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A NUMERICAL METHODOLOGY TO SOLVE THERMAL POLLUTION PROBLEMS

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Abstract. *The advances in computer technologies have expanded the capability for numerical simulation in science and engineering. This happens specially in environmental problems since their mathematical and computational complexity can grow very fast. Their solutions have required the development of appropriate mathematical models, numerical methodologies and algorithms to solve practical problems. A common environmental problem is the thermal pollution created by a thermal power plant where cold water is pumped into the plant and returned at elevated temperature. This relatively hot water is detrimental to aquatic life in rivers, lakes or bays. There are two approaches to deal with thermal pollution problems. In the near-field approach the problem is concerned with a very limited zone, near the discharge point. The other one is the far-field approach in which the main emphasis is on the effects of a perturbation at a considerable distance downstream. The purpose of this work is to provide a numerical methodology to solve thermal pollution problems efficiently in the far-field approximation. The Streamline Upwind Petrov-Galerkin Method provides the numerical stability of the finite element method. The solution of the algebraic linear system that arises from the finite element discretization is performed by a new method called Left Conjugate Gradient Method presented by Yuan, Golub and Plemmons. Its performance is compared with the most traditional methods for this type of problems, the GMRES Method.*

Keywords: *thermal pollution, convection-diffusion, iterative methods, finite element*

1. Introduction

In recent years water pollution in surface waters like rivers, lakes and coastal seas dominate discussions of environmental problems world-wide. This concern is motivated by the increasing in human activities in the last decade and the high cots of new technologies to obtain drinking water.

Modeling environmental problems is not an easy task due to the fact that they deal with large scale phenomenon for a long period of time. As an example, consider the impact of the installation of a power plant on a river ecosystem. Because of the discharge of hot water, even slightly higher than the original water temperature, factors like: low circulation regions of the river, bathymetry and seasonal variation of the air temperature can keep the water temperature higher for long distances and long periods of time which can promote and accelerate some chemical reactions and decrease the dissolved oxygen (DO), affecting the water quality and the river ecosystem.

The numerical model for the thermal pollution problem must satisfy some basic essential requirements in order to get a feasible computation. First of all, the finite element formulation should be stable enough to deal with thermal gradients that often appear in such problems. Here this is provided by the Streamline Upwind Petrov-Galerkin Method (SUPG) proposed by Brooks and Hughes, 1982, which has good stability and accuracy properties in the case of regular exact solution. The used finite element space is spanned by piecewise linear functions. The efficient solution of the resulting system of linear equations that arises from the discretization is the main focus of this work.

Solving this discrete problems requires the resolution of large, sparse and non-symmetric systems of linear equations for different scenarios. It is well known that iterative methods are the only affordable choice when dealing with large and sparse systems. In this work we evaluate the use of a new iterative method introduced by Yuan et al., 2000, called Left Conjugate Gradient method (LCG). We use a traditional method, in this case the GMRES(k) method introduced by Saad and Schultz, 1986, to compare with its performance.

The outline of this paper is as follows. In Section 2, the thermal pollution problem is presented and the numerical formulation used is derived. Section 3 presents the basic ideas of the Left Conjugate Gradient method

(LCG). Section 4 briefly presents the GMRES method. The numerical experiments are presented in Section 5 and, finally, Section 6 draws the final conclusions as well as the directions for further research.

2. Problem Statement

The thermal pollution problem can be modeled by the stationary convection-reaction-diffusion transport equation of the form

$$\boldsymbol{\nabla} \cdot (-\mathbf{K}\boldsymbol{\nabla}\phi) + \mathbf{u} \cdot \boldsymbol{\nabla}\phi + \sigma\phi = f \qquad \text{in} \quad \Omega, \tag{1}$$

with the following boundary conditions

$$\begin{aligned} \phi(\mathbf{x}) &= g(\mathbf{x}) \ , \qquad && \mathbf{x} \in \Gamma_g, \\ -\mathbf{K}\boldsymbol{\nabla}\phi \cdot \mathbf{n} &= q(\mathbf{x}) \ , \qquad && \mathbf{x} \in \Gamma_q, \end{aligned} \tag{2}$$

where the bounded domain $\Omega \in \Re^n$ has a smooth boundary $\Gamma = \Gamma_g \cup \Gamma_q$, $\Gamma_g \cap \Gamma_q = \emptyset$, with an outward unit normal $\mathbf{n}$. The unknown field $\phi = \phi(\mathbf{x})$ is the physical quantity to be transported by a flow, characterized by the given velocity field $\mathbf{u} = (u_1, \ldots, u_n)$, the diffusion tensor $\mathbf{K} = \mathbf{K}(\mathbf{x})$,the reaction term σ and the source term f. The functions $g(\cdot)$, $q(\cdot)$ are given data.

It is well known that if the boundary data $g(\cdot)$ is discontinuous there may be regions in Ω, where the solution ϕ varies dramatically. The width of such layers depends on the amount of diffusion present in the fluid flow, being very small for convection-dominated problems. In this case, the use of the standard Galerkin finite element method produces a globally oscillating approximate solution unless an extremely fine mesh is used, which most of the time leads to an unbearable computational cost for practical purposes. To resolve those sharp layers the SUPG method is used, which is presented in the next section.

2.1. Approximate Solution

Let us consider a finite element partition π^h of triangular elements Ω_e such that $\overline{\Omega} = \bigcup_{e=1}^{N_e} \overline{\Omega}_e$ and $\bigcap_{e=1}^{N_e} \Omega_e = \emptyset$, where N_e is the total number of elements in π^h. The chosen finite dimensional set of kinematically admissible functions and space of admissible variations are

$$\mathcal{S}^h = \left\{ \phi^h \in C^0\left(\Omega\right), \ \phi^h\big|_{\Omega_e} \in P_e^k \ , \ \phi^h\big|_{\Gamma_g} = g \right\} \tag{3}$$

and

$$\mathcal{V}^h = \left\{ \theta^h \in C^0\left(\Omega\right), \ \theta^h\big|_{\Omega_e} \in P_e^k \ , \theta^h\big|_{\Gamma_g} = 0 \right\}, \tag{4}$$

where P_e^k is the space of polynomials of degree less or equal to k and the subscript e denotes the restriction of a given function to the element Ω_e.

With these definitions, the Petrov-Galerkin approximation of the problem (1) consists of finding $\phi^h \in \mathcal{S}^h$ such that

$$G\left(\phi^h, \theta^h\right) + \sum_{e=1}^{N_e} \left(R_e\left(\phi^h\right), p_e^h\right)_{\Omega_e} = F\left(\theta^h\right), \tag{5}$$

$\forall \ \theta^h \in \mathcal{V}^h$, where

$$R_e\left(\phi^h\right) = \boldsymbol{\nabla} \cdot \left(-\mathbf{K}\boldsymbol{\nabla}\phi^h\right) + \mathbf{u} \cdot \boldsymbol{\nabla}\phi^h + \sigma\phi - f \qquad \text{in} \quad \Omega_e \tag{6}$$

is the residual of the approximate solution, with G and F defined as:

$$\begin{aligned} G\left(\phi^h, \theta^h\right) &= \left(\mathbf{u} \cdot \boldsymbol{\nabla}\phi^h, \theta^h\right) + \left(\mathbf{K}\boldsymbol{\nabla}\phi^h, \boldsymbol{\nabla}\theta^h\right) + \left(\boldsymbol{\sigma}\phi^h, \theta^h\right), \\ F\left(\theta^h\right) &= \left(f, \theta^h\right) + \left(q, \theta^h\right)_{\Gamma_q}. \end{aligned}$$

<u>**Remarks:**</u>

1. in the formulation (5), the space of weighting functions is constructed by adding to the standard Galerkin weighting function $\theta^h \in \mathcal{V}^h$ a perturbation p_e^h in each element Ω_e. Different choices of this perturbation generate different consistent Petrov-Galerkin methods;

2. the operator $G\left(\cdot, \cdot\right)$ stands for the Galerkin contribution to (5).

The SUPG method introduces a discontinuous perturbation in the streamline direction defined as

$$p_e^h = \tau_e^s \ \mathbf{u}_e \cdot \boldsymbol{\nabla}\theta^h \ , \qquad e = 1, \ldots, N_e \ , \tag{7}$$

where τ_e^s is the upwind function given by:

$$\tau_e^s = \frac{\xi_e h_e}{2|\mathbf{u}_e|} \tag{8}$$

with h_e being the characteristic element length in the streamline direction and ξ_e the non-dimensional numerical diffusivity as defined in Brooks and Hughes, 1982. Rewriting the variational formulation (5) we obtain:

$$G\left(\phi^h, \theta^h\right) + C\left(\phi^h, \theta^h\right) = \overline{F}\left(\theta^h\right) \ , \qquad \forall \ \theta^h \in \mathcal{V}^h \ , \tag{9}$$

where

$$C\left(\phi^h, \theta^h\right) \ = \ \sum_{e=1}^{N_e} \left\{ \left(\tau_e^s \ \mathbf{D}\boldsymbol{\nabla}\phi^h, \boldsymbol{\nabla}\theta^h\right)_{\Omega_e} - \left(\boldsymbol{\nabla} \cdot \mathbf{K}\boldsymbol{\nabla}\phi^h, \tau_e^s \ \mathbf{u}_e \cdot \boldsymbol{\nabla}\theta^h\right)_{\Omega_e} + \left(\boldsymbol{\sigma}\phi^h, \tau_e^s \ \mathbf{u}_e \cdot \boldsymbol{\nabla}\theta^h\right)_{\Omega_e} \right\}$$

and

$$\overline{F}\left(\theta^h\right) = F\left(\theta^h\right) + \sum_{e=1}^{N_e} \left(f, \tau_e^s \ \mathbf{u}_e \cdot \boldsymbol{\nabla}\theta^h\right)_{\Omega_e} \ . \tag{10}$$

In the above expression $\mathbf{D} = \mathbf{u}_e \otimes \mathbf{u}_e$, with $\otimes$ denoting the tensor product. It is exactly the quadratic term containing the tensor $\mathbf{D}$ which is responsible for the additional stability engendered by the SUPG method.

Substituting ϕ^h and θ^h in (9) leads to a system of linear equations that can be written as:

$$Ax = b \tag{11}$$

where x is the unknown vector, A is a non symmetric matrix and b is the source given vector. For practical interests, in special for 3D and transient problems, this system is solved by iterative methods. But to find the most effective method for the problem at hand is still a challenge. In the next section a new iterative method introduced by Yuan et al., 2000, is presented.

3. The Left Conjugate Gradient Method

The Left Conjugate Gradient method (LCG) proposed by Yuan et al., 2000, is different in nature from the Krylov subspace methods, such as GMRES and their variants. The main difference is that LCG method finds a basis of $I\!R^n$ that enables the exact solution of (11) to be expressed uniquely by solving a triangular system, instead of solving at each iteration a least square problem. Besides, LCG method can be applied in order to find the inverse of A.

Although LCG could be reduced to CG when the matrix is symmetric and positive definite, the method does not keep the conjugate orthogonality property in the non symmetric case. LCG also guarantees finite termination, in the absence of roundoff errors, but looses some short recurrence relations. The method is designed as follows.

The vectors $p_1, p_2, \ldots, p_n \in I\!R^n$ denotes the left conjugate gradient vectors in respect to A if, for $i, j = 1, \ldots, n$,

$$\begin{cases} p_i^T A p_j = 0, & \text{for} \quad i < j, \\ p_i^T A p_i \neq 0. \end{cases}$$

Suppose $p_1, \ldots, p_n$ are given LCG vectors. Analogous to the meaning of the residual defined by $r = b - Ax$ in CG method, that attends the optimally condition of a corresponding minimization problem (Golub, 1985), the residual r^*, evaluated on the exact solution x^* of (11) should obey

$$p_i^T r^* = 0, \quad \forall i = 1, \ldots, n. \tag{12}$$

Since $p_1, \ldots, p_n$ are linear independent vectors when A is nonsingular, let us consider

$$x^* = x_0 + \sum_{i=1}^{n} \alpha_i p_i,$$

for a given $x_0 \in I\!R^n$. Observe that x^* is uniquely determined by $p_1, \ldots, p_n$ and x_0. Thus, substituting x^* in (12), the following expressions can be derived, for $i = 1, \ldots, n$:

$$\begin{aligned} \alpha_i &= \frac{p_i^T r_{i-1}}{p_i^T A p_i}, \\ r_i &= b - Ax_i = r_{i-1} - \alpha_i A p_i, \\ x_i &= x_0 + \sum_{k=1}^{i} \alpha_k p_k = x_{i-1} + \alpha_i p_i. \end{aligned}$$

Let r_k and $p_1, \ldots, p_k$ be respectively the residual and the LCG vectors given at iteration k. Suppose the next LCG vector can be expressed by

$$p_{k+1} = r_k + \sum_{i=1}^{k} \beta_i p_i. \tag{13}$$

By definition of LCG vector, for all $1 \leq j < k+1$, we have

$$p_j^T A p_{k+1} = 0.$$

Pre-multiplying $p_j^T A$ in (13), $j = 1, \ldots, k$, we shall obtain the following recurrence formulas to generate a well defined p_{k+1}:

$q_0 = r_k$
for $i = 1, \ldots, k$
    $\beta_i = -\left(p_i^T A q_{i-1}\right) / \left(p_i^T A p_i\right)$
    $q_i = q_{i-1} + \beta_i p_i$
$p_{k+1} = q_k$.

Regarding the fact that A is neither a symmetric nor a positive definite matrix, the choice of the first direction must be such that $p_1^T A p_1 \neq 0$. The LCG algorithm with few modifications related to the convergence test is here reproduced:

LCG Algorithm

given A, b, x_0, p_1 such that $p_1^T A p_1 \neq 0$ and $\varepsilon > 0$
compute $r_0 = b - Ax_0$
set $k = 1$
while $k \leq n$ and $\|r_k\| > \varepsilon$
    $q_k = A^T p_k$
    $\alpha_k = (p_k^T r_{k-1})/(q_k^T p_k)$
    $x_k = x_{k-1} + \alpha_k p_k$
    $r_k = r_{k-1} - \alpha_k A p_k$
    $p_{k+1} = r_k$
    for $i = 1, \ldots k$
        $q_i = A^T p_i$
        $\beta_i = -(q_i^T p_{k+1})/(q_i^T p_i)$
        $p_{k+1} = p_{k+1} + \beta_i p_i$
    $k = k + 1$
end of while

Remarks:

- the total flops per iteration of the above algorithm is $2n^2 + (2k+4)n + 1$. In the case A is symmetric and positive definite, the algorithm obtains the A-conjugate gradients vectors of CG method;
- in Yuan et al., 2000, the LCG authors present also a variant of LCG method called Generalized LCG to overcome problems with skew symmetric matrices and general breakdown problems.

Here, the performance of the method just outlined is compared with the most traditional one used for non symmetric Computational Fluid Dynamics (CFD) problems, the GMRES method, that will be presented in the following section for the sake of clarity.

4. GMRES

The GMRES method, proposed by Saad and Schultz in 1986, has gained wide acceptance in solving systems coming from CFD problems due to the following properties:

- it never breaks down, unless the exact solution has already been achieved;
- the convergence is monotonic;
- assuming exact arithmetic, it converges in no more than n iterations.

The GMRES derives an approximate solution to x in the form $x = x_0 + z$, where x_0 is the initial guess and z comes from minimizing the residual $\|b - A(xo + z)\|$ over the Krylov subspace $span\left[r_0, Ar_0, A^2r_0, ..., A^k r_0\right]$, where here k is the dimension of the Krylov space and $r_0 = b - Ax_0$. The major known drawback of GMRES is that increasing k the amount of memory required per iteration increases linearly and the computational work increases quadratically. In order to control the amount of work and memory requirements a restarted version (GMRES(k)) is used. This means that after k orthogonalization steps all variables will be cleaned up and the solution obtained at this point will be taken as the initial solution for the next k steps. Unfortunately, there are some problems for which this version stagnates, failing convergence indenpendent of the value of k (Barret et al., 1994). The restarted version algorithm used here is the following:

GMRES(k) Algorithm

given A, b, x_0, k and $\varepsilon > 0$
repeat
    set $nsteps = 0$
    while $nsteps < k$
        (Arnoldi process)
        compute $r_0 = b - Ax_0$, $\beta = \|r_0\|$ and $v_1 = r_0/\beta$
        for $j = 1, \ldots, k$
            compute $w = Av_j$
            for $i = 1, \ldots, j$
                $h_{i,j} = (w, v_i)$
                $w = w - h_{i,j} v_i$
            compute $h_{j+1,j} = \|w\|$ and $v_{j+1} = w/h_{j+1,j}$.
        define $V_k = [v_1, \ldots, v_k]$ and $\bar{H}_k = \{h_{i,j}\}_{1 \le i \le j+1; 1 \le j \le k}$.
        (form the approximate solution)
        compute $x_k = x_0 + V_k\, y_k$,
        where $y_k = argmin_y \left\|\beta e_1 - \bar{H}_k\, y\right\|$ and $e_1 = [1, 0, \ldots, 0]^t$.
        $nsteps = nsteps + 1$
    end of while
    $x_0 = x_k$
until $\|r_k\| < \varepsilon$

5. Numerical Results

All the numerical experiments are performed using the iterative methods tolerance equal to 10^{-6}. The **first example** is a two-dimensional test problem with $0 \le x \le 1$, $0 \le y \le 1$, no source term, $u = (1, 1)^t$, $\mathbf{K} = 0.005$ and the following boundary conditions

$$\begin{array}{ll} \phi(x,0) = 0, & \\ \phi(0,y) = 1 & \text{if} \quad y \le 0.2, \\ \phi(0,y) = 0 & \text{if} \quad y \ge 0.4, \\ \phi(0,y) = 5\,(0.2 - y) + 1 & \text{if} \quad 0.2 \le y \le 0.4. \end{array} \tag{14}$$

This is a predominant convective transport problem and such boundary conditions generate two internal boundary layers, beginning at $y = 0.2$ and $y = 0.4$. The dimension of the Krylov space (k) is set equal to 5 for the GMRES method.

In Figure 1 the influence of the reaction factor σ in the convergence of the iterative methods are presented. Notice that the performance of the LCG method is better when σ is small, even in the presence of some oscillations. For higher σ values there are almost no oscillations but the performance of the LCG decreases. This behavior is probably due to the fact that as long as the reaction term becomes more relevant the system matrix A tends towards symmetry.

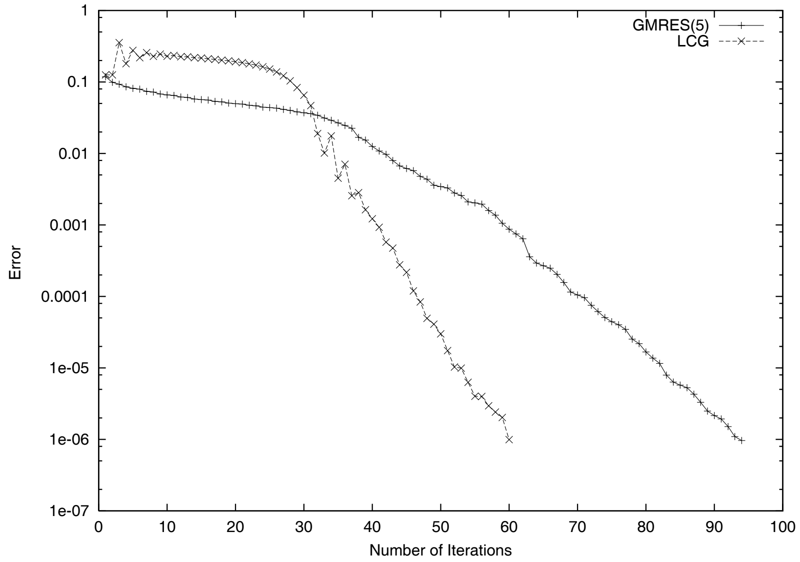

Figure 1: Example 1: convergence rate for GMRES(5) and LCG with $\sigma = 0$.

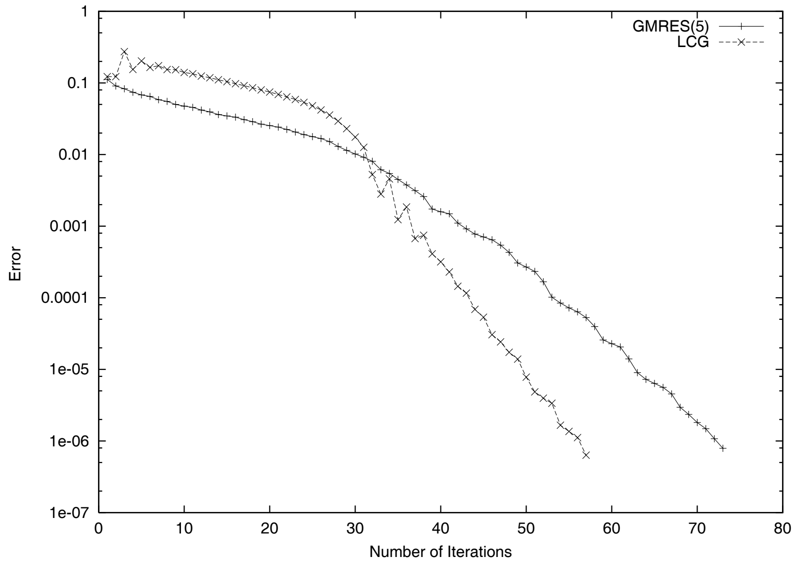

Figure 2: Example 1: convergence rate for GMRES(5) and LCG with $\sigma = 1$.

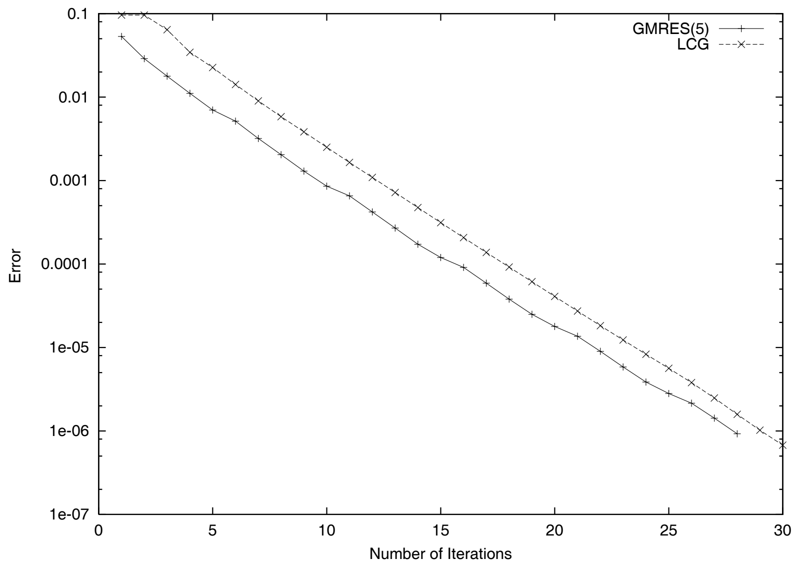

Figure 3: Example 1: convergence rate for GMRES(5) and LCG with $\sigma = 10$.

The **second and the third examples** simulate the problem of a discharge of a hot water in a river. For these examples, the water temperature is the variable modeled by equation (1). We used the same physical parameters used in Banks, 1994; Pirozzi and Zicarelli, 2000, presented in Table 1.

river velocity	$u_x = 0.3\ m/s$
thermal diffusivity	$\mathbf{K} = 25\ m/s^2$
air temperature	$\phi_{air} = 20^oC$
discharge temperature	$\phi_{in} = 30^oC$
surface transfer coefficient	$\sigma = 2.0 \times 10^{-5}s^{-1}$

Table 1: Parameters used in the one dimensional thermal problem

The second example is a one dimensional problem: the computational domain has 150km of length and the hot water discharge occurs at the origin, $x = 0$. Figure 4 presents the analytical and numerical steady state temperature profiles obtained using LCG, showing that they agree very well, even with the coarse mesh used. The temperature drops from 30^oC to 25^oC after 10km due to heat transfer from the river water to the air. After 50km the water temperature is approximately equal to the air temperature.

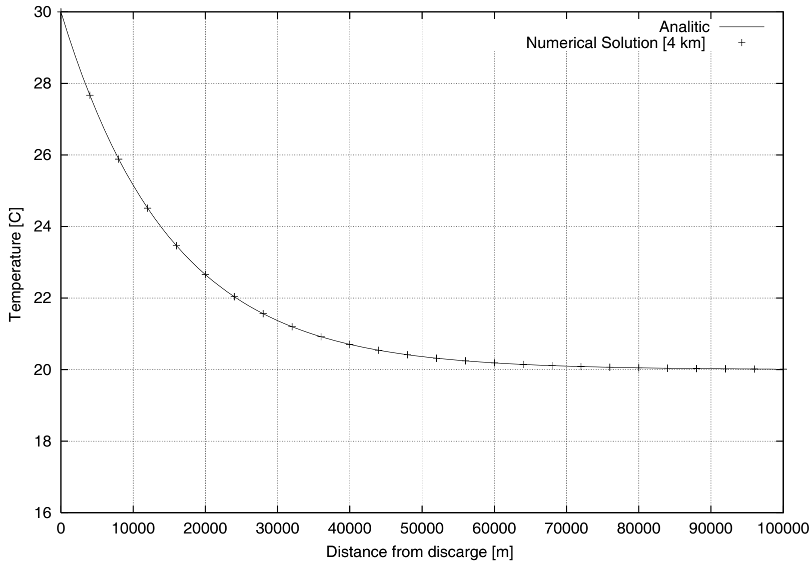

Figure 4: Example 2: comparison of analytical and numerical solutions with 4 km resolution.

The third example is a thermal pollution 2D problem. The computational domain is 100 km x 5 km, discretized using a regular mesh which resolution is 2 km x 1 km and considering the discharge inside of the domain. Figure 5 presents the temperature profile at the middle section. The discharge origin causes oscillations upwind to this point in the numerical solution for the Galerkin formulation, enforcing the necessity of a stable method.

The convergence rate of LCG and GMRES are presented in Figure 6, where we can notice that LCG takes less iterations than GMRES, even increasing the Krylov space dimension from 5 to 10 and 20. The last case, which doubles the memory requirements, leads to a small difference in the convergence history. The drawback of the LCG method is that, besides keeping the LCG vectors in memory, it needs an additional Matrix-vector product for the transpose product.

6. Conclusions

This work shows some computational experiments of combining a stable finite element method and two iterative methods to simulate thermal pollution problems. Even for the simple environmental problem considered here, the presence of steep gradients requires the use of a stable method, like SUPG, to get rid of global spurious oscillations. The system of linear equation originated from the finite element discretization is solved using a new method called LCG. Its performance is compared with the well known GMRES(k), concluding that it has superior convergence behavior. Like the initial version of GMRES, LCG consumes a lot of memory resource. However, this is a initial version of the LCG method and there are plenty of improvements to be done.

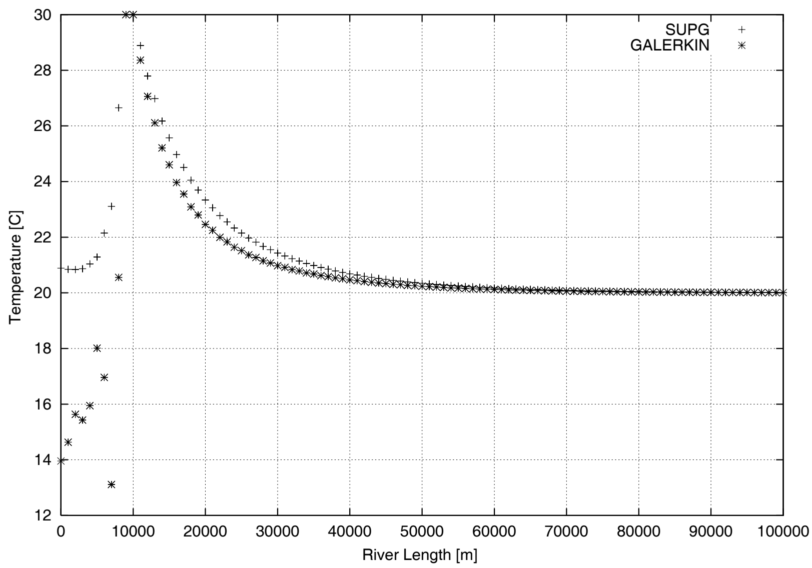

Figure 5: Example 3: comparison of the Galerkin and SUPG formulations for the middle section (2500 m).

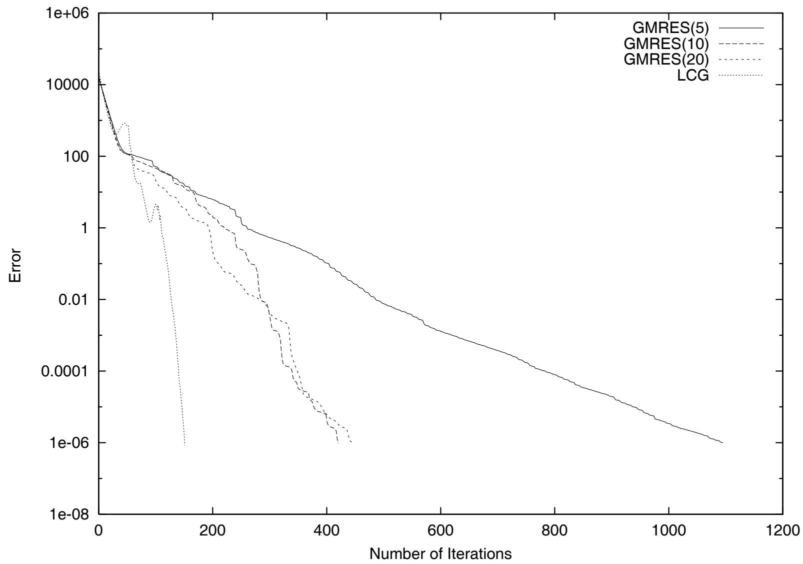

Figure 6: Example 3: convergence rate for LCG and GMRES(k), $k = 5, 10$ and 20.

7. Acknowledgments

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