MATHEMATICS DEPARTMENT

Numerical Experiences with Bi-CGSTAB on an Advection-Diffusion Problem

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The Bi-CGSTAB nonsymmetric linear solver has the attractive conjugate gradient-like properties of efficiency, low storage and no external parameters. However, unlike the conjugate gradient method, it has no minimisation property.

This report is concerned with performance of Bi-CGSTAB on the linear systems

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This report is concerned with the performance of the Bi-CGSTAB nonsymmetric solver on the linear systems which arise during one particular numerical solution method for advection-diffusion problems.

Many discretisation techniques for problems involving advection give rise to large, sparse, symmetric, positive definite matrix systems. These are ideally suited to solution by the conjugate gradient (CG) method which has the advantages that,

- 1. the only reference to the matrix in the system is a matrix-vector product,
- 2. the iterates are computed efficiently due to a three-term recurrence,
- 3. a bound on the error exists which guarantees monotonic convergence and,
- 4. unlike many other iterative methods (e.g. Chebychev acceleration [8]), no external parameters are required.

Many of the discretisation methods for advection-diffusion problems that lead to symmetric systems treat the advection explicitly, giving rise to either a stability restriction or decreased temporal accuracy (see e.g. Leismann Frind [13]). If the advection is treated implicitly, there is no formal stability restriction and good temporal accuracy can be obtained but, for a standard Bubnov-Galerkin finite element spatial discretisation, the coefficient matrix in the linear system is nonsymmetric, i.e.

=
$$(^T =)$$
 where $\mathbb{R}^{n \times n}$ is invertible and \mathbb{R}^n (1)

Due to the nonsymmetry, CG cannot be used to solve (1). But, since most matrices arising from standard spatial discretisation techniques are large and sparse, it is desirable to use a linear solver with properties 1 and 2. This precludes the use of direct methods based on Gaussian elimination except for cases where there is some special structure present. Ideally, the solver should also possess properties 3 and 4. There are many nonsymmetric solvers in the literature but, as yet, none satisfy all of these requirements.

CG may be used to solve (1) if the system is pre-multiplied by T to form the normal equations,

in which the coefficient matrix is symmetric and positive definite (SPD). There are cases where this approach is optimal (e.g. when — is unitary) but, in general, the coefficient matrix tends to be poorly conditioned and convergence is slow.

Most of the current popular iterative solvers are Krylov subspace methods. At the th iteration, these attempt to find the solution to (1) in a space $_0 + _i$ (where $_0 \mathbb{R}^n$ is the initial iterate and $_i$ is a Krylov subspace of dimension) by imposing the Petrov-Galerkin condition,

$$i$$
 i

where $_i$ is another space of dimension. The class of Krylov subspace methods include CG, the generalized minimal residual (GMR—S, Saad and Schultz [19]), quasi-minimal residual (QMR, Freund—Nachtigal [7]) and Bi-CGSTAB (van der Vorst [23]) methods.

based studies, where various methods are compared in practical situations (e.g. plasma turbulence modelling [1], groundwater flow [17], semiconductor device modelling [18]), have also shown that the relative performance of these methods depends on the situation.

Since so many comparisons of the different methods exist then, apart from some brief results for GMR S, Bi-CGSTAB is investigated in isolation in this work and the reader is left to use the available literature (e.g. the references cited in the previous paragraph) for general comparison purposes.

This report contains numerical results on the behaviour of Bi-CGSTAB when applied to the system arising from the discretisation of an advection-diffusion equation by the implicit Taylor-Galerkin method. This approach is used in [15] for transport problems arising in hydrology.

The next section contains a brief history of the development of Bi-CGSTAB, a review of some theoretical convergence results for Krylov subspace methods and a statement of the Bi-CGSTAB algorithm. Section 3 describes the nonsymmetric system used to test the solver in this work. Section 4 contains results on the performance of Bi-CGSTAB from numerical experiments under both moderate and harsh convergence criteria - the latter results indicate that rounding errors can lead to divergence. Some techniques for improving convergence behaviour are reviewed in Section 5 and a selection of these are

Bi-CGSTAB is an iterative method for approximating the solution to a linear system in which the matrix is nonsymmetric. It is a bi-orthogonalisation Krylov subspace method, i.e. given an initial iterate $_0$ \mathbb{R}^n , at the th iteration the method looks for an approximate solution $_i$ of (1) from a space,

$$_0 + \operatorname{span} _0 \quad _0 \quad ^2 \quad _0 \dots \quad ^{i-1} \quad _0$$

(where $_0 = _0$) by imposing the orthogonalisation,

$$_{i}\qquad _{0}\text{ (}\overset{T}{\text{ }})\text{ }_{0}\text{ (}\overset{T}{\text{ }})^{2}\text{ }_{0}\text{ }\ldots\text{ (}\overset{T}{\text{ }})^{i-1}\text{ }_{0}$$

In this section, the origin of Bi-CGSTAB is described. This is followed by an overview of convergence results for Krylov subspace methods, and a description of the particular form of the Bi-CGSTAB algorithm used.

In the CG method for SPD matrices, the residuals are mutually orthogonal, i.e.

$$(i_i) = 0 \quad (=)$$

and can be shown to satisfy the expression,

$$i = i()_0$$

where i() is a polynomial of degree (and i(0) = 1). A three-term recurrence relationship exists between these residuals, and it is the exploitation of this property that makes the algorithm economical in terms of both computing time and storage. This three-term recurrence relation arises from the close relationship of the algorithm with the symmetric Lanczos tridiagonalisation process (see e.g. Golub Van Loan [8] for a description of this relationship).

When is nonsymmetric, it is not possible to construct a three-term recurrence relationship of the type used in CG for the residuals. In this case, a possible approach is to base the solver on the Lanczos tridiagonalisation process - this is the origin of the earliest predecessor of Bi-CGSTAB, the bi-conjugate gradient method (Bi-CG) [5, 12].

In Bi-CG, the approximations are constructed in such a way that the residual vector, i, is orthogonal to a set of pseudo-residual vectors $\hat{j}_{(j=1,\dots,i-1)}$ and, vice versa, $\hat{i}_{(j=1,\dots,i-1)}$. This is accomplished by three-term recurrence relationships for the rows $\hat{i}_{(j)}$ and $\hat{j}_{(j)}$. The Bi-CG residual vectors are given by,

This inner product can be written as,

$$(i \hat{j}) = (j \hat{j}) i(j \hat{j}) = 0 \quad (i = j)$$

$$i \quad i \quad i \quad T$$

$$i \quad \frac{2}{i} \quad 0$$

$$i \quad \frac{2}{i} \quad i \quad i$$

 $i \qquad j \qquad T \qquad 0 \quad (j=1,...,i-1)$ $j \qquad \qquad j \qquad j \quad i$ $i \qquad \qquad 1 \qquad 2 \qquad i$

 1 If a solution exists, the process finds this in at most n iterations.

where **u** is the exact solution of the linear system, \mathbf{u}_i is the i^{th} iterate produced by the conjugate gradient method and $\|\cdot\|_A$ is the A-norm defined by,

$$\|\mathbf{w}\|_A = \sqrt{\mathbf{w}^T A \mathbf{w}}.$$

The class of Krylov subspace iteration methods to which GMR S belongs (i.e. \mathcal{K}_i as in CG and $\mathcal{L}_i = A\mathcal{K}_i$) possesses the optimality property,

$$\|\mathbf{r}_i\|_2 = \min_{\mathbf{w} \in \mathbf{u}_0 + \mathcal{K}_i} \|\mathbf{f} - A\mathbf{w}\|_2.$$

The existence of such a property guarantees that the residual is a monotonic function of the iteration number.

Unfortunately, the main theorem from Faber Manteuffel [4] states that CG-like methods with (i) a minimisation property and (ii) cheap short-term recurrence relationships exist only for special matrices. In general, CG-like methods possess either (i) or (ii) but not both, e.g. GMR S has (i) but can be expensive to implement (the work at each iteration grows linearly) while Bi-CG has (ii) but has no minimisation property.

An apparent exception is the quasi-minimal residual method which has three-term recurrence relationships and also minimises the residual in the norm, $\| _{i+1}^{-1} W_{i+1}^T \mathbf{r}_i \|_2$, at the i^{th} iteration (where — and W are matrices associated with the underlying nonsymmetric Lanczos process - see [6] for more detail). However, as the name suggests, QMR is not a true minimisation process; the residual is minimised in a norm that changes with each iteration. Because of this, QMR falls out of the scope of the Faber — Manteuffel theorem.

Since it is based on three-term recurrence relationships and possesses no quasiminimisation property, no convergence bounds exist for Bi-CGSTAB. Current knowledge of the practical behaviour of the method falls into two main categories:

- Investigations on the effects of the presence of extreme (large, small and negative) eigenvalues in the eigenspectrum of the coefficient matrix (e.g. for a comparison of this type with Bi-CG and CG-S, see Campos, filho Rollet [2]). These studies tend to use matrices constructed to generate a particular eigenspectrum.
- Comparisons with other solvers on matrices arising from the solution of practical problems (e.g. Peters [17]).

The work in this report uses a coefficient matrix whose properties are controlled by the physical values associated with the problem being solved and the size of the temporal and spatial discretisation used in the numerical approximation of the underlying differential equation, and examines the behaviour of the Bi-CGSTAB method in isolation as the parameters are varied.

There are many possible forms of the Bi-CGSTAB algorithm which are equivalent in exact arithmetic but which show different behaviour in finite precision. For this reason, the form of the Bi-CGSTAB algorithm used in this work is given in this section.

The following algorithm is similar to the one given by van der Vorst [23], but incorporates some of the modifications suggested in that original paper. This algorithm

searches iteratively for a solution to (1) where the matrix is preconditioned by .

is an initial iterate;
$$_{0} = _{}$$
; $_{0} = _{} = _{} = 1; _{1} = (_{0} _{0}); = _{} = _{} = ;$ do $_{} = 1 _{max} = (_{i} _{i-1})(_{}); = _{i-1} + (_{});$ (6)

$$i$$
 0 $i-1$

$$i+1$$
 0

The nonsymmetric system in this work arises from an implicit discretisation of the equation for contaminant transport in porous medium, a full description of the origin of this system being given in [15]. In this section a brief summary of the relevant parts of that work is presented; this includes a description of the partial differential equation being approximated, the discretisation used and a simple test case arising from the solution of a 1-D problem.

3.1 Governing Equation for Contaminant Transport in Porous Media

From [15], the mass balance equation for a contaminant in a saturated porous medium is,

$$\rho \phi \frac{\partial c}{\partial t} + (\rho \mathbf{q}) \cdot \nabla c = \nabla \cdot \phi \underline{\underline{\mathbf{D}}} \nabla (\rho c) \quad , \tag{11}$$

where $\rho = \rho(c)$ is fluid density, ϕ is the porosity, c is the (dimensionless) contaminant concentration, \mathbf{q} is the Darcy velocity and $\mathbf{\underline{D}}$ is the dispersion tensor.

In this work, ρ , ϕ , $\underline{\underline{\mathbf{D}}}$ and \mathbf{q} are taken to $\overline{\mathbf{be}}$ constant. With these simplifications (11) becomes the constant coefficient advection-diffusion equation,

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = \nabla \cdot \ \underline{\mathbf{D}} \nabla c \quad , \tag{12}$$

where $\mathbf{v} = \frac{\mathbf{q}}{\phi}$ is the average fluid velocity.

The advection-diffusion equation representing the contaminant mass balance is discretised by an implicit Taylor-Galerkin method - using (12) to replace the temporal derivatives in an approximate Taylor series expansion, and then performing a spatial discretisation by the standard Galerkin finite element method. This gives the same result as the Crank-Nicolson finite element method [17].

The fully discretised form of the contaminant mass balance equation is,

$$\frac{1}{\Delta t}A + \frac{1}{2}(B+C) \quad \mathbf{c}^{t+\Delta t} = \frac{1}{\Delta t}A - \frac{1}{2}(B+C) \quad \mathbf{c}^{t} - \mathbf{F},\tag{13}$$

where

$$A = \{A_{IJ}\}_{I,J=1,...,n}$$

$$B = \{B_{IJ}\}_{I,J=1,...,n}$$

$$C = \{C_{IJ}\}_{I,J=1,...,n}$$

$$\mathbf{F} = \{F_I\}_{I=1,...,n},$$

and

$$A_{IJ} = A_{IJ}^e = N_I N_J d\Omega^e$$

$$B_{IJ} = B_{IJ}^e = \nabla N_I \cdot \underline{\underline{\mathbf{D}}} \nabla N_J d\Omega^e$$

$$IJ = \begin{bmatrix} e & e & e & I & J & \Omega^e \end{bmatrix}$$
 $I = \begin{bmatrix} e & e & -\frac{c}{n} & I & \Gamma^e \end{bmatrix}$

where the superscript, $% \left(1\right) =\left(1\right) =\left($

In this section, the performance of Bi-CGSTAB on the linear systems arising from the test case in Section 3 is examined. As with CG, preconditioning is an important aspect of the behaviour of this method. However, this is not considered here - no preconditioning (i.e. =) is used in the moderate convergence tests (to allow a comparison with

-16

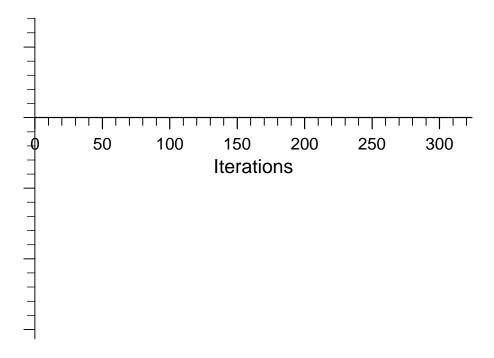
7

i 2

-c

 		_					
			_				

2 2	
166	



based) Bi-CGSTAB residuals and the true residuals (calculated by $\mathbf{r}_i^{true} = \mathbf{f} - A\mathbf{u}_i$), and also the iteration when this maximum occurs. These errors are quite small, so a total breakdown of the recursion process has not occurred; but the small discrepancy between the true and recursion residuals may indicate that the recursion process has been spoiled, leading to the convergence difficulties. Indeed, comparing Tables 2 and 3, the onset of divergence often coincides with the largest relative error in the residual.

Pe	ν	$\max_{i} \frac{\ \mathbf{r}_{i}^{true} - \mathbf{r}_{i}\ _{2}}{\ \mathbf{r}_{i}^{true}\ _{2}}$	Iteration
	0.5	8.22×10^{-3}	8
	1	2.51×10^{-3}	12
	2	2.54×10^{-3}	20
1	5	6.49×10^{-5}	36
	10	5.24×10^{-6}	56
	20	1.27×10^{-8}	70
	40	3.83×10^{-8}	375
	0.5	7.04×10^{-6}	8
	1	4.04×10^{-4}	13
	2	7.60×10^{-4}	20
5	5	1.94×10^{-7}	35
	10	1.32×10^{-10}	39
	20	3.29×10^{-11}	147
	40	1.09×10^{-10}	168

Table 3: Relative error in residuals

If Bi-CGSTAB is to be considered as a viable alternative to other nonsymmetric solvers for this problem, the convergence difficulties highlighted by the harsh convergence criterion tests must be overcome so that the solver is robust as well as efficient.

In this section, an attempt is made to prevent the divergent behaviour in the harsh convergence criterion tests highlighted by Figures 1 and 2. Some techniques for improving convergence behaviour currently in the literature are:

- it is known that the Lanczos tridiagonalisation process (which underpins three-term recurrence relationship methods) is unstable and prone to breakdown due to a loss of orthogonality between the Lanczos vectors [8]. To remedy this, the look-ahead Lanczos process of Parlett [16] allows the use of block pivots in the iteration steps where the scalar pivots of the standard Lanczos process is expected to encounter difficulties. This method is used in practical versions of QMR.

variants of Bi-CGSTAB (e.g. Bi-CGSTAB2 [9], Bi-CGSTAB() [20]) allow in the construction of $\tilde{}_i($) in (4) rather than the linear components, (1 $_j$), used in the original van der Vorst version. These methods attempt to avoid stagnation in the convergence history of Bi-CGSTAB which occurs when the eigenvalues are almost purely imaginary.

(Weiss Schönauer [24]) - an auxiliary sequence of vectors, \bar{a}_i , is generated from non-monotonic iterates, \bar{a}_i , by the recursion,

$$\begin{array}{rcl} -_{0} & = & _{0} \\ -_{i} & = & (1 & _{i})^{-}_{i-1} + _{i} & _{i} & (= 1 \ 2 \dots) \end{array}$$

where each is chosen to minimise,

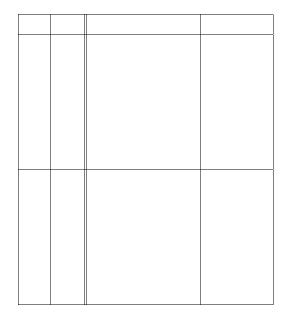
$$(1)^{-i-1} + i = 2$$

over \mathbb{R} . is given explicitly by,

$$_{i}=\begin{array}{cc} \frac{T}{i-1}(_{i}\quad _{i-1})\\ \\ \frac{1}{i}\quad _{i-1}\stackrel{2}{\stackrel{2}{\stackrel{}{\sim}}} \end{array}$$

where $_{i-1} = _{i-1}$. The vectors in the auxiliary sequence, $_{i}$, are iterates with monotone non-increasing residual.

- the Mismatch Theorem [22] indicates that a breakdown



Since a good initial iterate, $_0$, is available, a vector of random entries () is added to this to generate a new initial iterate $\tilde{~}_0$. The size of the random perturbation is controlled by scaling and a factor, ~, i.e.

$$\tilde{a}_0 = a_0 + a_0 = a_0 + a_0 = a_0 = a_0 + a_0 = a$$

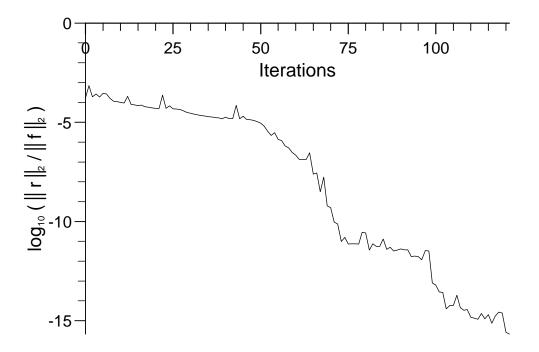
Table 5 shows the minimum residual achieved and the corresponding iteration number for the harsh convergence tests with different perturbation sizes.

			$=10^{-3}$			$=10^{-2}$			$=10^{-1}$	
		(2	$_2)_{min}$	Itn.	(2	$_2)_{min}$	Itn.	(2	$_2)_{min}$	Itn.
	0.5	2 80	10^{-16}	20	1 10	10^{-15}	20	1 31	10^{-14}	17
	1			25	5 03	10^{-16}	27	1 90	10^{-14}	25
	2			50			42	7 88	10^{-14}	41
1	5			89	1 12	10^{-14}	79	6 72	10^{-14}	69
	10	1 96	10^{-15}	129	2 59	10^{-14}	116	2 31	10^{-13}	138
	20	3 16	10^{-15}	400	5 23	10^{-14}	414	3 53	10^{-13}	224
	40	7 70	10^{-15}	413	2 36	10^{-15}	431	8 94	10^{-14}	469
	0.5			22	2 01	10^{-15}	24	1 51	10^{-14}	25
	1	2 18	10^{-15}	29	3 89	10^{-15}	25	1 46	10^{-14}	25
	2	4 98	10^{-15}	30	4 10	10^{-14}	30	5 83	10^{-13}	28
5	5	1 55	10^{-14}	72	1 15	10^{-13}	71	2 23	10^{-13}	107
	10	7 18	10^{-14}	135	6 48	10^{-14}	157	1 02	10^{-12}	149
	20	3 74	10^{-15}	258	2 50	10^{-13}	243	8 77	10^{-13}	239
	40	40	$24^{1}3$	10	152	$1^{-}5^{3}40$		243I)Aw	/SzHB8sF	10

"z(,67Xffi64ffffi

(1 (see !	Section	2.3)	which	are h	ighlighted	because	thev	may	he clo	se to zero	without
/	. 0	/ \	SCC 1	occuon.	4.9)	, willten	arc n	ngningnica	Decause	uncy	may	ne cro	SC TO ZCIT	WIGHOUG

	2	2 min	2	2 min	2	2 min	



the matrix, the more sensitive the process is to rounding errors. Thus, the optimum value of k for this problem is expected to decrease with n, ν and Pe (the latter is included because it also affects the amount of nonsymmetry in the matrix).

The requirement for the value k violates the desired property that the solver should require no external parameters (see Section 1).

From the operation in the Bi-CGSTAB algorithm where ρ is used as a denominator (got by combining (6) and (7)),

$$= _{i-1} + \frac{\rho_i}{\rho_{i-1}} \frac{\alpha}{\omega} (\qquad \omega).$$

and the definition of the round-off unit (14), rounding errors can be expected to occur in this operation if,

$$\epsilon > \frac{\rho_i}{\rho_{i-1}} \frac{\alpha}{\omega} \frac{(j) \quad \omega \quad (j)}{\sum_{i=1}^{i} (j)} > \frac{1}{\epsilon} \quad (1 \quad j \quad n), \tag{16}$$

where (j) is the j^{th} component of . The expression is undefined when a term in the residual vector is zero so these cases must be excluded. Hence a more suitable form of (16) is

$$i_{i-1}(j) = 0 \text{ and } \epsilon_{i-1}(j) > \beta_{i}(j) \quad \omega_{i}(j) > \frac{1}{\epsilon_{i-1}(j)} \quad (1 \quad j \quad n), \quad (17)$$

which is a possible restart criterion, requiring no external parameters other than the easily available round-off unit. However, experimental investigations show that in all the harsh convergence criterion tests, the monitor value is always well within the bounds which indicate round-off and there is no interesting behaviour in the monitor near the onset of convergence difficulties - hence (17) is of no use for this problem.

In the same way as round-off error in ρ_{i+1} is tested for in (17), round-off can be tested for in (0,) by combining (8) and (9) and using the definition of the round-off unit to give the possible restart criterion,

$$i_{i-1}(j) = 0 \text{ and } \epsilon_{i-1}(j) > \alpha_i(j) > \frac{1}{\epsilon_{i-1}(j)} \quad (1 \quad j \quad n).$$
 (18)

Again, experimental investigations show that this monitor is always well within the bounds for all the tests, and there are no significant features in the monitor near the onset of convergence difficulties, so this restart criterion is also of no use.

Joubert [10] uses restart criteria based on the occurrence of inner products as denominators in Bi-CG and CG-S. The general form of these criteria are that if (\cdot, A_{\cdot}) is used as a denominator then restart if,

$$\frac{(A)}{2A_2} f(\epsilon).$$

In [10], the tolerance has the form, $() = 10^{a} \frac{1}{2}$, where | is an integer.

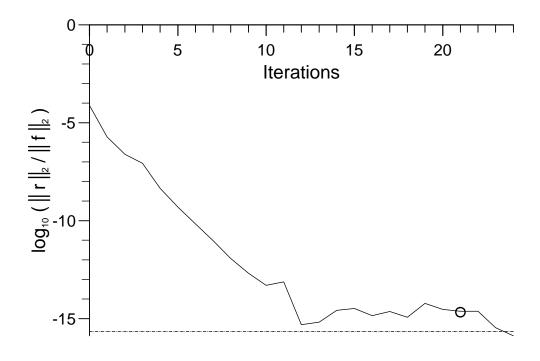
Since the inner product ($_0$) is used in Bi-CGSTAB (10) for the calculation of $_{i+1}$ then a possible restart criterion is,

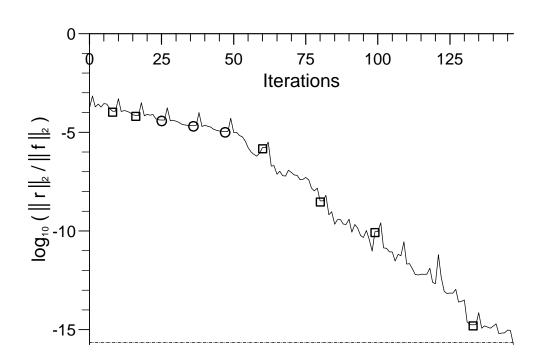
$$\frac{\left(\begin{array}{cc} 0 \end{array}\right)}{\left(\begin{array}{cc} 0 \end{array}\right)} \quad \left(\begin{array}{cc} 1\end{array}\right) \tag{19}$$

0

 $5 \quad \frac{1}{2}$

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