I3M-Montpellier - ANR MAIDESC

Bruno Koobus*

(∗) I3M, Université Montpellier 2, France

Réunion MAIDESC - 9 avril 2014 - INRIA Roquencourt

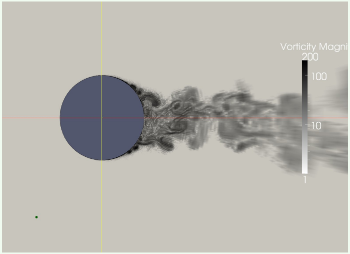
I3M - current work

- Test cases
- Multirate time-advancing
- A third order space-accurate scheme : CENO

Test cases

Test case 1

Circular cylinder at Reynolds 1M : three-dimensional flow with thin boundary layers, unsteady separated shear layers and vortex shedding.



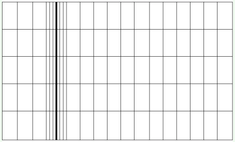
Circular cylinder (1.2M nodes), iso-contours of the vorticity magnitude.
Reynolds number = 1M, Mach number = 0.1, RANS/VMS-LES hybrid model.

$\Longrightarrow$ Evaluation of the performance of the multirate scheme, and CENO (and turbulence modeling...).

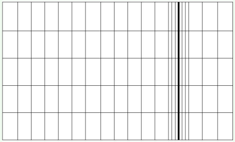
Test cases

Test case 2

Simulation of a moving contact discontinuity followed by the mesh (uniform pressure, uniform velocity, different density) with an ALE formulation :



time t1



time t2 > t1

$\Longrightarrow$ Evaluation of the efficiency of the multirate scheme.

Multirate schemes

Introduction

Many physical phenomena show multiple scales which require locally-refined meshes (with possibly mesh adaption), but **the time step required by the smallest details should not be applied to the larger details**. The **multirate time-advancing approach**, which allows to use **different time steps in the computational domain**, is a way to overcome this problem.

Some work has been made on these methods in the field of ODE (mostly) and PDE, but only few applications have been carried out in CFD...

The objective for Montpellier and INRIA Sophia-Antipolis is to **develop and implement a multirate scheme in the parallel scalable LES solver AIRONUM**. Test cases 1 and 2 will be used to assess the effectiveness of the proposed multirate approach.

Multirate schemes

Several methods for integrating stiff ODE

To speed-up numerical integration of ODE (including those deriving from the method of lines in PDE), three research directions have been followed in the last decades :

- **Multi-method schemes** : different integration schemes used for the stiff and non-stiff part of the solution.
- **Multi-order schemes** : same explicit method and same step size, but the order of the method is chosen according to the stiffness level of the solution.
- **Multirate schemes** : the same explicit or implicit method, with the same order, is applied to the solution, but the step size is chosen according to the stiffness level of the solution.
  Remark : Multirate and multi-method schemes can be mixed.

Multirate schemes

Works since 1960...

Rice (1960), Andrus (1979), Osher-Sanders (1983), Gear-Wells (1984), Löhner-Morgan-Zienkiewicz (1984), Rentrop (1985), Byrne-Hindmarsh (1987), Skelboe (1989), Jorgen-Skelboe (1992), Andrus (1993), Günther-Rentrop (1993), Biesiadecki-Skeel (1993), Ven-Niemann-Tuitman-Veldman (1997), Engstler-Lubich (1997), Maurits-Ven-Veldman (1998), Günther-Kvaerno-Rentrop (1999), Kvaerno-Rentrop (1999), Kato-Kataoka (1999), Skelboe (2000), Günther-Kvaerno-Rentrop (2001), Dawson-Kirby (2001), Bartel-Günther (2002), Kirby (2002), Logg (2003, 2004), Guennouni-Verhoeven-Maten-Beelen (2004), Piperno (2005), Savcenco-Hundsdorfer-Verwer (2007), Savcenco (2007), Constantinescu-Sandu (2007, 2008), Savcenco-Mattheij (2008), Schlegel-Knoth-Arnold-Wolke (2008), Jansson-Log (2008), Ly (2008), Debreu-Blayo (2008), Faille-Nataf-Willien-Wolf (2009), Constantinescu-Sandu (2009, 2010), Mugg (2012), Fok-Rosales (2012), Seny-Lambrechts-Comblen-Legat-Remacle (2012), Dawson-Trahan-Kubatko-Westering (2013).

Multirate schemes

Base integration methods to solve $\dot{y} = f(t,y)$

- **Linear multistep methods** (including one-step methods as degenerate cases) :

$$y_n = \sum_{i=1}^{K_1} \alpha_i y_{n-i} + h \sum_{i=0}^{K_2} \beta_i \dot{y}_{n-i}$$

where y_n approximates $y(t_n)$, $h = t_n - t_{n-1}$ and $\dot{y}_j = f(t_j, y_j)$

- **BDF methods** $(K_2 = 0, K_1 = q)$: $y_n = \sum_{i=1}^{q} \alpha_i y_{n-i} + h\beta_0 \dot{y}_n$
- **Adams methods** :

  - **explicit** of order q $(K_1 = 1, \alpha_1 = 1, K_2 = q-1, \beta_0 = 0)$: $y_n = y_{n-1} + h \sum_{i=1}^{q-1} \beta_i \dot{y}_{n-i}$

  - **implicit** of order q $(K_1 = 1, \alpha_1 = 1, K_2 = q-1)$: $y_n = y_{n-1} + h \sum_{i=0}^{q-1} \beta_i \dot{y}_{n-i}$

Multirate schemes

Base integration methods to solve $\dot{y} = f(t, y)$

- **Runge Kutta (RK) methods**
  - **r-stage explicit RK methods** : $y_n = y_{n-1} + \sum_{i=1}^{r} b_i k_i$

    with $\quad k_1 = hf(t_{n-1}, y_{n-1})$ and $k_i = hf(t_{n-1} + c_i h, y_{n-1} + \sum_{j=1}^{i-1} a_{ij} k_j) \quad (i = 2 \ldots r)$
  - **r-stage implicit RK methods** : $y_n = y_{n-1} + \sum_{i=1}^{r} b_i k_i$

    with $\quad k_i = hf(t_{n-1} + c_i h, y_{n-1} + \sum_{j=1}^{r} a_{ij} k_j) \quad (i = 1 \ldots r)$
  - **r-stage Rosenbrock methods** : $y_n = y_{n-1} + \sum_{i=1}^{r} b_i k_i$

    $$k_i = hf(t_{n-1} + c_i h, y_{n-1} + \sum_{j=1}^{i-1} a_{ij} k_j) + d_i h^2 \frac{\partial f}{\partial t}(t_{n-1}, y_{n-1}) + h \frac{\partial f}{\partial y}(t_{n-1}, y_{n-1}) \sum_{j=1}^{i} d_{ij} k_j$$

Multirate schemes

Base integration methods to solve $\dot{y} = f(t,y)$

- **r-stage explicit RK methods, representation in Butcher tableau** :

$$y_{n+1} = y_n + h\sum_{i=1}^{r} b_i k_i \text{ with } \quad k_i = f(t_n + c_i h, y_n + h\sum_{j=1}^{i-1} a_{ij}k_j)$$

$$\begin{array}{c|cccccc} c_1 = 0 & 0 & & & & \\ c_2 & a_{21} & & & & \\ c_3 & a_{31} & a_{32} & & & \\ \vdots & \vdots & \vdots & \ddots & & \\ c_r & a_{r1} & a_{r2} & \cdots & a_{r,r-1} & \\ \hline & b_1 & b_2 & \cdots & b_{r-1} & b_r \end{array} \quad \text{or shorter} \quad \begin{array}{c|c} c & A \\ \hline & b^T \end{array} \quad \text{or} \quad [A,b,c]$$

- **r-stage implicit RK methods, representation in Butcher tableau** :

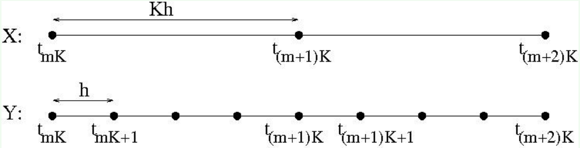
$$y_{n+1} = y_n + h\sum_{i=1}^{r} b_i k_i \text{ with } \quad k_i = f(t_n + c_i h, y_n + h\sum_{j=1}^{r} a_{ij}k_j)$$

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1r} \\ \vdots & \vdots & & \vdots \\ c_r & a_{r1} & \cdots & a_{rr} \\ \hline & b_1 & \cdots & b_r \end{array} \quad \text{or shorter} \quad \begin{array}{c|c} c & A \\ \hline & b^T \end{array} \quad \text{or} \quad [A,b,c]$$

Multirate schemes

Rice 1960, Multirate RK methods

$$\begin{array}{lll} \dot{x} = F(t,x,y) & x(t_0) = x_0, & x \text{ latent component} \\ \dot{y} = G(t,x,y) & y(t_0) = y_0, & y \text{ active component} \end{array}$$



Multirate schemes

Rice 1960, Multirate RK methods

Evaluation of $x_{(m+1)K}, x_{(m+2)K}, \dots$:

$$x_{(m+1)K} = x_{mK} + \sum_{i=1}^{3} b_i k_i$$

$$k_i = hF(t_{mK} + c_i Kh, x_{mK} + \sum_{j=1}^{i-1} a_{ij} k_j, y_{mK} + \sum_{j=1}^{i-1} a_{ij} h_j) \quad (i = 1 \dots 3)$$

$$h_i = hG(t_{mK} + c_i Kh, x_{mK} + \sum_{j=1}^{i-1} a_{ij} k_j, y_{mK} + \sum_{j=1}^{i-1} a_{ij} h_j) \quad (i = 1 \dots 2)$$

b_i, c_i, a_{ij} given by any RK3 method (work also done with RK4).

Multirate schemes

Rice 1960, Multirate RK methods

Evaluation of $y_{mK+j+1}, y_{mK+j+2}, \dots$:

$$y_{mK+j+1} = y_{mK+j} + \sum_{i=1}^{3} \alpha_i d_i(j) \quad \text{for} \quad 0 \le j \le K-1.$$

$$d_1(j) = hG(t_{mK+j}, x_{mK+j}, y_{mK+j})$$

$$d_2(j) = hG(t_{mK+j} + \mu_2 h, x_{mK+j} + \sum_{i=4}^{6} \lambda_i(j) k_{i-3}, y_{mK+j} + \gamma_{21} d_1(j))$$

$$d_3(j) = hG(t_{mK+j} + \mu_3 h, x_{mK+j} + \sum_{i=7}^{9} \lambda_i(j) k_{i-6}, y_{mK+j} + \gamma_{31} d_1(j) + \gamma_{32} d_2(j))$$

with extrapolation using previous k_i : $x_{mK+j} = x_{mK} + \sum_{i=1}^{3} \lambda_i(j) k_i \quad 1 \le j \le K-1,$

where several sets of parameters "$\alpha_i, \mu_i, \gamma_{ik}, \lambda_i(j)$" are determined so that :
option 1) local truncation error of integration formula for $y(t)$ is in $O(h^4)$
option 2) extrapolation parameters $\lambda_i(j)$ leads to an extrapolation truncation error in $O(h^4)$ and integration parameters are determined independantly.

Multirate schemes

Rice 1960, Multirate RK methods

Applications : 2 degrees of freedom problem of the type :

$$\frac{dx}{dt} = x/2 \quad x(0) = 1$$

$$\frac{dy}{dt} = x\cos(25t) \quad y(0) = 1/1250.5$$

Number of operations and functions evaluations :

	Add.	Mult.	F evaluation	G evaluation
Normal RK3	22K	28K	3K	3K
Multirate RK3	14(K+1)	17(K+1)	3	3K+2

Multirate schemes

Skelboe 1989, Multirate BDF methods

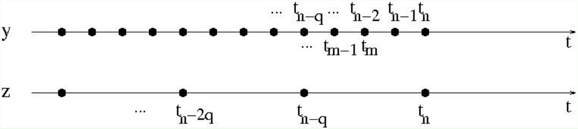
$$\dot{y} = f(t,y,z), \quad y(t_0) = y_0, \quad \text{fast subsystem}$$
$$\dot{z} = g(t,y,z), \quad z(t_0) = y_0, \quad \text{slow subsystem}$$

Fast subsystem integrated by a k-step BDF formula (BDF-k) with step length h :

$$y_m = \sum_{i=1}^{k} \alpha_i y_{m-i} + h\beta_0 f(t_m, y_m, z_m)$$

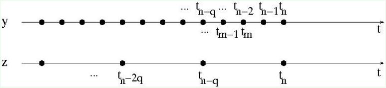
Slow subsystem integrated by the same BDF-k formula with step length $H = qh$:

$$z_n = \sum_{i=1}^{k} \alpha_i z_{n-qi} + qh\beta_0 f(t_n, y_n, z_n)$$



Multirate schemes

Skelboe 1989, Multirate BDF methods



Various strategies for the sequence of computation :

- **Fastest first algorithm**
  step 1) Integration of the fast subsystem from t_{n-q} to t_n (q steps) with extrapolated values $\tilde{z}_m$ ($n-q < m \le n$) based on $z_{n-kq}, \ldots, z_{n-q}$ (Newton, $\tilde{z}_m = \sum_{r=1}^{k} \tilde{\alpha}_{r,m-(n-q)} z_{n-rq}$).
  step 2) Integration of the slow subsystem from t_{n-q} to t_n (one step).
- **Slowest first algorithm**
  step 1) Integration of the slow subsystem from t_{n-q} to t_n (one step) with extrapolated value $\tilde{y}_n$ based on $y_{n-q-k+1}, \ldots, y_{n-q}$ (Newton).
  step 2) Integration of the fast subsystem from t_{n-q} to t_n (q steps) with interpolated values $\tilde{z}_m$ ($n-q < m < n$) based on $z_{n-(k-1)q}, \ldots, z_n$ (Newton, $\tilde{z}_m = \sum_{r=0}^{k-1} \tilde{\alpha}_{r,m-(n-q)} z_{n-rq}$).

Option : Waveform relaxation until convergence.

Multirate schemes

Skelboe 1989, Multirate BDF methods

Various strategies for the sequence of computation (continued) :

- **Implicit multirate algorithm**
  Interpolated values $\tilde{z}_m$ $(n-q<m<n)$ based on $z_{n-(k-1)q},\ldots,z_n$ where z_n computed by BDF-k with y_n computed by BDF-k.
  Integration from t_{n-q} to t_n $\Rightarrow$ solution of one large system of algebraic equations :

$$K\begin{pmatrix} Y_n \\ Z_n \end{pmatrix} = L\begin{pmatrix} Y_{n-q} \\ Z_{n-q} \end{pmatrix}$$

where

$$K=\begin{pmatrix} K_{yy} & K_{yz} \\ K_{zy} & K_{zz} \end{pmatrix}, \quad L=\begin{pmatrix} L_{yy} & L_{yz} \\ L_{zy} & L_{zz} \end{pmatrix},$$

$$Y_n=(y_n,y_{n-1},\ldots,y_{n-k+1})^T \text{ and } Z_n=(z_n,z_{n-q},\ldots,z_{n-(k-1)q})^T.$$

Multirate schemes

Skelboe 1989, Multirate BDF methods

Applications : 2×2 test problems for investigating the stability properties of the previous multirate algorithms (BDF-1 and BDF-2, interpolation of order 0 and 1).

Conclusion : These multirate methods not necessarily A-stable, even when based on A-stable integration formulas.

Multirate schemes

Günther-Rentrop 1993, Multirate ROW methods

Autonomous EDO (for the sake of clarity) :

$$\dot{y}(t) = f(y), \quad y(t_0) = y_0, \quad y \in \mathbb{R}^n$$

$$\Downarrow$$

$$\dot{y_S} = f_S(y_S, y_L), \quad y_S(t_0) = y_{S0}, \quad y_S \in \mathbb{R}^{n_S}, \quad \text{active subsystem}$$

$$\dot{y_L} = f_L(y_S, y_L), \quad y_L(t_0) = y_{L0}, \quad y_L \in \mathbb{R}^{n_L}, \quad \text{latent subsystem}$$

Multirate schemes

Günther-Rentrop 1993, Multirate ROW methods

- y_L integrated with ROW methods on one large time step H :

$$y_L^H(t_0+H) = y_{L0} + \sum_{i=1}^{s} c_i k_i$$

$$k_i = hf_L(\hat{y}_S(t_0+\alpha_i H), y_{L0} + \sum_{j=1}^{i-1} \alpha_{ij} k_j) + HJ_L \sum_{j=1}^{i} \gamma_{ij} k_j \ , \quad J_L = \frac{\partial f_L}{\partial y_L}(y_{S0}, y_{L0})$$

where $\alpha_i = \sum_{j=1}^{i-1} \alpha_{ij}$ and $\hat{y}_S(t)$ is an extrapolated value for $y_S(t)$.

- y_S integrated with ROW methods and m time steps $h = H/m$:

$$y_S^H(t_0+(\lambda+1)h) = y_{S0}(t_0+\lambda h) + \sum_{i=1}^{s} c_i l_i$$

$$l_i = hf_S(y_S(t_0+\lambda h) + \sum_{j=1}^{i-1} \alpha_{ij} l_j, \tilde{y}_L(t_0+\lambda h+\alpha_i)) + hJ_S \sum_{j=1}^{i} \gamma_{ij} l_j \ ,$$

$$J_S = \frac{\partial f_S}{\partial y_S}(y_S(t_0+\lambda h), \tilde{y}_L(t_0+\lambda h)), \ \text{for} \ \lambda = 0, 1, \ldots, m-1$$

where $\tilde{y}_L(t)$ is an extrapolated value for $y_L(t)$.

Multirate schemes

Günther-Rentrop 1993, Multirate ROW methods

Rational (1,1)-extrapolation scheme (Padé approximant) :

$$\hat{y}_{Si}(t_0+\bar{h}) = y_{Si}(t_0) + \frac{2\bar{h} f_{Si}(t_0)^2}{2f_{Si}(t_0) - \bar{h}\sum_{j=1}^{n_S} \frac{\partial f_{Si}}{\partial y_{Sj}}(y(t_0)) f_{Sj}(y(t_0)) - \bar{h}\sum_{j=n_S+1}^{n} \frac{\partial f_{Si}}{\partial y_{Lj}}(y(t_0)) f_{Lj}(y(t_0))}$$

$$\tilde{y}_{Li}(t_0+\bar{h}) = y_{Li}(t_0) + \frac{2\bar{h} f_{Li}(t_0)^2}{2f_{Li}(t_0) - \bar{h}\sum_{j=1}^{n_S} \frac{\partial f_{Li}}{\partial y_{Sj}}(y(t_0)) f_{Sj}(y(t_0)) - \bar{h}\sum_{j=n_S+1}^{n} \frac{\partial f_{Li}}{\partial y_{Lj}}(y(t_0)) f_{Lj}(y(t_0))}$$

Multirate schemes

Günther-Rentrop 1993, Multirate ROW methods

Applications : simulation of electric circuits (inverter chain)
$\Rightarrow$ stiff EDO (system of 250-4000 differential equations).

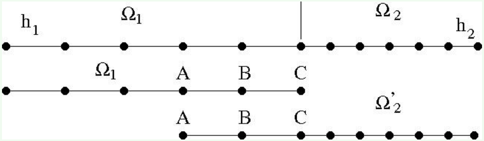
Results : implementation of a multirate 4-steps ROW method, A-stable, speedup up to 2.8 compared to a RK4 method.

Multirate schemes

Löhner-Morgan-Zienkiewicz 1984, Explicit multirate for hyperbolic problems

$$\frac{\partial U}{\partial t} + \nabla \cdot F(U) = 0 \quad \text{in } \Omega = \Omega_1 \cup \Omega_2,$$

with, for a given explicit scheme, an allowable time step Δt_1 in Ω_1 and $\Delta t_2 = \Delta t_1 / n$ in Ω_2.



1D model and a splitting into 2 subdomains

One global time step of the proposed multirate explicit scheme (for 2 subdomains) :

- Add to Ω_2 two grid points of Ω_1 $\rightarrow$ new subdomain Ω_2'.
- Specify a BC for U (free or fixed) at point C and advance one global time step Δt_1 in Ω_1.
- Specify a BC for U (free or fixed) at point A and advance n small time steps $\Delta t_2 = \Delta t_1 / n$ in Ω_2'.
- U_A is obtained from Ω_1, U_C from Ω_2', U_B = mean values obtained from Ω_1 and Ω_2'.

The same procedure can be performed with more than 2 subdomains splitting, and in the multidimensional case.

Multirate schemes

Löhner-Morgan-Zienkiewicz 1984, Explicit multirate for hyperbolic problems

Applications :

- Implementation of the proposed multirate scheme with a second order explicit FE scheme (Taylor-Galerkin method of Donea).
- Transient solution of a 1D shock tube problem (Sod).
- Transient solution of a 2D supersonic inviscid flow around a circular cylinder.
- Steady-state solution of a 2D supersonic inviscid flow past a wedge.
- Speedup of 2 between the multirate and single-rate scheme (2D supersonic wedge).

Multirate schemes

Kirby 2002, Multirate forward Euler for hyperbolic conservation laws

$$\frac{\partial y(t,x)}{\partial t} + \frac{\partial F(y(t,x))}{\partial x} = 0$$

$\Downarrow$ Semi-discretization

$$\dot{y}_i(t) = f_i(y_1(t), \ldots, y_n(t)), \quad i = 1, \ldots, n$$

$\Downarrow$ Partitioning in slow/fast components

$$\dot{y}_F = f_F(y_F, y_S) \quad \text{(fast solution subsystem, explicit Euler time step } \Delta t/m\text{)}$$

$$\dot{y}_S = f_S(y_F, y_S) \quad \text{(slow solution subsystem, explicit Euler time step } \Delta t\text{)}$$

Multirate schemes

Kirby 2002, Multirate forward Euler for hyperbolic conservation laws

A multirate scheme based on forward Euler steps

- y_F : m steps integration from t^n to t^{n+1}
  $$y_F^{n+\eta_k} = y_F^{n+\eta_{k-1}} + \sigma_k \Delta t f_F(y_F^{n+\eta_{k-1}}, y_S^n), \quad k = 1, \ldots, m-1$$
  $$y_F^{n+1} = y_F^{n+\eta_{m-1}} + \sigma_m \Delta t f_F(y_F^{n+\eta_{m-1}}, y_S^n)$$
- y_S : 1 step integration from t^n to t^{n+1}
  $$y_S^{n+1} = y_S^n + \Delta t f_S(y_F^n, y_S^n)$$

where $\sum_{k=1}^{m} \sigma_k = 1$ with $0 < \sigma_k \leq 1$,

$$\eta_l = \sum_{k=1}^{l} \sigma_k, \ \eta_0 = 0 \text{ and } t^{n+\eta_k} = t^n + \eta_k \Delta t.$$

Multirate schemes

Kirby 2002, Multirate forward Euler for hyperbolic conservation laws

- Results : the proposed multirate scheme satisfies the TVD property and a maximum principle under local CFL conditions, but only first order time accurate.

Multirate schemes

Sandu-Constantinescu 2007, Multirate RK for hyperbolic conservation laws

$$\frac{\partial y(t,x)}{\partial t} + \frac{\partial F(y(t,x))}{\partial x} = 0$$

$\Downarrow$ Semi-discretization

$$\dot{y}_i(t) = f_i(y_1(t), \ldots, y_n(t)), \quad i = 1, \ldots, n$$

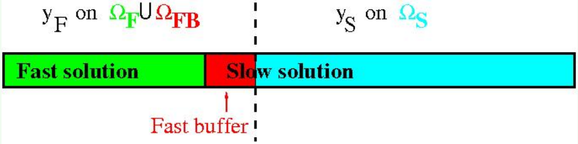
$\Downarrow$ Partitioning in slow/fast subsystems

$\dot{y}_F = f_F(y_F, y_S)$, fast subsystem ($\neq$ fast solution subsystem)

$\dot{y}_S = f_S(y_F, y_S)$, slow subsystem ($\neq$ slow solution subsystem)

Multirate schemes

Sandu-Constantinescu 2007, Multirate for hyperbolic conservation laws



Fast solution : solution with fast characteristic time ($\neq y_F$)
Slow solution : solution with slow characteristic time ($\neq y_S$)
Ω_F : fast characteristic time , small time step $\Delta t/m$ used in the multirate scheme
Ω_{FB} : slow characteristic time , but small time step $\Delta t/m$ used in the multirate scheme
Ω_S : slow characteristic time , large time step Δt used in the multirate scheme
y_F = fast solution $\cup$ fast buffer solution $\rightarrow$ small time step $\Delta t/m$
y_S = slow solution $\setminus$ fast buffer solution $\rightarrow$ large time step Δt

Ω_{FB} : important for the TVB property of the multirate scheme under local CFL conditions (size of fast buffer = half of stencil size).

Multirate schemes

Sandu-Constantinescu 2007, Multirate RK for hyperbolic conservation laws

Multirate partitioned RK scheme (2nd order accurate, conservative, nonlinearly stable) :

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array}$$ **Base method** (RK_B)

$$\begin{array}{c|cccc}
\frac{1}{m}c & \frac{1}{m}A & & & \\
\frac{1}{m}\mathbf{1}+\frac{1}{m}c & \frac{1}{m}\mathbf{1}b^T & \frac{1}{m}A & & \\
\vdots & \vdots & & \ddots & \\
\frac{m-1}{m}\mathbf{1}+\frac{1}{m}c & \frac{1}{m}\mathbf{1}b^T & \cdots & \frac{1}{m}\mathbf{1}b^T & \frac{1}{m}A \\
\hline
 & \frac{1}{m}b^T & \frac{1}{m}b^T & \cdots & \frac{1}{m}b^T
\end{array}$$

Fast method (RK_F) : $\dot{y}_F = f_F(y_F, y_S)$

$$\begin{array}{c|cccc}
c & A & & & \\
c & & A & & \\
\vdots & & & \ddots & \\
c & & & & A \\
\hline
 & \frac{1}{m}b^T & \frac{1}{m}b^T & \cdots & \frac{1}{m}b^T
\end{array}$$

Slow method (RK_S) : $\dot{y}_S = f_S(y_F, y_S)$

Same weight coefficients for RK_F **and** RK_S $\left(b_{F_i} = b_{S_i} = \frac{b_i}{m}\right)$: important for second order accuracy and conservation properties of the multirate scheme.

Multirate schemes

Sandu-Constantinescu 2007, Multirate RK for hyperbolic conservation laws

Case RK2 and m=2 :

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & 1/2 & 1/2 \end{array}$$

Base method ($\mathbf{RK_B}$)

$$\begin{array}{c|cccc} 0 & 0 & & & \\ 1/2 & 1/2 & 0 & & \\ 1/2 & 1/4 & 1/4 & 0 & \\ 1 & 1/4 & 1/4 & 1/2 & 0 \\ \hline & 1/4 & 1/4 & 1/4 & 1/4 \end{array}$$

Fast method ($\mathbf{RK_F}$)

$$\begin{array}{c|cccc} 0 & 0 & & & \\ 1 & 1 & 0 & & \\ 0 & 0 & 0 & 0 & \\ 1 & 0 & 0 & 1 & 0 \\ \hline & 1/4 & 1/4 & 1/4 & 1/4 \end{array}$$

Slow method ($\mathbf{RK_S}$)

$\mathbf{RK_B}$, $\mathbf{RK_F}$ and $\mathbf{RK_S}$ stages :

$\mathbf{RK_B}$ $(\dot{y} = f(y))$:

$$\begin{aligned} k^1 &= f(y^n) \\ y^{(1)} &= y^n + \Delta t\, k^1 \\ k^2 &= f(y^{(1)}) \\ y^{n+1} &= y^n + \frac{\Delta t}{2}(k^1 + k^2) \end{aligned}$$

$\mathbf{RK_F}$ $(\dot{y}_F = f_F(y_F, y_S))$:

$$\begin{aligned} k_F^1 &= f_F(y_F^n, y_S^n) \\ y_F^{(1)} &= y_F^n + \frac{\Delta t}{2} k_F^1 \\ k_F^2 &= f_F(y_F^{(1)}, y_S^{(1)}) \\ y_F^{(2)} &= y_F^n + \frac{\Delta t}{4} k_F^1 + \frac{\Delta t}{4} k_F^2 \\ k_F^3 &= f_F(y_F^{(2)}, y_S^n) \\ y_F^{(3)} &= y_F^{(2)} + \frac{\Delta t}{2} k_F^3 \\ k_F^4 &= f_F(y_F^{(3)}, y_S^{(3)}) \\ y_F^{n+1} &= y_F^n + \frac{\Delta t}{4}(k_F^1 + k_F^2 + k_F^3 + k_F^4) \end{aligned}$$

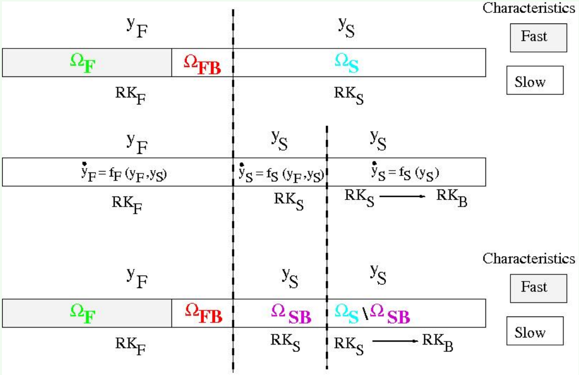
$\mathbf{RK_S}$ $(\dot{y}_S = f_S(y_F, y_S))$:

$$\begin{aligned} k_S^1 &= f_S(y_F^n, y_S^n) \\ y_S^{(1)} &= y_S^n + \Delta t\, k_S^1 \\ k_S^2 &= f_S(y_F^{(1)}, y_S^{(1)}) \\ y_S^{(2)} &= y_S^n \\ k_S^3 &= f_S(y_F^{(2)}, y_S^n) \\ y_S^{(3)} &= y_S^n + \Delta t\, k_S^3 \\ k_S^4 &= f_S(y_F^{(3)}, y_S^{(3)}) \\ y_S^{n+1} &= y_S^n + \frac{\Delta t}{4}(k_S^1 + k_S^2 + k_S^3 + k_S^4) \end{aligned}$$

At each stage of the multirate formula, evaluation of the flux functions at the same argument values : important for the conservation properties of the multirate scheme.

Multirate schemes

Sandu-Constantinescu 2007, Multirate RK for hyperbolic conservation laws



Ω_{SB} = slow buffer, f_S depends on y_F and y_S (size = $m \times$ half of stencil size).

Multirate schemes

Sandu-Constantinescu 2007, Multirate RK for hyperbolic conservation laws

Case RK2 and m=2 :

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & 1/2 & 1/2 \end{array}$$

Base method ($\mathbf{RK_B}$)

$$\begin{array}{c|cccc} 0 & 0 & & & \\ 1/2 & 1/2 & 0 & & \\ 1/2 & 1/4 & 1/4 & 0 & \\ 1 & 1/4 & 1/4 & 1/2 & 0 \\ \hline & 1/4 & 1/4 & 1/4 & 1/4 \end{array}$$

Fast method ($\mathbf{RK_F}$)

$$\begin{array}{c|cccc} 0 & 0 & & & \\ 1 & 1 & 0 & & \\ 0 & 0 & 0 & 0 & \\ 1 & 0 & 0 & 1 & 0 \\ \hline & 1/4 & 1/4 & 1/4 & 1/4 \end{array}$$

Slow method ($\mathbf{RK_S}$)

$\mathbf{RK_B}\ (\dot{y} = f(y))$:

$$\begin{aligned} k^1 &= f(y^n) \\ y^{(1)} &= y^n + \Delta t\, k^1 \\ k^2 &= f(y^{(1)}) \\ y^{n+1} &= y^n + \tfrac{\Delta t}{2}(k^1 + k^2) \end{aligned}$$

$\Omega_F \cup \Omega_{FB}$, $\mathbf{RK_F}\ (\dot{y}_F = f_F(y_F, y_S))$:

$$\begin{aligned} k_F^1 &= f_F(y_F^n, y_S^n) \\ y_F^{(1)} &= y_F^n + \tfrac{\Delta t}{2} k_F^1 \\ k_F^2 &= f_F(y_F^{(1)}, y_S^{(1)}) \\ y_F^{(2)} &= y_F^n + \tfrac{\Delta t}{4} k_F^1 + \tfrac{\Delta t}{4} k_F^2 \\ k_F^3 &= f_F(y_F^{(2)}, y_S^n) \\ y_F^{(3)} &= y_F^{(2)} + \tfrac{\Delta t}{2} k_F^3 \\ k_F^4 &= f_F(y_F^{(3)}, y_S^{(3)}) \\ y_F^{n+1} &= y_F^n + \tfrac{\Delta t}{4}(k_F^1 + k_F^2 + k_F^3 + k_F^4) \end{aligned}$$

Ω_{SB}, $\mathbf{RK_S}\ (\dot{y}_S = f_S(y_F, y_S))$:

$$\begin{aligned} k_S^1 &= f_S(y_F^n, y_S^n) \\ y_S^{(1)} &= y_S^n + \Delta t\, k_S^1 \\ k_S^2 &= f_S(y_F^{(1)}, y_S^{(1)}) \\ y_S^{(2)} &= y_S^n \\ k_S^3 &= f_S(y_F^{(2)}, y_S^n) \\ y_S^{(3)} &= y_S^n + \Delta t\, k_S^3 \\ k_S^4 &= f_S(y_F^{(3)}, y_S^{(3)}) \\ y_S^{n+1} &= y_S^n + \tfrac{\Delta t}{4}(k_S^1 + k_S^2 + k_S^3 + k_S^4) \end{aligned}$$

$\Omega_S \backslash \Omega_{SB}$, $\mathbf{RK_S} \rightarrow \mathbf{RK_B}\ (\dot{y}_S = f_S(y_S))$

$$\begin{aligned} k_S^1 &= f_S(y_S^n) \\ y_S^{(1)} &= y_S^n + \Delta t\, k_S^1 \\ k_S^2 &= f_S(y_S^{(1)}) \\ &\left\{ y_S^{(2)} = y_S^n \right\} \\ &\left\{ k_S^3 = f_S(y_S^n) = k_S^1 \right\} \\ &\left\{ y_S^{(3)} = y_S^n + \Delta t\, k_S^3 = y_S^{(1)} \right\} \\ &\left\{ k_S^4 = f_S(y_S^{(3)}) = k_S^2 \right\} \\ y_S^{n+1} &= y_S^n + \tfrac{\Delta t}{2}(k_S^1 + k_S^2) \end{aligned}$$

Multirate schemes

Sandu-Constantinescu 2007, Multirate RK for hyperbolic conservation laws

Properties of the proposed multirate partitioned RK scheme :

- second order accurate
- conservative
- nonlinear stable (positivity, maximum principle preserving, TVB)
- theoritical speedup (single rate/multirate) :

$$\text{Speedup} = \frac{m(N_{\Omega_F}+N_{\Omega_{FB}}+N_{\Omega_S})}{m(N_{\Omega_F}+N_{\Omega_{FB}}+N_{\Omega_{SB}})+N_{\Omega_S}-N_{\Omega_{SB}}} = \frac{m(N_{\Omega_F}+N_{\Omega_{FB}}+N_{\Omega_S})}{m(N_{\Omega_F}+N_{\Omega_{FB}}+N_{int}m\Delta)+N_{\Omega_S}-N_{int}m\Delta}$$

where N_{Ω_X}= number of nodes in Ω_X, Δ= half of stencil size, and N_{int}= number of interface nodes between $N_{\Omega_{FB}}$ and N_{Ω_S}.

  - for large m, decrease of speedup $\Rightarrow$ nested partitioning.
  - in practice, $N_{\Omega_{SB}} << min(N_{\Omega_F}+N_{\Omega_{FB}}, N_{\Omega_S})$

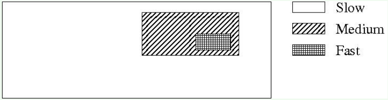
    $\Rightarrow$ Speedup $\simeq \frac{m(N_{\Omega_F}+N_{\Omega_{FB}}+N_{\Omega_S})}{m(N_{\Omega_F}+N_{\Omega_{FB}})+N_{\Omega_S}}$

    $\Rightarrow$ Speedup close to the ideal value of m if $N_{\Omega_F}+N_{\Omega_{FB}} << N_{\Omega_S}$.

Multirate time scheme

Sandu-Constantinescu 2007, Multirate RK for hyperbolic conservation laws

Nested partitioning :



Nested partitioning, example with 3 levels

- $N+1$ levels of partitioning, with time step requirement $\Delta t_j = \frac{\Delta t}{m^j}$, $j = 0, \ldots, N$.

  $$\Rightarrow \text{Speedup} = \left(m^N \sum_{j=0}^{N} L_j \right) \Big/ \left(\sum_{j=0}^{N} m^j L_j \right)$$

  where L_j = number of grid points associated to Δt_j (level j)
- If $L_{j+1} << L_j$, then Speedup $\simeq m^N$.

Multirate time scheme

Sandu-Constantinescu 2007, Multirate RK for hyperbolic conservation laws

Applications :

- multirate RK2 scheme with $m = 2$ $(\Delta t/2)$ and $m = 3$ $(\Delta t/3)$, 2 levels of partitioning.
- 1D advection equation (initial solutions : step, triangular and exponential shape), fixed and moving grids, 2nd order limited FV scheme.
- 1D burger equation (initial solutions : step and exponential shape), fixed grids, 3rd order TVD FV scheme.
- numerical solutions : 2nd order accurate, positive, obey the maximum principle, TVD, wiggle free; conservative time steps.
- Speedup (single rate/multirate, burger Eq.), fast region $\simeq 10$ % entire domain :

Time ratio	Single rate time (sec)	Multirate time (sec)	Experimental Speedup	Theoritical Speedup
$m = 2$	25.28	13.71	1.84	1.80
$m = 3$	36.73	15.07	2.43	2.45

Multirate time scheme

Sandu-Constantinescu 2009, Multirate Adams for hyperbolic conservation laws

Multirate explicit Adams : same solution component partitioning as for multirate RK schemes.

Semi-discretization of hyperbolic PDE's
$\Downarrow$
Partitioning in slow/fast subsystems

$$\dot{y}_F = f_F(y_F, y_S), \quad \text{fast subsystem}$$
$$\dot{y}_S = f_S(y_F, y_S), \quad \text{slow subsystem}$$

y_F integrated with small time step h at times $\ldots, t_{n-m}, t_{n-m+1}, t_{n-m+2}, \ldots, t_{n-1}, t_n, \ldots$:
$\ldots, y_F^{n-m}, y_F^{n-m+1}, y_F^{n-m+2}, \ldots, y_F^{n-1}, y_F^{n}, \ldots$

y_S integrated with large time step mh at times $\ldots, t_{n-3m}, t_{n-2m}, t_{n-m}, t_n, \ldots$:
$\ldots, y_S^{n-3m}, y_S^{n-2m}, y_S^{n-m}, y_S^{n}, \ldots$

Multirate time scheme

Sandu-Constantinescu 2009, Multirate Adams for hyperbolic conservation laws

Time integration from t_{n-m} to t_n by the multirate *explicit k-steps Adams*$^{(*)}$ scheme (fastest first strategy):

- Step 1, for $l = 1, \ldots, m$: $\quad y_F^{n-m+l} = y_F^{n-m+l-1} + h \sum_{i=1}^{k} \beta_i f_F(y_F^{n-m+l-i}, y_S^{n-im})$
- Step 2, $\quad y_S^n = y_S^{n-m} + h \sum_{i=1}^{k} \beta_i \left(\sum_{l=1}^{m} f_S(y_F^{n-m+l-i}, y_S^{n-im}) \right)$

  Remark : on $\Omega_S \backslash \Omega_{SB}$, $\quad \dot{y}_S = f_S(y_S) \quad \Rightarrow \quad y_S^n = y_S^{n-m} + mh \sum_{i=1}^{k} \beta_i f_S(y_S^{n-im})$

  (base explicit k-steps Adams scheme retrieved with an integration step of mh).

Evaluation of the flux functions with the same argument values and same weights β_i for y_F and y_S : important for the conservation properties and 2nd order accuracy of the multirate scheme.

$(*)$ *Base explicit k-steps Adams scheme* applied to $\dot{y} = f(y)$: $\quad y^n = y^{n-1} + h \sum_{i=1}^{k} \beta_i f(y^{n-i})$

Multirate time scheme

Sandu-Constantinescu 2009, Multirate Adams for hyperbolic conservation laws

Case of explicit 2-steps Adams and $m = 2$:

- $y_F^{n-1} = y_f^{n-2} + \frac{3h}{2} f_F(y_F^{n-2}, y_S^{n-2}) - \frac{h}{2} f_F(y_F^{n-3}, y_S^{n-4}),$
  $y_F^{n} = y_f^{n-1} + \frac{3h}{2} f_F(y_F^{n-1}, y_S^{n-2}) - \frac{h}{2} f_F(y_F^{n-2}, y_S^{n-4})$
- $$y_S^n = y_S^{n-2} + \frac{3h}{2}\Big(f_S(y_F^{n-1}, y_S^{n-2}) + f_S(y_F^{n-2}, y_S^{n-2})\Big) - \frac{h}{2}\Big(f_S(y_F^{n-2}, y_S^{n-4}) + f_S(y_F^{n-3}, y_S^{n-4})\Big)$$

  Remark : on $\Omega_S \backslash \Omega_{SB}$, $\quad \dot{y}_S = f_S(y_S) \quad \Rightarrow \quad y_S^n = y_S^{n-2} + \frac{3 \times 2h}{2} f_S(y_S^{n-2}) - \frac{2h}{2} f_S(y_S^{n-4})$

  (base explicit k-steps Adams scheme retrieved with an integration step of $2h$)

Multirate time scheme

Sandu-Constantinescu 2009, Multirate Adams for hyperbolic conservation laws

Properties of the proposed multirate explicit k-steps Adams scheme :

- second order accurate
- conservative
- nonlinear stable (positivity, maximum principle preserving, TVB)
- theoritical speedup (single rate/multirate) :

$$\text{Speedup} = \frac{m(N_{\Omega_F}+N_{\Omega_{FB}}+N_{\Omega_S})}{m(N_{\Omega_F}+N_{\Omega_{FB}}+N_{\Omega_{SB}})+N_{\Omega_S}-N_{\Omega_{SB}}} = \frac{m(N_{\Omega_F}+N_{\Omega_{FB}}+N_{\Omega_S})}{m(N_{\Omega_F}+N_{\Omega_{FB}}+N_{int}m\Delta)+N_{\Omega_S}-N_{int}m\Delta}$$

where N_{Ω_X}= number of nodes in Ω_X, Δ= half of stencil size, and N_{int}= number of interface nodes between $N_{\Omega_{FB}}$ and N_{Ω_S}.

  - for large m, decrease of speedup $\Rightarrow$ nested partitioning.
  - in practice, $N_{\Omega_{SB}} << min(N_{\Omega_F}+N_{\Omega_{FB}}, N_{\Omega_S})$

    $\Rightarrow$ Speedup $\simeq \frac{m(N_{\Omega_F}+N_{\Omega_{FB}}+N_{\Omega_S})}{m(N_{\Omega_F}+N_{\Omega_{FB}})+N_{\Omega_S}}$

    $\Rightarrow$ Speedup close to the ideal value of m if $N_{\Omega_F}+N_{\Omega_{FB}} << N_{\Omega_S}$.

Multirate time scheme

Sandu-Constantinescu 2009, Multirate Adams for hyperbolic conservation laws

Applications :

- multirate explicit 2-steps Adams scheme with $m = 2$ ($2h$) and $m = 3$ ($3h$), 2 levels of partitioning.
- 1D advection equation (initial solution : step shape), fixed grids, 3rd order limited FV scheme.
- 1D burger equation (initial solution : step ashape), fixed grids, 3rd order TVD FV scheme.
- numerical solutions : 2nd order accurate, positive, obey the maximum principle, TVD, wiggle free; conservative time steps.
- Speedup (single rate/multirate, advection Eq.), fast region $\simeq 10$ % entire domain :

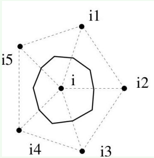
Time ratio	Single rate time (sec)	Multirate time (sec)	Experimental Speedup	Theoritical Speedup
$m = 2$	39.81	19.44	2.04	1.81
$m = 3$	39.81	14.22	2.79	2.50

Transition to order 3

Definition of the scheme (CENO)

Finite Volume approach (2D) :

$$\frac{d}{dt}\int_{C_i} u(x,y,t)dxdy + \int_{\partial C_i} \vec{f}(u(x,y,t)).\vec{n}ds = 0$$



$$\frac{d}{dt}\int_{C_i} u(x,y,t)dxdy + \sum_{k\in V(i)} \int_{\partial C_i \cap \partial C_k} \vec{f}(u(x,y,t)).\vec{n}ds = 0$$

Transition to order 3 (2)

Definition of the scheme (CENO)

Polynomial reconstruction :

Average of a function g over cell C_k : $\overline{g}^k = \frac{1}{area(C_k)} \int_{C_k} g(x,y)dxdy$

$$\text{We define} \quad P_i^n = \overline{u^n}^i + \sum_{\alpha \in I} c_{i,\alpha}^n \left[(X - X_{0,i})^\alpha - \overline{(X - X_{0,i})^\alpha}^i \right]$$

$\overline{P_i^n}^i = \overline{u^n}^i$ is satisfied.

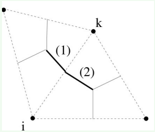
$c_{i,\alpha}^n$ chosen to minimize $H_i = \sum_{k \in N(i)} (\overline{P_i^n}^k - \overline{u^n}^k)^2$

$\Rightarrow$ Linear system with unknowns $c_{i,\alpha}^n$ (5 in 2D)

Transition to order 3 (3)

Definition of the scheme (CENO)

Flux evaluation :



Interfaces $C_i \cap \partial C_k$ between C_i and C_k, $(1) : \partial C_{ik}^{(1)}$ and $(2) : \partial C_{ik}^{(2)}$

$$\begin{aligned}
\int_{\partial C_i \cap \partial C_k} \vec{f}(u(x,y,t)).\vec{n}ds &= \sum_{l=1,2} \int_{\partial C_{ik}^{(l)}} \vec{f}(u(x,y,t)).\vec{n}ds \\
&= \sum_{l=1,2} \int_{\partial C_{ik}^{(l)}} \vec{f}(P_i(x,y,t)).\vec{n}ds \\
&= \sum_{m=1,2} \omega_m \vec{f}(P_i(x_{g_m,ik}^{(l)}, y_{g_m,ik}^{(l)}, t))\vec{\nu_{ik}}^{(l)}
\end{aligned}$$

Transition to order 3 (4)

Definition of the scheme (CENO)

Flux evaluation (2) :

$$\vec{f}(P_i(x^{(l)}_{g_m,ik}, y^{(l)}_{g_m,ik}, t)).\vec{\nu}_{ik} = \Phi(P_i(x^{(l)}_{g_m,ik}, y^{(l)}_{g_m,ik}, t), P_k(x^{(l)}_{g_m,ik}, y^{(l)}_{g_m,ik}, t), \vec{\nu}_{ik})$$

where Roe's scheme is used as approximate Riemann solver :

$$\Phi(u_1, u_2, \vec{\nu}) = \frac{\vec{f}(u_1) + \vec{f}(u_2)}{2}.\vec{\nu} - \frac{\gamma}{2}\left|\frac{\partial \vec{f}}{\partial u}\left(\frac{u_1+u_2}{2}\right).\vec{\nu}\right|(u_2 - u_1)$$

Application with mesh adaption

Scramjet, thesis of A. Carabias (INRIA Sophia and Rocquencourt)

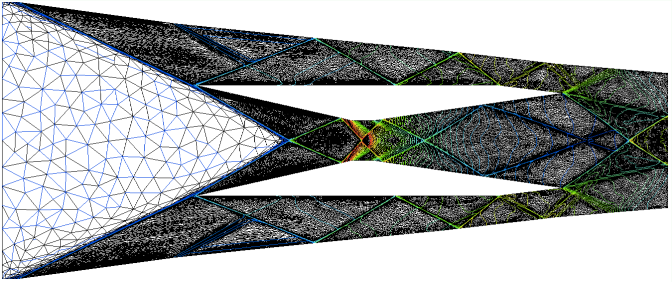


Figure: 2D anisotropic mesh adaption (31460 nodes), iso-contours of Mach number. Inlet Mach number = 3, CENO scheme.

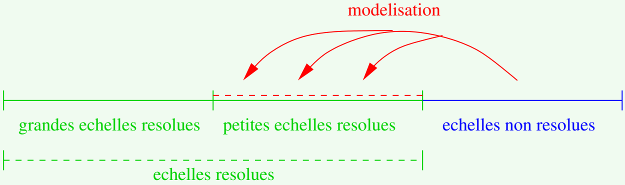
Thank you for your attention.

Appendix : Turbulence modeling

VMS-LES approach

Main features :

- Approach based on variational projections of the Navier-Stokes equations $\Rightarrow$ equations governing different scales of the solution (large resolved scales, small resoved scales, unresolved scales),
- Effects of the unresolved scales only modeled in the equations governing the small resolved scales :



Appendix : Turbulence modeling

VMS-LES approach (2)

The VMS-LES option chosen allows to take into account :

- the 3D compressible Navier-Stokes equations,
- unstructured meshes,
- a finite element/finite volume formulation,
- the scales separation with a simple and efficient procedure obtained from averaging on macro-cells,
- bluff body flows with vortex sheding.

Appendix : Turbulence modeling

RANS/VMS-LES hybrid model

- Central idea of this hybrid approach :
  - Solve the RANS equations in the whole domain,
  - Correct the mean flow field by adding fluctuations provided by a VMS-LES model in regions where the grid resolution is fine enough for VMS-LES.
- Basic ingredients of this hybrid approach :
  - a RANS model,
  - a VMS-LES model,
  - a blending function.

Appendix : Turbulence modeling

RANS/VMS-LES hybrid model (2)

$$\left(\frac{\partial W_h}{\partial t}, \mathscr{X}_i\right) + (\nabla \cdot F(W_h), \mathscr{X}_i, \Phi_i) = -\theta(\tau^{RANS}(W_h), \Phi_i) \\ -(1-\theta)(\tau^{LES}(W'_h), \Phi'_i)$$

where $\theta = tanh\left[\left(\frac{\Delta}{l_{RANS}}\right)^2\right]$

with $l_{RANS} = \dfrac{k^{3/2}}{\varepsilon}$ et Δ = local mesh size.

$$\Downarrow$$

$\Delta \ll l_{RANS}$: $\theta \to 0$ (VMS-LES mode)
$\Delta \gg l_{RANS}$: $\theta \to 1$ (RANS mode)