Using sparse matrices and splines-based interpolation in computational fluid dynamics simulations

Gianluca Argentini
Laboratorio di Computazione Avanzata
Riello Group, Legnago (VR), Italy

gianluca.argentini@riellogroup.com
Summary

- Position of the computational problem
- The method of splines-based interpolations
- The computation of the splines coefficients
- The computation of the splines values
- A principle of virtual equivalence
- Pros and cons of the method
Numerical problems for burners

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

- computation of fields of temperature, pressure and velocity in the combustion chamber
- correct design of the combustion head for an optimal efficiency of the flame
- computation of all the flows (air, oil, residual gases) in the burner components
- design of the optimal shape for ventilation fans
Limited area meteo model

Two recent floodings by violent meteorological events have induced to consider a service of weather forecasting,

the company has factories in two opposite side of the geographical zone interested by Euganei Hills.

Numerical Weather Prediction: based on mathematical models and numerical resolution of a PDEs system on the atmospheric fluid.

Streamlines over a hill from a raw version of EHLAM, Euganean Hills Limited Area Model.
Computational fluid dynamics

Numerical resolution of a system of PDEs for fluid flows is required:

- Navier-Stokes for velocity and pressure of flows
- diffusion-like equation for temperature field
- conservation law for mass and energy of multiphase fluids, i.e. liquid-gas oil components
- boundary conditions for the geometry of domain, e.g. combustion chamber

The computational model for burners is quite similar to that of NWP

Large use of distributed and parallelized computations on multiprocessor computers
Computational complexity analysis for a flow

**Simple example** for a detailed knowledge of the velocity-field of fluid particles in the combustion chamber, using a *flow-like grid*:

- $M$ 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*: good values are of order $10^3 - 10^4$

Using *finite difference* in a computational grid, for every time step the number of computational flops is of order $10^9$, and from Courant-Friedrichs-Lewy (CFL) condition, the time step must to be very small:

*computation and graphic rendering of one minute of flow is very CPU expensive (some Gflop/s) and RAM consuming (hundreds of Mbytes)*
Mathematical models and software

We have experimented three ways:

1. *commercial software*, based on finite elements method for a numerical resolution of Navier-Stokes equations; in general, the accuracy of solution is good, but the methods are not easy customizable and CPU-RAM expensive;

2. *cellular automata model* for the computation of velocity field, based on C or Fortran programs, very useful for generic geometries but RAM consuming; the treatment of the temperature is difficult;

3. *finite difference schema* for the complete system of equations, based on MATLAB or Fortran programs; the computation of the flow is complete, but for a realistic simulation we must verify CFL condition and stability criteria.
S. Wolfram (1986) has shown the equivalence between some cellular automata for fluids and Navier-Stokes equations. With some simple customized models of cellular automata we have obtained good geometrical description of flows, but we have noticed difficulties on:

1. correct treatment of boundary conditions;
2. computation of the temperature field;
3. huge consumption of CPUs and RAM.

\[ Re \sim k \log \rho \]
Finite difference schema model

PDEs system from Navier-Stokes equations, mass conservation law, first thermodynamics principle, fluid equation of state

unknowns: velocity vector, pressure, density, temperature

a generic shape of a burner component or the orography of a hill require a non-uniform computational grid

FD schema: Lax-Friedrichs (forward in time, centered in space)

*Example of computational complexity for a small simulation.* 3D box 50x25x25 cm, medium scalar velocity of fluid in each cartesian direction of combustion chamber 50 cm/sec, a space resolution of 0.5 cm: *what is a right time-step?* From CFL condition we have

\[
\text{time-step} < 0.5 \text{ cm} / 50 \text{ cm/sec} = 0.01 \text{ sec}
\]

\[O(10^{10}) \text{ flops and } 5 \text{ GB RAM for 1 real minute of simulation}\]
The method of FD and interpolations

Two problems:

1. time-step is too small and generates a lot of non useful snapshots per second;

2. RAM occupation is very large even in the case of limited simulations.

Suppose to accept 10 snapshots/second; from CFL condition we have

\[ \text{min space-step} = 0.1 \text{ sec} \times 50 \text{ cm/sec} = 5 \text{ cm} \]

For realistic resolution of single components and good graphic rendering, this value can be too high: for better final results, we have developed a method based on the interpolation of the computed values of FD solutions; we have experimented that CPUs effort and RAM occupation are lower than in the case of a fine grid simulation, without significant loss in the final resolution.
The method is based on two steps for the graphic rendering of fluid particles trajectories, after the numerical computation of Navier-Stokes or CA model:

1. interpolation by cubic splines of the geometric positions of the particles:

2. fine valuation of every cubic in a suitable set of time values $t_i$: 

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*Phases for interpolations*
Fitting the trajectories

Let $S$ the number of computed velocity vectors in a particle trajectory, $M$ the number of trajectories.

What method for interpolation of speed-points?

- Bezier-like is not realistic for rendering the divergence of velocity field
- Chebychev or Least-Squares-like are too rigid in the case of a customized application
- Polynomial-like is simple but often shows spurious effects as Runge phenomenon, p.e.:

We have obtained better results with a particular splines-based method.
Let $S = 3 \times N$ : a trajectory is divided into $N$ groups, each of 4 points. At every group the points are interpolated by three cubic polynomials imposing four analytical conditions:

- passage at $P_k$ point, $1 \leq k \leq 3$
- passage at $P_{k+1}$ point
- continuous slope at $P_k$ point
- continuous curvature at $P_k$ point

For smooth rendering and for avoiding excessive twisting of trajectories, the cubics $u_k$ are added to the Bezier curve $b$ associated to the four points:

$$v = \alpha b + \beta u_k \quad 0 < \alpha, \beta < 1$$
Finding the splines

We consider $\alpha = \beta = 0.5$

Let $b = As^3 + Bs^2 + Cs + D \ (0 \leq s \leq 1)$ the Bezier curve of control points $P_1,\ldots, P_4$; for every spline

$u_k = at^3 + bt^2 + ct + d \ (0 \leq t \leq 1)$

the coefficients can be computed by the system

$$(a, b, c, d) = T (P_{k+1}, P_k, B, C, 1)$$

(matrix-vector multiplication) where the matrix $T$ is constant:

$$T = \begin{pmatrix} 1 & -1 & -3 & -1 & -6 \\ 0 & 0 & 1 & 0 & 3 \\ 0 & 0 & 2 & 1 & 3 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix}$$
A global matrix for splines

We define the $G$ matrix:

$$G = \begin{pmatrix}
T & 0 & \ldots & 0 \\
0 & T & \ldots & 0 \\
\cdot & \cdot & \ldots & \cdot \\
0 & 0 & \ldots & T \\
\end{pmatrix}$$

($0$ is the $4 \times 5$ zero-matrix)

$G$ is a $4M \times 5M$ sparse matrix with density number $< 1/M$

if $b = (P_{k+1}, P_k, B_1, C_1, 1, \ldots, P_{k+1}, P_k, B_M, C_M, 1)$
we can compute for every two-points group the coefficients of cubic splines for all the $M$ trajectories:

$$\text{coeff} = G \ b$$
Flops and time execution for the splines

The theoretic number of floating point operations for computing the coefficients of all the splines in flow is $O(10 M^2 N)$

in a useful *not too small* simulation the $N, M$ values are of order $10^3 - 10^4$

the total number of flops is $O(10^{12})$

With a processor having a clock frequency of GHz order the total time can require *some hundreds of seconds*, which is a performance not very good for fast graphics; using

- *some mathematical libraries as LAPACK routines (Fortran calls or Matlab environment)*
- *distributed computation on a multinode cluster*

we have reached a computation time of *some tens of seconds*
Computing with Lapack

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

These are the results for single multiplication using 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 theoric $O(10^6)$ KB: $G$ can be stored in the processor cache.
Distributed computing

If we have \( p \) processors, with Mod\((M,p)\)=0, we can run faster the computation of splines distributing \( M/p \) rows of matrix \( G \) to every processor:

- Single Program Multiple Data method
- no communication among processes is involved; there is only a limited overhead for sending the rows of \( G \) to every processor
- tests with a Matlab multi-engine environment

From previous example, using 4 Xeon processors and \( N=10^3 \), the registered execution time for computing all the splines is about 12 seconds \((0.012 * 3 * 10^3 / 4 = 9 \text{ theoric})\):

\[
\text{time}_{\text{execution}} = \text{time}_{\text{cpu}} + \text{time}_{\text{overhead}}
\]
Now we would a fast method for computing the splines values in a set of parameter ticks with fine sampling.

Let $V + 1$ the number of ticks for each cubic spline valuation; then the ticks are $(0, 1/V, 2/V, \ldots, (V-1)/V, 1)$, and the values of parameter in the computation are their $(0, 1, 2, 3)$-th degree powers. The value of a cubic at $t_0$ can be viewed as a dot product:

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

This fact permits to consider a new constant $4 \times (V+1)$ matrix:

$$T = \begin{pmatrix}
0 & (1/V)^3 & \ldots & ((V-1)/V)^3 & 1 \\
0 & (1/V)^2 & \ldots & ((V-1)/V)^2 & 1 \\
0 & (1/V)^1 & \ldots & ((V-1)/V)^1 & 1 \\
1 & 1 & \ldots & 1 & 1
\end{pmatrix}$$
An eulerian view

This is the $M \times 4$ matrix $C$, each row is a spline between two points, and this for all the $M$ trajectories.

Then the $M \times (V+1)$ matrix product $V = C^T$ contains in each row the values of a cubic between two data-points, for all the $M$ trajectories (eulerian method: computation of all the trajectories at a predefined set of time ticks).

The theorinc number of floating point operations for computing all the cubics values for all the trajectories in flow is $O(10 \cdot MVN)$. 
Computing the values of splines

The matrices product is fast with Matlab incorporated Lapack routines: tests with Xeon 3.2 GHz processor, $M=10^4$ and $V=10$ show a time of 0.02 seconds for one multiplication;

if $N=10^2$, the time for computing the values of all the splines of a FD time-step (a snapshot of flow) is $0.02 \times 3 \times 10^2 = 6$ seconds

The black line is a real trajectory from FD computation; the red is the virtual line from splines method.

(at left the line has been shifted; trajectory of a gas particle in combustion chamber exiting from forced ventilation fan)
Assume that the splines method is equivalent to a Finite Difference method with a grid space-step defined by the value of $V$; from CFL:

\[
\text{time-step}_{\text{splines}} = L \times (3N)^{-1} \times s^{-1}, \quad \text{where } L \text{ is the linear length and } s \text{ the scalar speed of flow}
\]

\[
\text{time-step}_{\text{FD}} = L \times (3NV)^{-1} \times s^{-1}
\]

**Example** with $L=3\,\text{m}$, $M=10^4$, $N=10^2$, $s=30\,\text{cm/sec}$, $V=10$;

Report of total execution time (FD computation & graphics) for 1 minute of real simulation, 1 second between two snapshots, with four 3.2 GHz Xeon processors, for the two methods (Matlab parallel multi-engine environment):
Numerical considerations

\[ \text{time}_{\text{splines}} \approx 450 \text{ sec (FDc)} + 4500 \text{ sec (splines)} + 3000 \text{ sec (graphic rendering)} \approx 8000 \text{ sec} \]

\[ \text{RAM}_{\text{splines}} \text{ (total allocation)} \approx 1 \text{ GB for every flow snapshot} \]

\[ \text{time}_{\text{FD}} \approx 8000 \text{ sec (FDc)} + 2000 \text{ sec (graphic rendering)} \approx 10000 \text{ sec} \]

\[ \text{RAM}_{\text{FD}} \text{ (total allocation)} \approx 2 \text{ GB for every flow snapshot} \]

**Example** of graphic output for a \( V=4 \) grid step (\( \sim 2 \text{ mm space-step} \))

red = line from splines method (AB first spline, BC second spline)

black = points from full FD method
Pros and cons

The **spline method**:  

- reduces total time of computation and RAM allocation  
- is easily adaptable for a multiprocessor architecture  
- its graphic rendering gives results comparable with those of FD method  
- *it is limited to the design of particles trajectories and gives no information on other Navier-Stokes variables as pressure, temperature*  
- *it is not useful in the case of very small geometries (the interpolated trajectories can cut the small element of boundary)*  
- *its equivalence with a finer-grid FD method must to be mathematically justified*

Thank you  

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