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INCREASING THE CALCULATION SPEED OF AN ACCELERATION SCHEME FOR AN AGE-STRUCTURED DIFFUSION MODEL

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In this paper we propose an optimized algorithm, which is faster compared to previously described Modified Super-Time-Stepping (Modified STS) scheme for age-structured population models with diffusion. Keeping the accuracy of the Modified STS algorithm, we reduce its computational time almost two times, obtaining an additional speed-up. This makes the optimized method highly preferable for nonlinear and higher-dimensional problems.

1. Introduction. The Super-Time-Stepping (STS) scheme is proved to be a simple and very effective method which accelerates explicit time stepping schemes for parabolic problems [1]. Even though the method is quite old, it is not known by most of the people working in the computational PDE world. Pelovska [11] and Boyadzhiev [12] have applied it on equations of age-dependent population diffusion. While the analytical properties of such models have been extensively studied since years (see for instance [3, 4, 7] and the references therein), only several authors have dealt with the numerical study of age and space dependent population models. Kim [6], Kim-Park [5] and Milner [9] deal with nonlinear diffusion models. They propose some mixed numerical algorithms combining finite difference methods along characteristics and finite element methods in the spatial variables. In the case of linear fertility and mortality functions, Lopez and Trigiante [8] have developed a finite difference scheme for an age-dependent model with Dirichlet boundary conditions and linear population flux. Ayati [2] proposes a numerical method for a nonlinear model with nonlinear diffusion which allows the use of variable time steps and independent age and time discretization.

The authors' goal in this paper is to present an improved version of the Modified STS scheme (see [11, 12]) adapted for solving an age-dependent population model with linear spatial diffusion. Let $p(a,t,x)$ be the density of a population having age $a \in [0, a_+]$, where a_+ is the maximum age; $t \in (0,T]$ denotes time, where T is the final time; $x \in (0,1)$ denotes spatial position and $D > 0$ is the coefficient of diffusion. Then, following [4], a

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mathematical model describing the evolution of the population $p(a,t,x)$ starting at time $t=0$ with initial distribution

$$p(a,0,x) = p_0(a,x), \quad a \in [0,a_+],\ x \in (0,1) \tag{1.1}$$

is:

$$p_t + p_a + \mu(a)p = Dp_{xx}, \quad a \in [0,a_+],\ t \in (0,T],\ x \in (0,1), \tag{1.2}$$

where $\mu(a) \geq 0$ is the natural death rate of the species. We add to this model the birth process

$$p(0,t,x) = \int_0^{a_+} \beta(a)p(a,t,x)\ \mathrm{d}a, \quad t \in (0,T],\ x \in (0,1), \tag{1.3}$$

with $\beta(a) \geq 0$ representing the age specific fertility, and the following Dirichlet conditions on the boundary

$$p(a,t,0) = p(a,t,1) = 0, \quad a \in [0,a_+],\ t \in (0,T] \tag{1.4}$$

Aiming to present a more realistic case where the species are with a finite life span, we assume the maximum age a_+ to be finite (a $\in [0,a_+]$, where $a_+ < +\infty$) and we require that the survival probability

$$\pi(a) = e^{-\int_0^a \mu(\tau)\mathrm{d}\tau} \tag{1.5}$$

vanishes at a_+.

In order to approximate our model we shall use a first order method combined with the trapezoidal rule for the integral terms. In [10] it is shown that this creates problems every time when an evaluation of the mortality function at the right endpoint a_+ of the interval is required, since $\lim\limits_{a \to a_+} \mu(a) = \infty$. Following [10] we take

$$u(a,t,x) = \pi^{-1}(a)p(a,t,x) \tag{1.6}$$

and then substituting with the new variable $u(a,t,x)$ in the equations above, we obtain a reformulation of the discussed model

$$\begin{aligned}
&1)\ u_t + u_a = Du_{xx}, \quad a \in [0,a_+],\ t \in (0,T],\ x \in (0,1) \\
&2)\ u(0,t,x) = \int_0^{a_+} \beta(a)\pi(a)u(a,t,x)\ \mathrm{d}a, \quad t \in (0,T],\ x \in (0,1) \\
&3)\ u(a,0,x) = u_0(a,x), \quad a \in [0,a_+],\ x \in (0,1) \\
&4)\ u(a,t,0) = u(a,t,1) = 0, \quad a \in [0,a_+],\ t \in (0,T]
\end{aligned} \tag{1.7}$$

Using this form of the equations describing our model, we can apply a finite difference scheme, since the qualitative features of the model are preserved but there are no more problems with its numerical treatment (see [10] for details).

The aim of our article is to witness the Modified STS [11] theory on, namely to show how a bigger acceleration of this scheme can be obtained. We use some of the properties of its coefficients gaining more speed but preserving its accuracy, which is comparable to the accuracy of other first and even second order schemes as shown in [11].

2. Optimization of the Modified Super-Time-Stepping scheme. The Super-Time-Stepping algorithm [1] is an acceleration method for explicit schemes for parabolic problems. It relaxes the condition of stability at the end of each time step that is imposed for the normal explicit scheme and demands stability at the end of each super-step ΔT, consisting of K sub-steps $\tau_1, \tau_2, ..., \tau_K$ with different length. These sub-steps can be found by the following explicit formula

$$\tau_k = \tau \left((-1+\nu) \cos \left(\frac{(2k-1)\pi}{2K} \right) + 1 + \nu \right)^{-1}, \quad k = 1, \ldots, K \tag{2.1}$$

where τ is the time step for the explicit scheme (2.5), calculated in such a way that the CFL (stability) condition is satisfied; ν is a number in the interval $\left(0, \frac{\lambda_{\min}}{\lambda_{\max}}\right]$ with $\lambda_{\min}$ and $\lambda_{\max}$ being the smallest and the biggest eigenvalues respectively of the matrix A in (2.6). It implies that we can take larger time steps and consequently the total number of steps is reduced which speeds the computations up, compared with the standard explicit scheme. The inner steps have no approximation properties and can be chosen explicitly in such a way that stability is ensured over the super-step and we obtain a maximum duration of

$$\Delta T = \sum_{k=1}^{K} \tau_k \tag{2.2}$$

Inspired by the fact that along characteristics in the age-time direction the governing equation in (1.7) can be treated as parabolic differential equation (see [11] for details), we proceed as follows, introducing some convenient notation. We assume the step size in age identical to the step size in time and we choose $\tau > 0$ to be the age and time discretization parameter, where $\tau = \frac{a_+}{L}$ (L is the number of subintervals in age). We assume T is a multiple of a_+, so that we have $T = L_1 a_+ = L_1 L \tau = N\tau$, where L_1 is an integer and N is the total number of subintervals in time. Let $h = \frac{1}{M}$ be the discretization step in space, where M is the number of subintervals in space. Then for each time level $t^n = n\tau$, $n = 0, \ldots, N$ we have the following grid: $\Gamma = \{(a^j, x_i) : a^j = j\tau,\ j = 0, \ldots, L;\ x_i = ih,\ i = 0, \ldots, M\}$. With this notation, we approximate the directional derivative $\frac{\partial}{\partial t} + \frac{\partial}{\partial a}$, setting

$$\left(\frac{\partial}{\partial t} + \frac{\partial}{\partial a} \right) u(a^j, t^n, x_i) \approx \frac{\widehat{U}_i^{j+1} - U_i^j}{\tau}, \tag{2.3}$$

where the discrete function U_i^j is an approximation of the solution of (1.7) at time level t^n at grid point (a^j, x_i) and $\widehat{U}_i^{j+1}$ – at time level t^{n+1} at grid point (a^{j+1}, x_i).
An approximation of the Laplace operator is given by

$$U_{xx} = \frac{U_{i-1}^j - 2U_i^j + U_{i+1}^j}{h^2} \tag{2.4}$$

Consequently an approximation of problem (1.7) by an Euler explicit scheme (analogous to the one applied to the heat equation in [1]) is given by

$$\begin{aligned} &\widehat{U}_i^{j+1} = \frac{D\tau}{h^2} U_{i-1}^j + \left(1 - \frac{2D\tau}{h^2}\right) U_i^j + \frac{D\tau}{h^2} U_{i+1}^j, \\ &\qquad\qquad i = 1, \ldots, M-1;\ j = 0, \ldots, L-1 \\ &\widehat{U}_0^{j+1} = \widehat{U}_M^{j+1} = 0,\ j = 0, \ldots, L-1 \end{aligned} \tag{2.5}$$

or written in a more convenient form

$$\widehat{U}^{j+1} = AU^j,\ j = 0, \ldots, L-1 \tag{2.6}$$

where A is an $(M-1) \times (M-1)$ symmetric and three-diagonal matrix.

We couple (2.5) with the trapezoidal rule for the boundary condition (1.7, 2))

$$\widehat{U}_i^0 = \tau \sum_{j=1}^{L-1} \beta_j \pi(a_j) \widehat{U}_i^j + \frac{\tau}{2} \left[\beta_0 \pi(a_0) \widehat{U}_i^0 + \beta_L \pi(a_L) \widehat{U}_i^L \right], \quad i = 0, \ldots, M \tag{2.7}$$

At the initial time $t = 0$ we take $U_i^j = \dfrac{p_0(a^j, x_i)}{\pi(a^j)}$, $j = 0, \ldots, L$, $i = 0, \ldots, M$.

This scheme is easy to be implemented, but it is conditionally stable, i.e. it is stable if the time step is very small, namely $\tau \leq \dfrac{2}{\lambda_{\max}}$ ($\lambda_{\max}$ being the biggest eigenvalue of the matrix A in (2.6)). In order to overcome this drawback and to increase the efficiency of the method while keeping the accuracy at the same time, we adapt the STS scheme for parabolic problems (see [1]) to the age-structured model as shown on the graph:

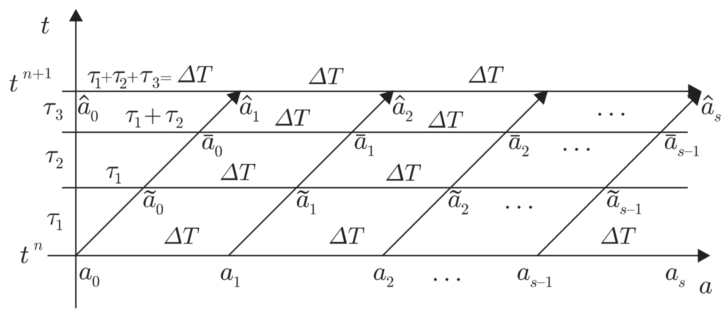

Fig. 1. One super-time-step with $K = 3$ intermediate steps

The figure above shows how one super-time-step looks like. The vertical and the horizontal axis present the time and the age distributions respectively; τ_k, $k = 1, \ldots, K$ are the inner-time-steps (on the graph we have taken $K = 3$). The similarity between Modified STS and STS is the way to move in time, i.e. the super-time-stepping. However, while moving in time, the same steps in age have to be done. This is the basic difference between STS for parabolic problems and the modification presented in [11]. In the modified scheme the solution at the boundary points is calculated, but not at the intermediate time levels (since it is not needed for the approximation of the solution in the next time levels – see Figure 1). Since there are age nodes at each time level (as shown on Figure 1), the "discrete solution" at the k^{th} inner time level $k = 1, \ldots, K-1$ is calculated as follows

$$\begin{aligned} \widehat{U}_i^j &= \frac{D\tau_k}{h^2}(U_{i-1}^j + U_{i+1}^j) + \left(1 - \frac{2D\tau_k}{h^2}\right) U_i^j, \\ & \qquad i = 1, \ldots, M-1; j = 0, \ldots, s-1 \\ \widehat{U}_0^j &= \widehat{U}_M^j = 0, \quad j = 0, \ldots, s-1, \end{aligned} \tag{2.8}$$

where U_i^j is the "discrete solution" at the $(k-1)^{\text{st}}$ time level and it is considered as known; $s = \dfrac{a_+ K}{T}$ is the number of age-nodes (see Figure 2), which depends on K, i.e. on the length of one super-step ΔT. The "discrete solution", calculated at these inner steps has no approximation properties and it is not outputted. The approximation only at the end level – K corresponding to t^{n+1} time level is used. It is found by formula (2.5), but with time step τ_K, i.e. $\tau = \tau_K$. As we mentioned before at this level the solution at the boundary point is calculated as well, by formula (2.7) and time step ΔT. This procedure is repeated until the end of the time interval.

In [11] it is proved that in some cases the Modified STS algorithm can speed up the explicit scheme more than K^2 times. Additional acceleration of the Modified STS can be achieved when using some of the properties of its coefficients, namely that the coefficients c_l^k, $k = 1, \dots, K$, $l = 0, \dots, k$ of the k^{th} inner level, can be obtained by the coefficients c_l^{k-1} of the previous, $(k-1)^{\text{st}}$ intermediate time level by the following recursive formulas

$$\begin{aligned} c_0^k &= (1 - 2\sigma_k)\, c_0^{k-1} + 2\sigma_k c_1^{k-1}, \\ c_l^k &= \sigma_k \left(c_{l-1}^{k-1} + c_{l+1}^{k-1}\right) + (1 - 2\sigma_k)\, c_l^{k-1}, \quad l = 1, \dots, k-1, \\ c_k^k &= \sigma_k c_{k-1}^{k-1}, \end{aligned} \tag{2.9}$$

where $\sigma_k = \dfrac{D\tau_k}{h^2}$, $c_l^{k-1} = 0$ for $l \geq k$ and we assume that in the beginning $c_0^0 = 1$, $c_l^0 = 0$, $l \geq 1$.

Using this dependence between c_l^k, $k = 1, \dots, K$, $l = 0, \dots, k$ and c_l^{k-1} and the fact, that the inner steps have no approximation properties (for the discrete solution), we can make only steps with length ΔT. Moreover, after one super step we have the following form of the Modified STS scheme

$$\widehat{U}_i^{j+1} = c_0^K U_i^j + \begin{cases} \displaystyle\sum_{l=1}^{i} c_l^K (U_{i+l}^j + U_{i-l}^j) + \sum_{l=i+1}^{K} c_l^K (U_{i+l}^j - U_{l-i}^j), \\ \qquad\qquad 1 \leq i \leq K-1 \\ \displaystyle\sum_{l=1}^{k} c_l^k (U_{i-l}^j + U_{i+l}^j), \quad K \leq i \leq M-K \\ \displaystyle\sum_{l=1}^{M-i} c_l^K (U_{i+l}^j + U_{i-l}^j) + \sum_{l=M-i+1}^{K} c_l^K (U_{i-l}^j - U_{2M-l-i}^j), \\ \qquad\qquad M-K+1 \leq i \leq M-1, \end{cases} \tag{2.10}$$

where $j = 0, \dots, s-1$ and c_k^K, $k = 0, \dots, K$ can be obtained explicitly by formula (2.9). In this way we present the solution at the new time level t^{n+1} as a linear combination of $2K + 1$ nodes of the previous time level and we reduce the number of the arithmetical operations we do. As it is shown in [12] the number of multiplications is reduced from $2K$ for the Modified STS to $K + 1$ for the optimized algorithm. Thus we save computational time while keeping the accuracy of the Modified STS scheme.

3. Performance on a linear test problem. In this section we investigate the performance of the optimized scheme on one exactly solvable test problem proposed in [11]. We consider a population with a finite age and for simplicity we take the maximum age of the individuals $a_+ = 1$. The mortality and the survival probability are $\mu(a) = 1/(1-a)$, $\pi(a) = 1 - a$ respectively. The initial conditions are given as follows

$$p_0(a, x) = e^{-\alpha^* a}(1 - a)\sin(\pi x), \tag{3.1}$$

where α^* is the intrinsic Malthusian parameter which determines the population growth. We assume the fertility $\beta(a) = \beta$ and by choosing an appropriate value of $\alpha^* = 2$, we calculate it by the following formula

$$p_0(0, x) = \int_0^{a_+} \beta(a)p_0(a, x)da, \tag{3.2}$$

which provides continuity of the solution $p(a, t, x)$. The solution of system (1.7) is given by

$$p(a, t, x) = e^{\alpha^*(t-a)}(1 - a)e^{-\pi^2 Dt} \sin(\pi x), \tag{3.3}$$

where $p(a, t, x)$ satisfies Dirichlet conditions on the boundary. We assume the diffusion constant $D = 1$ for simplicity. We vary the number of steps in space – M (we calculate τ in such a way that the CFL condition $\tau \leq \frac{h^2}{2D}$ for the explicit scheme to be satisfied – see (2.1) and the text below), the number of sub-steps – K and the value of the parameter ν, chosen as a random number in the interval (0,1) (see [11]). We trace the efficiency of the optimized algorithm and the Modified STS. We ran simulations on an ACER Aspire M3610 in double precision arithmetic and we took as final time $T = 3$.

We use the following convenient notation: K – number of intermediate steps per one super-step; M – number of discrete subintervals in space; CPU – time (in seconds); E_{abs} – the maximum L^∞ error; OS – optimized scheme; $MSTS$ – Modified STS scheme

The data reported in this table show, that the performance of the optimized scheme is better as CPU-time than the one of the Modified STS algorithm while their accuracy

Table 1. Efficiency comparison of OS and MSTS

M	K	ν	$E_{abs}(OS)$	$CPU(OS)$	$E_{abs}(MSTS)$	$CPU(MSTS)$	$\frac{CPU(MSTS)}{CPU(OS)}$
20	3	0.004	2.62E-002	0.062	2.62E-002	0.078	1.25
20	5	0.06	1.75E-002	0.059	1.75E-002	0.089	1.51
20	10	0.07	1.50E-002	0.031	1.50E-002	0.048	1.55
20	10	0.7	1.12E-003	0.25	1.12E-003	0.41	1.64
40	5	0.004	1.62E-002	0.36	1.62E-002	0.50	1.39
40	5	0.07	3.13E-003	18.41	3.13E-003	26.16	1.42
40	10	0.06	4.61E-003	0.71	4.61E-003	1.05	1.48
40	20	0.7	2.79E-004	3.51	2.79E-004	6.94	1.69
60	10	0.004	1.07E-002	0.48	1.07E-002	0.76	1.58
60	20	0.06	2.01E-003	2.33	2.01E-003	3.88	1.67
60	25	0.7	1.29E-004	21.18	1.29E-004	36.55	1.73
60	30	0.2	5.40E-004	4.58	5.40E-004	8.11	1.77
60	30	0.88	8.98E-005	21.48	8.98E-005	38.49	1.80
100	20	0.004	1.07E-002	2.13	1.07E-002	3.68	1.73
100	20	0.06	7.41E-004	31.04	7.41E-004	54.82	1.77
100	40	0.7	4.66E-005	170.8	4.66E-005	328.32	1.92
100	50	0.4	8.95E-005	73.82	8.95E-005	141.738	1.92
200	5	0.004	6.45E-004	1190.55	6.45E-004	2309.68	1.94
200	20	0.06	1.87E-004	1357.34	1.87E-004	2646.82	1.95
200	50	0.7	1.22E-005	1408.94	1.22E-005	2775.61	1.97

is the same. Taking less space nodes and sub-steps, and choosing ν comparatively small number (see $M = 20$, $K = 3$, $\nu = 0.004$ and $M = 40$, $K = 5$, $\nu = 0.004$) we do not improve much the efficiency of the Modified STS scheme. But we see that in this case the accuracy of the schemes is not good enough. Reducing the step size in x and increasing the number of the intermediate steps and the value of the damping factor ν, we obtain better accuracy (compare results for $M = 60$, $K = 30$, $\nu = 0.88$; $M = 100$, $K = 40$, $\nu = 0.7$; $M = 100$, $K = 50$, $\nu = 0.4$ and $M = 200$) and nearly two times bigger acceleration given by the optimized scheme. The conclusion is that the optimized algorithm [12] has several advantages – it is easy to implement, it preserves the good accuracy of the Modified STS [11] and it speeds this scheme up. Consequently, when we deal with higher-dimensional and nonlinear problems, when we run simulations with a large time span or we simply wish to gain high accuracy for less time, the application of the optimized algorithm is preferable.

Remark. The CPU-time of the Modified STS scheme given in the table above differs from the CPU-time of the same scheme presented in [11] (for the same values of the parameters) since the simulations were ran on different computers (an ACER TravelMate 6003LMi was used in [11]).

REFERENCES

[1] V. Alexiades, G. Amiez, P.-A. Gremaud. Super-Time-Stepping acceleration of explicit schemes for parabolic problems. *Communications in numerical methods in engineering*, **12** (1996), 31–42.

[2] B. Ayati. A variable time step method for an age-dependent population model with nonlinear diffusion. *Siam Journal of Numerical Analysis*, **37** (2000), No 5, 1571–1589.

[3] S. Busenberg, M. Iannelli. A degenerated nonlinear diffusion problem in age-structured population dynamics. *Nonlinear Analysis, Theory, Methods and Applications*, **7** (1983), No 12, 1411–1429.

[4] M. Gurtin. A system of equations for age-dependent population diffusion. *Journal of Theoretical Biology*, **40** (1973), 389–392.

[5] M.-Y. Kim, E.-J. Park. Mixed approximation of a population diffusion equation. *Computers Math. Applic.*, **30** (1995), No 12, 23–33.

[6] M.-Y. Kim. Galerkin methods for a model of population dynamics with nonlinear diffusion. *Numerical methods for partial differential equations*, **12** (1996), 59–73.

[7] M. Kubo, M. Langlais. Periodic solutions for a population dynamics problem with age-dependence and spatial structure. *Journal of Math. Biology*, **27** (1991), 363–378.

[8] L. Lopez, D. Trigiante. A finite-difference scheme for a stiff problem arising in the numerical solution of a population dynamical model with spatial diffusion. *Nonlinear Analysis, Theory, Methods and Applications*, **9** (1985), No 1, 1–12.

[9] F. A. Milner. A numerical method for a model of population dynamics with spatial diffusion. *Computers Math. Applic.*, **19** (1990), No 4, 31–43.

[10] G. Pelovska, M. Iannelli. Numerical methods for the Lotka-McKendrick's equation. *Journal of Comp. and Applied Math.*, **197** (2006), 534–557.

[11] G. Pelovska. An improved explicit scheme for age-dependent population models with spatial diffusion. *International Journal of Numerical Analysis and Modeling*, **5** (2008), No 3, 466–490.

[12] D. Boyadzhiev. Application of an acceleration scheme for an age-structured diffusion model. Proceedings of the Anniversary International Conference REMIA, 2010, 117–123.

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ПОВИШАВАНЕ НА ИЗЧИСЛИТЕЛНАТА СКОРОСТ НА УСКОРЕНА СХЕМА ЗА ВЪЗРАСТОВО СТРУКТУРИРАН ДИФУЗИОНЕН МОДЕЛ

Дойчин Бояджиев, Галена Пеловска

В статията се предлага оптимизиран алгоритъм, който е по-бърз в сравнение с по-рано описаната ускорена (модифицирана STS) диференчна схема за възрастово структуриран популационен модел с дифузия. Запазвайки апроксимацията на модифицирания STS алгоритъм, изчислителното времето се намаля почти два пъти. Това прави оптимизирания метод по-предпочитан за задачи с нелинейност или с по-висока размерност.