A Combined Compact Difference Scheme for Solving the Three-Dimensional Advection-Diffusion Equation

M. M. Rahman, K. A. M. Moinuddin and G. R. Thorpe

Centre for Environmental Safety and Risk Engineering College of Engineering and Science, Victoria University, Melbourne, Victoria 8001, Australia

Abstract

The advection-diffusion equation is ubiquitous in fluid mechanics. For example, it arises in equations that govern turbulence, heat and mass transfer, and these equations form the basis of computational fluid dynamics. However, numerical schemes for solving the governing equations are often inherently dispersive and this confounds the solutions, particularly when the effects of dispersion are to be quantified. In this work, we develop a combined compact difference scheme to solve the unsteady advection-diffusion equation in three-dimensions. Along with the Crank-Nicholson time discretization scheme, the combined compact difference scheme demonstrates sixth order accuracy in space and second order accuracy in time. The alternating direction implicit method has been used in time factorization in each direction. The scheme is unconditionally stable and significantly eliminates artificial diffusion from the solution that usually arises in lower order discretization schemes. The compactness of the scheme improves the computational efficiency compared to other higher order schemes. The work also discusses the boundary conditions, the correctness of which is sensitive to delicate mathematical formulation. Numerical experiments are performed on a generalized advection-diffusion problem defined in a cubic region subject to Dirichlet boundary conditions. A known analytical solution to the is used to evaluate the performance of the numerical scheme. The threedimensional combined compact scheme produces solutions that are in very close agreement with the analytical solutions when either convection or dispersive effects are dominant.

Introduction

The numerical simulation of the advection-diffusion equation (ADE) is omnipresent in computational fluid dynamics and heat transfer. Many physical phenomena are governed by this equation, therefore accurate, efficient and stable finite difference schemes to represent the ADE is vital for obtaining a reliable numerical solution. Furthermore, attempts to quantify the rate of dispersion in the flows may be confounded by the presence of artificial diffusion that arises when lower order discretization schemes are implemented. Researchers have invested considerable effort to develop discretization schemes with higher order accuracy. However in most cases, the solution involves large stencils which require solution of a denser system of equations that result in higher computational cost To overcome this issue, combined compact difference (CCD) schemes have been developed and used in the solution of many partial differential equations in recent years (Sun & Li 2014).

Gupta et al. (1984) presented a finite difference scheme with spatial fourth order accuracy for one dimensional (1D) ADE with a variable diffusion coefficient. This scheme has been extended to solve two-dimensional (2D) unsteady ADE by Spotz & Carey (2001). Nevertheless, the scheme involved nine nodes in the difference equation which render it computationally inefficient. Noye & Tan (1989) derived a set of higher order compact scheme (HOC) implicit schemes for solving 1D steady ADE with third and second order accuracy in space and time.

In pursuit of a computationally effective scheme Karaa & Zhang (2004) developed an unconditionally stable fourth order accurate HOC schemes with the standard (Paceman-Rachford) alternating direction implicit (PR-ADI) method to solve two-dimensional time dependent convection diffusion equation with a constant diffusion coefficient. It was later implemented for a 3D unsteady ADE by Karaa (2006). The computational efficiency of the scheme was superior to other fourth order schemes. The high order Padé ADI method (PDE-ADI) proposed by You (2006) demonstrates better fidelity of phase and amplitude than the PR-ADI and HOC-ADI method whilst maintaining a similar order of accuracy.

A series of HOC exponential finite difference schemes (EHOC-ADI) have been proposed by Tian & Dai (2007) to solve the 1D and 2D steady ADEs. This scheme has been revised to solve the 1D unsteady ADE by adapting the Padé approximation for temporal discretization by Tian & Yu (2011). Furthermore, Tian & Ge (2007) and Ge et al. (2013) have extended the approach for solving unsteady ADE in 2D and 3D Cartesian coordinates respectively. These methods have fourth order accuracy in the spatial domain and exhibit non-oscillatory behaviour. Other schemes with similar accuracy have been developed as rational HOC schemes with ADI method (RHOC-ADI) by Tian (2011) and Liao (2012). However, superior accuracy and computational efficiency as well as better phase and amplitude error characteristics have been demonstrated for the RHOC-ADI scheme over HOC-ADI, EHOC-ADI and PDE-ADI methods.

Most of the schemes discussed above are limited to comparatively low cell Peclet numbers and do not possess the same level of accuracy when convection becomes the dominant mechanism in the flow (Sun & Li 2014). To overcome this limitation the combined compact difference (CCD) scheme has been proposed by Chu & Fan (1998) for one and twodimensional steady ADE. The scheme is a sixth order spatially accurate implicit method. Sun & Li (2014) have used the CCD method combined with ADI method for solving the twodimensional unsteady convection diffusion equation. The three point stencil structure of the scheme facilitates high computational efficiency. In this work we develop a CCD-ADI scheme to solve the unsteady ADE in 3D Cartesian coordinate.

Development of the CCD scheme

To visualize the development of three point CCD scheme, we consider following one dimensional differential equation

$$\alpha(x)\frac{d^2\phi}{dx^2} + \beta(x)\frac{d\phi}{dx} + \gamma(x)\phi = f(x), \qquad 0 \le x < L \tag{1}$$

With boundary condition

$$\zeta_1(x)\phi(x) + \zeta_2(x) \frac{d\phi}{dx}(x) = g(x), \qquad x = 0, L$$
 (2)

Where α , β , γ , f, ζ_1 , ζ_2 and g are given functions. Discretising the one dimensional domain into a uniform grid $0 = x_1 < x_2 < \cdots \ldots < x_{N-1} < x_N = L$ with grid spacing h = L/N. Expanding any arbitrary function $\phi(x)$ and x_i , $i = 1, 2, \ldots, N$ using a Taylor series with up to the sixth derivative, we have

$$\phi(x_{i\pm1}) = \phi(x_i) \pm h\phi'(x_i) + \frac{h^2}{2}\phi''(x_i) \pm \frac{h^3}{6}\phi'''(x_i) + \frac{h^4}{24}\phi^{(4)}(x_i) \pm \frac{h^5}{120}\phi^{(5)}(x_i) + \frac{h^6}{720}\phi^{(6)}(x_i) + \mathcal{O}(h^7)$$
(3)

Similar expressions can be obtained by replacing $\phi(x_i)$ with $\phi'(x_i)$ and $\phi''(x_i)$

$$\phi'(x_{i\pm1}) = \phi'(x_i) \pm h\phi''(x_i) + \frac{h^2}{2}\phi'''(x_i) \pm \frac{h^3}{6}\phi^{(4)}(x_i) + \frac{h^4}{24}\phi^{(5)}(x_i) \pm \frac{h^5}{120}\phi^{(6)}(x_i) + \mathcal{O}(h^7)$$
(4)

$$\phi''(x_{i\pm 1}) = \phi''(x_i) \pm h\phi'''(x_i) + \frac{h^2}{2}\phi^{(4)}(x_i) \pm \frac{h^3}{6}\phi^{(5)}(x_i) + \frac{h^4}{24}\phi^{(6)}(x_i) + \mathcal{O}(h^7)$$
(5)

In order to express the variable with higher order truncation term, equations (3) - (5) can be manipulated to develop an expression of the variable combined with its first and second derivatives as follows-

$$\frac{\phi(x_{i+1}) - \phi(x_{i-1})}{2h} = \phi'(x_i) + \frac{h^2}{6}\phi'''(x_i) + \frac{h^4}{120}\phi^{(5)}(x_i) + O(h^6)$$

$$\frac{\phi'(x_{i+1}) + \phi'(x_{i-1})}{2} = \phi'(x_i) + \frac{h^2}{2}\phi'''(x_i) + \frac{h^4}{24}\phi^{(5)}(x_i) \qquad (6)$$

$$\phi''(x_{i+1}) - \phi''(x_{i-1}) = 2h\phi'''(x_i) + \frac{h^3}{3}\phi^{(5)}(x_i) + O(h^5)$$

$$\frac{\phi(x_{i+1}) - 2\phi(x_i) + \phi(x_{i-1})}{h^2} = \phi''(x_i) + \frac{h^2}{12}\phi^{(4)}(x_i) + \frac{h^4}{360}\phi^{(6)}(x_i) + O(h^6)$$

$$\frac{\phi'(x_{i+1}) - \phi'(x_{i-1})}{h^2} = \phi''(x_i) + \frac{h^2}{2}\phi^{(4)}(x_i) + \frac{h^4}{24}\phi^{(6)}(x_i) \qquad (7)$$

$$\frac{2h}{\phi''(x_{i+1}) + \phi''(x_{i-1})} = \phi''(x_i) + \frac{h^2}{2}\phi^{(4)}(x_i) + \frac{h^4}{24}\phi^{(6)}(x_i)$$

$$+ \mathcal{O}(h^6)$$

From equation (6) and (7), writing $\phi(x_i) = \phi_i$, the first and second derivative at point *i* can be expressed as

$$\phi'_{i} = \frac{15}{16h} [\phi_{i+1} - \phi_{i-1}] - \frac{7}{16} [\phi'_{i+1} + \phi'_{i-1}] + \frac{h}{16} [\phi''_{i+1} - \phi''_{i-1}] + \mathcal{O}(h^{6})$$
(8)

$$\phi_{i}^{\prime\prime} = \frac{3}{h^{2}} [\phi_{i+1} - 2\phi_{i} + \phi_{i-1}] - \frac{9}{8h} [\phi_{i+1}^{\prime} - \phi_{i-1}^{\prime}] \\ + \frac{1}{8} [\phi_{i+1}^{\prime\prime} + \phi_{i-1}^{\prime\prime}] + \mathcal{O}(h^{6})$$
(9)

Furthermore, equations (8) and (9) can be reorganized into the following form and dropping the truncation errors

$$\frac{15}{16h}\phi_{i-1} - \frac{15}{16h}\phi_{i+1} + \frac{7}{16}\phi_{i-1}' + \phi_i' + \frac{7}{16}\phi_{i+1}' + \frac{h}{16}\phi_{i-1}'' - \frac{h}{16}\phi_{i+1}'' = 0$$
(10)

$$-\frac{3}{h^2}\phi_{i-1} + \frac{6}{h^2}\phi_i - \frac{3}{h^2}\phi_{i-1} - \frac{9}{8h}\phi_{i-1}' + \frac{9}{8h}\phi_{i+1}' - \frac{1}{8}\phi_{i-1}'' + \phi_i'' - \frac{1}{8}\phi_{i+1}'' = 0$$
(11)

These equations are applicable at nodes i = 2, 3, ..., N - 1resulting a total of 2(N - 1) equations. For periodic boundaries $(\phi_1 = \phi_N, \phi'_1 = \phi'_N, \text{and } \phi''_1 = \phi''_N)$ the above equations (10) and (11) stands for i = 1. However, for non-periodic boundaries, to keep the three point structure at the boundaries, a pair of fifth order one sided CCD schemes is introduced as follows at x_1 and x_N (Chu & Fan 1998)

$$-\frac{31}{h}\phi_1 + \frac{32}{h}\phi_2 - \phi_3 + 14\phi_1' + 16\phi_2' + 2h\phi_1''$$
(12)
$$-4h\phi_2'' = 0$$

$$\frac{\frac{31}{h}\phi_N + \frac{32}{h}\phi_{N-1} - \phi_{N-2} + \frac{16\phi'_{N-1} + 14\phi'_N}{-4h\phi'_{N-1} + 2h\phi''_N} = 0$$
(13)

Furthermore, equations (1) and (2) can be written in discretized form as

$$\gamma_i \phi_i + \beta_i \phi'_i + \alpha_i \phi''_i = f_i, \qquad i = 1, 2, 3 \dots \dots, N$$
(14)

$$\zeta_1(0)\phi_1 + \zeta_2(0)\phi_1' = g(0) \tag{15}$$

$$\zeta_1(L)\phi_N + \zeta_2(L)\phi_N' = g(L) \tag{15}$$

The above system of equations can be organized into a triple tridiagonal system consisting of 3N equations (equation (10) and (11) for i = 2,3,...,N - 1 giving 2(N - 2) equations, equation (12) for i = 1 and (13) for i = N giving 2 equations, and equations (14) for i = 1,2,3,...,N and equation (15) for i = 1,N giving N + 2 equations) with 3N unknowns ($\phi_i, \phi'_i, and \phi''_i$ for i = 1,2,3,...,N). This system of linear equations can be solved by triple forward elimination and triple backward substitutions. A simpler version of the algorithm solves a twin tridiagonal system which appears while calculating first and second derivatives from a given function with the CCD method (discussion to appear in later section).

CCD Scheme for Three-Dimensional Advection-Diffusion Equation

The method outlined above has been developed for a onedimensional case. However, most of the cases we have to deal with are multidimensional. Consider a three-dimensional convection-diffusion equation with constant velocity \mathbf{p} , \mathbf{q} and \mathbf{r} and constant molecular diffusivity \mathbf{a} , \mathbf{b} and \mathbf{c} in the *x*, *y* and *z* directions respectively. The unsteady convection diffusion of any scalar ϕ can be expressed as

$$\frac{\partial \phi}{\partial t} + p \frac{\partial \phi}{\partial x} + q \frac{\partial \phi}{\partial y} + r \frac{\partial \phi}{\partial z}$$
$$= a \frac{\partial^2 \phi}{\partial x^2} + b \frac{\partial^2 \phi}{\partial y^2} + c \frac{\partial^2 \phi}{\partial z^2} + S, \qquad (16)$$
$$(x, y, z, t) \in \Omega \times (0, T]$$

Where Ω is a three dimensional domain in \mathbb{R}^3 in $[L_x \times L_y \times L_z]$. The initial condition is given by

$$\phi(x, y, z, 0) = \phi_0(x, y, z), \quad (x, y, z) \in \Omega$$
 (17)

and the boundary condition

$$\zeta_1 \phi(x, y, z, t) + \zeta_2 \frac{\partial \phi}{\partial \boldsymbol{n}}(x, y, z, t) = g(x, y, z, t),$$
(18)
(x, y, z) $\in \partial \Omega, t \in (0, T]$

In this case $\zeta_1 = 1$ and $\zeta_2 = 0$ corresponds to the Dirichlet boundary condition and $\zeta_1 = 0$ and $\zeta_2 = 1$ corresponds to the

Neumann boundary condition. \boldsymbol{n} is the outward unit normal vector of the domain.

The source terms S, ϕ_0 and g are given smooth functions. For convenience, let us define three finite difference operators

$$\mathcal{L}_{x} \equiv a \frac{\partial^{2}}{\partial x^{2}} - p \frac{\partial}{\partial x}; \ \mathcal{L}_{y} \equiv b \frac{\partial^{2}}{\partial y^{2}} - q \frac{\partial}{\partial y}; \ \mathcal{L}_{z} \equiv c \frac{\partial^{2}}{\partial z^{2}} - r \frac{\partial}{\partial z}$$

Hence equation (16) can be rewritten as

$$\frac{\partial \phi}{\partial t} = (\mathcal{L}_x + \mathcal{L}_y + \mathcal{L}_z)\phi + S \tag{19}$$

Using the Crank-Nicholson scheme, discretising the above equation in the time interval [0, *T*] with increment $\Delta t = T/N$ where *N* is the total number of time steps, we get

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = \frac{1}{2} \left(\mathcal{L}_x + \mathcal{L}_y + \mathcal{L}_z \right) (\phi^{n+1} + \phi^n) + S^{n+\frac{1}{2}} + \mathcal{O}(\Delta t^2)$$
(20)

Here ϕ^n is the approximation of $\phi(x, y, z, n\Delta t)$ for an arbitrary function $\phi(y, z, t)$. Collecting terms in ϕ^{n+1} and ϕ^n

$$\begin{pmatrix} 1 - \frac{\Delta t}{2} \mathcal{L}_{x} - \frac{\Delta t}{2} \mathcal{L}_{y} - \frac{\Delta t}{2} \mathcal{L}_{z} \end{pmatrix} \phi^{n+1} \\ = \begin{pmatrix} 1 + \frac{\Delta t}{2} \mathcal{L}_{x} + \frac{\Delta t}{2} \mathcal{L}_{y} + \frac{\Delta t}{2} \mathcal{L}_{z} \end{pmatrix} \phi^{n} \qquad (21) \\ + \Delta t S^{n+\frac{1}{2}} + \mathcal{O}(\Delta t^{3})$$

Further modification by factorization of the above equation gives (assuming all coefficients to be constant)

$$\begin{pmatrix} 1 - \frac{\Delta t}{2} \mathcal{L}_x \end{pmatrix} \left(1 - \frac{\Delta t}{2} \mathcal{L}_y \right) \left(1 - \frac{\Delta t}{2} \mathcal{L}_z \right) \phi^{n+1} = \left(1 + \frac{\Delta t}{2} \mathcal{L}_x \right) \left(1 + \frac{\Delta t}{2} \mathcal{L}_y \right) \left(1 + \frac{\Delta t}{2} \mathcal{L}_z \right) \phi^n + \Delta t S^{n+\frac{1}{2}} + \frac{\Delta t^2}{4} \mathcal{L}_x \mathcal{L}_y \mathcal{L}_z (\phi^{n+1} - \phi^n) + \mathcal{O}(\Delta t^3)$$

$$(22)$$

We note that the term $((\Delta t)^2/4)\mathcal{L}_{\chi}\mathcal{L}_{y}\mathcal{L}_{z}(\phi^{n+1} - \phi^n)$ on the RHS of the above equation has an order of accuracy of $\mathcal{O}(\Delta t^3)$ because $\phi^{n+1} - \phi^n \approx \Delta t$. Hence this term can be accumulated in the truncation error

$$\begin{pmatrix} 1 - \frac{\Delta t}{2} \mathcal{L}_x \end{pmatrix} \left(1 - \frac{\Delta t}{2} \mathcal{L}_y \right) \left(1 - \frac{\Delta t}{2} \mathcal{L}_z \right) \phi^{n+1} = \left(1 + \frac{\Delta t}{2} \mathcal{L}_x \right) \left(1 + \frac{\Delta t}{2} \mathcal{L}_y \right) \left(1 + \frac{\Delta t}{2} \mathcal{L}_y \right) \left(1 + \frac{\Delta t}{2} \mathcal{L}_z \right) \phi^n + \Delta t S^{n+\frac{1}{2}} + \mathcal{O}(\Delta t^3)$$

$$(23)$$

To discretise equation (16) we divide the domain Ω into a uniform grid with a grid size $\Delta y = L_x/(N_x - 1)$, $\Delta y = L_y/(N_y - 1)$ and $\Delta z = L_z/(N_z - 1)$ in the *x*, *y* and *z* directions respectively. Moreover, if we denote $\phi_{i,j,k}^n$ as an approximation of $\phi(x_i, y_j, z_k, t_n)$ for an arbitrary function $\phi(x, y, z, t)$ and dropping the truncation error the above equation is written as

$$\left(1 - \frac{\Delta t}{2} \mathcal{L}_x\right) \left(1 - \frac{\Delta t}{2} \mathcal{L}_y\right) \left(1 - \frac{\Delta t}{2} \mathcal{L}_z\right) \phi_{i,j,k}^{n+1}$$

$$= \left(1 + \frac{\Delta t}{2} \mathcal{L}_x\right) \left(1 + \frac{\Delta t}{2} \mathcal{L}_y\right) \left(1 + \frac{\Delta t}{2} \mathcal{L}_y\right) \left(1 + \frac{\Delta t}{2} \mathcal{L}_z\right) \phi_{i,j,k}^{n+\frac{1}{2}}$$

$$+ \frac{\Delta t}{2} \mathcal{L}_z \phi_{i,j,k}^{n} + \Delta t S_{i,j,k}^{n+\frac{1}{2}}$$

$$(24)$$

This equation can be solved by splitting the operators using D'Yakonov Alternating Directional Implicit scheme (D'yakonov 1963) and introducing two intermediate variables ϕ^{**} and ϕ^{*}

$$\left(1 - \frac{\Delta t}{2} \mathcal{L}_z\right) \phi_{i,j,k}^{**} = \left(1 + \frac{\Delta t}{2} \mathcal{L}_x\right) \left(1 + \frac{\Delta t}{2} \mathcal{L}_y\right) \left(1 + \frac{\Delta t}{2} \mathcal{L}_z\right) \phi_{i,j,k}^{n+\frac{1}{2}}$$

$$+ \frac{\Delta t}{2} \mathcal{L}_z\right) \phi_{i,j,k}^{n} + \Delta t S_{i,j,k}^{n+\frac{1}{2}}$$

$$(25)$$

$$\left(1 - \frac{\Delta t}{2} \mathcal{L}_{\mathcal{Y}}\right) \phi_{i,j,k}^* = \phi_{i,j,k}^{**}$$
⁽²⁶⁾

$$\left(1 - \frac{\Delta t}{2}\mathcal{L}_x\right)\phi_{i,j,k}^{n+1} = \phi_{i,j,k}^* \tag{27}$$

The above operation creates three one-dimensional equations which can be solved by the CCD method. The sixth order accurate CCD formulas (10) and (11) combined with boundary equations (12) and (13) can be used by replacing *h* with $\Delta x \Delta y$ and Δz to solve equations (25) - (27) respectively with an accuracy of $\mathcal{O}(\Delta x^6 + \Delta y^6 + \Delta z^6 + \Delta t^2)$

We have to calculate the right hand side of equation (25) which requires computing the first and second derivatives of $\phi_{i,j,k}^n$ with higher order accuracy beforehand. For periodic boundary conditions, equation (10)-(13) are sufficient to calculate ϕ'_i and ϕ''_i provided that ϕ_i are given. However for non-periodic boundary these equations provide 2(*N*-1) equations with 2*N* unknowns. Therefore we need two additional boundary CCD equations

$$\frac{7}{2h}\phi_1 - \frac{4}{h}\phi_2 + \phi_3 + \phi_1' + 2\phi_2' - h\phi_2'' = 0$$
(28)
$$\phi_{N-2} + \frac{4}{h}\phi_{N-1} - \frac{7}{2h}\phi_N + 2\phi_{N-1}' + \phi_N' + 4h\phi_{N-1}''$$
(29)
$$= 0$$

The boundary condition for ϕ^* and ϕ^{**} are calculated from the following equations for Dirichlet type boundaries.

$$\phi_{i,j,k}^* = \left(1 - \frac{\Delta t}{2} \mathcal{L}_x\right) g_{i,j,k}^{n+1} \tag{30}$$

$$\phi_{i,j,k}^{**} = \left(1 - \frac{\Delta t}{2}\mathcal{L}_{\mathcal{Y}}\right) \left(1 - \frac{\Delta t}{2}\mathcal{L}_{\mathcal{X}}\right) g_{i,j,k}^{n+1} \tag{31}$$

Numerical Experiments

We consider a prototypal partial differential equation (16) in a three-dimensional cubic domain $0 \le x, y, z \le 2$, for which the analytical solution is

$$\phi(x, y, z, t) = \frac{1}{(4t+1)^{\frac{3}{2}}} \exp\left(-\frac{(x-pt-0.5)^2}{a(4t+1)} -\frac{(y-qt-0.5)^2}{b(4t+1)} -\frac{(y-qt-0.5)^2}{b(4t+1)}\right)$$
(32)

The initial and Dirichlet boundary conditions are directly taken from the exact solution. For a uniform grid size ($\Delta x = \Delta y = \Delta z = 0.025$), we keep the diffusivity constant (a = b = 0.01) and vary the convection velocity p, q, r = 0.8, 8, 80, 800 to observe the effect of Peclet number ($Pe = p\Delta x/a$). The resulting solutions after time t = 1.25 sec are represented in Figure 1 (a-d) and Figure 2 (a-b).





Figure 1. Comparison between the exact and numerical solutions using the present method, 1(a) Pe = 2, 1(b) Pe = 20, 1(c) Pe = 200, 1(d) Pe = 2000 at z = 1.0

From Figure 1, it can be clearly observed that the CCD-ADI scheme developed in this paper generates results that are in close agreement with the analytical solution.



Figure 2. Comparison of the CCD-ADI solution with exact solution $0 \le x, y \le 2, t = 1.25$, Pe = 2; (a) z = 0.2, (b) z = 1.2

Furthermore, in Figure 2, it can be observed that the crosssectional area-averaged value of the quantity ϕ at two different zlocations (z = 0.2 and z = 1.2) are very closely matched with the analytical solution which again confirms the high degree of accuracy of the present scheme.

The temporal accuracy can be extended to fourth order by performing a Richardson extrapolation. The method can be shown to be unconditionally stable.

Conclusions

In this work, we have developed a sixth order spatially accurate and second order temporally accurate three-point compact combined difference scheme to solve the advection-diffusion equation in three dimensions. The numerical method is extremely robust, and it reproduces analytical solutions over a wide range of Peclet numbers with a high degree of fidelity.

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