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Diffusion-convection problems using boundary-domain integral formulation for non-uniform flows

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Abstract

The paper presents a new numarical approach for diffusion-convection problems in non-uniform velocity field employing fundamental solution of the corresponding steady-state difusion-convection equation with constant coefficients and an extreme concept of subdomain technique. Numerical example of steady state flow in two-dimensions is included to demostrate the accuracy present numerical technique.

Introduction

The diffusion-convection equation is one of the most basic governin equation describing the transport phenomena in classical physic. However, it is still very difficult to numerically solve this type of equation, when the convection term is dominant. Most of the common numerical methods give emphasis on algorithms to suppress the well-known problems of oscillation in numerical solution for high Pe number values [4]. Applications of the boundary-domain integral formulation is free from these problems due to the correct degree of "upwind" presented in the fundamental solution of the convection-diffusion equation [8].
A substantial number of different formulations by BEM for the diffusion-convection equation has appeared in the literature. Some of them have employed the elliptic or parabolic fundamental solution and treated the convective term as pseudo-sources [6], but they are useful only for low Pe, number values. Alternatively, the velocity field can be decomposed into an average and a variable part and the fundamental solution of the diffusion-convection equation used incorporating the average velocity. The variable part of field can be accouted for either by domain diskretization [5] or through DRM technique [7]. This approach is applicable for moderate Pe number values. For high Pe number values only for constant velocity field the BEM technique is developed [1].

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In the new algorithm for high Pe number values, the main restriction of the formulation, fact that the fundamental solution are only avaliable for equations with constant coefficients, is overcome by decomposition of the domain under consideration into subdomains, which allows the use of constant coefficients [9]. Such formulation drastically cuts down the computation of integrals and allows the use of the alternative solvers for sparse matrices.

Governing equation

Let us consider a general unsteady state nonlinear diffusion-convection equation describing time dependent transfer of an arbitrary scalar function $u(r,t)$ in a homogeneous and isotropic medium defined in solution domain $R = \Omega \times I$ representing the product of space Ω and time interval $I(t_0, t)$

$$\frac{\partial}{\partial x_j}\left(a_e \frac{\partial u}{\partial x_j}\right) - \frac{\partial u}{\partial t} - \frac{\partial v_j u}{\partial x_j} - k_e u + I_u = 0 \quad \text{in} \quad R \ , \tag{1}$$

where $v_j(r_k)$ is the local solenoidal velocity field. The variable $u(r_k)$ can be interpreted, e.g. as a temperature in heat transfer problems, concentration in dispersion processes, vorticity in fluid dynamics problems, turbulent kinetic energy in its transport equation etc., and will be refered to as a potential. The effective diffusivity $a_e(r_k, u)$, the effective reaction constant $k_e(r_k, u)$ and the source term $I_u(r_k, u)$ are some monotonic space and potential dependent functions. The effective diffusivity a_e and the reaction constant k_e can be always partitioned into a constant a_0 and a variable part $a_N(r_k, u)$

$$a_e = a_0 + a_N(r_k, u) \ . \tag{2}$$

$$k_e = k_0 + k_N(r_k, u) \ . \tag{3}$$

This permits rewriting eq. (1) as

$$a_0 \frac{\partial^2 u}{\partial x_j \partial x_j} - \frac{\partial u}{\partial t} - \frac{\partial v_j u}{\partial x_j} - k_0 \, u + \frac{\partial}{\partial x_j}\left(a_N \frac{\partial u}{\partial x_j}\right) - k_N \, u + I_u = 0 \quad \text{in} \quad R \ , \tag{4}$$

The eq. (4) represents a parabolic initial-boundary values problem, thus some boundary and initial conditions have to be known to complete the mathematical description of the problem, e.g. Dirichlet, Neumann or Cauchy type boundary conditions have to be prescribed on the part of the boundary Γ_1, Γ_2 and Γ_3 respectively

$$\begin{aligned} u &= \overline{u} && \text{on} \quad \Gamma_1 && \text{for} \quad t > t_0 \ , \\ \frac{\partial u}{\partial x_j} n_j &= \overline{\frac{\partial u}{\partial n}} && \text{on} \quad \Gamma_2 && \text{for} \quad t > t_0 \ , \\ \frac{\partial u}{\partial x_j} n_j &= \alpha_u (u - u_f) && \text{on} \quad \Gamma_3 && \text{for} \quad t > t_0 \ , \end{aligned} \tag{5}$$

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while the initial conditions are

$$u = \overline{u}_0 \quad \text{in} \quad \Omega \quad \text{at} \quad t = t_0 \ . \tag{6}$$

α_u is transfer coefficient between the fluid flow surface defined by the unit normal vector $\vec{n}$, and the surrounding ambient at the potential u_f.

Integral representation for the steady transport equation

Perhaps the most adequate and stable integral formulation regardless on Reynold's number values can be obtained by using the fundamental solution of diffusion-convective *PDE* with constant coefficients. The general steady-state transport including first order reaction can be governed by the equation

$$a_0 \frac{\partial^2 u}{\partial x_j \partial x_j} - \frac{\partial v_j u}{\partial x_j} - k_0 u + b = 0 \quad \text{in} \ \Omega \ , \tag{7}$$

where b stands for the pseudo-body force term. In order to developed an integral equation to the above *PDE*, a fundamental solution of eq. (7) is necessary. Since it exists only for the case of constant velocity fields, the variable velocity vector $v_j(r_k)$ has to be decomposed into an average constant vector $\overline{v_j}$ and perturbation vector $\tilde{v}_j$, such that [5]

$$v_j(r_k) = \overline{v}_j + \tilde{v}_j(r_k) \ , \tag{8}$$

This permits rewriting eq. (7) as

$$a_0 \frac{\partial^2 u}{\partial x_j \partial x_j} - \frac{\partial \overline{v}_j u}{\partial x_j} - k_0 \ u + \frac{\partial}{\partial x_j}\left(a_N \frac{\partial u}{\partial x_j}\right) - \frac{\partial \tilde{v}_j u}{\partial x_j} - k_N \ u + I_u = 0 \quad \text{in} \quad R \tag{9}$$

The above diferential formulation can now be transformed into an equivalent integral statement using a weighted residual technique or Green's theorems for scalar functions, resulting in the following integral formulation

$$c(\xi)u(\xi) + a_0 \int_\Gamma u \frac{\partial u^{*C}}{\partial n} d\Gamma = \int_\Gamma a_e \frac{\partial u}{\partial n} u^{*C} d\Gamma - \int_\Gamma u v_n u^{*C} d\Gamma +$$

$$+ \int_\Omega \left[\left(u\tilde{v}_j - a_N \frac{\partial u}{\partial x_j}\right) \frac{\partial u^{*C}}{\partial x_j} - (k_N \ u - I_u) u^{*C} \right] d\Omega \tag{10}$$

where $v_n = \overline{v}_n + \tilde{v}_n = v_i \cdot n_i$ and u^{*C} is now the fundamental solution of the diffusion-convective equation with constant coefficients [3], i.e. the solution of

$$a_0 \frac{\partial^2 u^{*C}}{\partial x_j \partial x_j} + \frac{\partial \overline{v_j} u^{*C}}{\partial x_j} - k_0 u^{*C} + \delta(\xi, s) = 0 \tag{11}$$

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where is

$$u^{*C} = \frac{1}{2\pi a_0} \exp\left(\bar{v}_j \cdot r_j / 2a_0\right) K_0(\mu r) \tag{12}$$

for 2D cases and

$$u^{*C} = \frac{1}{4\pi r\, a_0} \exp\left((\bar{v}_j \cdot r_j)/2a_0 - \mu r\right) \tag{13}$$

for 3D cases. K_0 is modified Bessel function of order zero and factor μ is

$$\mu^2 = \left[\left(\frac{\bar{v}}{2a_0}\right)^2 + \frac{k_0}{a_0}\right] ; \qquad \bar{v}^2 = \bar{v}_j \cdot \bar{v}_j \tag{14}$$

Notice, that in the domain integral only the convection due to the perturbation velocity field exists, making this approach combined with sub-structure technique the most promissible one for the numerical solution of general fluid flow problems for high Reynolds number values.

Integral representation for unsteady transport equation

Let us introduce left non-symmetric finite difference approximation of the time derivative in eq. (1)

$$\frac{\partial u}{\partial t} \cong \frac{u_F - u_{F-1}}{\tau} , \tag{15}$$

what permits rewriting eq. (4) as

$$a_0 \frac{\partial^2 u_F}{\partial x_j \partial x_j} - \frac{\partial v_j u_F}{\partial x_j} - \frac{1}{\tau} u_F - k_0\, u_F + \frac{\partial}{\partial x_j}\left(a_N \frac{\partial u}{\partial x_j}\right) - k_N\, u + I_u + \frac{1}{\tau} u_{F-1} = 0 \tag{16}$$

After decomposition of velocity vector the following integral representation can be obtained

$$c(\xi) u_F(\xi) + a_0 \int_\Gamma u_F \frac{\partial u^{*H}}{\partial n} d\Gamma = \int_\Gamma a_e \frac{\partial u_F}{\partial n}\, u^{*C} d\Gamma - \int_\Gamma u_F v_n u^{*C} d\Gamma$$

$$+ \int_\Omega \left[\left(u_F \tilde{v}_j - a_N \frac{\partial u_F}{\partial x_j}\right) \frac{\partial u^{*C}}{\partial x_j} - (k_N\, u_F - I_u)\, u^{*C}\right] d\Omega + \frac{1}{\tau} \int_\Omega u_{F-1} u^{*C} d\Omega \tag{17}$$

Parameter μ from (14) is now expanded for additional term

$$\mu^2 = \left[\left(\frac{\bar{v}}{2a_0}\right)^2 + \frac{k_0}{a_0} + \frac{1}{a_0\, \tau}\right] ; \tag{18}$$

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The boundary-domain integral eq. (17) is formally identical to eq (10) except for the additional initial conditions domain integral. Althought the complete implicit scheme is developed, Crank-Nicholson and others, can be simply formulated on the same manner.

Extreme concept of subdomain technique

Developed method is based on so called extreme concept of subdomain technique similar to that of finite volumes. Namely, in general fluid flow problem the velocity vector is changing its direction and its absolute values from one field point to another. The diffusion coeffitient, reaktion constant and the source term also usually depends from the point to point, so that the variable part in (4) becomes predominant for the whole domain. This problem is overcame by decomposition of the interesting domain into subdomains, which locally allow constant material properties and velocity vector (Fig. 1).

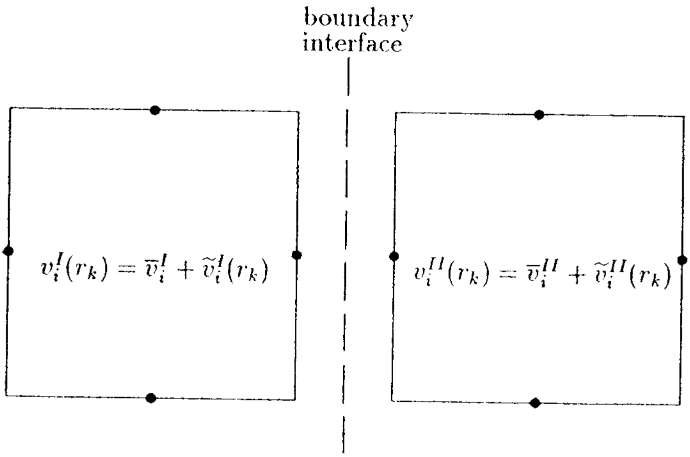

Fig.1: Extreme concept of subdomain technique

After discretisation, is one subdomain, described by integral formulation (10) or (17), surrounded by four constant boundary elements (Fig. 1). The domain integrals are captured by constant internal cell what follows next discret form for each subdomain respectively

$$[H]\{u\} = [G]\{\frac{\partial u}{\partial n}\} - [C]\{u\} - [G]\{\tilde{v}_n u\} + [B] \qquad (19)$$

Subdomains are connected at the interfaces throught the compatibility and equilibrium boundary conditions.

$$\{u\}^I = \{u\}^{II}; \qquad (20)$$

$$\{\frac{\partial u}{\partial n}\}^{I} = -\{\frac{\partial u}{\partial n}\}^{II} \tag{21}$$

This approach unlike all previous Boundary Element and Boundary-Domain methods provides us with extreme sparse matrix which allows an efficient use of powerfull iterative solvers.

Test example and discussion

The effectivity of single subdomain is tested for steady state transport on a simple example of one dimensional scalar transport [8]. Since the analytical solution for high Pe number values (over 100) is practically a step function, the comparison is done for outlet normal derivative of function. Results are given in Table 1. It is obviesly, that the accuracy of the solution depends only on exact calculation of integrals and is not dependent on the ratio of $\overline{v}/\kappa$.

Pe	Analytically	Numerically	Error (%)
10^2	100.0000	100.000	—
10^3	1000.000	1000.002	—
10^4	10000.000	10000.46	$4.6\ 10^{-3}$
10^5	100000.00	100050.8	$5.0\ 10^{-2}$
10^6	1000000.0	1004404.	0.44

Table 1: Comparison of normal derivatives at $x = L$ for different Pe

To study the applicability of the new numerical approach for a large practical problem with non-uniform velocity field, heat conditions in a five row in-line tubular heat exchanger were computed. Velocity field for Re=850 (based on maximal velocity) was taken from previous computations by Boundary-Domain Integral Method (BDIM) [2], where forced convection in tubular heat exchangers was examined. Figure 2 presents the new results for temperature distribution for Pe=600 (Pr=0.7), where it is clearly visible that cold fluid, which enters at left, gets heated up when passing through the bundle. The effect of recirculation zones between the tubes and behind the last tube can be noticed also in Nusselt number values for each row, as these decrease in the weak recirculation areas (Fig. 3). Comparison of experimental and numerical data obtained by classical [2] and alternative formulation for average Nu number is given in Table 2.

1 Conclusion

Boundary-domain integral method offers some important features in computational fluid dynamics. Due to the fundamental solutions more or less

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	Experimental	Classical f.[2]	Alternative f.
Nu	10.68	7.22	10.57

Table 2: Comparison of experimental and numerical data

transport process is transfered to the boundary, producing a very stable and accurate numerical scheme. In a numerical algorithm, for example based on Laplace's or diffusion Green's function, the diffusion is completely described by boundary integrals only, and for the convection the domain discretization is needed. Much more efficient numerical scheme can be formulated regardless of Reynolds number values for the diffusion-convective Green's function, where only the convection for the perturbation velocity field is governed by the domain integrals. Very straight forward formulation for the time dependent problems can be developed by using fundamental solution of steady-state diffusion-convection equation including first order reaction term and finite-difference approximation in time.

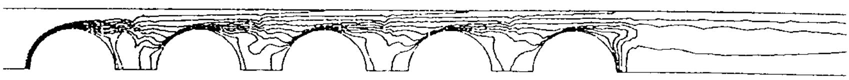

Figure 2: Temperature field for Re=850 and Pr=0.7

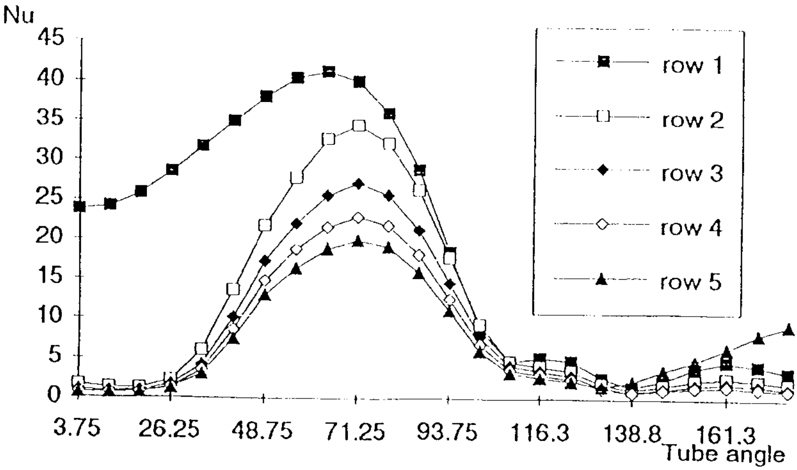

Figure 3: Local Nu numbers

At it is well known the system matrices resulting in boundary-domain technique are completely accupied at least in its original form and the Gauss direct solver has to be used, the consequences of these fact are enormous computation times and memory demands. The method can be drastically improved by using sub-domain technique and mixed-type boundary elements, which can be developed in extreme case to the concept of finite volume. Using sub-domain approach the sparsity patherns of system matrices are strongly improved, and the preconditioned conjugate gradient iterative methods can be succesfully used in very promising computation time and memory savings.

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