High Order Compact Finite Difference Schemes on Nonuniform Grids

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Mathematical Models

The first problem is defined by the parabolic equation:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - q(x)u + f(x,t), \tag{1}$$

and the second problem solves the Schrödinger equation

$$\frac{\partial u}{\partial t} - i\Big(\frac{\partial^2 u}{\partial x^2} - q(x)u\Big) = 0, \tag{2}$$

where t and x are time and space variables, $u(x,t)$ is a real valued function for the parabolic equation and a complex valued function for the Schrödinger equation.

We formulate the initial condition

$$u(x,0) = \phi(x), \quad a < x < b, \tag{3}$$

and the boundary conditions:

$$u(a,t) = 0, \quad u(b,t) = 0, \quad t > 0, \tag{4}$$

where ϕ is a known function.

Stability Results

Let us consider a general nonstationary problem formulated in the operator form

$$\frac{\partial u}{\partial t} = Au, \quad (x, t) \in D \times (0, T], \tag{5}$$

where the definition of A also includes boundary conditions. For the benchmark parabolic and Schrödinger problems we denote

$$Au := A_P u = \frac{\partial^2 u}{\partial x^2} - qu \quad \text{and} \quad Au := iA_P u,$$

respectively.

Let φ_j, $\widetilde{\lambda}_j$ be eigenfunctions and eigenvalues of operator A:

$$A\varphi_j = \widetilde{\lambda}_j \varphi_j.$$

In general, eigenvalues $\widetilde{\lambda}_j$ are complex numbers $\widetilde{\lambda}_j = \widetilde{\lambda}_{jR} + i\,\widetilde{\lambda}_{jI}$.

It is well-known, that the differential problem (5) is stable if

$$\widetilde{\lambda}_{jR} \le 0.$$

Let us denote eigenvalues of operator A_P as $\lambda_j = \lambda_{jR} + i\,\lambda_{jI}$. The stability region of the parabolic problem is defined by the inequality

$$\lambda_{jR} \leq 0 \tag{6}$$

and the stability region of the Schrödinger problem is defined by the inequality

$$\lambda_{jI} \geq 0. \tag{7}$$

Semi-discretization

Let Ω_t be a t-grid

$$\Omega_t = \{t^n : \ t^n = t^{n-1} + \tau_n, \ n = 1, \dots, N, \ t^N = T\},$$

where τ_n is the discretization step.

We introduce the backward difference quotient and the averaging operator with respect to t

$$\partial_{\bar{t}} U^n(x) = \big(U^n(x) - U^{n-1}(x)\big)/\tau_n,$$
$$U^{n-1/2}(x) = 0.5\big(U^n(x) + U^{n-1}(x)\big).$$

The differential problem (5) is approximated by the symmetrical Euler semi-discrete scheme

$$\partial_{\bar{t}} U^n = AU^{n-1/2}, \quad x \in D, \ \ n > 0, \tag{8}$$

The stability region of the semi-discrete scheme (8) coincides with the stability region of the differential equation (5)

High order FDS on the uniform grid

The space domain $[a, b]$ is covered by the discrete uniform grid

$$\bar{\Omega}_x = \{x_j : \; x_j = a + jh, \quad j = 0, \dots, J, \quad h = (b - a)/J\}$$

The following difference diffusion operator is defined

$$A_D^h U_j^n = (U_{j+1}^n - 2U_j^n + U_{j-1}^n)/h^2, \quad x_j \in \Omega_x,$$

for grid functions such that $U_0 = 0, \; U_J = 0$.

Let us approximate the parabolic problem (1) by the high order compact finite difference scheme

$$\left(I + \frac{h^2}{12}A_D^h\right)\left(U_{\bar t}^n + qU^{n-1/2} - f^{n-1/2}\right) = A_D^h U^{n-1/2},$$
$$U_0^n = U_J^n = 0. \qquad (9)$$

The Schrödinger problem (2) is approximated by the compact finite difference scheme

$$\left(I + \frac{h^2}{12}A_D^h\right)\left(U_{\bar t}^n + iqU^{n-1/2}\right) = iA_D^h U^{n-1/2},$$
$$U_0^n = U_J^n = 0. \qquad (10)$$

First we assume that $q(x) = q_0$ is constant and apply the spectral method to prove the stability with respect to the initial condition. Let $\{\lambda_l, \varphi_l(x)\}$, $\varphi_l(x_0) = 0$, $\varphi_l(x_J) = 0$, $1 \leq l < J$ be eigenpairs of the following eigenvalue problem

$$A_D^h \varphi_l = \lambda_l \varphi_l, \quad x_j \in \Omega_x.$$

We get for the Schrödinger problem the following relation for spectral coefficients c_l^n:

$$c_l^n = \frac{1 + h^2\lambda_l/12 - i\tau/2\big(- \lambda_l + q_0(1 + h^2\lambda_l/12)\big)}{1 + h^2\lambda_l/12 + i\tau/2\big(- \lambda_l + q_0(1 + h^2\lambda_l/12)\big)}\, c_l^{n-1}.$$

We see that $|c_l^n| = |c_l^{n-1}|$, $l = 1, \dots, J-1$ and the L_2 norm of the solution is conserved

$$\|U^n\| = \|U^{n-1}\|. \tag{11}$$

For the parabolic problem we get:

$$c_l^n = \frac{1 + h^2\lambda_l/12 - \tau/2\big(-\lambda_l + q_0(1 + h^2\lambda_l/12)\big)}{1 + h^2\lambda_l/12 + \tau/2\big(-\lambda_l + q_0(1 + h^2\lambda_l/12)\big)}\, c_l^{n-1}.$$

Since $\lambda_l < 0$ and $(1 + h^2\lambda_l/12) \geq 2/3$, then the inequality $|c_l^n| \leq |c_l^{n-1}|$ is valid. Thus the scheme (9) is stable in the L_2 norm:

$$\|U^n\| \leq \|U^{n-1}\|. \tag{12}$$

Non-uniform grids

We introduce a non-uniform spatial grid

$$\Omega_x = \{x_j : \ \ x_j = x_{j-1} + h_{j-\frac{1}{2}}, \ \ j = 1, \dots, J-1\}, \quad x_0 = a, \ \ x_J = b,$$
$$h_j = \frac{h_{j-\frac{1}{2}} + h_{j+\frac{1}{2}}}{2}, \quad h := \max_{1 \le j < J} (h_j).$$

Also we define the difference operators

$$\partial_x U_j := \frac{U_j - U_{j-1}}{h_{j-\frac{1}{2}}}, \quad A_D^h U_j := \frac{1}{h_j}\Big(\partial_x U_{j+1} - \partial_x U_j\Big), \quad x_j \in \Omega_x.$$

We define a high-order compact finite difference schemes on non-uniform grid for the parabolic problem (1)

$$\widetilde{B}^h \big(U^n_{\bar{t}} + qU^{n-1/2} - f^{n-1/2} \big) = A^h_D U^{n-1/2}, \tag{13}$$

and for the Schrödinger problem (2)

$$\widetilde{B}^h \big(U^n_{\bar{t}} + iqU^{n-1/2} \big) = iA^h_D U^{n-1/2}. \tag{14}$$

Here the operator $\widetilde{B}_h$ is defined as

$$\widetilde{B}^h U_j := \alpha_j U_{j-1} + (1 - \alpha_j - \beta_j) U_j + \beta_j U_{j+1},$$

$$\alpha_j = \frac{h^2_{j-\frac{1}{2}} + h_{j+\frac{1}{2}} (h_{j-\frac{1}{2}} - h_{j+\frac{1}{2}})}{12 h_j h_{j-\frac{1}{2}}}, \quad \beta_j = \frac{h^2_{j+\frac{1}{2}} + h_{j-\frac{1}{2}} (h_{j+\frac{1}{2}} - h_{j-\frac{1}{2}})}{12 h_j h_{j+\frac{1}{2}}}.$$

It follows directly from the construction of this compact finite difference scheme that for sufficiently smooth solutions the approximation error is of order

$$\mathcal{O}(\tau^2 + h^4).$$

Stability analysis of compact high-order finite difference schemes is much more complicated. The main challenges are connected to two properties of operators A_D^h, $\widetilde{B}^h$:

First, the operator $\widetilde{B}^h$ is not symmetric.

Second, these two operators do not commute.

Stability of FDS for the Schrödinger problem

General necessary and sufficient spectral stability conditions can be obtained by considering the generalized eigenvalue problem

$$A_D^h V = \lambda \widetilde{B}^h V, \quad V_0 = V_J = 0. \tag{15}$$

The characteristic equation has only real coefficients, then complex eigenvalues (if they exist) make a pair $\lambda_R \pm i\lambda_I$, where $\lambda_I > 0$. In this case it follows from the A stability region of the symmetrical Euler scheme (7) that scheme (14) is not A stable for the Schrödinger problem.

A. Zlotnik have investigated the stability of this FDS applying the energy method.
The skew-part of the operator $\widetilde{B}^h$ is analysed and three conditions are derived which are sufficient in order to prove the ρ-stability of the FDS (14).
The most restrictive among these conditions requires the time step to be not too small

$$\tau \geq C_0 h.$$

This condition can be considered as a regularization technique to guarantee the ρ-stability

$$\|U^n\| \leq (1 + c\tau)\|U^{n-1}\|.$$

Let us consider the spectral stability factor ρ, corresponding to the eigenvector for which the imaginary part of the eigenvalue is the largest

$$\rho = \frac{1 + \widetilde{\tau}\lambda_I + i\widetilde{\tau}\lambda_R}{1 - \widetilde{\tau}\lambda_I - i\widetilde{\tau}\lambda_R}, \quad \widetilde{\tau} = \frac{\tau}{2}.$$

Then, after simple computations we get

$$|\rho|^2 = 1 + \frac{4\widetilde{\tau}\lambda_I}{(1 - \widetilde{\tau}\lambda_I)^2 + \widetilde{\tau}^2\lambda_R^2}.$$

The analysis of the obtained estimate shows that this condition requires that a nonclassical “converse” restriction on grid steps $h \leq c_0\tau$ must be satisfied.

Critical grids

Such critical space grids Ω_x are constructed by using two level approach:

First a brute force search algorithm is applied to find small size J_0 critical space grids.

Then a family of grids with $J = KJ_0$ is constructed in such a way, that if λ_j is an eigenvalue of the small size problem, then $\lambda_j K^2$ is an eigenvalue of the large size J eigenvalue problem (15).

Finite element scheme

We use local quadratic elements as basis functions: local piecewise linear (hat) functions

$$\varphi_j(x) = \begin{cases} (x - x_{j-1})/h_{j-\frac{1}{2}}, & x_{j-1} \le x \le x_j, \\ (x_{j+1} - x)/h_{j+\frac{1}{2}}, & x_j \le x \le x_{j+1}, \\ 0, \quad \text{otherwise}, \end{cases} \qquad j = 1, \dots, J-1,$$

and local piecewise quadratic functions

$$\varphi_{j-\frac{1}{2}}(x) = \begin{cases} 4(x - x_{j-1})(x_j - x)/h^2_{j-\frac{1}{2}}, & x_{j-1} \le x \le x_j, \\ 0, \quad \text{otherwise}, \; j = 1, \dots, J. \end{cases}$$

We write the discrete solution $U^n(x)$ in the usual way as

$$U^n(x) = \sum_{j=1}^{J-1} U_j^n \varphi_j(x) + \sum_{j=1}^{J} U_{j-\frac{1}{2}}^n \varphi_{j-\frac{1}{2}}(x). \qquad (16)$$

Applying the standard Galerkin method we approximate the parabolic problem (1) by the following FEM scheme:

$$B_F^h U_{\bar{t}}^n = A_{DF}^h U^{n-\frac{1}{2}} - Q_F^h U^{n-\frac{1}{2}} + F^{n-\frac{1}{2}}, \tag{17}$$

and the Schrödinger problem (2):

$$B_F^h U_{\bar{t}}^n = i\big(A_{DF}^h U^{n-\frac{1}{2}} - Q_F^h U^{n-\frac{1}{2}}\big), \tag{18}$$

The following three properties are valid for the obtained compact finite-difference scheme (17).

1. B_F^h, $(-A_{DF}^h)$ and Q_F^h are SPD operators.

2. For the Schrödinger equation (2) the special energy conservation law is valid:

$$(B_F^h U^n, U^n) = (B_F^h U^{n-1}, U^{n-1}).$$

3. Due to the super-convergence property, the discrete solution converges at the grid points as $O(\tau^2 + h^4)$. The same super-convergence rate is valid at points $x_{j-\frac{1}{2}} = \frac{1}{2}(x_{j-1} + x_j)$

From equation

$$B_{j-\frac{1}{2},j-1} U^n_{j-1,\bar{t}} + B_{j-\frac{1}{2},j-\frac{1}{2}} U^n_{j-\frac{1}{2},\bar{t}} + B_{j-\frac{1}{2},j} U^n_{j,\bar{t}} = A_{j-\frac{1}{2},j-\frac{1}{2}} U^{n-\frac{1}{2}}_{j-\frac{1}{2}} - Q_{j-\frac{1}{2},j-1} U^{n-\frac{1}{2}}_{j-1} - Q_{j-\frac{1}{2},j-\frac{1}{2}} U^{n-\frac{1}{2}}_{j} - Q_{j-\frac{1}{2},j} U^{n-\frac{1}{2}}_{j} + F^{n-\frac{1}{2}}_{j-\frac{1}{2}},$$

the solution $U^n_{j-\frac{1}{2}}$ is expressed as a linear combination:

$$U^n_{j-\frac{1}{2}} = a_{j-\frac{1}{2}} U^n_{j-1} + b_{j-\frac{1}{2}} U^n_j + c_{j-\frac{1}{2}} U^{n-1}_{j-1} + d_{j-\frac{1}{2}} U^{n-1}_j + e_{j-\frac{1}{2}} U^{n-1}_{j-\frac{1}{2}} + f_{j-\frac{1}{2}}$$

Then a modified system with a tridiagonal matrix is obtained and a standard factorization algorithm can be applied.

Computational experiments

Consider the linear Schrödinger equation (2) with zero potential function $q = 0$. The initial and boundary conditions correspond to the exact solution

$$u(x,t) := \sqrt{\frac{i}{i-4t}} \exp\left[(-ix^2 - 4x + 16t)/(i-4t)\right]. \tag{19}$$

We simulate the movement of a Gaussian wave for $(x,t) \in [-X, X] \times [0, T]$, where $X = 10$ and $T = 0.5$.

The first grid mimics the structure of adaptive grids. It is more dense at the center of the domain and becomes coarser closer to the ends of the domain:

$$h_{\frac{J}{2}\pm(j-\frac{1}{2})} = \big(2j/J + 0.5\big)h, \quad j = 1, \ldots, J/2.$$

In Table 1 we present errors and experimental convergence rates of the discrete solutions of high-order compact finite difference scheme (14) and FEM scheme (18).

TABLE : Errors ϵ_{FDS}, ϵ_{FEM} and convergence rates ρ_{FDS}, ρ_{FEM} for the discrete solutions of high-order compact finite difference scheme (14) and the FEM scheme (18) for adaptive grids.

J	N	ϵ_{FDS}	ρ_{FDS}	ϵ_{FEM}	ρ_{FEM}
100	50	9.400e-2	—	3.497e-2	—
140	100	2.230e-2	4.066	8.464e-3	4.093
200	200	5.533e-3	4.107	2.122e-3	3.992
280	400	1.404e-3	3.957	5.206e-4	4.054
400	800	3.431e-4	4.065	1.314e-4	3.966

The second family of the nonuniform grids is defined using pseudo-random number generator. The space grid steps are defined as

$$h_{j-\frac{1}{2}} = (\alpha + r_{j-\frac{1}{2}})h, \quad j = 1, \dots, J,$$

here $0 < r_{j-\frac{1}{2}} \leq 1$ are pseudo-random numbers, α is a regularization parameter and h is a scaling constant.

TABLE : Errors ϵ_α and convergence rates ρ_α for the discrete solutions of high-order compact finite difference scheme (14) when random nonuniform grids are used, regularization parameters $\alpha = 0.1, 0.25$.

J	N	$\epsilon_{0.25}$	$\rho_{0.25}$	$\epsilon_{0.1}$	$\rho_{0.1}$
100	50	1.574e-1	—	1.952e-1	—
140	100	4.697e-2	3.489	6.080e-2	3.366
200	200	1.031e-2	4.374	1.338e-2	4.368
280	400	2.987e-3	3.575	3.942e-3	3.526
400	800	6.360e-4	4.463	8.160e-4	4.545

TABLE : Errors ϵ_α and convergence rates ρ_α for the discrete solutions of high-order compact finite element scheme (18) when random nonuniform grids are used, regularization parameters $\alpha = 0.1, 0.25$.

J	N	$\epsilon_{0.25}$	$\rho_{0.25}$	$\epsilon_{0.1}$	$\rho_{0.1}$	N	$\epsilon_{0.1}$	$\rho_{0.1}$
100	50	2.41e-2	—	1.735e-2	—	400	3.197e-2	—
140	100	3.69e-3	5.41	2.126e-3	6.04	800	1.114e-2	3.04
200	200	1.28e-3	3.05	7.14e-4	3.15	1600	2.432e-3	4.39
280	400	1.80e-4	5.66	1.49e-4	4.52	3200	8.03e-4	3.20
400	800	6.00e-5	2.81	3.90e-5	3.87	6400	1.67e-4	4.53

We present results of computational experiments for a grid when the high-order finite difference scheme (14) is non-stable.

First applying the brute force search strategy a critical grid $\overline{\Omega}_h^0$ with the nodes $0 = x_0^0 < \ldots < x_{J_0}^0 = X$ is obtained for some small size J_0. For such a grid the generalized eigenvalue problem (15) has at least one pair of complex eigenvalues.

Next we construct the family of grids $\overline{\Omega}_h^{0,K}$, $K \geq 1$ with the space steps defined as

$$h_{kJ_0+j-\frac{1}{2}} = h^0_{j-\frac{1}{2}} h, \quad j = 1, \ldots, J_0, \;\; k = 2l, \;\; l = 0, \ldots, K/2-1,$$
$$h_{kJ_0+j-\frac{1}{2}} = h^0_{J_0-j+\frac{1}{2}} h, \quad j = 1, \ldots, J_0, \;\; k = 2l-1, \;\; l = 1, \ldots, K/2.$$

In Table we present errors of the discrete solutions of finite difference scheme (14) and FEM scheme (18).

The basic grid $\overline{\Omega}_h^0$ has the size $J_0 = 14$ and $K = 40$.

As it follows from the theoretical analysis the scheme (14) starts to be non-stable for sufficiently small discrete steps τ.

TABLE : Errors ϵ_N for the discrete solutions of high-order compact finite difference scheme (14) and finite element scheme (18). A critical grid is used in computations.

	N=1000	N=1200	N=1400	N=1600	N=1800
FDS	0.000248	0.002327	0.02783	0.3251	3.4825
FEM	7.613-5	4.119-5	2.010-5	6.473-6	5.082-6

Stability analysis for the parabolic problem

As it follows from the analysis given above, the stability domain of the high-order finite difference scheme (13) is defined by estimates

$$\operatorname{Re} \lambda_j \leq 0,$$

where λ_j are eigenvalues of problem (15).
Now the critical task is to find examples of nonuniform grids such that for some eigenvalue $\operatorname{Re} \lambda_j > 0$

Theorem

Let us consider the homogeneous equation with the given initial condition V:

$$\widehat{B} Y_{\bar{t}}^{n} + \widehat{A} Y^{n-1/2} = 0, \quad n = 1, \ldots, N, \quad Y^0 = V, \tag{20}$$

where $\widehat{A}$ is a self-adjoint positive operator $\widehat{A} = \widehat{A}^* > 0$. Then the condition

$$\widehat{B} > 0 \tag{21}$$

is necessary and sufficient for the validity of the stability estimates

$$(\widehat{A} Y^n, Y^n) \leq (\widehat{A} Y^{n-1}, Y^{n-1}) \leq \ldots \leq (\widehat{A} Y^0, Y^0). \tag{22}$$

For small sizes J of Ω_x we attempted to find nonuniform grids when matrix $\widetilde{B}^h$ has at least one eigenvalue with a negative real part.

The search procedure for all tested values J returned back many grids satisfying this requirement. Thus in general stability estimate (22) in weighted $\widehat{A}$ norm is not strictly valid for the scheme (13).

But this fact do not forbid the discrete scheme (13) to be ρ-stable in some other norm.

We have applied the brute force search method to find critical grids Ω_x when eigenvalue problem (15) has solutions with $\mathrm{Re}\,\lambda_j > 0$.

For the smaller size $J = 8$ we generated all possible grids, when the relative values of grid steps varied as

$$\widetilde{h}_{j-\frac{1}{2}} = k, \quad k = 1, \ldots, 12, \quad j = 1, \ldots, 8,$$

For the larger size $J = 14$ we generated all possible grids, when the relative values of grid steps varied as

$$\widetilde{h}_{j-\frac{1}{2}} = k, \quad k = 1, \ldots, 6, \quad j = 1, \ldots, 14.$$

In both experiments we have not identified any critical grid.

The obtained computational results can be explained by the following two properties of the eigenvalue problem (15).

First, a perturbation due to discretization error is done around non-zero eigenvalue of the differential operator, thus the amplitude of such perturbations should be sufficiently large in order to change a sign of the eigenvalue.

Second, the eigenvectors corresponding to the first eigenvalues are smooth and they are well approximated on any non-uniform grid.

We note, that this situation is very different from the case of the Schrödinger problem.