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Fire Science & Technology

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SIERRA/Fuego validation works for DNS, LES, and solid pyrolysis models

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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SIERRA/Thermal-Fluid/Fuego

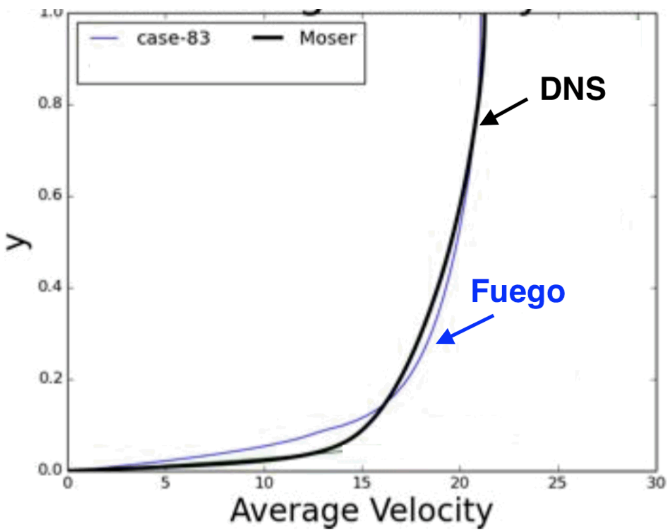
- SIERRA: Sandia's engineering mechanics simulation code suite
  - Solid mechanics: Adagio, Presto
  - Structural dynamics: SD
  - Thermal-fluid: Aria, Arpeggio, Aero, **Fuego**, Syrinx
  - Tools: Encore, Percept, STK, & python scripts
- Fuego: low-Ma, turbulent combustion flow solver
  - Various RANS and LES models
    - Smagorinsky-type and K_{SGS} LES models
  - Two turbulent combustion models
    - EDC with fast chemistry and flamelet
  - Unstructured (co-located)
    - Requires some level of numerical dissipation; prefers hexahedron
  - Finite element
  - Insufficient amount of LES validation works has been performed

List of Validation Works

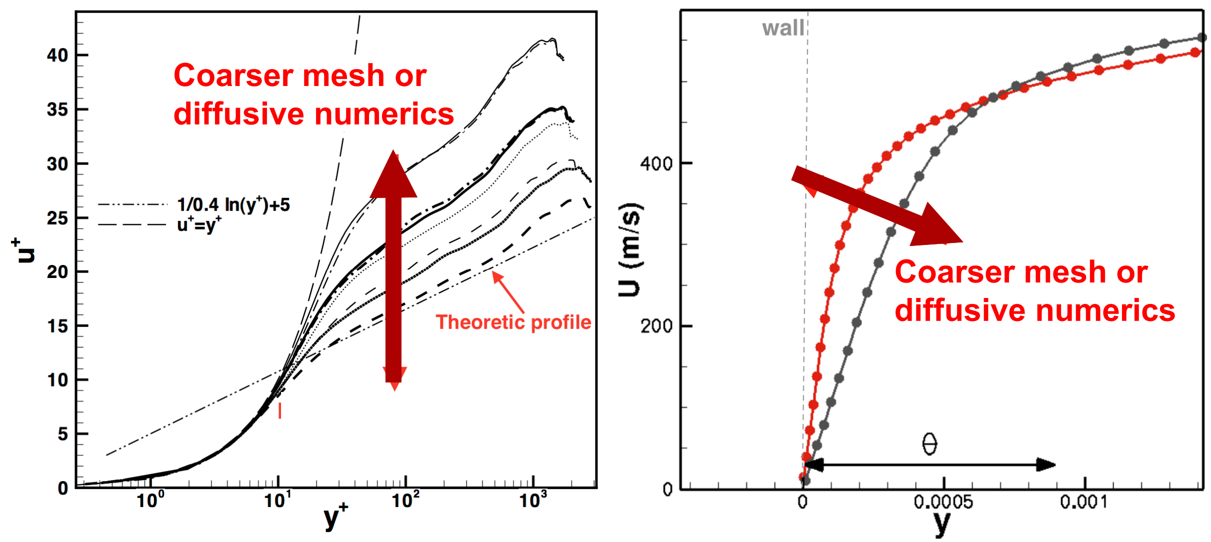
- DNS
  - Channel
  - Pipe
- LES
  - Channel
  - Round jet
- Solid combustion
  - TGA
  - Heated panel

Previous Channel LES

- LES without wall model was tested on a channel using wall-resolved mesh
  - Result was similar to that from coarse resolution or diffusive numerics
  - Not enough efforts were made to fix or understand why



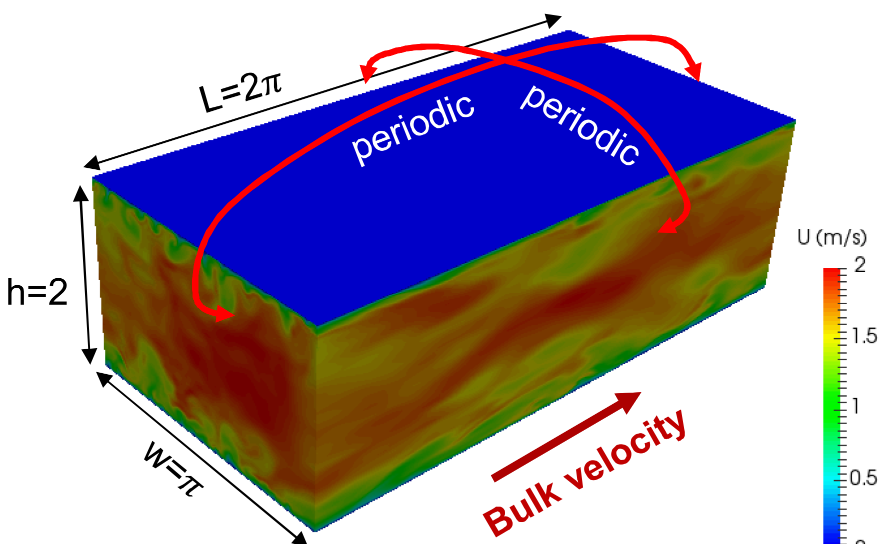
Channel LES without wall model (SAND2015-7938)



Known effect of resolution and numerics in turbulent boundary layer (H. Koo thesis)

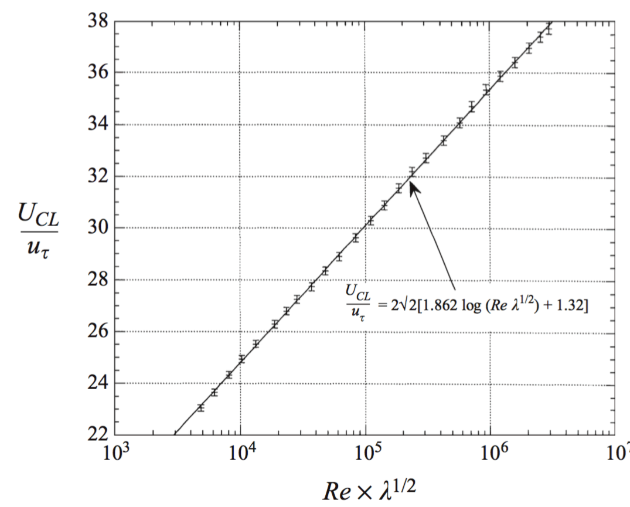
DNS of a Channel

- Target Re_b~13000, Re_τ~400
  - $Re_b=\rho U_{mean}h/\mu$; $Re_\tau=\rho U_\tau(h/2)/\mu$
  - $h=Re_\tau^+$; half height is 400+
  - I.C.: laminar profile + randomness
  - Central differencing is used
  - Collect statistics after flow becomes statistically stationary



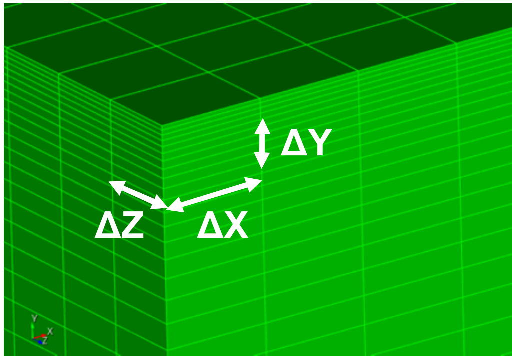
Re vs Re$_\tau$

J. Kim, 2011

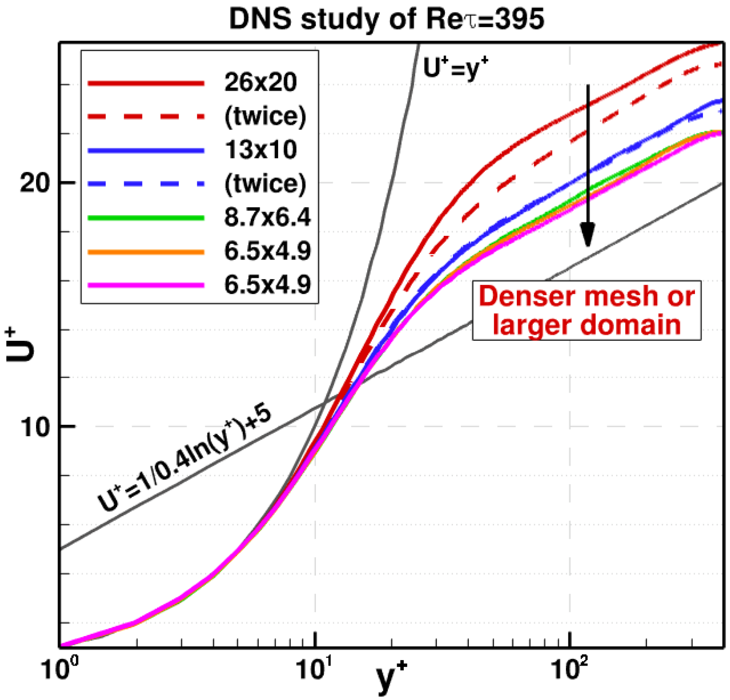


Structured Mesh

- Denser mesh or larger domain improves the result
- Mean velocity does not reach theoretical profile
- Cell aspect ratio could be the reason, near wall or at the center



ΔX	ΔY (+)	ΔZ	Mesh	Re_b	Re_τ
26	1.08-40	20	0.4M, 96x72x64	21500	391
Twice the domain size			1.7M	17400	392
13	0.68-40	10	2.0M, 192x80x128	16700	403
Twice the domain size			7.9M	16200	394
8.7	0.68-40	6.4	4.5M, 288x80x196	15700	398
6.5	1.08-40	4.9	7.1M, 384x72x256	15400	393
6.5	0.68-40	4.9	7.9M, 384x80x256	15500	392



Layered Mesh

- Denser mesh or larger domain improves the result
- Mean velocity does not reach theoretical profile
- Cell aspect ratio could be the reason, near wall or at the center
- Wedge-shape cell layers are placed to ensure cell AR < 6 everywhere

ΔX	ΔY (+)	ΔZ	Mesh	[illegible]	[illegible]
26	1.08-40	20	0.4M, 96x72x64	[illegible]	[illegible]
Twice the domain size			1.7M	[illegible]	[illegible]
13	0.68-40	10	2.0M, 192x80x128	[illegible]	[illegible]
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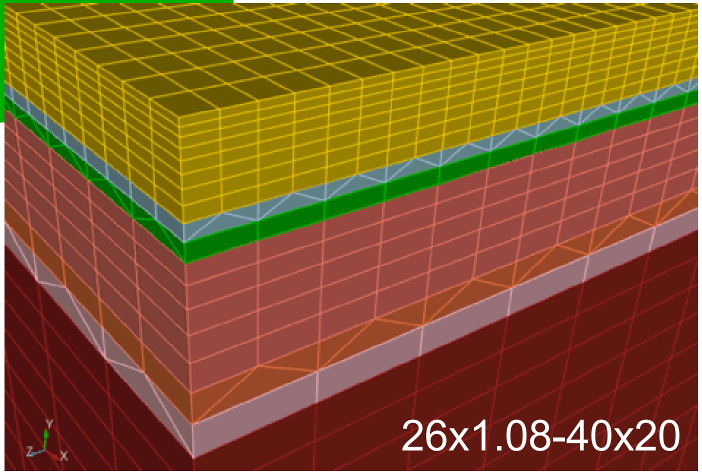
6.5 -26	1.08-40	4.9-20	4.0M, layered	12300	400

Near wall resolution: 6.5x1.08-40x4.9



Layered Mesh

- Denser mesh or larger domain improves the result
- Mean velocity does not reach theoretical profile
- Cell aspect ratio could be the reason, near wall or at the center
- Wedge-shape cell layers are placed to ensure cell AR < 6 everywhere
- Result now matches to other channel DNS

ΔX	ΔY (+)	ΔZ	Mesh	Re_b	Re_τ
26	1.08-40	20	0.4M, 96x72x64	21500	391
Twice the domain size			1.7M	17400	392
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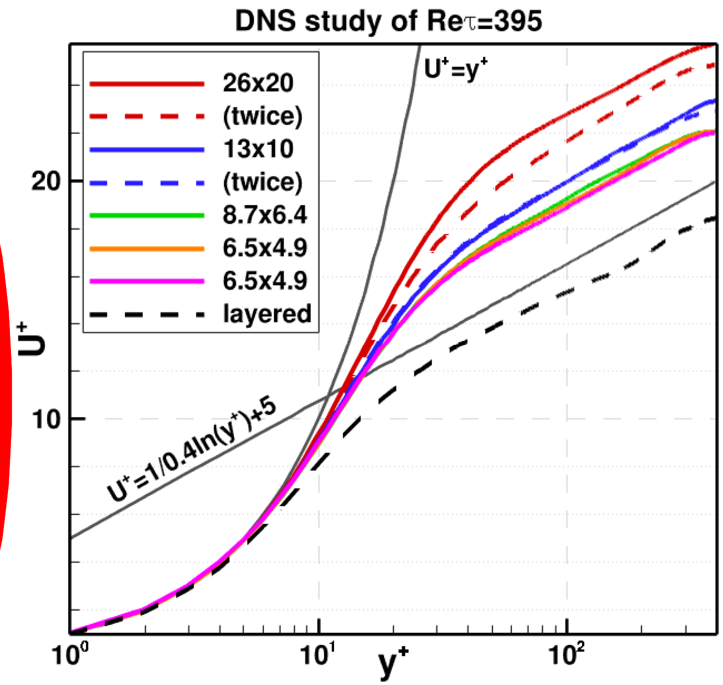
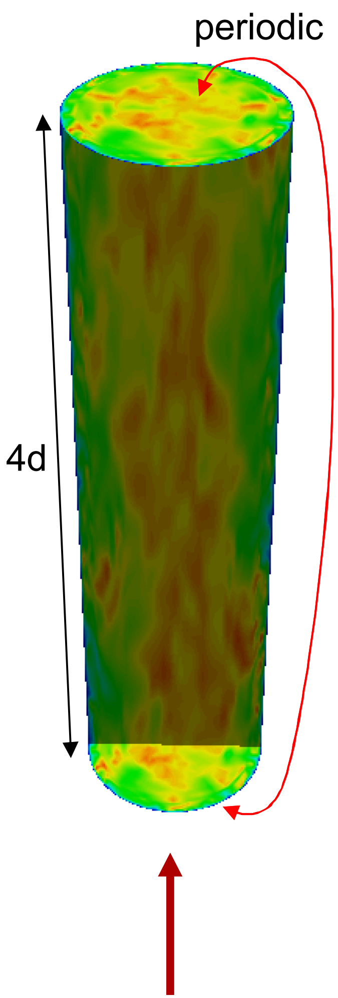


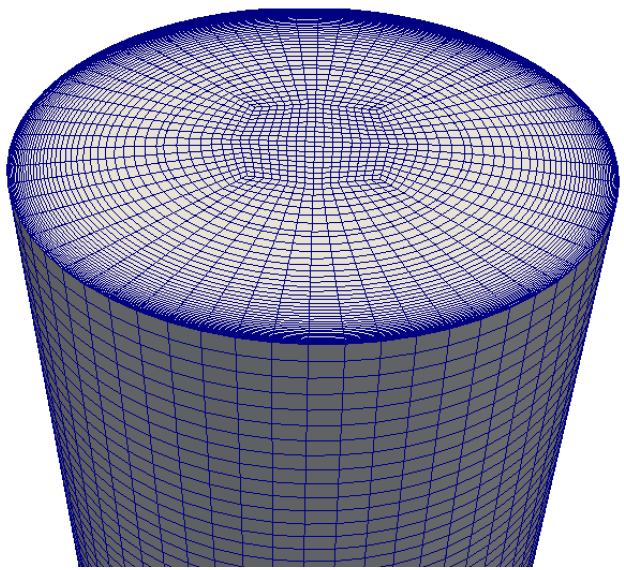
DNS of a Pipe

Sandia National Laboratories

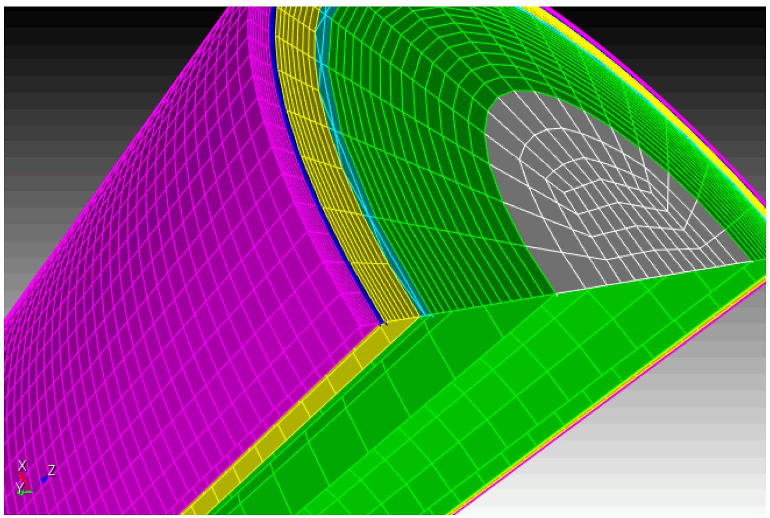


nx	nr	nθ	Total
128	~50	64	0.4M
256	~55	128	1.8M
64-256	~50	32-128	0.5M (layered)
128-512	~55	64-256	2.0M (layered)

0.4M mesh



Layered 0.5M mesh



Similar Behavior

nx	nr	nθ	Total
128	~50	64	0.4M
256	~55	128	1.8M
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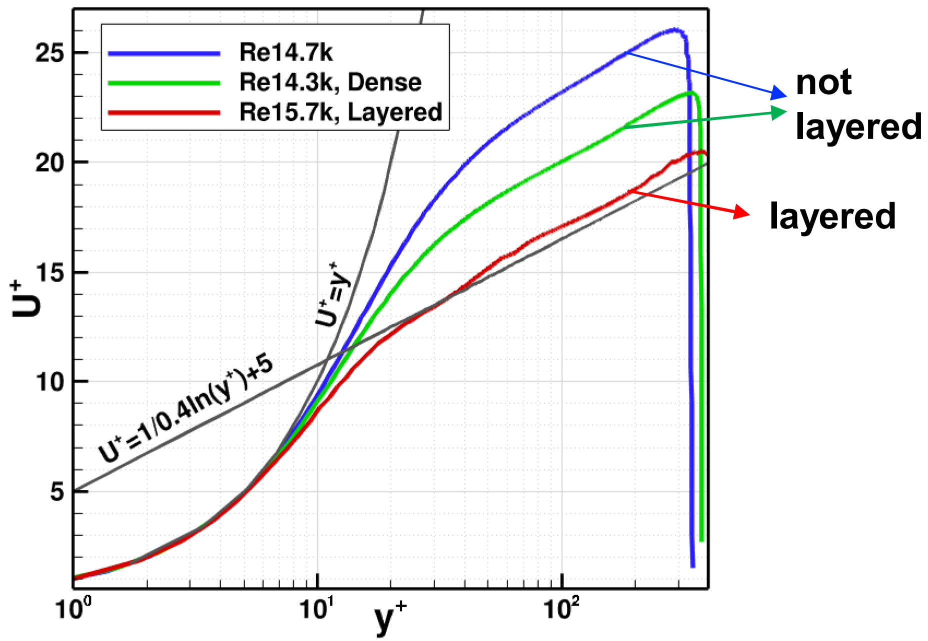
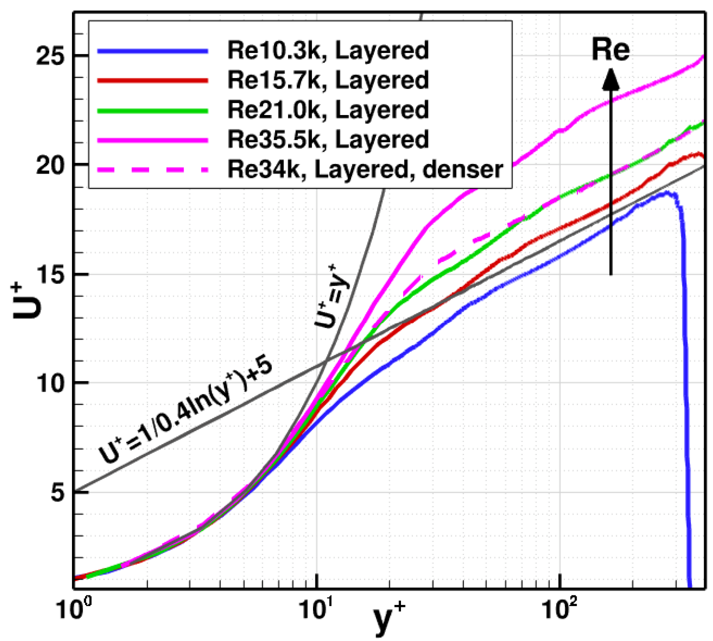




Summary so far

- DNS was performed on canonical problems
  - Being a generalized solver, mesh requirement is tighter
  - Sensitive to grid aspect ratio
  - Theoretical velocity profiles were obtained with a layered mesh

LES on Wall-Bounded Flows

- K_{SGS} model solves transport equation of subgrid kinetic energy

$$\int \frac{\partial \bar{\rho} k^{\mathrm{sgs}}}{\partial t} \mathrm{d}V + \int \bar{\rho} k^{\mathrm{sgs}} \tilde{u}_j n_j \mathrm{d}S = \int \frac{\mu_t}{\sigma_k} \frac{\partial k^{\mathrm{sgs}}}{\partial x_j} n_j \mathrm{d}S + \int \left(P_k^{\mathrm{sgs}} - D_k^{\mathrm{sgs}}\right) \mathrm{d}V$$

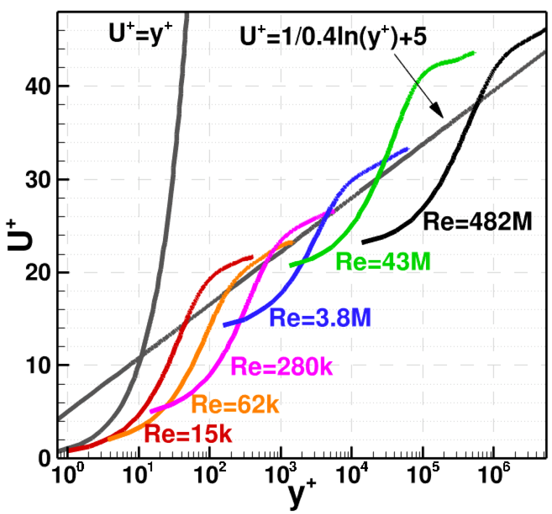
$$\mu_t = \rho C_\mu \Delta k^{sgs \frac{1}{2}}$$

cf> Smagorinsky-type: $\mu_t = \rho \left(C_s \Delta\right)^2 |\tilde{S}|$

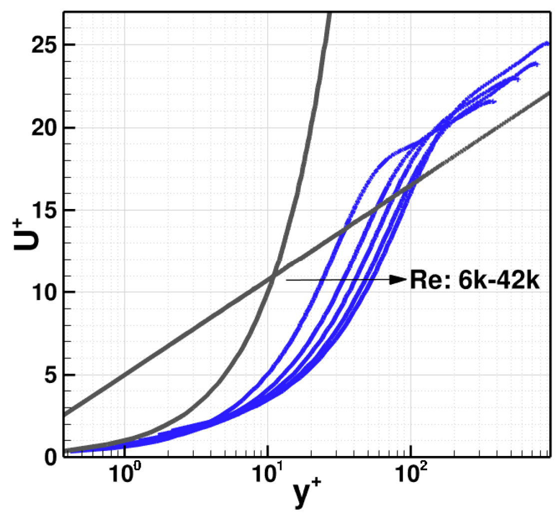
  - An equilibrium wall model is available with K_{SGS} model

- Velocity approaches log-law profile even at large Re

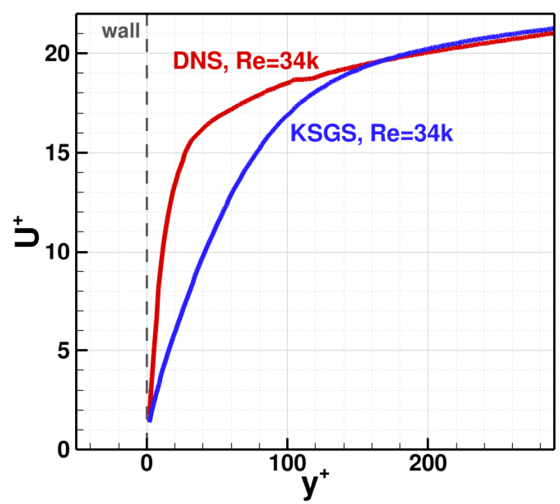
Channel



Pipe



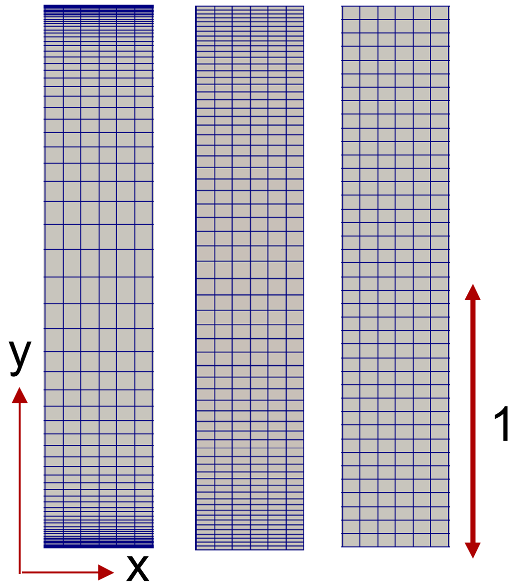
Pipe, not in log scale

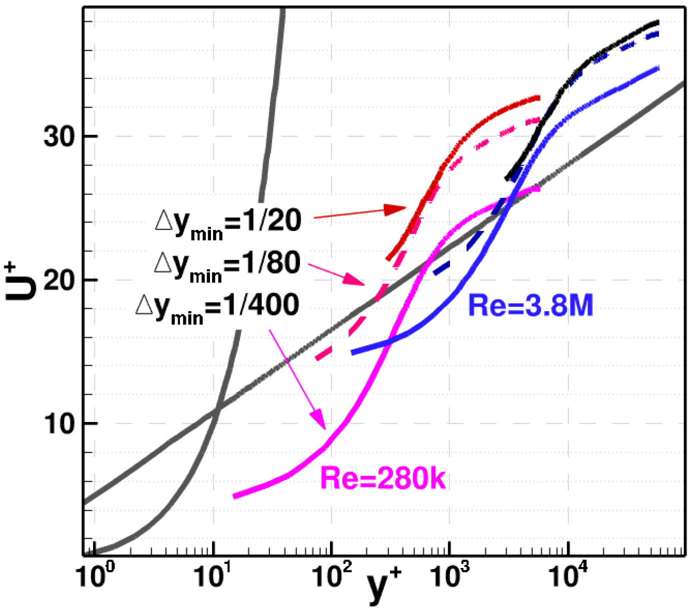


Resolution Yield Test

- For K_{SGS}, wall shear stress reduces to below expected value without a wall resolved mesh
  - Coarse resolution results are still acceptable

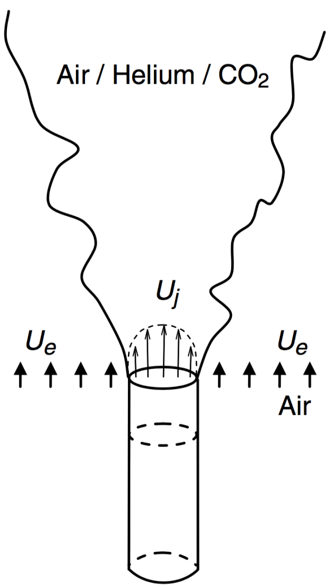
Δy_{min}= 1/400, 1/80, 1/20

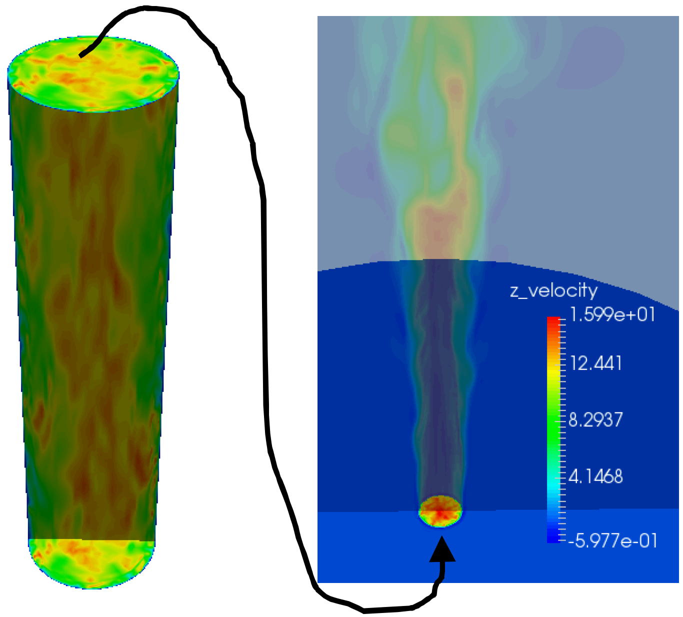




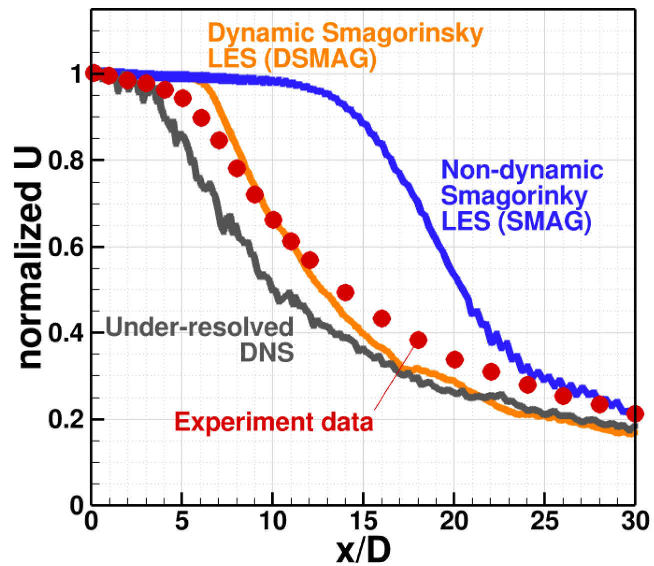
LES on a Jet

- Fully developed turbulent pipe is incorporated into a jet LES
  - Many jet experiments use a long pipe to eliminate BC uncertainties
  - Useful for comparing near exit profiles, predicting lift-off flame for a moderate Re jet
- Dynamic Smag. found superior than other approaches





Time-varying inflow boundary condition from a fully-developed turbulent pipe



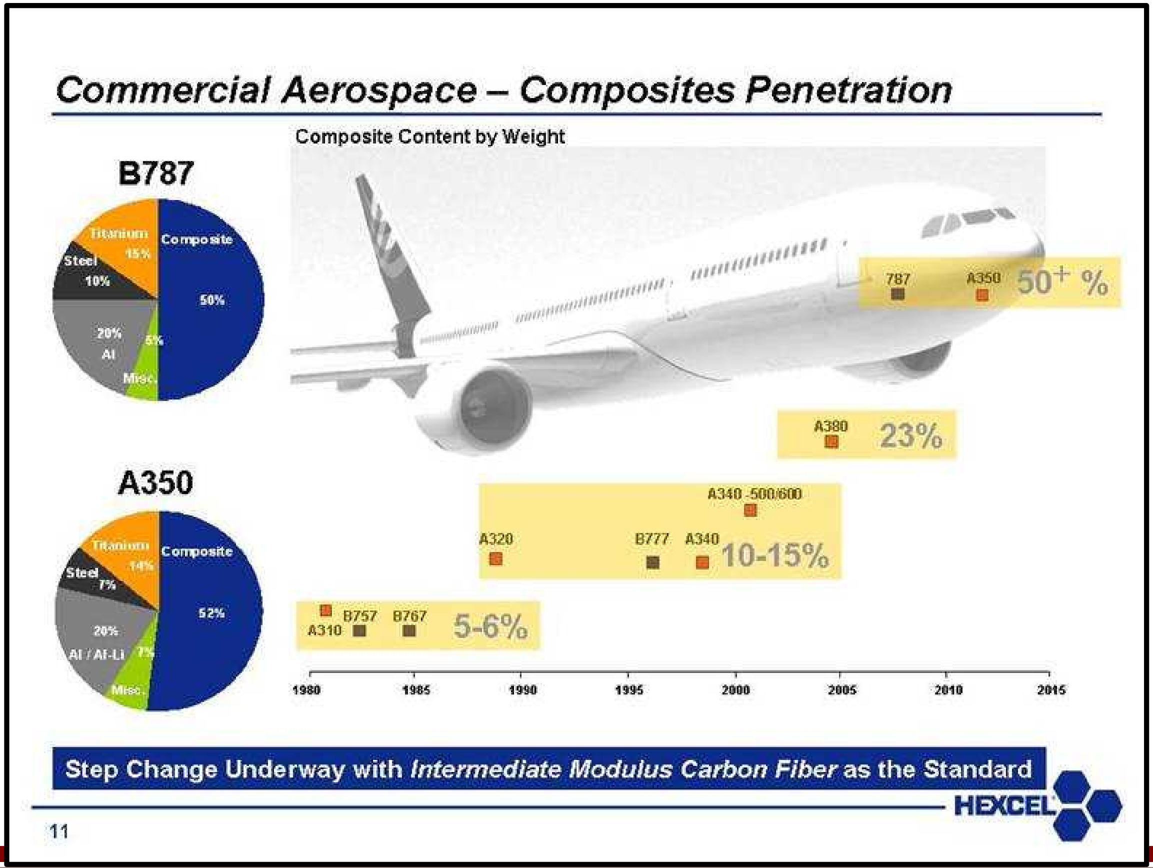
Centerline velocity

Summary so far

- DNS was performed on canonical problems
  - Being a generalized solver, mesh requirement is tighter
  - Sensitive to grid aspect ratio
  - Theoretical velocity profiles were obtained with a layered mesh
- LES models work as expected
  - K_{SGS} performance is not too sensitive to the mesh resolution near wall, thereby can be used for a wide range of problems
  - Jet breakdown is well predicted using dynamic Smagorinsky model

Composites in the Aviation Industry

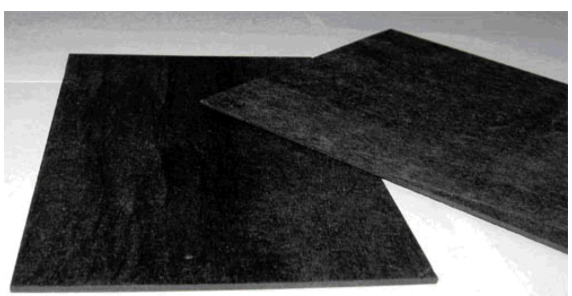
- Modern aircraft uses increasing quantities of composites
  - Reduce weight while preserving strength
  - Lower fuel consumption: efficiency ↑, emission ↓



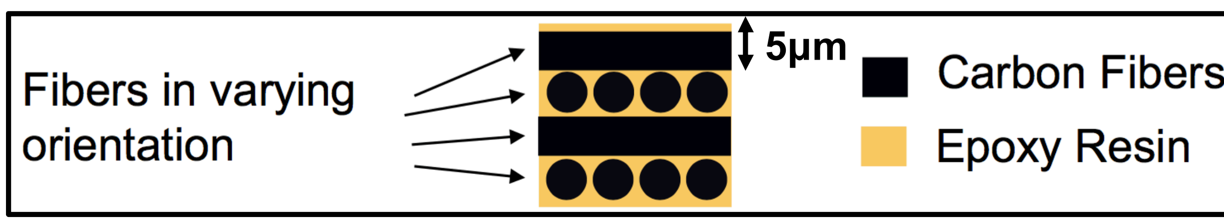
from hexcel.com

Composites in the Aviation Industry

- Modern aircraft uses increasing quantities of composites
  - Reduce weight while preserving strength
  - Lower fuel consumption: efficiency ↑, emission ↓
- Carbon fiber-epoxy materials are heavily used in new design
  - 65% carbon fiber, 35% epoxy resin
  - Fabric (woven) or uni-tape sheets, in multiple layers thick
  - Woven CYTEC 977-3, cured in 1 atm oven with IM7 fibers, is tested

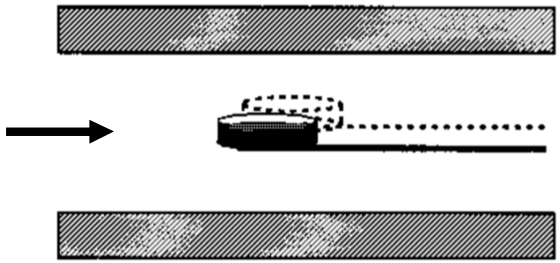


from utsi.edu

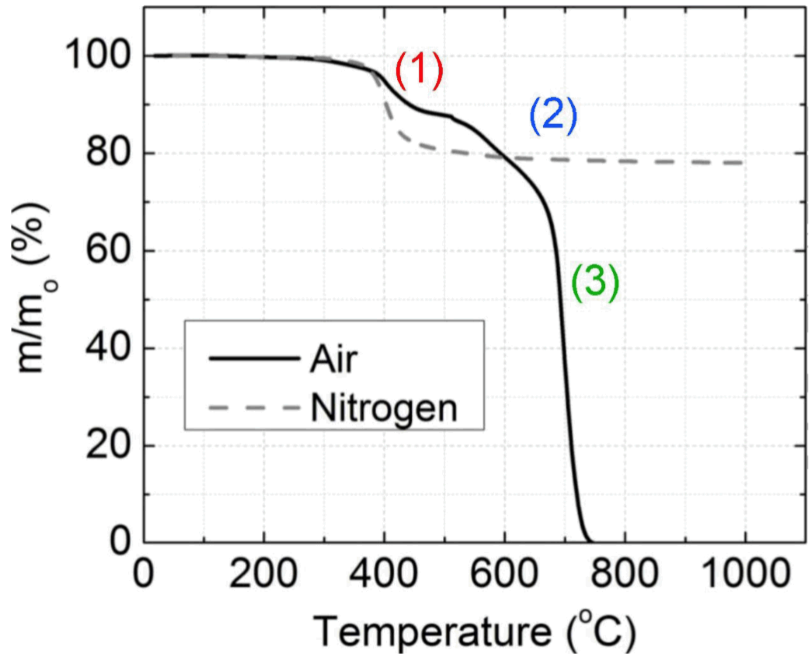


TGA Study

- $20^oC/min$
- Epoxy pyrolysis generates gaseous fuel and char
- In air, epoxy oxidizes before char and carbon fiber



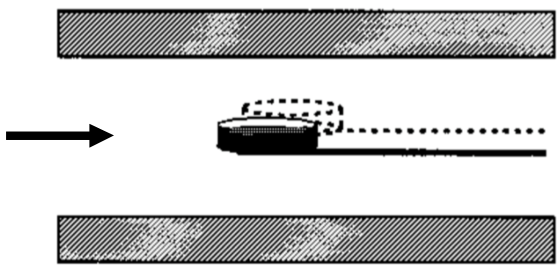
Dodd et al. (2013), Brown et al. (2012)



(1) Epoxy Decomposition (both Thermal and Oxidative Pyrolysis) and Char Formation
(2) Slow Char Oxidation
(3) Carbon Fiber Oxidation

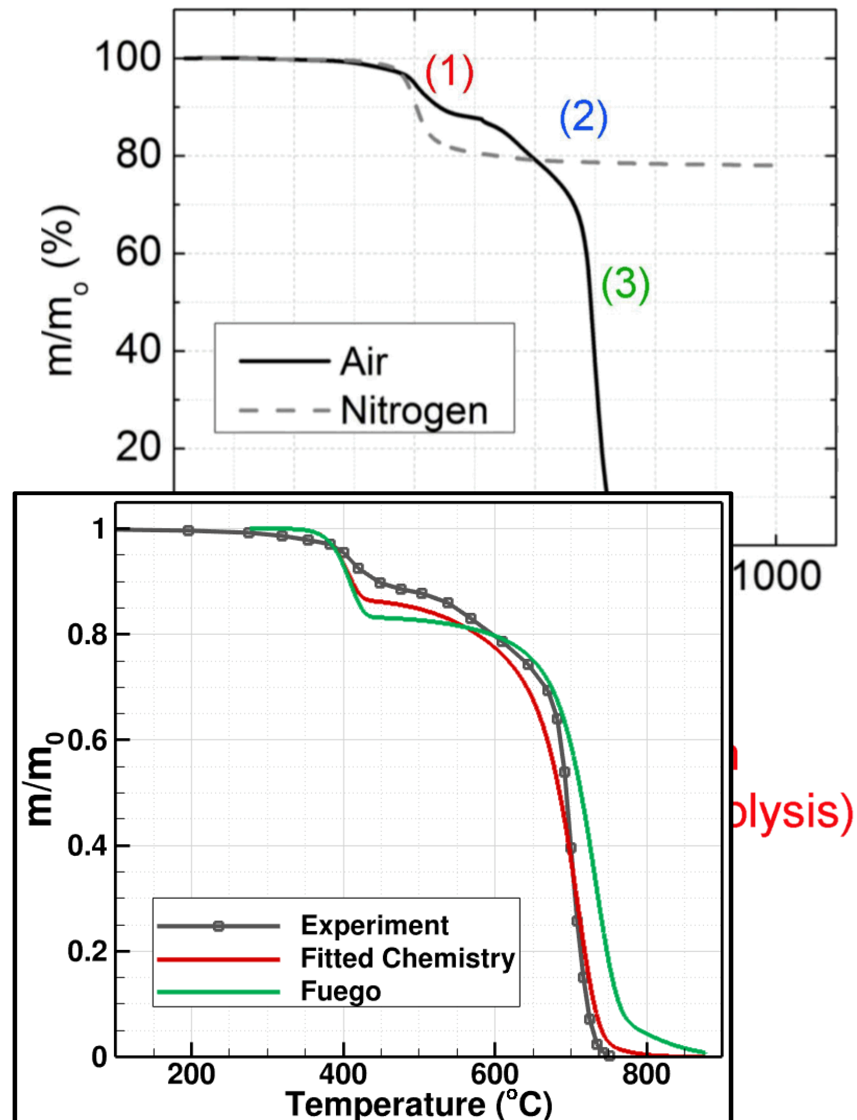
TGA Study

- 20°C/min
- Epoxy pyrolysis generates gaseous fuel and char
- In air, epoxy oxidizes before char and carbon fiber



- Fuego solid combustion does not match the fitted chemistry
  - Why?

Dodd et al. (2013), Brown et al. (2012)



Reaction Mechanism

- Fitted mechanism with the TGA (Dodd et al. 2013)
- For a solid-gas reaction, defining pre-exponent factor needs a caution

Gas species: $$\frac{\partial \rho_g Y_{CH_4}}{\partial t} + \nabla \cdot (\rho_g \mathbf{u} Y_{CH_4} + \rho_g D \nabla Y_{CH_4}) = \dot{\omega_{EDC}} + 0.5\dot{\omega_1} + \dot{\omega_2}$$

Solid composition: $$\frac{d\rho_s Y_{epoxy}}{dt} = -\dot{\omega_1} - \dot{\omega_2}$$

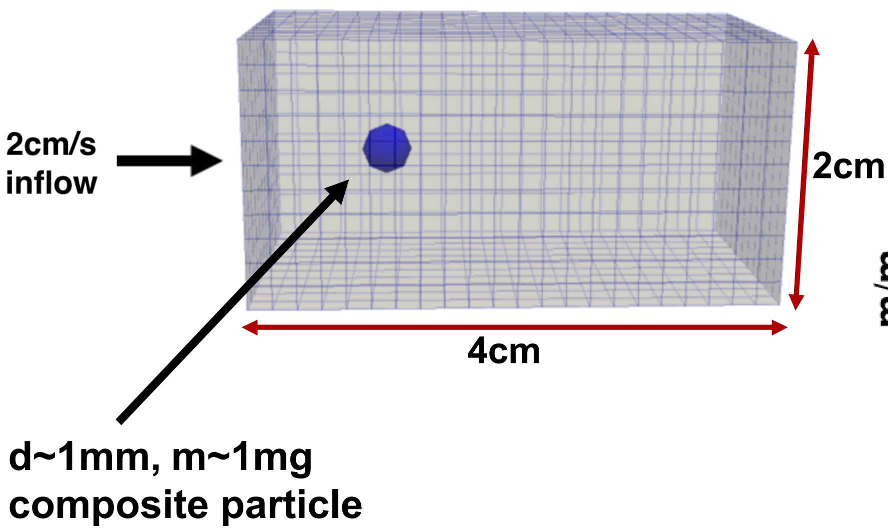
Reaction rates: $$\dot{\omega_1} = \rho_s Y_{r,s} A e^{-E_a/RT}$$

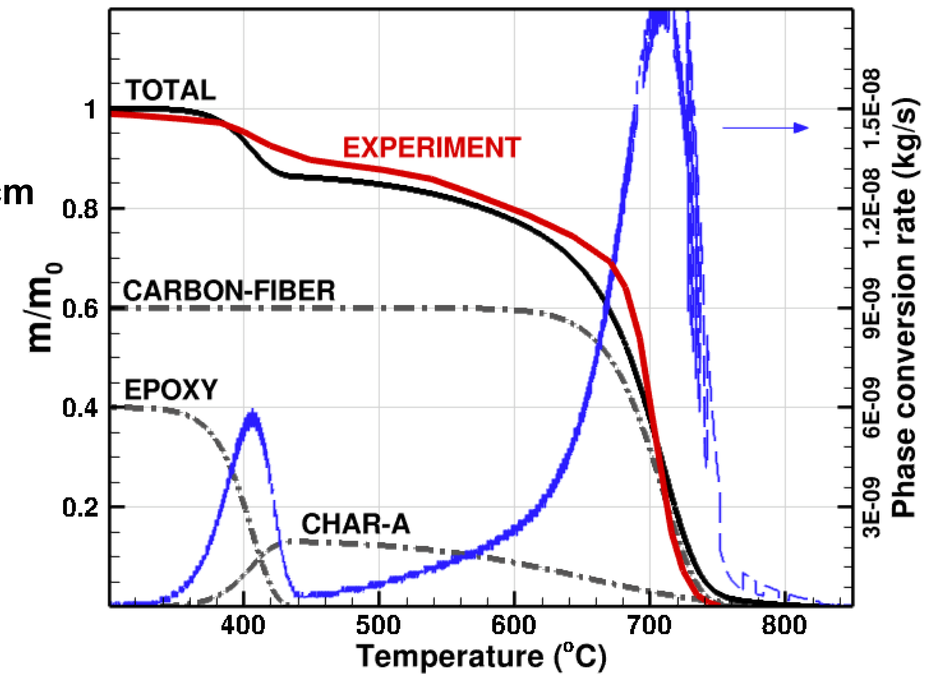
$$\dot{\omega_{2-5}} = \rho_s Y_{r,s} \rho_g Y_{r,g} A e^{-E_a/RT}$$

1 pyrolysis	Epoxy → 0.5 CharA + 0.5 CH_4	A=3.33E15, E_a/R=27200
2 oxid.	Epoxy + O_2 → CharB + CH_4	A=5.3E15/ρ_g, E_a/R=27200
3 oxid.	CharA + O_2 → Residue + CO	A=7.58E2/ρ_g, E_a/R=10000, ΔH=12730kJ/kg
4 oxid.	CharB + O_2 → Residue + CO	A=7.58E2/ρ_g, E_a/R=10000, ΔH=12730kJ/kg
5 oxid.	Carbon-Fiber + O_2 → Residue + CO_2	A=3.79E15/ρ_g, E_a/R=38000, ΔH=24770kJ/kg

TGA Simulation

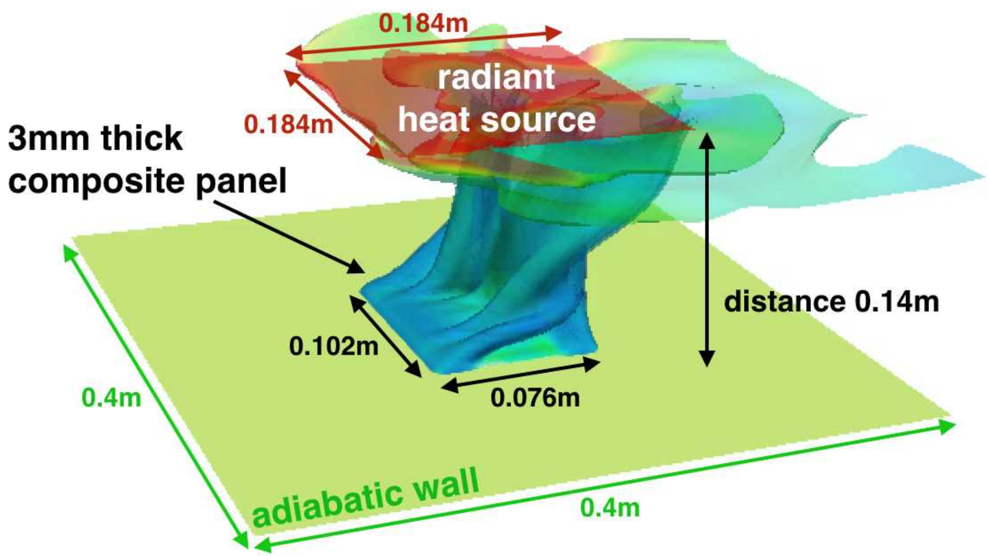
- An immovable Lagrangian particle represents TGA sample
- Fuego result closely matches to the TGA of air at 20°C/min

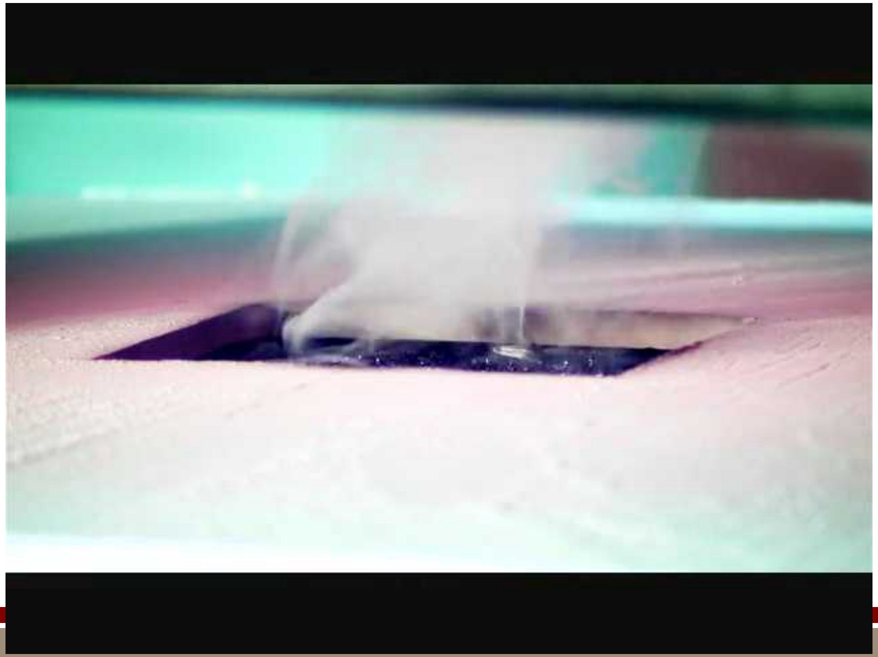




Composite Panel Experiment

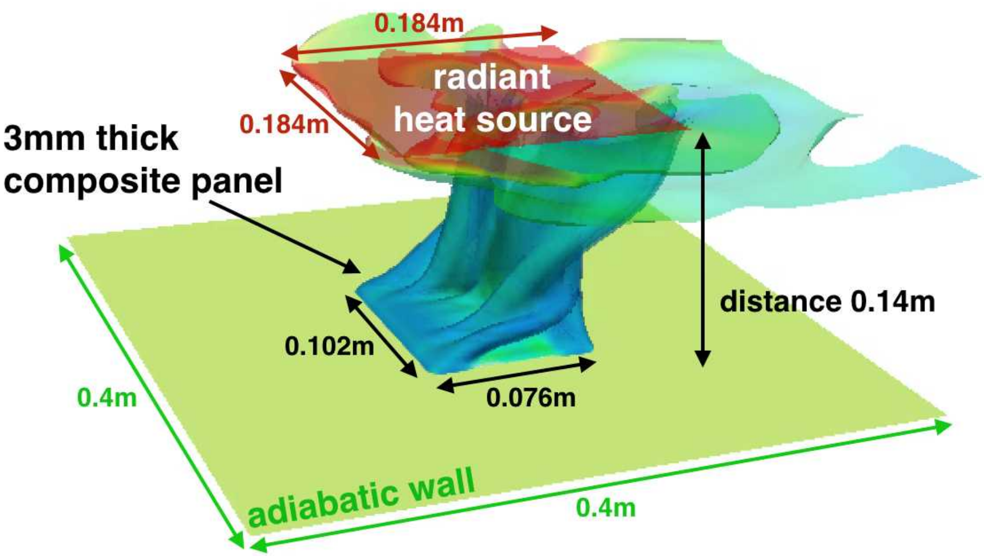
- Exposed composite panel degrades under a radiant heat (Hubbard et al., 2011)
  - Upper panel is heated up to 800°C
  - Duration of visible gasification (smoke) and backside panel temperature profiles are available



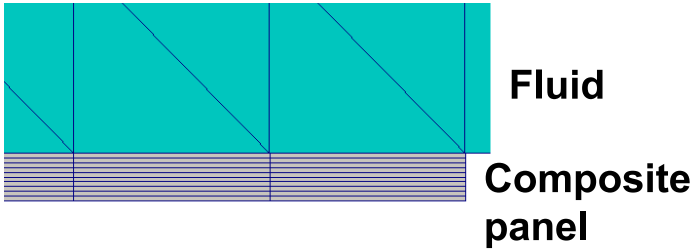


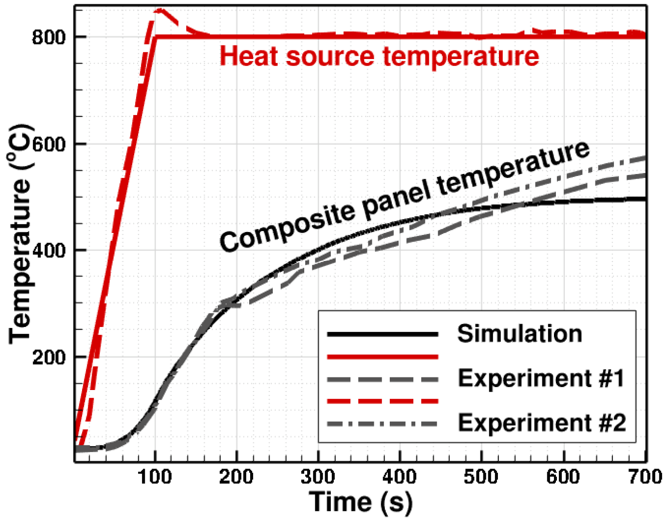
Composite Panel Experiment

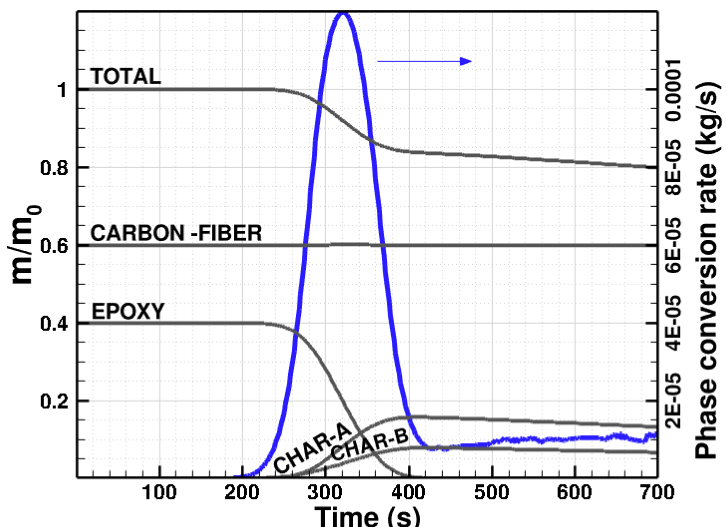
- Exposed composite panel degrades under a radiant heat (Hubbard et al., 2011)
  - Upper panel is heated up to 800^{o}C
  - Duration of visible gasification (smoke) and backside panel temperature profiles are available
- Directional BC: panel is discretized normal to the wall
  - Mesh size ~ 5mm, total 0.1M grid; no gas-phase reaction



Side view:







Smoke duration

Smoke in the experiments

Summary

- DNS was performed on canonical problems
  - Being a generalized solver, mesh requirement is tighter
  - Sensitive to grid aspect ratio
  - Theoretical velocity profiles were obtained with a layered mesh
- LES models work as expected
  - KSGS performance is not too sensitive to the mesh resolution, thereby can be used for a wide range of problems
  - Jet breakdown is well predicted using dynamic Smagorinsky model
- Composite pyrolysis and oxidation procedures were verified
  - Reaction parameter definitions were revisited
  - Solid mass response and heat transfer on the panel were correctly predicted
  - Detailed composition of the gas phase release needs further work
    - So does missing physics such as swelling