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IMPLEMENTATION OF SECOND MOMENT CLOSURE TURBULENCE MODEL FOR INCOMPRESSIBLE FLOWS IN THE INDUSTRIAL FINITE ELEMENT CODE N3S

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SYNTHÈSE :

Cette note traite de l'introduction d'un modèle de turbulence au second moment (modèle des contraintes de Reynolds) dans un code industriel aux éléments finis N3S mis au point à Electricité de France.

La réalisation numérique du modèle dans le N3S sera détaillée en 2D et 3D. On donne certains détails concernant les calculs aux éléments finis et les méthodes de résolution. On donnera ensuite des résultats y compris une comparaison entre le modèle standard k-epsilon, le modèle R.S.M. et les données expérimentales pour un cas test.

EXECUTIVE SUMMARY :

This paper deals with the introduction of a second moment closure turbulence model (Reynolds Stress Model) in an industrial finite element code, N3S, developed at Electricité de France.

The numerical implementation of the model in N3S will be detailed in 2D and 3D. Some details are given concerning finite element computations and solvers. Then, some results will be given, including a comparison between standard k-ε model, R.S.M. model and experimental data for some test case.

Implementation of 3D Second Moment Closure Turbulence Model for incompressible flows in the Finite Element Code N3S.

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Introduction

The "Direction des Etudes et Recherches" of EDF has been working since 1982 on N3S, a 3D finite element (F.E.) code for simulating turbulent incompressible [1], dilatabie [2] or compressible flows [3], including eventually free surface effects [4] and moving domain [5]. This code has been developed under quality assurance procedures, and is used for many industrial applications (internal flows [6], external flows [7], turbomachinery [8], thermal problems [9]).
Nowadays, better predictions are needed for the more and more complex turbulent flows which are studied (see [6] for example). So, second moment closure models are now a good answer to these industrial requirements, in a part because of the recent increasing power of computers.
This work presents the implementation of such a model in N3S, based on the work of Launder, Reece and Rodi [10], on the experience of using this model in finite volume codes developed at EDF [11], and on the implementation which has already been done in 2D in 1994 [12].

1. Presentation of the equations and of $(\overline{u_i u_j} - \varepsilon)$ model

1.1. *General presentation of the problem*

The equations governing the fluid motion in a regular open bounded subset Ω of $\mathbf{R}^N$ (N = 2 or 3) and over a time interval [0,T] are the Reynolds-averaged Navier-Stokes equations :

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} - \frac{\partial \overline{u_i u_j}}{\partial x_j} + \nu \Delta U_i \qquad (1)$$

(capital letters represent mean values, small letters fluctuations and $\overline{(.)}$ a statistical average. U, p, ρ, and ν are the mean velocity, pressure, density and viscosity respectively)

Many applied computations of turbulent flows still use the eddy viscosity model :

$$\overline{u_i u_j} = -\nu_t \left(\frac{\partial U_j}{\partial x_i} + \frac{\partial U_i}{\partial x_j}\right) + \frac{2}{3} k \delta_{ij} \qquad (2)$$

Eddy viscosity is defined as: $\nu_t = C_\mu \frac{k^2}{\varepsilon}$, where $k = \frac{1}{2}\overline{u_i u_i}$ is the turbulent kinetic energy, and ε its dissipation. They are modelled by transport equations with on the right hand side production, destruction and diffusive transport respectively :

$$\frac{Dk}{Dt} = P - \varepsilon + d_k \qquad (3)$$

$$\frac{D\varepsilon}{Dt} = \frac{\varepsilon}{k}(c_{\varepsilon 1} P - c_{\varepsilon 2}\varepsilon) + d_\varepsilon \qquad (4)$$

For some flows of the thermal convection type, we assume that density variations with temperature θ are small enough to be taken into account with the Boussinesq approximation. The energy equation gives the evolution of the temperature θ which satisfies a convection diffusion equation. It is also possible to take into account more important thermal effects which lead to consider Navier-Stokes problem with varying density ρ. This modelling is operational in the code today [6].

1.2. *The* $(\overline{u_i u_j}$ - $\varepsilon)$ *model*

The standard second moment closure (see [13], [14]) is expressed as :

$$\frac{D\overline{u_i u_j}}{Dt} = P_{ij} + \phi_{ij} + d_{ij} - \varepsilon_{ij} \qquad (5)$$

No approximation is made for the transport term or the production term P_{ij}, dissipation is assumed to be isotropic at high Reynolds number, $\varepsilon_{ij} = \frac{2}{3}\varepsilon\,\delta_{ij}$, where ε is obtained by the transport equation :

$$\frac{D\varepsilon}{Dt} = c_{\varepsilon 1}\frac{\varepsilon}{k}P - c_{\varepsilon 2}\frac{\varepsilon^2}{k} + c_\varepsilon \frac{\partial}{\partial x_i}\left(\frac{k}{\varepsilon}\overline{u_i u_j}\frac{\partial \varepsilon}{\partial x_j}\right) \qquad (6)$$

The turbulent transport d_{ij} has a minor contribution to the budget and is modelled by a gradient diffusion term, so much of the modelling effort is devoted to the pressure-strain correlation which is modelled by an algebraic expression, function of stresses and velocity gradients.

The simplest linear model or "Isotropization of production" is :

$$\phi_{ij} = \phi_{ij_1} + \phi_{ij_2} + \phi_{ij}^{w} \tag{7}$$

$$\phi_{ij_1} = -c_1 \; a_{ij} \; \varepsilon \tag{8}$$

$$\phi_{ij2} = -c_2 \; dev(P_{ij}) \tag{9}$$

A wall reflection term is added to account for pressure reflection at solid walls [15] :

$$\phi_{ij}^{w} = c_1^{w} \frac{\varepsilon}{k} (\overline{u_k u_m} n_k n_m \delta_{ij} - \frac{3}{2} \overline{u_k u_i} n_k n_j - \frac{3}{2} \overline{u_k u_j} n_k n_i) \; f_w(\frac{l}{y})$$
$$+ c_2^{w} (\phi_{km2} n_k n_m \delta_{ij} - \frac{3}{2} \phi_{ki2} n_k n_j - \frac{3}{2} \phi_{kj2} n_k n_i) \; f_w(\frac{l}{y}) \tag{10}$$

where l is a turbulent caracteristic length, y the normal distance to the wall, n_i the component of the normal to the wall.

The following values of the constant are chosen :

c_S	c_ε	$c_{\varepsilon 1}$	$c_{\varepsilon 2}$	c_1	c_2	c_1^w	c_2^w
0.22	0.18	1.44	1.90	1.8	0.6	0.5	0.3

We stress again that the production term P_{ij} is exact:

$$P_{ij} = -\overline{u_k u_j} \frac{\partial U_i}{\partial x_k} - \overline{u_k u_i} \frac{\partial U_j}{\partial x_k} \tag{11}$$

This is an important issue in the case of streamline curvature, body forces (rotation or buoyancy) and when distortion is not restricted to simple shear. In a plan compression like impinging flows the normal stresses make the following contribution to the production :

$$P_n = -\overline{u^2} \frac{\partial U}{\partial x} - \overline{v^2} \frac{\partial V}{\partial y} = (\overline{v^2} - \overline{u^2}) \frac{\partial U}{\partial x} \; ,$$

This term is generally overestimated by far, when using the k-ε model which yields : $P_n = 4 \nu_t \left(\frac{\partial U}{\partial x} \right)^2$

2. Implementation in finite element code N3S

2.1. *Time discretization*

Time discretization of scalar equations of convection diffusion plus source terms as well as Navier-Stokes equations is done obtained by a fractional step scheme. The convection step is processed by a characteristics method and the diffusion or Stokes steps thanks to an implicit Euler scheme.
Convection step : the k^{th}-order characteristics scheme consists in computing an approximation at time t^{n+1} in [0,T] of the total derivative of any scalar quantity $C(U_i, \overline{u_iu_j}, \varepsilon, \theta)$ with the help of a k^{th}-order backward differentiation scheme integrated along the characteristics curve defined on the time interval $[t^{n-k+1}, t^{n+1}]$.
Diffusion and Stokes step : we can now compute C^{n+1} which denotes an approximation at time t^{n+1} by solving a diffusion problem (or a Stokes problem for velocity U and pressure p) by a classical k^{th}-order centered differentiation scheme. The coupled diffusion plus source terms step on U_i, $\overline{u_iu_j}$, ε will be detailed after.
A theoretical analysis of the whole scheme has been done in [16]. In N3S code, the 1st-order and 2nd-order schemes have been implemented for the k-ε model.

2.2. *Treatment of the coupling diffusion plus source terms step*

The numerical difficulties of SMC associated with replacing the stabilizing turbulent diffusion term, $\nu_t \frac{\partial^2 U_i}{\partial x_{k^2}}$ in the momentum equation by an explicit source term , $-\frac{\partial \overline{u_iu_j}}{\partial x_j}$, has certainly delayed the progress from eddy viscosity to SMC in engineering codes.

It is only the production term in the stress equation (involving velocity gradients) that introduces a coupling between adjacent momentum nodes. This coupling must be preserved by an implicit discretization similar to that of the pressure-velocity coupling in the Navier-Stokes equation

Let δU_i, $\delta\overline{u_iu_j}$, $\delta\varepsilon$, δp be the increments of all variables between time steps n and n+1, i.e. $\delta U_i = U_i^{n+1} - U_i^n$; we define also the "diffused velocity" δU_i^D.
All variables at time step n are known, the increments are given by :

$$\frac{\delta U_i^D}{\Delta t} = -\frac{\partial \overline{u_iu_j^n}}{\partial x_i} - \frac{1}{\rho}\frac{\partial p^n}{\partial x_i} - \frac{\partial \overline{\delta u_i u_j}}{\partial x_i} \qquad (12)$$

(explicit) (implicit)

$$\frac{\delta\overline{u_i u_j}}{\Delta t} = P_{ij}^{n} + \phi_{ij}^{n} + d_{ij}^{n} - \varepsilon^{n}\frac{2}{3}\delta_{ij} + \delta P_{ij} + \delta\phi_{ij} + \delta d_{ij} - \frac{2}{3}\delta\varepsilon\ \delta_{ij} \tag{13}$$

On the right hand side of Eq. 13 the first line is the explicit balance of the stress equation, and the second line is the implicit contribution of the increments which is discretized as follows:

$$\delta P_{ij} = -\overline{u_k u_j}^{n}\frac{\partial \delta U_i}{\partial x_k} - \overline{u_k u_i}^{n}\frac{\partial \delta U_j}{\partial x_k} \tag{14}$$

$$\delta\phi_{ij} = -C_2 dev(\delta P_{ij}) - C_1 dev(\overline{\delta u_i u_j})\frac{\varepsilon^{n}}{k^{n}} \tag{15}$$

$$\delta d_{ij} = \frac{\partial}{\partial x_k}\left(\left[C_s\frac{k}{\varepsilon}\overline{u_k u_l}\right]^{n}\frac{\partial}{\partial x_l}\overline{\delta u_i u_j}\right) \tag{16}$$

where the deviator of the Reynolds stress tensor is defined by $dev(\overline{u_i u_j}) = \overline{u_i u_j} - \frac{1}{3}\overline{u_n u_n}\delta_{ij} = k\ a_{ij}$, and it's anisotropy tensor by $a_{ij} = (\overline{u_i u_j}/k - \frac{2}{3}\delta_{ij})$.

Eq. 14 will ensure the velocity-stress coupling. Eq. 15 allows for inter-stress coupling while Eq. 16 is a diffusion operator which naturally must be implicit to ensure spacial coupling. Other terms coming from the linearization (but that do not contribute to the stability) are left out (e.g. the increment associated with the diffusion coefficient in Eq. 16).

The mean velocity increment and the pressure increment are obtained at the last stage of the scheme by using a Chorin-Temam algorithm [18], which ensure the incompressibility :

$$\begin{cases} \dfrac{\rho}{\Delta t}\delta U_i + \dfrac{\partial \delta p}{\partial x_i} = 0 \\ -\dfrac{\partial(\delta U_i)}{\partial x_i} = \dfrac{\partial(U_i^{D})}{\partial x_i} \end{cases} \tag{17}$$

2.3. *Space discretization*

The finite element method is based on a classical weak formulation on the stationnary problem obtain after the advection step. The unstructured meshes

use triangles or tetrahedra with a mixed formulation for the velocity and the pressure so as to get the Stokes problem well posed.
In order to satisfy the Brezzi-Babuska condition, the elements available in the N3S code are P1-P2 or P1-isoP2 elements. In most industrial cases, we use the P1-isoP2 element (linear discretization for the velocity on each subelement). The velocity mass-matrix can be mass-lumped without diminishing the global spatial precision. This leads to more simple calculations, particularly in the case of varying density.

2.4. *Finite element calculation*

One important part of the time in standard F. E. code is needed for F.E. calculation — obtained with Gauss formula numerical integration —, and assembling of the different matrices (varying in time with the eddy viscosity) and r.h.s. In N3S, only triangle in 2D and tetrahedron in 3D are kept. These elements, named simplicial elements, have interesting properties which allow us to compute the elementary terms (matrix and r.h.s.) by hand ; for example, the mass-matrix of linear triangle is directly obtained by :

$$\left[\int_T \psi_i \psi_j d\omega\right]_{I,J} = \frac{S}{12}\begin{vmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{vmatrix} \quad \text{(analog in 3D)}$$

where S is the surface of the element.
Based on this idea, we have developed a formal pre-processor adapted for all elementary matrix and r.h.s. calculations, PREFN3S. For one type of matrix or r.h.s., all the elementary terms are then computed in a single loop whose length is the total number of elements — this loop is fully vectorized on a CRAY supercomputer—.
For example, we give after the computational time on a CRAY Y-MP for a diffusion matrix calculation (806 217 non zero terms, the mesh is composed of 70 000 tetrahedra with 100 000 velocity nodes)

Method	Gauss	PREFN3S	Speed-up
Elementary calculation	18.4 s	0.17s	108

2.5. *Boundary conditions*

Boundary conditions depend on the type of boundary which is to be dealt with :
- for the inlet Γ_{in} of the Ω fluid domain, forced constrained conditions (Dirichlet) are used on all the variables ;
- for the outlet Γ_{out} of the Ω fluid domain, normal stress calculated by using pressure at previous time step for the velocity and vanishing flux conditions (homogeneous Neumann) for all other quantities are used ;
- for walls Γ_w a modelling based on the analysis of the boundary layer on a flat plate is used. For velocity, the normal component satisfies an impermeability condition (u.n = 0, where n is the exterior normal to the

wall). This condition is completed by a friction condition on the tangential stress ($\sigma.\tau = -\rho\, u_*^2$, where u_* is computed with the so-called logarithmic law). Concerning.the turbulent quantities $\overline{u_i u_j}$, ε , we can express each of it by using the friction velocity u_*. In a local frame related to the wall, this condition can be written as follows :

$$\begin{bmatrix} \overline{u_1u_1} & \overline{u_1u_2} & 0 \\ \overline{u_1u_2} & \overline{u_2u_2} & 0 \\ 0 & 0 & \overline{u_3u_3} \end{bmatrix} = u_*^2 \begin{bmatrix} 5.1 & -1. & 0. \\ -1. & 1. & 0. \\ 0. & 0. & 2.1 \end{bmatrix} \text{ and } \varepsilon = \frac{u_*^3}{\kappa y}$$

2.6. *Solvers*

2.6.1. After the space discretization, we obtain for the Eq. 12 to Eq. 16 a non symetrical linear system. This system is solved by a conjugate residual method which is efficient for non-symmetric linear systems and easy to implement. Let Y be a vector comprising all increments of variables at all nodes ; then, the system to solve is:

$$\frac{1}{\Delta t} Y = B^n + \underline{\underline{A}}.Y \tag{18}$$

where B^n is the explicit balances and $\underline{\underline{A}}.Y$ the coupling of increments. Assembly of the very large matrix $\underline{\underline{A}}$ would be complex and time-consuming (time-dependent coefficients). But this is not necessary since a conjugate residual algorithm is applied to Eq. 18. This is an iterative procedure; let the approximate solution at iteration k be known : $Y^k = (\delta U_i^k, \delta\overline{u_i u_j}^k, \delta\varepsilon^k)$.
It is then simple to compute the residual R^k :

$$R^k = \frac{1}{\Delta t} Y^k - B^n - \underline{\underline{A}}.Y^k \tag{19}$$

(improvement of matrix vector product needed for $\underline{\underline{A}}.Y^k$ have been done by using sophisticated storage mode [17]).
The next iteration is defined by $Y^{k+1} = \alpha\, Y^k + \beta\, Y^{k-1}$ where the scalars a and b are computed as functions of scalar products of R^k , R^{k-1} and Y^k. α and β are optimized so that R^{k+1} will be minimal.
Finally, with the this incremental formulation and conjugate residual it is easy to switch from linear to more sophisticated models.
2.6.2. The space discretization of pressure-continuity step (Eq. 17) leads to a symmetrical matrical system :

$$\begin{bmatrix} M & B^t \\ B & 0 \end{bmatrix} \begin{bmatrix} \delta U \\ \delta P \end{bmatrix} = \begin{bmatrix} 0 \\ S \end{bmatrix} \tag{20}$$

where M is the mass-matrix, B the divergence-matrix, B^t the gradient-matrix. If we mass-lump the mass-matrix and eliminate the velocity in Eq. 20, we obtain the equivalent system :

$$-[BM^{-1}B^t][\delta P] = [S] \quad (21)$$

$$[\delta U] = -[M^{-1}B^t][\delta P] = [S] \quad (22)$$

In this case, the laplacian like pressure matrix $[BM^{-1}B^t]$ can be easily built. It can be solved either by a classical Preconditioned Conjugate Gradient algorithm, or a direct solver by using a complete Cholesky factorization. An efficient sparse Cholesky factorization scheme has been especially developped [19], which provides a significant reduction of the total CPU time needed for solving the pressure-continuity step, and gives a divergence of the velocity field close to zero.

3. A 2D application : flow around cylinders

We consider here a flow inside a tube bundle (ERCOFTAC/IAHR test case, 1993 [20]). After the first odd rows of tubes the flow becomes periodic and the computation can be reduced to a minimal inter-tube spacing using symmetries and periodic inlet-outlet conditions (see fig. 1). Though the numerical approach to this important problem of cross-flow in a tube bank seems feasible, the k-ε model does not permit to replace experimental studies. The mean flow pattern is easily reproduced because it is dominated by inertia and pressure forces when the gaps are narrower or equal to the tube diameter.This flow is interesting because periodicity makes it free of inlet conditions.

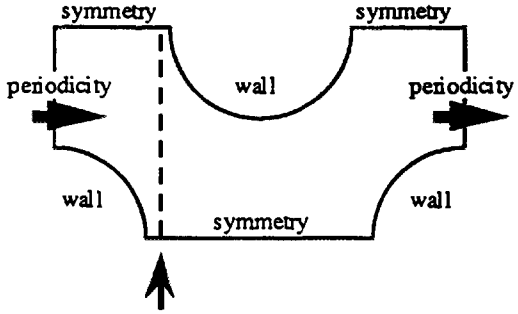

Figure 1 : computational domain for the flow in a staggered tube bundle

The level of turbulence depends only on equilibrium between production P_k and dissipation ε. The former term along the impinging axis is modeled in the k-ε approach by $P_{k\varepsilon} = 4\nu_t\left(\frac{\partial U}{\partial x}\right)^2$, but it is exact in the RSM : $P_{R_{ij}\varepsilon} = -\left(\overline{u_y^2}-\overline{u_x^2}\right)\frac{\partial U}{\partial x}$

Thus $P_{k\varepsilon}$ is always positive and becoming very large near the stagnation point whereas $P_{Rij\text{-}\varepsilon}$ stays null whatever the rate of strain as long as the turbulence stays isotropic. By integration the k-ε model gives an over-estimation of k by 100% ! The standard R_{ij}-ε though still gives some positive production because the axial fluctuation is larger than the longitudinal one while the experiment curiously exhibits the opposite. On the whole, in opposition to the k-ε the standard R_{ij}-ε model gives an under-estimation of k and a good prediction of the shear stresses (fig. 2).

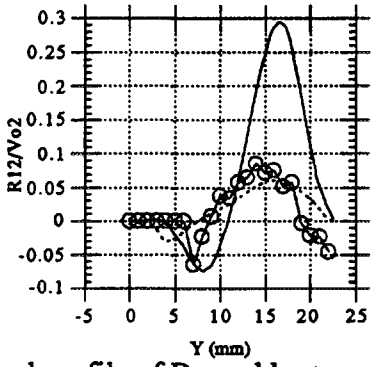

Figure 2: vertical profile of Reynolds stress R_{12} at section Xr
— : N3S computation k-epsilon model, o : experiment,
--- : N3S computation R_{ij}-epsilon model.

Further improvement can be obtained by using a simple modification of the ε equation :

$$\frac{\partial \varepsilon}{\partial t} + \overline{U}_k \frac{\partial \varepsilon}{\partial x_k} = C_{\varepsilon 1} \frac{\varepsilon}{k} P - C_{\varepsilon 2} \frac{\varepsilon^2}{k} + C_\varepsilon \frac{\partial}{\partial x_k} \left(\frac{k}{\varepsilon} \overline{u_k u_l} \frac{\partial \varepsilon}{\partial x_l} \right)$$

In anisotropic flows Launder et al. [21] suggest a dependence of the ε equation constants in terms of the anisotropy tensor invariants :

$$C_{\varepsilon 1} = 1 \, , \, C_{\varepsilon 2} = \frac{1.92}{1 + 0.6 \sqrt{A_2}\, A}$$

$$a_{ij} = \left(\overline{u_i u_j} \, / k - \frac{2}{3} d_{ij} \right) ,$$

$$A_2 = a_{ik} a_{ki}, \quad A_3 = a_{ik} a_{km} a_{mi}, \quad A = 1 - \frac{9}{8} (A_2 - A_3)$$

On fig. 3 we see a very significant improvement on turbulence level at section Xr using this modification of the of the ε equation.

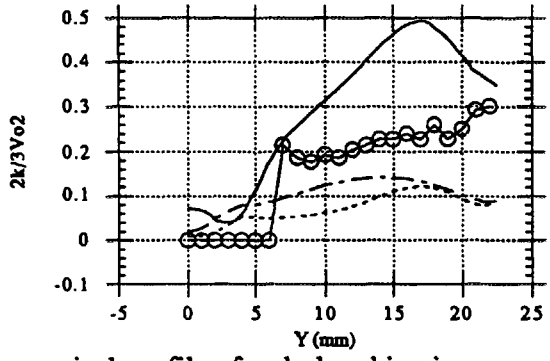

Figure 3 : vertical profile of turbulent kinetic energy at section Xr
— : N3S computation k-epsilon model, o : experiment,
--- : N3S computation R_{ij}-epsilon model,
— - —: N3S computation R_{ij}-epsilon model with modification on ε equation.

4. 3D applications

Some three dimensional application will be presented at the conference :
• validation of the implementation on the turbulent channel flow,
• developing flow in a curved rectangular duct [22].

5 Conclusion

In this paper, the feasability to implement in a finite element code a turbulent model such as R_{ij}-ε model has been presented. One important result is that the efficient algorithm which is used can extend easily to more sophisticated R_{ij}-ε model such as so-called "cubic" models. Now, coupling with temperature are being developed.

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