Direct Numerical Simulation of Turbulence-Combustion Interaction

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What is DNS in combustion?

- Fluid mechanics: solve Navier-Stokes equations to determine one realization of the flow
  - All lengthscales and timescales are resolved
  - Limited to low-to-moderate Reynolds numbers (10^3 - 10^4)
  - Cost scales roughly as Re^3
- DNS in combustion: include chemistry, mass and energy conservation
  - Usual simplifications in 3D reacting flows
    - Reduced/small chemical networks (mechanisms)
    - Simple transport
    - No radiation
    - Single phase flow
  - Not all “possible” timescales are captured in general
- No single investigator can implement all the physics and numerics while achieving peak performance in modern hardware.
  - Heavy use of libraries for chemistry/transport (Chemkin, Cantera)

Equations

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

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = \frac{-(\nabla \cdot \boldsymbol{P})}{\rho} + \sum_{i=1}^{N} Y_i \boldsymbol{f}_i$$

$$\rho \frac{\partial u}{\partial t} + \rho\, \mathbf{v} \cdot \nabla u = -\nabla \cdot \boldsymbol{q} - \boldsymbol{P} : (\nabla \mathbf{v}) + \rho \sum_{i=1}^{N} Y_i \boldsymbol{f}_i \cdot \boldsymbol{V}_i$$

$$\frac{\partial Y_i}{\partial t} + \mathbf{v} \cdot \nabla Y_i = \frac{\omega_i}{\rho} - \frac{[\nabla \cdot (\rho Y_i \boldsymbol{V}_i]}{\rho}, \; i = 1, \ldots N.$$

$$\boldsymbol{P} = \left[p + \left(\frac{2}{3}\mu - \kappa \right) (\nabla \cdot \mathbf{v}) \right] \mathbf{U} - \mu \left[(\nabla \mathbf{v}) + (\nabla \mathbf{v})^T \right]$$

$$q = -\lambda \nabla T + \rho \sum_{i=1}^{N} h_i Y_i \boldsymbol{V}_i + R^o T \sum_{i=1}^{N} \sum_{j=1}^{N} \left(\frac{X_j D_{T,i}}{W_i D_{ij}} \right) (\boldsymbol{V}_i - \boldsymbol{V}_j) + \boldsymbol{q}_R$$

$$\nabla X_i = \sum_{j=1}^{N} \left(\frac{X_i X_j}{D_{ij}} \right) (\boldsymbol{V}_j - \boldsymbol{V}_i) + (Y_i - X_i) \left(\frac{\nabla p}{p} \right) + \frac{\rho}{p} \sum_{j=1}^{N} Y_i Y_j (\boldsymbol{f}_i - \boldsymbol{f}_j) +$$

$$+ \sum_{j=1}^{N} \left[\left(\frac{X_i X_j}{\rho D_{ij}} \left(\frac{D_{T,j}}{Y_j} - \frac{D_{T,i}}{Y_i} \right) \right) \right] \left(\frac{\nabla T}{T} \right), \quad i = 1, \ldots, N.$$

$$p = \rho R^o T \sum_{i=1}^{N} \left(\frac{Y_i}{W_i} \right), \quad u = \sum_{i=1}^{N} h_i Y_i - \frac{p}{\rho}$$

$$h_i = h_i^o + \int_{T^o}^{T} c_{p,i}\, dT, \quad i = 1, \ldots, N$$

$$X_i = \frac{(Y_i / W_i)}{\sum_{j=1}^{N} (Y_j / W_j)}, \quad i = 1, \ldots, N$$

Chemistry

$$\omega_i = W_i \sum_{k=1}^{M} \left(\nu''_{i,k} - \nu'_{i,k}\right) B_k T^{\alpha\kappa} e^{-\left(E_k / R^o T\right)} \prod_{j=1}^{N} \left(\frac{X_j p}{R^o T}\right)^{\nu'_{j,k}} \quad , \quad i = 1, \ldots, N,$$

Nr.	Reaction	B mole, cm^3, sec	n	E kJ/mole
1.1 H_2/O_2 Chain Reactions				
1f	$O_2+H \rightarrow OH+O$	2.000E+14	0.00	70.30
1b	$OH+O \rightarrow O_2+H$	1.568E+13	0.00	3.52
2f	$H_2+O \rightarrow OH+H$	5.060E+04	2.67	26.30
2b	$OH+H \rightarrow H_2+O$	2.222E+04	2.67	18.29
3f	$H_2+OH \rightarrow H_2O+H$	1.000E+08	1.60	13.80
3b	$H_2O+H \rightarrow H_2+OH$	4.312E+08	1.60	76.46
4f	$OH+OH \rightarrow H_2O+O$	1.500E+09	1.14	0.42
4b	$H_2O+O \rightarrow OH+OH$	1.473E+10	1.14	71.09
1.2 HO_2 Formation and Consumption				
5f	$O_2+H+M' \rightarrow HO_2+M'$	2.300E+18	-0.80	0.00
5b	$HO_2+M' \rightarrow O_2+H+M'$	3.190E+18	-0.80	195.39
6	$HO_2+H \rightarrow OH+OH$	1.500E+14	0.00	4.20
7	$HO_2+H \rightarrow H_2+O_2$	2.500E+13	0.00	2.90
8	$HO_2+OH \rightarrow H_2O+O_2$	6.000E+13	0.00	0.00
9	$HO_2+H \rightarrow H_2O+O$	3.000E+13	0.00	7.20
10	$HO_2+O \rightarrow OH+O_2$	1.800E+13	0.00	-1.70
1.3 H_2O_2 Formation and Consumption				
11	$HO_2+HO_2 \rightarrow H_2O_2+O_2$	2.500E+11	0.00	-5.20
12f	$OH+OH+M' \rightarrow H_2O_2+M'$	3.250E+22	-2.00	0.00
12b	$H_2O_2+M' \rightarrow OH+OH+M'$	1.692E+24	-2.00	202.29
13	$H_2O_2+H \rightarrow H_2O+OH$	1.000E+13	0.00	15.00
14f	$H_2O_2+H \rightarrow H_2+HO_2$	1.700E+12	0.00	15.70
14b	$H_2+HO_2 \rightarrow H_2O_2+H$	1.150E+12	0.00	80.88

Nr.	Reaction	B mole, cm^3, sec	n	E kJ/mole
1.4 Recombination Reactions				
15	$H+H+M' \rightarrow H_2+M'$	1.800E+18	-1.00	0.00
16	$OH+H+M' \rightarrow H_2O+M'$	2.200E+22	-2.00	0.00
17	$O+O+M' \rightarrow O_2+M'$	2.900E+17	-1.00	0.00
2. CO/CO_2 Mechanism				
18f	$CO+OH \rightarrow CO_2+H$	4.400E+06	1.50	-3.10
18b	$CO_2+H \rightarrow CO+OH$	4.956E+08	1.50	89.76
3.1 CH Consumption				
19	$CH+O_2 \rightarrow CHO+O$	3.000E+13	0.00	0.00
20	$CO_2+CH \rightarrow CHO+CO$	3.400E+12	0.00	2.90
3.2 CHO Consumption				
21	$CHO+H \rightarrow CO+H_2$	2.000E+14	0.00	0.00
22	$CHO+OH \rightarrow CO+H_2O$	1.000E+14	0.00	0.00
23	$CHO+O_2 \rightarrow CO+HO_2$	3.000E+12	0.00	0.00
24f	$CHO+M' \rightarrow CO+H+M'$	7.100E+14	0.00	70.30
24b	$CO+H+M' \rightarrow CHO+M'$	1.136E+15	0.00	9.97
3.3 CH_2 Consumption				
25f	$CH_2+H \rightarrow CH+H_2$	8.400E+09	1.50	1.40
25b	$CH+H_2 \rightarrow CH_2+H$	5.830E+09	1.50	13.08
26	$CH_2+O \rightarrow CO+H+H$	8.000E+13	0.00	0.00
27	$CH_2+O_2 \rightarrow CO+OH+H$	6.500E+12	0.00	6.30
28	$CH_2+O_2 \rightarrow CO_2+H+H$	6.500E+12	0.00	6.30

Nr.	Reaction	B mole, cm^3, sec	n	E kJ/mole
3.4 CH_2O Consumption				
29	$CH_2O+H \rightarrow CHO+H_2$	2.500E+13	0.00	16.70
30	$CH_2O+O \rightarrow CHO+OH$	3.500E+13	0.00	14.60
31	$CH_2O+OH \rightarrow CHO+H_2O$	3.000E+13	0.00	5.00
32	$CH_2O+M' \rightarrow CHO+H+M'$	1.400E+17	0.00	320.00
3.5 CH_3 Consumption				
33f	$CH_3+H \rightarrow CH_2+H_2$	1.800E+14	0.00	63.00
33b	$CH_2+H_2 \rightarrow CH_3+H$	3.680E+13	0.00	44.30
34	$CH_3+H+(M) \rightarrow CH_4+(M)$ k_∞ k_0	2.108E+14 6.257E+23	0.00 -1.80	0.00 0.00
35	$CH_3+O \rightarrow CH_2O+H$	7.000E+13	0.00	0.00
36	$CH_3+CH_3+(M) \rightarrow C_2H_6+(M)$ k_∞ k_0	3.613E+13 1.270E+41	0.00 -7.00	0.00 11.56
37	$CH_3+O_2 \rightarrow CH_2O+OH$	3.400E+11	0.00	37.40
38f	$CH_4+H \rightarrow CH_3+H_2$	2.200E+04	3.00	36.60
38b	$CH_3+H_2 \rightarrow CH_4+H$	8.391E+02	3.00	34.56
39	$CH_4+O \rightarrow CH_3+OH$	1.200E+07	2.10	31.90
40f	$CH_4+OH \rightarrow CH_3+H_2O$	1.600E+06	2.10	10.30
40b	$CH_3+H_2O \rightarrow CH_4+OH$	2.631E+05	2.10	70.92
4.1 C_2H Consumption				
41f	$C_2H+H_2 \rightarrow C_2H_2+H$	1.100E+13	0.00	12.00
41b	$C_2H_2+H \rightarrow C_2H+H_2$	5.270E+13	0.00	119.95
42	$C_2H+O_2 \rightarrow CHCO+O$	5.000E+13	0.00	6.30

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29	$CH_2O+H \rightarrow CHO+H_2$	2.500E+13	0.00	16.70
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31	$CH_2O+OH \rightarrow CHO+H_2O$	3.000E+13	0.00	5.00
32	$CH_2O+M' \rightarrow CHO+H+M'$	1.400E+17	0.00	320.00
3.5 CH_3 Consumption				
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34	$CH_3+H+(M) \rightarrow CH_4+(M)$ k_∞ k_0	2.108E+14 6.257E+23	0.00 -1.80	0.00 0.00
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Nr.	Reaction	B mole, cm^3, sec	n	E kJ/mole
5.3 C_3H_5 Consumption				
69f	$C_3H_5 \rightarrow C_3H_4+H$	3.980E+13	0.00	293.10
69b	$C_3H_4+H \rightarrow C_3H_5$	1.267E+13	0.00	32.48
70	$C_3H_5+H \rightarrow C_3H_4+H_2$	1.000E+13	0.00	0.00
5.4 C_3H_6 Consumption				
71f	$C_3H_6 \rightarrow C_2H_3+CH_3$	3.150E+15	0.00	359.30
71b	$C_2H_3+CH_3 \rightarrow C_3H_6$	2.511E+12	0.00	-34.69
72	$C_3H_6+H \rightarrow C_3H_5+H_2$	5.000E+12	0.00	6.30
5.5 C_3H_7 Consumption				
73	$n\text{-}C_3H_7 \rightarrow C_2H_4+CH_3$	9.600E+13	0.00	129.80
74f	$n\text{-}C_3H_7 \rightarrow C_3H_6+H$	1.250E+14	0.00	154.90
74b	$C_3H_6+H \rightarrow n\text{-}C_3H_7$	4.609E+14	0.00	21.49
75	$i\text{-}C_3H_7 \rightarrow C_2H_4+CH_3$	6.300E+13	0.00	154.50
76	$i\text{-}C_3H_7+O_2 \rightarrow C_3H_6+HO_2$	1.000E+12	0.00	20.90
5.6 C_3H_8 Consumption				
77	$C_3H_8+H \rightarrow n\text{-}C_3H_7+H_2$	1.300E+14	0.00	40.60
78	$C_3H_8+H \rightarrow i\text{-}C_3H_7+H_2$	1.000E+14	0.00	34.90
79	$C_3H_8+O \rightarrow n\text{-}C_3H_7+OH$	3.000E+13	0.00	24.10
80	$C_3H_8+O \rightarrow i\text{-}C_3H_7+OH$	2.600E+13	0.00	18.70
81	$C_3H_8+OH \rightarrow n\text{-}C_3H_7+H_2O$	3.700E+12	0.00	6.90
82	$C_3H_8+OH \rightarrow i\text{-}C_3H_7+H_2O$	2.800E+12	0.00	3.60

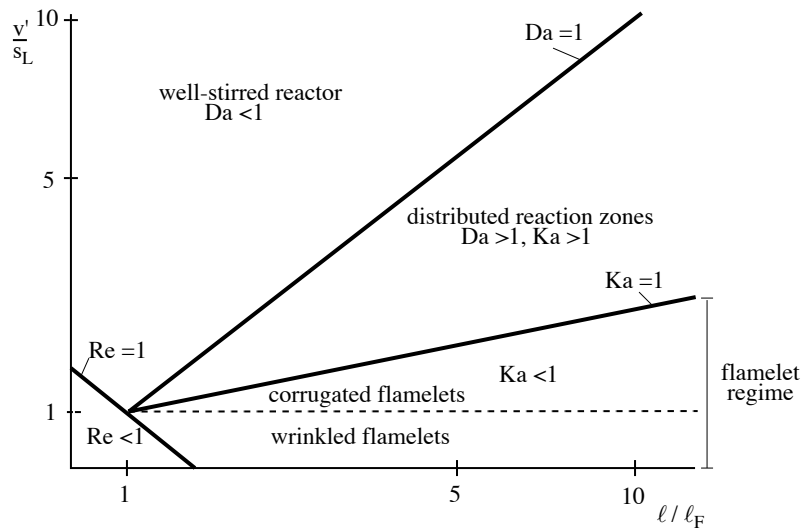
$[M'] = 6.5[CH_4]+6.5[H_2O]+1.5[CO_2]+0.75[CO]+0.4[O_2]+0.4[N_2]+1.0[Other]$

Problem

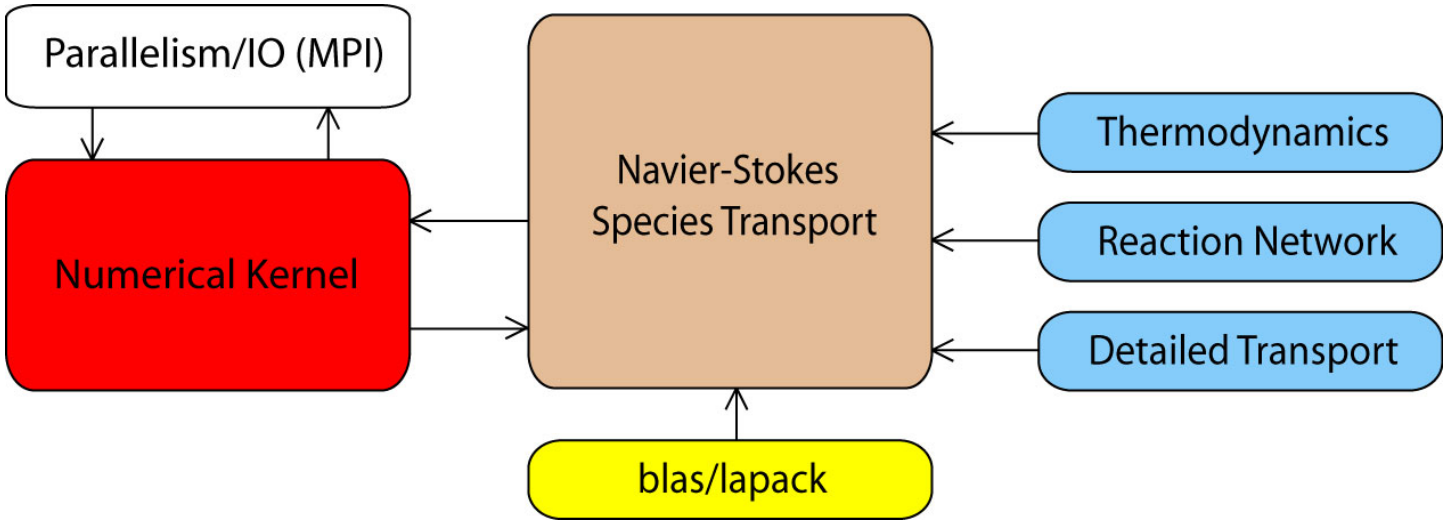
- There is no spatial or temporal scale separation
- In general, everything is coupled: small scales with large scales, heat release with momentum, composition with thermodynamics
- Practical (device level) simulations are accomplished by imposing an affordable computational cost (filtering) and modeling the nonlinear interaction terms that result: large-eddy simulation (LES)
- The most successful use of DNS is to gain understanding of the turbulence-combustion interaction regimes, which do produce “high-fidelity” closures for LES
- DNS is usually setup to investigate combustion regimes in turbulent flows:
  - ignition kernels,
  - flames,
  - flame edges (tribrachial flames),
  - flameless combustion
- What are the effects of unstationarity on the combustion structure?
- Is there a change in the turbulence structure due to heat release?
- DNS can be a powerful technique applied to laboratory controlled flames, where statistically steady state can be achieved and direct comparisons can be made
  - turbulent lifted jet flames and Bunsen flames

Turbulence-combustion interaction

- With the fluid dynamical lengthscale (Kolmogorov) η and a combustion lengthscale l (flame thickness), there are three regimes
  - i) l « η little fluid dynamical interaction, one way heat release coupling only
  - ii) l ~ η strong fluid dynamical interaction (most challenging regime)
  - iii) l » η little combustion interaction at the Kolmogorov scale
- Because turbulence involves a hierarchy of scales, third regime almost always presents interaction but at a larger scale than η
- Details of the interaction depend on the combustion regime: premixed, nonpremixed or partially premixed



Classical DNS code

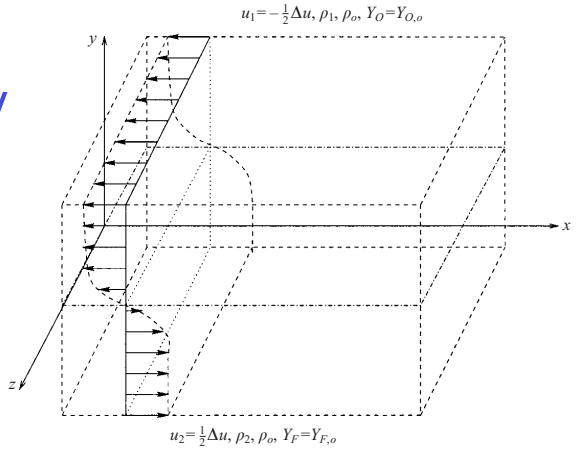


- Transport terms (second order derivatives) are very important in combustion
- Need to use high order methods: 4th, 6th, or 8th
- Conservation of mass, energy are very important in combustion
- Low numerical dissipation is preferred in turbulence simulations
- Stiff integrator to remove short timescales in the chemistry

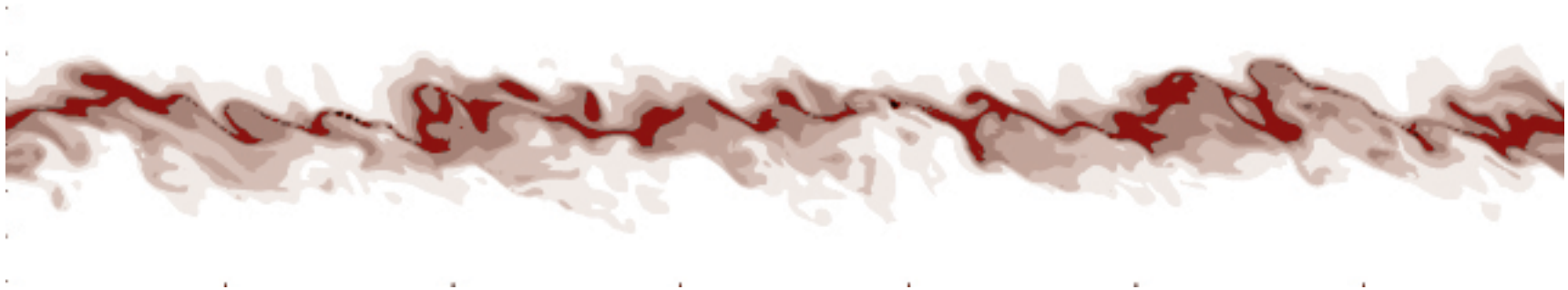
- It used to be the case that one could encapsulate most of the hardware performance issues within the BLAS/LAPACK subroutines
- This is proving harder now with new systems
- Mostly, hardware change too fast for us to evolve accordingly
- Performance issues are spilling back at the level of the Solver ■ and Parallelism □

Effect of heat release on turbulence

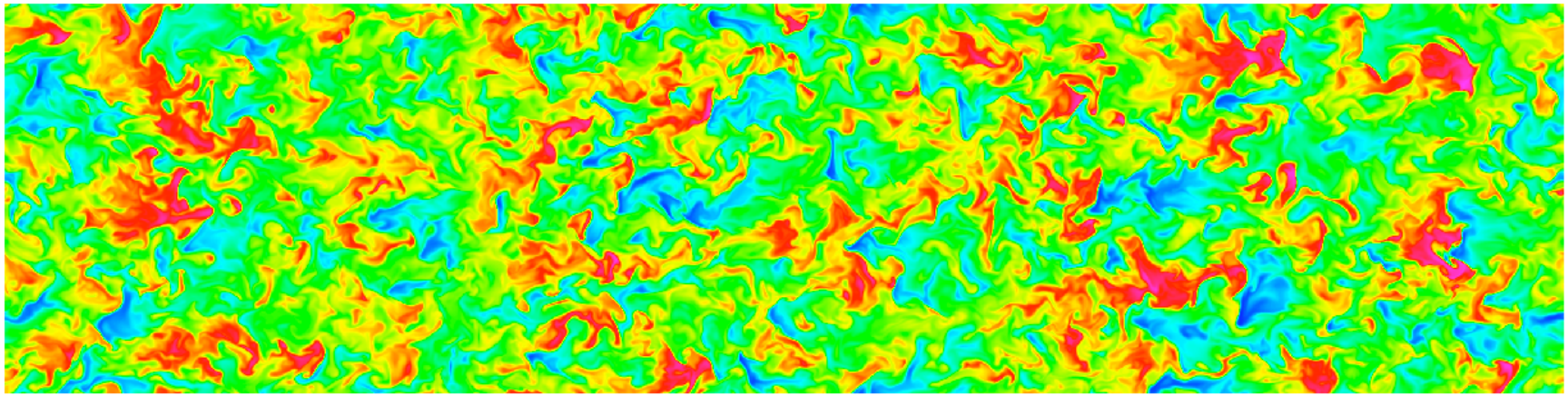
- Consider nonpremixed turbulent combustion
- Simplify chemistry to the infinitely-fast regime (one-way coupling)
- One-step Methane-Air and Hydrogen-Air
- 1 - 5 x 10^8 grid cells
- Re = 5000 - 10,000



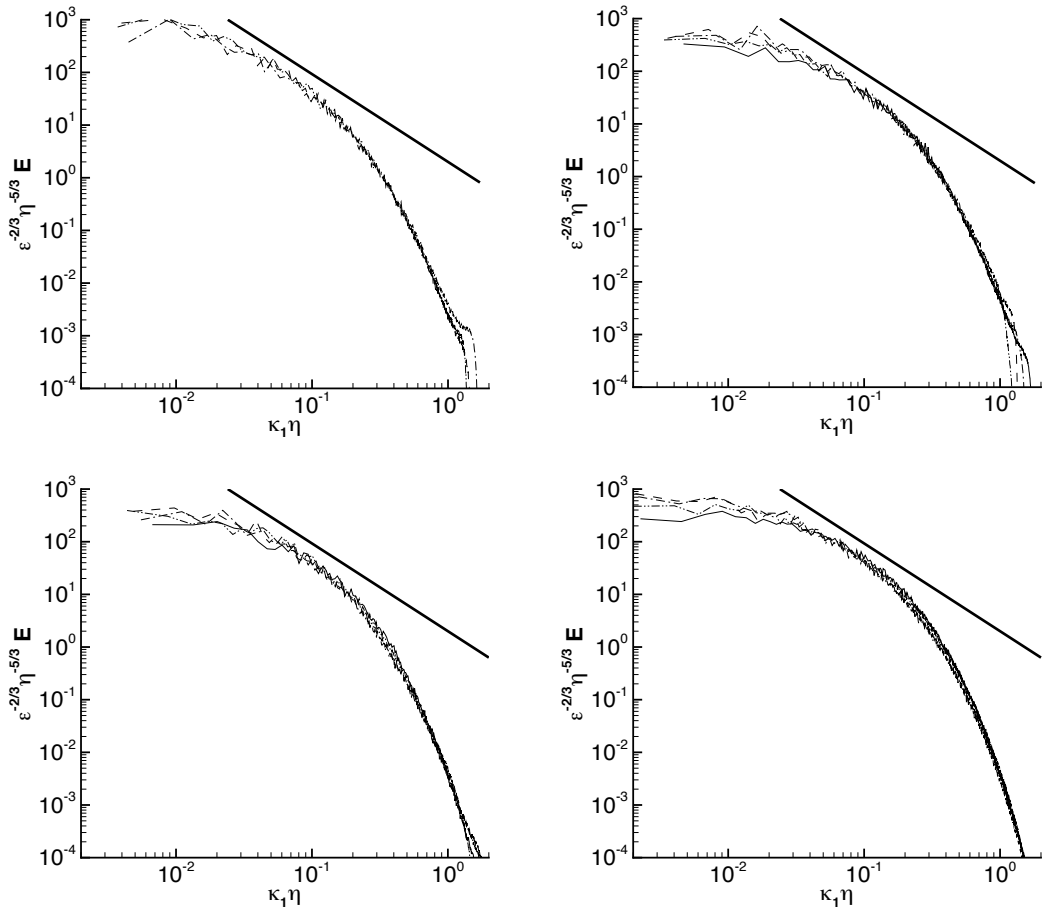
temperature

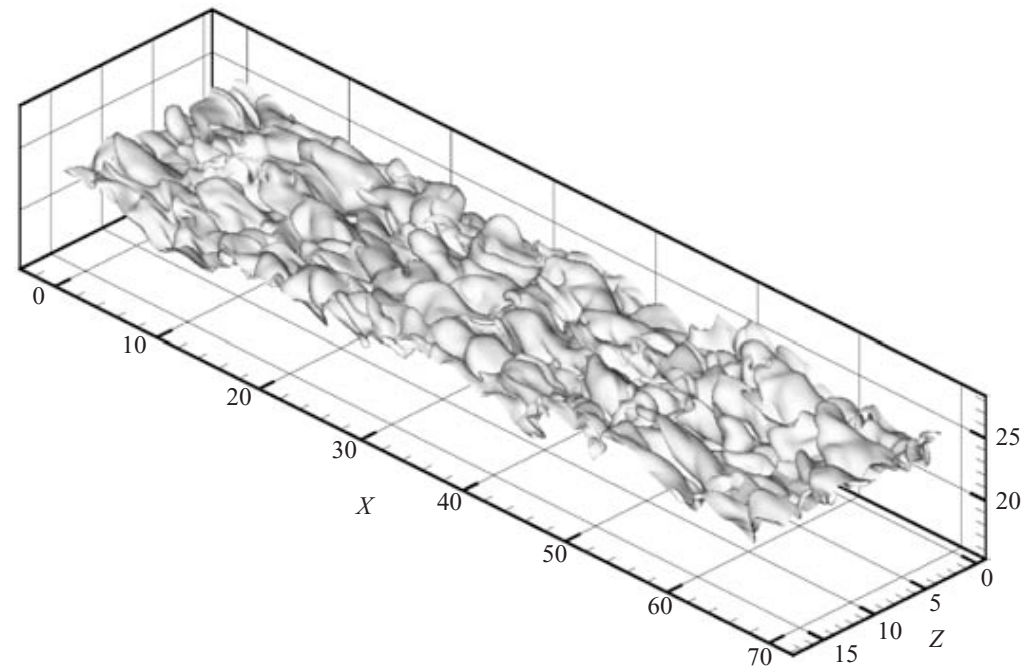


mixture fraction



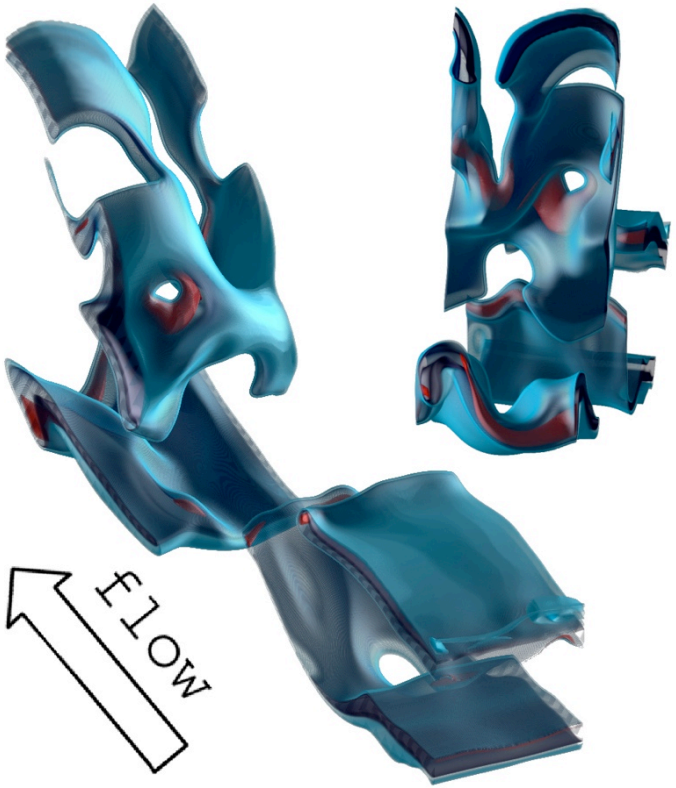
Energy spectra



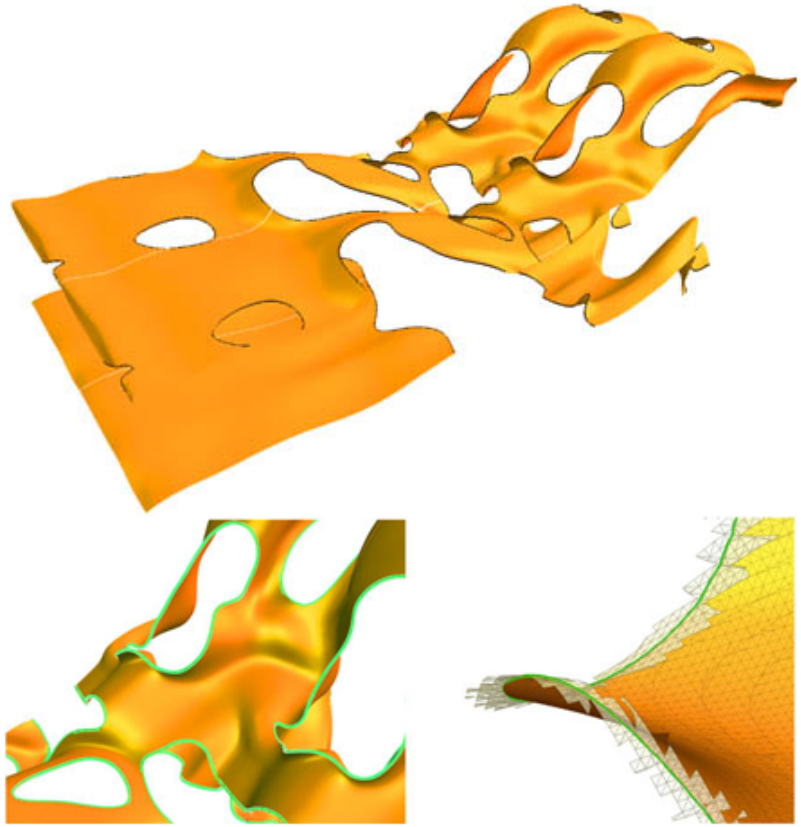


- Heat release does not seem to affect the inertial and dissipation subranges of the turbulent flow (Knaus & Pantano 2008)
- This validates our current models in the high heat release regime, which are based on incompressible turbulence

Jet flame stabilization and edge flames



hydrogen atom



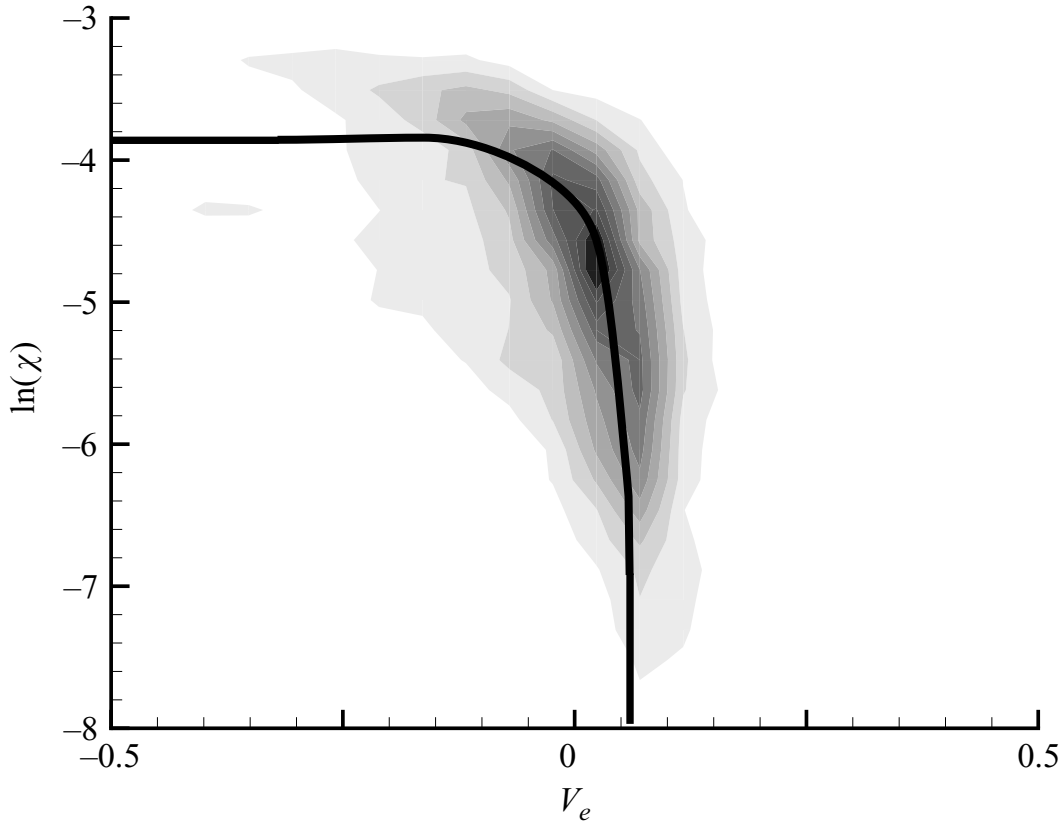
flame surface

- Simulation of methane-air jet flame (3D) using 4 step reduced chemistry

$$
\begin{aligned}
CH_4 + 2H + H_2O &= CO + 4H_2 && (I),\\
CO + H_2O &= CO_2 + H_2 && (II),\\
H + H + M &= H_2 + M && (III),\\
O_2 + 3H_2 &= 2H + 2H_2O && (IV),
\end{aligned}
$$

- Re=3000, 10^8 grid points, 1.2 10^9 DOF

Unstationary effects



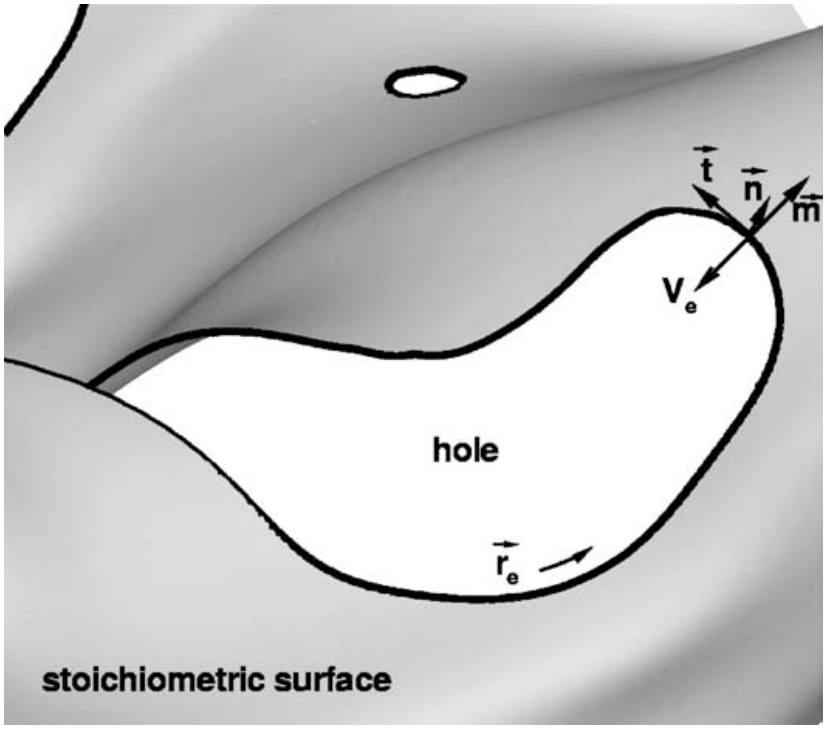


Fig. 1. Geometrical sketch of a flame hole and its associated local orthogonal coordinate system.

- Flame edges experience substantial unstationary effects, even at the modest Reynolds number of this simulation
- Models can incorporate this information

Future algorithms

- additive time integrators for stiff systems (ASIRK, IMEX, ...)

$$\dot{y} = f(y) + g(y),$$

explicit → f, implicit → g

- global Newton methods
- adaptive mesh refinement
- implicit geometry and fictitious domain methods for interface problems
  - immersed interface method (Leveque & Li 1994), Lee & Leveque 2003)
  - immersed boundary method (Lai & Peskin 1998)
  - Lagrange multiplier/penalty (Glowinski *et al.* 2001)

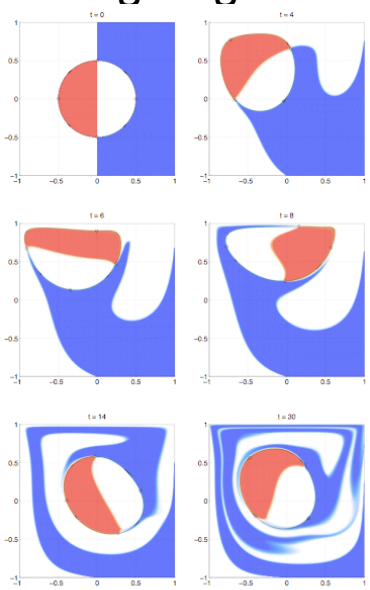
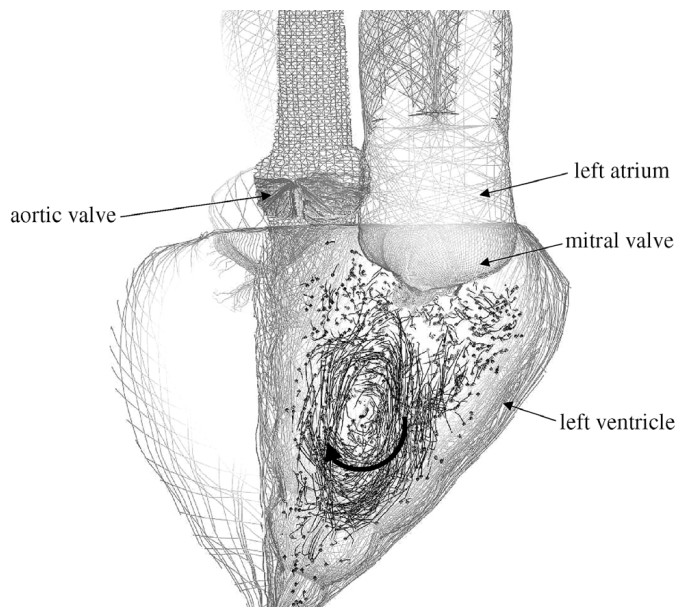


FIG. 8.10. *Stretched membrane in a lid-driven cavity.*



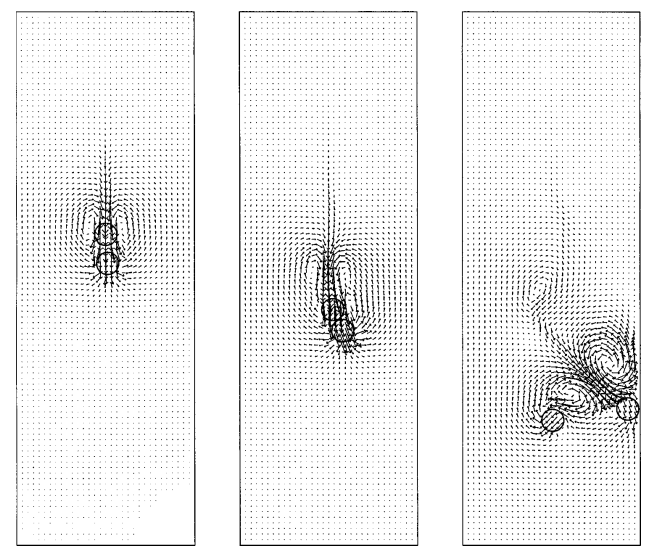


FIG. 8.12. Disks positions and flow field visualization at $t = 0.15$, 0.2, and 0.3 ($\rho_s = 1.5$, $\nu = 10^{-2}$, $h_\Omega = 1/384$, $\Delta t = 5 \times 10^{-4}$). Wave-like equation treatment of the advection.

Challenges

- Numerical issues
  - high-pressure (all Mach number), high-order, conservative, low dissipation formulation
  - gas-liquid, high-order, conservative, stable formulation
    - requires DNS-accurate Lagrangian tracking of interface
  - stochastic (pdf) coupling for soot and possibly sprays
  - temporal and numerical discretization error control
- Chemistry
  - automatic mechanism reduction
  - are chemical mechanism time accurate in unstationary flames?
  - chemical parameters uncertainty effects
- Thermodynamics
  - general equation of state
  - phase transition: evaporation and cavitation

- Immediate challenge: high-pressure regime
- Next 5-10 years: two-phase flow regime