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A robust and reliable approach to nonlinear dynamical problems

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Abstract

A new approach, which utilizes Gaussian Lagrange distributed approximating functionals (LDAFs) for evaluating spatial derivatives to high accuracy is proposed for solving nonlinear dynamical problems. Three different nonlinear problems (Burgers' equation, a nonlinear Fokker–Planck equation and the Korteweg–de Vries equation) are used to demonstrate the usefulness and test the accuracy of the method. It is found that the present approach is robust for a variety of different nonlinear dynamical problems, and, using equivalent parameters, is the most accurate available method for the problems which we have examined. © 1998 Elsevier Science B.V.

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Nonlinear partial differential equations (PDE's) are ubiquitous in science and engineering, with applications ranging from statistical physics to aerodynamics, and to ecology. Analytical solutions to nonlinear equations are available for only a few special cases. Analytical approximations (e.g., asymptotic expressions) are commonly used, and are profitable for providing a conceptual understanding of various nonlinear systems. However, in contrast to linear PDE's, there is no universal analytical procedure applicable to all possible nonlinear equations. Usually, the validity of each approach is limited to one or, at most, a few particular models. However, significant progress has been made in recent years in the numerical solution of such equations. One of the major driving forces behind the recent advances in the understanding of nonlinear phenomena has undoubtedly been the accessibility of even more powerful digital computers for performing calculations rapidly and efficiently.

Thus, the study of numerical methods for solving nonlinear PDE's is an extremely important contemporary research field. There are two major classes of methods currently being employed, namely, global methods (e.g., spectral and pseudospectral methods) and local methods (e.g., finite elements and finite differences). For a linear system with relatively simple boundary conditions, such as the Schrödinger equation describing quantum dynamics, various spectral and pseudospectral methods [1–7] are powerful in terms of accuracy, minimizing the number of grid points required, and achieving computational efficiency. For nonlinear systems, the superposition principle is no longer valid, and spectral methods are not as simple

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or robust to use as in linear cases for dealing with complex boundary conditions and geometries. Local methods, such as various finite element [8–10] and finite difference methods [11–17], are more easily implemented in these instances, and therefore are often the method of choice. In general, however, global methods, when applicable, are more accurate than local methods.

In this letter we introduce a reliable and robust approach (the Gaussian Lagrange distributed approximating functional [18] or GLDAF) that, as a local spectral method, has the accuracy of a global approach but also has the simplicity and flexibility of a local method for solving various nonlinear partial differential equations. It provides the most accurate numerical results to date (although very similar to those obtained using our earlier Hermite DAFs [19] for appropriately chosen parameters) for several different types of nonlinear partial differential equations, including Burgers'equation [21], a nonlinear Fokker–Planck equation [16] and the Korteweg–de Vries (KdV) equation [22]. We present detailed results for these after we outline the GLDAF method. To simplify our presentation, we restrict ourselves to one-dimensional cases, but the approach is general, and is being applied to other multi-dimensional problems.

The GLDAFs have been proposed [18] as a computational tool for approximating physically realizable functions in their domain of definition, with controllable accuracy. GLDAFs can be regarded as members of generalized delta sequences, and in the appropriate limit of a GLDAF-parameter, the GLDAF tends to a Dirac delta function [23,24]. In contrast to the Dirac delta function, and the commonly used Gaussian test functions, the GLDAF is a very powerful and simple tool for numerical applications. The GLDAF already has been shown [18] to provide controllable accuracy, up to the computer round-off limit, both for the linear Schrödinger eigenvalue problem and for the wave packet propagation of the linear Ornstein–Uhlenbeck Fokker–Planck equation. We now give a brief summary of the GLDAF.

The Dirac delta function, $\delta(x-x')$, has the properties

$$F(x) = \int_{-\infty}^{\infty} \delta(x-x')F(x')dx' , \tag{1}$$

$$\frac{d^l F(x)}{dx^l} = F^{(l)}(x) = \int_{-\infty}^{\infty} \delta^{(l)}(x-x')F(x')dx' . \tag{2}$$

However, these relations are of little numerical utility for practical computations because they cannot be approximated directly by quadrature. One way to view the GLDAF is as an element in a sequence of well-behaved L^2 functions that behave like the Dirac delta function when applied to bandlimited functions, but whose action on a function can be approximated discretely.

The GLDAF is defined [18] as

$$\delta_{M,\sigma}(x-x_k) = CP_{M,k}(x)w_\sigma(x-x_k) \tag{3}$$

on the domain $\mathbb{R}^1$, where C is determined by

$$\int dx\, \delta_{M,\sigma}(x-x_k) = 1 . \tag{4}$$

In Eq. (3), $P_{M,k}(x)$ is the polynomial

$$P_{M,k}(x) = \prod_{i=1}^{M/2}(x-x_k+i\Delta)(x-x_k-i\Delta) , \tag{5}$$

where Δ is the (uniform) grid spacing. (One can also use a nonuniform grid by appropriately modifying the polynomial, $P_{M,k}(x)$.) The weight $w_\sigma(x-x_k)$ is chosen to be a (non-negative) rapidly decaying function, and in particular as a Gaussian function,

$$w_\sigma(x-x_k) = e^{-(x-x_k)^2/2\sigma^2} , \tag{6}$$

in the present work. For more details, the reader is referred to Ref. [18].

The value of a function F at a grid point x_g can be accurately represented by the GLDAF through the "discrete convolution"

$$F(x_g) \approx \Delta \sum_{k=g-W}^{g+W} \delta_{M,\sigma}(x_g-x_k)F(x_k) , \tag{7}$$

where $2W+1$ is the band width of the GLDAF.

The qth derivative of the GLDAF is analytically expressed as

$$\delta^{(q)}_{M,\sigma}(x-x_k) = C\sum_{t=0}^{q}\frac{q!}{q!(q-t)!} \times P^{(t)}_{M,k}(x)w^{(q-t)}_\sigma(x-x_k) . \tag{8}$$

This can be used to approximate the qth derivative of a function on a grid point x_g as

$$F^{(q)}(x_g) \approx \Delta \sum_{k=g-W}^{g+W} \delta^{(q)}_{M,\sigma}(x_g - x_k) F(x_k) . \qquad (9)$$

Eqs. (7) and (9) are obvious discrete analogues of Eqs. (1) and (2) for the Dirac delta function. Eqs. (7) and (9) provide the tools for solving PDE's.

To solve nonlinear equations by a time propagation method, a robust numerical scheme is required, which also achieves computational efficiency. The GLDAF approach can be combined with any number of explicit or implicit time propagation schemes, such as Runge–Kutta and/or Crank–Nicholson [20]. However, we shall illustrate the GLDAF method by the particularly simple strategy of employing a Taylor expansion in time, using the PDE to simplify the evaluation of the time derivatives. Let us consider a general class of nonlinear equations of the form

$$\frac{\partial f(x,t)}{\partial t} = L(x,t,f(x,t))f(x,t) = L(t)f(x,t) , \qquad (10)$$

where in the second equality, $L(t)$ represents both the explicit *and* implicit time dependences. The Taylor's expansion of Eq. (10) is giving by

$$\begin{aligned} f(x,t+\tau) &= \sum_{n=0} \frac{\tau^n}{n!}\frac{\partial^n}{\partial t^n} f(x,t) \\ &\approx f(x,t_0) + \tau L(t) f(x,t) \\ &\quad + \frac{\tau^2}{2!}[L^2(t) + L_t'(t)] f(x,t) \\ &\quad + \frac{\tau^3}{3!}[L^3(t) + L(t)L_t'(t) \\ &\quad + 2L_t'(t)L(t) + L_{tt}''] f(x,t) + \cdots , \end{aligned} \qquad (11)$$

and it is this equation that we use for the present computations. Numerical tests indicate that a truncation at the term which is linear in τ is good for sufficiently small τ's. However, for a larger τ it is necessary to retain terms of higher order in τ in order to achieve the desired accuracy and numerical stability. We have confirmed that the Runge–Kutta scheme provides results which are extremely close to those obtained with the Taylor expansion, but the latter provides a physical picture of various contributions.

For a given time t, the GLDAF representation of Eq. (11) is constructed according to Eqs. (7) and (9). The robust nature of the GLDAF method is here illustrated by applying it to three nonlinear equations, namely Burgers' equation [21], a nonlinear Fokker–Planck equation [16] and the KdV equation [22]. In the present computations, we choose $M = 80$, $W = 40$ and $\sigma = 3.173\Delta$, for all cases.

Burgers' equation [21], given by

$$\frac{\partial u}{\partial t} = -u\frac{\partial u}{\partial x} + \frac{1}{\mathrm{Re}}\frac{\partial^2 u}{\partial x^2} , \qquad (12)$$

is a nonlinear partial differential equation modeling a velocity field, where $u(x,t)$ is the dependent variable simulating the velocity and Re is the Reynolds number characterizing the "fluid viscosity". The competition between the nonlinear advection and the viscous diffusion is controlled by the value of Re in Burgers' equation, and thus determines the qualitative behavior of the solution. There is an analogy between Burgers' equation and the Navier–Stokes equation in the forms of the nonlinear advection and the viscous diffusion terms. The analytical solvability of Burgers' equation makes it an important test model for computational fluid dynamics (CFD), and it is customary to test new methods in CFD by first applying them to Burgers' equation [9,25–28].

We consider Eq. (12) using the following initial-boundary conditions:

$$\begin{aligned} &u(x,0) = \sin(\pi x) , \\ &u(0,t) = u(1,t) = 0 . \end{aligned} \qquad (13)$$

The exact solution [29] for this problem is available in a series form which is readily computable for the parameter range Re ≤ 100. For the parameter Re = 100, the present GLDAF calculations use three sets of grid points (25, 35 and 45 uniformly spaced points for interval [0,1]), with a time increment of $\tau = 0.01$ and a second order Taylor expansion. The function values at grid points outside this region are generated by an antisymmetric extension with respect to the boundaries. The maximum absolute errors (L_∞) for all sets of grid points at four different times are listed in Table 1. It is interesting to compare the present results with the earlier accurate numerical results recently obtained using the generalized boundary element method by Kakuda and Tosaka [10]. These authors used 100

Table 1
L_∞ errors of the numerical solutions for Burgers' equation

t	K–T	Present		
		$N = 25$	$N = 35$	$N = 45$
0.4	2.6(−2)	1.6(−2)	3.6(−3)	1.1(−3)
0.8	2.9(−2)	2.6(−2)	6.6(−3)	1.4(−3)
1.2	1.8(−2)	8.0(−3)	1.2(−3)	1.9(−4)
3.0	6.9(−3)	4.5(−5)	2.3(−5)	2.2(−5)

elements, up to 6 iterations and the same time increment as ours ($\tau = 0.01$). The errors in both methods are very small. The present results, although obtained using fewer grid points, are from ten to a few hundred times more accurate than those of Kakuda and Tosaka [10] (K–T).

It is well known that solving Burgers' equation with a high Reynolds number is extremely challenging due to shock wave fronts produced by the nonlinear steepening of the momentum wave [9,10,30]. Most numerical methods are not reliable for such computations because of the occurrence of spurious oscillations, as has been shown by Jamet and Bonnerot [30]. The present approach provides oscillation-free solutions for Reynolds numbers as high as 10^5.

In order to demonstrate further the usefulness, test the accuracy and explore the limitations of the GLDAF method for other types of nonlinear problems, we next consider a benchmark nonlinear Fokker–Planck equation,

$$\frac{\partial f(x,t)}{\partial t} = \frac{\partial[(\omega x + \theta\langle x(t)\rangle) f(x,t)]}{\partial x} + D\frac{\partial^2 f(x,t)}{\partial x^2}, \tag{14}$$

where the moment $\langle x(t)\rangle$ is determined by the instantaneous distribution

$$\langle x(t)\rangle = \int_{-\infty}^{\infty} x f(x,t)\, dx, \tag{15}$$

and ω, θ and D are constant. Assuming an initial spatial distribution of the form

$$f(x,0) = \delta(x - x_0), \tag{16}$$

the exact solution to Eq. (14) is

Table 2
Errors of the numerical solutions for the nonlinear Fokker–Planck equation

t	$\tau = 0.02$		$\tau = 0.01$	
	L_2	L_∞	L_2	L_∞
0.2	1.3(−3)	2.1(−3)	1.0(−3)	1.2(−3)
0.6	9.9(−5)	1.5(−4)	1.7(−5)	2.3(−5)
1.0	3.6(−5)	5.1(−5)	1.2(−5)	1.3(−5)
1.5	2.1(−5)	2.3(−5)	6.4(−6)	7.8(−6)
2.0	1.2(−5)	1.6(−5)	4.8(−6)	6.1(−6)

$$f(x,t) = \frac{1}{\sqrt{2\pi\sigma(t)}} \exp\left[-\frac{(x - \langle x(t)\rangle)^2}{2\sigma(t)}\right], \tag{17}$$

where $\langle x(t)\rangle$ and $\sigma(t)$ are given by

$$\langle x(t)\rangle = x_0\, e^{-(\omega+\theta)t} \tag{18}$$

and

$$\sigma(t) = \frac{D}{\omega}\left(1 - e^{-2\omega t}\right). \tag{19}$$

It is noted that the nonlinear structure in this problem is typical for statistical mechanical problems and is different from that of Burgers' equation. Eq. (14) has been used as a test problem [16] for a nonlinear, self-consistent dynamical mean field model [31,32] for describing the control and regulation of a biological system.

We choose $D = 0.1$, $\omega = 1$, $\theta = 1$, $x_0 = 0.82$, $\tau = 0.01, 0.02$ and a third order Taylor expansion for the present calculations. The function values at grid points outside the region where the solution is desired are set identically to zero. A total of 31 evenly spaced grid points are used in the solution region. Because the initial distribution is a delta function, we start the calculation at $t_0 = 0.1$ using the analytically known solution at this time (see Eq. (17)). The L_2 and L_∞ errors of our numerical solutions for a few times are listed in Table 2. It is seen that the present GLDAF approach provides highly accurate results. Another measure of the accuracy is obtained by calculating the relative second moment (M_2) errors for different times. The GLDAF approach gives smaller relative M_2 errors than does a K-point Stirling interpolation formula [16].

Finally, the present GLDAF approach is also tested for the soliton wave problem which is described by the (modified) KdV equation [22],

Table 3
Errors of the numerical solutions for de KdV equation

t	L_2	L_∞
1.0	6.30(−10)	4.03(−10)
3.0	4.59(−09)	1.41(−09)
6.0	5.05(−09)	1.83(−09)
9.0	4.88(−09)	1.45(−09)
12.0	5.08(−09)	1.86(−09)
15.0	5.06(−09)	1.58(−09)
18.0	5.53(−09)	2.02(−09)
21.0	5.66(−09)	2.11(−09)
24.0	6.56(−09)	2.53(−09)
27.0	8.18(−09)	3.57(−09)
30.0	9.13(−09)	3.64(−09)

$$\frac{\partial u(x,t)}{\partial t} = -6\,[u(x,t)]^2\,\frac{\partial u(x,t)}{\partial x} - \frac{\partial^3 u(x,t)}{\partial x^3}, \tag{20}$$

with the initial soliton wave

$$u(x,0) = 2\eta \mathrm{sech}(2\eta x) \tag{21}$$

and analytical solution

$$u(x,t) = 2\eta\,\mathrm{sech}\left[2\eta(x - 4\eta^2 t)\right]. \tag{22}$$

Note that this nonlinear equation differs from Burgers' equation and the Fokker–Planck equation in that it contains a third order spatial derivative.

We choose $\eta = 0.5$, $\Delta = 0.2$, $\tau = 0.001$ and a fourth order Taylor expansion for this computation. The function values at grid points outside the solution region of interest are set identically to zero. As shown in Table 3, our GLDAF results for this system are accurate up to 9 significant figures. Limits on the length of letters prevent us from going into the details of a comparison with other methods; see Ref. [33].

To summarize, we have presented a robust and reliable approach for solving a variety of nonlinear dynamical problems. Our basic approach is to use the LDAF to provide an accurate and localized spatial discretization and use a simple Taylor expansion (or any other standard scheme) for the time evolution. The robust nature of the present approach is illustrated by its generality. It provides a single framework for solving many different types of nonlinear problems, as has been demonstrated. Furthermore, for every problem we have examined, our method is more accurate than those available in the literature, for comparable grid and time mesh sizes. The robustness of the present approach has also been demonstrated through its accurate treatment of high Reynolds number cases of Burgers' equation, for which other numerical methods have difficulty [10,30].

References

[1] S.A. Orszag, J. Comput. Phys. 37 (1980) 79.
[2] B.A. Finlayson, The Method of Weighted Residuals and Variational Principles (Academic Press, New York, 1972).
[3] D.O. Harris, G.G. Engerholm, W.D. Gwinn, J. Chem. Phys. 43 (1965) 1515.
[4] B. Shizgal, J. Comput. Phys. 41 (1981) 309.
[5] J.V. Lill, G.A. Parker, J.C. Light, Chem. Phys. Lett. 89 (1982) 483.
[6] W. Yang, A.C. Peet, Chem. Phys. Lett. 153 (1988) 98.
[7] D.W. Schwenke, D.G. Truhlar, in: Computing Methods in Applied Sciences and Engineering, R. Glowinski, A. Lichnewsky, eds. (SIAM, Philadelphia, PA, 1990).
[8] O.C. Ziekiewicz, The Finite Element Method in Engineering Science (McGraw-Hill, London, 1971).
[9] E. Varoglu, W.D.L. Finn, Int. J. Numer. Methods Eng. 16 (1980) 171.
[10] K. Kakuda, N. Tosaka, Int. J. Numer. Methods Eng. 29 (1990) 245.
[11] P.D. Lax, Commun. Pure Appl. Math. 6 (1953) 231.
[12] G.E. Forsythe, W.R. Wasow, Finite Difference Methods for Partial Differential Equations (Wiley, New York, 1967).
[13] J.S. Chang, G. Cooper, J. Comput. Phys. 6 (1970) 1.
[14] E.W. Larson, C.D. Levermore, G.C. Pomraning, J.G. Sanderson, J. Comput. Phys. 61 (1985) 359.
[15] E.M. Epperlein, J. Comput. Phys. 112 (1994) 291.
[16] A.N. Drozdov, M. Morillo, Phys. Rev. E 54 (1996) 931.
[17] D.W. Schwenke, S.L. Mielke, D.G. Truhlar, Theor. Chem. Acta 79 (1991) 241.
[18] G.W. Wei, D.S. Zhang, D.J. Kouri, D.K. Hoffman, Phys. Rev. Lett. 79 (1997) 775.
[19] D.K. Hoffman, N. Nayar, O.A. Sharafeddin, D.J. Kouri, J. Phys. Chem. B 95 (1991) 299.
[20] W.H. Press, B.P. Flannery, S.A. Teukolsky, W.T. Vetterling, Numerical Recipes (Cambridge Univ. Press, Cambridge, 1986).
[21] J. Burgers, A Mathematical Model Illustrating the Theory of Turbulence, Advances in Applied Mechanics (Academic Press, New York, 1948).
[22] Korteweg de Vries, Phil. Mag. 39 (1895) 422.
[23] D.K. Hoffman, G.W. Wei, D.S. Zhang, D.J. Kouri, Phys. Rev. E, in press.
[24] G.W. Wei, S.A. Althorpe, D.S. Zhang, D.J. Kouri, D.K. Hoffman, Phys. Rev. A, in press
[25] J. Caldwell, P. Wanless, A.E. Cook, Appl. Math. Modelling 5 (1981) 189.
[26] P. Bar-Yoseph, E. Moses, U. Zrahia, A.L. Yarin, J. Comput. Phys. 119 (1995) 62.

[27] R. Arina, C. Canuto, J. Comput. Phys. 105 (1993) 290.
[28] S. Biringen, A. Saati, J. Aircraft. 27 (1990) 90.
[29] J.D. Cole, Q. Appl. Math. 9 (1951) 225.
[30] P. Jamet, R. Bonnerot, J. Comput. Phys. 18 (1975) 21.
[31] K. Kometani, H. Shimizu, J. Stat. Phys. 13 (1975) 473.
[32] R.C. Desai, R. Zwanzig, J. Stat. Phys. 19 (1978) 1.
[33] G.W. Wei, D.S. Zhang, D.J. Kouri, D.K. Hoffman, in preparation.
[34] P. Givi, in: Turbulent Reacting Flows, P.A. Libby, F.A. Williams, eds. (Academic Press, New York, 1994).