Computer-Based Compartment Fire Modeling

3ème École des Sciences des Incendies et Applications (ESIA) – June 1 2022

Arnaud Trouvé

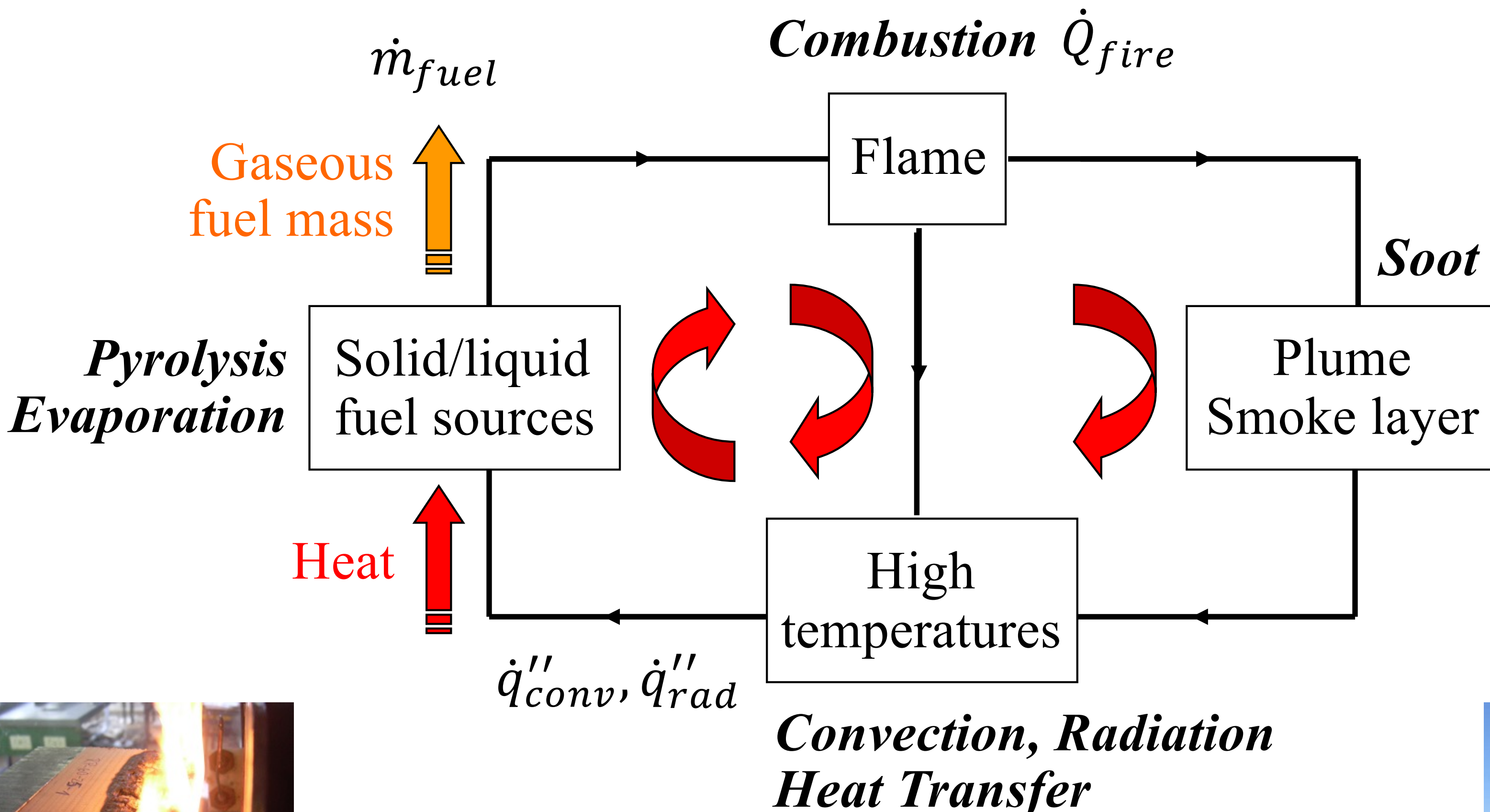
Department of Fire Protection Engineering
University of Maryland, College Park MD (USA)

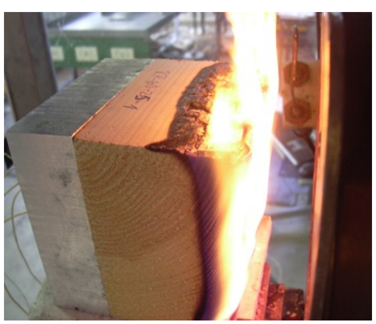
Compartment Fire Modeling

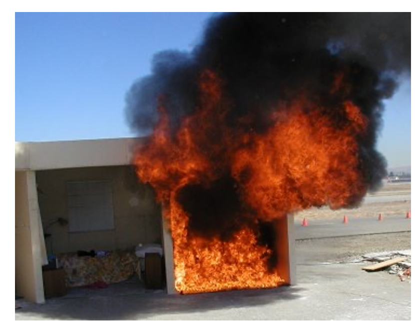
- Outline
  - **Brief Review of Compartment Fire Dynamics**
  - Fire Modeling Landscape
  - Computational Infrastructure
  - Physical Modeling
  - Examples

Fire Dynamics

- **Main features**: fire is an uncontrolled combustion process characterized by a thermal feedback loop



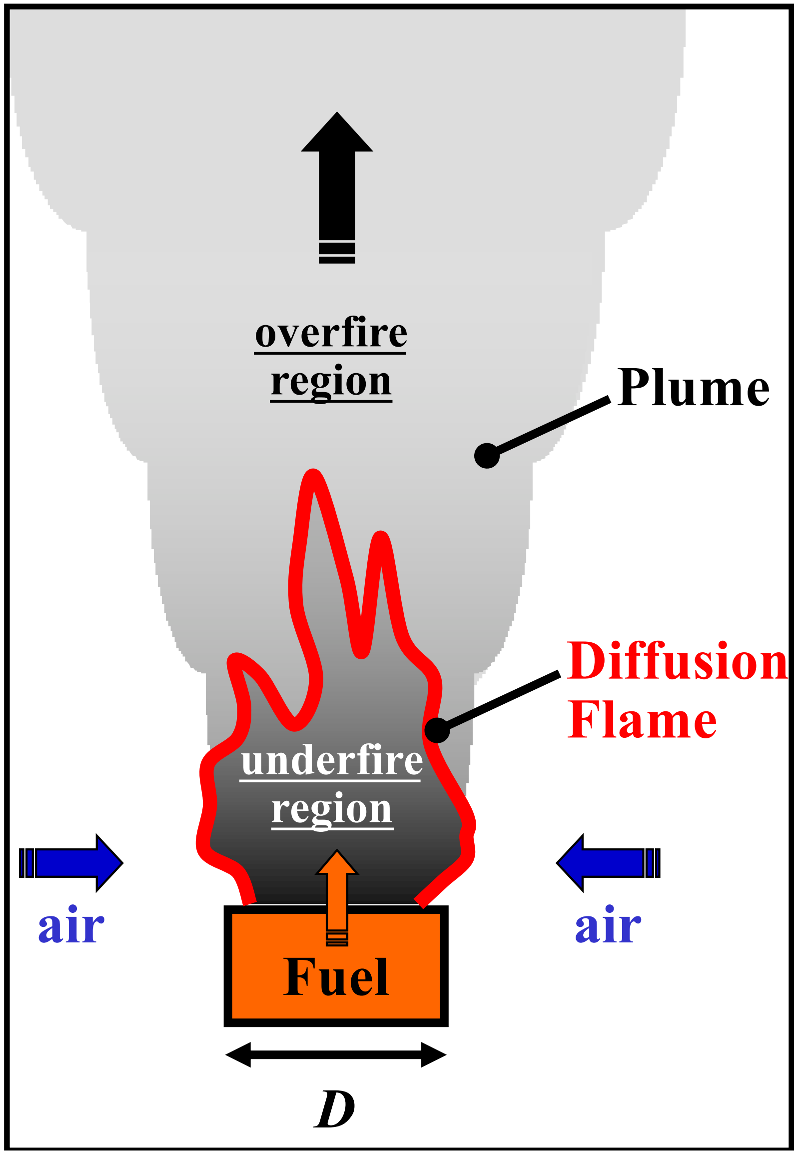




Fire Dynamics

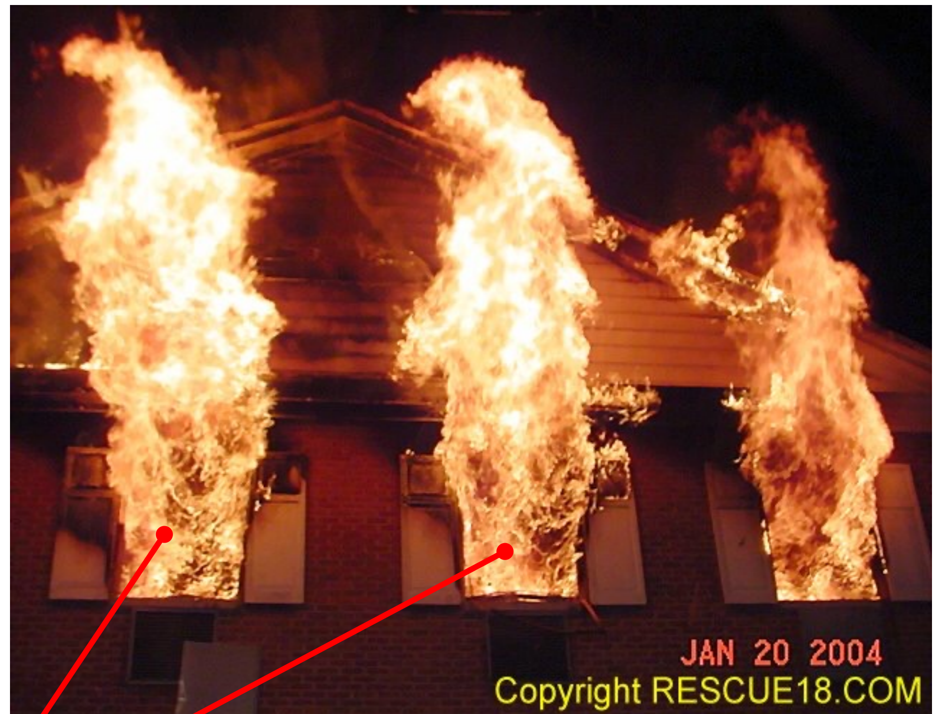
- **Main features**: fire is a buoyancy-driven, relatively-slow, non-premixed combustion process
  - *Example*: pool fire configuration
    - Fuel source velocity is small (a few cm/s)
    - Buoyancy effects accelerate the flow up to several m/s; flow regime corresponds to moderate turbulence intensities
    - Flame corresponds to diffusion combustion and to a thin reaction sheet where fuel and air meet in stoichiometric proportions
    - Long residence times and large length scales promote soot formation and radiation losses

$$\chi_{rad} = (\dot{Q}_{rad}/\dot{Q}_{fire}) \sim 0.3$$



Fire Dynamics

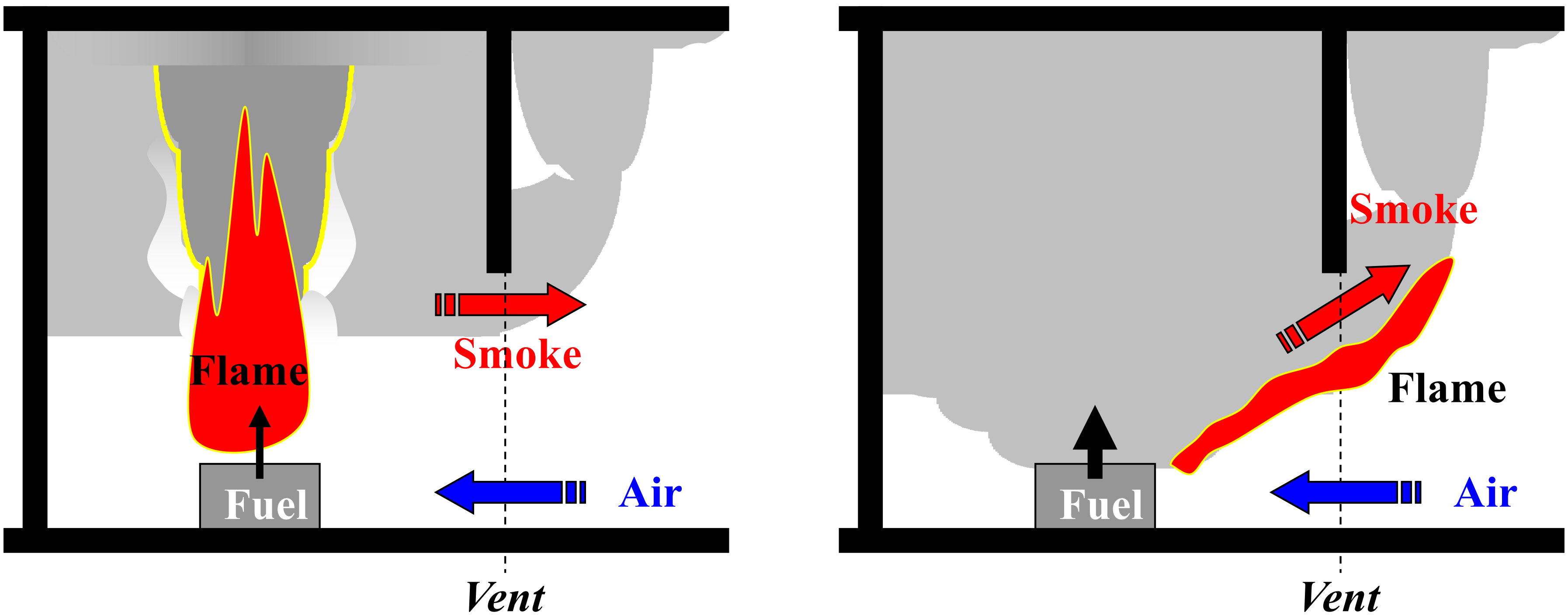
- **Main features**: in compartment fires, combustion can evolve to under-ventilated (*i.e.*, fuel-rich) conditions



Flames extending out of the compartment of fire origin

Fire Dynamics

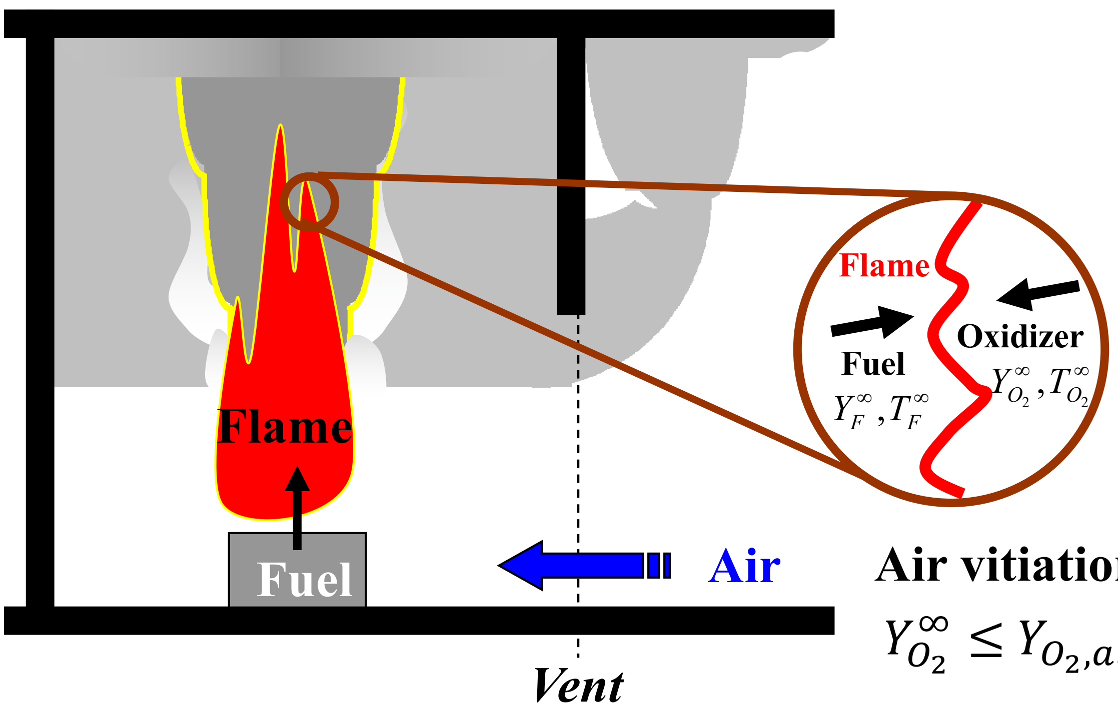
- **Main features**: in compartment fires, combustion can evolve to under-ventilated (*i.e.*, fuel-rich) conditions
  - Flame location: (1) near the fuel source; (2) near the vents



(1) Over-ventilated combustion, (2) Under-ventilated combustion

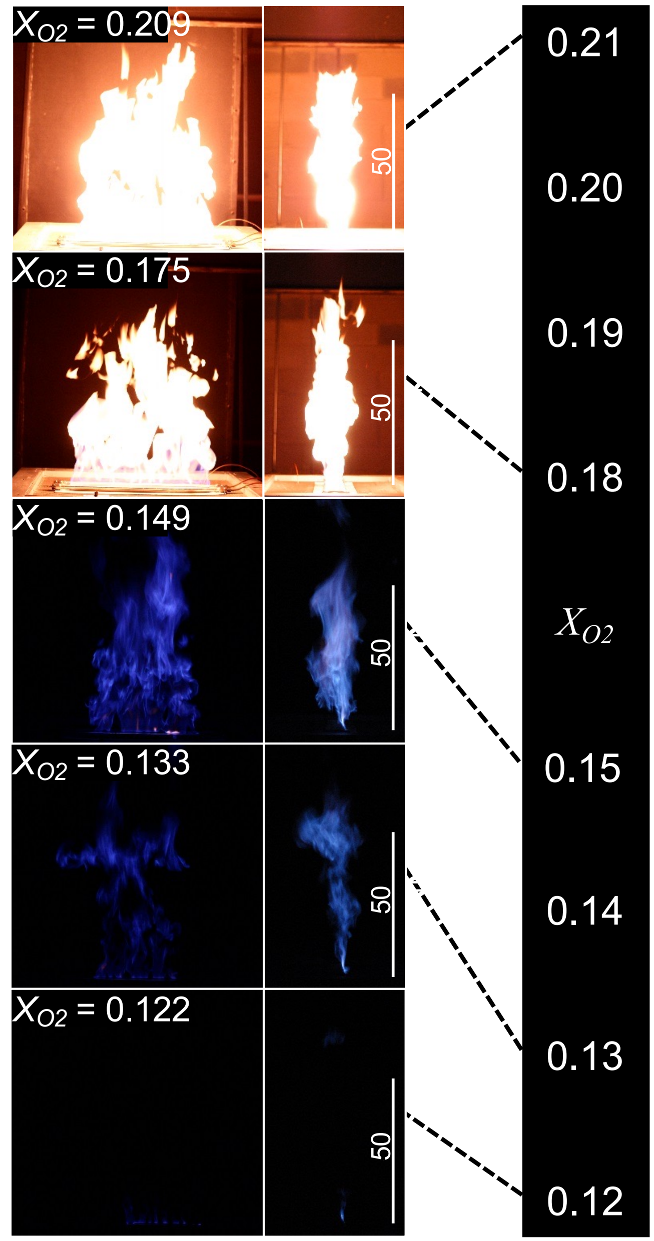
Fire Dynamics

- **Main features**: in compartment fires, combustion can evolve to under-ventilated (*i.e.*, fuel-rich) conditions
  - Oxygen starvation reduces the flame intensity and promotes flame extinction



Air vitiation

$Y_{O_2}^\infty \leq Y_{O_2,air}$



Fire Dynamics

- **Main features**: in compartment fires, radiation plays a dominant role in the thermal feedback to fuel sources

$$G_{UL} = \varepsilon_{UL} \times (\sigma T_{UL}^4)$$

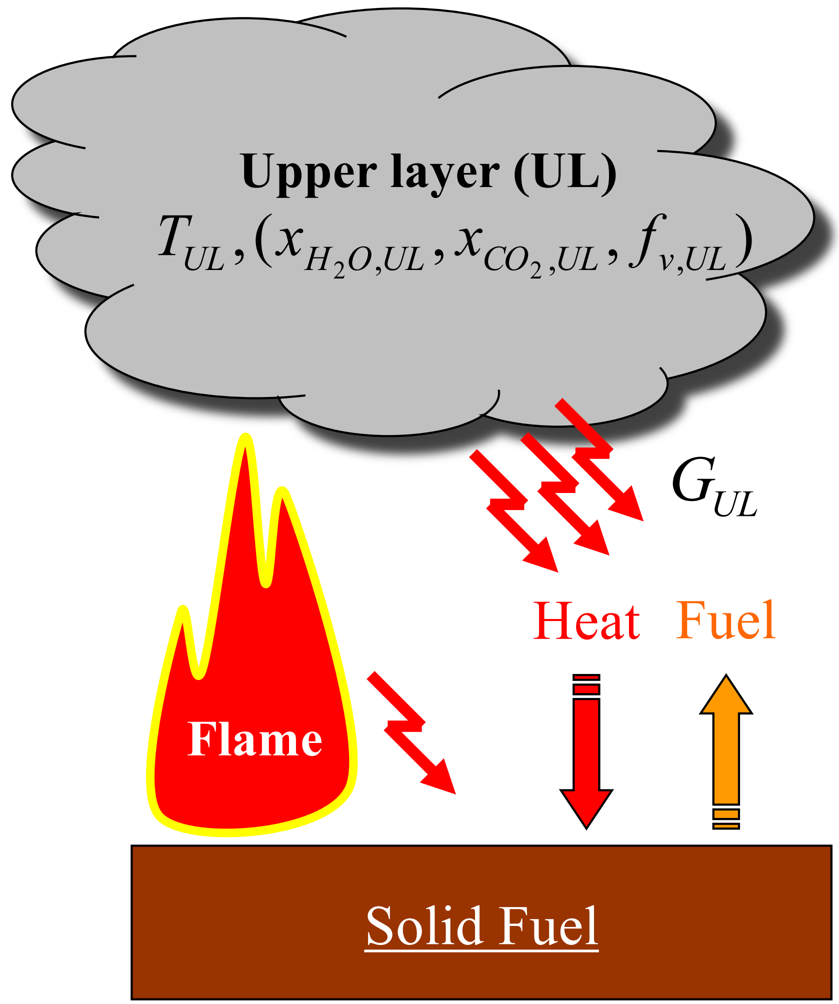
emissive power (G_{UL})   **emissivity** (ε_{UL})

$$\varepsilon_{UL} = 1 - \exp(-\kappa_{UL} \times d_{UL})$$

Planck mean absorption coefficient (κ_{UL})   **mean beam length** (d_{UL})

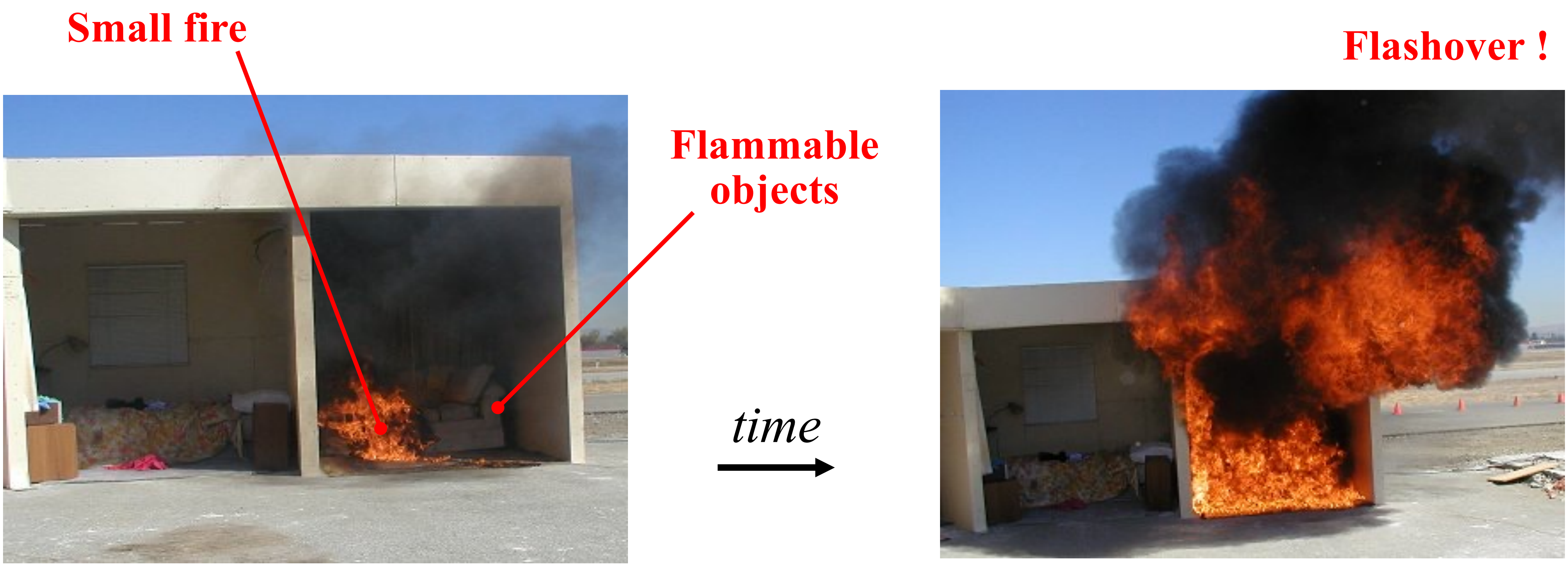
$$\kappa_{UL}(T_{UL}, (x_{H_2O,UL}, x_{CO_2,UL}, f_{v,UL}))$$

gas radiation ($x_{H_2O,UL}, x_{CO_2,UL}$)   **soot radiation** ($f_{v,UL}$)



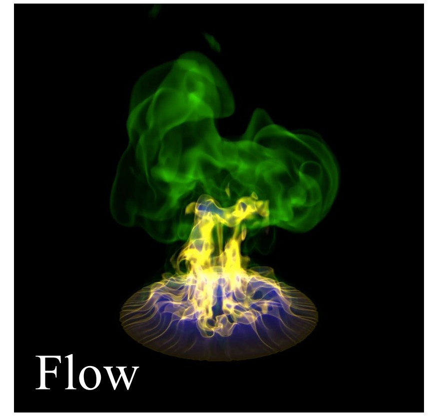
Fire Dynamics

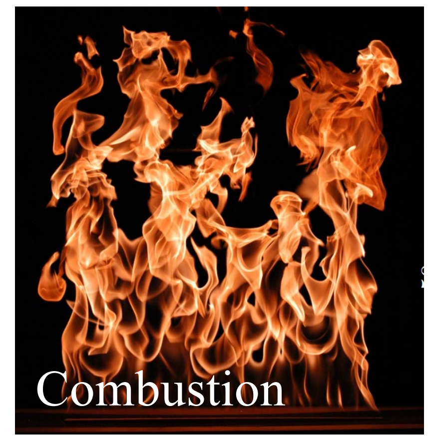
- **Main features**: in compartment fires, radiation plays a dominant role in the thermal feedback to fuel sources
  - Possible transition to *flashover* (rapid series of radiation-driven ignition events involving all flammable objects/materials present in the fire room)

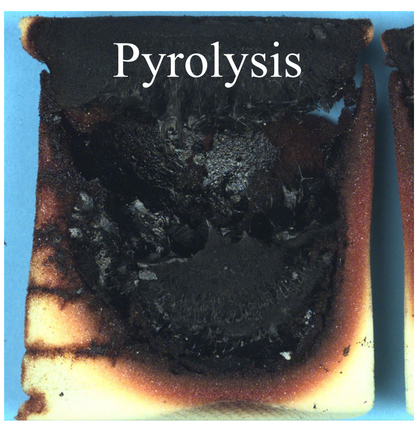


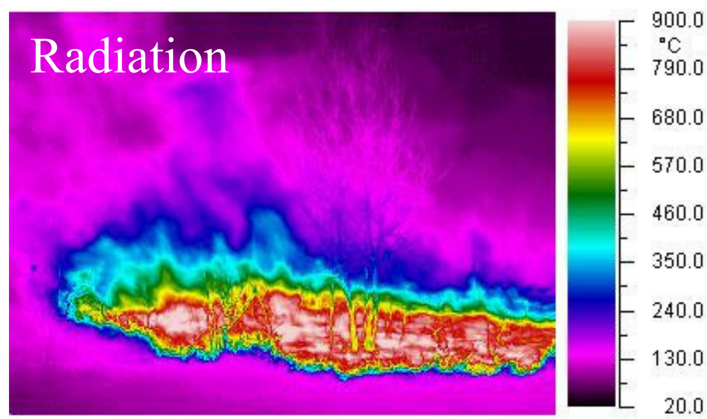
Fire Dynamics

- **Main features**: fire is an uncontrolled combustion process characterized by a thermal feedback loop
  - Buoyancy-driven turbulent flow
  - Non-premixed combustion
    - Including possible oxygen-limited conditions leading to flame extinction/re-ignition phenomena
    - Including soot formation
  - Thermal radiation
    - Including possible transition to flashover
  - Pyrolysis









Fire Dynamics

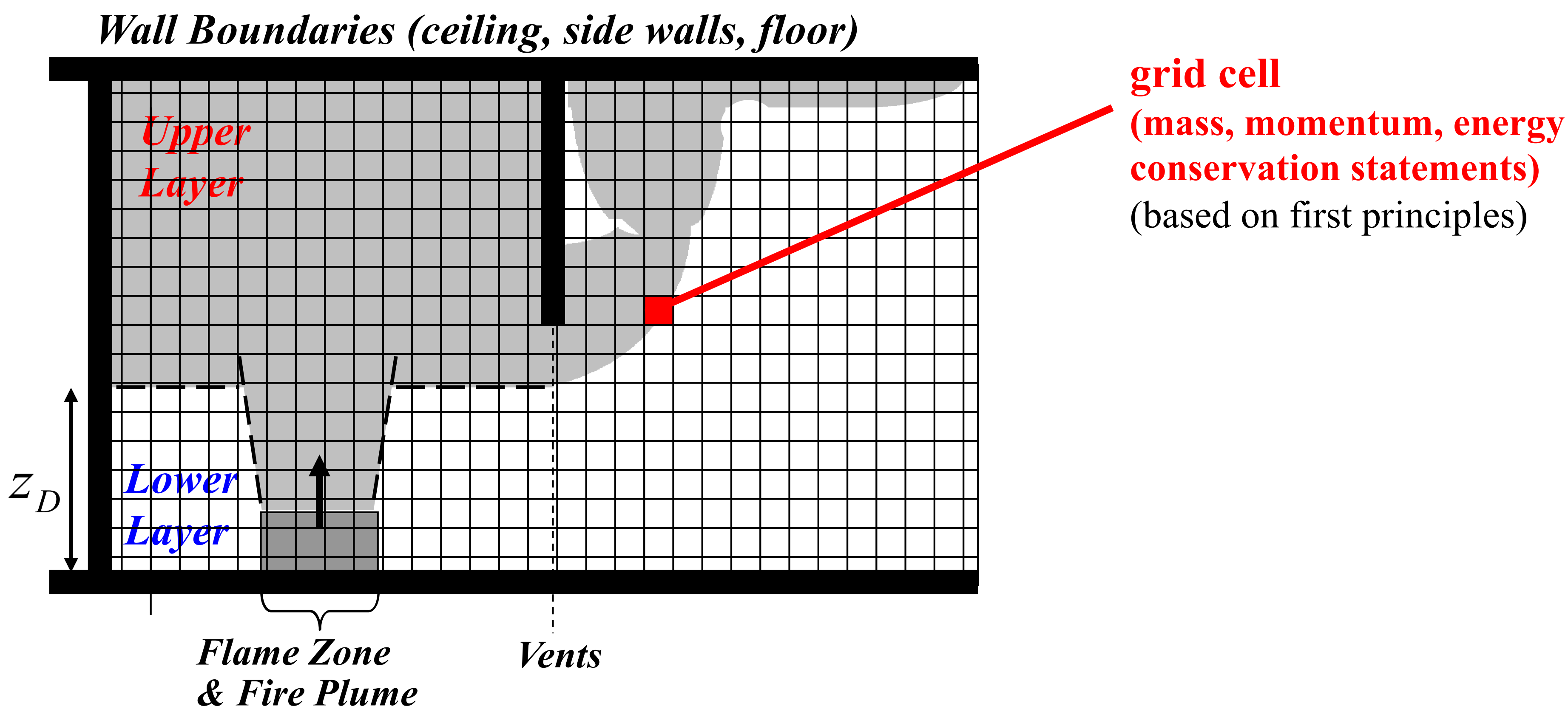
- Three different components in a computational model aimed at fire applications
  - Computational Fluid Dynamics (CFD) flow/combustion solver
    - Heat release by combustion and heat transfer by convection
  - Radiation solver
    - Heat transfer by radiation (electromagnetic energy)
  - Solid phase pyrolysis solver
    - Heat transfer by conduction and possible thermal degradation of materials

Compartment Fire Modeling

- Outline
  - Brief Review of Compartment Fire Dynamics
  - **Fire Modeling Landscape**
  - Computational Infrastructure
  - Physical Modeling
  - Examples

Fire Modeling Landscape

- CFD modeling
  - A spatially-resolved description of compartment fires



Fire Modeling Landscape

- CFD modeling
  - History
    - An approximately 25-years-old activity
    - Widespread use by different fire safety stakeholders (including researchers and practicing engineers)
  - Landscape
    - No commercial software
    - Software with limited distribution: JASMINE (Building Research Establishment, UK), KAMELEON (Norwegian University of Science and Technology/SINTEF, Norway), SMARTFIRE (University of Greenwich, UK), SOFIE (University of Cranfield, UK)
    - Open-source software: FDS (NIST, USA), FireFOAM (FM Global, USA), ISIS (IRSN, France)

Fire Modeling Landscape

- CFD modeling
  - Applications
    - Performance-based design (compartmentation performance, evacuation performance, smoke management, fire suppression systems, structural resistance, *etc*)
    - Forensic applications
    - Risk analysis
    - Fire-fighter training
    - Sensor-driven real-time emergency management
    - Research (scientific studies of fire dynamics)

Compartment Fire Modeling

- Outline
  - Brief Review of Compartment Fire Dynamics
  - Fire Modeling Landscape
  - **Computational Infrastructure**
  - Physical Modeling
  - Examples

Computational Infrastructure

- CFD-based fire modeling (field modeling)
  - A branch in a wider class of simulation tools known as Computational Fluid Dynamics (CFD)
  - CFD infrastructure requires:
    - **Mathematical models** to describe relevant physics
      - ✓ First principles (conservation of mass, momentum, energy)
    - **Numerical algorithms** to solve mathematical models
      - ✓ Partial Differential Equations (PDE) solvers
      - ✓ Mesh generators
    - **Computer power** to enable numerical algorithms
      - ✓ Massively parallel computers
      - ✓ Graphics Processing Unit (GPU) computers

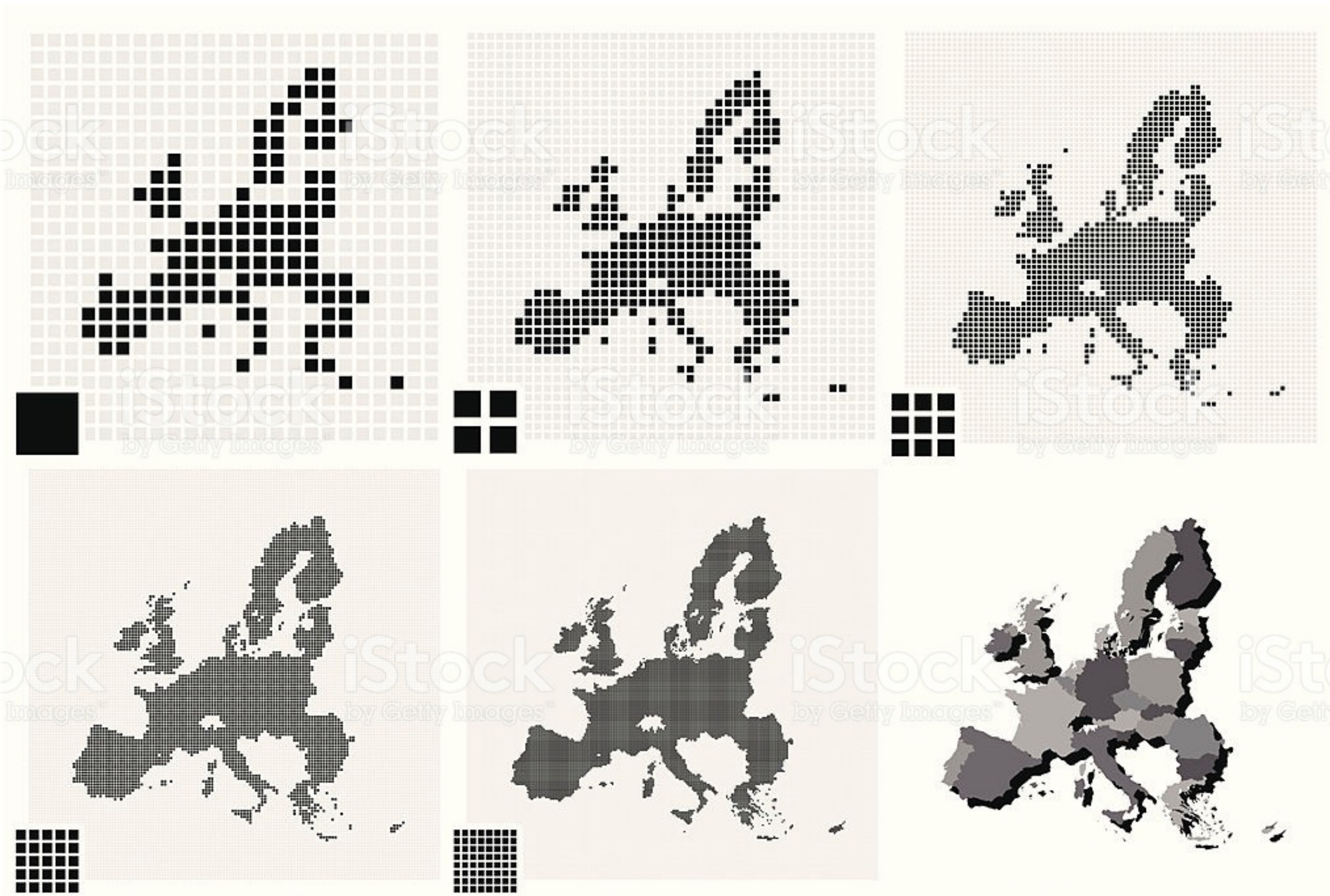
Computational Infrastructure

- Mathematical modeling (Direct Numerical Simulation – DNS)

$$
\begin{cases}
\dfrac{\partial \rho}{\partial t} + \dfrac{\partial}{\partial x_j}(\rho u_j) = 0 \\[2ex]
\dfrac{\partial}{\partial t}(\rho Y_k) + \dfrac{\partial}{\partial x_j}(\rho Y_k u_j) = \dfrac{\partial}{\partial x_j}(\rho D_k \dfrac{\partial Y_k}{\partial x_j}) + \dot{\omega}_k, \quad 1 \le k \le N_S \\[2ex]
\dfrac{\partial}{\partial t}(\rho u_i) + \dfrac{\partial}{\partial x_j}(\rho u_i u_j) = -\dfrac{\partial p}{\partial x_i} + \dfrac{\partial \tau_{ij}}{\partial x_j} + \rho g_i, \quad 1 \le i \le 3 \\[2ex]
\dfrac{\partial}{\partial t}(\rho h) + \dfrac{\partial}{\partial x_j}(\rho h u_j) = \dfrac{\partial p}{\partial t} + u_j \dfrac{\partial p}{\partial x_j} + \tau_{ij} \dfrac{\partial u_i}{\partial x_j} - \dfrac{\partial q_j}{\partial x_j} \\[2ex]
p = \rho R T (\sum_{k=1}^{N_s} \dfrac{Y_k}{M_k})
\end{cases}
$$

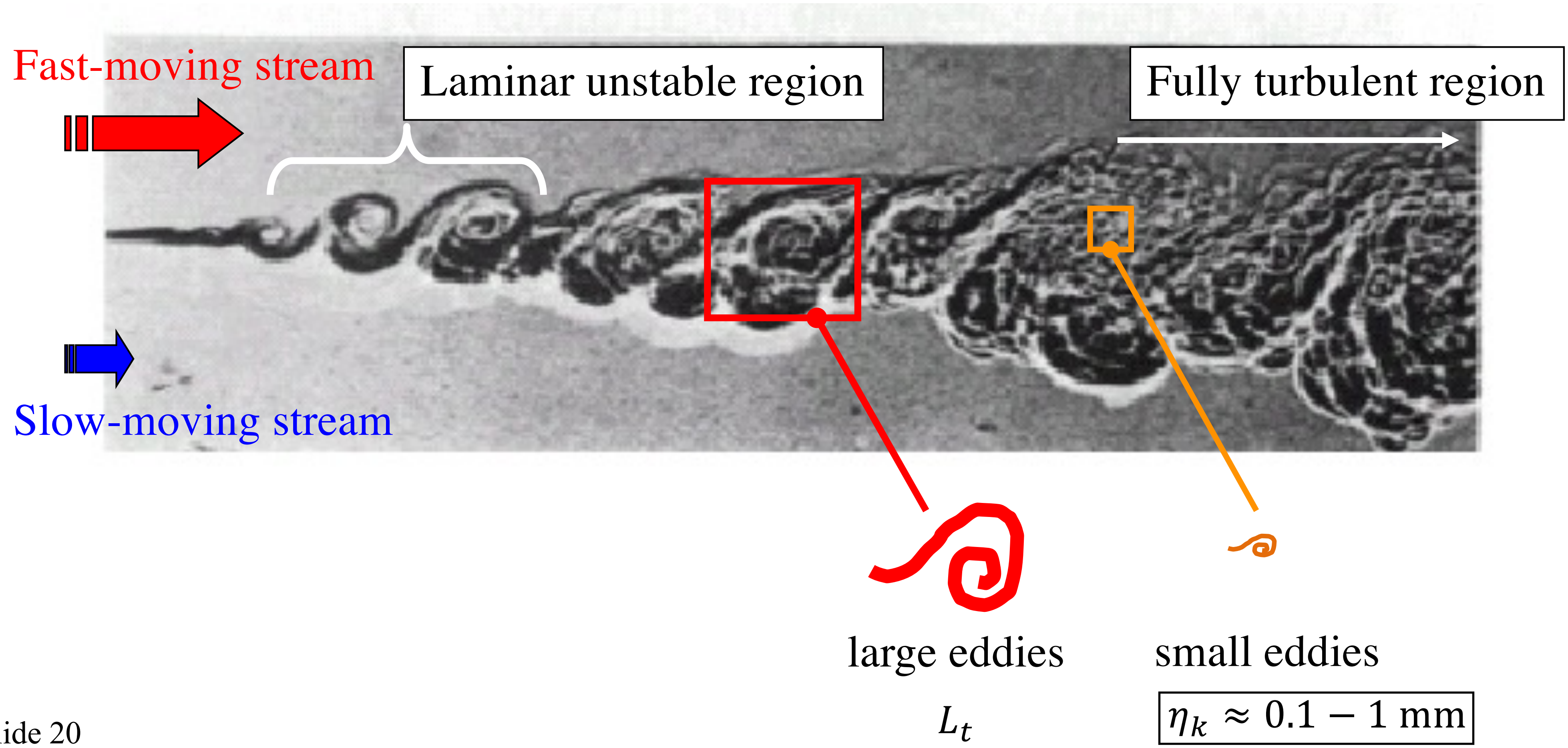
Computational Infrastructure

- Resolution requirements
  - How many pixels (*i.e.* computational cells)?



Computational Infrastructure

- Mathematical modeling (DNS)
  - Characteristic length scales
    - Turbulence viewed as a multi-scale problem



Computational Infrastructure

- Mathematical modeling (DNS)
  - Computational grid requirement
    - Large eddies (macro-scales)
      - ✓ Turbulent rms velocity (m/s): u'
      - ✓ Integral length scale (m): L_t
      - ✓ Turbulent Reynolds number:

$$\mathrm{Re}_t = \frac{\rho u' L_t}{\mu} = \frac{u' L_t}{\nu}$$

    - Small eddies (micro-scales, also called Kolmogorov scales)
      - ✓ Kolmogorov velocity (m/s):

$$v_K = u' \times (\mathrm{Re}_t)^{-1/4}$$

      - ✓ Kolmogorov length scale (m):

$$\eta_K = L_t \times (\mathrm{Re}_t)^{-3/4}$$

Computational Infrastructure

- Mathematical modeling (DNS)
  - Computational grid requirement
    - Example: pool fire, $\dot{Q} = 1$ MW; $D = 1$ m

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

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

$$\boxed{\Delta x_{DNS} \approx 0.4 \text{ mm}}$$ **Grid requirement based on flow**

Computational Infrastructure

- Mathematical modeling (DNS)
  - Characteristic length scales
    - Combustion viewed as a stiff problem

Lecoustre *et al*. (2014) *Combust. Flame*

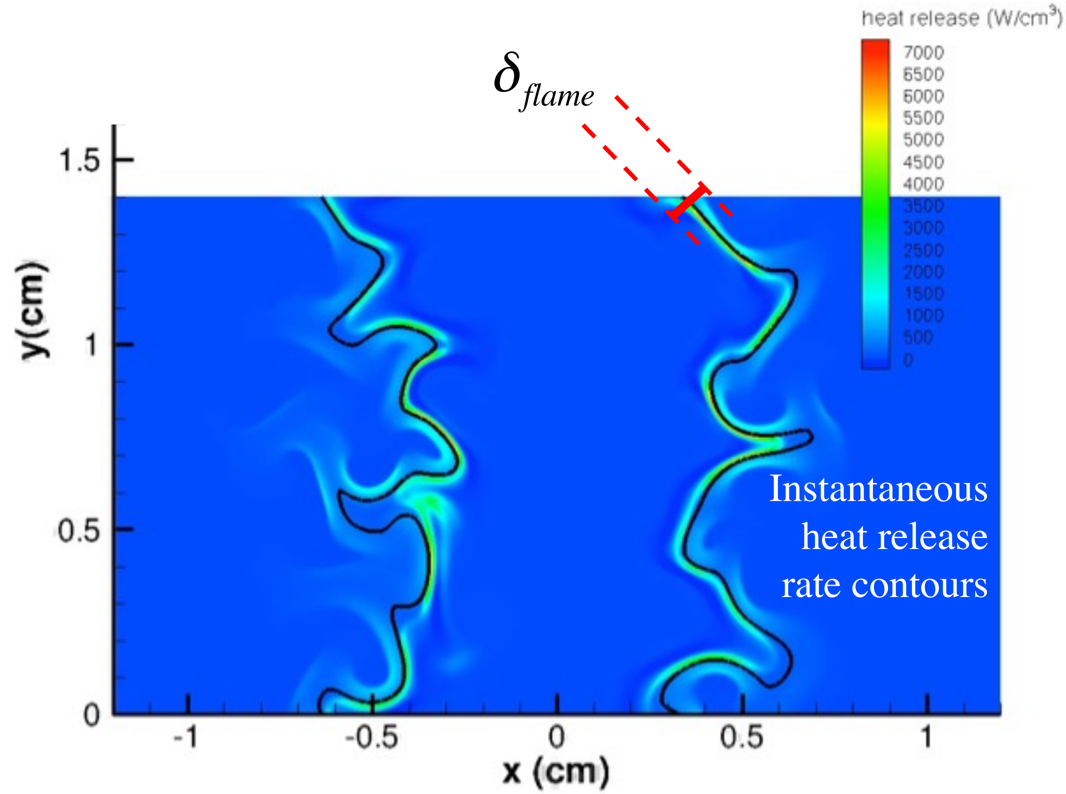
Strained laminar diffusion flame theory

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

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

$$\boxed{\Delta x_{DNS} \approx 0.1\ \text{mm}}$$

Grid requirement based on flame



Computational Infrastructure

- Mathematical modeling (DNS)
  - Characteristic length scales
    - Thermal radiation viewed as a stiff problem

Experimental observations

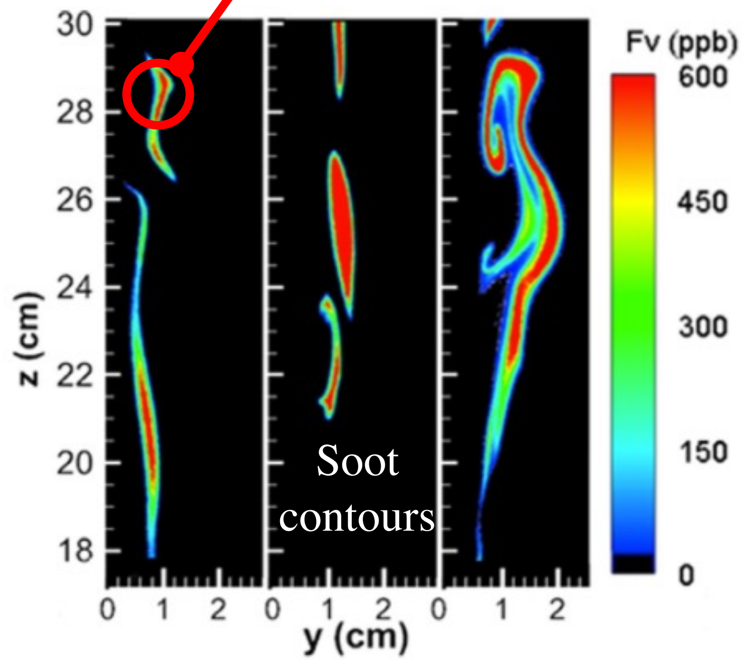
$\delta_{soot} \approx 1$ mm

$\Delta x_{DNS} \approx 0.1$ mm

Grid requirement based on radiation

δ_{soot}

δ_{soot}



Valencia *et al.*
Proc. Combust. Inst. 2016

Computational Infrastructure

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

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

Computational Infrastructure

- Mathematical modeling (Large Eddy Simulation – LES)

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j) = 0$$

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{Y}_k) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{Y}_k\tilde{u}_j) = -\frac{\partial \lambda_{kj}}{\partial x_j} + \frac{\partial}{\partial x_j}\overline{(\rho D_k \frac{\partial Y_k}{\partial x_j})} + \overline{\dot{\omega}'''_k}, \quad 1 \le k \le N_S$$

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{u}_i) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_i\tilde{u}_j) = -\frac{\partial T_{ij}}{\partial x_j} - \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \overline{\tau_{ij}}}{\partial x_j} + \bar{\rho} g_i, \quad 1 \le i \le 3$$

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{h}) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{h}\tilde{u}_j) = -\frac{\partial Q_j}{\partial x_j} + \frac{\partial \bar{p}}{\partial t} + \overline{u_j \frac{\partial p}{\partial x_j}} + \overline{\tau_{ij}\frac{\partial u_i}{\partial x_j}} - \frac{\partial \overline{\dot{q}''_j}}{\partial x_j}$$

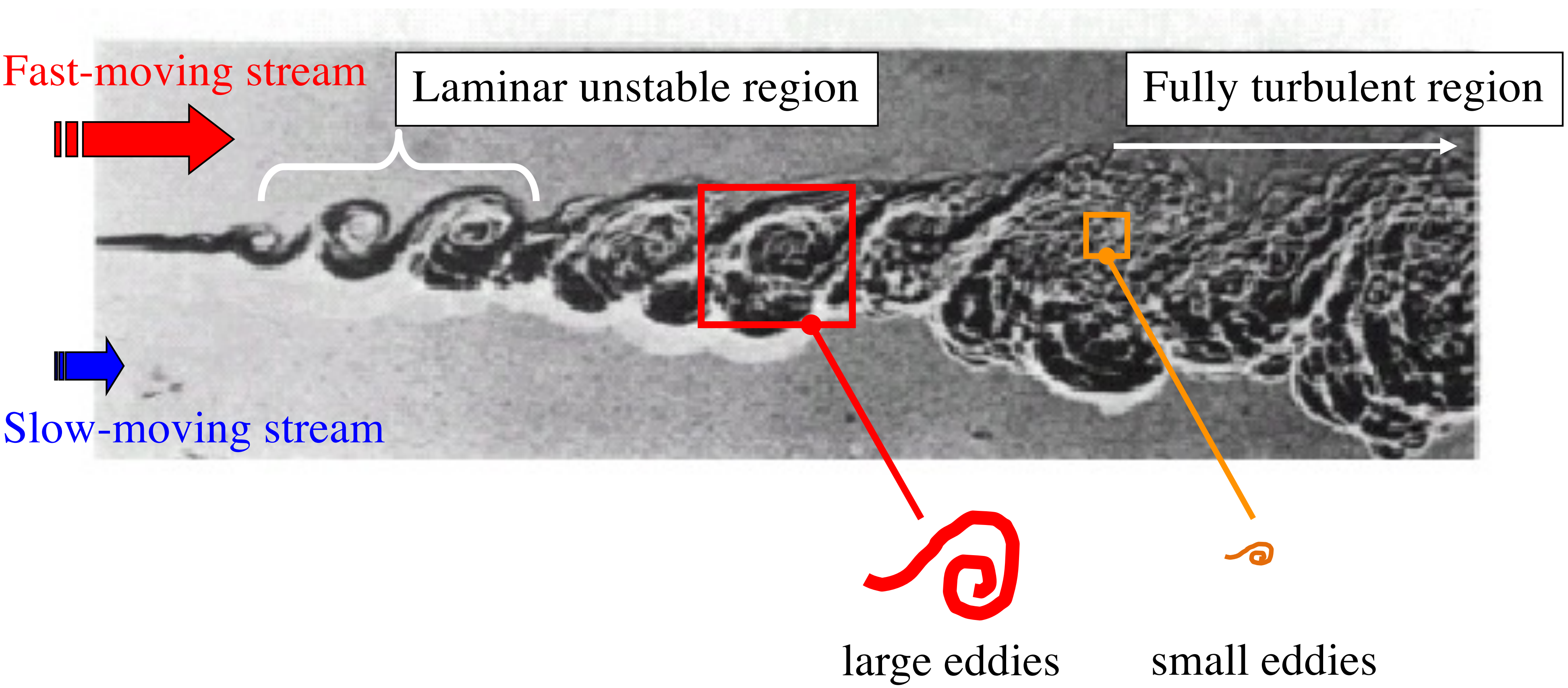
$$\bar{p} = \bar{\rho} R \tilde{T} \sum_{k=1}^{N_s} \frac{\tilde{Y}_k}{M_k} + R \sum_{k=1}^{N_s} \frac{(\overline{\rho T Y_k} - \bar{\rho}\tilde{T}\tilde{Y}_k)}{M_k}$$

Computational Infrastructure

- Mathematical modeling (Large Eddy Simulation – LES)
  - Mathematical formulation applied to LES-filtered (*i.e.* computational-grid-cell-averaged) quantities; requires models to describe unresolved (subgrid-scale) physics
    - Models to describe turbulent fluxes: $\lambda_{kj}, T_{ij}, Q_j$
    - Models to describe turbulent combustion: $\bar{\dot{\omega}}_k'''$
    - Models to describe thermal radiation transport: $\bar{\dot{q}}_{rad}''' = -\partial/\partial x_j(\bar{\dot{q}}_j'')$

Computational Infrastructure

- Mathematical modeling (LES)
  - Computational grid requirement
    - Turbulence viewed as a multi-scale problem



Computational Infrastructure

- Mathematical modeling (LES)
  - Computational grid requirement (fine-grained LES)
    - Example: pool fire, $\dot{Q} = 1$ MW; $D = 1$ m

$$L_t \approx 0.5 \times D = 0.5 \text{ m}$$

$$\Rightarrow \quad \boxed{\Delta x_{LES} \approx \frac{L_t}{10} = 0.05 \text{ m} \approx 100 \times \Delta x_{DNS}}$$

Computational Infrastructure

- Mathematical modeling
  - Direct Numerical Simulation (DNS)
    - Grid-resolved scales: $L_t, \eta_K, \delta_{flame}, \delta_{soot}$

$$\Delta x_{DNS} \approx \eta_K$$
$$\Delta x_{DNS} \approx (\delta_{flame}/10)$$
$$\Delta x_{DNS} \approx (\delta_{soot}/10)$$
$$\Longrightarrow \boxed{\Delta x_{DNS} = O(0.1\text{ mm})}$$

  - 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 Infrastructure

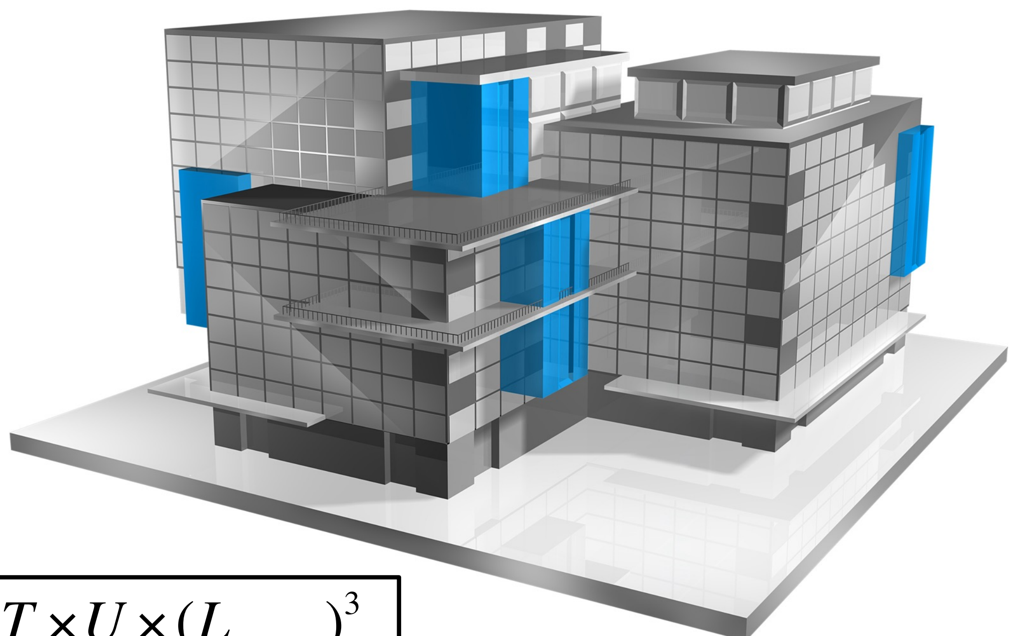
- Mathematical modeling (LES)
  - Computational grid requirement (coarse-grained LES)
    - Example: fire in a large building system

Space: $(L_{system})^3$

$$\frac{\text{CPU cost}}{N_{\Delta t}(N_{\Delta x}N_{\Delta y}N_{\Delta z})} = O(100\,\mu s)$$

$$N_{\Delta x} \sim N_{\Delta y} \sim N_{\Delta z} = (\frac{L_{system}}{\Delta x})$$

$$N_{\Delta t} = (\frac{T}{\Delta t}) = (\frac{T}{CFL \times (\Delta x / U)})$$



$$\text{CPU cost} \times (\Delta x)^4 = O(100\,\mu s) \times (\frac{T \times U \times (L_{system})^3}{CFL})$$

Computational Infrastructure

- Mathematical modeling (LES)
  - Computational grid requirement (coarse-grained LES)
    - Example: fire in a large building system

$L_{system} = 50 \text{ m}$

$U = 10 \text{ m/s}$

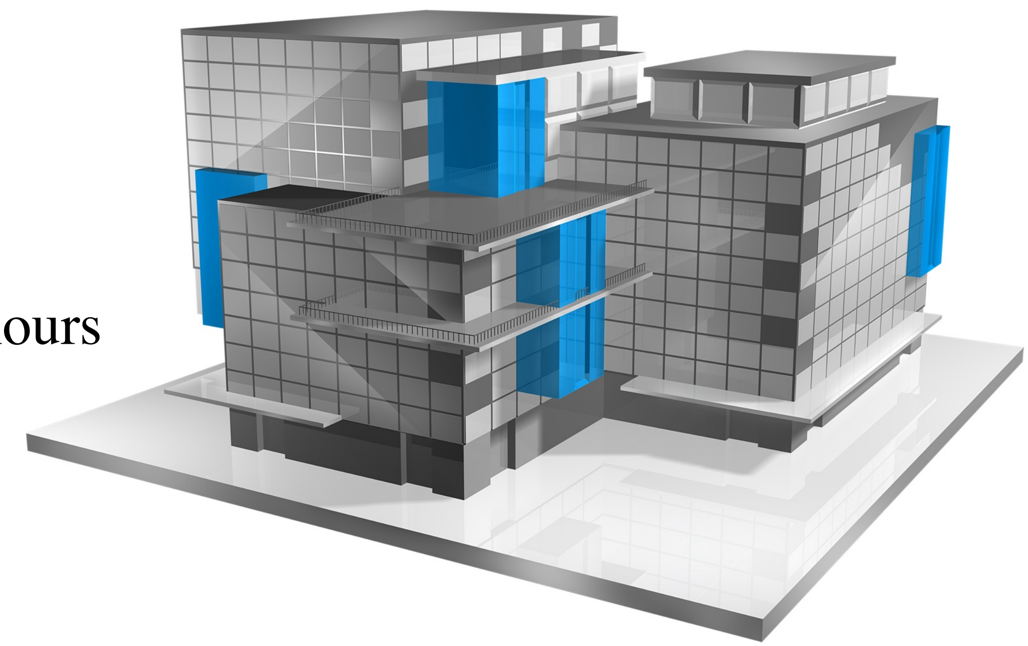
$T = 10 \text{ minutes}$

$\text{CPU cost} = 24 \times 32 \text{ PEs} = 768 \text{ hours}$

$CFL = 0.5$

$\Rightarrow \boxed{\Delta x \sim 0.5 \text{ m}}$

$(N_{\Delta x} N_{\Delta y} N_{\Delta z}) \sim 1 \; Million$



Computational Infrastructure

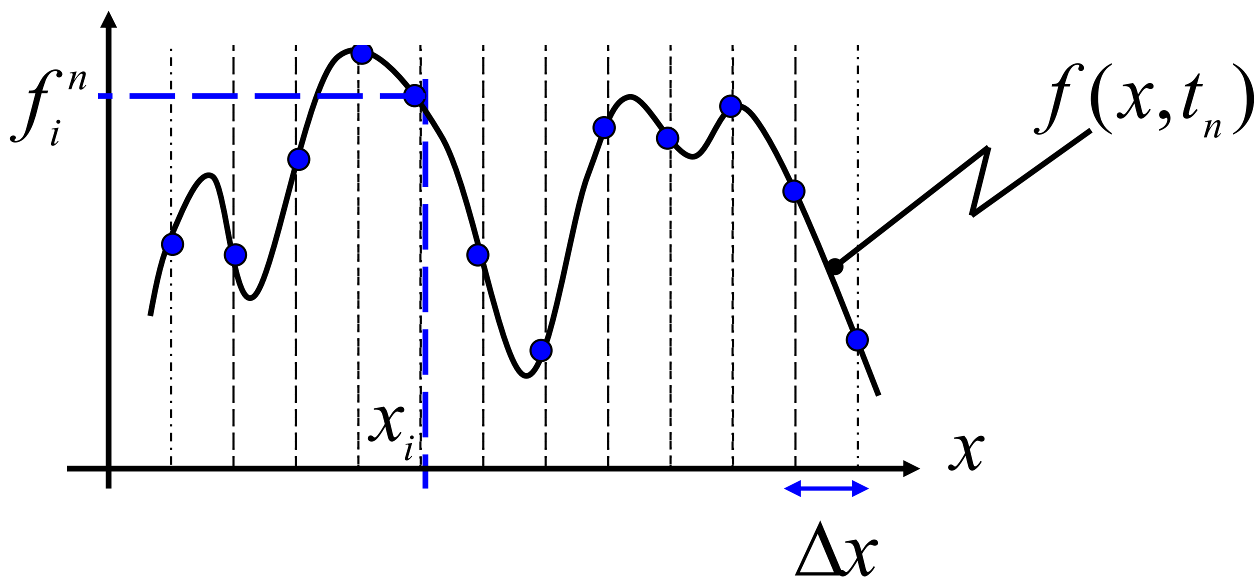
- Computational modeling
  - Going from a mathematical model to a numerical algorithm

    Model problem

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} = D\frac{\partial^2 f}{\partial x^2}$$

  - **Discretization**: describe continuous function *f(x,t)* as a set of discrete numbers corresponding to values taken by *f* at prescribed space and time locations

$$f_i^n = f(x_i, t_n)$$



Computational Infrastructure

- Computational modeling
  - Going from a mathematical model to a numerical algorithm

    Model problem

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} = D\frac{\partial^2 f}{\partial x^2}$$

  - Formulation of discretized equations: describe original partial differential equations (PDEs) as a set of algebraic operations (additions, subtractions, multiplications, divisions) that can be performed by a computer

$$\underbrace{\frac{f_i^{n+1} - f_i^n}{\Delta t}}_{unsteady} + u\underbrace{\frac{f_{i+1}^n - f_{i-1}^n}{2\Delta x}}_{convection} = D\underbrace{\frac{f_{i+1}^n + f_{i-1}^n - 2f_i^n}{(\Delta x)^2}}_{diffusion}$$

Computational Infrastructure

- Computational modeling
  - PDE solvers

<u>Model problem</u>

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} = D\frac{\partial^2 f}{\partial x^2}$$

Computational domain

$L_x = 20\,\mathrm{m}$

Initial conditions

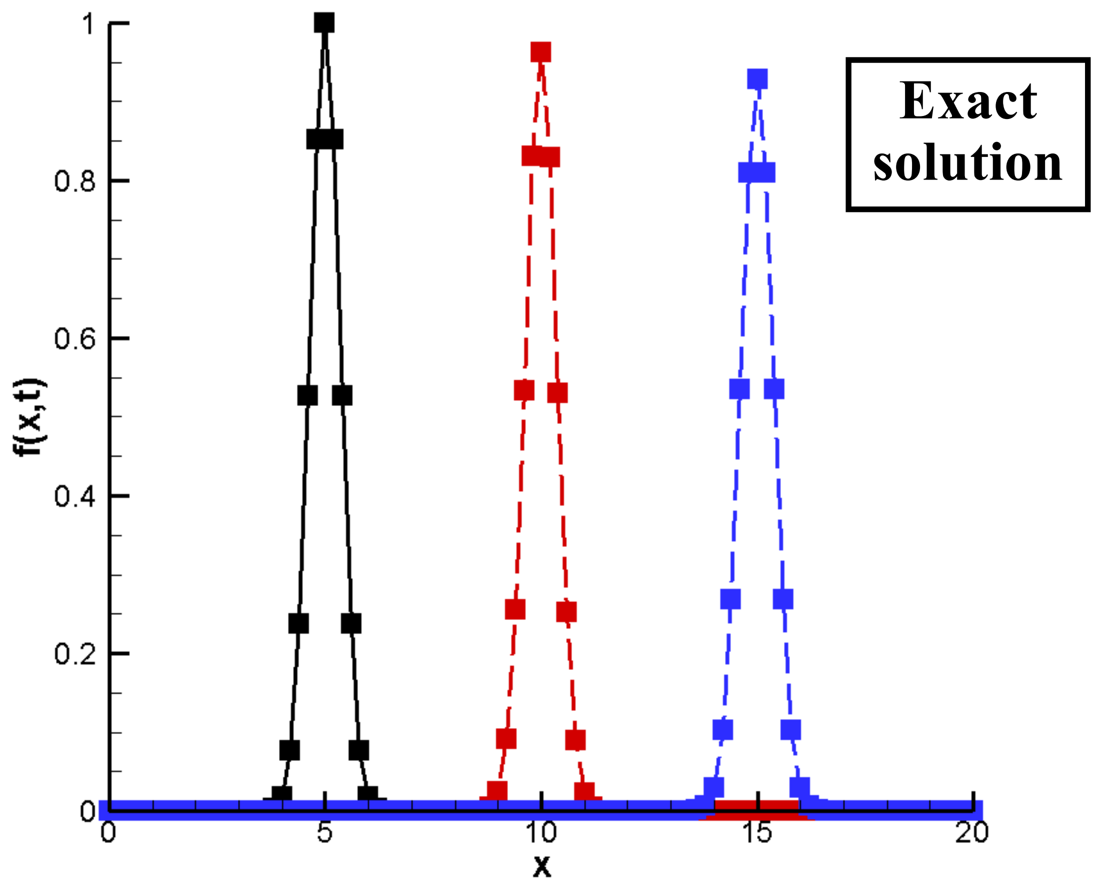
$f(x, t=0) = \exp(-\frac{(x-x_0)^2}{\sigma_0^2})$

$x_0 = 5\,\mathrm{m}$; $\sigma_0 = 0.5\,\mathrm{m}$

Parameters

$u = 1\,\mathrm{m/s}$; $\delta_0 = 2\sigma_0 = 1\,\mathrm{m}$

$\mathrm{Re} = \frac{u \times \delta_0}{D} = 1000$; $D = 10^{-3}\,\mathrm{m^2/s}$



Computational Infrastructure

- Computational modeling
  - PDE solvers

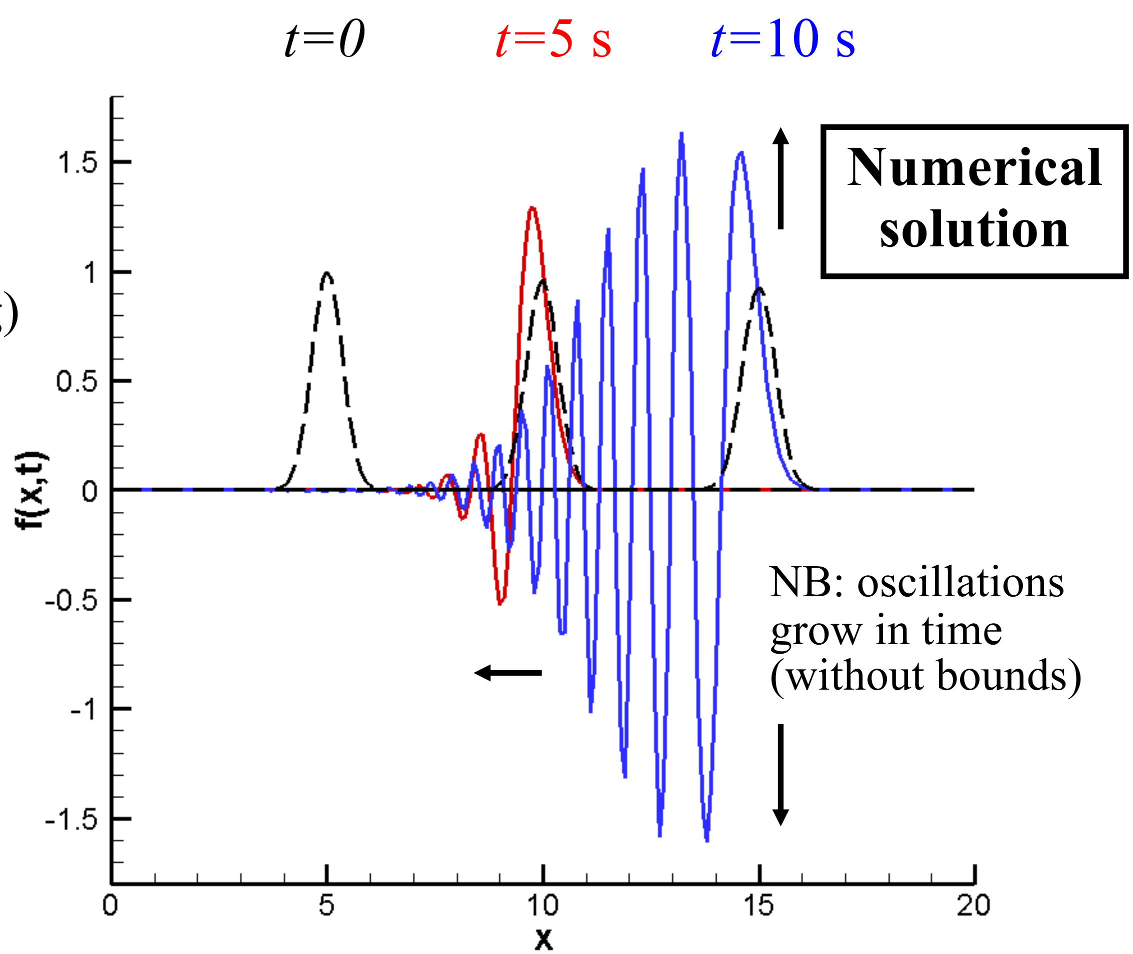
<u>Model problem</u>

EECD scheme
(Euler/explicit, central-differencing)

$$\Delta x = (\delta_0 / 10) = 0.1 \text{ m}$$

$$\Delta t = 0.2 \times (\Delta x / u) = 0.02 \text{ s}$$

unstable solution!
(unphysical)



Computational Infrastructure

- Computational modeling
  - PDE solvers

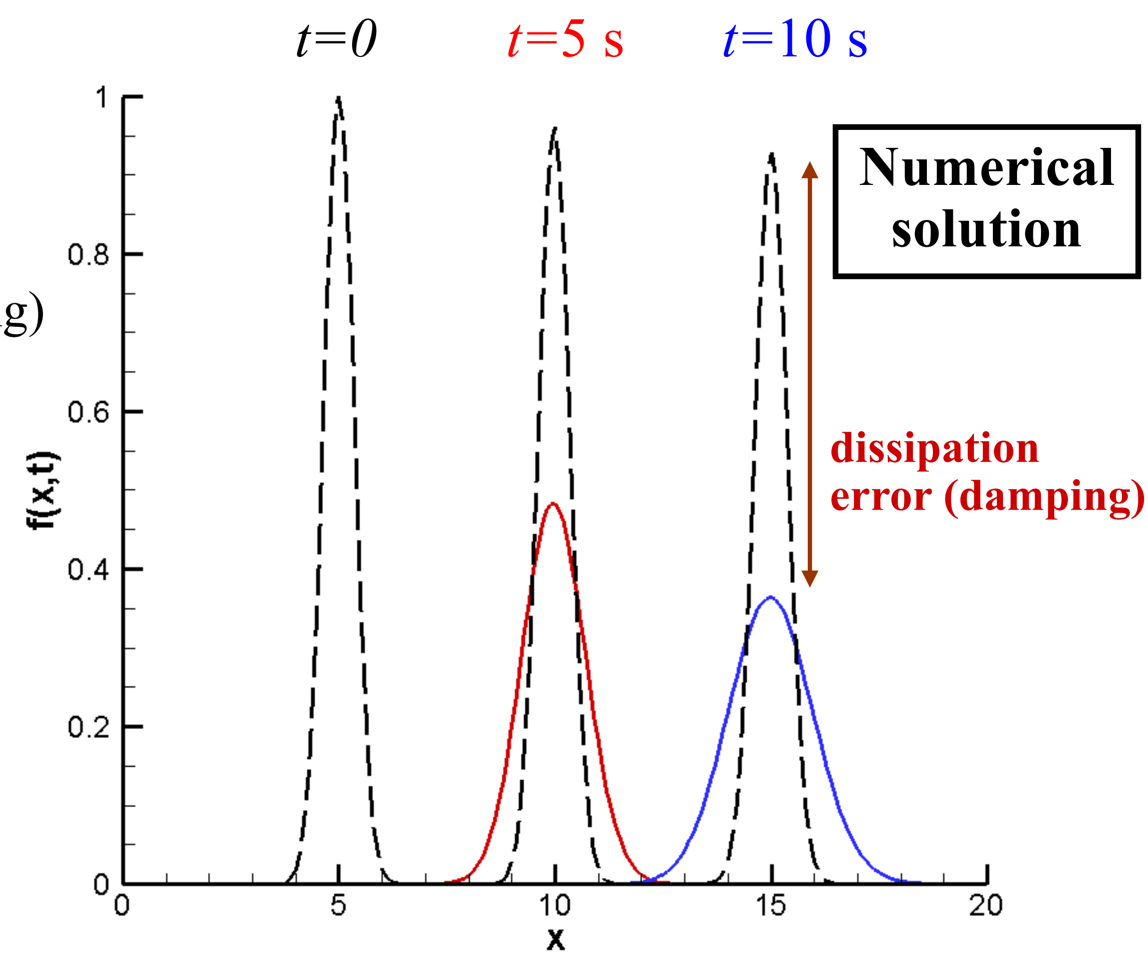
    Model problem

EEUD scheme
(Euler/explicit, upwind-differencing)

$$\Delta x = (\delta_0 / 10) = 0.1 \text{ m}$$

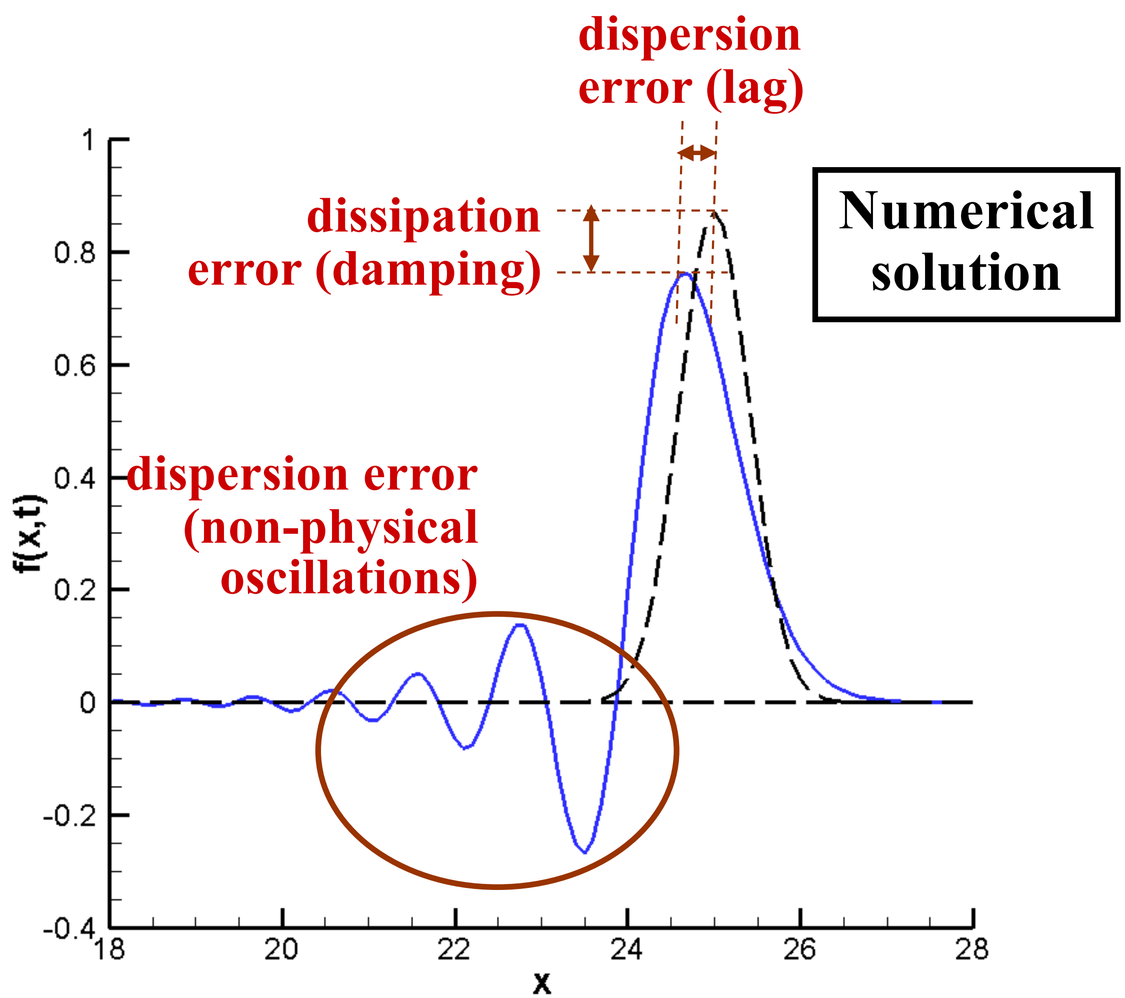
$$\Delta t = 0.2 \times (\Delta x / u) = 0.02 \text{ s}$$

stable solution
positive solution
(physical but) **inaccurate**



Computational Infrastructure

- Computational modeling
  - PDE solvers
  - Numerical errors



Computational Infrastructure

- Computational modeling
  - PDE solvers

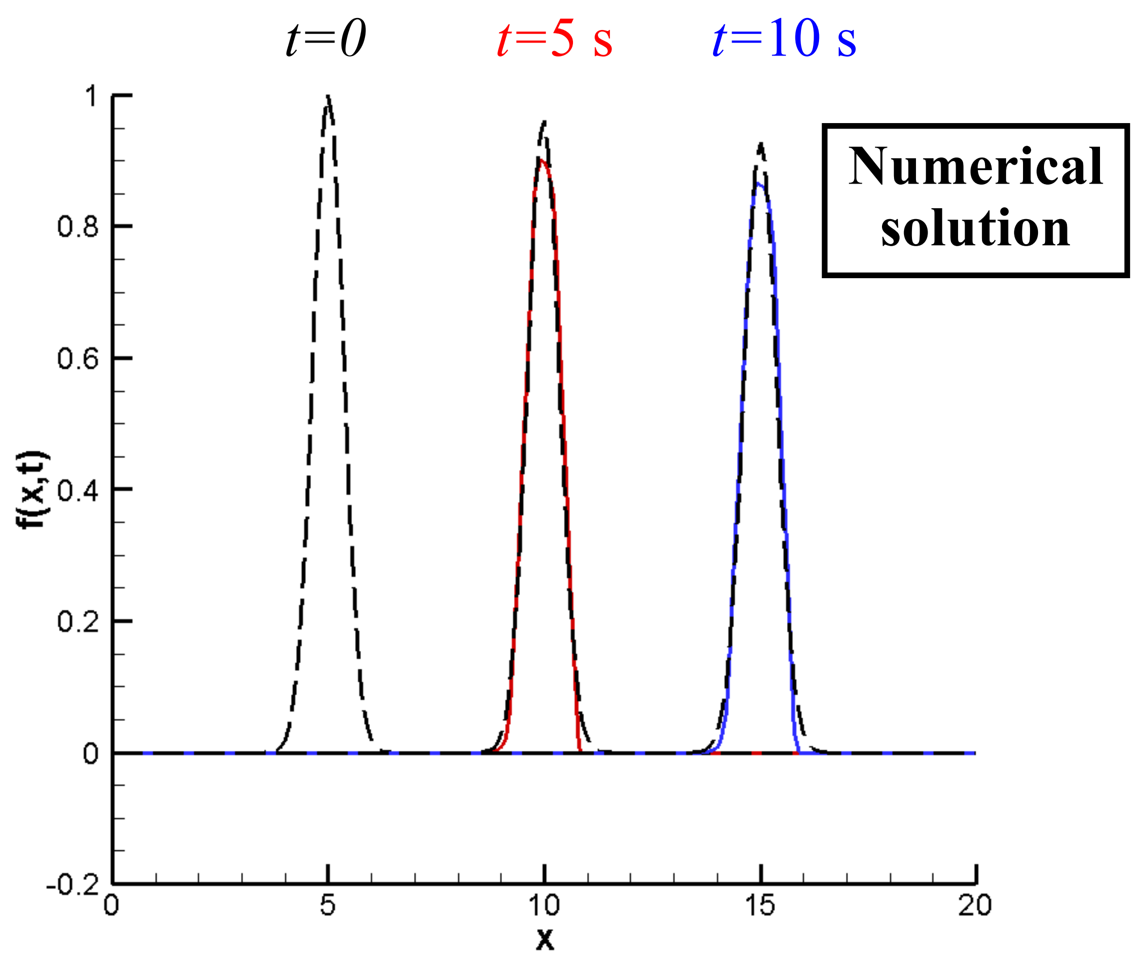
<u>Model problem</u>

TVD scheme
(Total Variation Diminishing)

$$\Delta x = (\delta_0 / 10) = 0.1 \text{ m}$$

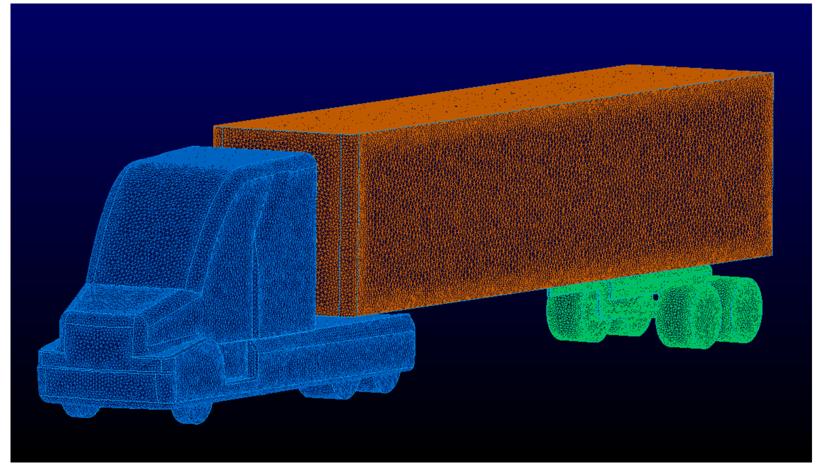
$$\Delta t = 0.2 \times (\Delta x / u) = 0.02 \text{ s}$$

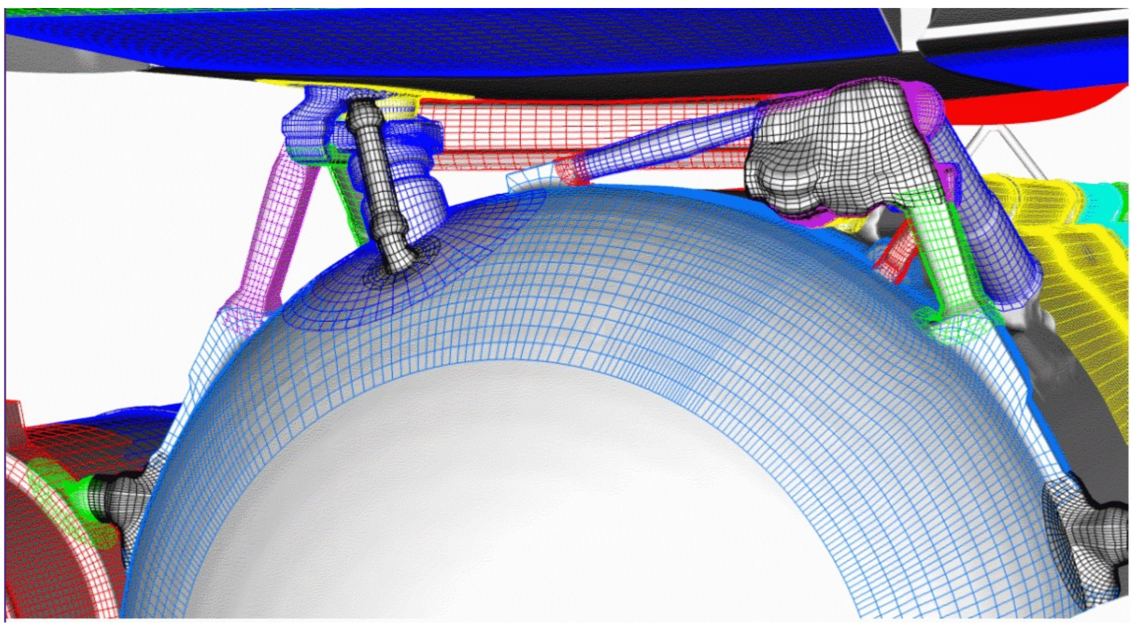
stable solution
physical and accurate
(and positive)



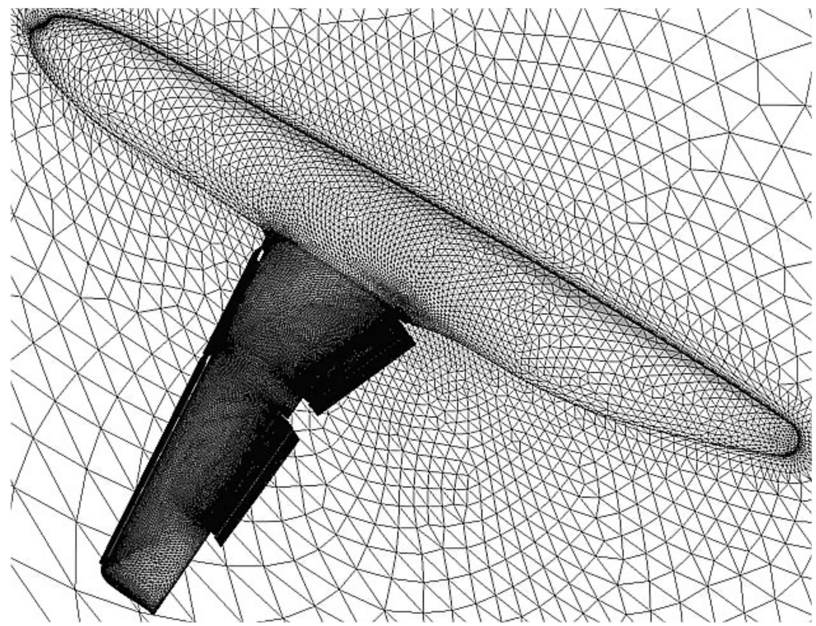
Computational Infrastructure

- Computational modeling
  - Mesh generators





Multiblock-structured grid

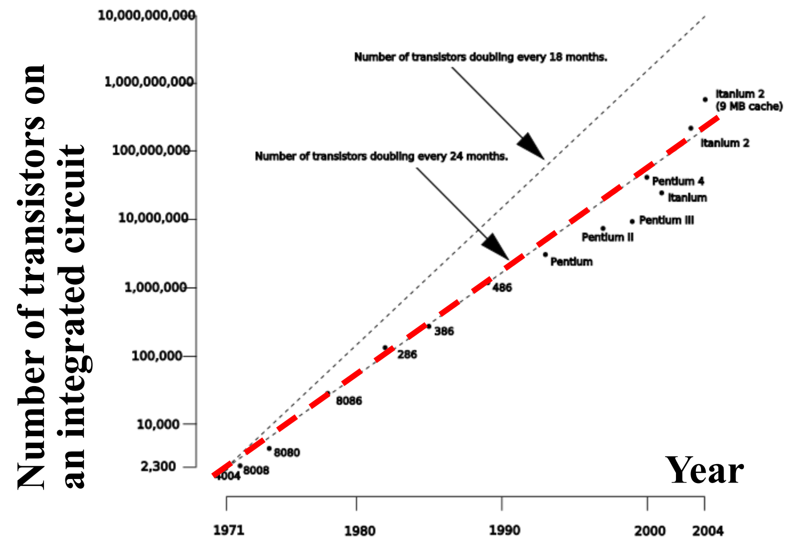


Unstructured grid

Computational Infrastructure

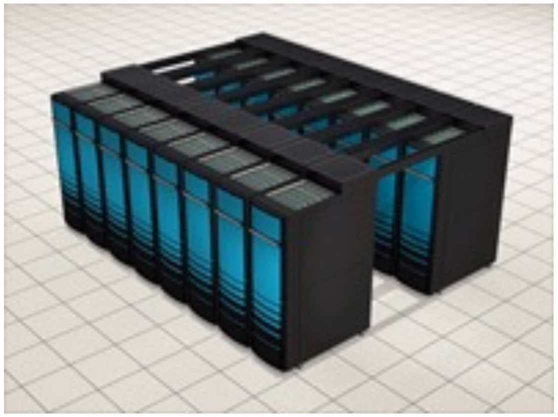
- Computer power
  - ➢ Cyber-infrastructure (CI): Information Technologies for computation, storage, communication, and data processing services, driven by:
    - Fast development of computer and network technologies
    - Dissemination of these technologies on a global scale
    - Rapid decrease in cost (< $1/MFlops)

Moore's law



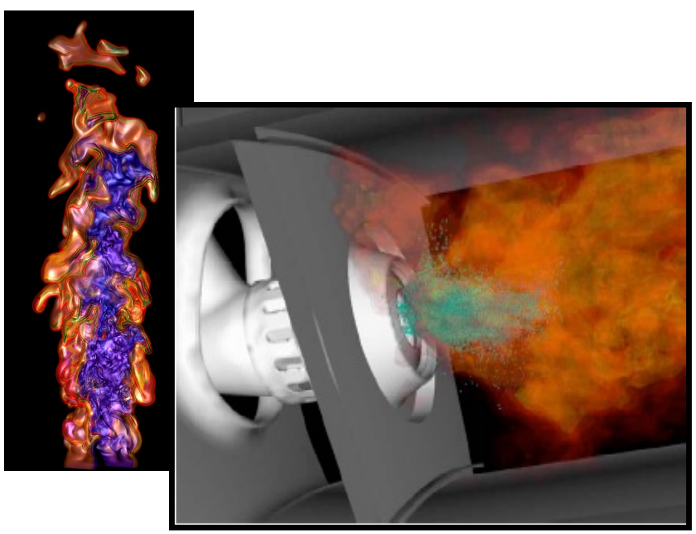
Computational Infrastructure

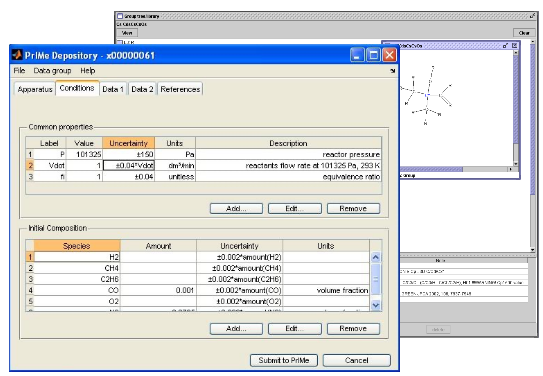
- Computer power
  - Current status of CI technologies
    - High-performance computing (HPC) facilities (Government Research Laboratories, Universities)
      - ✓ Massively parallel processing systems with computational rates ~ 1 Exa (10^{18}) Flops
    - Small-to-mid-scale computing facilities (Businesses)
      - ✓ Medium-scale parallel computing systems (clusters)
    - Grid infra-structure (coupling of distributed and heterogeneous computational resources and data stores via high-speed networks)
      - ✓ Cloud computing



Computational Infrastructure

- Computer power
  - Changes brought by CI technologies
    - Development of computational research as a new scientific approach
    - Development of computational research as a new engineering approach
    - Development of open-source data and software digital libraries





Compartment Fire Modeling

- Outline
  - Brief Review of Compartment Fire Dynamics
  - Fire Modeling Landscape
  - Computational Infrastructure
  - **Physical Modeling**
    - **Turbulence**
    - Combustion
    - Radiation
    - Pyrolysis
  - Examples

Modeling of Turbulent Flow

- Modeling of convective transport

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{u}_i) + \underbrace{\frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_i\tilde{u}_j)}_{\text{grid-resolved convective transport}} = \underbrace{-\frac{\partial T_{ij}}{\partial x_j}}_{\text{subgrid-scale convective transport}} - \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \overline{\tau_{ij}}}{\partial x_j} + \bar{\rho} g_i$$

$$T_{ij} = \overline{\rho u_i u_j} - \bar{\rho}\tilde{u}_i\tilde{u}_j$$

requires modeling

Modeling of Turbulent Flow

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

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

  - Closure expression for μ_t

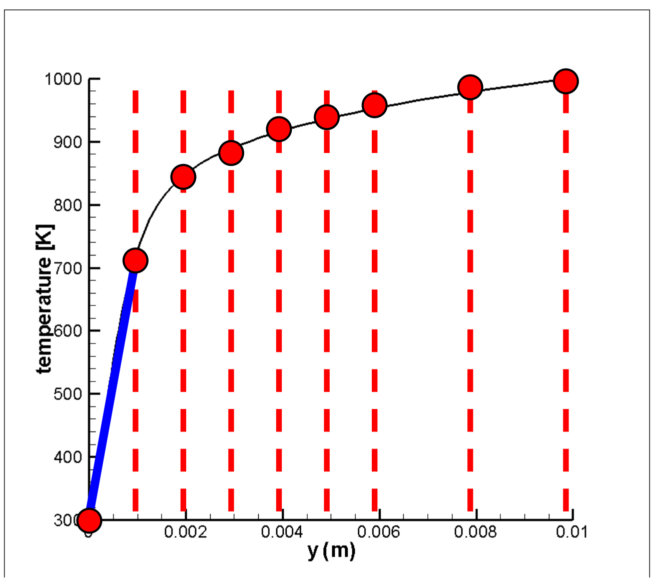
$$\boxed{\mu_t = \bar{\rho}(C_{\mu_t}\Delta)\sqrt{k_{SGS}}} \text{ where } \Delta = \left(\Delta x_1 \Delta x_2 \Delta x_3\right)^{1/3}$$

  - Closure expression for k_{SGS}
    - Models: Smagorinsky; Deardorff (FDS); *k*-equation (FireFOAM); WALE; *etc*

Modeling of Turbulent Flow

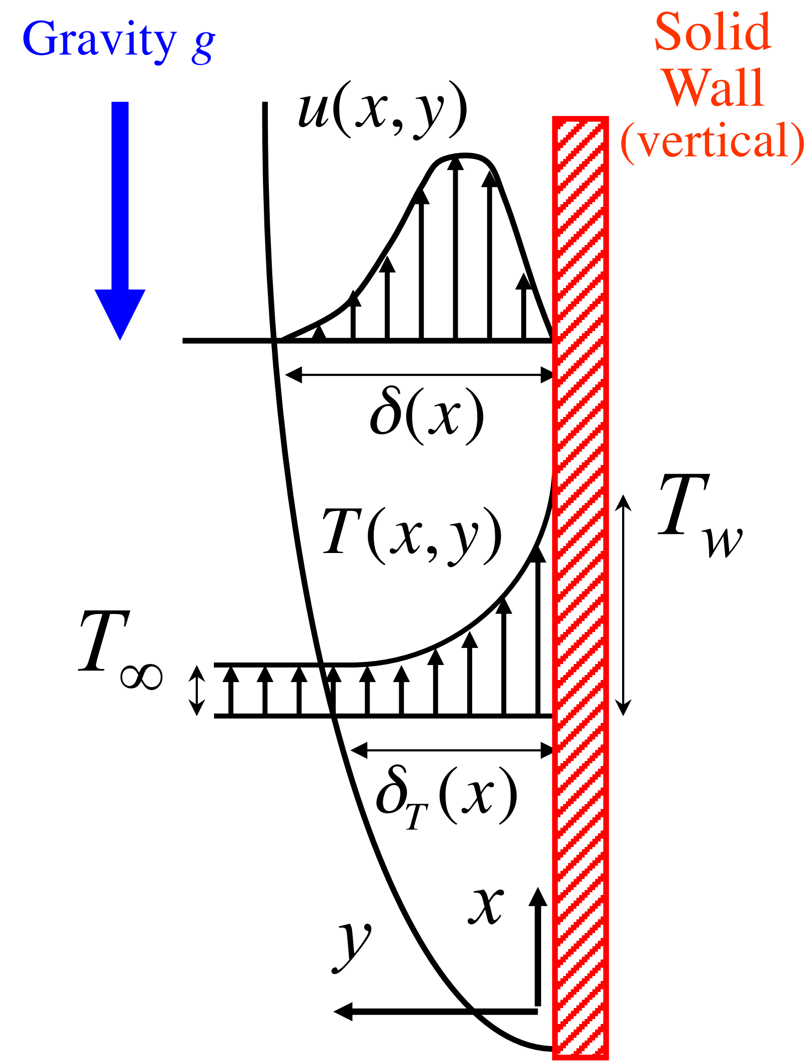
- Limitations of current subgrid-scale turbulence models
  - No suitable treatment of boundary layer effects:
    - Sharp gradients of temperature at the wall surface need to be evaluated in order to calculate the wall convective heat flux

$$\dot{q}''_{w,c} = -k \left. \frac{\partial T}{\partial y} \right|_{y=0}$$



Wall-resolved LES

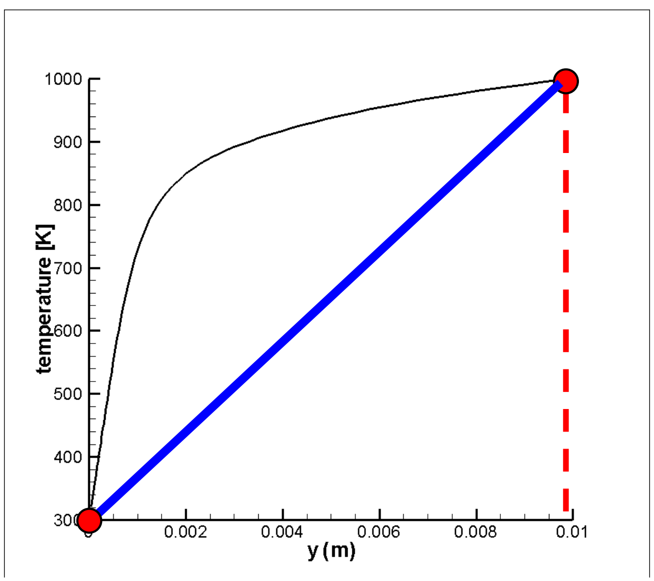
$\Delta y = O(1\ \mathrm{mm})$



Modeling of Turbulent Flow

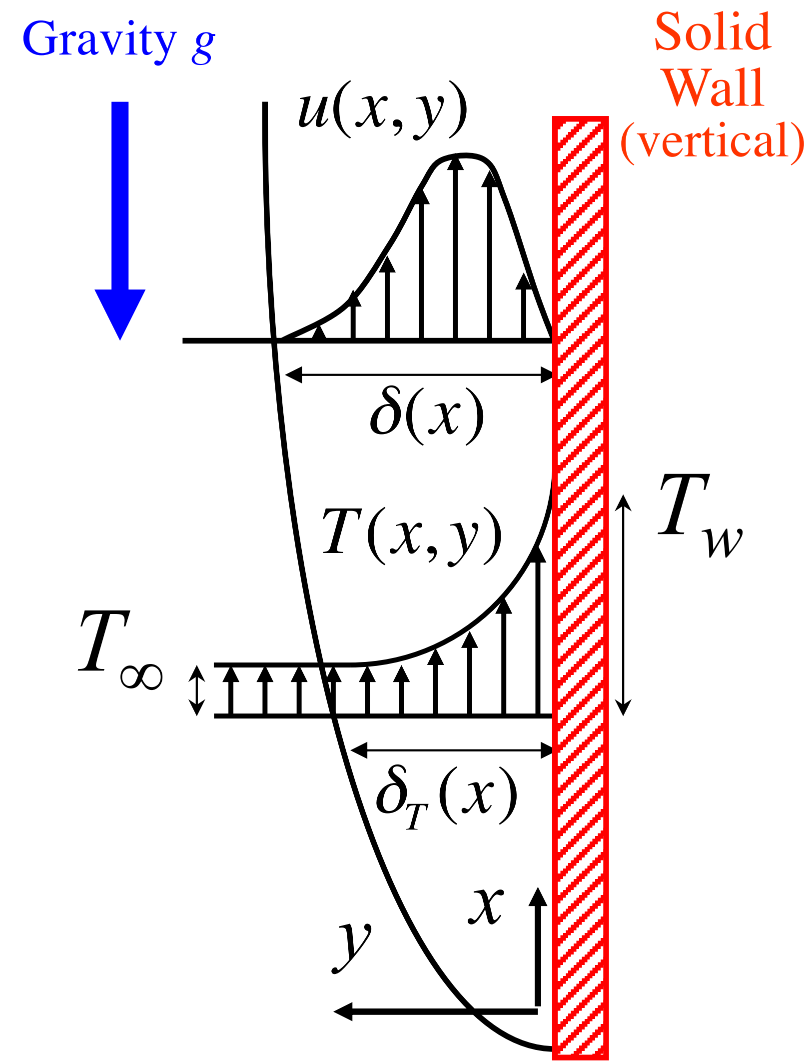
- Limitations of current subgrid-scale turbulence models
  - No suitable treatment of boundary layer effects:
    - Sharp gradients of temperature at the wall surface need to be evaluated in order to calculate the wall convective heat flux

$$\dot{q}''_{w,c} = -k \frac{\partial T}{\partial y}\bigg|_{y=0}$$



Wall-modelled LES

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



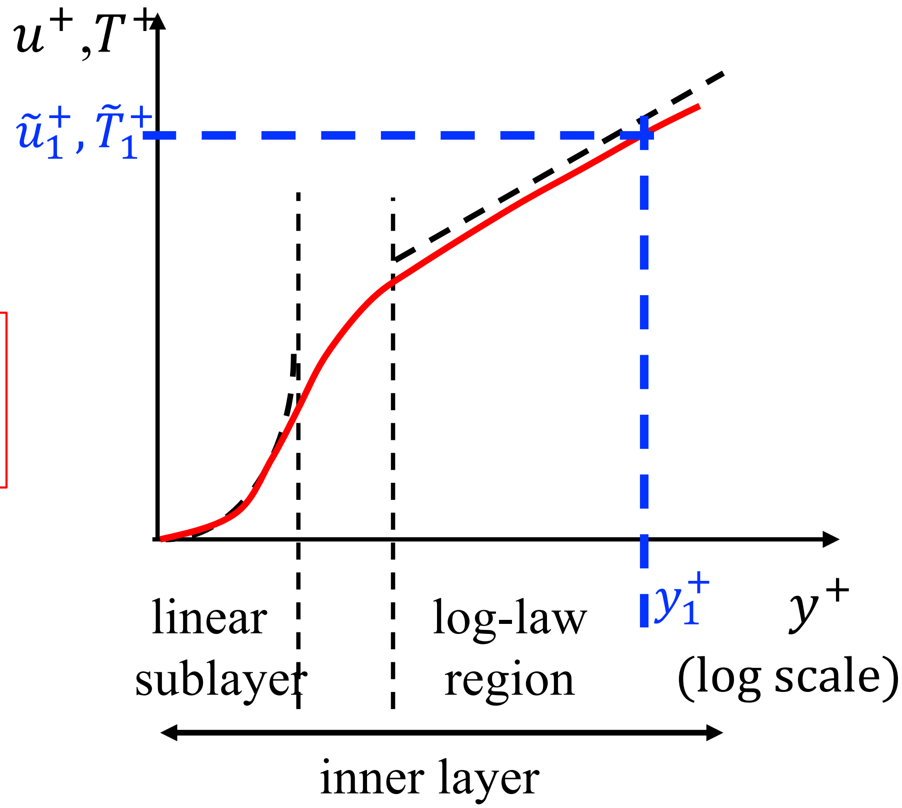
Modeling of Turbulent Flow

- Limitations of current subgrid-scale turbulence models
  - Traditional approach to wall modeling
    - ✓ First off-wall grid node located inside the log-law region
    - ✓ Implicit equation for u_τ

$$\tilde{u}_1^+ = \frac{1}{\kappa}\text{Log}(y_1^+) + C_1$$

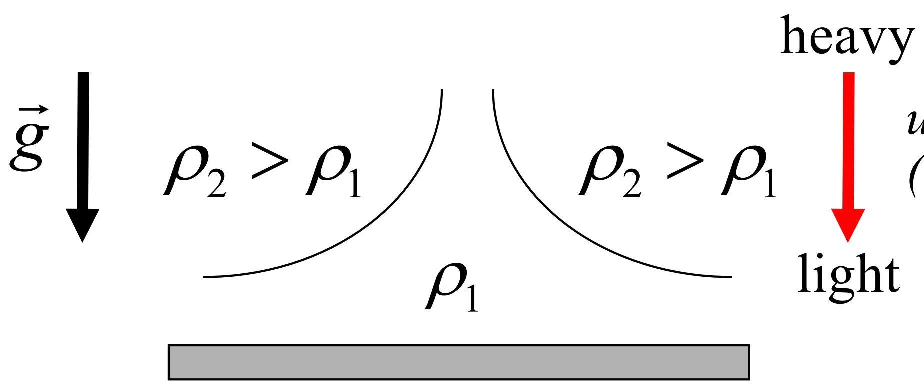
    - ✓ Equation for $\dot{q}_w''$

$$\frac{(\rho c_p u_\tau)(T_w - \tilde{T}_1)}{\dot{q}_w''} = \frac{1}{\kappa_\theta}\text{Log}(y_1^+) + C_\theta$$

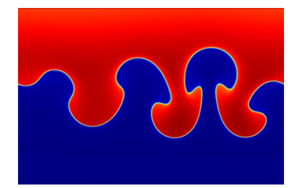


Modeling of Turbulent Flow

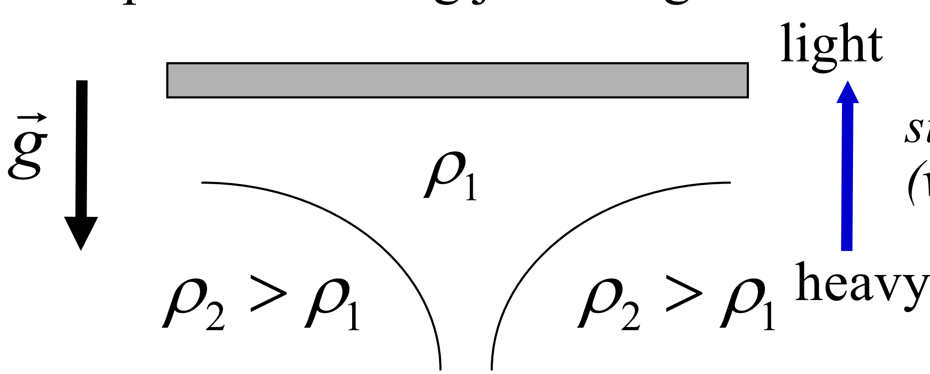
- Limitations of current subgrid-scale turbulence models
  - No treatment of buoyancy effects: Rayleigh-Taylor instabilities; reverse cascade of turbulent kinetic energy
    - Example of a pool fire configuration



unstable stratification
(will promote mixing)



    - Example of a ceiling jet configuration



stable stratification
(will prevent mixing)

Compartment Fire Modeling

- Outline
  - Brief Review of Compartment Fire Dynamics
  - Fire Modeling Landscape
  - Computational Infrastructure
  - **Physical Modeling**
    - Turbulence
    - **Combustion**
    - Radiation
    - Pyrolysis
  - Examples

Modeling of Combustion

- Modeling of chemical reaction rates

$$\frac{\partial}{\partial t}(\overline{\rho}\tilde{Y}_k) + \frac{\partial}{\partial x_j}(\overline{\rho}\tilde{Y}_k\tilde{u}_j) = -\frac{\partial \lambda_{kj}}{\partial x_j} + \frac{\partial}{\partial x_j}\overline{(\rho D_k \frac{\partial Y_k}{\partial x_j})} + \underbrace{\overline{\dot{\omega}'''_k}}_{\substack{\text{mass reaction rate} \\ \text{(grid-scale} \\ \text{and subgrid-scale)}}}$$

requires modeling

Modeling of Combustion

- Modeling of chemical reaction rates
  - Fuel composition is often unknown in fire problems: use a representative surrogate fuel (wood, plastic, foam, fabric, *etc*)
  - 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) model

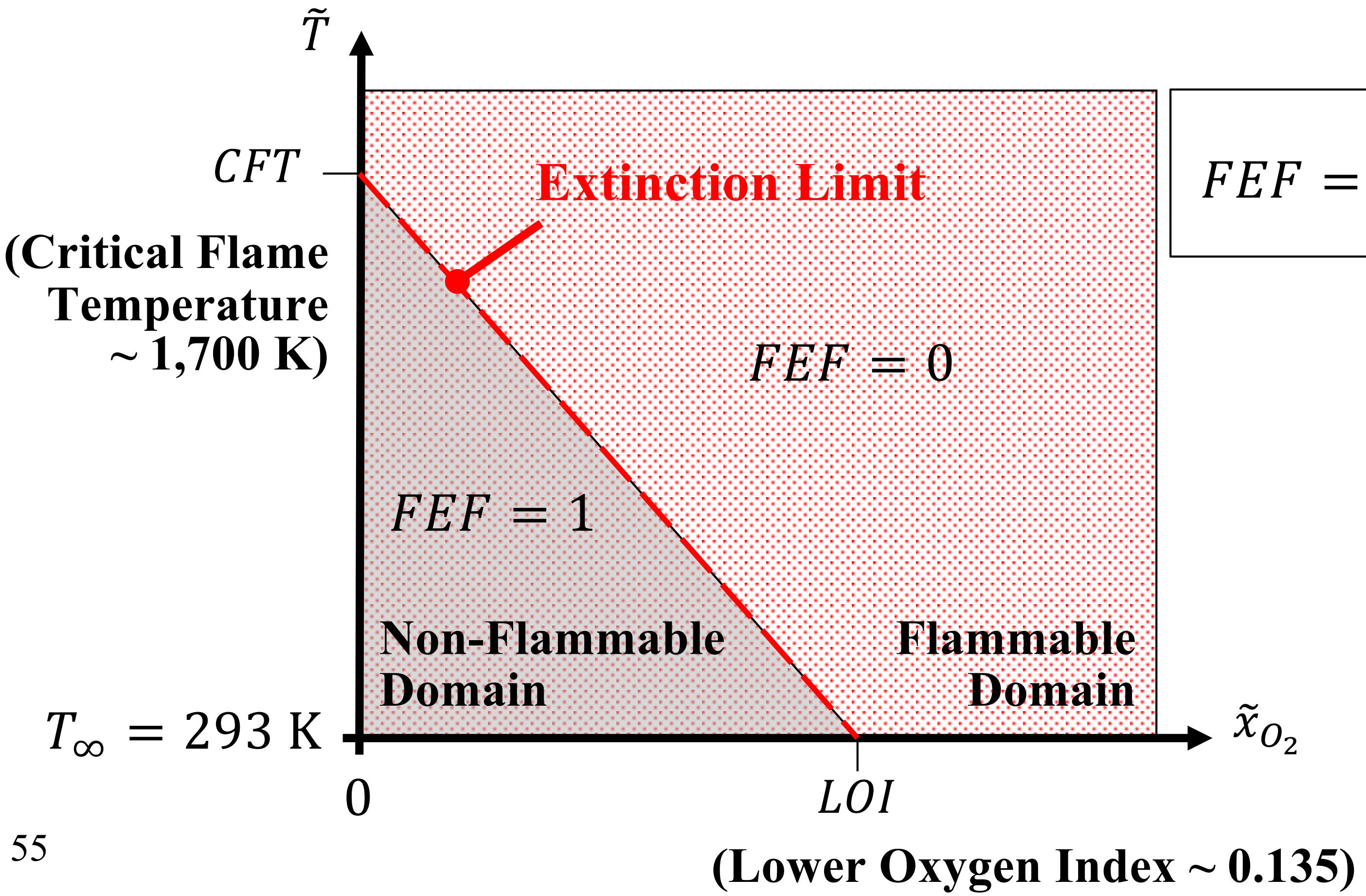
$$\boxed{\overline{\dot{\omega}_F'''} = \bar{\rho} \times \frac{\min(\tilde{Y}_F; \tilde{Y}_{O_2}/r_s)}{\tau_t}} \quad \text{where} \quad \tau_t = C_{\tau_t} \times (\frac{\bar{\rho}\Delta^2}{\mu_t})$$

Modeling of Combustion

- Limitations of current combustion models
  - No treatment of extinction effects
    - Extinction by oxygen depletion in under-ventilated compartment fires or by evaporative cooling in fires weakened by water-based suppression systems
  - No treatment of ignition effects
    - Possible re-ignition of fuel-air mixture following extinction
    - Ignition of flammable vapor-air mixtures in explosion scenarios (*e.g.*, backdraft)
  - No treatment of toxic products emission (soot, *CO*, *HCN*, *etc*)

Modeling of Combustion

- Limitations of current combustion models
  - Current treatment of extinction effects (FDS)
    - Flammability map based on a critical value of the flame temperature for extinction, $FEF = function(\tilde{x}_{O_2}, \tilde{T})$



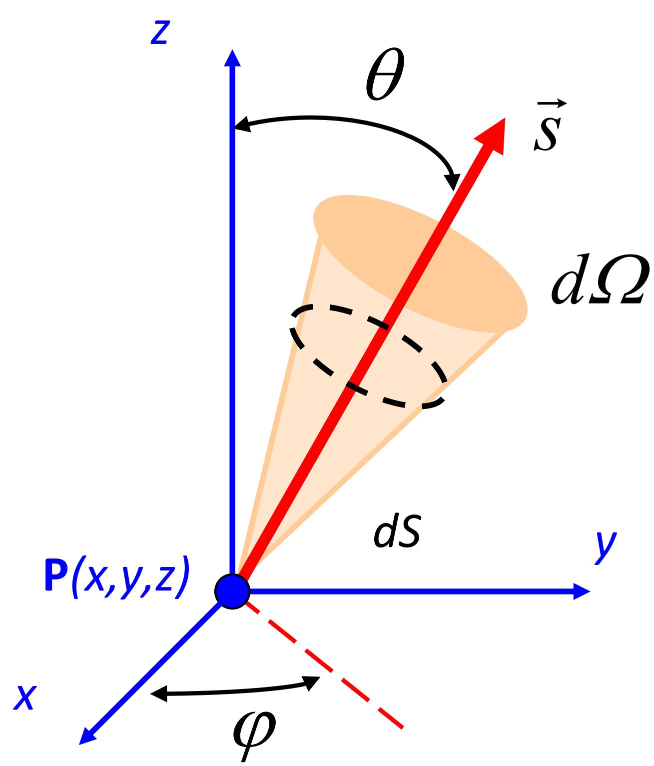
$$FEF = H\left(\frac{CFT - \tilde{T}}{CFT - T_\infty} - \frac{\tilde{x}_{O_2}}{LOI}\right)$$

Compartment Fire Modeling

- Outline
  - Brief Review of Compartment Fire Dynamics
  - Fire Modeling Landscape
  - Computational Infrastructure
  - **Physical Modeling**
    - Turbulence
    - Combustion
    - **Radiation**
    - Pyrolysis
  - Examples

Modeling of Thermal Radiation

- Modeling of radiative cooling/heating
  - Theoretical framework
    - Decomposition of angular space (hemisphere) into discrete viewing directions and elementary viewing areas (solid angles)



Viewing direction:

$$\vec{s} = \begin{cases} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{cases}$$

Elementary solid angle:

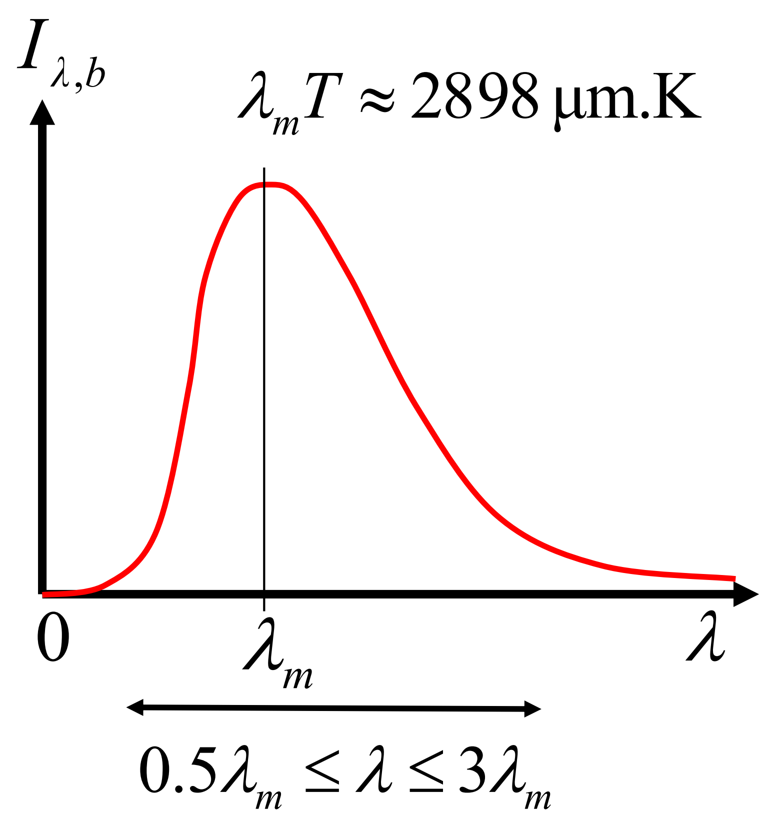
$$d\Omega = \sin\theta \, d\theta \, d\varphi$$

Modeling of Thermal Radiation

- Modeling of radiative cooling/heating
  - Theoretical framework
    - Description of radiation energy as electromagnetic wave energy with spectral-dependent properties
    - Black body radiation

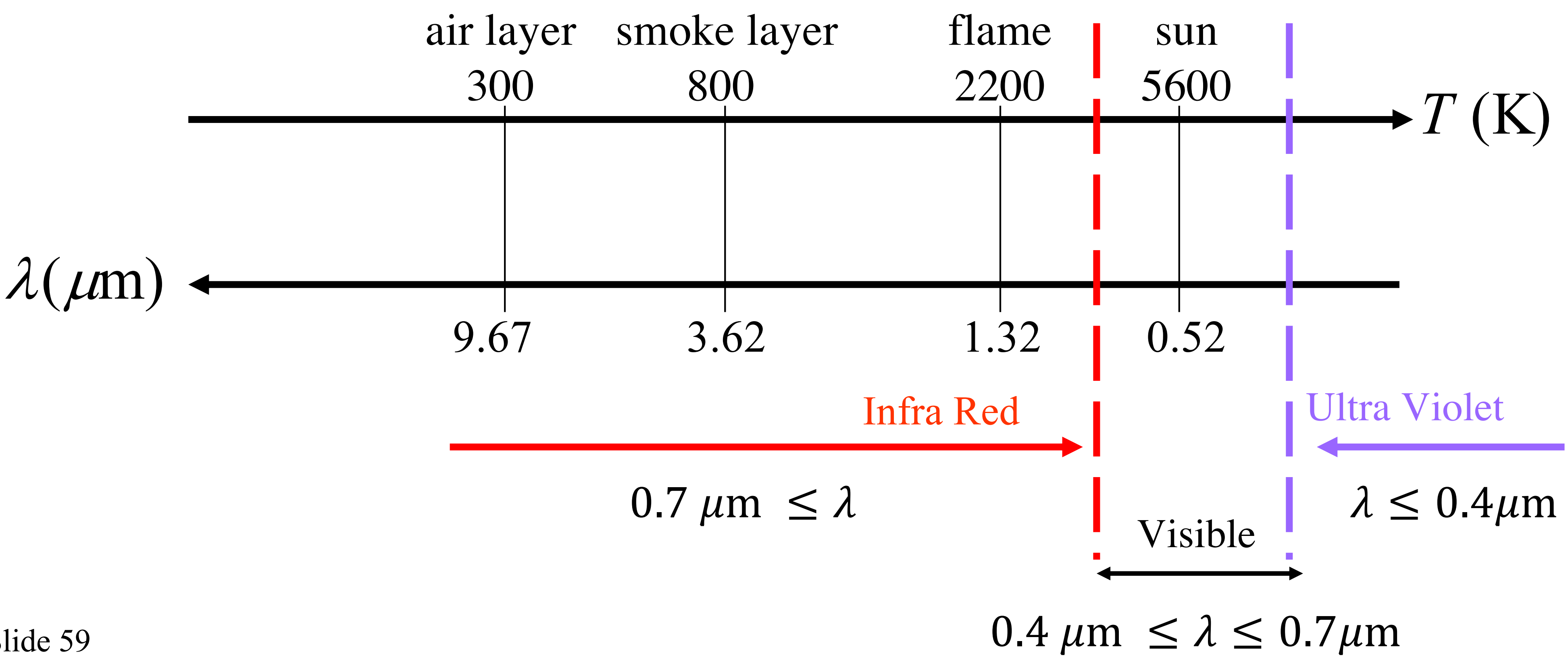
$$I_{\lambda,b}(\lambda,T) = \frac{2hc_0^{\,2}T^5}{(\lambda T)^5\left[\exp\left(\frac{hc_0}{k(\lambda T)}\right)-1\right]}$$

$$\boxed{I_b = \int_0^\infty I_{\lambda,b}\,d\lambda = \frac{\sigma T^4}{\pi}}$$



Modeling of Thermal Radiation

- Modeling of radiative cooling/heating
  - Theoretical framework
    - Description of radiation energy as electromagnetic wave energy with spectral-dependent properties

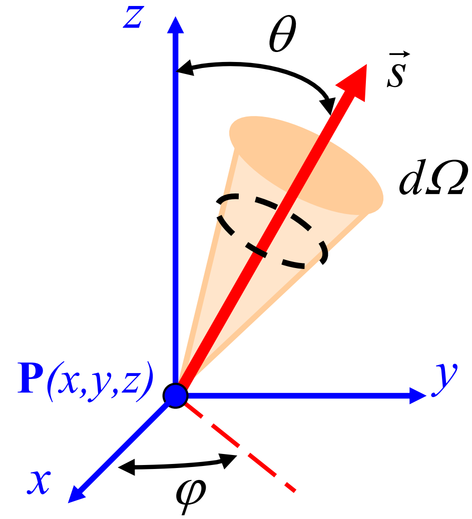


Modeling of Thermal Radiation

- Modeling of radiative cooling/heating
  - Radiative transfer equation (RTE) (assumed grey medium)

$$I(P,\vec{s}):\quad \nabla I.\vec{s} = \kappa\left(\frac{\sigma T^4}{\pi}\right) - \kappa I$$

emission absorption



$$\kappa(T,(x_{H_2O}, x_{CO_2}, f_v))$$

$$\dot{q}'''_{rad} = -\int_{4\pi\ \mathrm{sr}} (\nabla I.\vec{s})d\Omega = -4\kappa(\sigma T^4) + \kappa \times \int_{4\pi\ \mathrm{sr}} I d\Omega$$

- Solution methods for the RTE: Discrete Ordinate Method (DOM); Discrete Transfer Method (DTM); Monte Carlo Method (MCM)

Modeling of Thermal Radiation

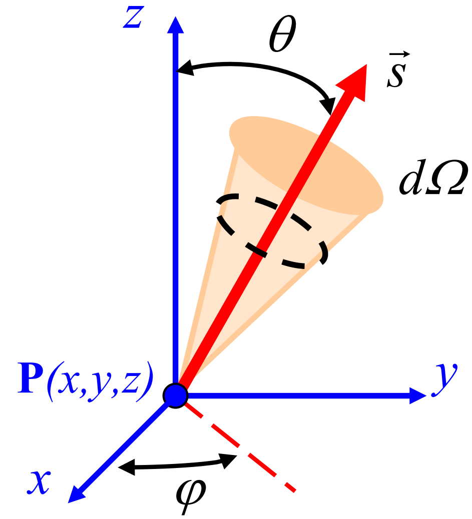
- Modeling of radiative cooling/heating
  - Radiative transfer equation (LES framework)

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

Emission   Absorption

(grid-scale & subgrid-scale)

requires modeling



$$\bar{\dot{q}}'''_{rad} = -4\overline{\kappa(\sigma T^4)} + \overline{\kappa \times \int_{4\pi\ \mathrm{sr}} I d\Omega}$$

Modeling of Thermal Radiation

- Modeling of radiative cooling/heating
  - Closure model for the RTE (LES framework): the prescribed global radiant fraction (PGRF) approach

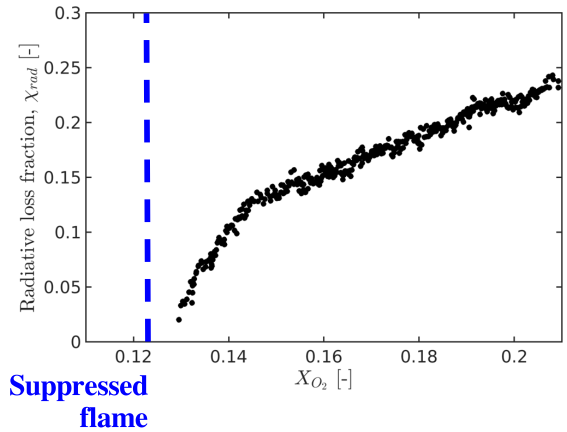
$$\nabla \bar{I}.\vec{s} = \boxed{\chi_{rad}^{g}} \times \left(\frac{\dot{q}'''_{comb}}{4\pi}\right), \quad \text{if } \dot{q}'''_{comb} > 0$$

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

- Global radiant fraction χ_{rad}^{g} is treated as an input quantity to the fire model and is user-prescribed

Modeling of Thermal Radiation

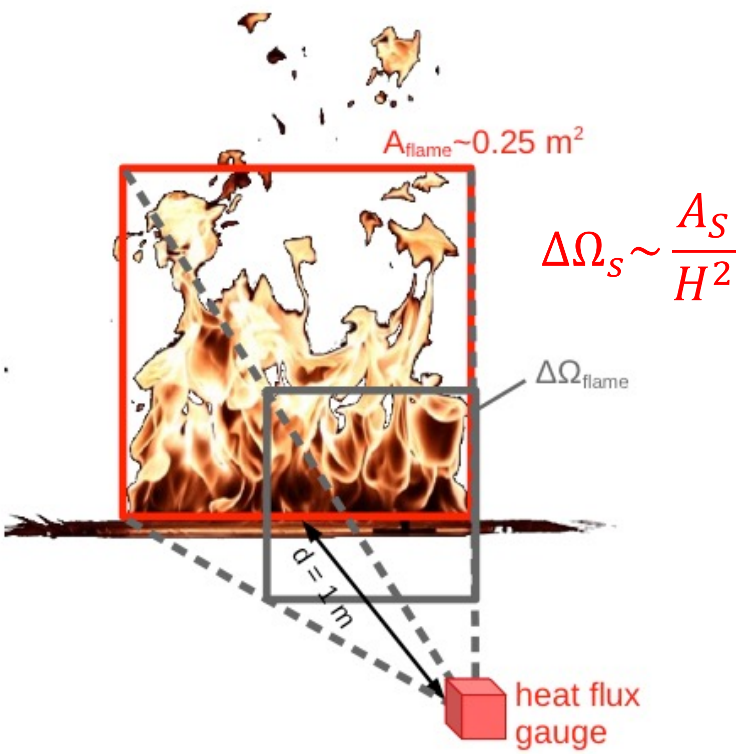
- Limitations of current radiation models
  - The PGRF approach remains approximate (does not work in scenarios in which the flame structure changes and the radiant fraction is not constant)

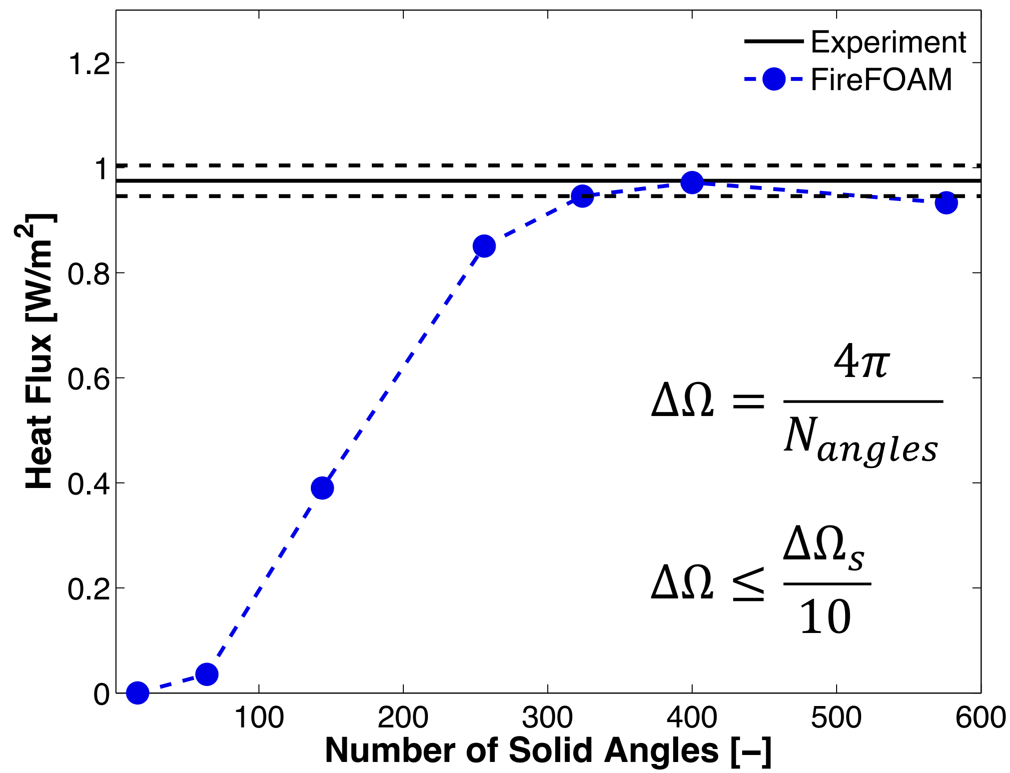


  - Radiation properties depend on soot volume fraction: the radiation model requires a soot model
  - No treatment of spectral effects (assumed grey medium)
  - Accuracy of DOM and DTM controlled by discretization of angular space and typically decreases in the far-field (ray effect)
    - Solution methods for the RTE are computationally expensive (typically multiplies the cost of CFD by a factor of at least 2)

Modeling of Thermal Radiation

- Control of numerical accuracy (DOM, DTM)
  - The solution of the RTE is a function of spatial location and angular direction; the accuracy of the RTE solution is controlled by the number of angles used in the decomposition of angular space





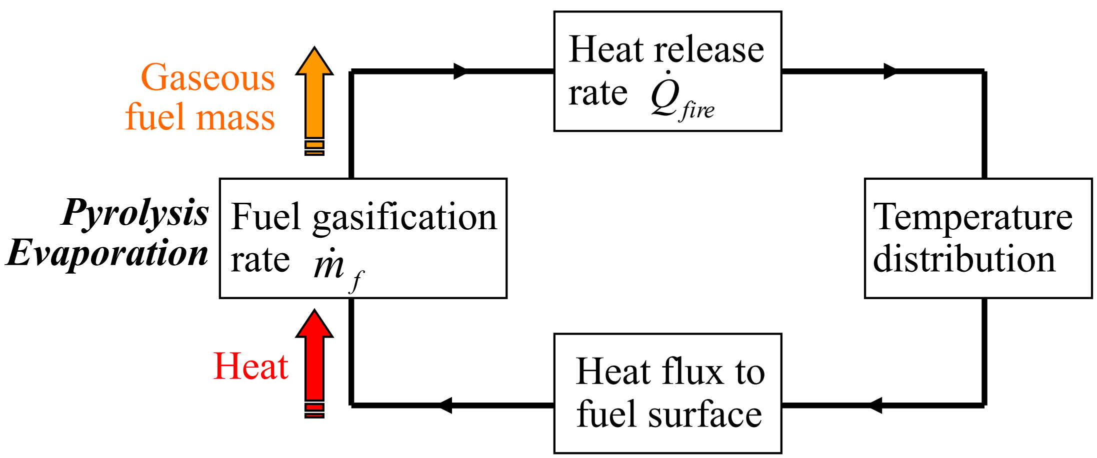
(Vilfayeau et al. (2016) *Fire Safety J.*)

Compartment Fire Modeling

- Outline
  - Brief Review of Compartment Fire Dynamics
  - Fire Modeling Landscape
  - Computational Infrastructure
  - **Physical Modeling**
    - Turbulence
    - Combustion
    - Radiation
    - **Pyrolysis**
  - Examples

Modeling of Pyrolysis

- Modeling of the fuel mass loss rate (MLR)
  - Two different approaches
    - ***Empirical*** approach: prescribed MLR; predicted ignition time
    - ***Advanced*** approach: MLR predicted from gas-to-solid thermal feedback and finite rate decomposition kinetics

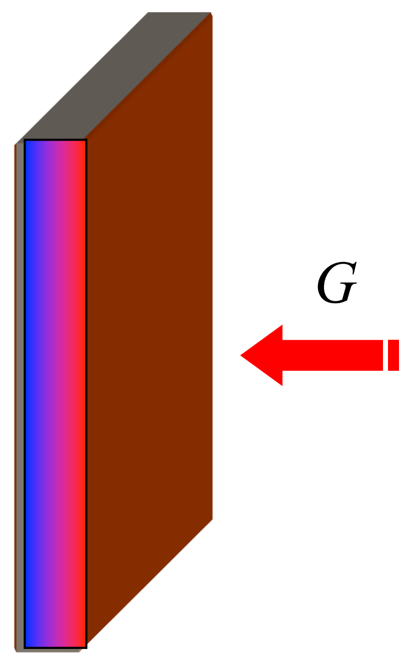


Modeling of Pyrolysis

- Modeling of the fuel mass loss rate (MLR)
  - Advanced approach
    - Finite-rate chemical kinetic model: explicit treatment of thermal decomposition chemistry
    - Thermal degradation across flammable solid described by a local 1D problem in the direction normal to the exposed solid surface

$$\underbrace{-k_s \frac{\partial T_s}{\partial x}(0,t)}_{\substack{\text{heat flux to solid interior} \\ \text{(conduction)}}} = \overbrace{\underbrace{-\varepsilon G + \varepsilon\sigma(T_s(0,t)^4 - T_\infty^4)}_{\text{radiation}} + \underbrace{h(T_s(0,t) - T_\infty)}_{\text{convection}}}$$

thermal feedback
(challenge: need to be evaluated accurately)



Modeling of Pyrolysis

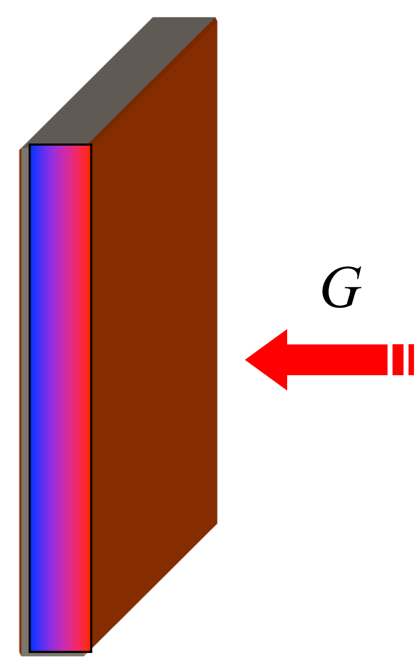
- Modeling of the fuel mass loss rate (MLR)
  - Advanced approach
    - Finite-rate chemical kinetic model: explicit treatment of thermal decomposition chemistry
    - Sequence of 4 chemical reactions (example)

(Drying) $(1\ kg\ wet\ solid)$
$$\rightarrow (\eta_{H_2O,Rd}\ kg\ water\ vapor) + (\eta_{ds,Rd}\ kg\ dry\ solid)$$

(Thermal pyrolysis) $(1\ kg\ dry\ solid)$
$$\rightarrow (\eta_{f,Rp}\ kg\ fuel) + (\eta_{c,Rp}\ kg\ char)$$

(Oxidative pyrolysis) $(1\ kg\ dry\ solid) + \left(\eta_{O_2,Rop}\ kg\ O_2\right)$
$$\rightarrow \left(\eta_{f,Rop}\ kg\ fuel\right) + \left(\eta_{c,Rop}\ kg\ char\right)$$

(Char oxidation) $(1\ kg\ char) + \left(\eta_{O_2,Rco}\ kg\ O_2\right)$
$$\rightarrow (\eta_{p,Rco}\ kg\ products) + (\eta_{a,Rco}\ kg\ ash)$$



Modeling of Pyrolysis

- Modeling of the fuel mass loss rate (MLR)
  - Advanced approach
    - Arrhenius reaction rates (Lautenberger & Fernandez-Pello, *Combust. Flame* **156**:1503-1513, 2009)

$$\dot{m}'''_{Rd}\Delta V = \left(\frac{\rho_{s,ws}(1-\psi_{ws})x_{ws}\Delta V}{\left(\rho_{s,ws}(1-\psi_{ws})x_{ws}\Delta V\right)_{\Sigma}}\right)^{n_{Rd}} \left(\rho_{s,ws}(1-\psi_{ws})x_{ws}\Delta V\right)_{\Sigma} \times A_{Rd}\exp\left(-\frac{E_{Rd}}{RT_s}\right)$$

$$\dot{m}'''_{Rp}\Delta V = \left(\frac{\rho_{s,ds}(1-\psi_{ds})x_{ds}\Delta V}{\left(\rho_{s,ds}(1-\psi_{ds})x_{ds}\Delta V\right)_{\Sigma}}\right)^{n_{Rp}} \left(\rho_{s,ds}(1-\psi_{ds})x_{ds}\Delta V\right)_{\Sigma} \times A_{Rp}\exp\left(-\frac{E_{Rp}}{RT_s}\right)$$

Modeling of Pyrolysis

- Modeling of the fuel mass loss rate (MLR)
  - Advanced approach
    - Arrhenius reaction rates (Lautenberger & Fernandez-Pello, *Combust. Flame* **156**:1503-1513, 2009)

$$\dot{m}'''_{Rop}\Delta V = \left(\frac{\rho_{s,ds}(1-\psi_{ds})x_{ds}\Delta V}{(\rho_{s,ds}(1-\psi_{ds})x_{ds}\Delta V)_{\Sigma}}\right)^{n_{Rop}} (\rho_{s,ds}(1-\psi_{ds})x_{ds}\Delta V)_{\Sigma} \times \left(\frac{Y_{g,O_2}}{Y_{g,O_2,air}}\right)^{n_{O_2,Rop}} \times A_{Rop} exp\left(-\frac{E_{Rop}}{RT_s}\right)$$

$$\dot{m}'''_{Rco}\Delta V = \left(\frac{\rho_{s,c}(1-\psi_{c})x_{c}\Delta V}{(\rho_{s,c}(1-\psi_{c})x_{c}\Delta V)_{\Sigma}}\right)^{n_{Rco}} (\rho_{s,c}(1-\psi_{c})x_{c}\Delta V)_{\Sigma} \times \left(\frac{Y_{g,O_2}}{Y_{g,O_2,air}}\right)^{n_{O_2,Rco}} \times A_{Rco} exp\left(-\frac{E_{Rco}}{RT_s}\right)$$

Modeling of Pyrolysis

- Modeling of the fuel mass loss rate (MLR)
  - Advanced approach
    - Governing equations (Lautenberger & Fernandez-Pello, *Combust. Flame* **156**:1503-1513, 2009)

$$\frac{\partial}{\partial t}(\rho_{s,ws}(1-\psi_{ws})x_{ws}\Delta V) = -\dot{m}'''_{Rds}\,\Delta V$$

$$\frac{\partial}{\partial t}(\rho_{s,ds}(1-\psi_{ds})x_{ds}\Delta V) = +\eta_{ds,Rd}\dot{m}'''_{Rd}\,\Delta V - \dot{m}'''_{Rp}\,\Delta V - \dot{m}'''_{Rop}\,\Delta V$$

$$\frac{\partial}{\partial t}(\rho_{s,c}(1-\psi_{c})x_{c}\Delta V) = +\eta_{c,Rp}\dot{m}'''_{Rp}\,\Delta V + \eta_{c,Rop}\,\dot{m}'''_{Rop}\,\Delta V - \dot{m}'''_{Rco}\,\Delta V$$

$$\frac{\partial}{\partial t}(\rho_{s,a}(1-\psi_{a})x_{a}\Delta V) = +\eta_{a,Rco}\dot{m}'''_{Rco}\,\Delta V$$

$$\frac{\partial}{\partial t}\left(\bar{\rho}_g Y_{g,O_2}\bar{\psi}\Delta V\right) + \frac{1}{\phi}\frac{\partial}{\partial \zeta}\left(\phi\,\dot{m}''_{\zeta}Y_{g,O_2}\right)\Delta V$$
$$= \frac{1}{\phi}\frac{\partial}{\partial \zeta}\left(\phi\,\bar{\psi}\bar{\rho}_g\bar{D}_g\,\frac{\partial Y_{g,O_2}}{\partial \zeta}\right)\Delta V - \eta_{O_2,Rop}\dot{m}'''_{Rop}\,\Delta V - \eta_{O_2,Rco}\dot{m}'''_{Rco}\,\Delta V$$

Modeling of Pyrolysis

- Modeling of the fuel mass loss rate (MLR)
  - Advanced approach
    - Governing equations (Lautenberger & Fernandez-Pello, *Combust. Flame* **156**:1503-1513, 2009)

$$\dot{m}''_{\zeta} = -\frac{\bar{K}}{\nu_g} \times \frac{\partial p}{\partial \zeta}$$

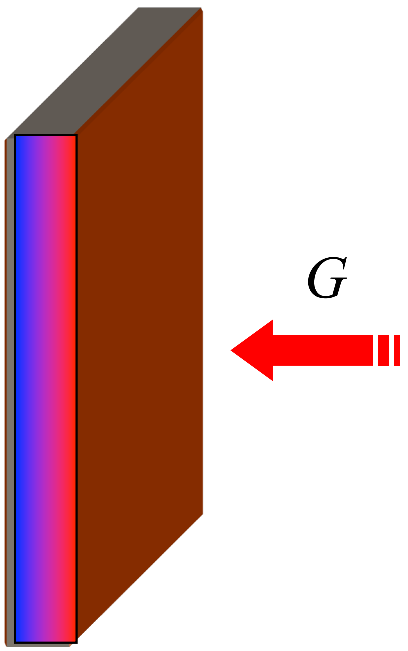
$$\frac{\partial}{\partial t}(\frac{M_g}{RT_g} p\bar{\psi}\Delta V) = \frac{1}{\phi}\frac{\partial}{\partial \zeta}(\phi\,\frac{\bar{K}}{\nu_g}\frac{\partial p}{\partial \zeta})\Delta V + \dot{m}'''_{sg}\,\Delta V$$

$$\left(\bar{\rho}_s\bar{c}_s(1-\bar{\psi}) + \bar{\rho}_g\bar{c}_{p,g}\bar{\psi}\right)\frac{\partial T_s}{\partial t}\Delta V + \dot{m}''_{\zeta}\bar{c}_{p,g}\,\frac{\partial T_s}{\partial \zeta}\Delta V = \frac{1}{\phi}\frac{\partial}{\partial \zeta}(((1-\bar{\psi})\bar{k}_s + \bar{\psi}\bar{k}_g)\phi\,\frac{\partial T_s}{\partial \zeta})\Delta V + \dot{q}'''_{hrr}\,\Delta V$$

Modeling of Pyrolysis

- Modeling of the fuel mass loss rate (MLR)
  - Advanced approach
    - Fuel mass loss rate

$$\dot{m}''_f = \int_{depth} (\eta_{f,Rp}\, \dot{m}'''_{Rp} + \eta_{f,Rop}\, \dot{m}'''_{Rop})\, d\zeta$$



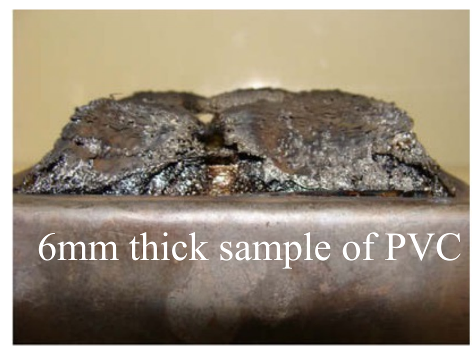
Modeling of Pyrolysis

- Modeling of the fuel mass loss rate (MLR)
  - Advanced approach
    - Input data

Thermal properties of wet solid	$\rho_{s,ws}, k_{s,ws}, c_{s,ws}, \varepsilon_{ws}$
Thermal properties of dry solid	$\rho_{s,ds}, k_{s,ds}, c_{s,ds}, \varepsilon_{ds}$
Thermal properties of char	$\rho_{s,c}, k_{s,c}, c_{s,c}, \varepsilon_{c}$
Thermal properties of ash	$\rho_{s,a}, k_{s,a}, c_{s,a}, \varepsilon_{a}$
Porosity and permeability of wet solid	ψ_{ws}, K_{ws}
Porosity and permeability of dry solid	ψ_{ds}, K_{ds}
Porosity and permeability of char	ψ_{c}, K_{c}
Porosity and permeability of ash	ψ_{a}, K_{a}
Drying reaction	$A_{Rd}, E_{Rd}, n_{Rd}, \Delta H_{Rd}, \eta_{ds,Rd}$
Thermal pyrolysis reaction	$A_{Rp}, E_{Rp}, n_{Rp}, \Delta H_{Rp}, \eta_{c,Rp}$
Oxidative pyrolysis reaction	$A_{Rop}, E_{Rop}, n_{Rop}, n_{O_2,Rop}, \Delta H_{Rop}, \eta_{c,Rop}, \eta_{O_2,Rcp}$
Char oxidation reaction	$A_{Rco}, E_{Rco}, n_{Rco}, n_{O_2,Rco}, \Delta H_{Rco}, \eta_{a,Rco}, \eta_{O_2,Rco}$

Modeling of Pyrolysis

- Modeling of the fuel mass loss rate (MLR)
  - Advanced approach
    - Many of the model parameters cannot be measured and remain unknown
    - Model parameters determined by comparison between model predictions and experimental results from micro-scale tests (*e.g.* thermogravimetric analysis) and bench-scale tests (*e.g.*, cone calorimeter, Fire Propagation Apparatus)
    - This comparison often uses optimization methods



6mm thick sample of PVC

Modeling of Pyrolysis

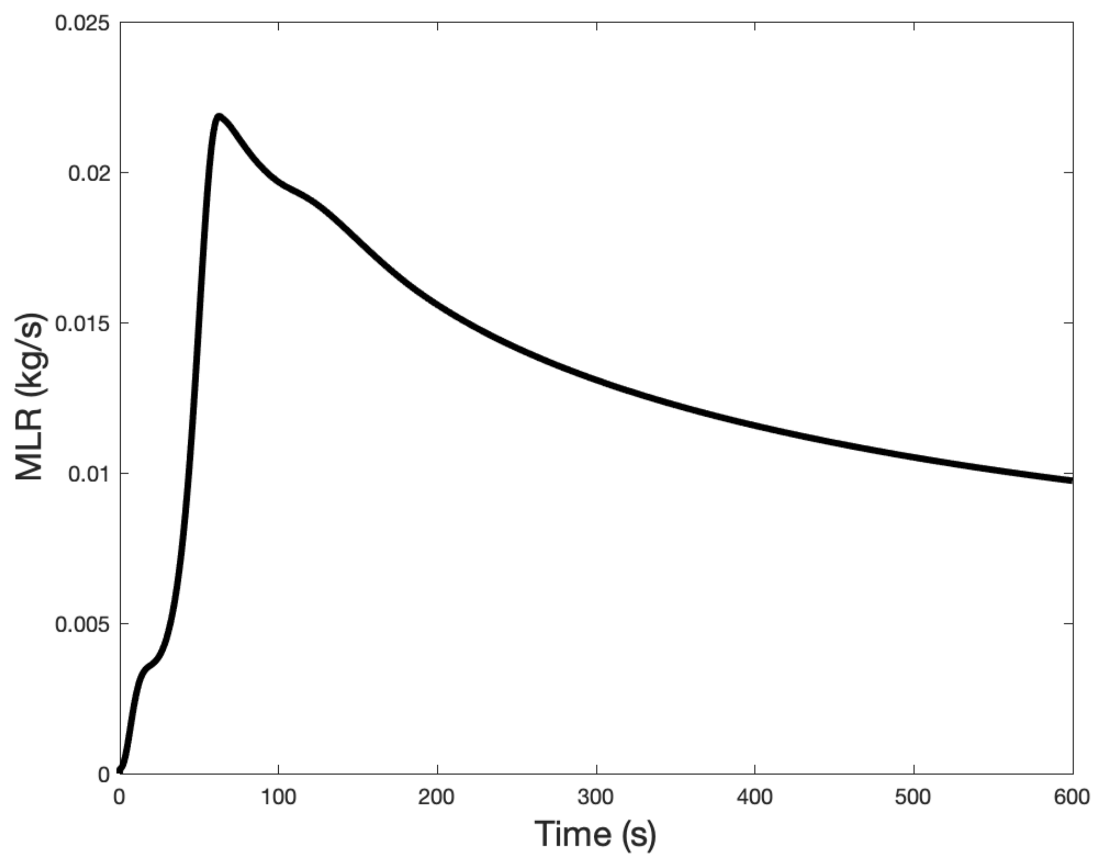
- Modeling of the fuel mass loss rate (MLR)
  - Advanced approach
    - *Example*: white pine (Lautenberger & Fernandez-Pello, *Combust. Flame* **156**:1503-1513 (2009)

$\Delta = 3.8$ cm

$G = 40$ kW/m^2

$x_{O_2,g} = 0.21$

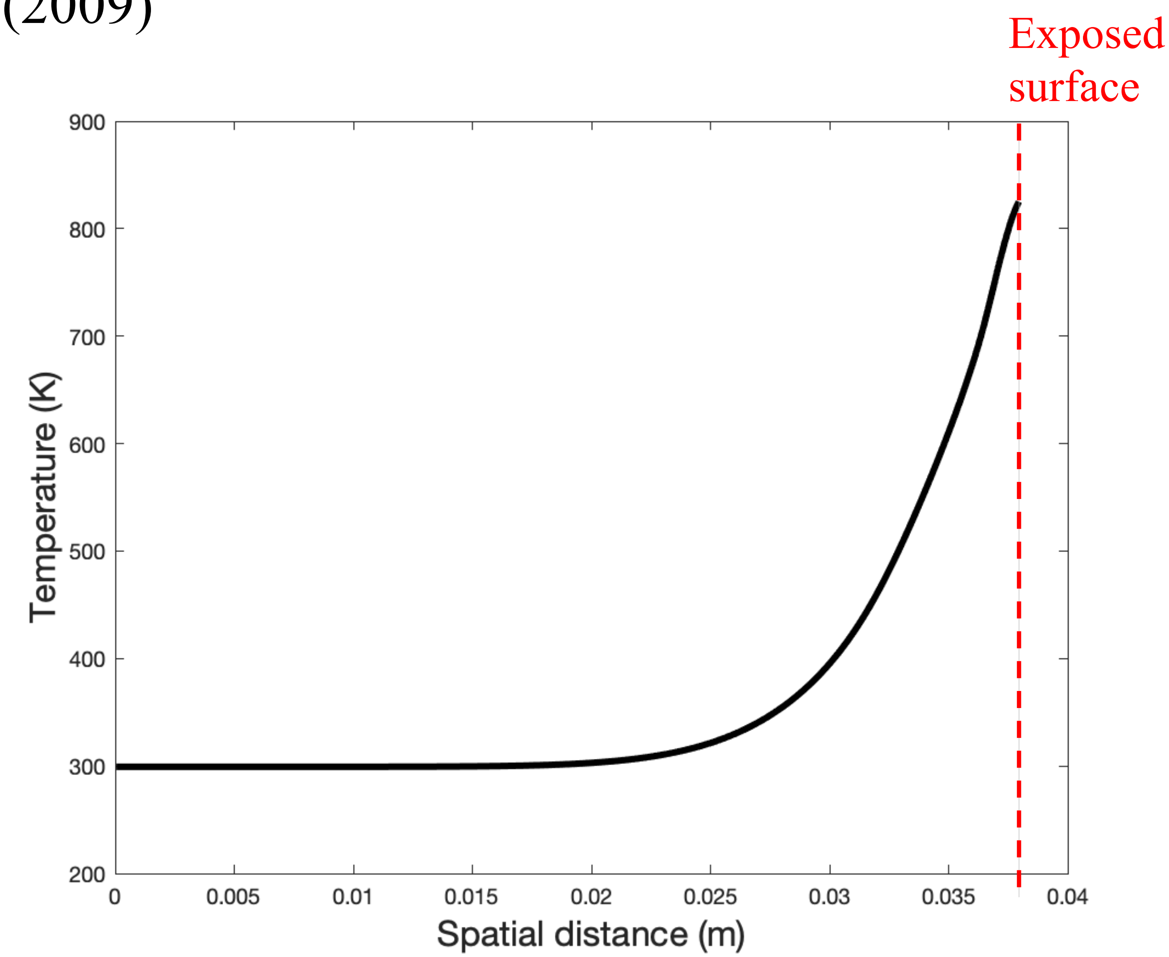
$t = 100$ s



Modeling of Pyrolysis

- Modeling of the fuel mass loss rate (MLR)
  - Advanced approach
    - *Example*: white pine (Lautenberger & Fernandez-Pello, *Combust. Flame* **156**:1503-1513 (2009)

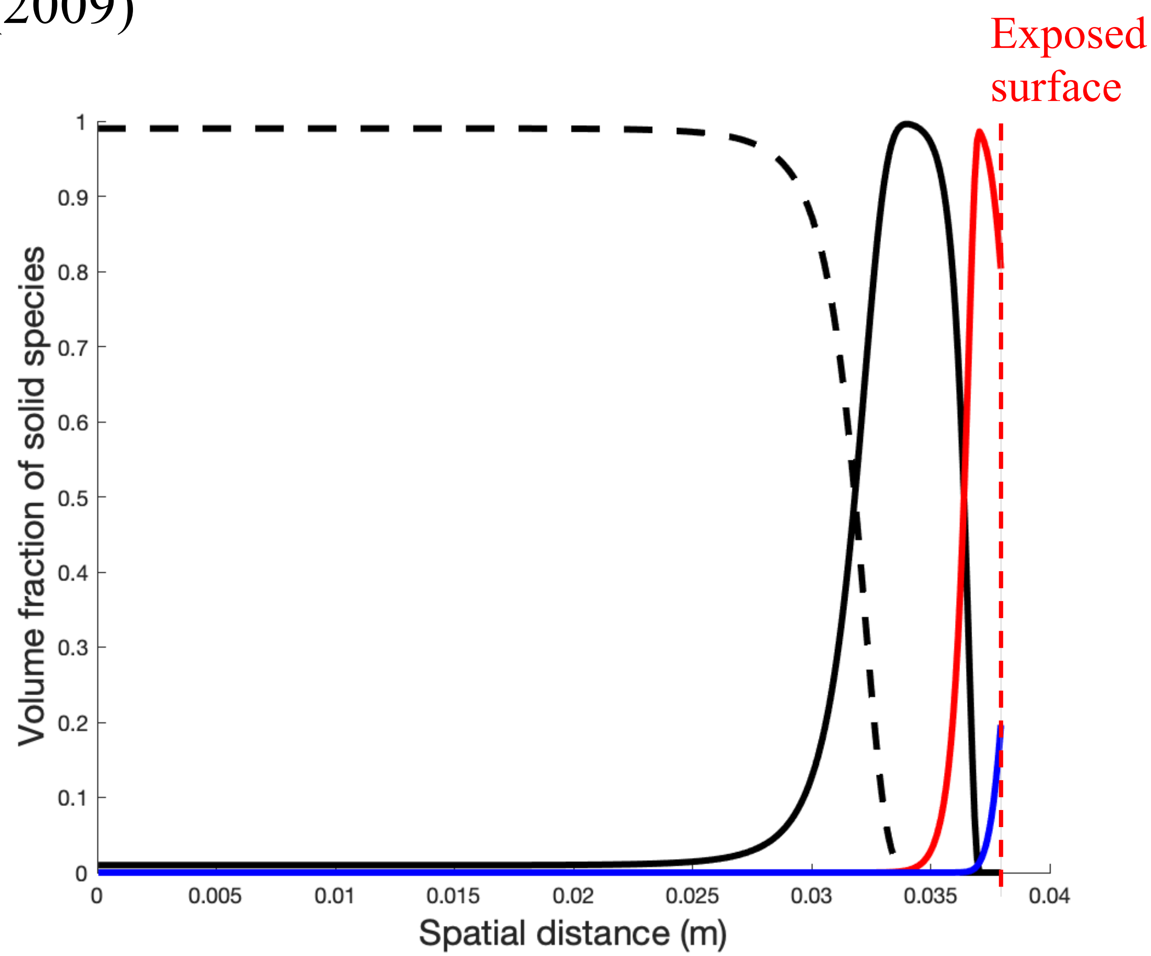
$\Delta = 3.8$ cm
$G = 40$ kW/m^2
$x_{O_2,g} = 0.21$
$t = 100$ s



Modeling of Pyrolysis

- Modeling of the fuel mass loss rate (MLR)
  - Advanced approach
    - *Example*: white pine (Lautenberger & Fernandez-Pello, *Combust. Flame* **156**:1503-1513 (2009)

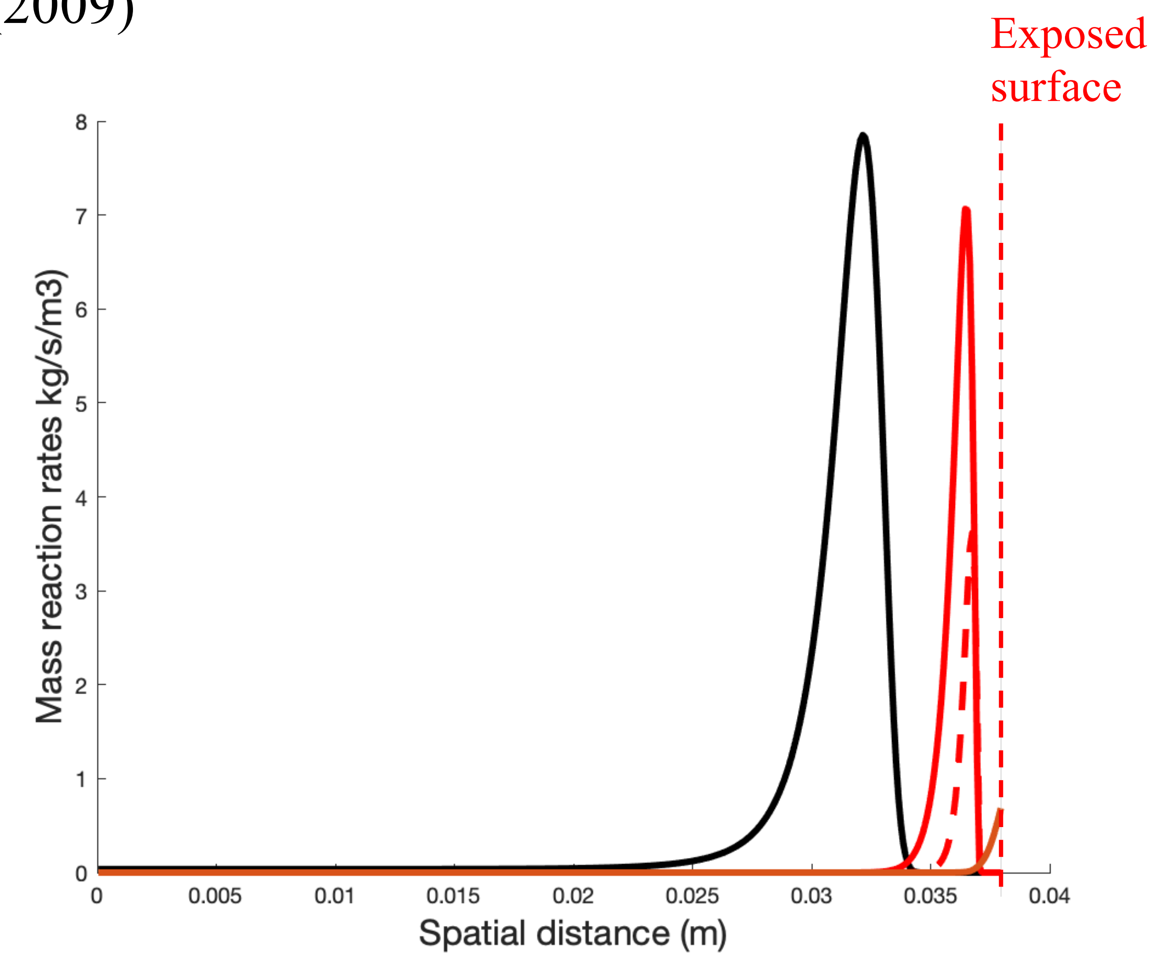
$\Delta = 3.8$ cm
$G = 40$ kW/m^2
$x_{O_2,g} = 0.21$
$t = 100$ s



Modeling of Pyrolysis

- Modeling of the fuel mass loss rate (MLR)
  - Advanced approach
    - *Example*: white pine (Lautenberger & Fernandez-Pello, *Combust. Flame* **156**:1503-1513 (2009)

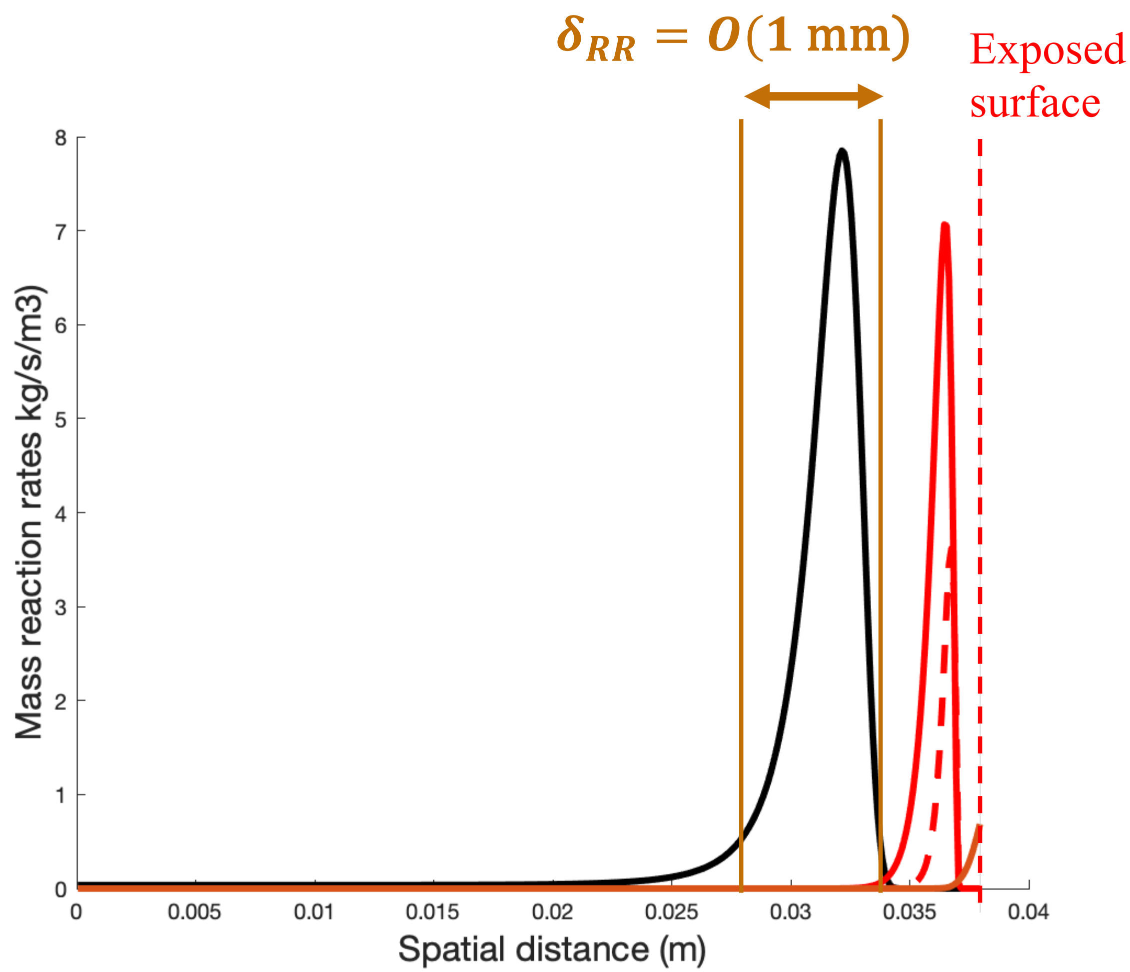
$\Delta = 3.8$ cm
$G = 40$ kW/m^2
$x_{O_2,g} = 0.21$
$t = 100$ s



Modeling of Pyrolysis

- Control of numerical accuracy
  - The accuracy of the solution of the solid phase equations is controlled by the spatial resolution

$$\Delta x_s \leq 100 - 200\ \mu m$$



Compartment Fire Modeling

- Outline
  - Brief Review of Compartment Fire Dynamics
  - Fire Modeling Landscape
  - Computational Infrastructure
  - Physical Modeling
  - **Examples**

Examples

- **Solvers**

	FireFOAM[1]	FDS[2]
Scheme	Second-order accurate, finite volume solver with implicit time integration	Second-order accurate, finite difference solver with explicit time integration
Turbulence	*k*-eqn model (default), dynamic Smagorinsky, WALE, Deardorff	Deardorff (default), dynamic Smagorinsky
Combustion	Global combustion eqn, Eddy Dissipation Model (EDM)	Global combustion eqn, Eddy Dissipation Model (EDM)
Radiation	DOM-FVM (prescribed radiant fraction, grey medium model, WSGG model)	DOM-FVM (prescribed radiant fraction, grey medium model, wide band model)
Soot	Flamelet-based model	Soot yield model
Pyrolysis	1D solid phase model	1D solid phase model
Mesh	Structured and unstructured grid	Structured (Cartesian) grid

[1] FM Global (USA), FireFOAM, Available from: https://github.com/fireFoam-dev

[2] NIST (USA), FDS, Available from: https://pages.nist.gov/fds-smv/

Examples

- Fine-grained LES (research-level) (FireFOAM)
  - UMD experiment on flame suppression by inert gas
  - Flame structure: $L_f \sim 0.5$ m; $L_{eddy} \sim$ O(1-10 cm); $U_{eddy} \sim$ O(1 m/s)

(Vilfayeau, White, Sunderland, Marshall, Trouvé, *Fire Safety J.*, 2016)

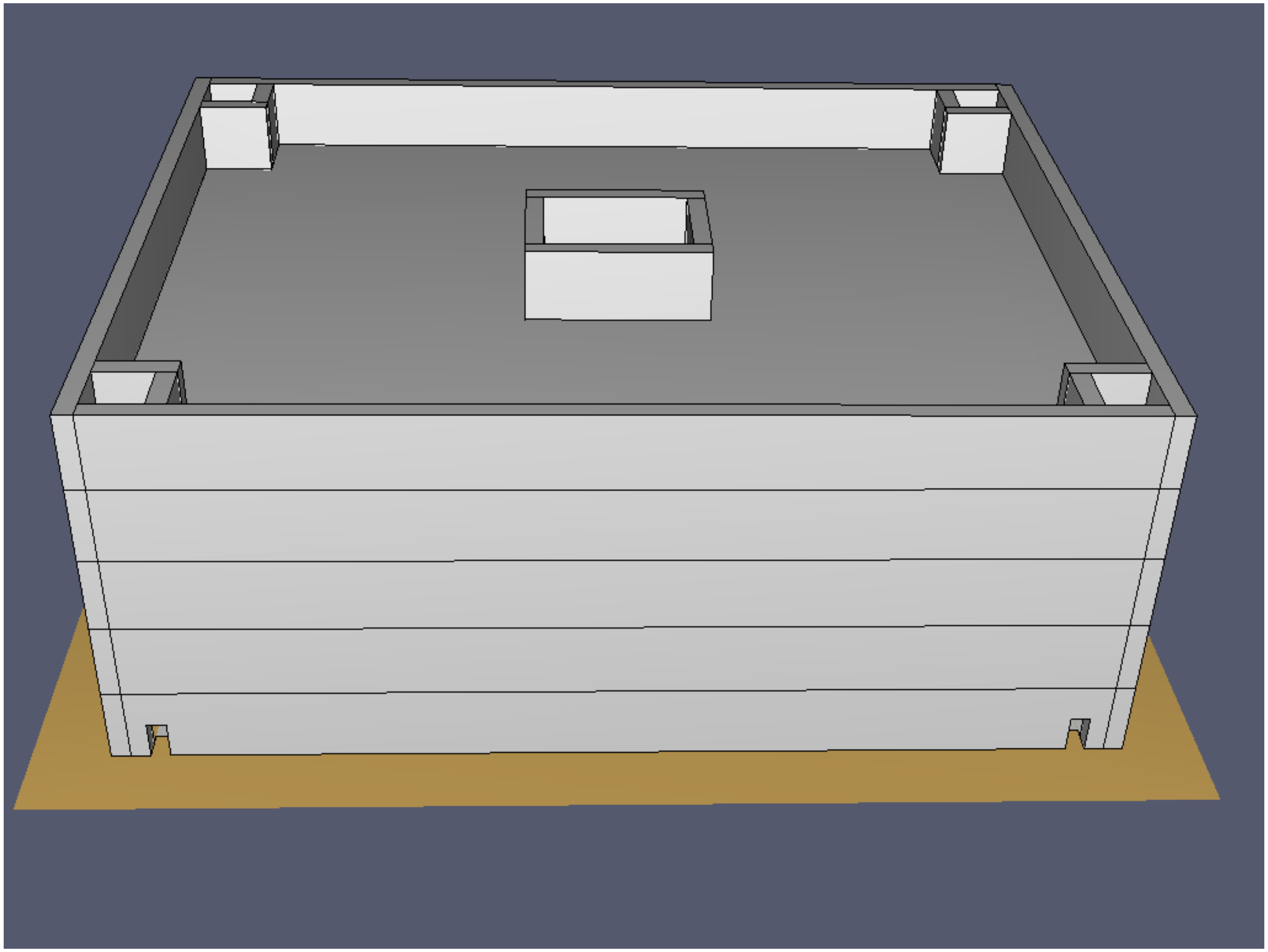
Examples

- Fine-grained LES (research-level) (FireFOAM)
  - Univ. Waterloo/NIST experiment on structure of pool fires
  - Flame structure: $L_f \sim 0.5$ m; $L_{eddy} \sim O(1\text{-}30\ \text{cm})$; $U_{eddy} \sim O(1\ \text{m/s})$

(Ahmed & Trouvé, submitted to *Combust. Flame*, 2020)

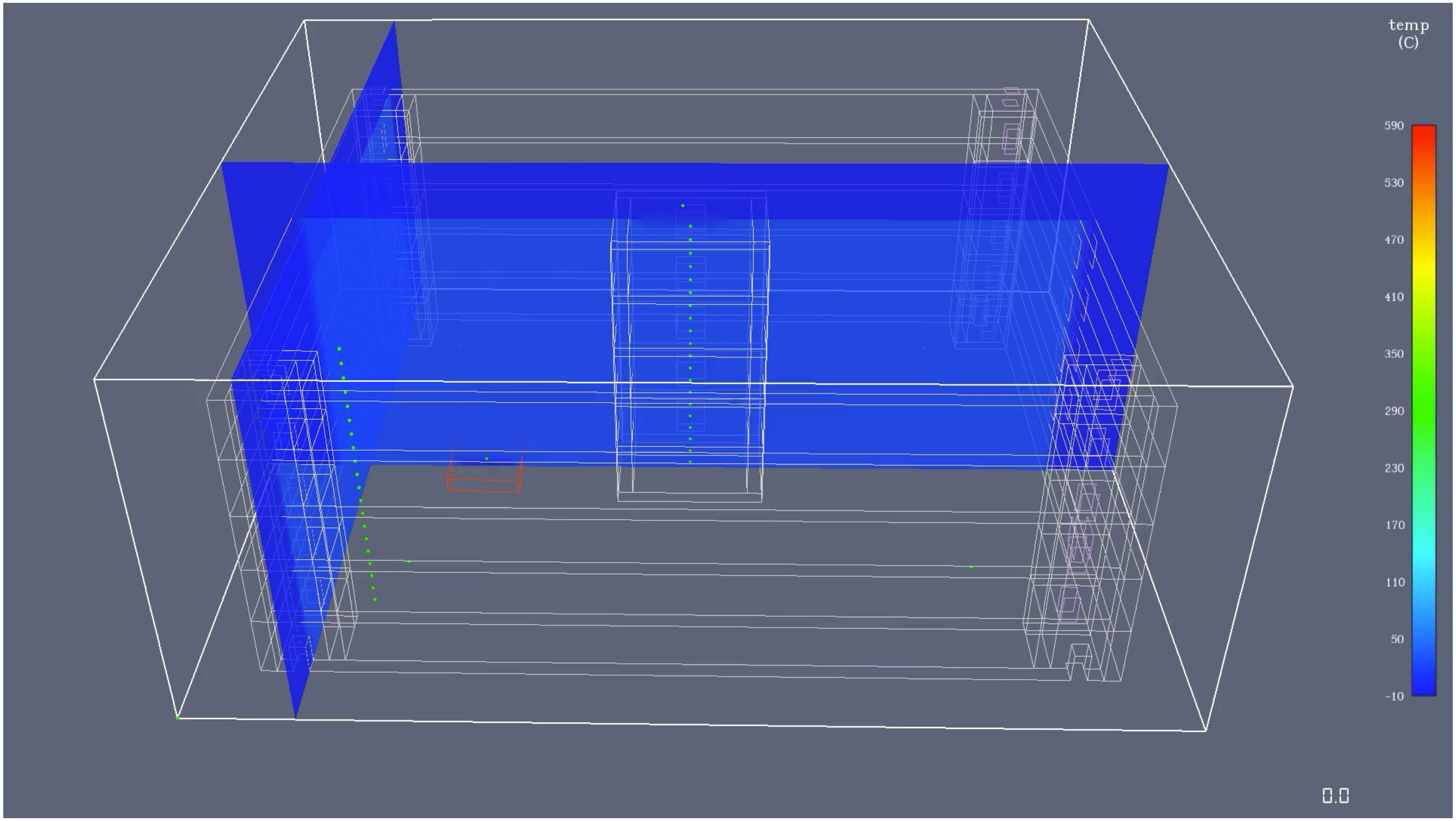
Examples

- Coarse-grained LES (engineering-level) (PyroSim/FDS)
  - Study of fire smoke dynamics in commercial 5-story building
  - Building: $L \sim O(10\text{s m})$; pressure effects; leakage paths



Examples

- Coarse-grained LES (engineering-level) (PyroSim/FDS)
  - Study of fire smoke dynamics in commercial 5-story building
  - Building: $L \sim O(10s\ m)$; pressure effects; leakage paths



Conclusion

- Fire modeling has experienced a remarkable growth in the past two decades
  - Fueled in particular by the development of FDS (and also now FireFOAM) and the development of open-source CFD software
  - Fire models have become routine fire safety engineering tools
- Fire modeling features several technical challenges
  - Modeling of complex (solid) fuel sources (pyrolysis processes)
  - Relatively slow, buoyancy-driven flow
  - Combustion with flame extinction/ignition
  - Boundary layer flames
  - Soot formation
  - Spectrally-resolved radiation and turbulence-radiation interactions
  - Water spray
  - Flame and smoke chemistry effects (toxicity)

Conclusion

- Organizational challenge
  - The fire modeling community is small, fragmented, geographically dispersed, without a history of well-defined standards and without a consensus on well-defined objectives
  - There is a need for a coordinated effort to organize and strengthen the fire modeling community
- MaCFP
  - The IAFSS Working Group on Measurement and Computation of Fire Phenomena (the MaCFP Working Group) (*http://www.iafss.org/macfp/*)
    - A recent initiative endorsed by the International Association for Fire Safety Science (IAFSS, *http://www.iafss.org*)
    - A forum between experimentalists and modelers to establish a common framework around the topic of CFD validation
    - A regular series of workshops
    - A list of community-approved experiments
    - A data repository (*https://github.com/MaCFP*)