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Multirate time advancing for high Reynolds LES

E. Itam*, B. Koobus*

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*I3M, Université de Montpellier, Montpellier, France
emmanuelle.itam@univ-montp2.fr, koobus@math.univ-montp2.fr

Abstract

A new multirate scheme based on control volume agglomeration is proposed for the solution of the compressible Navier-Stokes equations possibly equipped with turbulence models. The method relies on a prediction step where large time steps are performed with an evaluation of the fluxes on macro-cells for the smaller elements for stability purpose, and on a correction step in which small time steps are employed only for the smaller elements.

Keywords: Multirate time advancing, volume agglomeration, explicit scheme, unstructured grid, bluff body flow, compressible Navier-Stokes equations.

1 Introduction

A frequent configuration in mesh adaptation combines an explicit time advancing scheme for accuracy purpose and a computational grid with a very small portion of much smaller elements than in the remaining mesh. Examples of such situations are isolated traveling shock and large eddy simulation of high Reynolds number flows around bluff bodies where very thin boundary layers and vortices of much more important size need to be captured.
For such configurations, explicit time advancing schemes with global time stepping are too costly. In order to overcome this problem, the multirate time stepping approach represents an interesting alternative. The objective of such schemes, which allow to use different time steps in the computational domain, is not to penalize the advancement in time of unsteady solutions through the use of small global time steps imposed by the smallest elements such as those constituting the boundary layers.
Numerous works were made on multirate methods in the field of ODE, see for example [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12], but only few works were conducted on multirate time advancing schemes for the solution of PDE and hyperbolic conservation laws [13, 14, 15, 16, 17, 18], and rare applications were performed in Computational Fluid Dynamics (CFD) [17, 18]. Therefore, there is still much work to do to provide a viable multirate method for CFD applications. In this work, we propose a new multirate scheme based on control volume agglomeration which is well suited to our numerical framework using a mixed finite volume/finite element formulation. The method relies on a prediction step where large time steps are used with an evaluation of the fluxes performed on the macro-cells for the smaller

elements, and on a correction step in which small time steps are employed only for the smaller elements. Target applications are three-dimensional unsteady flows modeled by the compressible Navier-Stokes equations equipped with turbulence models and discretized on unstructured possibly deformable meshes.

2 Multirate time advancing by volume agglomeration

In this section, we present the multirate time advancing scheme based on volume agglomeration which is currently developing for the solution of the three-dimensional compressible Navier-Stokes equations.

We first define the inner zone and the outer zone, the coarse grid, and the construction of the fluxes on the coarse grid, ingredients on which our multirate time advancing scheme is based.

- **Definition of the Inner and Outer zones** :
  - Let Δt be the global time step over the computational domain
  - We define the **outer zone** as the set of cells for which the explicit scheme is stable for a time step $K\Delta t$ ($K \in \mathbb{N}^*$), and the **inner zone** as its complement
  - These zones are defined through the local time steps computed on each node.

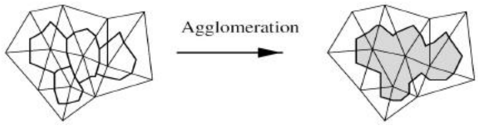
- **Definition of the coarse grid** :
  - **Objective** :
    * Advancement in time is performed with time step $K\Delta t$
    * Advancement in time preserves accuracy in the outer zone (space order of 3, Runge-Kutta 4)
    * Advancement in time is consistent in the inner zone
  - The **coarse grid** is defined as the set of the macro cells in the inner zone union the set of the fine cells in the outer zone
  - **Method** :
    * We advance in time the chosen explicit scheme (Runge-Kutta 4 for exemple) on the coarse grid with $K\Delta t$ as time step
    * A fluxes smoothing can be performed on the macro cells for stability purpose.

- **Construction of the flux on the coarse grid**
  - The nodal fluxes Ψ_i are assembled on the fine cells (as usual)
  - Fluxes are summed on the macro cells I (inner zone) :

$$\Psi^I = \sum_{k \in I} \Psi_k$$

  - Possibly smoothing of the coarse flux (inner zone) :

$$\Psi^I = (\sum_{K \in \mathcal{V}(I)} \Psi^K vol^K)/(\sum_{K \in \mathcal{V}(I)} vol^K)$$



fine cells i   macro cell I

The multirate algorithm is then based on a **prediction step** and a **correction step** as defined hereafter :

Step 1 (prediction step) :
The solution is advanced in time with time step $K\Delta t$, using a Runge-Kutta explicit scheme for example, on the macro cells in the inner zone and on the fine cells in the outer zone :
For $\alpha = 1, RKstep$

$$\begin{array}{lll} \text{outer zone :} & vol_i w_i^{(\alpha)} & = vol_i w_i^{(0)} \ + \ b_\alpha K\Delta t \ \Psi_i^{(\alpha-1)} \\ \text{inner zone :} & vol^I w^{I,(\alpha)} & = vol^I w^{I,(0)} \ + \ b_\alpha K\Delta t \ \Psi^{I,(\alpha-1)} \\ & w_i^{(\alpha)} \ = \ w^{I,(\alpha)} & \text{for } i \in I \end{array}$$

EndFor α.

Step 2 (correction step) :

- The unknowns are frozen in the outer zone
- These unknowns (in the outer zone) are interpolated (those useful for the next point)
- In the inner zone, using these interpolated values, the solution is advanced in time with the chosen explicit scheme and time step Δt
- The complexity, proportional to the number of points in the inner zone, is mastered.

3 Application

The multirate algorithm introduced in the previous section was implemented in the parallel CFD code AIRONUM shared by INRIA Sophia-Antipolis, LEMMA company and university of Montpellier. Special attention was paid to issues related to parallelism, and in particular to the evaluation of the fluxes on the macro cells located at the boundary between neighboring subdomains.

As a very first application of our multirate approach, the tandem cylinders benchmark at Reynolds number 1.66×10^5 is considered. This test case is challenging since several complex flow features need to be captured around multiple bodies (stagnation zones, boundary layers, shear layers, separations, laminar-turbulent transition, recirculations, vortex sheddings, wakes). Furthermore, small cells are necessary for a proper prediction of the very thin boundary layers, which implies very small global time steps so that classical explicit calculations become very costly. The application of our multirate scheme to the tandem cylinders benchmark is also made more difficult by the fact that we use a hybrid turbulence model based on RANS and VMS-LES approaches, so that additional equations associated with turbulent variables need to be advanced in time.

The instantaneous vorticity field around the tandem cylinders predicted by our hybrid RANS/VMS-LES model is depicted in Figure 1. The Q-criterion isosurfaces are shown in Figure 2. Both Figures illustrate the complex flow features and the very small structures that need to be captured by the numerical model and the turbulence model, which renders this simulation particularly challenging.

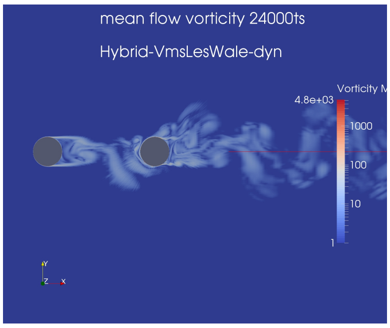


Figure 1: Tandem cylinders at Reynolds number 1.66×10^5 : instantaneous vorticity field.

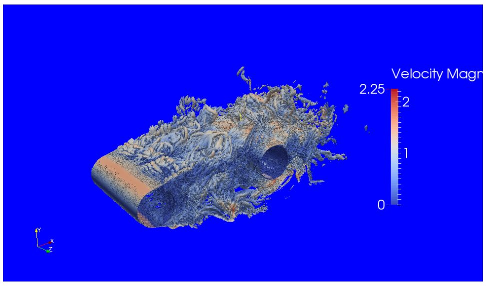


Figure 2: Tandem cylinders at Reynolds number 1.66×10^5 : instantaneous Q-criterion isosurfaces.

Two meshes were used for this study : a coarse mesh which contains 2.6 million nodes and 15 million tetrahedra, and a fine mesh with 16 million nodes and 96 million tetraedra.

Coarse mesh :

The computational domain is decomposed into 192 subdomains. When integer K, used for the definition of the inner and outer zones, is set to 2, 5 and 10, the percentage of nodes located in the inner zone is 4%, 16% and 25%, respectively.

The lift curve obtained by the multirate scheme with $K = 10$ and the explicit scheme corresponding to half of a period of vortex shedding for the first cylinder is given in Figure 3. The underlying explicit scheme is the 4-stage Runge-Kutta method and the CFL number was set to 1. Each simulation was left running over an elapsed time of 40 hours. A number of 192 cores on a BULL cluster was used to perform these computations. One can check that the response given by the two schemes is the same, as expected, except for the oscillations at the top of the lift curve for the multirate method that are due to a not properly controlled restart in the simulation. The number of time steps is 15284 for the multirate scheme and 132531 for the classical explicit scheme. From Figure 3, an improvement in the efficiency of about 14% is observed when the multirate scheme is used in our parallel solver. This rather slight improvement in efficiency can be explained by the fact that some of the subdomains almost contain only inner nodes so that workload is not equally shared by each computer core when the proposed multirate approach is used. Indeed, in our parallel strategy which is based on a decomposition of the computational domain in subdomains, designed to minimize the inter-core communications, and on a message passing parallel programming (MPI) model, each subdomain is assigned to a computer core. It is clear that in order to further increase the efficiency of the multirate approach in our parallel computing framework, the domain decomposition needs to be adapted.

Based on the fact that the cost per node in these explicit simulations is essentially due to the computation of the convective and diffusive fluxes, we can deduce that, for the multirate simulation that was performed and which involves $K = 10$ and 25% of the nodes located in the inner zone, the benefit-cost ratio between the multirate scheme and the classical 4-stage Runge-Kutta method would be 3 from a sequential point of view.

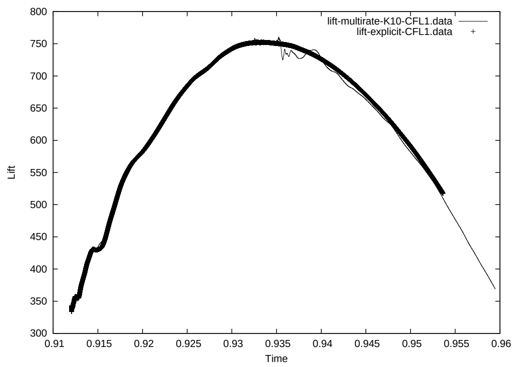


Figure 3: Coarse mesh - Tandem cylinders at Reynolds number 1.66×10^5 : lift curve for the first cylinder, multirate scheme (K=10) and explicit RK4 scheme, corresponding to an elapsed time of 40 hours.

In a second step, the multirate simulation is carried out with K=5 for the same benchmark, which means that the RK4 scheme is now performed with time steps $5\Delta t$ and Δt for the nodes located in the outer zone and the nodes located in the inner zone, respectively. The lift curve obtained by the multirate scheme with $K = 5$ and $K = 10$ for the first cylinder is depicted in Figure 4. Both simulations were left running over an elapsed time of 20 hours, which allows to simulate a quarter of a period of vortex shedding with a CFL number set to 1. One can notice that the response is similar, as expected, for both values of K, and that the efficiency is improved by 8.8% when the multirate scheme is used with $K = 10$ in our parallel solver. From a sequential point of view, we can also deduce that the cost of the multirate scheme with $K = 5$ and $K = 10$ would be of the same order.

Fine mesh :

The computational domain is decomposed into 768 subdomains. When integer K, used for the definition of the inner and outer zones, is set to 5, 10 and 20, the percentage of nodes

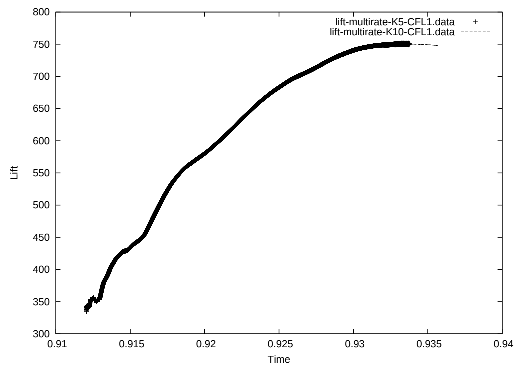


Figure 4: Coarse mesh - Tandem cylinders at Reynolds number 1.66×10^5 : lift curve for the first cylinder, multirate scheme with K=5 and K=10, corresponding to an elapsed time of 20 hours.

located in the inner zone is 18%, 24% and 35%, respectively.

The lift curve obtained by the multirate scheme with $K = 5$, $K = 10$, and $K = 20$, and by the explicit scheme, is shown in Figure 5. The underlying explicit scheme is the 4-stage Runge-Kutta method and the CFL number was set to 1. Each simulation was left running over an elapsed time of 1 hour. A number of 768 cores on a BULL cluster was used to perform these computations.

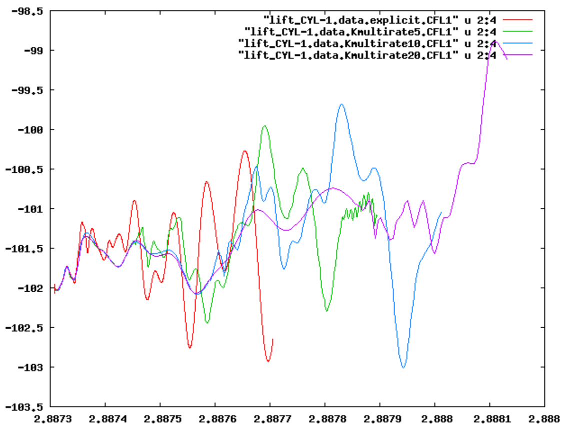


Figure 5: Fine mesh - Tandem cylinders at Reynolds number 1.66×10^5 : lift curve for the first cylinder, multirate scheme ($K = 5$, $K = 10$, $K = 20$) and explicit RK4 scheme, corresponding to an elapsed time of 1 hour.

One can observe that the lift curves quickly become different between the various options because of differences in the time step size and the rapidly fluctuating small scales that can be captured by this fine mesh. These differences affect the instantaneous solution but should not affect the flow statistics. From this Figure, an improvement in the efficiency of a factor slightly greater than 2 is observed when the multirate option is used with $K = 20$

compared to the classical 4-stage Runge-Kutta explicit scheme. For $K = 5$ and $K = 10$ this improvement becomes 1.5 and 1.8, respectively (see Figure 6). The better efficiency observed with the fine mesh compared to the coarse mesh is certainly due to a better distribution of the workload among the cores when the multirate approach is used.

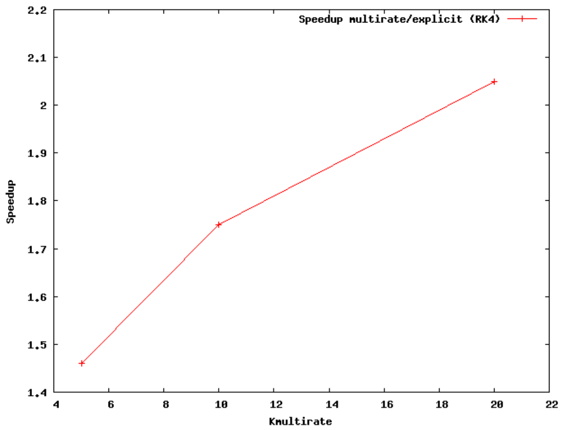


Figure 6: Fine mesh - Tandem cylinders at Reynolds number 1.66×10^5 : speedup multirate/explicit (RK4)

As for the coarse mesh, the benefit-cost ratio between the multirate scheme and the classical 4-stage Runge-Kutta method would be 3 from a sequential point of view.

4 Conclusion

A new multirate strategy is proposed in this work. The method is based on control volume agglomeration, and relies on a prediction step where large time steps are used and where the fluxes for the smaller elements are evaluated on macro cells for stability purpose. A correction step follows in which only the smaller elements are advanced in time with a small time step. Preliminary results are given which show that the proposed multirate strategy can be applied in complex CFD problems such as the prediction of three-dimensional flows around bluff bodies with complex hybrid turbulence models. Nevertheless, there is still work to do to obtain an efficient multirate method in a parallel numerical framework. Indeed, we need to improve the domain decomposition into subdomains, which is at the present time designed to minimize the inter-core communications, so that workload becomes (almost) equally shared by each computer core when the proposed multirate strategy is used.

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