

求解 Klein-Gordon 方程的新型 快速紧致时间积分方法

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[摘要] 构建了基于 Hermite 插值的快速紧致时间积分方法求解 Klein-Gordon 方程. 该方法先在空间方向上采用四阶紧致差分格式离散得到了一个半离散格式. 然后结合离散正弦变换和常数变易公式给出了半离散格式之解的显示时间积分表示式, 并对积分中的非线性源项采用 Hermite 插值逼近, 得到了一个全离散格式. 仅需利用前两个时间步的计算结果, 就可获得空间和时间方向均为四阶精度的高效算法. 数值模拟的结果验证了该方法的有效性.

[关键词] Klein-Gordon 方程, 紧致差分格式, Hermite 插值, 离散正弦变换

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A New Fast Compact Time Integrator Method for Solving Klein-Gordon Equations

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Abstract: This paper is intended to devise a fast compact time integration method based on Hermite interpolation for solving Klein-Gordon equations. The spatial discretization is carried out using the fourth-order compact difference scheme, leading to a semi-discrete problem. Then the solution is expressed explicitly by means of the discrete sine transform and the constant variation formula. Finally, the Hermite interpolation is used to approximate the nonlinear source term, yielding a fully discrete scheme. In particular, if the function values and the derivative function values at two latest historic instants are used for interpolation, we can derive a fourth-order scheme in space and time together. The numerical results verify the effectiveness of the method.

Key words: Klein-Gordon equation, compact difference scheme, Hermite interpolation, discrete sine transform

Klein-Gordon 方程是一类典型的非线性波动方程, 在理论和应用物理的许多领域, 如非线性光学、固体物理和量子场论^[1-2]中有广泛应用. 本文考虑如下 Klein-Gordon 方程:

$$\begin{cases} u_{tt} = D\Delta u + g(u) + f(\mathbf{x}, t), & \mathbf{x} \in \Omega, t > 0, \\ u(\mathbf{x}, 0) = u_0(\mathbf{x}), \quad u_t(\mathbf{x}, 0) = v_0(\mathbf{x}), & \mathbf{x} \in \Omega, \\ u(\mathbf{x}, t) = u^b(\mathbf{x}, t), & \mathbf{x} \in \partial\Omega, t \in [0, T], \end{cases} \quad (1)$$

式中, $\Omega \subset \mathbf{R}^2$ 是有界矩形区域, $D > 0$ 是扩散系数, g 是非线性函数, f 是外源函数.

近年来已有学者对 Klein-Gordon 方程发展了各种数值方法. 例如差分法^[3-4], 边界元法^[5], 微分求积法^[6]等. 然而这些现有的数值方法要么精度有限, 要么计算复杂度大, 因此很有必要发展求解该问题的高效计算方法. 最近, 作者在文献[7]中借鉴积分因子方法^[8-13]的思想提出了一种快速紧致时间积分法(FCTI)用于数值求解任意阶发展方程. 该方法在空间方向使用紧致差分格式离散, 然后在时间方向上基于快速离散正

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弦变换和常数变易公式获得任意阶发展方程的显式表达式,再利用 Lagrange 插值近似非线性源项,导出了一类高效求解方法. 本文将使用前文方法数值求解 Klein-Gordon 方程(1),但用 Hermite 插值代之以 Lagrange 插值来处理非线性源项,从而得到更为高效的数值求解方法. 此时,仅需利用前两个时间步的计算结果,就可获得空间和时间方向均为四阶精度的高效算法. 数值实验验证了所提算法的高效性.

1 空间离散:紧致差分格式

设 $\Omega = \{x_b < x < x_e, y_b < y < y_e\}$. 对 Ω 作矩形划分,在 x 和 y 方向的剖分步长分别为 $h_x = (x_e - x_b)/N_x$ 和 $h_y = (y_e - y_b)/N_y$. 相应的网格点记为

$$(x_i, y_j) = (x_b + ih_x, y_b + jh_y), 0 \leq i \leq N_x, 0 \leq j \leq N_y.$$

用 $u_{i,j} = u_{i,j}(t) \approx u(x_i, y_j, t)$ 表示空间半离散解. 类似地,用 $u_{i,j}^{xx}$ 和 $u_{i,j}^{yy}$ 分别表示空间半离散解的二阶偏导数 $u_{xx}(x_i, y_j, t)$ 和 $u_{yy}(x_i, y_j, t)$. 参照文献[7]引入以下符号:

$$U = (u_{i,j})_{(N_x-1) \times (N_y-1)}, \quad U^{xx} = (u_{i,j}^{xx})_{(N_x-1) \times (N_y-1)}, \quad U^{yy} = (u_{i,j}^{yy})_{(N_x-1) \times (N_y-1)}.$$

给定正整数 p , 记

$$R_{p \times p} = \begin{bmatrix} -2 & 1 & & \\ 1 & -2 & \ddots & \\ & \ddots & -2 & 1 \\ & & 1 & -2 \end{bmatrix}, \quad G_{p \times p} = \begin{bmatrix} 10 & 1 & & \\ 1 & 10 & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & 10 \end{bmatrix},$$

$$A_x = \frac{1}{12} G_{(N_x-1) \times (N_x-1)}, \quad B_x = \frac{D}{h_x^2} R_{(N_x-1) \times (N_x-1)},$$

$$A_y = \frac{1}{12} G_{(N_y-1) \times (N_y-1)}, \quad B_y = \frac{D}{h_y^2} R_{(N_y-1) \times (N_y-1)}.$$

并定义如下两个算子:

$$(A_x \otimes U)_{i,j} = \sum_{l=1}^{N_x-1} (A_x)_{i,l} u_{l,j}, \quad (A_y \otimes U)_{i,j} = \sum_{l=1}^{N_y-1} (A_y)_{j,l} u_{i,l}.$$

使用四阶紧致差分格式进行空间离散^[14-15]:

$$\frac{1}{12}(u_{i-1,j}^{xx} + 10u_{i,j}^{xx} + u_{i+1,j}^{xx}) = \frac{1}{h_x^2}(u_{i-1,j} - 2u_{i,j} + u_{i+1,j}),$$

$$\frac{1}{12}(u_{i,j-1}^{yy} + 10u_{i,j}^{yy} + u_{i,j+1}^{yy}) = \frac{1}{h_y^2}(u_{i,j-1} - 2u_{i,j} + u_{i,j+1}),$$

式中, $i=1, 2, \dots, N_x-1, j=1, 2, \dots, N_y-1$, 从而得到方程(1)的如下空间半离散化格式:

$$U''(t) - (A_x^{-1} \otimes B_x \otimes U + A_y^{-1} \otimes B_y \otimes U) = R(t, U(t)) =: \mathcal{F}(U) + W(t), \quad (2)$$

式中,

$$\mathcal{F}(U) = (g(u_{i,j}(t)))_{(N_x-1) \times (N_y-1)}, \quad W(t) = (f(x_i, y_j, t)) + A_x^{-1} \otimes U_{x02} + A_y^{-1} \otimes U_{y02}.$$

这里 $U_{x02} = (u_{i,j}^{x02})_{(N_x-1) \times (N_y-1)}, U_{y02} = (u_{i,j}^{y02})_{(N_x-1) \times (N_y-1)}$ 定义为

$$u_{i,j}^{x02} = \begin{cases} \frac{D}{h_x^2} u_{0,j} + \frac{D}{12} (u^b)^{yy}_{0,j} - \frac{1}{12} ((u^b)''_{0,j} - g(u^b_{0,1}) - f(x_0, y_j, t)), & i=1, 1 \leq j \leq N_y-1, \\ \frac{D}{h_x^2} u_{N_x,j} + \frac{D}{12} (u^b)^{yy}_{N_x,j} - \frac{1}{12} ((u^b)''_{N_x,j} - g(u^b_{N_x,1}) - f(x_{N_x}, y_j, t)), & i=N_x-1, 1 \leq j \leq N_y-1, \\ 0 & \text{其他,} \end{cases}$$

$$u_{i,j}^{y02} = \begin{cases} \frac{D}{h_y^2} u_{i,0} + \frac{D}{12} (u^b)^{xx}_{i,0} - \frac{1}{12} ((u^b)''_{i,0} - g(u^b_{i,0}) - f(x_i, y_0, t)), & j=1, 1 \leq i \leq N_x-1, \\ \frac{D}{h_y^2} u_{i,N_y} + \frac{D}{12} (u^b)^{xx}_{i,N_y} - \frac{1}{12} ((u^b)''_{i,N_y} - g(u^b_{i,N_y}) - f(x_i, y_{N_y}, t)), & j=N_y-1, 1 \leq i \leq N_x-1, \\ 0 & \text{其他,} \end{cases}$$

经直接计算可知,在方程(2)中出现的相关矩阵存在以下谱分解:

$$A_x = P_x \tilde{D}_{a,x} P_x^{-1}, \quad A_y = P_y \tilde{D}_{a,y} P_y^{-1}, \quad B_x = P_x \tilde{D}_{b,x} P_x^{-1}, \quad B_y = P_y \tilde{D}_{b,y} P_y^{-1},$$

式中, P_x 和 P_y 是由文献[8]给出的正交矩阵. $\tilde{D}_{a,x}, \tilde{D}_{a,y}, \tilde{D}_{b,x}, \tilde{D}_{b,y}$ 是相应的特征值组成的对角阵,即

$$\begin{aligned} \tilde{D}_{a,x} &= \text{diag}(d_1^{a,x}, d_2^{a,x}, \dots, d_{N_x-1}^{a,x}), & \tilde{D}_{a,y} &= \text{diag}(d_1^{a,y}, d_2^{a,y}, \dots, d_{N_y-1}^{a,y}), \\ \tilde{D}_{b,x} &= \text{diag}(d_1^{b,x}, d_2^{b,x}, \dots, d_{N_x-1}^{b,x}), & \tilde{D}_{b,y} &= \text{diag}(d_1^{b,y}, d_2^{b,y}, \dots, d_{N_y-1}^{b,y}). \end{aligned}$$

又记 $H = (h_{i,j})_{(N_x-1) \times (N_y-1)}$,

$$h_{i,j} = d_i^{b,x}/d_i^{a,x} + d_j^{b,y}/d_j^{a,y}.$$

在方程(2)左侧乘以 P_x^{-1} , 右侧乘以 P_y^{-T} 可得

$$\bar{U}''(t) - H \odot \bar{U} = \bar{R}(t, \bar{U}), \quad (3)$$

式中, $\bar{U} = P_y^{-1} \odot P_x^{-1} \odot U$, $\bar{R}(t, \bar{U}) = P_y^{-1} \odot P_x^{-1} \odot R(t, U(t))$. 运算符“ \odot ”表示矩阵的点乘. 易知, (3) 中每个 (i, j) -元素都是一个独立的常微分方程, 因此可以通过常数变易公式求得其解. 具体而言, 假设 $g_{i,j}(t)$ 是以下齐次方程之解

$$\begin{cases} y'' - h_{i,j}y = 0, & t \in (0, T), \\ y(0) = 0, & y'(0) = 1. \end{cases}$$

则注意到 $h_{i,j} < 0$, 从而易知

$$g_{ij}(t) = \frac{\sin \sqrt{-h_{ij}} t}{\sqrt{-h_{ij}}}, \quad \bar{g}_{ij}(t) = \cos \sqrt{-h_{ij}} t.$$

定义 $\mathbf{g}(t) = (g_{ij}(t))_{(N_x-1) \times (N_y-1)}$, $\mathbf{g}'(t) = (g'_{ij}(t))_{(N_x-1) \times (N_y-1)}$. 设 $\mathbf{V}(t) = \mathbf{U}'(t)$. 则使用文献[7]中相同办法, 利用常数变易公式可知问题(3)之解可显式表示为

$$\begin{cases} \bar{U}(t) = \mathbf{g}'(t) \odot \bar{U}_0 + \mathbf{g}(t) \odot \bar{V}_0 + \int_0^t \mathbf{g}(t-\tau) \odot \bar{R}(\tau, \bar{U}(\tau)) d\tau, \\ \bar{V}(t) = H \odot \mathbf{g}(t) \odot \bar{U}_0 + \mathbf{g}'(t) \odot \bar{V}_0 + \int_0^t \mathbf{g}'(t-\tau) \odot \bar{R}(\tau, \bar{U}(\tau)) d\tau, \end{cases} \quad (4)$$

式中, $\bar{U}_0 = P_y^{-1} \odot P_x^{-1} \odot (u_0(x_i, y_j))$, $\bar{V}_0 = P_y^{-1} \odot P_x^{-1} \odot (v_0(x_i, y_j))_{(N_x-1) \times (N_y-1)}$.

2 时间离散: 时间积分和非线性源项离散

给定正整数 N_t , 设 $\Delta t = T/N_t$. 对时间区间 $[0, T]$ 做均匀剖分: $t_m = m\Delta t, m=0, 1, \dots, N_t$. 由(4)可得如下时间递进计算格式:

$$\begin{aligned} U_{m+1} &= P_y \odot P_x \odot (\mathbf{g}'(\Delta t) \odot (P_y^{-1} \odot P_x^{-1} \odot U_m) + \mathbf{g}(\Delta t) \odot (P_y^{-1} \odot P_x^{-1} \odot V_m) + Q_0^R), \\ V_{m+1} &= P_y \odot P_x \odot (H \odot \mathbf{g}(\Delta t) \odot (P_y^{-1} \odot P_x^{-1} \odot U_m) + \mathbf{g}'(\Delta t) \odot (P_y^{-1} \odot P_x^{-1} \odot V_m) + Q_1^R), \end{aligned}$$

式中,

$$\begin{aligned} Q_0^R &= \int_0^{\Delta t} \mathbf{g}(\Delta t - \tau) \odot \bar{R}(t_m + \tau, \bar{U}(t_m + \tau)) d\tau, \\ Q_1^R &= \int_0^{\Delta t} \mathbf{g}'(\Delta t - \tau) \odot \bar{R}(t_m + \tau, \bar{U}(t_m + \tau)) d\tau. \end{aligned}$$

当 $r=0, 1, 2, 3$ 时, 记

$$\phi_{i,j}^{(r,0)} = \int_0^{\Delta t} g_{i,j}(\Delta t - \tau) \left(\frac{\tau}{\Delta t} \right)^r d\tau, \quad \phi_{i,j}^{(r,1)} = \int_0^{\Delta t} g'_{i,j}(\Delta t - \tau) \left(\frac{\tau}{\Delta t} \right)^r d\tau.$$

为了得到 U_{m+1} 和 V_{m+1} 可计算的全离散格式, 利用 U, V 在时刻 t_{m-1}, t_m 得到的计算值, 在子区间 $[t_m, t_{m+1}]$ 上构造三次 Hermite 插值多项式 $P_3(\tau)$ 逼近 $\bar{R}(t_m + \tau, \bar{U}(t_m + \tau))$:

$$P_3(\tau) = P_1(\tau) \bar{R}(t_m, \bar{U}_m) + P_2(\tau) \bar{R}'(t_m, \bar{U}_m) + P_3(\tau) \bar{R}(t_{m-1}, \bar{U}_{m-1}) + P_4(\tau) \bar{R}'(t_{m-1}, \bar{U}_{m-1}),$$

式中,

$$P_1(\tau) = 1 - \frac{3\tau^2}{\Delta t^2} - \frac{2\tau^3}{\Delta t^3}, \quad P_2(\tau) = \tau + \frac{2\tau^2}{\Delta t} + \frac{\tau^3}{\Delta t^2}, \quad P_3(\tau) = \frac{3\tau^2}{\Delta t^2} + \frac{2\tau^3}{\Delta t^3}, \quad P_4(\tau) = \frac{\tau^2}{\Delta t} + \frac{\tau^3}{\Delta t^2}.$$

定义

$$S_{(s,p)}(\Delta t) = (\alpha_{i,j}^{(s,p)}(\Delta t))_{(N_x-1) \times (N_y-1)}, \quad s=0,1,2,3,$$

式中,

$$\begin{aligned} \alpha_{i,j}^{(0,p)}(\Delta t) &= \phi_{i,j}^{(0,p)} - 3\phi_{i,j}^{(2,p)} - 2\phi_{i,j}^{(3,p)}, & \alpha_{i,j}^{(1,p)}(\Delta t) &= \Delta t\phi_{i,j}^{(1,p)} + 2\Delta t\phi_{i,j}^{(2,p)} + \Delta t\phi_{i,j}^{(3,p)}, \\ \alpha_{i,j}^{(2,p)}(\Delta t) &= 3\phi_{i,j}^{(2,p)} + 2\phi_{i,j}^{(3,p)}, & \alpha_{i,j}^{(3,p)}(\Delta t) &= \Delta t\phi_{i,j}^{(2,p)} + \Delta t\phi_{i,j}^{(3,p)}, \end{aligned}$$

在此基础上,就可以得到求解(1)的 Hermite 型快速紧致时间积分方法如下:

$$\begin{aligned} U_{m+1} &= P_y \circledast P_x \circledast (g'(\Delta t) \odot (P_y^{-1} \circledast P_x^{-1} \circledast U_m) + g(\Delta t) \odot (P_y^{-1} \circledast P_x^{-1} \circledast V_m) + Q_{(3)}^{(0,R)}), \\ V_{m+1} &= P_y \circledast P_x \circledast (H \odot g(\Delta t) \odot (P_y^{-1} \circledast P_x^{-1} \circledast U_m) + g'(\Delta t) \odot (P_y^{-1} \circledast P_x^{-1} \circledast V_m) + Q_{(3)}^{(1,R)}), \end{aligned}$$

式中,

$$Q_{(3)}^{(p,R)} = \bar{R}(t_m, \bar{U}_m) \odot S_{(0,p)} + \bar{R}'(t_m, \bar{U}_m) \odot S_{(1,p)} + \bar{R}(t_{m-1}, \bar{U}_{m-1}) \odot S_{(2,p)} + \bar{R}'(t_{m-1}, \bar{U}_{m-1}) \odot S_{(3,p)}.$$

设 $N = \max(N_x, N_y)$, 基于 FFT 算法实现以上数值解法, 易知在每一时间步总的计算复杂度是 $O(N^2 \log(N))$.

3 数值实验

在本节中,通过数值算例讨论快速紧致时间积分 Hermite 格式的收敛性和效率. 在方程(1)中,选取 $g(u) = u - u^3$ 以及适当的函数使得精确解为

$$u(t, x, y) = \cos(x) \cos(y) \sin(t).$$

取空间区域为 $\Omega = (-1, 2\pi - 1)^2$, 求解时间为 $T = 1$. 此时相应的边界条件是非齐次的. 在表 1 中列出了 U 和 V 在不同时空剖分网格下的 L_2 和 L_∞ 误差、收敛率和 CPU 时间. 从中可以看出该方法在空间和时间方向上都达到了四阶收敛率. 就 CPU 时间而言, 从表中可以发现, 由于使用了 FFT 算法, 即使在空间网格非常细的情况下, CPU 时间也非常小.

表 1 在最终时刻 $T=1$ 的误差、收敛率以及 CPU 时间
Table 1 Numerical errors, convergence rates and the CPU times at $T=1$

$(N_x \times N_y) \times N_t$	U				V				
	L_2 Error	CR	L_∞ Error	CR	L_2 Error	CR	L_∞ Error	CR	CPU
空间离散精度测试									
$4^2 \times 1\ 024$	2.1613e-02	—	5.8036e-03	—	5.8434e-02	—	1.5296e-02	—	0.90
$8^2 \times 1\ 024$	1.3554e-03	4.00	4.4258e-04	3.71	3.5547e-03	4.04	1.1517e-03	3.73	0.94
$16^2 \times 1\ 024$	8.4687e-05	4.00	2.7608e-05	4.00	2.2083e-04	4.01	7.1746e-05	4.00	1.03
$32^2 \times 1\ 024$	5.2867e-06	4.00	1.7632e-06	3.97	1.3767e-05	4.00	4.5649e-06	3.97	2.25
$64^2 \times 1\ 024$	3.3030e-07	4.00	1.1007e-07	4.00	8.5988e-07	4.00	2.8498e-07	4.00	6.22
$128^2 \times 1\ 024$	2.0642e-08	4.00	6.8780e-09	4.00	5.3734e-08	4.00	1.7806e-08	4.00	15.81
$256^2 \times 1\ 024$	1.2904e-09	4.00	4.3071e-10	4.00	3.3582e-09	4.00	1.1276e-09	3.98	79.16
时间离散精度测试									
$512^2 \times 8$	6.4931e-05	—	2.1414e-04	—	2.6551e-03	—	9.4541e-03	—	4.19
$512^2 \times 16$	4.9810e-06	3.70	1.9299e-05	3.47	2.9187e-04	3.19	1.0484e-03	3.17	8.24
$512^2 \times 32$	3.6095e-07	3.79	1.4138e-06	3.77	2.7199e-05	3.42	8.4010e-05	3.64	16.47
$512^2 \times 64$	2.4085e-08	3.91	9.2117e-08	3.94	2.0038e-06	3.76	5.6418e-06	3.90	32.98
$512^2 \times 128$	1.5739e-09	3.94	5.5840e-09	4.04	1.3079e-07	3.94	3.7520e-07	3.91	64.42
$512^2 \times 256$	1.4894e-10	3.40	3.7756e-10	3.89	8.3482e-09	3.97	2.3937e-08	3.97	126.74

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