### CHEMISTRY AND LES / DNS

How do we include realistic chemistry in DNS/LES codes?

Look at kinetics from the point of view of the turbulent code developers:

- **HOW MANY INDEPENDENT SPECIES?** -> more memory
- **HOW MANY REACTIONS?** -> more CPU time

1/ **BRUTE FORCE**
2/ **TABULATION METHODS OF FULL SCHEMES**
3/ **REDUCED SCHEMES**

High Performance Computation of 3D reacting flows
VARIABLES: 5 (for flow) + N (for species)

We need to solve at each time step, at each point:
- Density
- Velocities
- Temperature
- All species $Y_k$, for $k = 1$ to $N$

And all equations are coupled:

$M$ reactions taking place between the $N$ species

In general, in a turbulent 3D code, it is quite difficult to use large values of $N$ and $M$. Today:
- In DNS codes, $N=20$ to $100$; $M=10$ to $40$
- In LES codes, $N=6$ to $20$, $M=1$ to $4$

The brute force method: no compromise!

Solve at each time step, at each point, the equations for:
- Density
- Velocities
- Temperature
- all $Y_k$’s, for $k = 1$ to $N$

No assumption needed and no limitation except for the validity of the chemical scheme itself and the cost.

In practice, this works for:
- DNS and LES of H2 flames with full chemistry
- DNS of certain hydrocarbon flames (see Sandia team)
- 0D codes where mixing is supposed to be infinitely fast (see CHEMKIN, CANTERA, etc)
- 1D codes (laminar premixed flame, diffusion flame)
DNS of H2/O2 flame with 19 reactions and 9 species:

PhD A. Ruiz, 2012, CERFACS
See also J. Chen team at Sandia

DNS of lifted ethylene/air jet flame
22 species, 18 global reactions
All other methods: compromise!

Solve at each time step, at each point, the conservation equations for:
- Density
- Velocities
- Temperature
- One or two independent variables (usually $c$ and $z$)
- All other species $Y_k$ are functions of these two variables and are not solved for

$\Rightarrow$ TABULATION!

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**Manifolds in combustion (S. Pope)**

Even though all species are ‘independent’ variables and should be computed separately, the examination of mass fraction trajectories in most flames shows that, in composition space, most points fall on a manifold of limited size.

Instead of $N$ independent variables, the whole system can be described with much less variables.
Steady flamelet manifold projected onto the N2–CO2–CO mass fraction space, color-coded by temperature. The oxidizer is air; the fuel is methane/air 1:3 by volume; 1 bar; both streams at 300K. Green curve: extinction conditions; the black curve: stoichiometric mixture. (from M. Ihme, see S.B. Pope / Proceedings of the Combustion Institute 34 (2013) 1–31)

Not all manifolds are 'good' manifolds:

Assumption of universality of manifolds in combustion

Assume that ALL flames (laminar or turbulent) follow the same manifold:

Measure this manifold in laminar cases and then use if for all other flames

Which variables should be used to describe the manifold?

The most intuitive ones are:
- The progress variable $c$
- The mixture fraction $z$

For flames with heat losses, the total enthalpy is added

Defining the progress variable can be difficult. In most hydrocarbon flames, use:

\[
\frac{c}{c = \frac{Y_C - Y_C^\text{fresh}}{Y_C^\text{burnt} - Y_C^\text{fresh}}} \quad Y_c = Y_{CO} + Y_{CO2}
\]
Example for the reaction rate:

Manifold assumption

\[ \dot{\omega}(Y_1, Y_2, Y_3\ldots Y_k) = \dot{\omega}_1(c, z) \]

\[ \dot{\omega}_1(c, z) = \dot{\omega}_2(c, z) \]

Manifold universality assumption

\[ \dot{\omega}(Y_1, Y_2, Y_3\ldots Y_k) = \dot{\omega}_2(c, z) \]

Manifold assumption

Tabulation procedure

Take a laminar flame. Build a table with \(c\) and \(z\) as entries and the reaction rate as output.

In the 3D code add two conservation equations: one for \(c\) and one for \(z\). From \(c\) and \(z\), read the reaction rate in the table and get the reaction rate.
Bonus: if you have $c$ and $z$, you can read tables to have ALL species:

Tables can be extended to include all other species:

NO=$f(c,z)$
CO=$f(c,z)$
OH=$f(c,z)$

Just by post processing the computation, all species can be extracted. You pay to solve for 2 quantities ($c$ and $z$) but you obtain $N$ species.

Caution: this does not work very well for species such as NO which live in the burnt gases where $c$ goes from 0.95 to 0.99 and the tabulation is not precise.

Universality of manifolds?

If you tabulate a flame using PSR in 0D for autoigniting mixtures, is this sufficient for real flames?

Can we use a tabulation written for a diffusion flame in a premixed flame?

Which tabulation must be used in a partially premixed flame?

Can we really assume that the same manifold holds in laminar AND turbulent flames?
Example of tabulation based methods

Two cases where theory can prove simply that tabulation methods work and only one variable is needed:

- the diffusion flame with infinitely fast chemistry: using \( z \)
- the perfectly premixed flame using \( c \)

Cases where tabulation methods work but need two variables, usually \( c \) and \( z \)

Cases where tabulation methods don’t work: usually, real combustors...

THE SIMPLEST TABULATION: DIFFUSION FLAMES WITH INFINITELY FAST CHEMISTRY: 1 species, 0 reaction!

If all Lewis numbers are equal to unity, if pressure is constant, if only two streams feed the combustion chamber, the flow is adiabatic and chemistry is infinitely fast, we have already seen that all variables depend only on the mixture fraction \( z \).
A 3D code for diffusion flames with infinitely fast chemistry:

Solve at each time step, at each point, the conservation equations for:
- Density
- Velocities
- Mixture fraction \( z \)

All other species are directly given by \( z \) using the \( z \) diagram.

CAUTION: works only if... chemistry is infinitely fast. And if you have only two streams feeding the combustor (otherwise \( z \) does not exist)

Extensions of this simple case to real flames - Tabulation in a non-premixed flame:

Even if the previous assumptions are not satisfied, assume that:
- \( Y_k \) and \( T \) are functions of \( z \) in both cases
- and this function is the same!
We measure it in the laminar case and use it in the turbulent cases
Typical problem: stabilization of diffusion flames

**NEVER USE TABULATED FLAMES VS \( z \) ONLY IN A FLAME FOR WHICH YOU ARE NOT SURE THAT CHEMISTRY IS FAST AND THE FLAME IS IGNIITED EVERYWHERE.**

**IN THE REAL WORLD:**
- WORKS ONLY FOR H\(_2\) FLAMES
- FOR ALL OTHERS, IT IS DANGEROUS

Even if the flame is’ ignited’, it might be far from infinitely fast chemistry conditions:

**DNS of turbulent diffusion flame:**

**Y\(_{\text{fuel}}\)**

**Y\(_{\text{oxy}}\)**

Infinitely fast chemistry lines

Doom, Hou and Mahesh, JCP 226, 2007
Experiments say the same thing:

Barlow and Franck PCI, 27, 1998, 1027

STRETCH: a required extension for most flames:

DNS and experiments show that the flame structure does not depend on $z$ only: an additional parameter must be introduced: this is flame stretch (or scalar dissipation)
A required extension for diffusion flames:

The laminar diffusion flame is a stretched flame and stretch (or equivalently scalar dissipation) controls its structure. Most tabulation methods add scalar dissipation $\chi$ in the table which becomes 2D: all variables are:

$$f(z, \chi)$$

While $\chi$ is unambiguously defined for the laminar flame used to create the tabulation, its evaluation in a LES is more difficult.

ANOTHER SIMPLE ‘TABULATION’: PERFECTLY PREMIXED LEAN FLAMES. 1 species, 1 reaction

Here ‘tabulation’ is actually something which can be demonstrated using theory and we did it before in ‘Basics’:

1- Assume that the flame is so lean that only the fuel limits the reaction rate. Only $Y_F$ needs to be tracked

$$q_1 = A_1 \left( \frac{\rho Y_{CH_4}}{W_{CH_4}} \right)^{n_{1F}} \left( \frac{\rho Y_{O_2}}{W_{O_2}} \right)^{n_{1O}} \exp \left( -\frac{E_a}{RT} \right)$$

Almost constant
2- Assume that the Mach number is small, pressure is constant, Lewis=1. Theory says that in this case, temperature $T$ and fuel mass fraction $Y_F$ are linked by:

$$\frac{T - T_1}{T_2 - T_1} + \frac{Y_F}{Y_F^1} = 1$$

Only one independent variable gives everything. Usually take $c$:

$$c = \frac{T - T_1}{T_2 - T_1} = 1 - \frac{Y_F}{Y_F^1}$$

- Most classical theories for turbulent premixed flames are indeed based on methods using $c$ only.

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**Tabulation in 3D premixed flames:**

Solve at each time step, at each point, the conservation equations for:
- Density, velocities + Progress variable $c$ (also called theta by many authors): with one source term for $c$
- Here, obviously, the expression for the reaction rate is valid for laminar AND turbulent flames

$$\frac{\dot{\omega}_F}{Y_F^1} = B_1 T^{\beta_1} e^{-\beta/\alpha} \rho(1 - \Theta) \exp \left( -\frac{\beta(1 - \Theta)}{1 - \alpha(1 - \Theta)} \right)$$

This is the simplest manifold formulation... It can be extended:
We assume that:
• $Y_k$ and $T$ are functions of $c$ in these two flames
• the functions are the same

A nice numerical feature of tabulation:

A tabulation method will provide reaction rates obtained from reading a data base:

$$\dot{\omega} = f(c)$$

This expression will always a physically reasonable reaction rate

A method based on Arrhenius rates will provide reaction rates from the Arrhenius expression:

$$\dot{\omega} = A Y_f^{n_F} Y_O^{n_O} \exp(-T_a/T)$$

This expression might provide non physical values when small numerical errors develop on mass fractions or temperatures
With a direct impact on resolution:

A tabulation method will usually require less resolution points inside the flame front because it is much less sensitive to numerical errors (typically dispersive effects due to the resolution of species by the 3D solver) than a method using Arrhenius rates.

Extensions of tabulation methods

Perfectly premixed lean flames and infinitely fast chemistry situations are not sufficient to address all real flames.

Extensions have been developed to handle more flame regimes.

The first and most natural extensions are based on two variables:
- The progress variable \( c \)
- The mixture fraction \( z \)
GENERALIZED TABULATIONS (FPI, FGM): 2 independent variables $c$ and $z$

Solve at each time step, at each point, the conservation equations for:
- Density
- Velocities
- Progress variable $c$ and mixture fraction $z$: with one source term for $c$

All species $Y_k$ and temperature are tabulated as function of $z$ and $c$. The trick is to know in WHICH laminar flames this tabulation is used.
+ : we have all the other species: complex chemistry is included.
- : it is a ‘frozen’ complex chemistry. The links between $Y_k$ and $(z,c)$ are fixed and obtained on canonical laminar flames.

CAUTION: works only if... flow is adiabatic and is fed by two streams only.

FPI: CORIA, EM2C
FGM: EINDHOVEN
ISAT: CORNELL

THE SUCCESS OF TABULATIONS

Tabulation methods have been developed with significant success in the last five years (see Cornell, EM2C or Eindhoven papers).

They have been applied to canonical cases (purely premixed adiabatic flames, pure diffusion flames, constant pressure, constant inlet temperature, two-feed system).
THE LIMITS OF TABULATIONS

In real systems, taking into account:

- Variable pressure (such as in a piston engine)
- A variable dilution
- Cases where more than two streams enter the chamber (so that a mixture fraction \( z \) cannot be defined)
- Non adiabatic cases

leads to tabulation methods which become difficult and heavy.

In most cases finding the relevant flame on which to tabulate data becomes also quite arduous...

Tabulation in a real flame (premixed/diffusion):

Yk and T may depend on \( z \) and \( c \) but:
- Which \( z \) ? (more than two inlets here) -> we’ll need two or more \( z \)'s
- Which flamelet to tabulate them ? A premixed or a diffusion one ?
Tabulation in a flame with heat losses:

Heat losses are important here

6% Fuel (pure)

Yk and T will depend on z and c and heat losses. The table becomes big... And the choice of the flamelet to tabulate almost impossible.

Tabulation in a piston engine:

In a piston engine, we will have the same problems + new ones:
- The tabulation must account for variable pressure
- Most engines use EGR (exhaust gas recirculation): must account for dilution by burnt gas
- The tabulation must account for variable fresh gas temperature

Now Yk and T are functions of:
z1, z2, c, P, Dilution, Heat losses....

• The data base becomes too big to fit on local memories
• The choice of the flamelet for the construction of the data base becomes impossible

GOING TO REDUCED SCHEMES BECOMES ATTRACTIVE!
REDUCED SCHEMES: 5 to 10 species, 2 to 10 reactions

Solve at each time, at each point, the conservation equations for:
- Density
- Velocities
- Temperature
- Chemical species $Y_k$

All species are solved independently. More general but stiffer and more expensive than tabulation methods. No limitation EXCEPT for the quality of the reduced scheme!! (and that is a big one!)

Can work with non adiabatic flows, multiple streams feeding the combustor.
Requires the development of reduced schemes!

THE QUEST FOR REDUCED SCHEMES

The search for simple chemical schemes started long ago:

This is a fitting exercise: if we have a single step reaction, we can fit four parameters. How many flame properties can we fit with 4 adjustable constants?

Answer: not that many if we have only one reaction and we keep the reaction constants...constant. But if we start tuning the reactions constants?
Then we need to choose ‘objectives’. For example if we compute a turbulent premixed flame at a fixed equivalence ratio, we want the reduced scheme to match:

- Adiabatic flame temperature
- Laminar flame speed
- CO2 and CO mass fractions in the burnt gases

We use a full chemical scheme as a reference to tune the reduced scheme (this means we need one !) over our ‘objectives. These objective flames must be simple enough to be computed with the full scheme.

Main idea: it is very difficult to build a reduced scheme which matches ALL properties of a full scheme over ALL conditions of pressure, composition and temperature. But it is much easier to match certain properties of a full scheme with a reduced scheme only in a limited range of conditions.
Similarities between tabulation methods and reduced schemes:

• In tabulation methods, we assume that the manifold in composition space found in a turbulent flame is similar to the one found in a laminar flame.

• In reduced schemes, we assume that a scheme which performs correctly for a set of laminar flames (the ‘objectives’) will perform correctly in turbulent flames.

Both approaches rely on flamelet concepts. They are based on similar physical ideas.

Differences between tabulation methods and reduced schemes:

Their implementation is different:

• Tabulation methods use the true trajectories measured in laminar flames and use a reduced number of variables (usually c and/or z) to describe the manifold. We follow the manifold rigorously but we follow ONLY this specific one. An adiabatic manifold won’t be able to incorporate heat losses for example.

• Reduced schemes use more independent species and assume that the explicit reaction rates they use are general enough to describe chemistry. Since they have more independent species, they are not limited to one manifold. For example, the effects of heat losses (radiation) are directly taken into account.
TYPICAL RESULTS USING A SINGLE-STEP SCHEME:

\[
\text{CH}_4 + 2(\text{O}_2 + a \text{ N}_2) \rightarrow \text{CO}_2 + 2 \text{ H}_2\text{O} + 2a \text{ N}_2
\]

\[
q_1 = A_1 \left( \frac{\rho Y_{\text{CH}_4}}{W_{\text{CH}_4}} \right)^{n_1F} \left( \frac{\rho Y_{\text{O}_2}}{W_{\text{O}_2}} \right)^{n_{1O}} \exp \left( -\frac{E_{a_1}}{RT} \right)
\]

Figure 3.3 - Adiabatic temperature as a function of the equivalence ratio for a mixture initially at temperature \( T_f = 320 \text{ K} \). Comparison between 5 (solid line), 6 (dashed line) and 53 (symbols) species.

1-step: \( T_{\text{in}} = 630 \text{ K} \) \( P = 1 \text{ atm} \) \( \Phi_0 = 0.5 \)

<table>
<thead>
<tr>
<th>ELEMENTS</th>
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<tr>
<td>H</td>
<td>O</td>
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<td></td>
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<td>H\text{2}O</td>
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<td>N\text{2}</td>
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<th>REACTIONS</th>
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<tbody>
<tr>
<td>CH\text{4} + 2O\text{2} \rightarrow CO\text{2} + 2H\text{2}O</td>
</tr>
<tr>
<td>FORD / CH\text{4} 1.7602 /</td>
</tr>
<tr>
<td>FORD / O\text{2} 1.2867 /</td>
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<td>END</td>
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WHY CARRY 30 SPECIES AND 300 REACTIONS IF YOU ARE ONLY INTERESTED IN FLAME SPEED AND TEMPERATURE FOR A FIXED OPERATING POINT?
1-step: $T_{in}=630K$ $P=1$ atm $\Phi_0=0.5$

NEVER FORGET THAT THE ERROR MARGIN ON CHEMISTRY AND FLAME SPEED IS NOT SMALL:

Single step chemistry
BUT WE CAN DO BETTER:
• ADD ONE SPECIES (CO) -> CH4, O2, CO2, H2O, N2, CO
• AND ONE REACTION: CO + 1/2 O2 <-> CO2

Figure 3.3 - Adiabatic temperature as a function of the equivalence ratio for a mixture initially at temperature $T_i = 320$ K: comparison between 5 (solid line), 6 (dashed line) and 53 (symbols) species.

2-step: $T_{in}=630K$ P=1 atm $\Phi_0=0.5$

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<th>H</th>
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<tr>
<td>SPECIES</td>
<td>CH4</td>
<td>O2</td>
<td>CO</td>
<td>CO2</td>
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<td>END</td>
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<tr>
<td>REACTIONS</td>
<td>CH4 + 1.5O2 =&gt; CO + 2H2O</td>
<td>5.82549E+15</td>
<td>0.0</td>
<td>35626.0</td>
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<tr>
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<td>FORD / CH4 0.9441 / FORD / O2 1.1441 / CO+0.5O2 = CO2</td>
<td>1.30028E+13</td>
<td>0.0</td>
<td>20684.0</td>
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<tr>
<td></td>
<td>FORD / CO 1.00 / RORD / CO 0.00 / FORD / O2 0.50 / RORD / O2 0.00 / END</td>
<td></td>
<td></td>
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2-step: $T_{in}=630K$ $P=1atm$ $\Phi_0=0.5$

This method works well if we want to compute one case only (fixed pressure, fixed temperature, etc). Can we do better?
EXTENSION TO A WIDER RANGE OF EQUVALENCE RATIO AND CONDITIONS:

Tune each constant as a function of equivalence ratio:


- Franzelli et al Comb. Flame 157, 1364. MODIFY ONLY PREEXPONENTIAL CONSTANTS

\[ q_1 = A_1 \left( \frac{\rho Y_{CH_4}}{W_{CH_4}} \right)^{n_{1F}} \left( \frac{\rho Y_{O_2}}{W_{O_2}} \right)^{n_{1O}} \exp \left( -\frac{E_{a1}}{RT} \right) \]

A1 becomes A1(ϕ) where ϕ is the local equivalence ratio

Example for methane: the BFER scheme (exists also for kerosene)

The 2S_CH4_BFER mechanism is composed of six species (CH\(_4\), O\(_2\), CO\(_2\), CO, H\(_2\)O et N\(_2\)) and takes into account two reactions:

\[
\begin{align*}
CH_4 + 1.5 \, O_2 & \rightarrow CO + 2 \, H_2O \quad (13) \\
CO + 0.5 \, O_2 & \leftrightarrow CO_2 \quad (14)
\end{align*}
\]

- first reaction: it controls the flame speed and the ignition delay;
- second reaction: it is needed to predict burnt gas temperature for rich mixtures.

Validated for a wide range of pressure 1 \( atm < P < 10 \, atm \), initial temperature 300 \( K < T_f < 800 \, K \) and equivalence ratio 0.7 < \( \phi < 1.6 \).

The general methodology described in B. Franzelli, E. Riber, M. Sanjose and T. Ponsot, A two-step chemical scheme for kerosene-air premixed flames, Combust. Flame, 157 (2010) 1364-1373 has been used to build this scheme.
A two-step scheme for CH4/air flames (Franzelli et al CF 157, 1364):

Works for lean and rich flames, over a wide range of pressures and temperatures
Exists also for kerosene/air flames

The + and - of reduced schemes:

+: cheap
+: no assumption on regime: will work for premixed, diffusion, non adiabatic, etc
+: intuitive: no need to make assumptions on corresponding flamelet to tabulate
+: the user knows the limits of his scheme

-: cannot be used if no data is available on chemistry
-: might need more and more species and reactions to reach goals:
  Ex:
  - to have flame speeds: one reaction and 5 species
  - to have adiabatic flame temperatures: two reactions and 6 species
  for CH4 / air flames but sometimes ... More!
FOR CH4/O2 FLAMES, YOU MUST HAVE A SCHEME WHICH HANDLES CH4, O2, CO, CO2, H2O, H2, O AND H TO HAVE THE PROPER THERMOCHEMISTRY

CONSTRUCTING REDUCED SCHEMES:

In practice: how do you choose the coefficients of the reactions? This is an optimization problem. We have to determine $4^N$ coefficients where $N$ is the number of reactions:

$$q_1 = A_1 \left( \frac{\rho Y_{CH_4}}{W_{CH_4}} \right)^{n_{1F}} \left( \frac{\rho Y_{O_2}}{W_{O_2}} \right)^{n_{1O}} \exp \left( -\frac{E_{a1}}{RT} \right)$$

Finding these $4^N$ coefficients can be done:
- By hand, trying to avoid modifying coefficients which are known from elementary reactions when possible
- Automatically using optimization methods.
Genetic optimization of reduced schemes for a methane/air 2 step mechanism

- Constraints on laminar flame structure:
  - $\phi = 0.5, 0.8, 1.0$
  - targets: GRI-Mech 3.0
- 15 individuals / generation
- 200 generations
- Operators:
  - boundary mutation
  - whole/simple non-uniform mutation
  - Whole/simple arithmetical crossover

Global convergence

Over constrained

12 constraints

8 Arrhenius law parameters to fit

2nd Activation Energy convergence
Methane 2 step mechanism: 2S/CH4/CM2

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<tbody>
<tr>
<td>$\text{CH}_4 + \frac{3}{2}\text{O}_2 \rightarrow \text{CO} + 2\text{H}_2\text{O}$</td>
<td>2E15</td>
<td>0.9</td>
<td>1.1</td>
<td>35000</td>
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<tr>
<td>$\text{CO} + \frac{1}{2}\text{O}_2 \rightarrow \text{CO}_2$</td>
<td>2E09</td>
<td>1.0</td>
<td>0.5</td>
<td>12000</td>
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</tbody>
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**Flame temperature**

**Flame speed**

The + and - of reduced schemes:

+: cheap
+: no assumption on regime: will work for premixed, diffusion, non adiabatic, etc
+: intuitive: no need to make assumptions on corresponding flamelet to tabulate
+: the user knows the limits of his scheme

-: cannot be used if no data is available on chemistry
-: might need more and more species and reactions to reach goals:
  - to have flame speeds: one reaction and 5 species
  - to have adiabatic flame temperatures
  - to have NO: add Zeldovich
  - to have autoignition times
  - to have soot

-: kinetics experts not interested: they prefer building high-precision schemes with 10000 reactions!
-: reduced schemes validated using the idea that if they work for simple canonical flames, they will also work in turbulent cases. May not be true
SPATIAL RESOLUTION CONSTRAINTS

Choosing a chemical scheme is not the most critical part. Having one more species to solve for is not difficult. What is difficult is:

- having to resolve a flame front or the variations of one species in a flame front which is very thin
  \( \rightarrow \) small cell sizes

- having to solve a very stiff reaction
  \( \rightarrow \) small time steps

STIFFNESS AND NUMERICAL ISSUES

Reduced schemes are sometimes stiff...
Exponents can become negative!

\[
q_1 = A_1 \left( \frac{\rho Y_{\text{CH}_4}}{W_{\text{CH}_4}} \right)^{n_{1F}} \left( \frac{\rho Y_{\text{O}_2}}{W_{\text{O}_2}} \right)^{n_{1O}} \exp \left( -\frac{E_{a1}}{RT} \right)
\]

\[
s_L(P) = s_L(P_0) \left( \frac{P}{P_O} \right)^{n_{1F} + n_{1O} - 2}
\]

A ‘naive’ exploration of the values needed for the exponents \( n_{1F} \) and \( n_{1O} \) might end up with non physical values.
HIGH PERFORMANCE COMPUTING AND COMBUSTION

For 3D LES (and of course for DNS too), CPU time is a major issue

Parallel computing has been the major revolution in this field ten years ago: combustion is one of the most represented fields on the largest world machines (see for example ASCI projects)

WHICH EQUATIONS?

- The Navier Stokes equations (5 + N-1 unknowns: density, velocities and energy, N species). Partial differential equations -> non local, intense communication required
- Kinetics : N = 10 to 300 species reacting through 3000 reactions (everything local)
- Heat transfer through the walls, radiation, noise, soot
- All these flows are turbulent
WHAT DO WE COMPUTE?

**FINITE VOLUME CODES USING DOMAIN DECOMPOSITION AND MPI.**

Typically 100 Mcells with 20 to 100 variables at each cell (3 velocities, density, energy + 5 to 90 species) over 1000000 time steps. -> $10^{16}$ unknowns

WHAT ABOUT PARALLELISM?

**THE NAVIER STOKES EQUATIONS ARE ‘EMBARRASINGLY DIFFICULT’ TO PARALLELIZE -> THIS PROBLEM HAS BEEN IDENTIFIED AND IS REMODELING OUR COMMUNITY IN LARGER COLLABORATIVE TEAMS.**

**THIS IS NOT A ‘ONE-PROFESSOR ONE-CODE’ SHOW ANY MORE BECAUSE THE CODES ARE USED FOR INDUSTRY APPLICATIONS ON A DAILY BASIS.**
The SUCCESS scientific group
SUCCESS was created in 2012 to help the promotion of super-computing in the area of Computational Fluid Dynamics (CFD) for complex geometries. It is coordinated by the CORIA lab and is composed of 8 French public labs.

Our objectives
- Distribute in the labs research HPC codes for CFD in complex geometries
- Ensure the training of users
- Manage the development roadmap
- Share databases of high-resolution simulations
- Promote super-computing

The codes

**AVBP**
A massively-parallel finite-volume and finite-element 3D code for the simulation of compressible turbulent reactive and two-phase flows.

**YALES2**
A massively-parallel finite-volume 3D code for the simulation of turbulent reactive and two-phase flows at low-Mach number.

Some facts
- 8 French public labs
- Around 120 researchers and students
- 2 PRACE proposals accepted over the recent years

70

AVBP strong scaling examples

```
65536  ANL INTREPID, Bluegene P
57344  PRACE/TGCC, CURIE, BullX
49152  GENCI/CINES, JADE, SGI Altix ICE
40960  PRACE/SC, JUQUEEN, Bluegene Q
32768  INCITE/ARNL, INTREPID, Bluegene P
24576  HLRS/PRACE, HERMIT, CRAY XE6
16384  Ideal
8192   
```

1 billion cells (BG/Q)
ORGANIZATION OF THE FRENCH NUMERICAL COMBUSTION COMMUNITY

Example of organization: the AVBP ‘club’

Laboratories:
- IMFT (Toulouse)
- CORIA (Rouen)
- EM2C (Centrale Paris)
- IRPHE (Marseille)
- TUM (Munich)
- TU Eindhoven
- TWENTE
- MADRID
- ONERA
- Univ. Pau

Users:
- SNECMA (Villaroche)
- TURBOMECA (Bordes)
- SNECMA (Vernon)
- SPS (Bordeaux)
- RENAULT
- PSA
- ALSTOM
- ANSALDO
- SIEMENS
- FERRARI
- AIR LIQUIDE
- GAZ DE FRANCE

CERFACS
Institut Français du Pétrole

Code

Needs

Models

Code

STANFORD

INCITE
(Argonne)

Computer companies + Computing centers: CEA, Barcelona, GENCI
THIS PROGRESS IN HPC FOR COMBUSTION IMPACTS COMBUSTION SCIENCE:

- long course on turbulent combustion during this school

BUT : if we can perform DNS everywhere… we will not need turbulent combustion models !

Same evolution observed about RANS:

- who does high-order turbulence models today ?
- who does analytical methods ?

Is this good ? We will still need to understand what is going on.