Computational Aspects of a Numerical Model for Combustion Flow

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Position of the problem

Design, development and engineering of industrial power burners have strong mathematical requests:

- numerical resolution of a PDEs system involving *Navier-Stokes* equations for velocity and pressure fields, *energy conservation* law for temperature field, *Fick’s* law for diffusion of all the chemical species in the combustion chamber;
- geometrical design of the combustion head for a correct shape and optimal efficiency of *flame*;
- geometrical design of *ventilation fans* and computation of a correct air inflow for optimal combustion.

![Combustion head and chamber for burner.](image)

Computational complexity analysis for a flow (1)

*Simple example* for a detailed knowledge of the velocity field of fluid particles in the combustion chamber:

- **M** is the number of flow streamlines to compute;
- **S** is the number of geometrical points for every streamline.

High values for **M** are important for a *realistic simulation* of the flow, high values for **S** are important for a fine *graphic resolution*: minimal values are of order $O(10^3 - 10^4)$.

Suppose to use a 3D grid 10 x 10 x 1000 cm (hence **M** = 100, **S** = 1000), a medium value $v_i = 50$ cm/sec for every cartesian component of velocity vector field, and a space resolution $h = 0.5$ cm.
Computational complexity analysis for a flow (2)

For numeric resolution of time-dependent advective PDEs, the Courant-Friedrichs-Lewy (CFL) condition gives an upper limit for the time step:

\[ \Delta t \leq \frac{c}{v} \]

where \( c \) is a constant, usually \( \leq 1 \), depending on the used numeric method, and \( v = \sup |v_j| \). The quantity \( \frac{c}{h} \) is called CFL number. Let \( c = 1 \); then

\[ \Delta t \leq \frac{0.5 \text{ cm}}{0.05 \text{ sec}} = 0.01 \text{ sec.} \]

As consequence, for 1 real minute of simulation the flops are of order \( O(10^{10}) \) and the occupation of RAM is \( O(10^3) \) GB: the computation is CPU expensive, RAM consuming and produces a lot of useless data (100 snapshots of the flow every second).

A Finite Differences method and Interpolations

In the effort of minimize the relevance of these problems, we have studied a numeric model based on

- a Finite Differences schema with a not too restrictive CFL condition;
- an appropriate interpolation of the numeric FD velocity-field for a finer resolution without modifying the grid step.

This model gives a numeric solution comparable with the solutions based on finer grids: we present an estimate of its goodness and a mathematical justification.

The FD method is based on Lax-Friedrichs schema:

- discretization in time: \( \partial_t u^n_j = \frac{1}{\Delta t}(u^{n+1}_j - u^n_j) \), where \( u^n_j \leftarrow \frac{1}{3}(u^{n+1}_{j+1} + u^n_j + u^{n-1}_j) \) (for a better approximation we compute the mean on three values, two in LF original form);
- discretization in space: \( \partial_x u^n_j = \frac{1}{\Delta x}(u^n_{j+1} - u^n_{j-1}) \);

where \( u \) is a velocity component, \( n \) the time step, \( j \) a value on the cartesian coordinate \( x \).
Computational aspects of Lax-Friedrichs schema

For this schema the CFL condition has constant $c = 1$; the Finite Elements method with the same schema for discretization in time has a more restrictive constant $c < 1$.

If $K \in \mathbb{R}^+$, $K \leq \frac{1}{2}$, we can define the norm $\|u\| = K \sup_j |u_j|$; then the modified LF schema is strongly stable: $\|u^n\| \leq \|u^{n-1}\| \forall n \in \mathbb{N}$; hence there is not the blowing up of the numeric solution.

Suppose we want to compute at most 10 snapshots for every second; then, in the hypothesis $v = 50$ cm/sec as the previous example, from

$$v \Delta t \leq h$$

we must use as minimum a grid step $h = 5$ cm.

This case gives $S = 200$, the total flops for 1 minute of simulation is now of order $O(10^8)$ and the occupation of RAM is of order $O(10^{-2})$ GB.

The gain is of order $O(10^2)$.

The grid step $h = 5$ cm is too big for a good resolution of streamlines for flows into the combustion head: for better final results, it can be useful a method based on interpolations of the computed LF values.

Interpolation of trajectories (1)

Every streamline of LF solution is divided into $N$ couples of points, $\{(P_1, P_2), (P_2, P_3), \ldots, (P_{N-1}, P_N)\}$, so that $S = N + 1$.

We use for every couple a cubic polynomial (spline) imposing the following four analytical conditions ($v$ is the LF solution):

- passage at $P_k$ point, $1 \leq k \leq N - 1$;
- passage at $P_{k+1}$ point;
- the first derivative at $P_k$ is equal to $v_k$;
- the first derivative at $P_{k+1}$ is equal to $v_{k+1}$.

In this way we can construct a set of class $C^1$ new trajectories; we want to estimate

1. the overload for finding and valuating all the cubics;
2. the difference compared to the real LF solution of the smaller grid step.
Interpolation of trajectories (2)

For simplicity, consider a single component of a cubic:
\[ s(t) = at^3 + bt^2 + ct + d, \text{ where } 0 \leq t \leq 1; \]
if \( T \) is the \( 4 \times 4 \) matrix
\[
T = \begin{pmatrix}
2 & -2 & 1 & 1 \\
-3 & 3 & -2 & -1 \\
0 & 0 & 1 & 0 \\
1 & 0 & 0 & 0
\end{pmatrix}
\]
and \((p_1, p_2, v_1, v_2)\) is the vector of cartesian coordinates and velocities components of points \( P_1 \) and \( P_2 \), we have
\[(a, b, c, d) = T(p_1, p_2, v_1, v_2).\]

Interpolation of trajectories (3)

We define the \( 4M \times 4M \) global matrix
\[
G = \begin{pmatrix}
T & 0 & \ldots & 0 \\
0 & T & \ldots & 0 \\
\vdots & \ldots & \ddots & \vdots \\
0 & 0 & \ldots & T
\end{pmatrix}
\]
where \( 0 \) is the \( 4 \times 4 \) zero-matrix. Then
- \( G \) is a sparse matrix with density number \( \leq \frac{1}{M} \);
- if \( p = (p_{(1,1)}, p_{(1,2)}, \ldots, v_{(M,1)}, v_{(M,2)}) \), we can compute the cubics, between two points, for all the \( M \) trajectories by the product \( Gp \).
Interpolation of trajectories (4)

The theorric number of flops for computing the coefficients of all the splines is of
order $O(10M^2N)$. If $M = 10^4$ and $N = 10^3$, the total number of flops is $O(10^{12})$.

With a single processor having a clock frequency of $O(1)$ GHz, the total time
can require some hundreds of seconds, a performance not very good for practical
purposes; using

- some mathematical libraries as LAPACK routines with Fortran calls or Matlab environment,
- distributed computation on a multinode cluster,

we have reached a computation time of some tens of seconds.

Example: Matlab has internal Lapack level 3 BLAS routines for fast matrix-
matrix multiplication and treatment of sparse matrices.

Interpolation of trajectories (5)

![Matrix-vector multiplication](image)

Perfomances for a single $Gp$ multiplication using an Intel Xeon 3.2 GHz with
1 MB internal cache: for $M=10^4$ the memory occupied by the sparse version of
$G$ is only $O(10^2)$ KB instead of theorric $O(10^6)$: $G$ can be stored in processor
cache.
Computation of splines values (1)

Now we need a fast method for computing the splines values in a set of parameter ticks with fine sampling.

Let $r \in \mathbb{N}^+$ the number of ticks for each cubic: then the values of the parameter $t$ in these ticks are $(0, \frac{1}{r}, \frac{2}{r}, ..., \frac{r-1}{r}, 1)$; the value of a cubic at $t_0$ is a scalar product:

$$at_0^3 + bt_0^2 + ct + d = (a, b, c, d) \cdot (t_0^3, t_0^2, t_0, 1).$$

Consider the constant $4 \times (r + 1)$ matrix $R$ and the $(M \times 4)$ matrix $C$:

$$R = \begin{pmatrix} 0 & \left(\frac{1}{r}\right)^3 & \cdots & \left(\frac{r-1}{r}\right)^3 & 1 \\ 0 & \left(\frac{1}{r}\right)^2 & \cdots & \left(\frac{r-1}{r}\right)^2 & 1 \\ 0 & \left(\frac{1}{r}\right)^1 & \cdots & \left(\frac{r-1}{r}\right)^1 & 1 \\ 1 & 1 & \cdots & 1 & 1 \end{pmatrix}$$

$$C = \begin{pmatrix} a_1 & b_1 & c_1 & d_1 \\ a_2 & b_2 & c_2 & d_2 \\ \vdots & \vdots & \vdots & \vdots \\ a_M & b_M & c_M & d_M \end{pmatrix}$$

Computation of splines values (2)

Then the $M \times (r + 1)$ matrix $CR$ contains for each row the values of a cubic between two points, for all the trajectories ( eulerian method: computation of all the position and velocity at a fixed instant). The flops for one multiplication are of order $O(Mr)$.

Tests with Xeon 3.2 GHz processor, $M = 10^4$, $r = 10$ and GNU Fortran77 show a time of 0.01 seconds for a multiplication.

With $N = 10^2$, the time for computing the values of all the splines of a single time step is 4.5 seconds (theoric for 3D: $0.01 \times 10^2 \times 3 = 3$ secs).

If $p$ is the number of available processors and $\text{mod}(M, p) = 0$, the computation can be parallelized distributing $\frac{M}{p}$ rows of matrix $C$ to each processor: there is no need of communication among processes.

A version of High Performance Fortran on a SMP system with 4 ItaniumII processors shows a quasilinear speedup for $M$, $N$ of order $O(10^3)$.
Time for computation

These are the total time of computation for the two methods in the case of a cylinder of length $L = 1$ m, a flow with a max. speed $v = 10$ cm/sec, $M = 10^4$, $r = 10$ and 1 minute of real simulation. The space grid is $h = \frac{L}{10N}$.

Estimate of LF+interpolations vs normal LF (1)

But what is the difference between the modified LF solution and normal LF solution?

Consider the one-dimensional case. Let $u=(u_k)$ the solution of normal LF schema with grid step $h$ and initial value $u_0$; $w=(w_m)$ the solution of normal LF schema with grid step $s \times h$, $s \in \mathbb{N}^+$, and initial value $w_0 \subset u_0$; $v=(v_n)$ the solution of modified LF schema obtained by interpolation of $w$ and valuation on $s$ points per cubic; for a cubic, let $v_k$, $k \leq s$, the value of $v$ at $t=\frac{k}{s}$ and $u_k$ the value of $u$ at the corresponding node of the finer grid; $\frac{v\Delta t}{h}$ the CFL number and $N$ the $N$-th time step. Let

$$M_0 = \max_{|m-n|=1} |u_{0,m} - u_{0,n}|$$

Then it is possible to prove this result:

**Theorem 1** If $M_0 > 0$, there are two positive constants $A$ and $B$ such that

$$|v_n - u_n| \leq (A + Bs)M_0 \sum_{i=0}^{N} \left(\frac{v\Delta t}{2h}\right)^i \quad \forall n \in \{\text{grid indexes}\}, \forall N \in \mathbb{N}.$$
Estimate of LF+interpolations vs normal LF  \(2\)

The CFL number \(\frac{\Delta t}{\Delta t_h}\) is usually indicated by \(\lambda v\). From the previous theorem it follows:

**Corollary 1** If \(\lambda v < 2\), then

\[
|v_n - u_n| < \frac{2(A + Bs)M_0}{2 - \lambda v}.
\]

The CFL condition satisfies the hypothesis of the corollary.
Hence, for a realistic solution from the LF+interpolations model, the conditions are:

- a small \((\ll 2)\) CFL number,
- a not too big number \(s\) of valuations for the cubics; note that \(s\) has the inverse logical meaning of the previous \(r\) parameter.

Note that if \(M_0\) is very big, as in the case of very caotic flows, the LF+interpolations solution can be not very realistic.

Estimate of LF+interpolations vs normal LF  \(3\)

Testing the estimate: example for one-dimensional non linear Navier-Stokes equation, \(\lambda v = 1\), \(s = 10\), after \(N = 10^5\) time steps; graphic of the error between LF+interpolations and normal LF solutions.

In this case it can be shown that \(A = 8\), \(B = 2\) is a first, not optimized, approximation for the two constants. The picture shows that the estimate is correct but large.
Conclusions

The numeric LF schema can be modified using the interpolations method so that:

- the time spent on computation is much lower than the time of the LF based on the corresponding finer grid;
- the computation can be parallelized on multiprocessors environment with very reduced need of communication;
- the error on normal LF solution can be estimated and depends on the initial value $u_0$ of the problem;
- the estimate is compatible with CFL condition.

Thanks