Measurement and Computation of Fire Phenomena (*MaCFP*)

Review of Current Standards for CFD Verification and Validation

First MaCFP Workshop, Lund University – June 10-11, 2017

Randall McDermott (NIST, USA)

Arnaud Trouvé (University of Maryland, USA)

NIST National Institute of Standards and Technology U.S. Department of Commerce

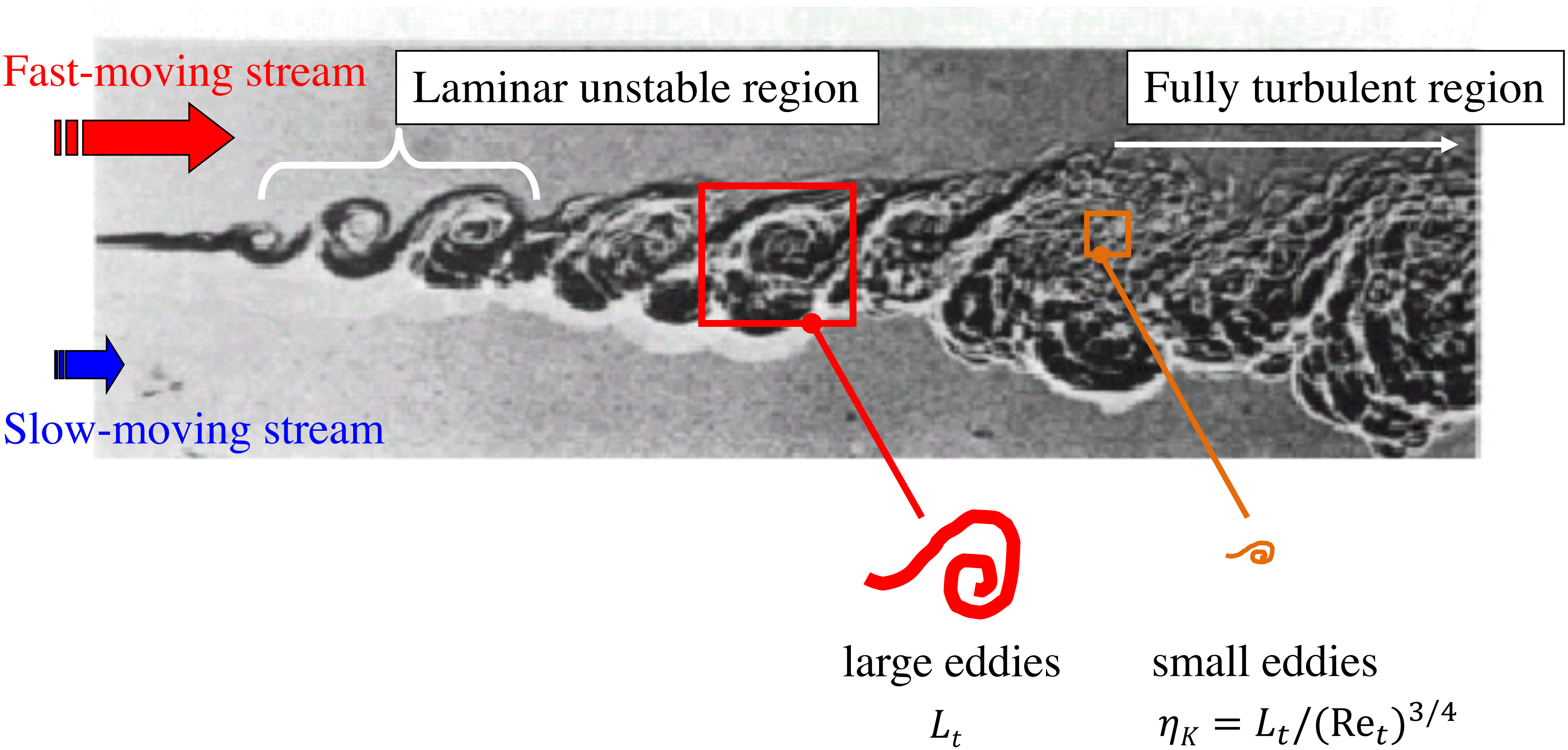
UNIVERSITY OF MARYLAND

CFD-based Fire Modeling

- **Outline**
  - Computational grid design
  - Subgrid-scale (SGS) modeling
    - Baseline SGS models used in FDS and FireFOAM
  - Code Verification
  - Model Validation

Characteristic Length Scales

- **Turbulent flow**



Characteristic Length Scales

- **Turbulent flow**
  - Example: pool fire, $\dot{Q} = 1$ MW; $D = 1$ m

$$\left.\begin{array}{l}\left.\begin{array}{l}\bar{u}_{CL,\max} \approx 1.9 \times (\dot{Q}/1000)^{1/5} = 7.6 \text{ m/s} \\ u' \approx 0.3 \times \bar{u}_{CL,\max} = 2.3 \text{ m/s}\end{array}\right\} \\ L_t \approx 0.5 \times D = 0.5 \text{ m}\end{array}\right\} \Rightarrow \mathrm{Re}_t = \frac{u' L_t}{\nu} \approx \frac{2.3 \times 0.5}{10^{-4}} \approx 11500$$

$$\Rightarrow \boxed{\eta_K = \frac{L_t}{(\mathrm{Re}_t)^{3/4}} = \frac{0.5}{(11500)^{3/4}} = 0.4 \text{ mm}} \quad \text{(Kolmogorov scaling)}$$

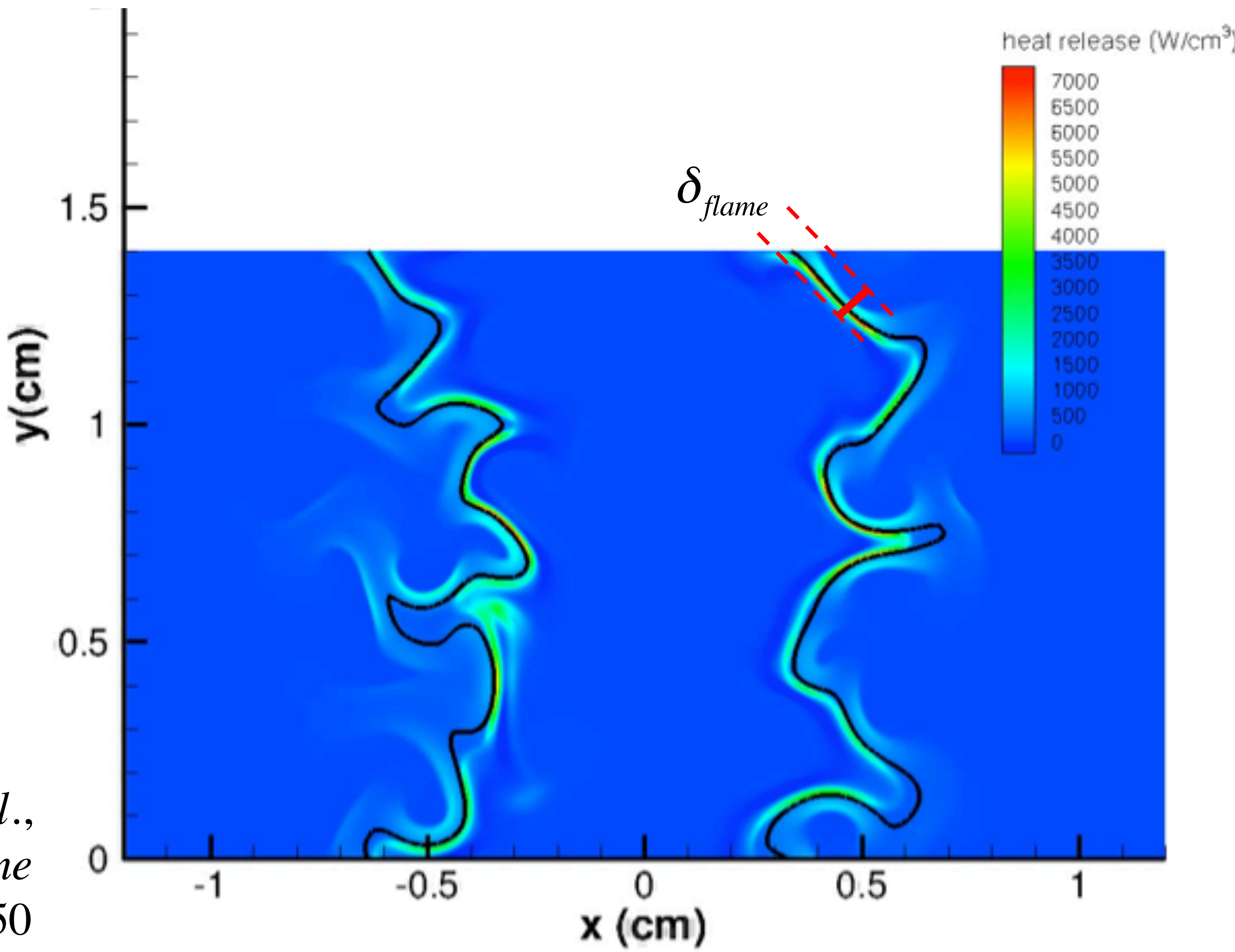
Characteristic Length Scales

- **Turbulent flame**

Strained laminar flame theory

$$\delta_{flame} \sim \sqrt{D_{th,st} / \chi_{st}}$$

$$\boxed{\delta_{flame} \approx 1 \text{ mm}}$$



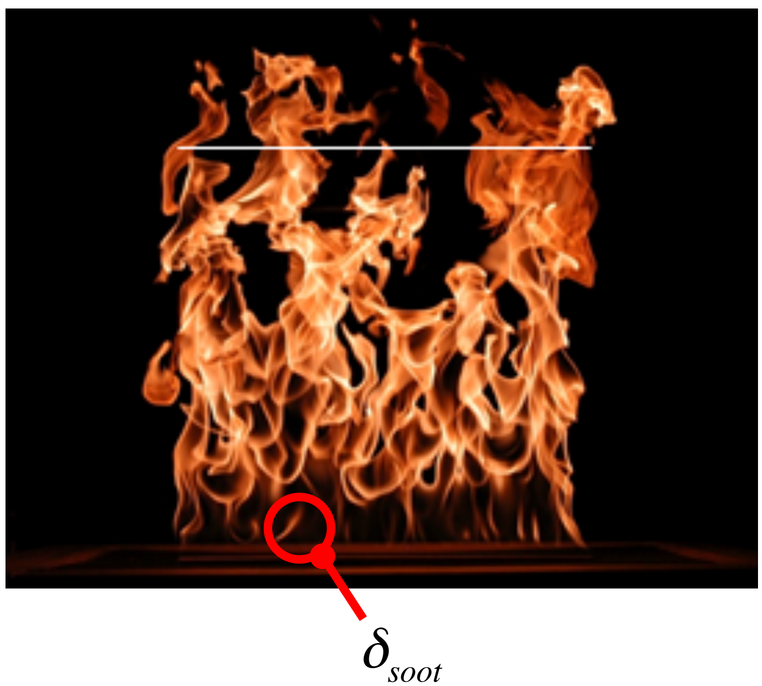
Lecoustre *et al.*, *Combust. Flame* **161** (2014) 2933-2950

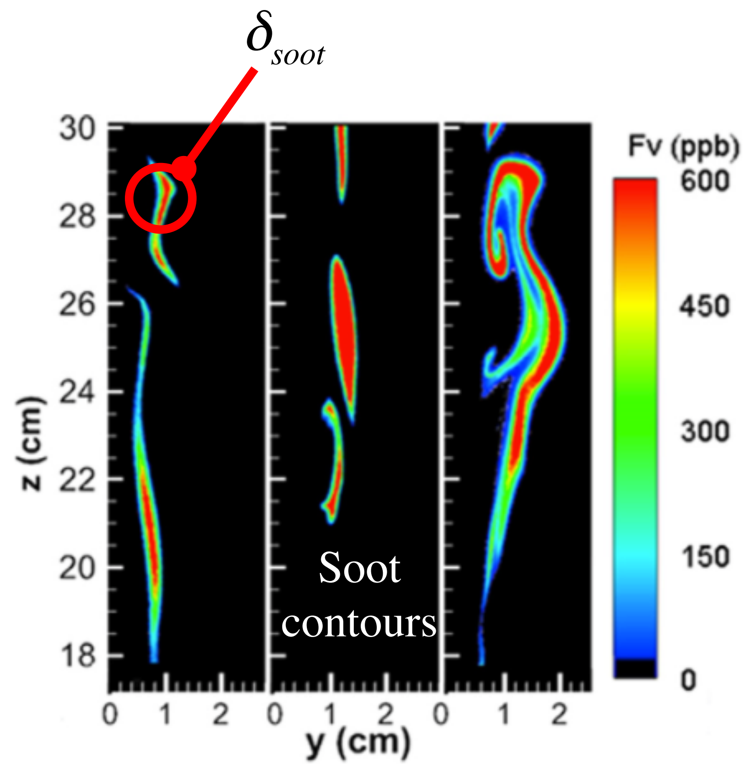
Characteristic Length Scales

- **Thermal radiation**

Experimental observations

$\delta_{soot} \sim 1$ mm





Valencia *et al*., *Proc*. *Combust*. *Inst*. **36** (2017) 3219-3226

Computational Grid Design

- **Computational grid requirement**
  - Direct Numerical Simulation (DNS)
    - Grid-resolved scales: $L_t, \eta_K, \delta_{flame}, \delta_{soot}$

$$\left.\begin{array}{l} \Delta x_{DNS} \approx \eta_K \\ \Delta x_{DNS} \approx (\delta_{flame}/10) \\ \Delta x_{DNS} \approx (\delta_{soot}/10) \end{array}\right| \Longrightarrow \boxed{\Delta x_{DNS} = O(0.1\ \text{mm})}$$

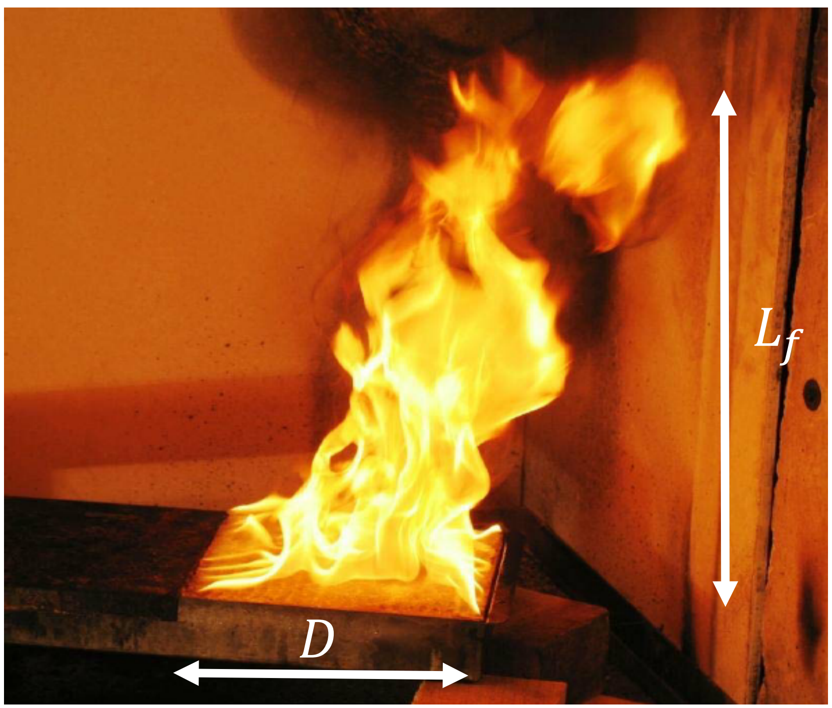
  - Large Eddy Simulation (LES)
    - Grid-resolved scales: L_t

$$\boxed{\Delta x_{LES} \approx (L_t/10)}$$

    - Unresolved scales: $\eta_K, \delta_{flame}, \delta_{soot}$

Computational Grid Design

- **Computational grid requirement**
  - Large Eddy Simulation (LES) $\Delta x_{LES} \approx (L_t/10)$
    - Traditional view point: $L_t \approx 0.5\times D$



Example: pool fire, $\dot{Q} = 22.6$ kW, $D = 0.3$ m

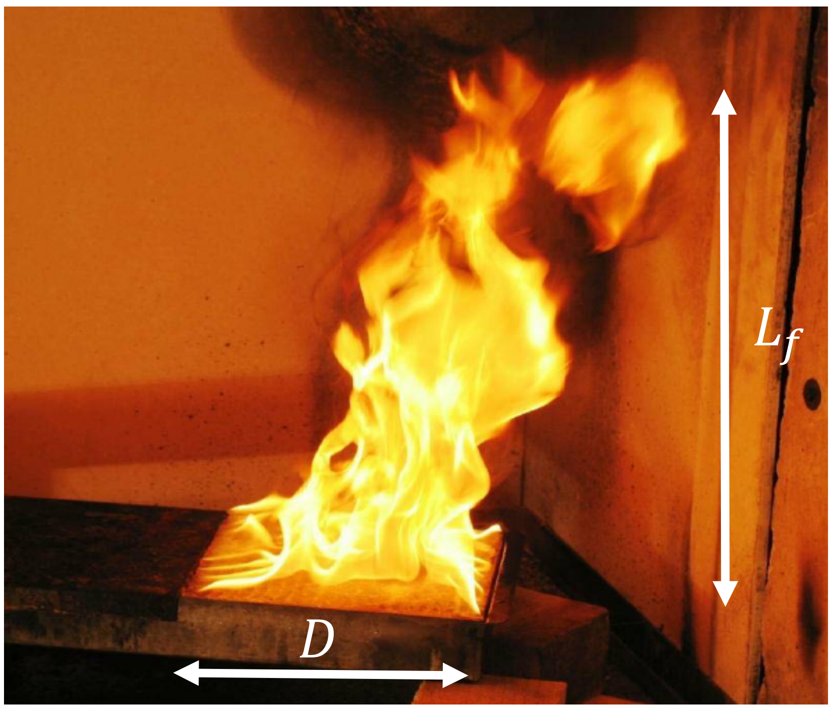
$$Q^* = \frac{\dot{Q}}{(\rho_\infty c_{p,\infty} T_\infty)\sqrt{gD}D^2} \approx 0.4$$

$$L_f = 3.7\times Q^{*2/5}\times D - 1.02\times D \approx 0.5 \text{ m}$$

$$\Rightarrow \Delta x_{LES} \approx (D/20) \approx 1.5 \text{ cm}$$

Computational Grid Design

- **Computational grid requirement**
  - Large Eddy Simulation (LES) $\Delta x_{LES} \approx (L_t/10)$
    - Alternative view point: $L_t \approx 0.5 \times D$



Example: pool fire, $\dot{Q} = 22.6\ \mathrm{kW}, D = 0.3\ \mathrm{m}$

$$L_f = 3.7 \times D^* - 1.02 \times D$$

$$D^* = \left(\frac{\dot{Q}}{(\rho_\infty c_{p,\infty} T_\infty)\sqrt{g}}\right)^{2/5} \approx 0.2\ \mathrm{m}$$

$$\Longrightarrow \boxed{\Delta x_{LES} \approx (D^*/10) \approx 2\ \mathrm{cm}}$$

Computational Grid Design

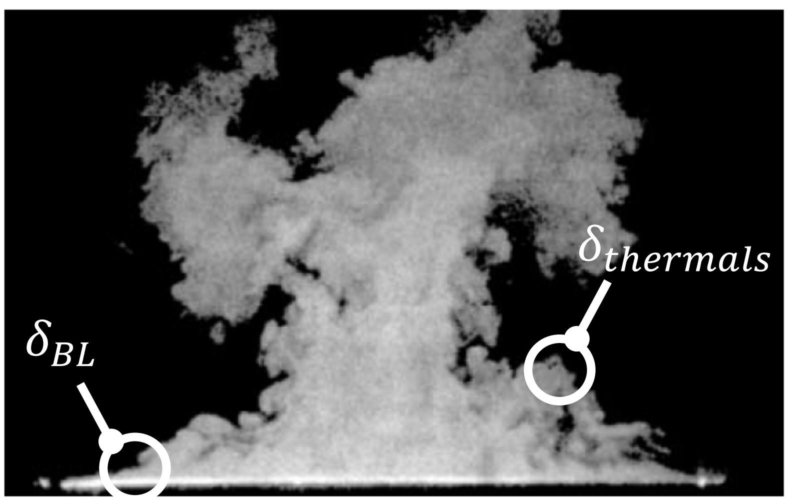
- **Computational grid requirement**
  - Large Eddy Simulation (LES) $\Delta x_{LES} \approx (L_t/10)$
    - In addition, flame base features a thin boundary layer: $\delta_{BL} \approx 1$ cm

$\Rightarrow \Delta x_{LES} \approx (\delta_{BL}/10) \approx 1$ mm

Computational Grid Design

Review of MaCFP target experiments

- Pool-like configurations with strong Rayleigh-Taylor instabilities (puffing motion, bubble and spike structures – thermals)
  - Category 1: Sandia Helium Plume
  - Category 2: Flames Sandia Methane and Hydrogen Flames
  - Category 3: Waterloo Methanol Pool Flame



- Grid resolution required to resolve large-scale flow features

$$\Delta x_{LES} = O(1\text{ cm})$$

- Grid resolution required to resolve boundary layer at flame base and vertical thermals

$$\Delta x_{LES} = O(1\text{ mm})$$

Computational Grid Design

Review of MaCFP target experiments

- Boundary layer flame configurations
  - Category 4: FM Global Vertical Wall Flames

$\delta_{BL} = O(1\text{ cm})$

- Grid resolution required to resolve boundary layer and wall gradients

$\Delta x_{LES} = O(1\text{ mm})$

Computational Grid Design

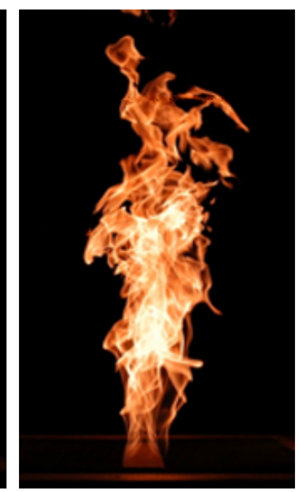
- **Review of MaCFP target experiments**
  - Configurations with no obvious small-scale feature
    - Category 2: NIST McCaffrey Natural Gas Flames

$$\Delta x_{LES} = (S/20) \approx O(1\ \mathrm{cm})$$

    - Category 5: UMD Methane and Propane Line Flames

$$\Delta x_{LES} = (W/20) \approx O(1\ \mathrm{mm})$$

Front view



Side view

Subgrid-Scale Modeling

Turbulence

- Classical LES treatment: gradient transport model for turbulent fluxes featuring a turbulent viscosity μ_t

$$T_{ij} = -\mu_t \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial \tilde{u}_k}{\partial x_k} \right) + \frac{2}{3} \delta_{ij} \bar{\rho} k_{SGS}$$

- Closure expression for μ_t

$$\boxed{\mu_t = \bar{\rho} (C_{\mu_t} \Delta) \sqrt{k_{SGS}}} \quad \text{where} \quad \Delta = \left(\Delta x_1 \Delta x_2 \Delta x_3 \right)^{1/3}$$

- Closure expression for k_{SGS}
  - Models: **modified Deardorff** (FDS); (constant-coefficient or dynamic) ***k*-equation** (FireFOAM)

Subgrid-Scale Modeling

Combustion

- Global combustion equation (no chemistry)

$$C_nH_mO_p + \{n + (m/4) - (p/2)\}O_2 \rightarrow nCO_2 + (m/2)H_2O$$

- Closure expression for reaction rate: **Eddy Dissipation Model** (EDM) (FDS, FireFOAM)

$$\boxed{\overline{\dot{\omega}_F'''} = \bar{\rho} \times \frac{\min(\tilde{Y}_F; \tilde{Y}_{O_2}/r_s)}{\tau_t}} \quad \text{where} \quad \tau_t = C_{\tau_t} \times (\frac{\bar{\rho}\Delta^2}{\mu_t})$$

  - Plus correction to treat laminar combustion (correction applies in regions where the flow is laminar)

Subgrid-Scale Modeling

Radiation

- Radiative transfer equation (RTE) (assumed grey medium)

$$\nabla\bar{I}.\vec{s} = \overline{\kappa(\frac{\sigma T^4}{\pi})} - \overline{\kappa I}$$

Emission **Absorption**

- Closure model for RTE: the prescribed **global radiant fraction** approach (FDS, FireFOAM)

$$\nabla\bar{I}.\vec{s} = C \times \bar{\kappa}(\frac{\sigma\tilde{T}^4}{\pi}) - \bar{\kappa}\bar{I},\ \text{if}\ \dot{q}'''_{comb} > 0$$

$$\nabla\bar{I}.\vec{s} = \bar{\kappa}(\frac{\sigma\tilde{T}^4}{\pi}) - \bar{\kappa}\bar{I},\ \text{if}\ \dot{q}'''_{comb} = 0$$

$$\nabla\bar{I}.\vec{s} = \chi_{rad} \times (\frac{\dot{q}'''_{comb}}{4\pi}),\ \text{if}\ \dot{q}'''_{comb} > 0$$

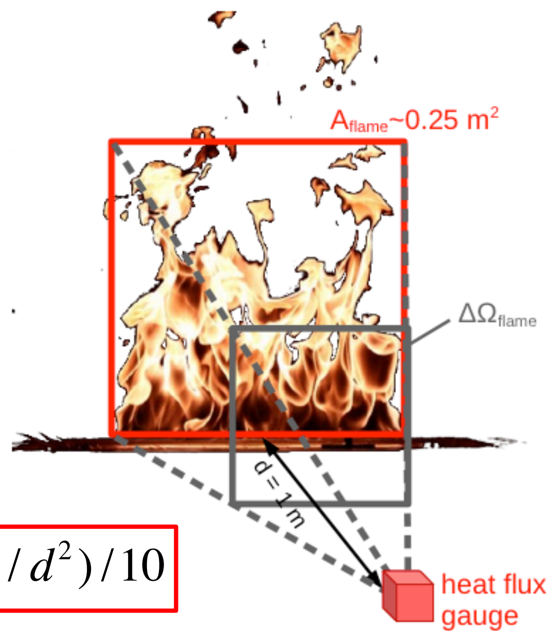
$$\nabla\bar{I}.\vec{s} = 0,\ \text{if}\ \dot{q}'''_{comb} = 0$$

Subgrid-Scale Modeling

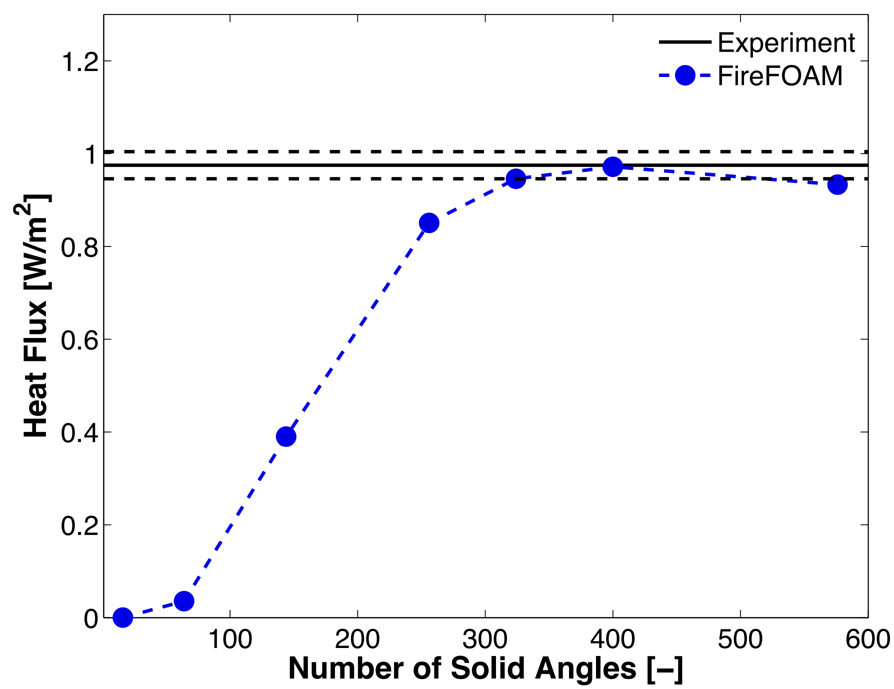
- **Challenges**
  - Turbulence
    - Deardorff, *k*-equation models formulated for high-Reynolds number, momentum-driven flow but fires often feature **moderate-Reynolds number**, **buoyancy-driven flow**
  - Combustion
    - EDM model does not describe **ignition/extinction**; modifications of EDM have been proposed to treat flame extinction for simulations of under-ventilated fires or suppressed fires
  - Radiation
    - The prescribed global radiant fraction approach remains approximate but more fundamental approaches require a treatment of **spectral effects** and a **soot model**

Subgrid-Scale Modeling

- **Challenges**
  - Radiation
    - RTE solved with Discrete Ordinate Method (DOM); accuracy of DOM is controlled by discretization of angular space and typically decreases in the far-field (ray effect)

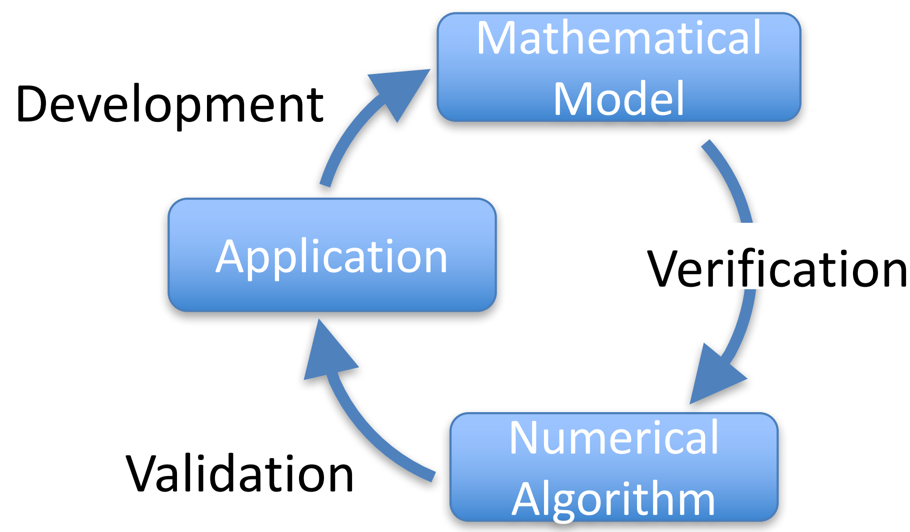


$$\Delta\Omega_{DOM} \approx (A_{flame} / d^2)/10$$



CFD-based Fire Modeling

- **Outline**
  - Computational grid design
  - Subgrid-scale (SGS) modeling
  - Code Verification
    - Manufactured solutions
    - Continuous integration
  - Model Validation
    - Calibration vs. Validation
    - Validation Metrics
    - Uncertainty Quantification
    - Quality Assurance
    - Application Space: Statistically stationary flows; Forecasting



Adapted from W.L. Oberkampf and C.J. Roy. Verification and Validation in Scientific Computing. Cambridge, 2010.

Manufactured Solutions

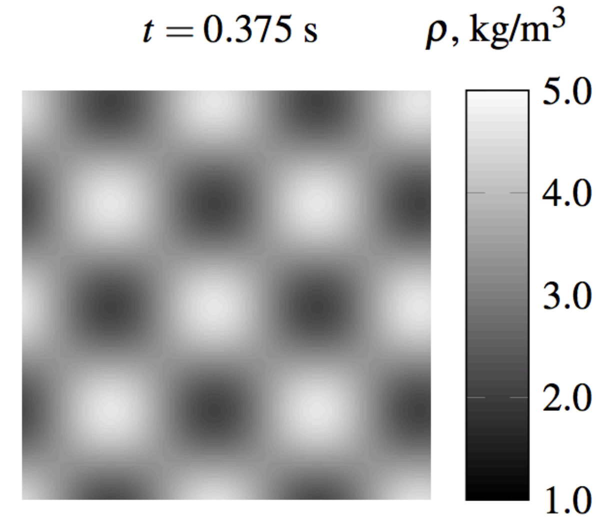
$$Z(x,y,t) = \frac{1+\sin(\pi k\hat{x})\sin(\pi k\hat{y})\cos(\pi\omega t)}{(1+\frac{\rho_0}{\rho_1})+(1-\frac{\rho_0}{\rho_1})\sin(\pi k\hat{x})\sin(\pi k\hat{y})\cos(\pi\omega t)}$$

$$\rho(x,y,t) = \left(\frac{Z(x,y,t)}{\rho_1}+\frac{1-Z(x,y,t)}{\rho_0}\right)^{-1}$$

$$u(x,y,t) = u_f + \frac{\rho_1-\rho_0}{\rho(x,y,t)}\left(\frac{-\omega}{4k}\right)\cos(\pi k\hat{x})\sin(\pi k\hat{y})\sin(\pi\omega t)$$

$$v(x,y,t) = v_f + \frac{\rho_1-\rho_0}{\rho(x,y,t)}\left(\frac{-\omega}{4k}\right)\sin(\pi k\hat{x})\cos(\pi k\hat{y})\sin(\pi\omega t)$$

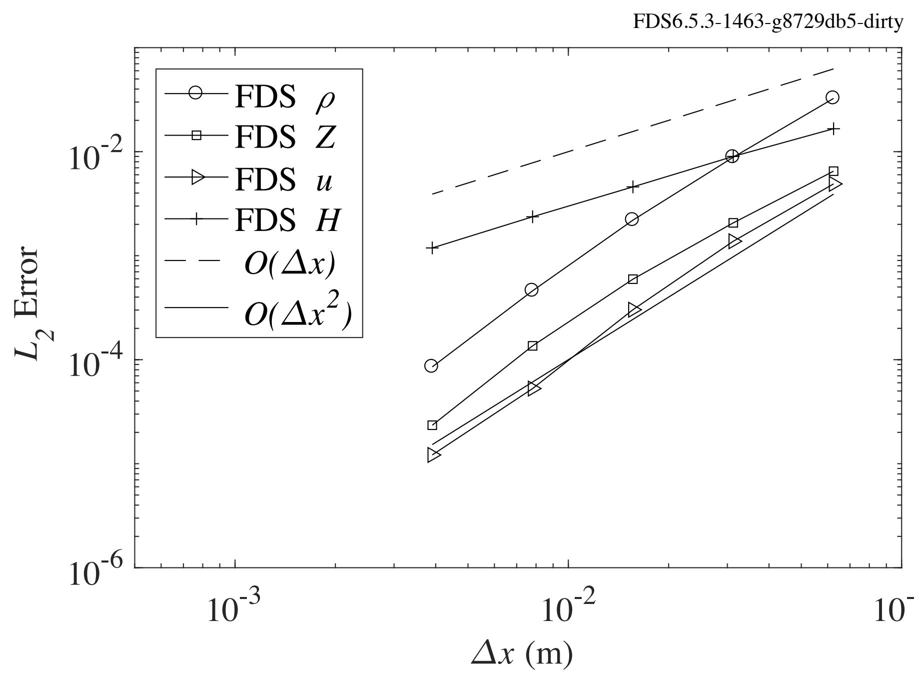
$$H(x,y,t) = \frac{1}{2}(u(x,y,t)-u_f)(v(x,y,t)-v_f)$$



$$\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\mathbf{u}) = \dot{Q}_\rho$$

$$\frac{\partial(\rho Z)}{\partial t}+\nabla\cdot(\rho Z\mathbf{u})-\nabla\cdot(\rho D\nabla Z) = \dot{Q}_Z$$

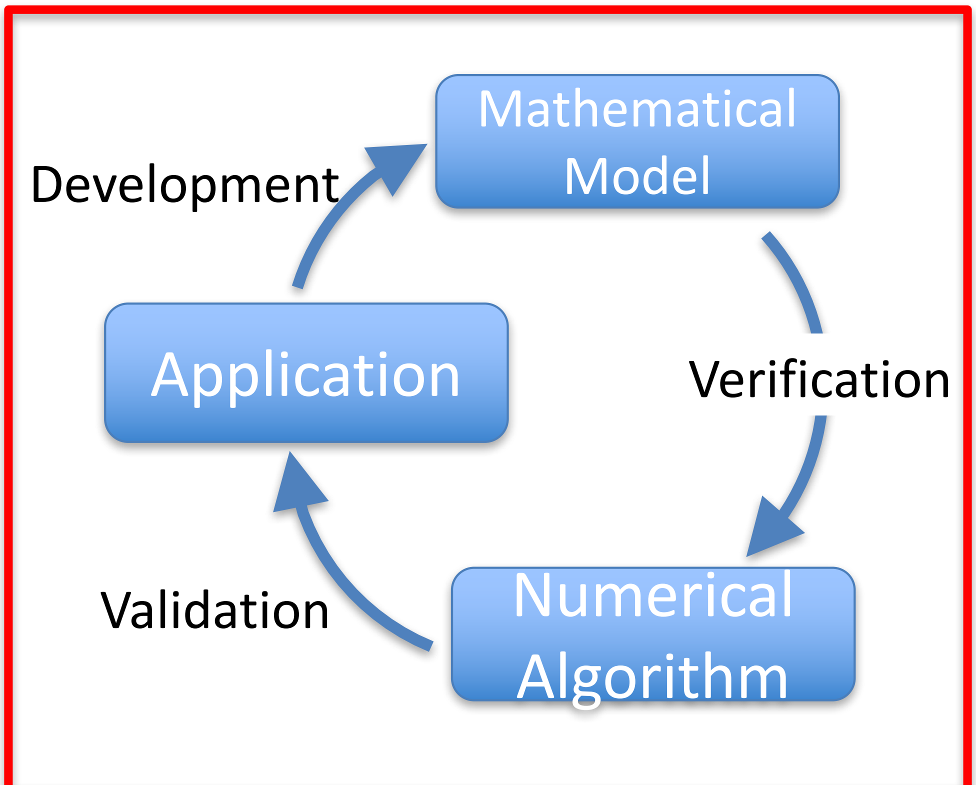
$$\frac{\partial\mathbf{u}}{\partial t}-\mathbf{u}\times(\nabla\times\mathbf{u})+\nabla H-\tilde{p}\nabla(1/\rho)-\frac{1}{\rho}\nabla\cdot\mathrm{T} = \dot{Q}_{\mathbf{u}}$$



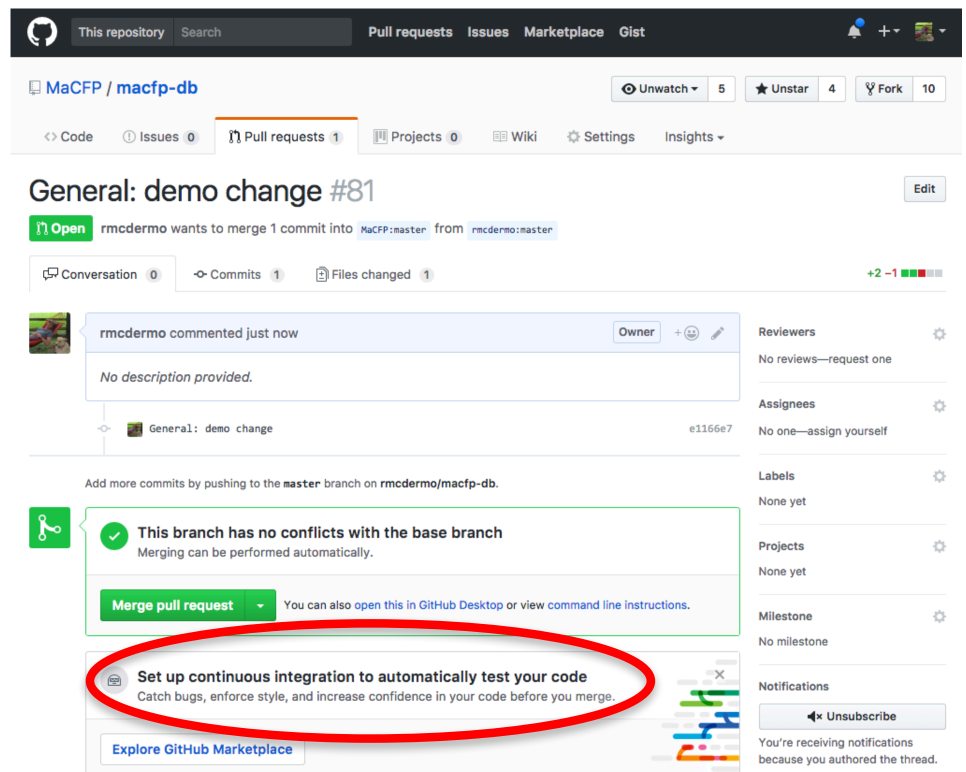
L. Shunn, F. Ham, P. Moin. Verification of variable-density flow solvers using manufactured solutions. Journal of Computational Physics, 231:3801-3827, 2012.

Continuous Integration

1. Version control
2. Unit tests
3. Software quality assurance (SQA)



GitHub



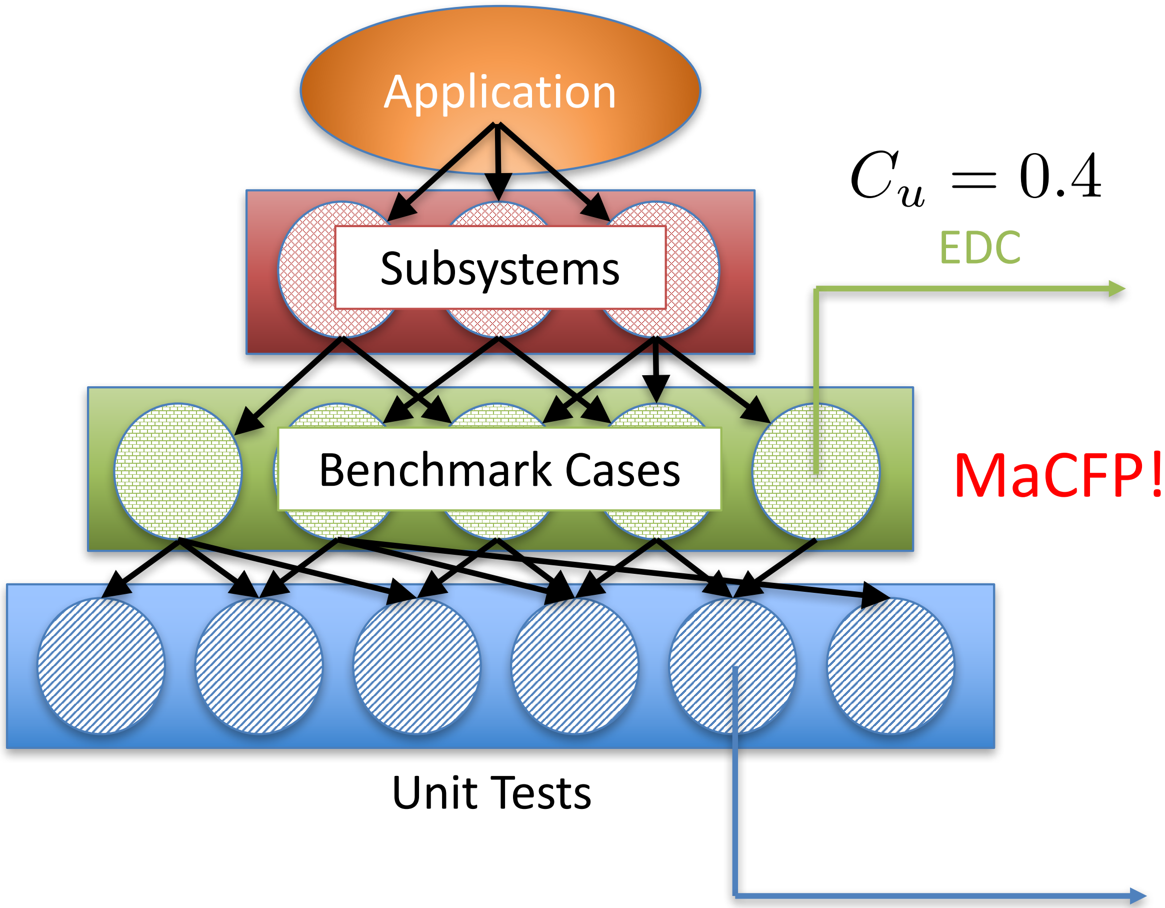
Model Validation

- W.L. Oberkampf, M.F. Barone (2006) Measures of agreement between computation and experiment: validation metrics. *J Comput Phys,* 217:5-36.
- K. McGrattan, B. Toman (2011) Quantifying the predictive uncertainty of complex numerical models. *Metrologia,* 48:173-180.
- R. McDermott, G. Rein. (2016) Special Issue on Fire Model Validation. *Fire Technology,* 52:1-4.

Contributors:

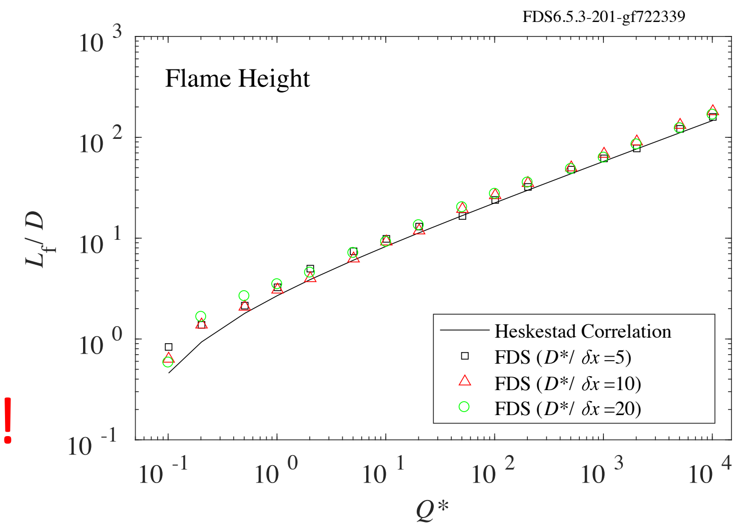
P. Ayala	K. Hartl	J. Li	F. Pimont	C.-H. Tang
G. Baker	Y. Hasemi	D. Lignell	G. Rein	G. Vigne
M. Bruns	R. Hintze	C.Y. Lin	P. Reneke	P. Wang
A. Cantizano	C. Hoffman	R. Linn	E. Ronchi	C. Weinschenk
J. Cranfield	G. Hsiano	N. Liu	S. Scott	C. Werner
A. Dodd	T.-C. Huang	K. McGrattan	C. Sieg	C. Zhang
K. Erickson	Z. Jozefik	W. Mell	J. Silva	J. Ziegler
O. Ezekoye	D. Kamikawa	E. Monson	A. Smits	
M. Finney	A. Kerstein	D. Nilsson	M. Spearpoint	
J. Floyd	E. Kuligowski	K. Overholt	S. Stoliarov	
C. Gutierrez-Montes	M. Larsen	R. Peacock	J. Suo-Anttila	

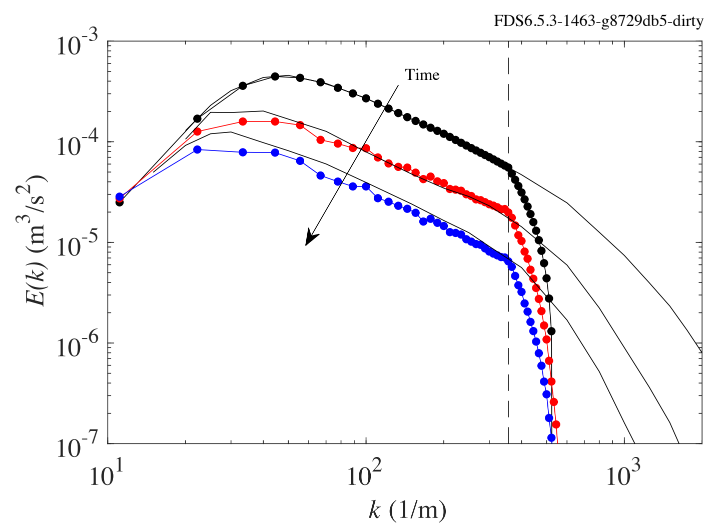
Calibration vs. Validation



$$C_u = 0.4$$

$$C_\nu = 0.1$$

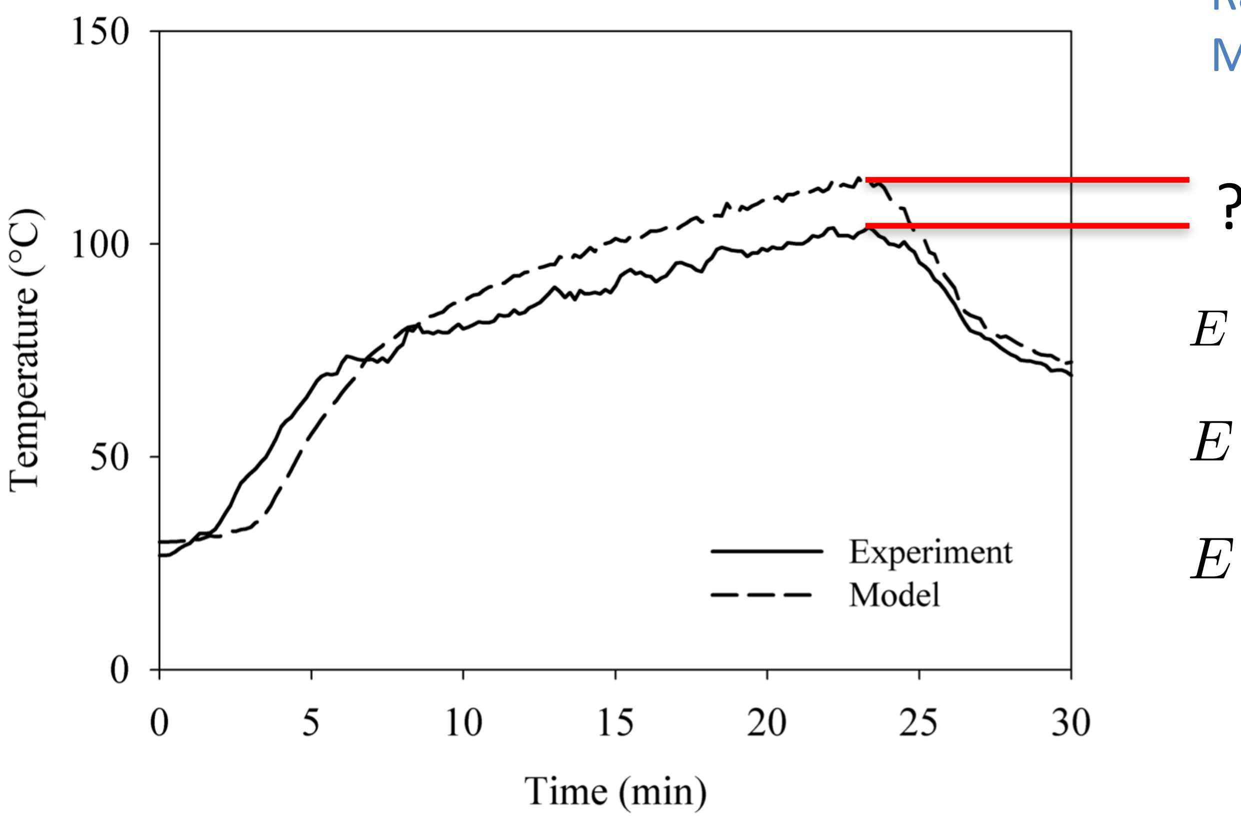




Adapted from W.L. Oberkampf and C.J. Roy. Verification and Validation in Scientific Computing. Cambridge, 2010.

Validation Metrics

Many possible choices!
What are you interested in?
Second-order statistics?
Rates of change?
Might be dictated by AHJ



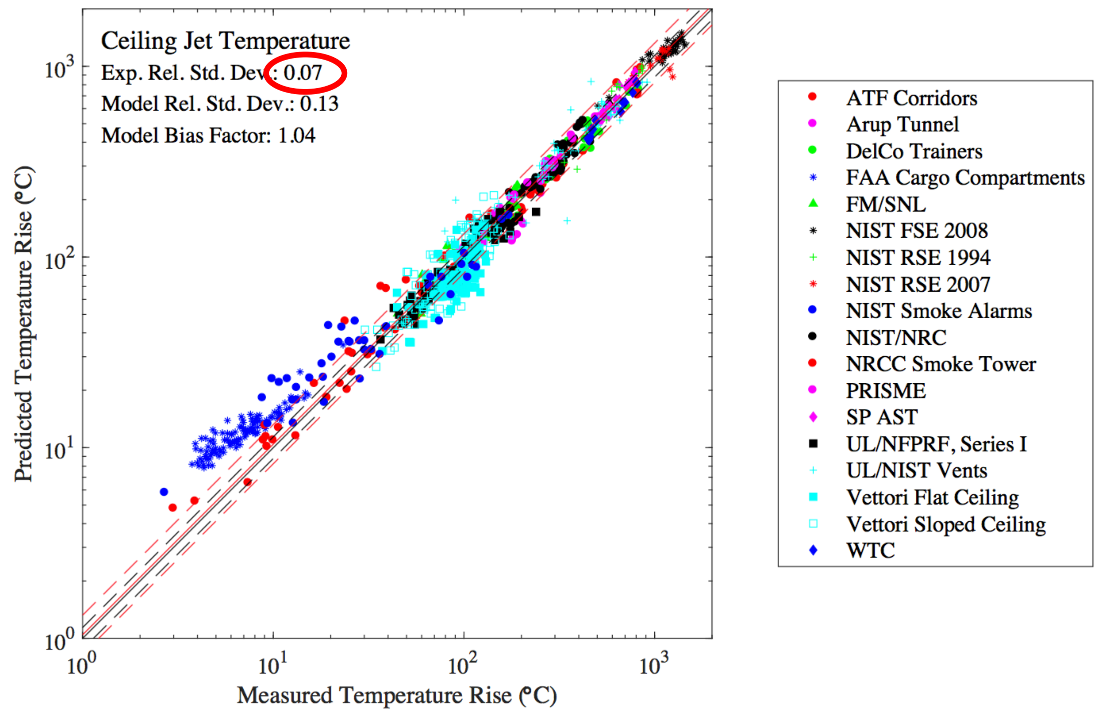
$$E = |\max(T_{exp}) - \max(T_{mod})|$$

$$E = \|I(T_{exp}) - I(T_{mod})\|_2$$

$$E = \|I(T_{exp}) - I(T_{mod})\|_\infty$$

Uncertainty Quantification

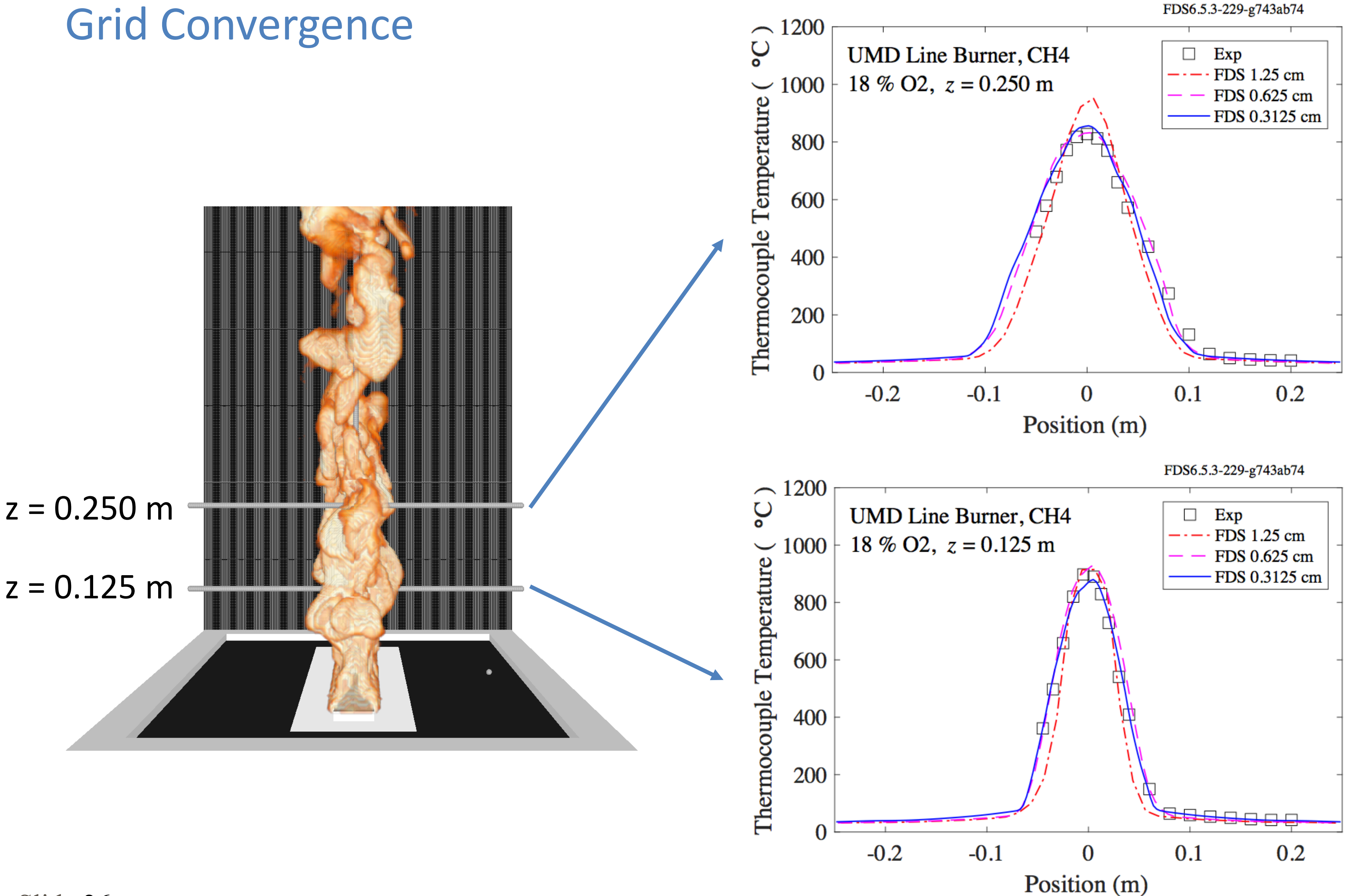
Output Quantity	Measurement Uncertainty	Propagated Input Uncertainty	Combined Uncertainty, $\widetilde{\sigma}_E$
Gas and Solid Temperatures	0.05	0.05	0.07
HGL Depth	0.05	0.00	0.05
Gas Concentrations	0.02	0.08	0.08
Smoke Concentration	0.14	0.13	0.19
Pressure, Closed Compartment	0.01	0.21	0.21
Pressure, Open Compartment	0.01	0.15	0.15
Velocity	0.07	0.03	0.08
Heat Flux	0.05	0.10	0.11
No. Activated Sprinklers	0.00	0.15	0.15
Sprinkler Activation Time	0.00	0.06	0.06
Cable Failure Time	0.00	0.12	0.12
Smoke Alarm Activation Time	0.00	0.34	0.34



- Helpful in capturing general trends and steering development
- Choice of metric can cloud conclusions
- Care should be taken to understand conditional uncertainties

Quality Assurance

Grid Convergence

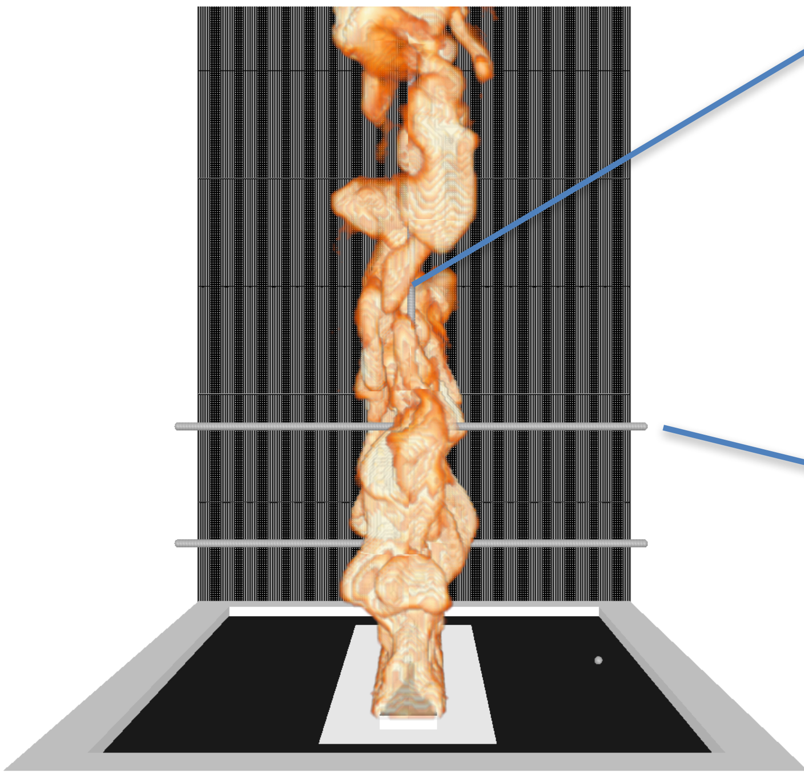


Quality Assurance

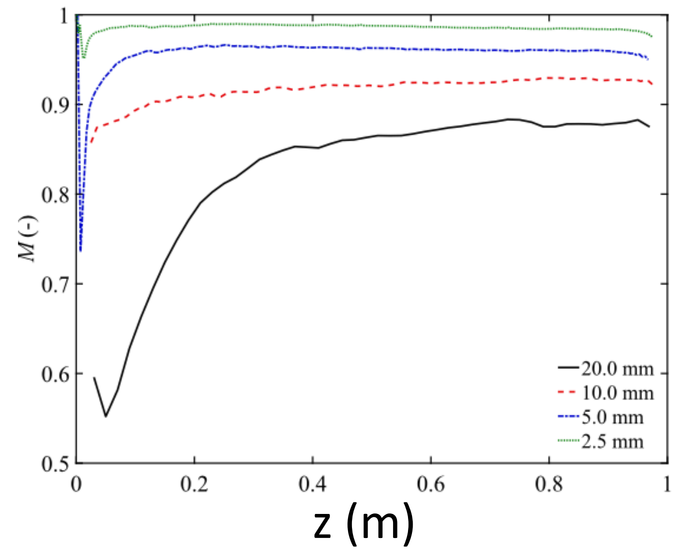
A Posteriori Resolution Metrics

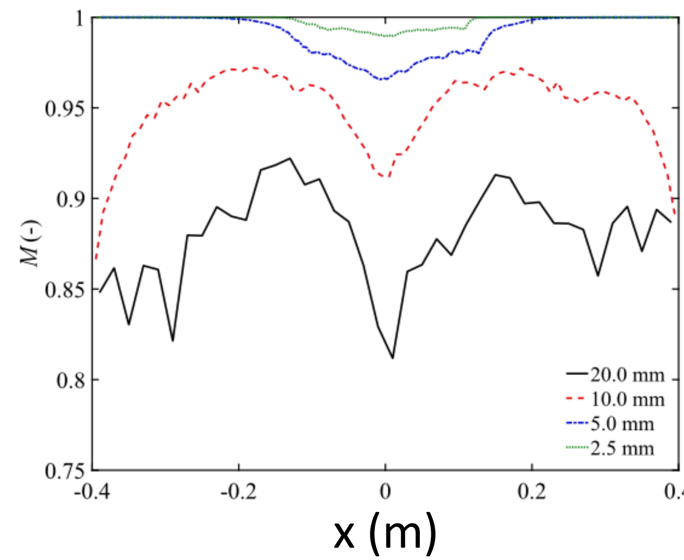
"Pope criterion"

$$M = \frac{k_t}{k_t + k_{sgs}}$$



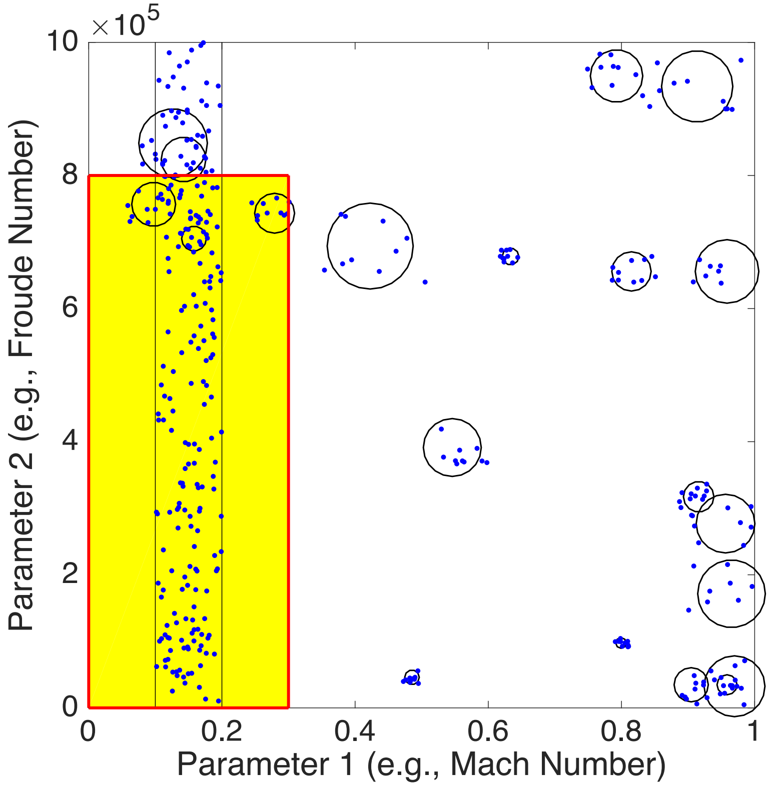
J.P. White et al. Fire Safety Journal, 2017.

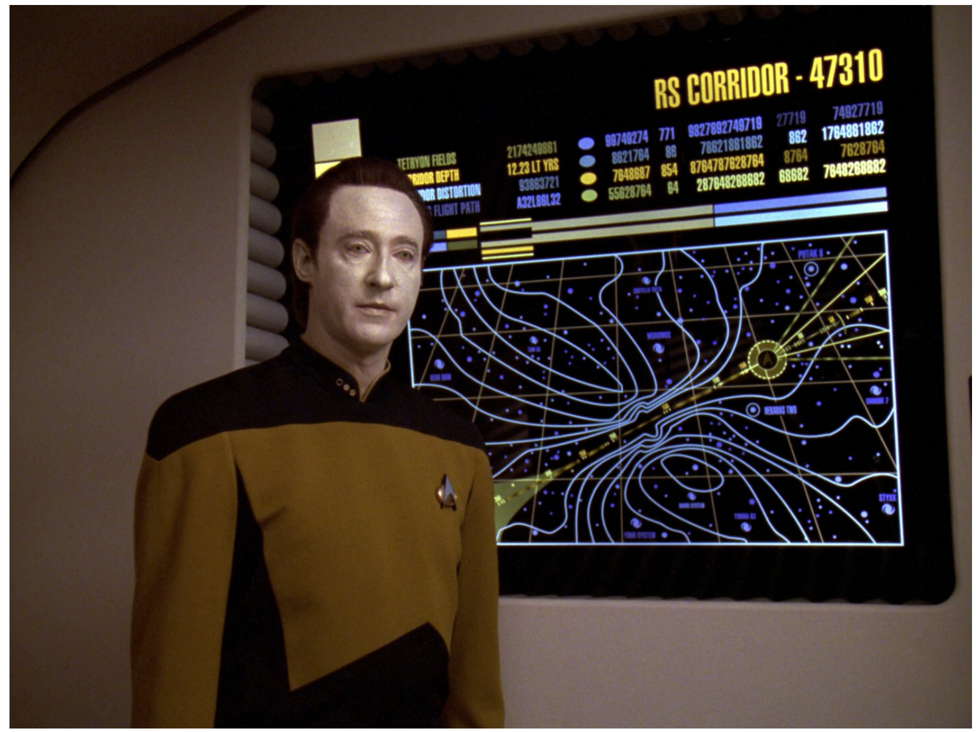




S.B. Pope. Ten questions on the large-eddy simulation of turbulent flows. New Journal of Physics, 6:35, 2004.

Application Space





"Application space is *N*-dimensional and infinite in volume."

Experimental data

Theoretical applicability

Class of problem

A goal: Quantify model uncertainty outside of regions where data already exists, and reduce that uncertainty to required levels.

Questions?