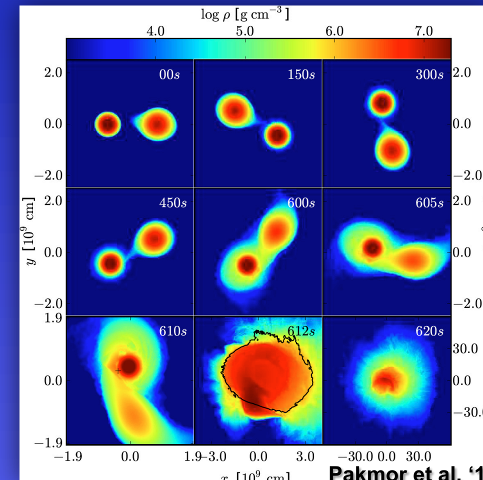
Single-degenerate, Chandrasekhar-mass white dwarf explosion



Single-degenerate, sub-Chandrasekhar-mass explosion



Double-degenerate merger



Critical velocity of gas expansion into vacuum

$$U_{crit} = \sqrt{\frac{2}{\gamma-1}}c_s > c_s, \text{ for degenerate relativistic plasmas } \gamma \sim 1.23 - 5/3$$

- Observations: virtually all stellar material undergoes combustion
- In order to burn supersonically expanding outer layers, a supersonic combustion front is required -> ***detonation***
- Detonation must form in an ***1) unconfined*** (no walls/boundaries), ***2) turbulent*** environment.

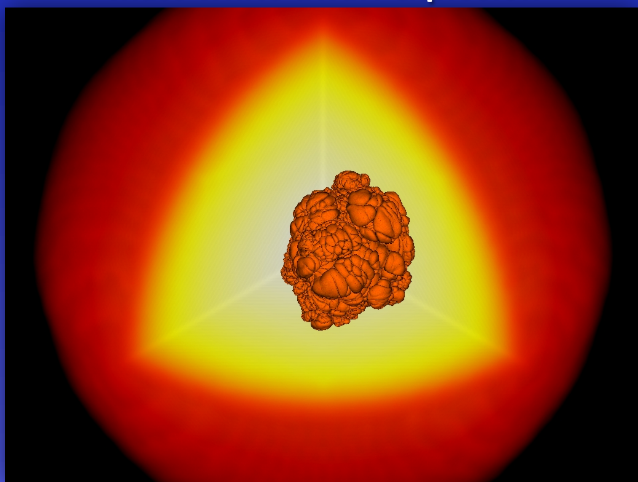
Lack of understanding of the mechanisms of detonation formation under such conditions is one of the main theoretical challenges of SN Ia theory

Extreme combustion regime: fast turbulence, large range of scales (Re)

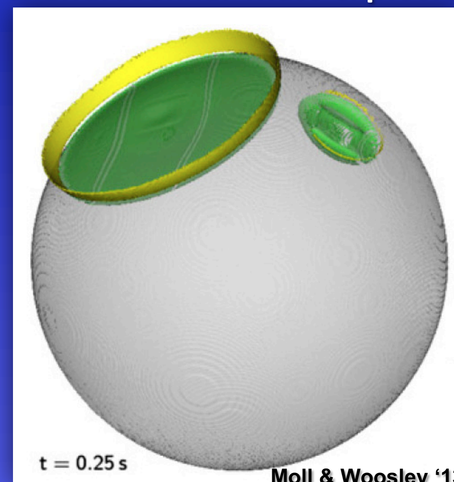
Thermonuclear Type Ia supernovae

Modern explosion models

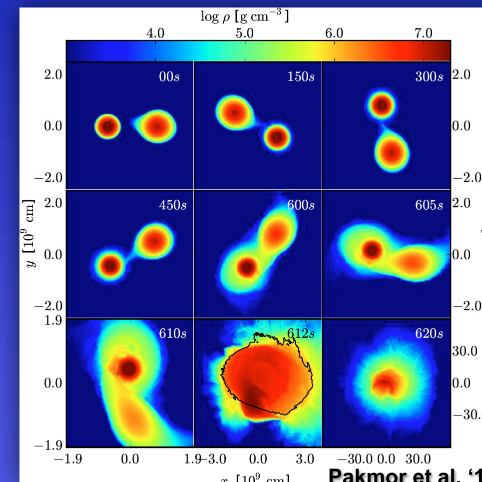
Single-degenerate, Chandrasekhar-mass white dwarf explosion



Single-degenerate, sub-Chandrasekhar-mass explosion



Double-degenerate merger



Unconfined Deflagration-to-DetonationTransition

Buncefield incident (2005)

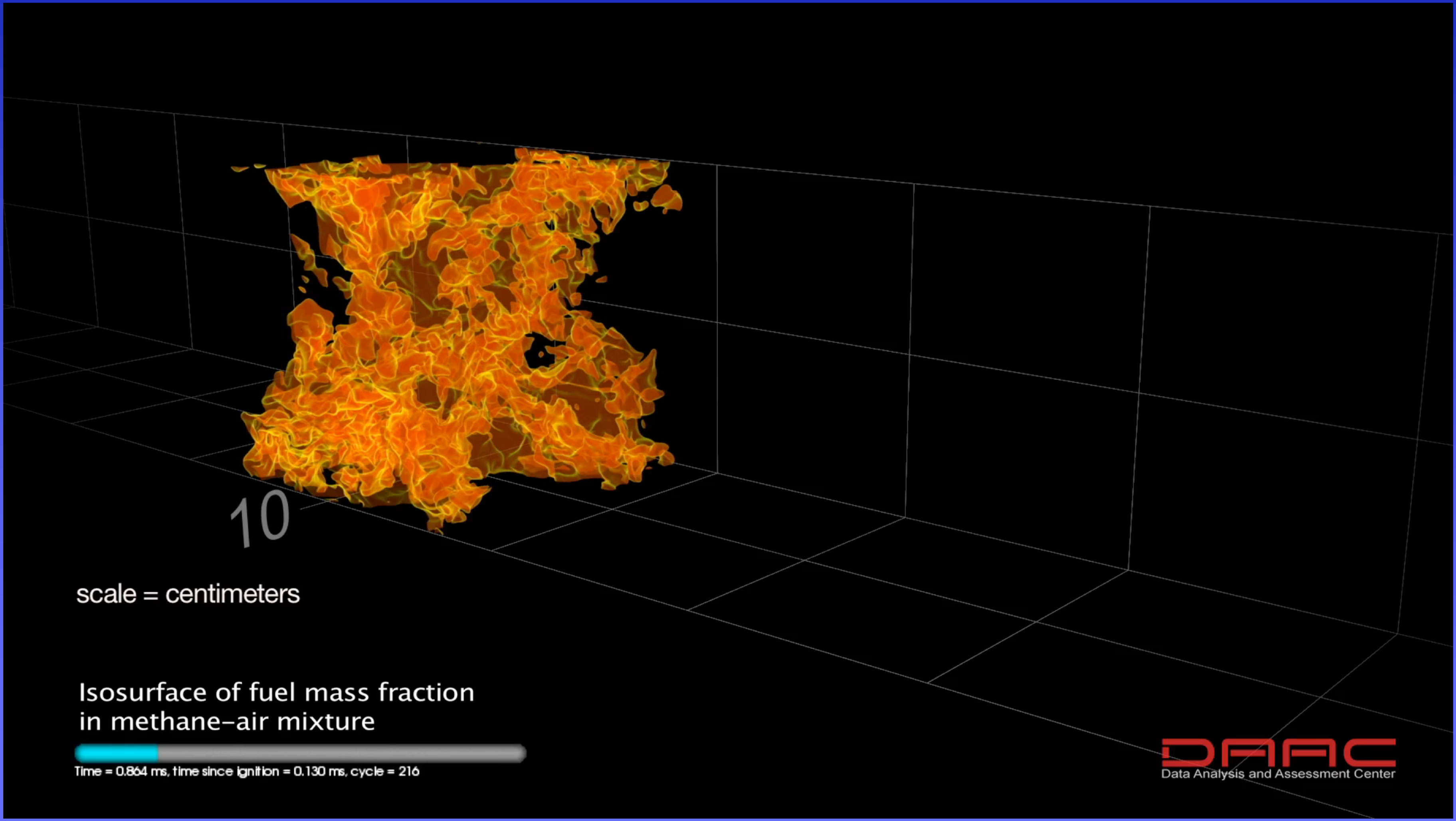
Jaipur incident (2009)

Fukushima incident (2011)

Extreme regime of high-speed reacting turbulence

Spontaneous deflagration-to-detonation transition

Poludnenko, Gardiner, & Oran PRL (2011); Poludnenko PoF (2015)



Extreme regime of high-speed reacting turbulence

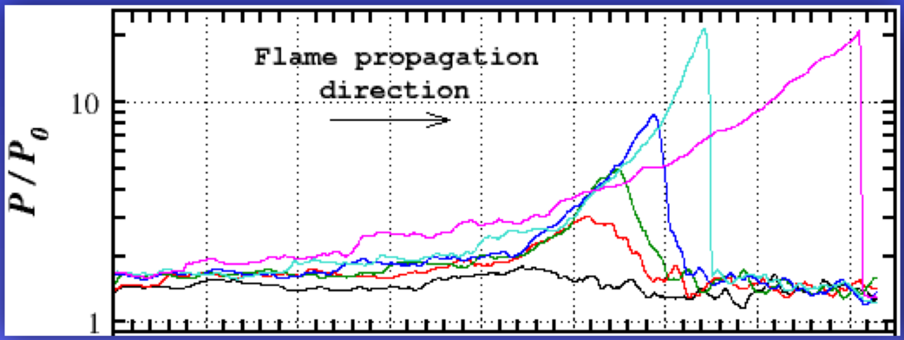
Spontaneous deflagration-to-detonation transition

AYP, Gardiner, & Oran PRL (2011); AYP PoF (2015)

Compressibility may arise because:

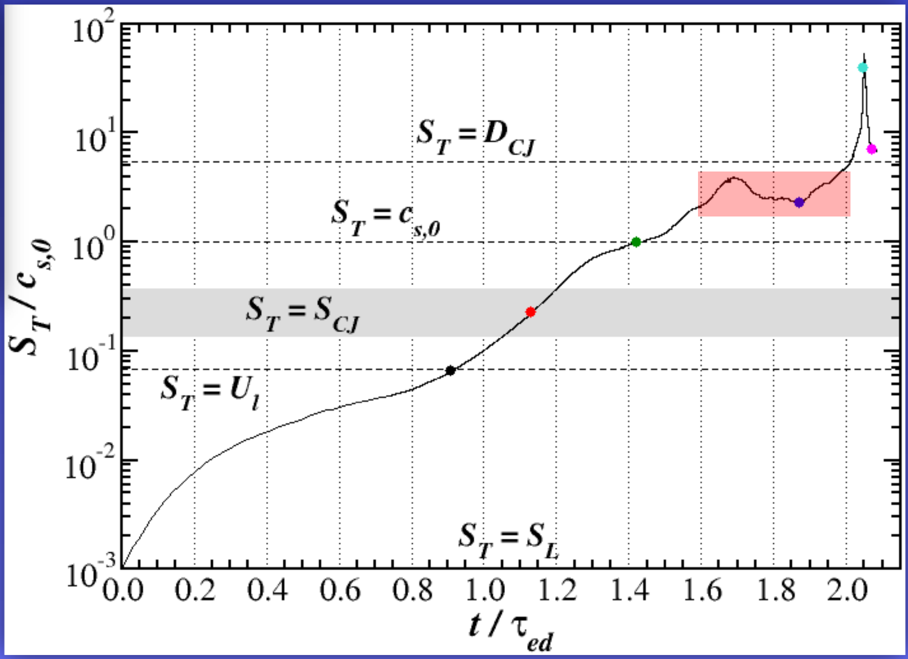
- ✓ ***the flow is fast:*** pressure gradients created by the flow: $Ma = \frac{U'}{c_s}$
- ✓ ***the reaction wave is fast:*** pressure gradients *(pressure increase!)* created by the combustion itself

$$CJ = \frac{S_T}{S_{CJ}} = \alpha\, Ma, \quad S_{CJ} = \frac{c_s}{\alpha}$$ **: Chapman-Jouguet deflagration speed**



Significant flame acceleration leading to DDT as the flame burning speed, S_T, approaches and then exceeds S_{CJ}

There was a period of ~ 0.14 ms of quasi-steady turbulent flame propagation with the speed of ~ 1 km/s (~ 14 cm)!

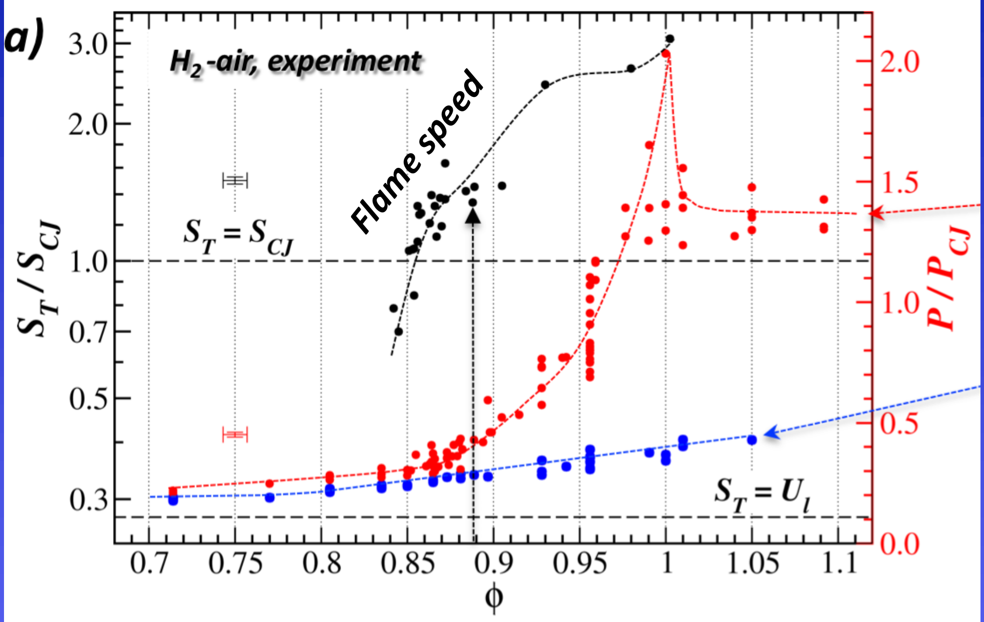


Aerospace Engineering, Texas A&M University

Is there experimental evidence of these effects?

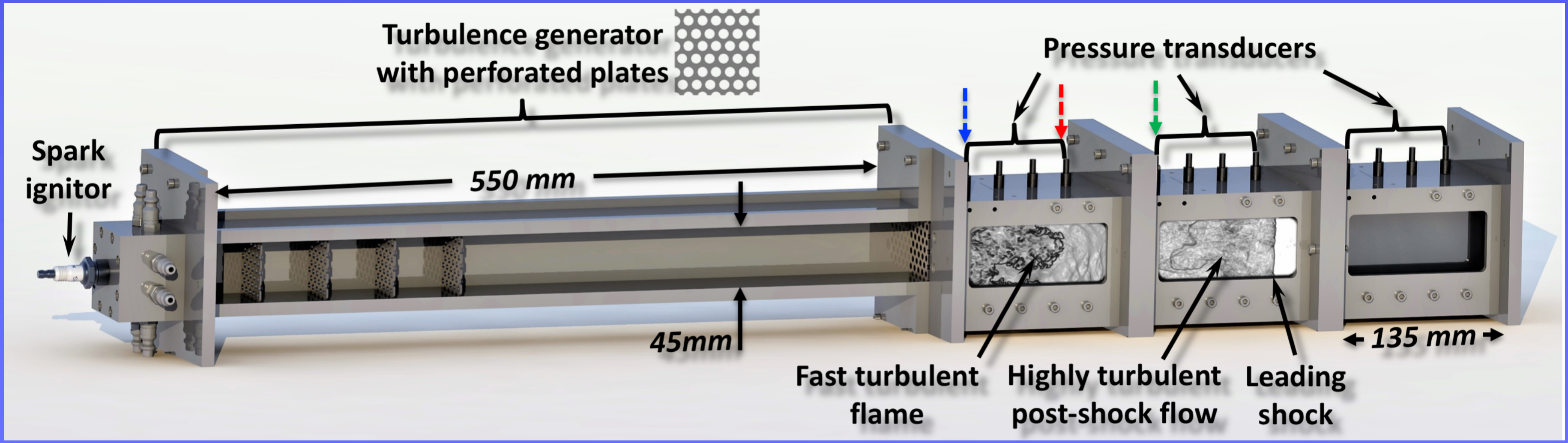
Turbulent Shock Tube, Kareem Ahmed, Univ. Central Florida

AYP+ Science (2019)
Chambers+ Comb. Flame (2019)



Flame-generated pressure

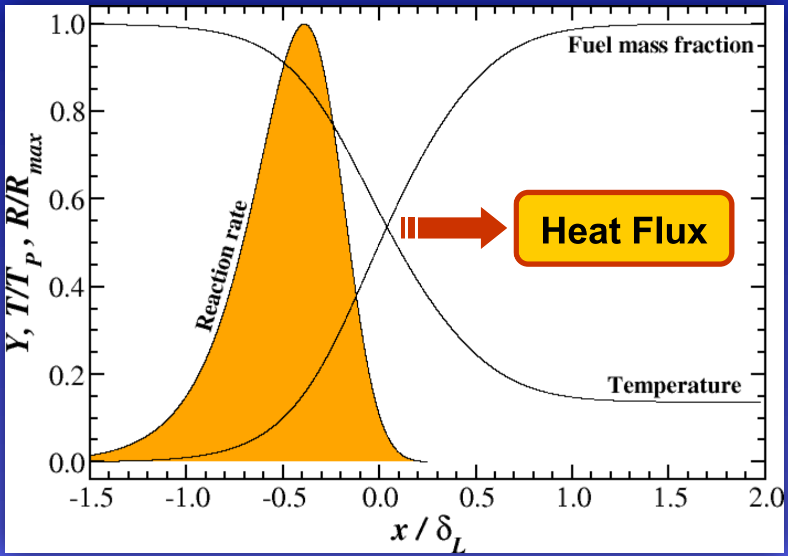
Global shock



Physical model

Athena - R$_{eacting}$ *F*$_{low}$ $_E$*X*$_{tensions}$

- **EOS (energy relaxation method)**
  - ideal gas
  - real gas (NASA 7-coefficient polynomials)
  - relativistic degenerate plasma (ideal-gas fully ionized ions, photons, relativistic degenerate electrons, electron-positron pairs, *Timmes & Arnett 99*)
- **Thermal conduction**
  - molecular (simplified T-dependent and real-gas)
  - degenerate electron (Timmes 00)
  - radiative (optically thick in degenerate electron gas)
- **Species diffusion and viscosity**
  - molecular (simplified T-dependent and real-gas)
- **Reaction kinetics**
  - *Chemical:*
    - ✓ Multiple single-step models
    - ✓ H_2 / H_2+CO / C1-C3 / n-dodecane / Cat C1 / Cat A2 / C_2H_4O / …
    - ✓ *Arbitrary kinetics via automatic code generator*
  - *Thermonuclear:* 13 isotope α-network from $^4He \Rightarrow {}^{56}Ni$



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

$$\frac{\partial (\rho \mathbf{U})}{\partial t} + \nabla \cdot (\rho \mathbf{U} \otimes \mathbf{U}) + \nabla P = \nabla \cdot \Pi + \mathcal{F} + \ldots$$

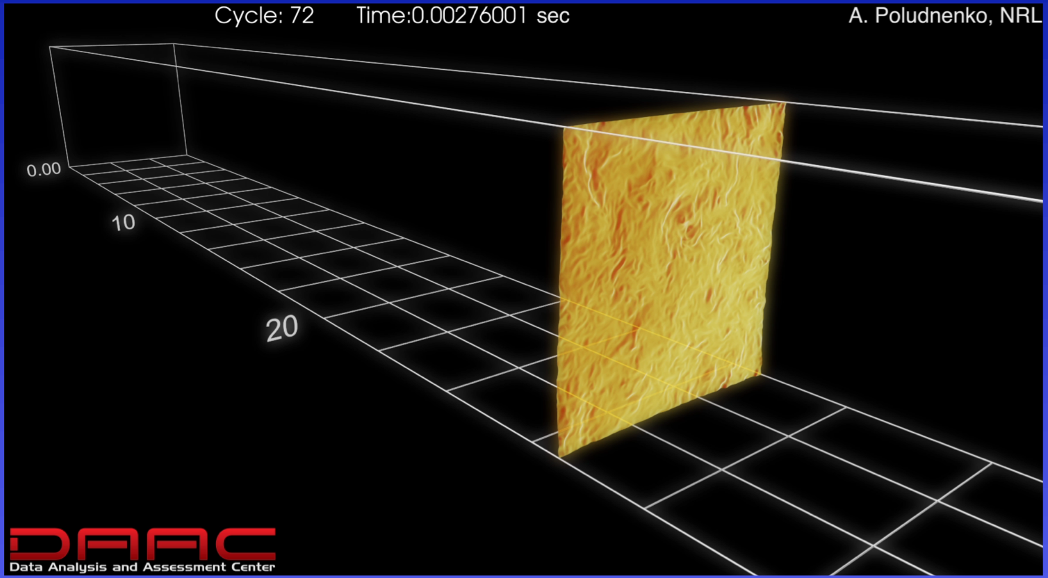
$$\frac{\partial E}{\partial t} + \nabla \cdot ((E+P)\mathbf{U}) - \nabla \cdot (K \nabla T) = \dot{S} + \nabla \cdot (\Pi \cdot \mathbf{U}) + \ldots$$

$$\frac{\partial (\rho Y)}{\partial t} + \nabla \cdot (\rho Y \mathbf{U}) - \nabla \cdot (\rho D \nabla Y) = \rho \dot{Y}$$

Chemical vs thermonuclear combustion

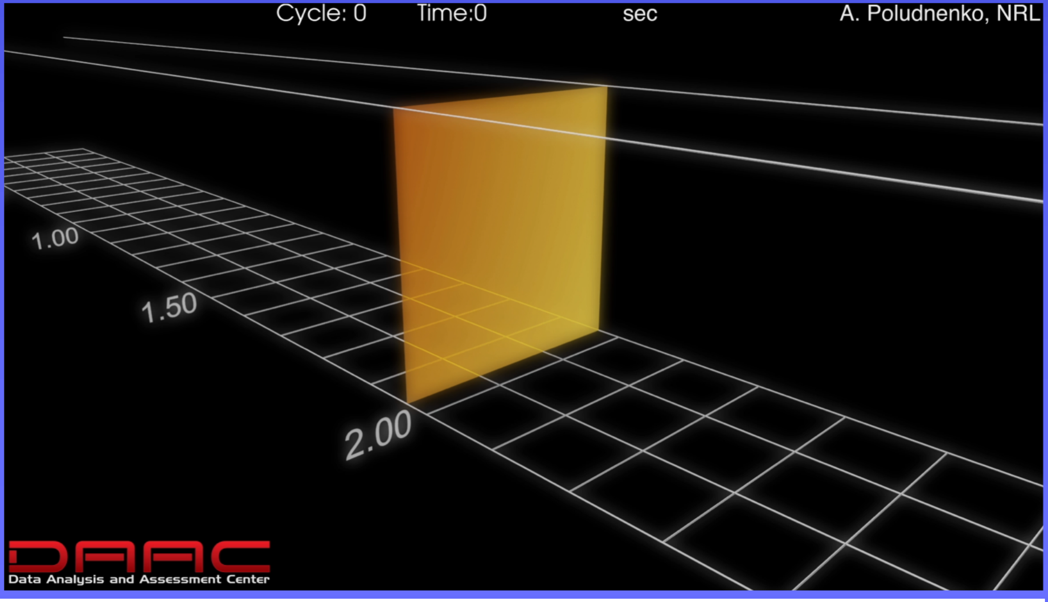
Chemical flame

- ***Stoichiometric H_2-air at 1 bar***
- Single-step chemistry
- Laminar flame width: ***3.2×10^{-2} cm***
- Laminar flame speed: ***1.5×10^{2} cm/s***
- Domain: ***4 cm × 4 cm × 132 cm***
- Simulation time: ***10 ms***
- **Domain/flame width: 85**
- **Damköhler number: 2.3**
- **Karlovitz number: 2.8**



Thermonuclear flame

- ***Pure ^{12}C at $\rho = 10^8$ g/cm^3***
- 13-isotope α-chain network
- Laminar flame width: ***3.6×10^{-3} cm***
- Laminar flame speed: ***2.3×10^{6} cm/s***
- Domain: ***0.3 cm × 0.3 cm × 5 cm***
- Simulation time: ***127 ns***
- **Domain/flame width: 128**
- **Damköhler number: 7.2**
- **Karlovitz number: 1.0**



Chemical vs. thermonuclear combustion

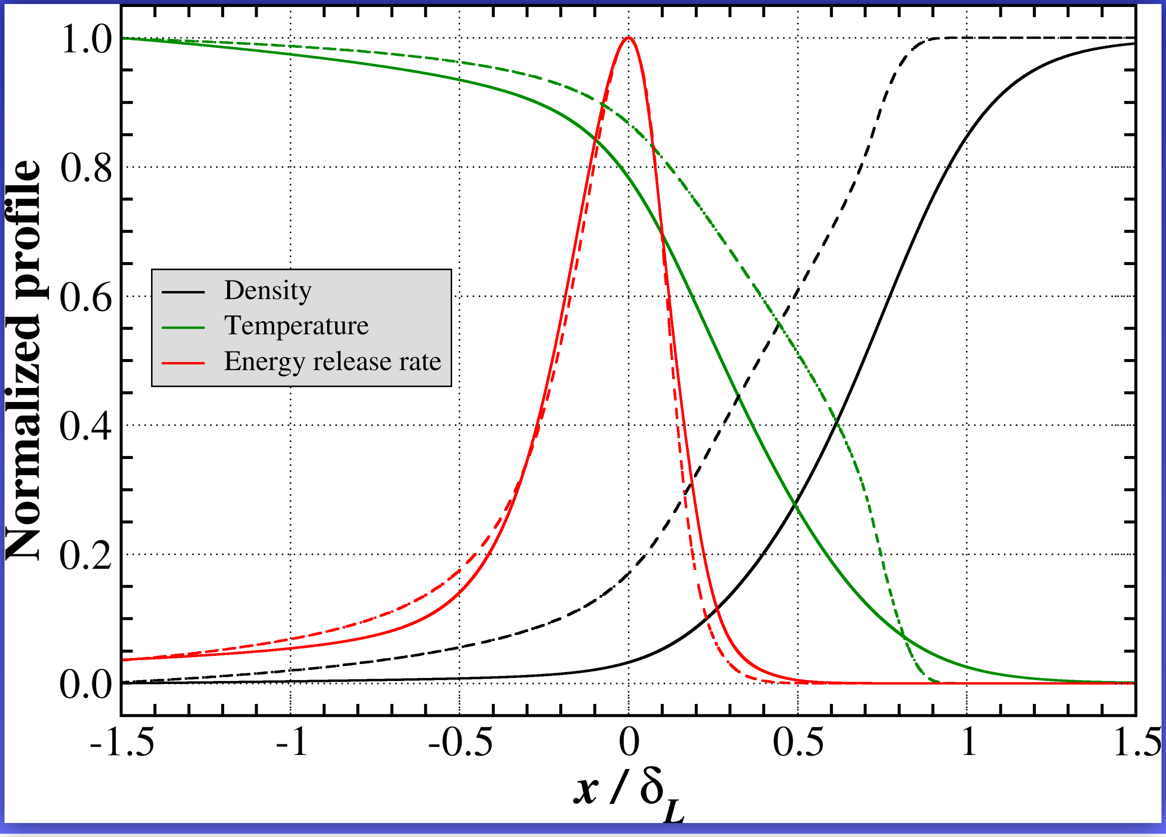
Comparison of the laminar flame structure in:

- stoichiometric jet-fuel/air – reduced mechanism, 1 bar (solid lines)

Laminar flame speed: 35 cm/s, *width: 0.04 cm*

- *50/50 $^{12}C/^{16}O$* – 13-isotope α-network, $\rho = 5\times10^{7}$ g/cm^3 (dashed lines)

Laminar flame speed: 1 km/s, *width: 0.05 cm*



Does this mechanism apply to thermonuclear flames?

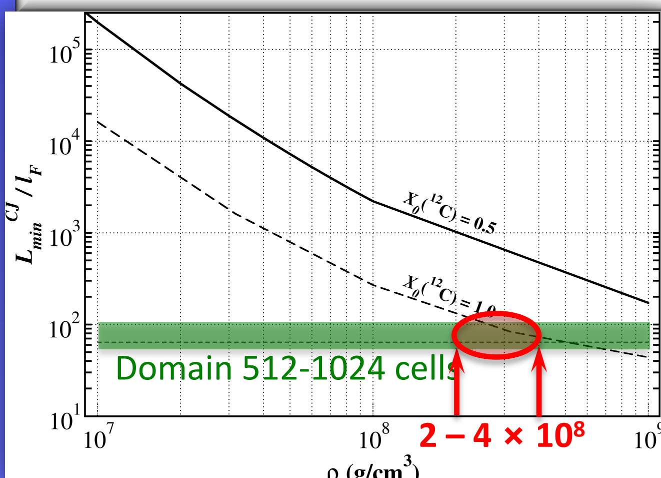
Critical conditions for DDT

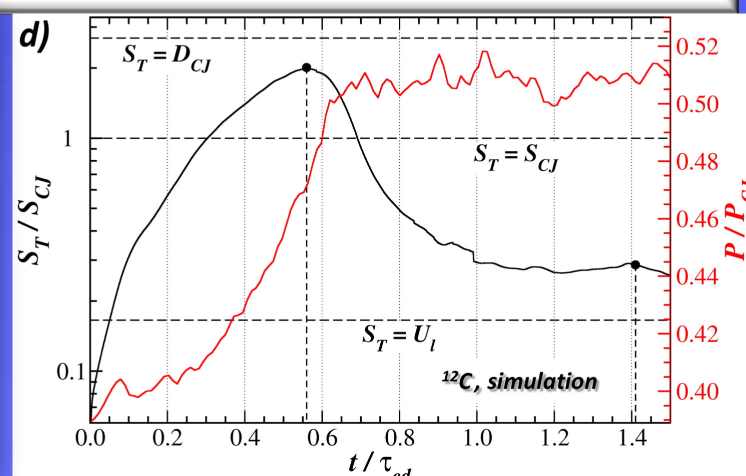
AYP+ Science (2019)

Minimum turbulent flame width	***Minimum integral velocity***, under 2 assumptions:
$L_{CJ}^{\min} = \dfrac{l_F c_s}{\alpha I_M S_L}$, $I_M = 1$ for Le = 1	➢ Kolmogorov cascade, $U_\lambda \sim \lambda^{1/3}$ ➢ Maximum flame surface density, $U_\delta \sim \alpha I_M S_L$ $U_l^{min} = (\alpha I_M S_L)^{2/3} c_s^{1/3}$

^{12}C flame, $\rho = 4\times10^8$ g/cc, $X_C = 1.0$

Domain width = L_{CJ}^{min}	$L_{CJ}^{min} = 0.02 \times 0.02 \times 0.34$ cm	
^{12}C zone width, δ_L	1.6×10^{-4} cm	4.1 cells
Laminar flame speed, S_L	1.15×10^{7} cm/s	**1.7% of $c_{s,0}$**
CJ deflagration speed, S_{CJ}	4.8×10^{8} cm/s	**69% of $c_{s,0}$**
Turbulent integral velocity, $U_l = 4U_{CJ}$	8×10^{7} cm/s	**12% of $c_{s,0}$**





What does all this mean for SN Ia?

AYP+ Science (2019)

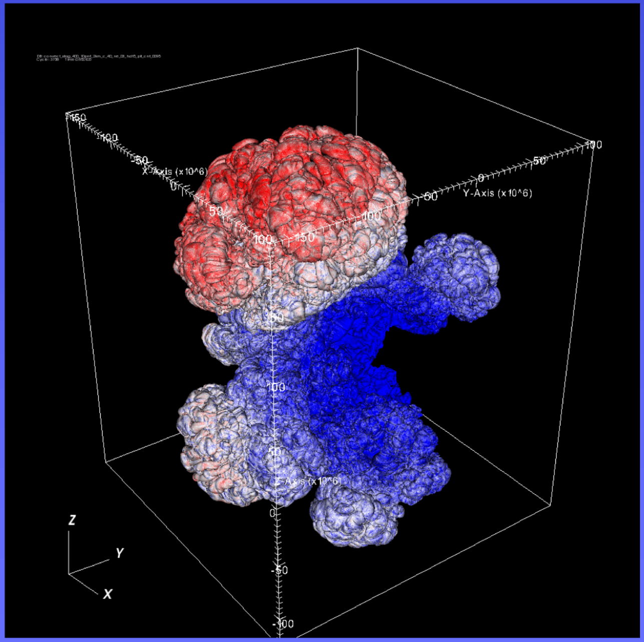
Classical Chandrasekhar-mass explosion scenario

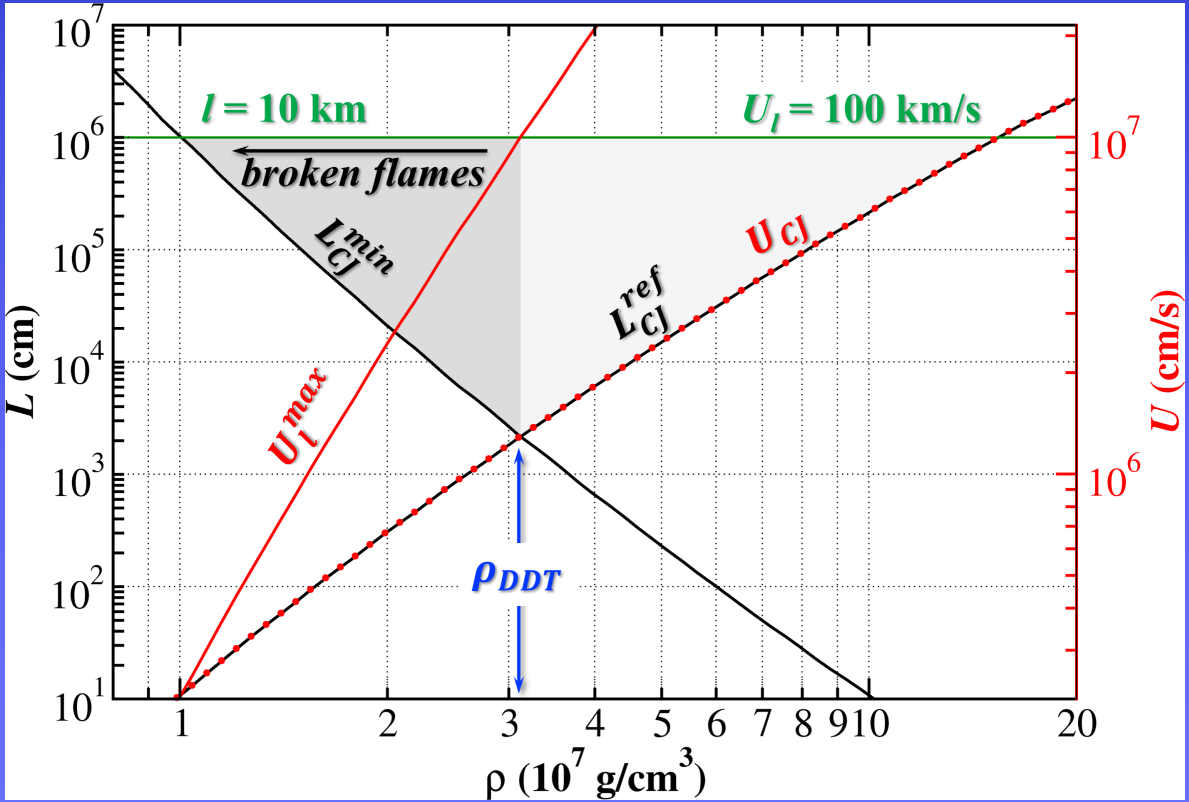
Maximum probability of the transition density (50/50 C/O)

$\rho_{DDT} \approx 3\times10^{7}\, g/cc$ ***(No free parameters in the model !)***

Probability of DDT in 10 x 10 x 10 km region: 10^{10} !!!

Future work: other compositions and explosion scenarios





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Some future development in Athena and Athena++

Yoram Kozak & Sai Sandeep Dammati (Texas A&M), Chris Stone (PETTT)

Multi-phase flows

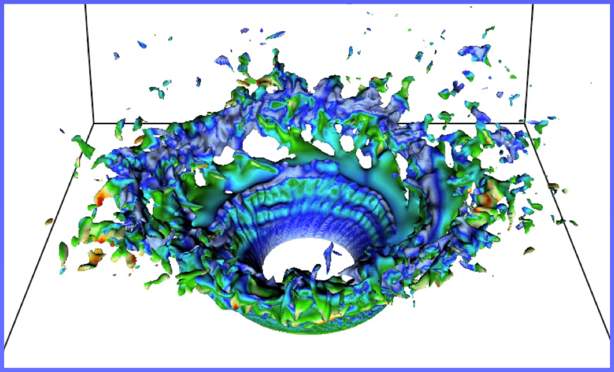
- ✓ Massive particles with feedback
- ✓ Atomization
- ✓ Evaporation
- ✓ Surface burning
- ✓ Electric charge / plasma effects

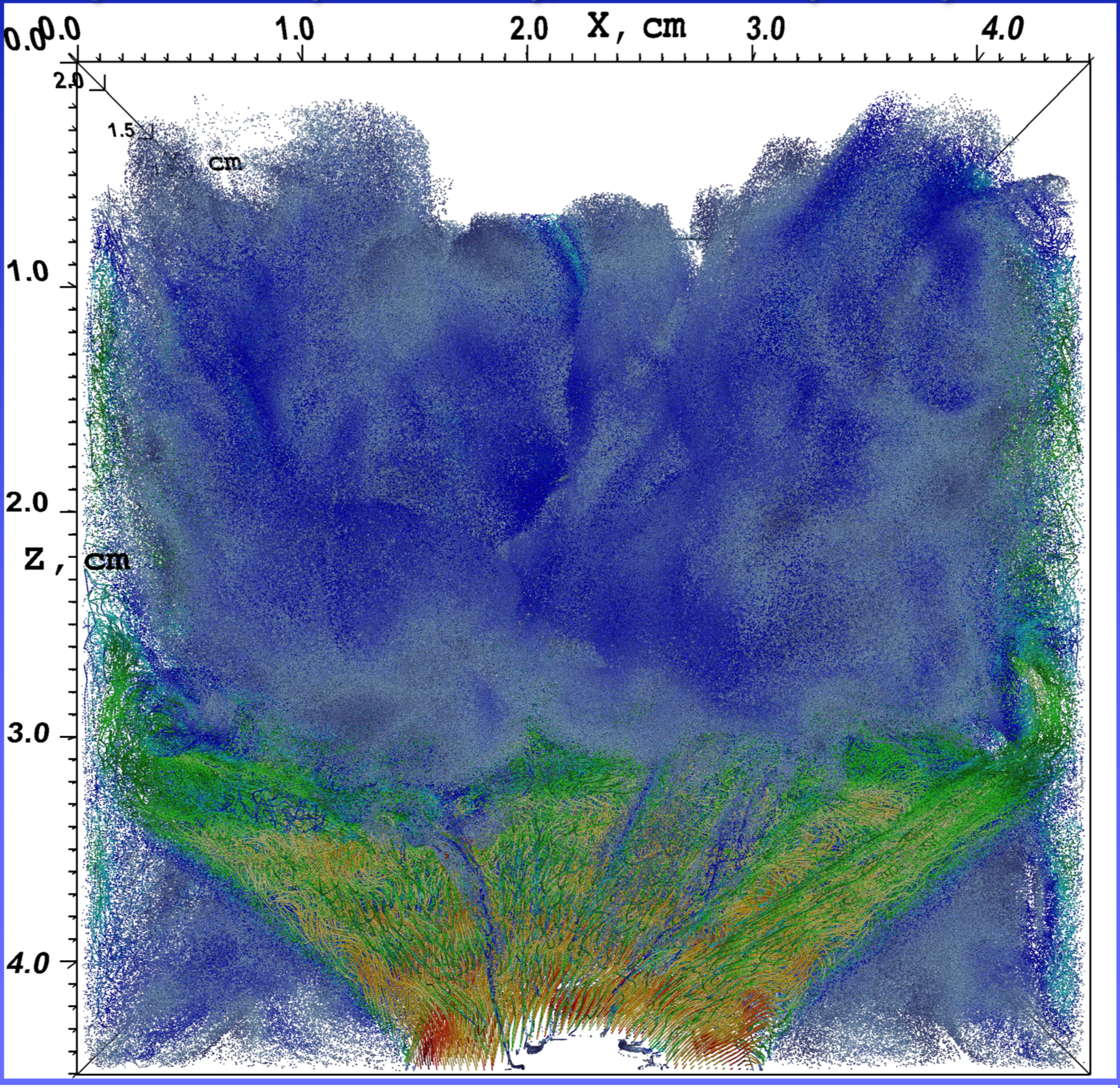
Complex geometries

- ✓ Ghost-cell immersed boundaries
- ✓ Multi-block capability

Large-Eddy Simulation Models

- ✓ Explicit / implicit filtering
- ✓ Turbulence SGS models





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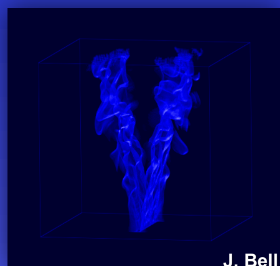

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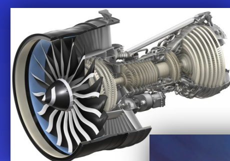


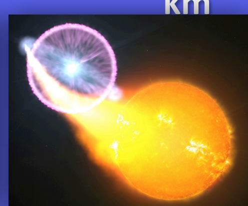
Propulsion and power generation


Industrial accidents

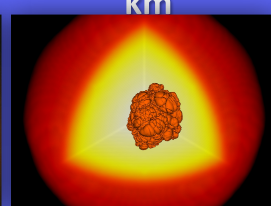
Thank you!

10^5 cm 1km | 10^6 cm 10 km | 10^7 cm 100 km | 10^8 cm 1000 km | 10^{11} cm 1 solar radius | 10^{14} cm 10 au | 10^{19} cm 10 ly | … | …

Neutron star X-ray bursts

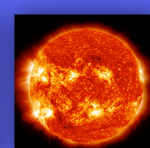
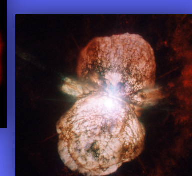
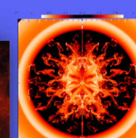


Classical novae



Type Ia supernovae

Explosive burning

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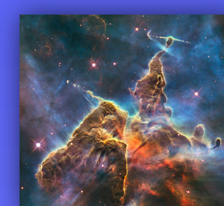
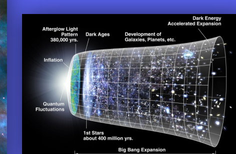


Star-forming regions

Dust formation



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Electroweak phase transition