Analysis of Chemical Structure using CSP applied to Triple Flames of Methane and *n*-Heptane

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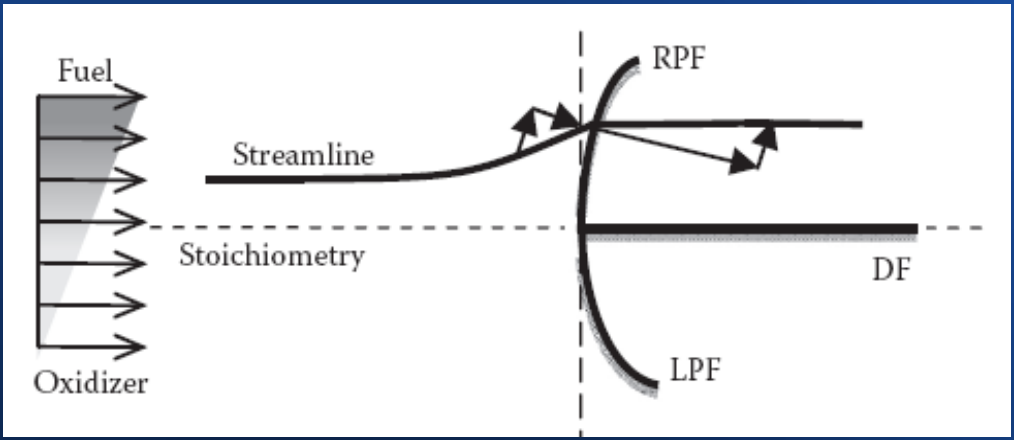
Overview

- Introduction to reacting flow studied
- Numerical model
- CSP analysis introduction
- Global CSP information
- Reaction network
- Explosive modes

Triple Flame Structure

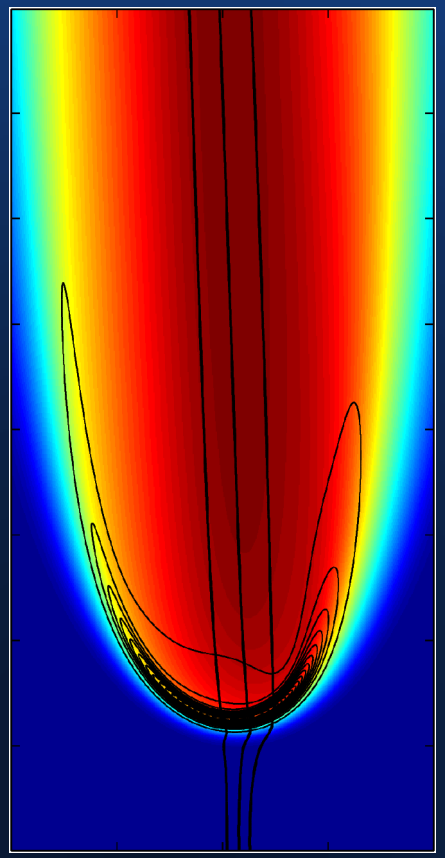


from: Suk Ho Chung, in 'Combustion Phenomena', CRC Press (2009)

- Triple flames are important flame structures in premixed and non-premixed systems
- Idealized picture: Lean and rich premixed flames and trailing diffusion flame meet at triple point
- Branches can be folded into the diffusion flame

Methane/Air Triple Flame

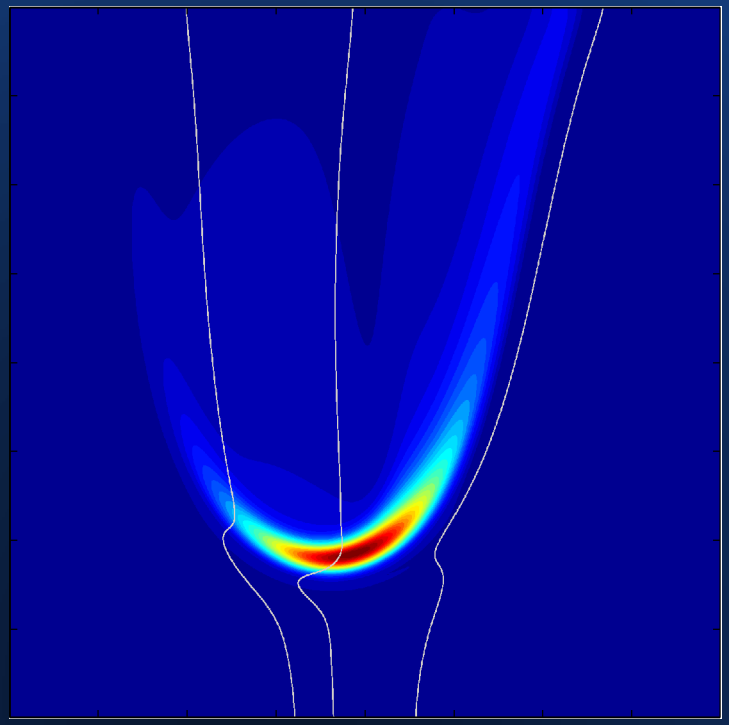
Temperature, heat-release rate,
0.9/1.0/1.1 x stoichiometric mixture fraction



- Non-premixed CH_4/air mixing layer
- Uniform inflow velocity
- GRI3.0
  (53 species, 325 reactions)
- 1.6 x 3.2 cm^2
- 1024 x 2048 cells
- Constant propagation speed

n-Heptane/Air Triple Flame

Heat-release rate,
mixture fraction of φ=0.5/1.0/2.5



- Partially-premixed *n*-C_7H_{16}/air mixing layer, φ=3.5 at right boundary
- Uniform inflow velocity
- Curran et al.
  (560 species, 2538 reactions)
- 0.4 x 0.4 cm^2
- 512 x 512 cells
- Constant propagation speed

Numerical Model

Zero-Mach-number approximation:

$$\partial_t \rho + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{v}) = 0$$

$$\partial_t T + \boldsymbol{v} \cdot \boldsymbol{\nabla} T = \frac{1}{\mathrm{RePr}} \frac{\boldsymbol{\nabla} \cdot (\lambda \boldsymbol{\nabla} T)}{\rho c_p} - \frac{1}{\mathrm{ReSc}} \sum_i \frac{c_{p,i} \left(\boldsymbol{\Gamma_i} \cdot \boldsymbol{\nabla} T \right)}{\rho c_p} + \mathrm{Da} \frac{\omega_T}{\rho c_p}$$

$$\partial_t \rho = -\frac{\rho}{T} \partial_t T - \rho \bar{W} \sum_i \frac{1}{W_i} \partial_t Y_i$$

density

$$\partial_t (\rho Y_i) + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{v} Y_i) = -\frac{1}{\mathrm{ReSc}} \boldsymbol{\nabla} \cdot (\boldsymbol{\Gamma_i}) + \mathrm{Da}\, \omega_i$$

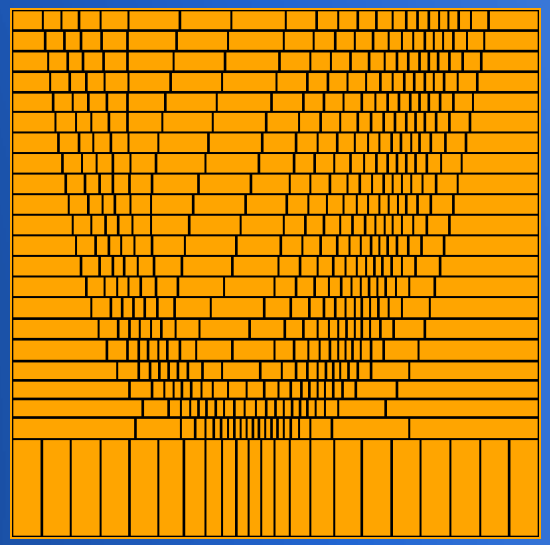
mass fractions

$$\partial_t (\rho \boldsymbol{v}) + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{v} \boldsymbol{v}) = -\boldsymbol{\nabla} p + \frac{1}{\mathrm{Re}} \boldsymbol{\nabla} \cdot \boldsymbol{\Phi}$$

momentum

Numerical Model

- Franklin of NERSC (National Energy Research Scientific Scientific Computing Center), Lawrence Berkeley National Laboratory
- Cray XT4, 9,572 nodes, each quad-core AMD Opteron, 38,128 cores



- Mixed mode MPI/OpenMP
- Load balance by dynamic repartitioning of the domain
- Load dominated by integrator of chemical source term
- 22 x 22 partitions, 484 processors, 1,936 cores

CSP Analysis

$$\frac{d\boldsymbol{w}}{dt} = \boldsymbol{L}(\boldsymbol{w}) + \boldsymbol{g}(\boldsymbol{w}) = \boldsymbol{f}(\boldsymbol{w})$$

Time evolution

$$\{\boldsymbol{a}_i, \boldsymbol{b}^i\}_{i=1}^{N}$$

$$\boldsymbol{g} = \sum_k \boldsymbol{S}_k R^k(\boldsymbol{w})$$

Chemical source term

CSP vectors, here:
Eigenvectors of Jacobian

$$\boldsymbol{f} = \boldsymbol{f}_s + \boldsymbol{f}_r = \sum_{r=1}^{M} \boldsymbol{a}_r h^r + \sum_{s=M+1}^{N} \boldsymbol{a}_s h^s$$

Fast and slow modes

$$\tau_i = |\lambda_i|^{-1}$$

$$\tau_1 < \ldots < \tau_M << \tau_{M+1} < \ldots < \tau_N$$

Time scales

$$\left| \tau_{M+1} \sum_{r=1}^{M} a_r^i h^r \right| < w_{\text{error}}^i$$

Dimension *M* of manifold

CSP Analysis

$$\boldsymbol{f} = \boldsymbol{f}_s + \boldsymbol{f}_r = \sum_{r=1}^{M} \boldsymbol{a}_r h^r + \sum_{s=M+1}^{N} \boldsymbol{a}_s h^s$$

CSP right-hand side

$$h^i = \boldsymbol{b}^i \cdot (\boldsymbol{L} + \boldsymbol{g}) = \sum_{j=1}^{N} b_j^i L_j + \sum_{k=1}^{R} (\boldsymbol{b}^i \cdot \boldsymbol{S}_k) R^k$$

Mode amplitudes

$$P_k^i = \frac{(\boldsymbol{b}^i \cdot \boldsymbol{S}_k) R^k}{\sum_{j=1}^{N} \left| b_j^i L_j \right| + \sum_{k'=1}^{R} \left| (\boldsymbol{b}^i \cdot \boldsymbol{S}_{k'}) R^{k'} \right|}$$

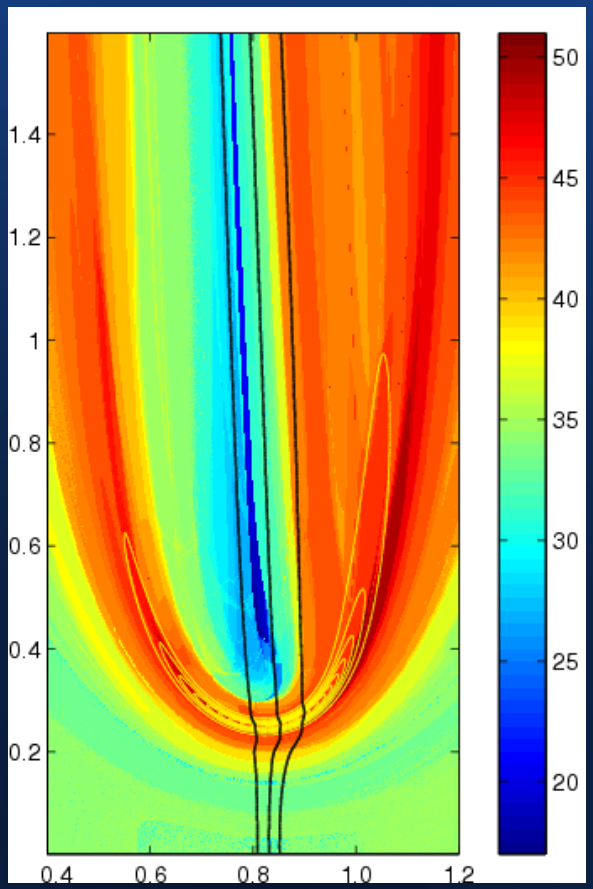
Participation Index reaction *k* in mode *i*

Importance Index reaction *k* for species *m*

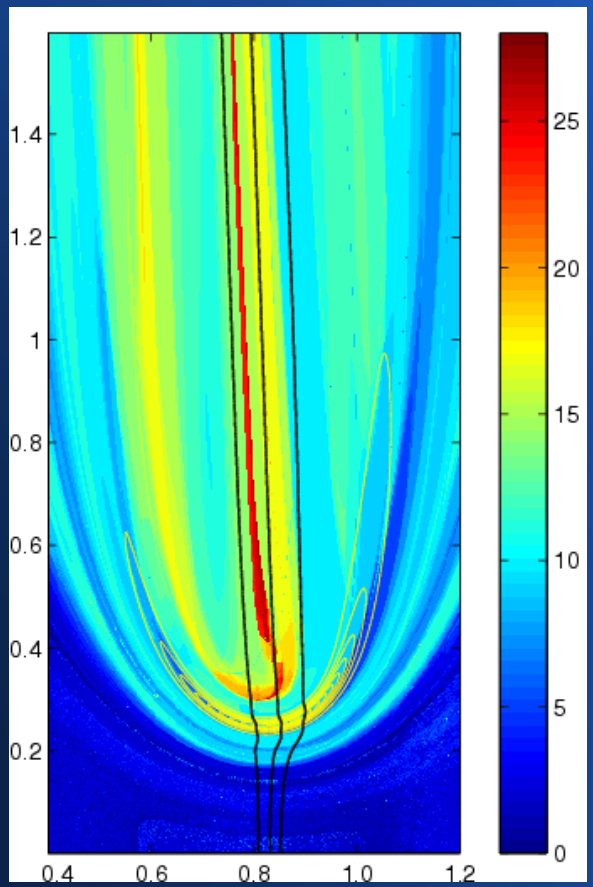
$$I_k^m = \frac{\sum_{i=M+1}^{N} a_i^m (\boldsymbol{b}^i \cdot \boldsymbol{S}_k) R^k}{\sum_{j=1}^{N} \left| \sum_{i=M+1}^{N} a_i^m (b_j^i L_j) \right| + \sum_{k'=1}^{R} \left| \sum_{i=M+1}^{N} a_i^m (\boldsymbol{b}^i \cdot \boldsymbol{S}_{k'}) R^{k'} \right|}$$

Global CSP Information, CH_4/air

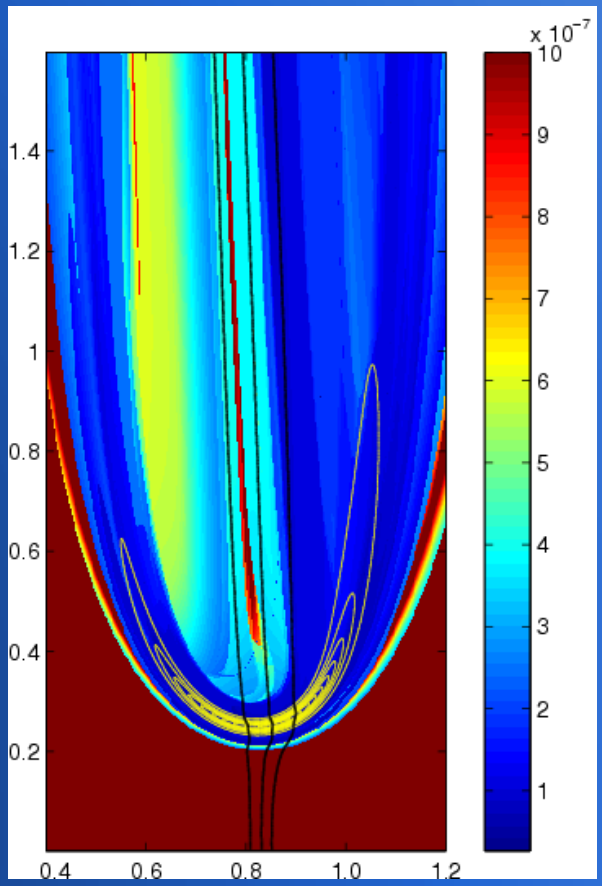
Number active modes



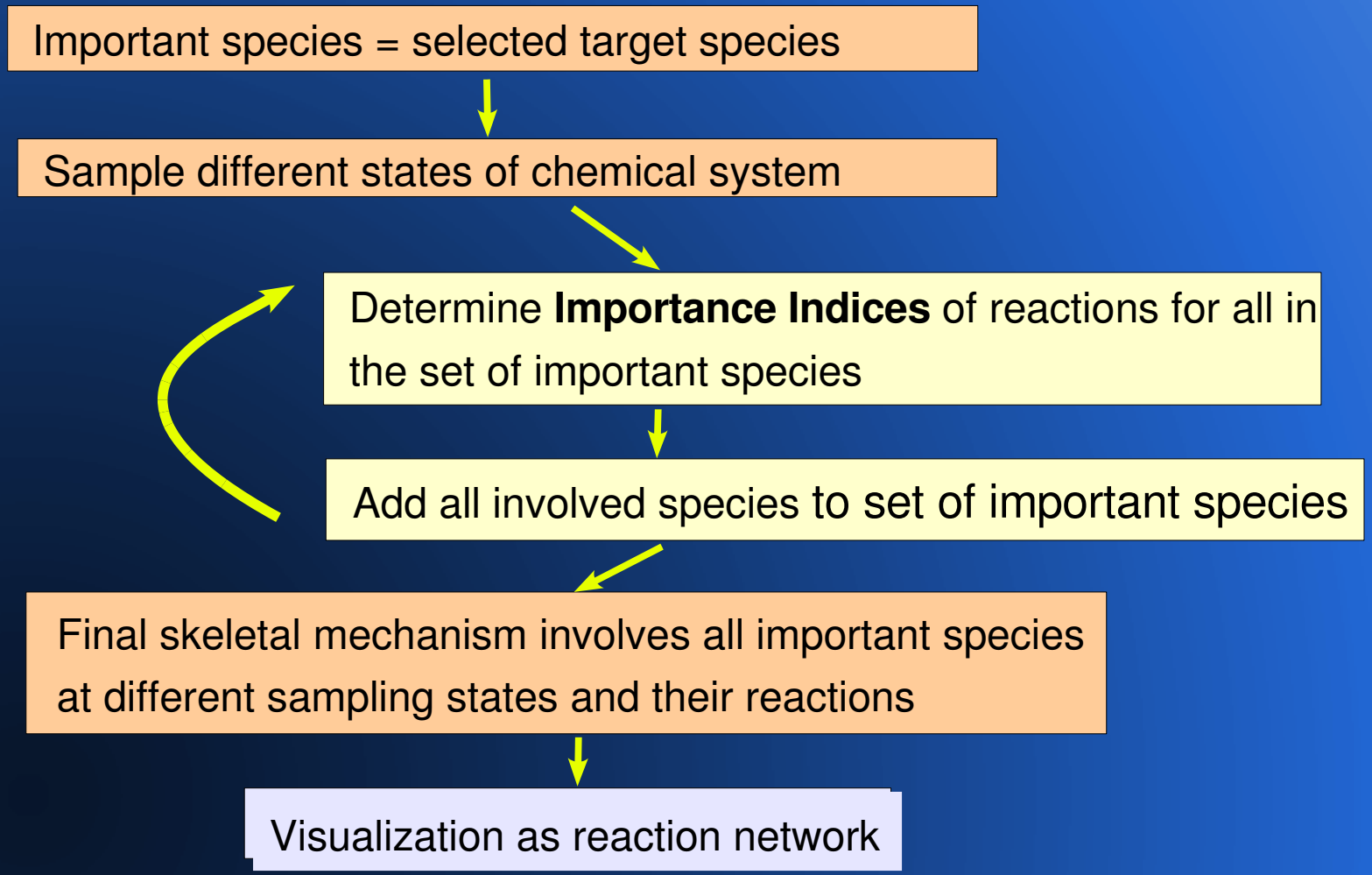
Number exhausted modes



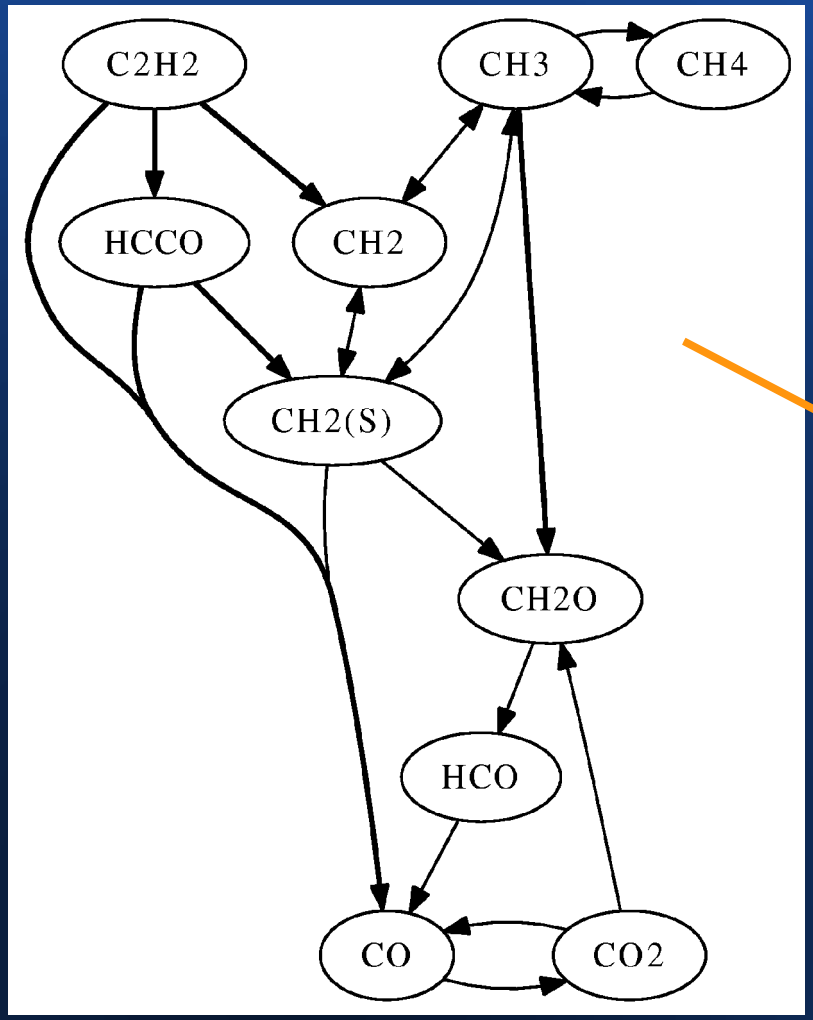
Driving time scale τ_{M+1}



Skeletal Mechanism Generation

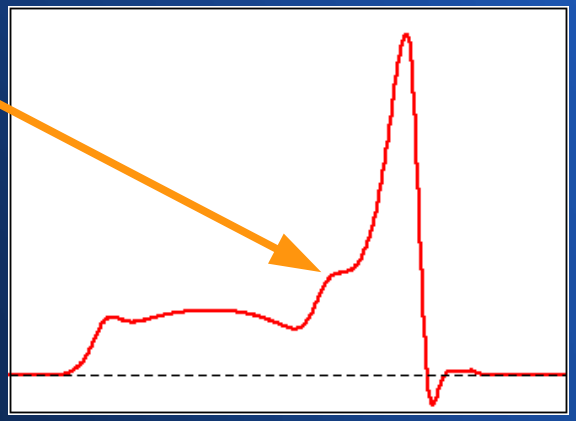


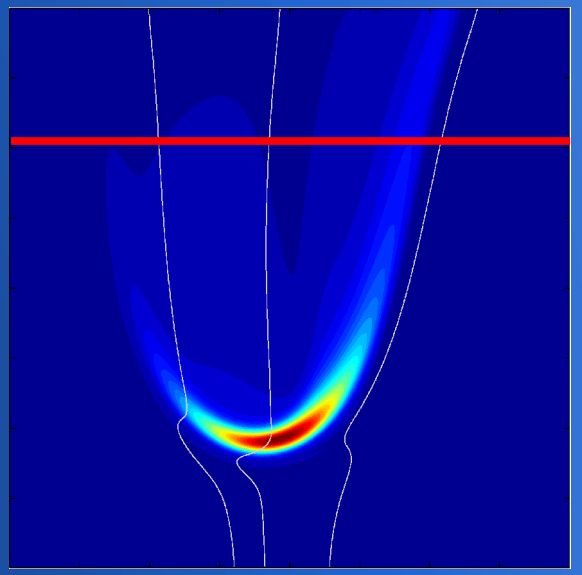
Local Reaction Network, *n*-heptane



- C_2H_2 and CH_3 together with H_2 and CO "fuel" the diffusion flame

Heat-release rate

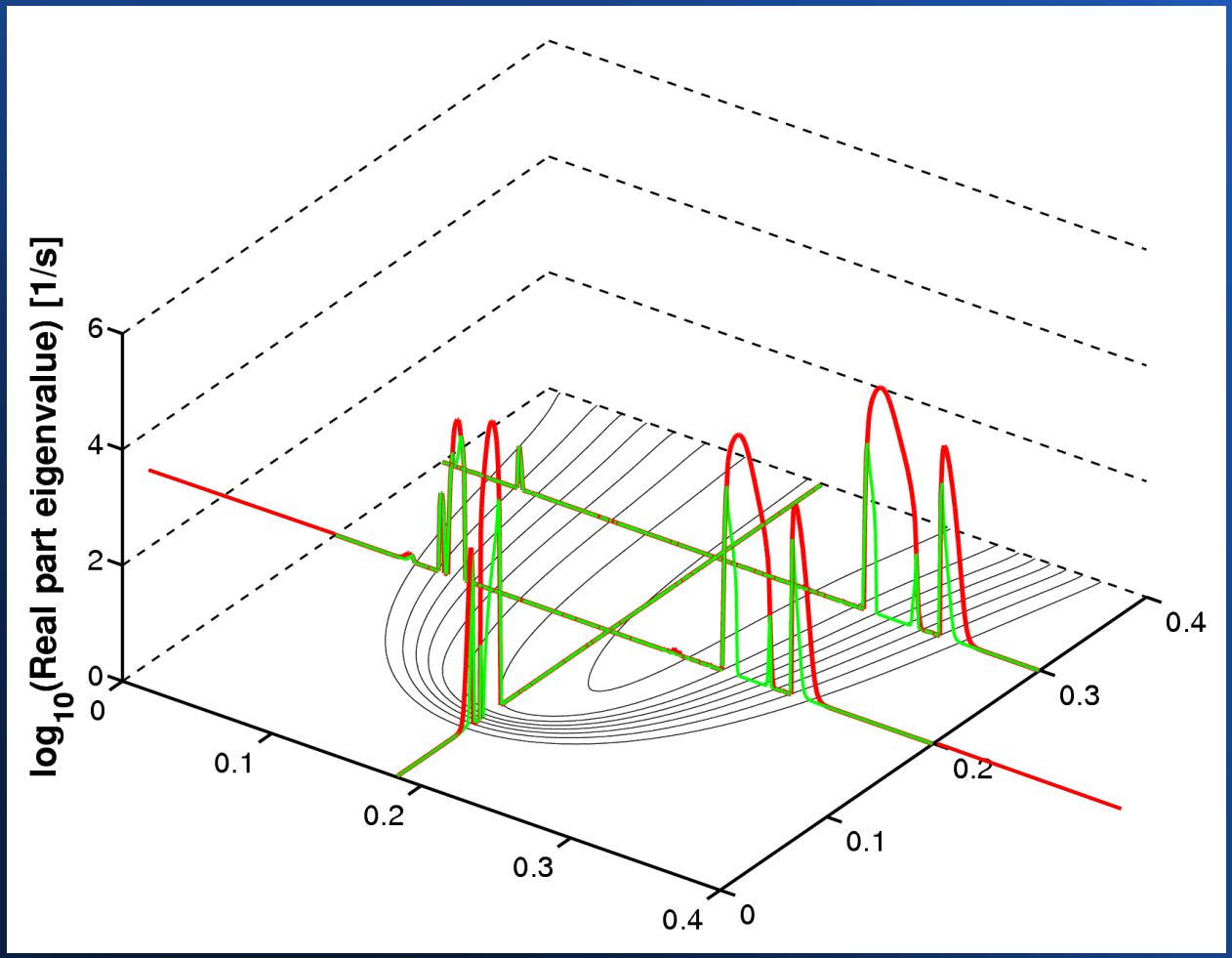




Explosive Modes

- Andrei Kazakov et al.
  - Two-stage ignition of *n*-heptane
- Wei Liu et al.
  - Counterflow ignition of methane, ethylene and CH_4/H_2
- Tianfeng Lu et al.
  - 3D-DNS turbulent lifted H_2 jet flame in heated coflow
- Dimitris Goussis et al.
  - Model reduction Circadian cycle, two-stage ignition *n*-heptane
- Habib Najm et al.
  - CH_4/air edge flame structure

Explosive Modes, *n*-heptane



- 2 explosive regions 1200K-1800K and 600K-800K
- 2 modes each

Explosive Modes, *n*-heptane

$$Q_m^{\exp} = a_{\exp}^m b_m^{\exp}$$

CSP pointer

T, O_2, C_3H_6, C_2H_x

T, CO_2, H_2O, O_2, H_2

$C_7H_{15}O_2$-*2*, $C_7H_{15}O_2$-*3*,
T, *n*C_7ket*24*, *n*C_7ket*35*

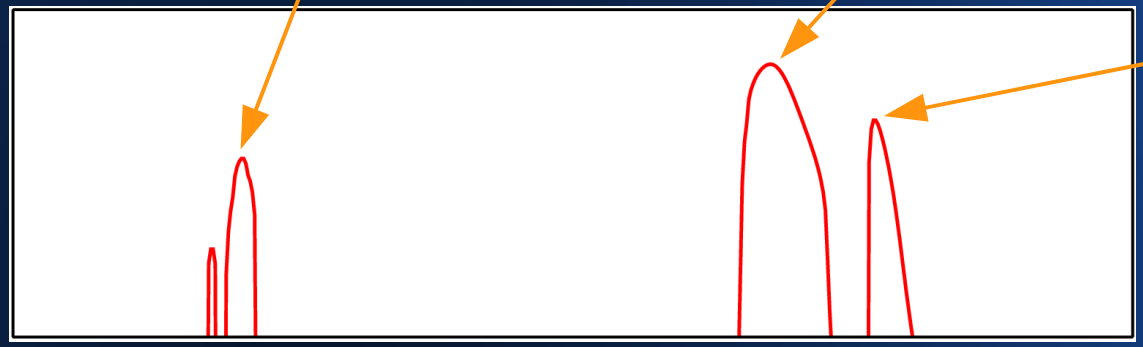
Explosive Modes, *n*-heptane

$$P_k^{\exp} \propto (b^{\exp} \cdot S_k) R^k$$

Participation Index

(+) $H+O_2 \rightarrow O+OH$
$CO+OH \rightarrow CO_2+H$
$HO_2+H \rightarrow 2OH$

(-) $H+O_2+M \rightarrow HO_2+M$
$HO_2+OH \rightarrow H_2O+O_2$
$O+OH \rightarrow H+O_2$

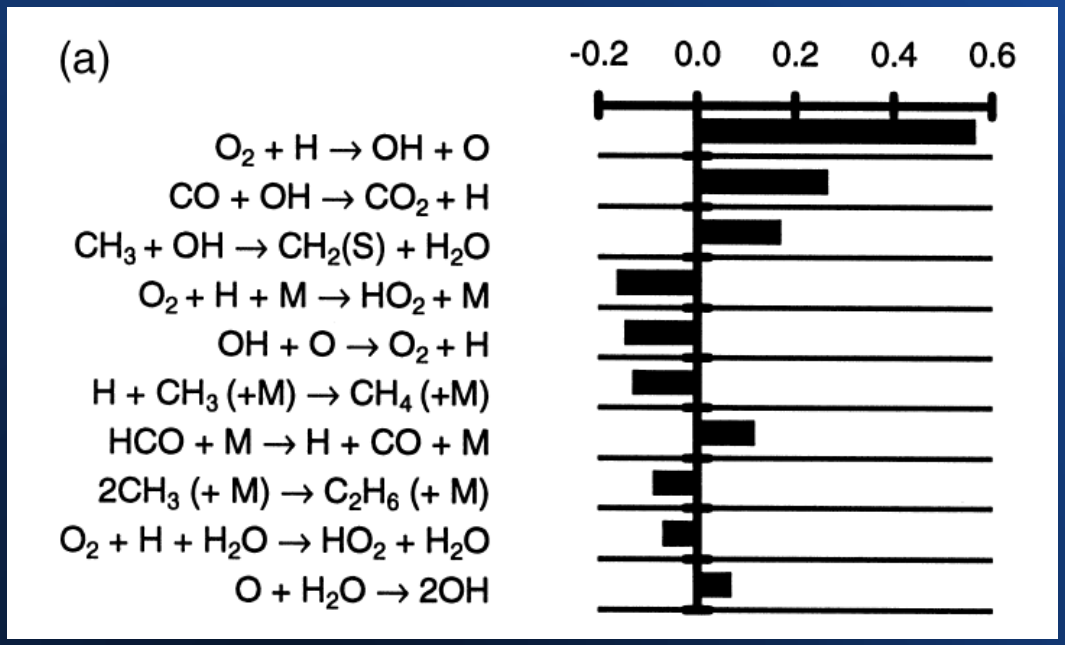


(+) $H+O_2 \rightarrow O+OH$
$C_2H_3+O_2 \rightarrow CH_2CHO+O$
$CH_3+H_2 \rightarrow CH_4+H$

(+) $C_7H_{15}O_2\text{-}x \rightarrow C_7H_{14}OOHx\text{-}y$
$C_7H_{14}OOHx\text{-}y+O_2 \rightarrow C_7H_{14}OOHx\text{-}yO_2$
$C_7H_{14}OOHx\text{-}yO_2 \rightarrow nC_7ketxy+OH$

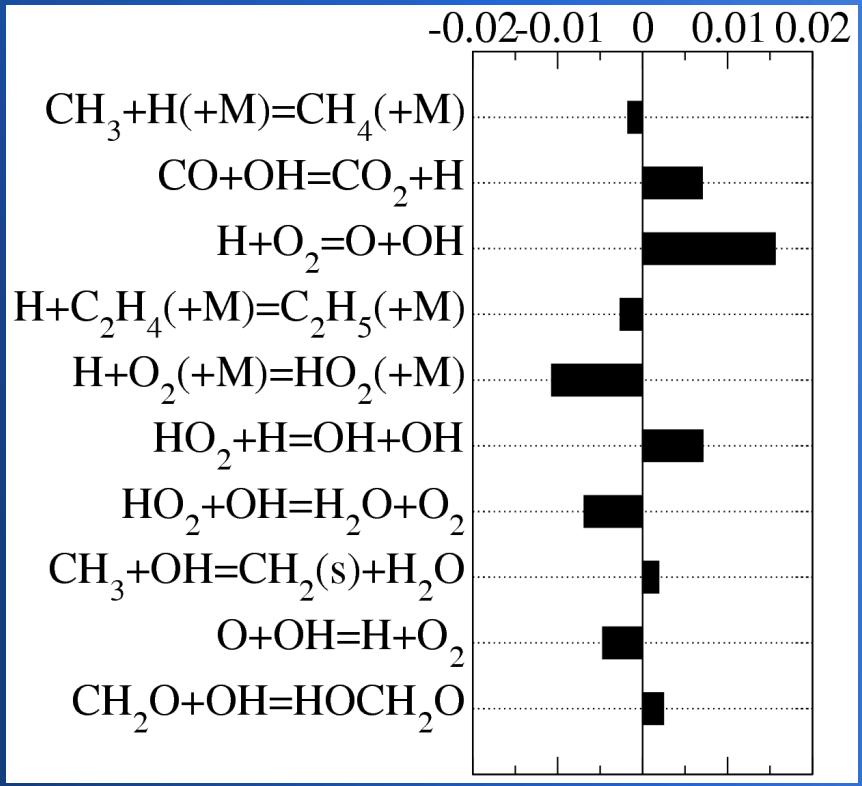
Explosive Modes, *n*-heptane

Sensitivity coefficients wrt. flame velocity, CH_4/air flame φ=0.61



Hughes et al. (2001)

Participation Index, *n*-heptane, lean branch, main explosive mode



Explosive Modes

Time Scale Importance Index

D.A. Goussis et al.:

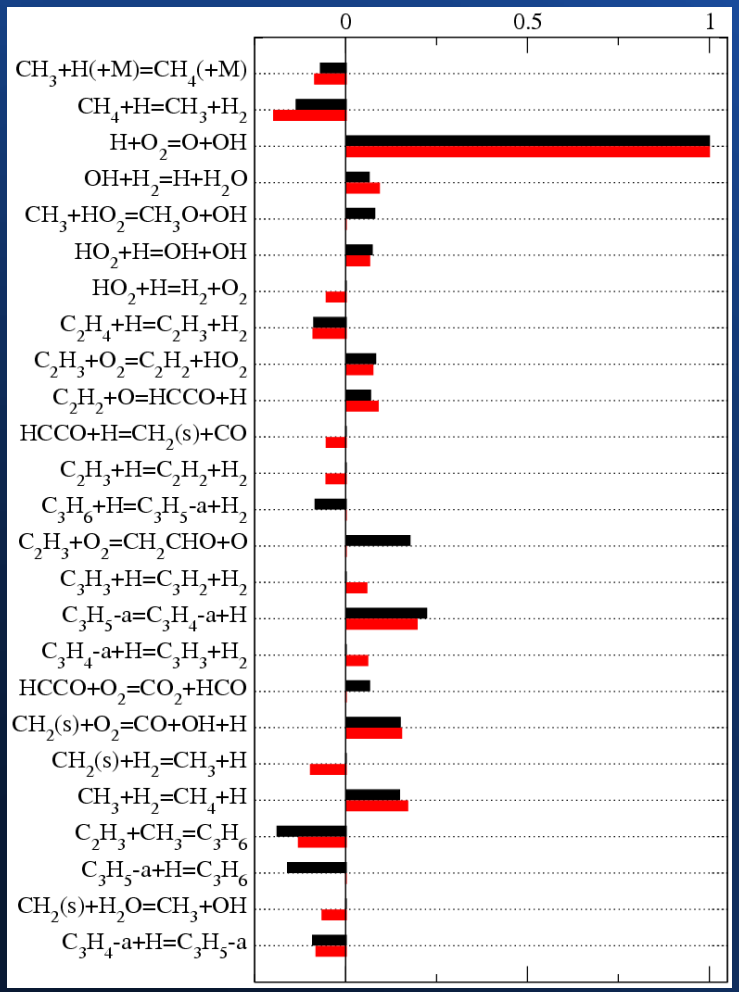
$$\lambda_i = \boldsymbol{b}^i \boldsymbol{J} \boldsymbol{a}_i$$

$$\boldsymbol{J} = \sum_{k=1}^{R} \boldsymbol{\nabla} \left(\boldsymbol{S}_k R^k \right)$$

$$J_k^{\exp} = \frac{\boldsymbol{b}^{\exp} \boldsymbol{\nabla} \left(\boldsymbol{S}_k R^k \right) \boldsymbol{a}_{\exp}}{\sum_{k'=1,R} \left| \boldsymbol{b}^{\exp} \boldsymbol{\nabla} \left(\boldsymbol{S}_{k'} R^{k'} \right) \boldsymbol{a}_{\exp} \right|}$$

$$J_k^{\exp} \propto \left(\boldsymbol{a}_{\exp} \cdot \boldsymbol{\nabla} R^k \right) \left(\boldsymbol{b}^{\exp} \cdot \boldsymbol{S}_k \right)$$

Explosive Modes, *n*-heptane



- Comparison Participation Index (black) and Time Scale Importance Index (red)
- Main explosive mode in rich branch
- Major contributions agree

Conclusions and Future Work

- CSP analysis valuable post-processing tool
- Examples:
  - Reaction networks
  - Time scale analysis
  - Model reduction
  - Identification of important processes
  - Explosive mode analysis

Conclusions and Future Work

- Study different reacting flows
- Explosive modes:
  - Relation to Sensitivity Analysis
  - Difference between Participation Index analysis and Time Scale Importance Index
  - Importance and physical meaning of slow Explosive Modes