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by

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Abstract

We present the stationary and transient complete flux schemes for the advection-diffusion-reaction equation. In the first scheme, the numerical flux is derived from a local BVP for the corresponding stationary equation. The transient scheme is an extension, since it includes the time derivative in the flux computation. The resulting semidiscretisation is an implicit ODE system, which has much smaller dissipation and dispersion errors than the semidiscretisation based on the stationary flux, at least for smooth problems. Both schemes are validated for a test problem.

Keywords. Advection-diffusion-reaction equation, flux, finite volume method, integral representation flux, numerical flux, dissipation and dispersion errors. **AMS subject classifications.** 65M99, 76M12.

1 Introduction

Conservation laws are ubiquitous in continuum physics, they occur in disciplines like fluid mechanics, combustion theory, plasma physics, semiconductor theory etc. These conservation laws are often of advection-diffusion-reaction type, describing the interplay between different processes such as advection or drift, diffusion or conduction and (chemical) reaction or recombination/generation.

The numerical solution of these equations requires accurate and robust space discretisation and time integration methods and efficient (iterative) solution methods for the resulting algebraic system. In this paper we address the first two topics for the model equation

$$\frac{\partial\varphi}{\partial t} + \frac{\partial}{\partial x} \left(u\varphi - \varepsilon \frac{\partial\varphi}{\partial x} \right) = s, \tag{1.1}$$

where u is the advection velocity, $\varepsilon \ge \varepsilon_{\min} > 0$ a diffusion/conduction coefficient and s a source term. The unknown $\varphi(x,t)$ can be, e.g., the temperature or a species mass fraction of a reacting gas mixture. Associated with (1.1) we introduce the flux f defined by

$$f := u\varphi - \varepsilon \frac{\partial \varphi}{\partial x}.$$
(1.2)

For space discretisation we use the finite volume method (FVM) [1] in combination with the complete flux (CF) scheme for the numerical fluxes [2, 4]. For stationary equations, the CF approximation is based on the solution of a local boundary value problem for the entire equation and is therefore an extension of exponentially fitted schemes, which are based on the corresponding constant coefficient, homogeneous

equation; see e.g. [5]. The CF approximation is second order accurate, even for strongly advection dominated flow, and gives rise to a tridiagonal system.

In this paper we consider the extension to time-dependent equations. A first obvious choice would be to combine the stationary CF approximation with a suitable time integration method. We refer to this flux approximation as the stationary complete flux (SCF) scheme. However, for strong advection, the space discretisation error reduces to first order. Therefore, we propose to include the time derivative $\partial \varphi / \partial t$ already in the numerical approximation of the flux. More precisely, we put the time derivative in the source term and solve the corresponding quasi-stationary BVP. The resulting scheme, referred to as the transient complete flux (TCF) scheme, does not have this drawback, and moreover, has usually much smaller dissipation and dispersion errors than the SCF scheme.

We have organised our paper as follows. The SCF scheme is briefly summarised in Section 2 and its extension to time-dependent equations is presented in Section 3. The SCF and TCF semidiscretisations are analysed in terms of dissipation and dispersion in Section 4. The performance of both schemes is demonstrated in Section 5, and finally in Section 6, we present a summary and conclusions.

2 Numerical approximation of the stationary flux

In this section we present the complete flux scheme for the stationary equation, which is based on the integral representation of the flux. The derivation is a summary of the theory in [2, 4].

The stationary conservation law can be written as df/dx = s with the flux f defined in (1.2). In the FVM we cover the domain with a finite number of control volumes (cells) I_j of size Δx . We choose the grid points x_j , where the variable φ has to be approximated, in the cell centres, the so-called cell centred approach; see e.g. [6]. Consequently, we have $I_j := [x_{j-1/2}, x_{j+1/2}]$ with $x_{j+1/2} := \frac{1}{2}(x_j + x_{j+1})$. Integrating the equation over I_j and applying the midpoint rule for the integral of s, we obtain the discrete conservation law

$$F_{j+1/2} - F_{j-1/2} = s_j \,\Delta x,\tag{2.1}$$

where $F_{j+1/2}$ is the numerical approximation of the flux f at the interface at $x = x_{j+1/2}$ and where $s_j := s(x_j)$.

The integral representation of the flux $f_{j+1/2} := f(x_{j+1/2})$ at the cell edge $x_{j+1/2}$ located between the grid points x_j and x_{j+1} is based on the following model boundary value problem (BVP) for the variable φ

$$\frac{\mathrm{d}}{\mathrm{d}x} \left(u\varphi - \varepsilon \frac{\mathrm{d}\varphi}{\mathrm{d}x} \right) = s, \quad x_j < x < x_{j+1}, \tag{2.2a}$$

$$\varphi(x_j) = \varphi_j, \quad \varphi(x_{j+1}) = \varphi_{j+1}.$$
 (2.2b)

We like to emphasize that $f_{j+1/2}$ corresponds to the solution of the *inhomogeneous* BVP (2.2), implying that $f_{j+1/2}$ not only depends on u and ε , but also on the source term s. It is convenient to introduce the variables λ , P, Λ and S for $x \in (x_j, x_{j+1})$ by

$$\lambda := \frac{u}{\varepsilon}, \quad P := \lambda \Delta x, \quad \Lambda(x) = \int_{x_{j+1/2}}^{x} \lambda(\xi) \, \mathrm{d}\xi, \quad S(x) := \int_{x_{j+1/2}}^{x} s(\xi) \, \mathrm{d}\xi. \tag{2.3}$$

Here, P and Λ are the Peclet function and Peclet integral, respectively, generalising the well-known (numerical) Peclet number. Integrating the differential equation (2.2a) from $x_{i+1/2}$ to x we get the



Figure 1: Green's function for the flux for P > 0 (left) and P < 0 (right).

integral balance $f(x) - f_{j+1/2} = S(x)$. Using the definition of Λ in (2.3), it is clear that the flux can be rewritten as $f = -\varepsilon e^{\Lambda} d(\varphi e^{-\Lambda})/dx$. Substituting this into the integral balance and integrating from x_j to x_{j+1} we obtain the following expression for the flux

$$f_{j+1/2} = f_{j+1/2}^{(h)} + f_{j+1/2}^{(i)},$$
(2.4a)

$$f_{j+1/2}^{(h)} = -\left(e^{-\Lambda_{j+1}}\varphi_{j+1} - e^{-\Lambda_{j}}\varphi_{j}\right) / \int_{x_{j}}^{x_{j+1}} \varepsilon^{-1} e^{-\Lambda} \,\mathrm{d}x,$$
(2.4b)

$$f_{j+1/2}^{(i)} = -\int_{x_j}^{x_{j+1}} \varepsilon^{-1} e^{-\Lambda} S \, \mathrm{d}x \, / \int_{x_j}^{x_{j+1}} \varepsilon^{-1} e^{-\Lambda} \, \mathrm{d}x, \tag{2.4c}$$

where $f_{j+1/2}^{(h)}$ and $f_{j+1/2}^{(i)}$ are the homogeneous and inhomogeneous part, corresponding to the homogeneous and particular solution of (2.2), respectively.

In the following we assume that u and ε are constant; extension to variable coefficients is discussed in [2, 4]. In this case we can determine all integrals in (2.4b). Moreover, substituting the expression for S(x) in (2.4c) and changing the order of integration, we can derive an alternative expression for the inhomogeneous flux. This way we obtain

$$f_{j+1/2}^{(h)} = -\frac{\varepsilon}{\Delta x} \left(B(P)\varphi_{j+1} - B(-P)\varphi_j \right), \tag{2.5a}$$

$$f^{(i)}(x_{j+1/2}) = \Delta x \int_0^1 G(\sigma; P) s(x_j + \sigma \Delta x) \,\mathrm{d}\sigma, \quad \sigma(x) := \frac{x - x_j}{\Delta x}.$$
(2.5b)

Here $B(z) := z/(e^z - 1)$ is the Bernoulli function and $G(\sigma; P)$ the Green's function for the flux, given by

$$G(\sigma; P) = \begin{cases} \frac{1 - e^{-P\sigma}}{1 - e^{-P}} & \text{for } 0 \le \sigma \le \frac{1}{2}, \\ -\frac{1 - e^{P(1-\sigma)}}{1 - e^{P}} & \text{for } \frac{1}{2} < \sigma \le 1; \end{cases}$$
(2.6)

see Figure 1.

Next, we give the numerical flux $F_{j+1/2}$. For the homogeneous component $F_{j+1/2}^{(h)}$ we simply take (2.5a), i.e., $F_{j+1/2}^{(h)} = f_{j+1/2}^{(h)}$. Note that for dominant diffusion ($|P| \ll 1$) the integral (average) of

 $G(\sigma; P)$ is small, whereas for dominant advection $(|P| \gg 1) G(\sigma; P)$ has a clear bias towards the upwind side of the interval. For this reason we replace s(x) in (2.5b) by its upwind value $s_{u,j+1/2}$, i.e., $s_{u,j+1/2} = s_j$ if $u \ge 0$ and $s_{u,j+1/2} = s_{j+1}$ if u < 0, and evaluate the resulting integral exactly. This way we obtain

$$F_{j+1/2} = F_{j+1/2}^{(h)} + \left(\frac{1}{2} - W(P)\right) s_{u,j+1/2} \Delta x,$$
(2.7)

where $W(z) := (e^z - 1 - z)/(z(e^z - 1))$. From this expression it is clear that the inhomogeneous component is only of importance for dominant advection. We refer to (2.7) as the complete flux (CF) scheme, as opposed to the homogeneous flux (HF) scheme for which we only take into account $F_{j+1/2}^{(h)}$. Finally, substituting (2.7) in (2.1) we obtain the discretisation

$$\frac{1}{\Delta x} \left(F_{j+1/2}^{(h)} - F_{j-1/2}^{(h)} \right) = \left(\frac{1}{2} + W(|P|) \right) s_j + \left(\frac{1}{2} - W(|P|) \right) s_{j(u)},$$
(2.8)

where $j(\mathbf{u})$ is the index of the grid point upwind of j, i.e., $j(\mathbf{u}) = j - 1$ if $u \ge 0$ and $j(\mathbf{u}) = j + 1$ if u < 0.

3 Extension to time-dependent conservation laws

In this section we present the extension of the complete flux scheme to time-dependent conservation laws.

Equation (1.1) can be written as $\partial \varphi / \partial t + \partial f / \partial x = s$. Integrating this equation over the control volume I_j and applying the midpoint rule to the integrals of $\partial \varphi / \partial t$ and s, we obtain the semidiscrete conservation law

$$\dot{\varphi}_j \Delta x + F_{j+1/2} - F_{j-1/2} = s_j \Delta x,$$
(3.1)

where $\dot{\varphi}_j = \mathrm{d}\varphi_j/\mathrm{d}t$. Note that the numerical flux $F_{j+1/2}$ still depends on t.

For the numerical flux $F_{j+1/2}$ in (3.1) we have two options. First, we can simply take the stationary flux (2.7); henceforth referred to as the SCF scheme. Alternatively, we can take into account $\partial \varphi / \partial t$ if we determine the numerical flux from the following quasi-stationary BVP

$$\frac{\partial}{\partial x} \left(u\varphi - \varepsilon \frac{\partial \varphi}{\partial x} \right) = s - \frac{\partial \varphi}{\partial t}, \quad x_j < x < x_{j+1}, \tag{3.2a}$$

$$\varphi(x_j) = \varphi_j, \quad \varphi(x_{j+1}) = \varphi_{j+1}.$$
(3.2b)

Thus, we have a modified source term $\tilde{s} := s - \partial \varphi / \partial t$. Repeating the derivation in the previous section, we obtain

$$F_{j+1/2} = F_{j+1/2}^{(h)} + \left(\frac{1}{2} - W(P)\right) \left(s_{u,j+1/2} - \dot{\varphi}_{u,j+1/2}\right) \Delta x.$$
(3.3)

This flux contains the upwind value $\dot{\varphi}_{u,j+1/2}$ of the time derivative and is referred to as the transient complete flux (TCF) scheme. Analogous to the stationary case, we conclude that inclusion of the time derivative is only of importance for dominant advection.

Combining the expression in (3.3) with the semi-discrete conservation law (3.1) we find

$$\left(\frac{1}{2} + W(|P|)\right)\dot{\varphi}_{j} + \left(\frac{1}{2} - W(|P|)\right)\dot{\varphi}_{j(\mathbf{u})} + \frac{1}{\Delta x} \left(F_{j+1/2}^{(\mathbf{h})} - F_{j-1/2}^{(\mathbf{h})}\right) = \left(\frac{1}{2} + W(|P|)\right)s_{j} + \left(\frac{1}{2} - W(|P|)\right)s_{j(\mathbf{u})}.$$

$$(3.4)$$

Finally, we have to apply a suitable time integration method to (3.4) for which we will take the trapezoidal rule.

4 Dissipation and dispersion of the semidiscrete system

It is interesting to compare the SCF and TCF semidiscretisations in terms of dissipation (damping) and dispersion. Therefore, consider the constant coefficient homogeneous equation

$$\frac{\partial\varphi}{\partial t} + u\frac{\partial\varphi}{\partial x} = \varepsilon\frac{\partial^2\varphi}{\partial x^2}.$$
(4.1)

In the following we assume that $u \ge 0$; the analysis for $u \le 0$ is similar. Following [3], we look for a planar wave solution

$$\varphi(x,t) = e^{i(\kappa x - \omega t)},\tag{4.2}$$

where κ is the wave number and ω is the frequency. Substituting (4.2) in (4.1) we obtain the dispersion relation

$$i\omega(\kappa) = iu\kappa + \varepsilon\kappa^2. \tag{4.3}$$

The frequency ω determines the time evolution of the solution (4.2). Comparing the (exact) solution of (4.1) at two consecutive time levels, we can define the amplification factor $g = g(\kappa)$ as follows

$$g(\kappa) := \varphi(x, t_{n+1}) / \varphi(x, t_n) = e^{-i\omega\Delta t},$$
(4.4)

where $t_n := n\Delta t$ (n = 0, 1, 2, ...) and $\Delta t > 0$ is the time step. Note that g is independent of x. Combining the relations (4.3) and (4.4) we find the following amplification factor for equation (4.1), i.e.,

$$g(\psi) = e^{-d\psi^2} e^{-ic\psi}, \qquad (4.5)$$

with $d := \varepsilon \Delta t / \Delta x^2$ the diffusion number, $c := u \Delta t / \Delta x$ the Courant number and $\psi := \kappa \Delta x$ the phase angle $(0 \le \psi < \pi)$.

We will now compute the amplification factors of the SCF and TCF semidiscretisations and compare these to (4.5). First, consider the SCF semidiscretisation of equation (4.1), which coincides with the HF semidiscretisation, given by

$$\dot{\varphi}_j \,\Delta x + \frac{\varepsilon}{\Delta x} B^- \left(\varphi_j - \varphi_{j-1}\right) - \frac{\varepsilon}{\Delta x} B^+ \left(\varphi_{j+1} - \varphi_j\right) = 0,\tag{4.6}$$

with $B^{\pm} := B(\pm P)$. Substituting $\varphi(x_j, t)$, with φ defined in (4.2), we obtain the discrete dispersion relation

$$i\omega(\kappa) = iu\kappa \frac{\sin\psi}{\psi} + \varepsilon\kappa^2 \frac{1}{2} (B^+ + B^-) \left(\frac{\sin\psi/2}{\psi/2}\right)^2 =: iu\kappa\xi + \varepsilon\kappa^2\eta.$$
(4.7)

The variables ξ and η in the right hand side define the deviation of ω from the expression in (4.3). From (4.4) and (4.7) we obtain the following expression for the amplification factor, i.e.,

$$q(\psi) = \mathrm{e}^{-d\psi^2 \eta} \mathrm{e}^{-\mathrm{i}c\psi\xi}.$$
(4.8)

To quantify dissipation and dispersion, we define the (relative) amplitude error ϵ_a and the (relative) phase error ϵ_f as follows:

$$\epsilon_{\rm a}(\psi) := 1 - e^{d\psi^2(1-\eta)}, \quad \epsilon_{\rm f}(\psi) := 1 - \xi.$$
(4.9)



Figure 2: The amplitude error (left) and the phase error (right). Parameter values are P = 1 (top), P = 50 (bottom) and c = 1.

Plots of ϵ_a and ϵ_f are given in Figure 2 (solid lines).

Next, consider the TCF semidiscretisation of (4.1), which reads

$$\left(\frac{1}{2} - W^{+}\right)\dot{\varphi}_{j-1}\,\Delta x + \left(\frac{1}{2} + W^{+}\right)\dot{\varphi}_{j}\,\Delta x + \frac{\varepsilon}{\Delta x}B^{-}\left(\varphi_{j} - \varphi_{j-1}\right) - \frac{\varepsilon}{\Delta x}B^{+}\left(\varphi_{j+1} - \varphi_{j}\right) = 0, \quad (4.10)$$

with $W^+ := W(P)$. Note that substituting $W^+ = \frac{1}{2}$ in (4.10) we recover the SCF semidiscretization (4.6). Once more substituting $\varphi(x_i, t)$ we find the discrete dispersion relation

$$i\omega(\kappa) = \frac{\varepsilon}{\Delta x^2} \frac{-B^+(e^{i\psi} - 1) + B^-(1 - e^{-i\psi})}{(\frac{1}{2} - W^+)e^{-i\psi} + (\frac{1}{2} + W^+)} =: iu\kappa\xi + \varepsilon\kappa^2\eta.$$
(4.11)

This relation implicitly defines the factors ξ and η . After a tedious computation we find

$$\xi = \frac{\sin\psi}{\psi} \frac{\cos^2\psi/2 + F_1(P)\sin^2\psi/2}{\cos^2\psi/2 + 4W^2(P)\sin^2\psi/2},$$
(4.12a)

$$\eta = \left(\frac{\sin\psi/2}{\psi/2}\right)^2 \frac{\cos^2\psi/2 + F_2(P)\sin^2\psi/2}{\cos^2\psi/2 + 4W^2(P)\sin^2\psi/2},\tag{4.12b}$$

where the functions $F_1(z)$ and $F_2(z)$ are defined by

$$F_1(z) := 2W(z) - \left(B(z) + B(-z)\right) \frac{2W(z) - 1}{z}, \quad F_2(z) := W(z) \left(B(z) + B(-z)\right). \quad (4.12c)$$

The corresponding amplification factor is given in (4.8). Combining (4.9) with (4.12) we can determine the amplitude and phase errors, which are shown in Figure 2 (dashed lines).

From these figures we conclude the following. For dominant diffusion, i.e. small P, the TCF scheme has slightly smaller amplitude and phase errors than the SCF scheme. On the other hand, for dominant

5 NUMERICAL EXAMPLE

advection, i.e. large P, the amplitude and phase errors of the TCF scheme are significantly smaller than those of the SCF scheme, at least for low wave number modes with typically $0 \le \psi \le \frac{1}{2}$. For smooth solutions this can always be attained if we choose Δx small enough. However, for high wave number modes, say $2 \le \psi \le \pi$, the dispersion error of the TCF scheme is large. Therefore, spurious oscillations cannot be excluded for nonsmooth solutions with steep interior/boundary layers.

5 Numerical example

In this section we apply the SCF and TCF schemes to a model problem to asses their (order of) accuracy. We consider both diffusion-dominated and advection-dominated flow.

Consider the test equation [6]

$$\frac{\partial \varphi}{\partial t} + u \frac{\partial \varphi}{\partial x} - \varepsilon \frac{\partial^2 \varphi}{\partial x^2} = s, \quad s(x,t) = \beta^2 \varepsilon \cos\left(\beta(x-ut)\right), \quad 0 < x < 1, \quad t > 0.$$
(5.1)

Initial and boundary condition are chosen such that the exact solution is given by

$$\varphi(x,t) = \cos\left(\beta(x-ut)\right) + e^{-\alpha^2 \varepsilon t} \cos\left(\alpha(x-ut)\right).$$
(5.2)

We take the following parameter values: $\alpha = 4\pi$, $\beta = 2\pi$, u = 1.1 and $\varepsilon = 2 \times 10^{-2}$ (dominant diffusion) or $\varepsilon = 10^{-8}$ (dominant advection). Furthermore, we choose $\Delta x = \Delta t =: h$. To determine the accuracy of a numerical solution we compute the average error $e_h := h ||\varphi - \varphi^*||_1$ at t = 1, where φ^* denotes the exact solution restricted to the grid, as a function of the reciprocal grid size h^{-1} . Table 1 shows e_h and the reduction factors $e_h/e_{h/2}$. Clearly, for $\varepsilon = 2 \times 10^{-2}$, $e_h/e_{h/2} \rightarrow 4$ for $h \rightarrow 0$ for both the SCF and TCF scheme, and consequently, both schemes display second order convergence behaviour for $h \rightarrow 0$. The numerical errors are approximately the same for both schemes. However, the situation is quite different for the case $\varepsilon = 10^{-8}$. In this case $e_h/e_{h/2} \rightarrow 2$ for $h \rightarrow 0$ for the SCF scheme, which means that the method is only first order convergent. The TCF-scheme still displays second convergence behaviour. Obviously, the TCF-solution is in this case much more accurate than the SCF-solution.

	$\varepsilon = 2 \times 10^{-2}$				$\varepsilon = 10^{-8}$			
	SCF		TCF		SCF		TCF	
h^{-1}	e_h	$e_h/e_{h/2}$	e_h	$e_h/e_{h/2}$	e_h	$e_h/e_{h/2}$	e_h	$e_h/e_{h/2}$
20	$7.479 \cdot 10^{-2}$	3.36	$1.415 \cdot 10^{-2}$	2.72	$3.879 \cdot 10^{-1}$	1.26	$2.430 \cdot 10^{-2}$	3.69
40	$2.224 \cdot 10^{-2}$	3.81	$5.197 \cdot 10^{-3}$	3.33	$3.070 \cdot 10^{-1}$	1.50	$6.586 \cdot 10^{-3}$	3.87
80	$5.843 \cdot 10^{-3}$	3.94	$1.563 \cdot 10^{-3}$	3.66	$2.046 \cdot 10^{-1}$	1.71	$1.703 \cdot 10^{-3}$	3.93
160	$1.482 \cdot 10^{-3}$	3.98	$4.268 \cdot 10^{-4}$	3.83	$1.200 \cdot 10^{-1}$	1.84	$4.333 \cdot 10^{-4}$	3.97
320	$3.723 \cdot 10^{-4}$	3.99	$1.114 \cdot 10^{-4}$	3.92	$6.532 \cdot 10^{-2}$	1.92	$1.092 \cdot 10^{-4}$	3.98
640	$9.324 \cdot 10^{-5}$	4.00	$2.844 \cdot 10^{-5}$	3.96	$3.411 \cdot 10^{-2}$	1.96	$2.742 \cdot 10^{-5}$	3.99
1280	$2.333 \cdot 10^{-5}$		$7.186 \cdot 10^{-6}$		$1.743 \cdot 10^{-2}$		$6.868 \cdot 10^{-6}$	

Table 1: Average errors and error quotients.

Finally, we show in Figure 3 the SCF and TCF numerical approximations of the highly oscillatory solution with $\alpha = 4\pi$ and $\beta = 20\pi$. The TCF scheme is superior to the SCF scheme; the TCF solution for $N = h^{-1} = 160$ control volumes is much better than the SCF solution on a 16 times finer grid! The SCF solution is damped too much due to the large dissipation error. Notice that the TCF solution for N = 160 has a little phase shift compared to the exact solution, due to the dispersion error. However, for N = 320 this phase shift has disappeared.

6 CONCLUDING REMARKS



Figure 3: Highly oscillatory numerical solutions of (5.1). Parameter values are $\alpha = 4\pi$, $\beta = 20\pi$, u = 1.1 and $\varepsilon = 10^{-8}$. Number of control volumes: N = 2560 (left) and N = 160 (right).

6 Concluding remarks

In this paper we have presented the SCF and TCF schemes for the advection-diffusion-reaction equation. The SCF scheme is based on the solution of a local boundary value problem, excluding the time derivative $\partial \varphi / \partial t$. As an extension of this scheme, we proposed the TCF scheme, where the time derivative is included in the flux computation. The resulting semidiscretisation is an implicit ODE system, which has much smaller dissipation and dispersion errors than the SCF scheme, at least for smooth solutions. The performance of both schemes is demonstrated for a model problem. We conclude that for dominant diffusion there is not much difference between both schemes, however, for dominant advection, the space discretisation error of the SCF scheme reduces to first order, whereas the TCF scheme is still second order accurate. In contrast to the SCF scheme, for nonsmooth solutions spurious oscillations cannot be excluded in the TCF scheme due to the large dispersion errors of the scheme. These have to be controlled by a (dissipative) time integration method. This is topic of current research.

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