Towards Parallel CFD computation for the ADAPT framework

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Abstract. In order to run Computational Fluid Dynamics (CFD) codes on large scale infrastructures, parallel computing has to be used because of the computational intensive nature of the problems. In this paper we investigate the ADAPT platform where we couple flow Partial Differential Equations and a Poisson equation. This leads to a linear system which we solve using direct methods. The implementation deals with the MUMPS parallel multi-frontal direct solver and mesh partitioning methods using METIS to improve the performance of the framework. We also investigate, in this paper, how the mesh partitioning methods are able to optimize the mesh cell distribution for the ADAPT solver. The experience gained in this paper facilitates the move to the 3D version of ADAPT and the move to a Service Oriented view of ADAPT as future work.

Keywords: Unstructured mesh, Mesh partitioning, Parallel direct solver, Multi-frontal method, MUMPS, METIS, Multi-physics, Multi-scale and Multilevel Algorithms.

1 Introduction and context of the work

In the last recent decades CFD (Computational Fluid Dynamics) used to play an important role in industrial designs, environmental impact assessments and academic studies. The aim of our work is to fully parallelize an unstructured adaptive code for the simulation of 3D streamer propagation in cold plasmas. As a matter of fact, the initial sequential version of the Streamer code needs up to one month for running typical benchmarks.

The generation of streamer discharges is described by coupling electrostatic to the motion of charged particles (electrons, positive and negative ions). The electrostatic is represented by a Poisson equation for the electric potential and the motion of particles is described by a set of convection-diffusion-reaction equations.

We aim to parallelize both the linear solver issued from the Poisson equation and the evolution equation using domain decomposition and mesh adaptation at 'the same time'. To our knowledge this is the first time that such a challenge
is considered. Intuitively speaking, separating the two steps may add delays because we need to synchronize them and to align the execution time on the slowest processor. Considering the two steps simultaneously offers the potential to better overlap different computational steps.

Other authors have tackled the parallelization of either the linear solvers or the evolution equation usually without mesh adaptation. In [1] the authors consider the parallelization of a linear system of electromagnetic equation on non adaptive unstructured mesh. Their time integration method leads to the resolution of a linear system which requires a large memory capacity for a single processor.

In [2] the authors introduce a parallel code which was written in C++ augmented with MPI primitives and the LIS (Linear Iterative Solver) library. Several numerical experiments have been done on a cluster of 2.40 GHz Intel Xeon, with 12 GB RAM, connected with a Gigabit Ethernet switch. The authors note that a classical run of the sequential version of their code might easily exceed one month of calculation. The improvement of the parallel version is due to the parallelization of three parts of the code: the diagonalization of the Schrödinger matrix, advancing one step in the Newton—Raphson iteration, and the Runge–Kutta integrator.

The authors in [3] focused only on the parallelization of a linear solver related to the discretization of self-adjoint elliptic partial differential equations and using multigrid methods.

It should also be mentioned that authors in [4] have successfully studied similar problems to those presented in this paper. The associated linear systems have been solved using iterative Gmres and CG solvers [5]. One difference is that in our work we consider direct methods based on LU decomposition using the MUMPS solver.

Moreover, the direct solution methods generally involve the use of frontal algorithms in finite element applications. The advent of multi—frontal solvers has greatly increased the efficiency of direct solvers for sparse systems. They make full use of high performance software layers such as invoking level 3 Basic Linear Algebra Subprograms (BLAS) [6,7] library. Thus the memory requirement is greatly reduced and the computing speed greatly enhanced. Multi—frontal solvers have been successfully used both in the context of finite volume, finite element methods and in power system simulations.

The disadvantage of using direct solvers is that the memory size increases much more quickly than the problem size itself. To circumvent this problem, out-of-core multi—frontal solvers have been developed which have the capability of storing objects of the resolution on the disk during factorization. Another viable alternative is to use direct solvers in a distributed computing environment. MUMPS [8,9] is among the fastest parallel general sparse direct solvers available under public domain.

In order to deal with complex geometries and fluid flows, a large number of mesh cells should be used. Therefore the parallel computing paradigm has to be introduced for coping with this large number of mesh cells. In the paral—
In the parallel computing field, several factors, such as the load balancing, the number of neighboring sub-domains and the halo cells (cells which are at the boundary of sub-domains), affect the performance. A well balanced load has the potential to reduce the amount of waiting processors and the partitioning method can optimize the distribution of the mesh cells across processors, thus it will improve the performance of the parallel application too.

In this paper, we also use METIS [10], an open source mesh partitioning software, and we incorporate it into the streamer code of ADAPT [11], to solve the evolution PDE, in order to study the impact of mesh partitioning on the parallel version of ADAPT that we are currently developing.

Moreover we carry out experiments using the parallel multi—frontal direct solver (MUMPS) with matrices extracted from the streamer code of the ADAPT platform. The general strategy is as follows. The linear system of equations is evaluated on different processors corresponding to the local grid assigned to the processor. The right hand side vector is assembled on the host processor and it is injected into the MUMPS solver. At the last step of the MUMPS solver, the solution is assembled centrally on the host processor. This solution is then broadcast to all the processors. We discuss later the pro and cons of such a strategy.

The organization of the paper is the following. In section 2 we introduce the aim of the ADAPT platform and its positioning. In section 3 we discuss about parallel approaches to solve evolution equation coupled with Poisson equation, show the strategy to parallelize our code and do some experiments with METIS. In section 4 we analyze different parts of our code in terms of speedup and efficiency and we provide numerical results that show the efficiency our work. Section 5 concludes the paper.

2 The ADAPT framework

2.1 Overview

ADAPT [11] is an object oriented platform for running numerical simulations with a dynamic mesh adaptation strategy and coupling between finite element and finite volume methods.

ADAPT, as a CFD (Computational Fluid Dynamics) software package, has been developed for realizing numerical simulation on an unstructured and adaptive mesh for large scale CFD applications.

In this paper, in order to tackle the long running time necessary for numerical simulation, we study the MUMPS and METIS toolkits and we integrate them into the ADAPT framework. In fact we perform code coupling between the two main steps of the studied problem.

The existing ADAPT implementation is a sequential C++ code for each phenomenon, and the code requires a huge CPU time for executing a 3D simulation. For example, the 3D streamer code may run up to 30 days before returning results, for this reason we decided to parallelize the code. This paper is an important step into this direction.
2.2 Working environment

To realize all the experiments (sequential and parallel) we worked on the MAGI cluster\footnote{http://www.univ-paris13.fr/calcul/wiki} which is located at the University of Paris 13, and also on the Ada cluster of Idris\footnote{http://www.idris.fr}, one of the national computing facility in France.

3 Parallel approach

In this paper, we parallelize the evolution equation coupled with the Poisson equation, written as:

\[
\begin{align*}
\frac{\partial u}{\partial t} + F(V,u) &= S, \\
\Delta P &= b.
\end{align*}
\]

(1)

given that \( F(V,u) = \text{div}(u\vec{V}) - \Delta u \), \( S = 0 \), and \( V = \nabla P \), the previous system gives:

\[
\begin{align*}
\frac{\partial u}{\partial t} + \text{div}(u\vec{V}) &= \Delta u, \\
\Delta P &= b.
\end{align*}
\]

(2)

The first equation is discretized using the finite volume method on an unstructured triangular mesh. The time-integration of the transport equation is performed using an explicit scheme. The discretized form of Poisson equation leads to a linear algebraic system. We obtain the following set of equations:

\[
\begin{align*}
\pi^n + 1 &= \pi^n - \frac{\Delta t}{\mu_i} \sum_{j=1}^{m} u_{ij} \vec{V}_{ij} \vec{n}_{ij} |\sigma_{ij}| + \frac{\Delta t}{\mu_i} \sum_{j=1}^{m} \nabla u_{ij} \vec{n}_{ij} |\sigma_{ij}| \\
&\quad \quad \text{Rez}_{\text{conve}} \quad \quad \text{Rez}_{\text{dissip}} \\
A\vec{P}^n &= \vec{b}^n
\end{align*}
\]

(3)

where \( m \) is the number of faces of volume \( \mu_i \), \( \vec{n}_{ij} \) is the unit normal vector of the face \( \sigma_{ij} \) (face between volumes \( \mu_i \) and \( \mu_j \)) and \( |\sigma_{ij}| \) is its length. Other variables denoted by subscript \( ij \) represent variables on the face \( \sigma_{ij} \).

A is a large sparse matrix, the coefficients of the matrix depend only on the grid topology.

**Computation of \( u_{ij} \):** In figure\footnote{http://www.idris.fr} we took the example when the mesh is splitted into two subdomains, and we compute \( u_{ij} \) on the face \( \sigma_{ij} \). For a given face \( \sigma_k \), suppose \( T_i \) and \( T_j \) are respectively the cells at the left and right of \( \sigma_k \). Let’s note \( \sigma_k = \sigma_{ij} \) and \( u_k = u_{ij} \). The algorithm\footnote{http://www.idris.fr} shows how the \( u_{ij} \) is computed on face \( \sigma_{ij} \).
**Algorithm 1**: Compute \( u_{ij} \) on face \( ij \)

1. F: number of faces;
2. for \( k := 1 \) to \( F \) do
3.  if \( \text{dot}(V_k.n_k) \geq 0 \) then
4.     \( u_k = u_i \);
5.  end
6.  else
7.     if \( \sigma_k \) is inner faces then
8.         \( u_k = u_j \);
9.     end
10.    else if \( \sigma_k \) is halo faces then
11.         \( u_k = u_h \); /* \( u_h \) : halo value sent by neighbor subdomain */
12.    end
13.  end
14. end

**Computation of \( \nabla u_{ij} \)**: In figure 3 we take the same mesh, and we compute \( \nabla u_{ij} \) of the face \( \sigma_{ij} \). The algorithm 2 shows how the \( \nabla u_{ij} \) is computed on volume \( \mu_{ij} \).

The diamond cell in \( 2 \) is constructed by connection of centers of gravity \((i, j)\) of cells \( T_i, T_j \) which shares the face \( \sigma_{ij} \) and its endpoints \( A, B \).

\[
\nabla u_{ij} = \frac{1}{2\mu(D_{\sigma_{ij}})}[(u_A - u_B)\vec{n}_{LR}\sigma_{LR} + (u_j - u_i)\vec{n}_{ij}\sigma_{ij}] \quad (4)
\]

**Computation of the linear system**: The system is solved directly by LU decomposition with an implementation for sparse matrices. We use the Intel MKL library\(^2\) solvers and UMFPACK\(^\text{12}\).

Note that in traditional approaches, one splits the mesh to solve both the evolution equation and the linear system in each sub-domain using iterative methods with added communications. In our work we use the same methodology in partitioning the mesh but the linear system is solved with a direct method.

\(^2\) https://software.intel.com/en-us/intel-mkl#pid-3374-836
Algorithm 2: Compute value at node \( u_{\text{node}} \)

\[
\begin{align*}
1 & \quad u_{\text{node}}: \text{double}; \\
2 & \quad N : \text{number of nodes}; \\
3 & \quad \text{Alpha} : \text{weight coming from the least square method}; \\
4 & \quad \text{for } n:=1 \text{ to } N \text{ do} \\
5 & \quad \quad \text{for } c:=1 \text{ to inner cells around node } n \text{ do} \\
6 & \quad \quad \quad u_{\text{node}}(n)+ = \text{Alpha} * u_j(c); \\
7 & \quad \quad \text{end} \\
8 & \quad \quad \text{for } m:=1 \text{ to halo cells around node } \text{do} \\
9 & \quad \quad \quad u_{\text{node}}(n)+ = \text{Alpha} * u_h(m); \\
10 & \quad \quad \text{end} \\
11 & \quad \text{end} \\
12 & \quad \text{return } u_{\text{node}}; 
\end{align*}
\]

Fig. 3: Computation of \( \nabla u_{ij} \) in mesh splitted into two subdomains
Algorithm 3: Compute $\nabla u_{ij}$ on face $ij$

1. $F$: number of faces;
2. $\nabla u$: Vector2d;
3. for $k := 1$ to $F$ do
   4. $A$: first node of face;
   5. $B$: second face node;
   6. $i$: center of gravity of cell $T_i$;
   7. $j$: center of gravity of cell $T_j$;
   8. $mes = \frac{1}{2} \mu (D_{ij})$;
   9. if Inner faces then
      10. $\nabla u(k) = mes \times (u_{node}(A) - u_{node}(B)) \nabla LR|\sigma_{LR}| + (u_j - u_i) \nabla T_{ij}|\sigma_{ij}|$;
   11. end
   12. else if Halo faces then
      13. $\nabla u(k) = mes \times (u_{node}(A) - u_{node}(B)) \nabla LR|\sigma_{LR}| + (u_h - u_i) \nabla T_{ih}|\sigma_{ih}|$;
   14. end
15. end
16. return $\nabla u$;

Parallelization: For the parallelization of CFD simulations, ADAPT employs the domain decomposition method. The 2D unstructured mesh in Figure 4 was decomposed into eight subdomains using the METIS algorithm, these partitions have approximately the same size that we may consider as a good property because the workload will be balanced on the homogenous processors of our platform.

Algorithm 4 on page 10 provides with a piece of pseudocode that shows how the parallelization is done in the streamer code according to the coupling of
evolution equation with Poisson equation. We can see that most parts of the
code are parallel ones (line 19, line 9 to 11 and line 22 to 26) except reading
and splitting mesh in the beginning and between lines 14 and 15. Indeed, at this
step, we construct matrix $A$ (eq. 2) that will be used to solve the linear system
in line 19. Matrix $A$ is computed one time because it depends only on the mesh.

Our contribution will serve in the future to tackle the 3D version of streamer
which includes the same type of equations, same strategy to solve the linear
system. The difference is the structure of the grid because we will work with
Tetrahedra instead of triangles, which will make the problem much more com-
plcicated due to big differences in handling the mesh in the 3D case.

Algorithm 4: Algorithm of parallel ADAPT

\begin{verbatim}
W:double;
if rank==0 then /* for the master processor */
  Read mesh data;
  Split mesh with METIS;
  Distribute mesh to all processors;
end
W=0;
for each rank do /* for each processor */
  Initialize conditions and create constants;
  Send the informations of halos cells to neighbor subdomains;
  Apply boundary conditions;
end
if rank==0 then
  Construct matrix of linear system;
  Split the matrix and send part of each processor;
end
for each iteration do
  for all rank do /* for all processors */
    Solve linear system using MUMPS;
  end
  for each rank do
    Send the informations of halos cells to neighbor subdomains;
    Apply boundary conditions;
    Compute fluxes of convection, diffusion and source term;
    Update solution :
      $W^{n+1} = W^n + \Delta t * (rez\_conv + rez\_dissip + rez\_source)$;
  end
  Save results in parallel way using Paraview;
end
\end{verbatim}
4 Application to streamer equations

When non-ionized or low ionized matter is exposed to high intensity electric field, non-equilibrium ionization processors (so-called discharges or streamers) occur. Because of the reactive radicals they emit, streamers are used for the treatment of contaminated media like exhaust gasses, polluted water or bio-gas.

4.1 The governing equation

The streamer consists of a convection-diffusion-reaction for the electron density, an ordinary differential equation for the positive ion density coupled by the Poisson’s equation for the electric potential. The model is given by the following equations:

\[
\frac{\partial n_e}{\partial t} + \text{div}(n_e \vec{v}_e - D_e \vec{\nabla} n_e) = S_e, \tag{5}
\]

\[
\frac{\partial n_i}{\partial t} = S_e, \tag{6}
\]

\[
\Delta V = -\epsilon \left( n_i - n_e \right), \tag{7}
\]

\[
\vec{E} = -\vec{\nabla} V, \tag{8}
\]

Where \( V \) is a potential of electric field \( E \), \( \epsilon \) is the dielectric constant, \( e \) the electron charge, \( n_e \) and \( n_i \) are the number densities of electrons and positive ions, the drift velocity of electrons is \( v_e = v_e(E) \) and \( D_e = D_e(E, v_e) \) is the diffusion coefficient. The source terms depend on the electron drift velocity and the electron density \( S_e = S_e(v_e, n_e) \).

4.2 Numerical method

The equations of the model are discretized using the finite volume method on an unstructured triangular mesh. The time-integration of the transport equations is performed using an explicit scheme. The discretized form of Poisson’s equation consists of a linear algebraic system that is solved with a direct method at each time step during the time-integration. We approximate the equation for the electron density (eq. 3) by the following finite volume method:

\[
\frac{\partial n_e}{\partial t} + \frac{1}{\mu(T)} \int_{\partial T} (n_e \vec{v}_e - D_e \vec{\nabla} n_e) \vec{n} \, ds = S_e \tag{9}
\]

where \( \mu(T) \) is the volume of the cell \( T \), \( \vec{n} \) the outward unit normal vector to the faces of the cell \( T \).

The Poisson’s equation (eq. 5) is discretized by a central type approximation which leads to a system of linear equation, as follows:

\[
A_n \vec{V}^{n+1} = \vec{b}^{n+1} \tag{10}
\]
A is a matrix of coefficients, $\vec{V}$ is a vector of unknowns (its dimension is equaled to the total number of cells) and $\vec{b}$ is a vector of right hand side.

### 4.3 Parallel results

Table 1 summarize our results. The speedup in this example shows a good scalability of the present method for solving the convection-diffusion equation coupled with Poisson equation problems using mesh with 529240 cells. For practical applications, the computation time could be reduced from 49h54min (one computing core) down to 5min (1024 computing cores). This test is made on MAGI cluster at Paris13.

| Compute cores | Total          | Convection     | Diffusion      | Linear solver     |
|---------------|----------------|----------------|----------------|-------------------|
| 1             | 49 h 54 min 48 s | 02 h 51 min 04 s | 13 h 06 min 00 s | 33 h 57 min 44 s  |
| 2             | 25 h 06 min 27 s | 01 h 22 min 57 s | 06 h 41 min 02 s | 17 h 02 min 27 s  |
| 4             | 12 h 34 min 35 s | 00 h 42 min 07 s | 03 h 22 min 04 s | 08 h 30 min 24 s  |
| 8             | 06 h 27 min 18 s | 00 h 22 min 13 s | 01 h 46 min 26 s | 04 h 18 min 38 s  |
| 16            | 03 h 39 min 45 s | 00 h 12 min 37 s | 01 h 01 min 40 s | 02 h 25 min 26 s  |
| 32            | 01 h 50 min 50 s | 00 h 08 min 03 s | 00 h 29 min 17 s | 01 h 13 min 29 s  |
| 64            | 01 h 01 min 41 s | 00 h 03 min 59 s | 00 h 17 min 05 s | 00 h 40 min 36 s  |
| 128           | 00 h 32 min 44 s | 00 h 01 min 52 s | 00 h 08 min 22 s | 00 h 22 min 29 s  |
| 256           | 00 h 18 min 16 s | 00 h 01 min 02 s | 00 h 04 min 34 s | 00 h 12 min 39 s  |
| 512           | 00 h 10 min 07 s | 00 h 00 min 33 s | 00 h 02 min 52 s | 00 h 06 min 42 s  |
| 1024          | 00 h 05 min 14 s | 00 h 00 min 18 s | 00 h 01 min 33 s | 00 h 03 min 23 s  |

**Scalability measurement:** There are two basic ways to measure the scalability of parallel algorithms:

(a) Strong scaling with a fixed problem size but the number of processing elements are increased.
(b) Weak scaling with problem size and compute elements increasing concurrently.

The speedup is defined as

$$sp = \frac{t_b}{t_N},$$

and the ideal speedup, $sp_{ideal}$, is naturally equivalent to the number of compute cores. Therefore, the strong scaling efficiency can also be calculated by

$$s_p \frac{sp}{sp_{ideal}}.$$
which shows how far is the measured speedup from the ideal one.

In this work, the strong scaling measurement is employed and the scaling efficiency is calculated by:

$$\frac{t_b N}{t_N N_b} \times 100, \quad N \geq N_b$$

where \(t_b\) is the wall clock time of a base computation, \(N_b\) is the number of compute cores used for the base computation, \(t_N\) is the wall clock time of a computation with \(N\) compute cores.

Figures 5 and 6 illustrate the speedup and the strong scaling efficiency in the computations of our illustrate example with \(t_b\) the wall clock times by one compute core. A more detailed injection into the data of this example provides interesting information about the computational efficiency of the individual parts of the parallel simulation. The results of the strong scaling tests, plotted in Fig 6, depict that the parallel speedup of the different parts increases up to 1024 computational cores, so our parallel strategy shows its efficiency.

![Fig. 5: Speedup of different parts of streamer code using mesh with 529240 cells](image)

**4.4 Comparison between sequential and parallel code**

In Figure 7 a comparison is made between sequential 2D streamer code and parallel counterpart. We can also observe the propagation of streamer in two cases:
Fig. 6: Efficiency of different parts of streamer code using mesh with 529240 cells

Fig. 7: Plasma discharge in sequential code (left) and parallel one (right)

| Mesh configuration           | Compute cores | Execution time     |
|------------------------------|---------------|--------------------|
| Mesh using 43674 elements    | 1             | 4h30min            |
| Mesh using 529240 elements  | 1, 64         | 150h15min, 03h59min|

Table 2: Comparison between sequential and parallel code
more the mesh is fine more the results are accurate (without oscillations). In table 2, the parallel code takes the same running time (using 64 MPI processors) as the sequential code but the input size is 12 times greater.

To conclude, our strategy although not classical shows to be very efficient, and provides with relevant properties regarding performance.

5 Conclusions and future work

In this work, we have introduced an effective parallelization of the ADAPT platform for CFD applications. We present the parallelization of the convection-diffusion equation and the linear system. The originality of this work is to solve linear system using a direct method whereas existing studies mainly use iterative methods to solve linear system in this kind of problems. The workflow is realized: (1) using external tools such as METIS for mesh partitioning in order to enable the computational load balance for the global assembly, (2) using MPI to assure communication, (3) using MUMPS solver to solve the system of linear equations. The current approach with MUMPS shows significant advantages in terms of avoiding the problems of pre-conditioners, and doesn’t need a lot of iterations to converge to the solution. In summary, the most important advantages of the presented scheme are:

- Efficient memory usage distribution over computer nodes,
- Good scalability to solve convection-diffusion equation,
- Stable, fast and good scalability of linear solvers provided by MUMPS.

We observe that the campaign of numerical tests provides expected results, meaning that our parallel implementation goes into the right direction at the moment.

For the future, we plan to investigate in depth the mesh partitioning problems and to conduct experiments with specific tools. We may target PAMPA [13] and the question is how such tool can impact the overall performance of ADAPT software. The challenge is to mix mesh partitioning and dynamic mesh adaptations. How to manage load balancing in this context? When dealing with three dimensional problems, the question is even more critical. At least, as explained in the discussion section our current work will serve for solving 3D streamer problems and a service oriented view of the ADAPT framework.

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