# High order relaxed schemes for nonlinear reaction diffusion problems

DOI: 10.1685/CSC060163

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#### Abstract.

Different relaxation approximations to partial differential equations, including conservation laws, Hamilton-Jacobi equations, convection-diffusion problems, gas dynamics problems, have been recently proposed. The present paper focuses onto diffusive relaxed schemes for the numerical approximation of nonlinear reaction diffusion equations. High order methods are obtained by coupling ENO and WENO schemes for space discretization with IMEX schemes for time integration, where the implicit part can be explicitly solved at a linear cost. To illustrate the high accuracy and good properties of the proposed numerical schemes, also in the degenerate case, we consider various examples in one and two dimensions: the Fisher-Kolmogoroff equation, the porous-Fisher equation and the porous medium equation with strong absorption.

Keywords: Degenerate reaction diffusion problems, relaxation schemes, porous-Fisher equation, Fisher-Kolmogoroff equation.

## 1. Introduction

The main purpose of this work is to approximate solutions of a nonlinear, possibly degenerate, reaction-diffusion equation of the form

(1) 
$$\frac{\partial u}{\partial t} = D\Delta(p(u)) + g(u)$$

for  $x \in \Omega \subseteq \mathbb{R}^d$ ,  $d \ge 1$ ,  $t \ge 0$ , with initial condition,  $u(x,0) = u_0(x)$  and with suitable boundary conditions, where the function p is a non-decreasing Lipschitz continuous function defined on  $\mathbb{R}$ . The equation is degenerate if p(0) = 0 and in this case the solutions often become non-smooth in finite time, developing fronts and discontinuities. Finally, the coefficient D is a diffusivity coefficient and the function g(u) is the reaction term.

Equations like (1) are relevant in describing biological and physical processes and are involved in the modelling of population growth and dispersal, of waves of concentration of chemical substances in living organisms, of the motion of viscous fluids (see e.g.<sup>8</sup>). Also, systems of equations like (1), coupled via the reaction terms, are capable of modelling the cyclic Belousov-Zhabotinskii reactions and the pattern formation on the wings of butterflies and the coat of mammals (see<sup>9</sup> and references therein).

This paper is organized as follows. In section 2 we introduce the relaxation approximation of nonlinear diffusion problems, in section 3 we describe the fully discrete relaxed numerical scheme in the reaction-diffusion case. In section 4 we report several numerical tests, both in one and two space dimensions.

# 2. Relaxation approximation of nonlinear diffusion

The schemes proposed in the present work are based on the same framework of the well-known relaxation approximation introduced in<sup>5</sup> for hyperbolic conservation laws. In the case of the nonlinear diffusion operator in (1), an additional variable  $\vec{v}(x,t) \in \mathbb{R}^d$  and a positive parameter  $\varepsilon$  are introduced and the following relaxation system is obtained:

(1) 
$$\begin{cases} \frac{\partial u}{\partial t} + \operatorname{div}(\vec{v}) = g(u) \\ \frac{\partial \vec{v}}{\partial t} + \varphi^2 \nabla p(u) = -\frac{1}{\varepsilon} \vec{v} + \left(\varphi^2 - \frac{D}{\varepsilon}\right) \nabla p(u) \end{cases}$$

Now, formally, in the small relaxation limit,  $\varepsilon \to 0^+$ , system (1) approximates to leading order equation (1). The parameter  $\varphi$  is introduced in order to have bounded characteristic velocities and to avoid a singular differential operator as  $\varepsilon \to 0^+$ .

Finally the non linearity in the convective term is removed, as in standard relaxation schemes, introducing another scalar variable w(x,t) and rewriting the system as:

(2) 
$$\begin{cases} \frac{\partial u}{\partial t} + \operatorname{div}(\vec{v}) = g(u) \\ \frac{\partial \vec{v}}{\partial t} + \varphi^2 \nabla w = -\frac{1}{\varepsilon} \vec{v} + \left(\varphi^2 - \frac{D}{\varepsilon}\right) \nabla w \\ \frac{\partial w}{\partial t} + \operatorname{div}(\vec{v}) = -\frac{1}{\varepsilon} (w - p(u)) \end{cases}$$

Formally, as  $\varepsilon \to 0^+$ ,  $w \to p(u)$ ,  $v \to -\nabla p(u)$  and the original equation is recovered.

In the previous system the parameter  $\varepsilon$  has physical dimensions of time and represents the so-called relaxation time. Furthermore, w has the same dimensions as u, while each component of  $\vec{v}$  has the dimension of u times a velocity; finally  $\varphi$  is a velocity. The inverse of  $\varepsilon$  gives the rate at which v decays onto  $-\nabla p(u)$  in the evolution of the variable  $\vec{v}$  governed by the stiff second equation of (2).

Equations (2), originally introduced in<sup>10</sup> for the purely diffusive case, form a semilinear hyperbolic system with a stiff source term. The characteristic velocities of the hyperbolic part are given by  $0, \pm \varphi$ . The parameter  $\varphi$  allows to move the stiff terms  $\frac{D}{\varepsilon} \nabla p(u)$  to the right hand side, without losing the hyperbolicity of the system.

We point out that degenerate parabolic equations often model physical situations where free boundaries and discontinuities are relevant: we expect that schemes for hyperbolic systems will be able to reproduce faithfully these details of the solution. One of the main properties of (2) consists in the semilinearity of the system, that is all the nonlinear terms are in the (stiff) source terms, while the differential operator is linear. Hence, the solution of the convective part requires neither Riemann solvers nor the computation of the characteristic structure at each time step, since the eigenstructure of the system is constant in time. Moreover, the relaxation approximation does not exploit the form of the nonlinear function p and hence it gives rise to a numerical scheme that, to a large extent, is independent of it, resulting in a very versatile tool.

We also anticipate here that, in the relaxed case (i.e.  $\varepsilon = 0$ ), the stiff source terms can be integrated solving a system that is already in triangular form and then it does not require iterative solvers.

#### 3. Relaxed numerical schemes

## 3.1. Relaxed IMEX schemes

We extend here the schemes studied in,<sup>3</sup> including the reaction term. For simplicity, here we describe the one-dimensional case, the generalization being straightforward.

We observe that system (2) is in the form

$$\frac{\partial z}{\partial t} + \frac{\partial f(z)}{\partial x} = g(z) + \frac{1}{\epsilon}h(z)$$

where  $z = (u, v, w)^T$ ,  $f(z) = (v, \varphi^2 w, v)^T$ ,  $g(z) = (g(u), 0, 0)^T$  and  $h(z) = (0, -v + (\varepsilon \varphi^2 - D)w_x, p(u) - w)^T$ . When  $\varepsilon$  is small, the presence of both non-stiff and stiff terms, suggests the use of IMEX schemes.<sup>2,6,11</sup> In the problems considered here, the reaction term g(u) is not stiff and hence we treat it with the explicit portion of the IMEX scheme.

First we consider a semi-discrete form for time integration. Let's assume for simplicity a uniform time step  $\Delta t$  and denote with  $z^n$  the numerical approximation of the variable z at time  $t_n = n\Delta t$ , for  $n = 0, 1, \ldots$  In our case a  $\nu$ -stages IMEX scheme reads

(1) 
$$z^{n+1} = z^n - \Delta t \sum_{i=1}^{\nu} \tilde{b}_i \left[ \frac{\partial f}{\partial x}(z^{(i)}) + g(z^{(i)}) \right] + \frac{\Delta t}{\varepsilon} \sum_{i=1}^{\nu} b_i h(z^{(i)})$$

where the stage values are computed as

(2) 
$$z^{(i)} = B^{(i)} + \frac{\Delta t}{\varepsilon} a_{i,i} h(z^{(i)})$$

for

(3) 
$$B^{(i)} = z^n - \Delta t \sum_{k=1}^{i-1} \tilde{a}_{i,k} \left[ \frac{\partial f}{\partial x} (z^{(k)}) + g(z^{(k)}) \right] + \frac{\Delta t}{\varepsilon} \sum_{k=1}^{i-1} a_{i,k} h(z^{(k)})$$

Here  $(a_{ik}, b_i)$  and  $(\tilde{a}_{ik}, \tilde{b}_i)$  are a pair of Butcher's tableaux<sup>4</sup> of, respectively, a diagonally implicit and an explicit Runge-Kutta schemes.

In this work we use the so-called relaxed schemes, that are obtained by formally letting  $\varepsilon \to 0$  in (1). For these the computation of the first stage, that is (2) with i = 1,

(4) 
$$\begin{bmatrix} u^{(1)} \\ v^{(1)} \\ w^{(1)} \end{bmatrix} = \begin{bmatrix} u^n \\ v^n \\ w^n \end{bmatrix} + \frac{\Delta t}{\varepsilon} a_{1,1} h \left( \begin{bmatrix} u^{(1)} \\ v^{(1)} \\ w^{(1)} \end{bmatrix} \right)$$

implies that  $h(z^{(2)}) = 0$ , which is equivalent to

$$u^{(1)} = u^n$$
  $w^{(1)} = p(u^{(1)})$   $v^{(1)} = \frac{\partial w^{(1)}}{\partial x},$ 

Now the second stage, i = 2, reads

$$z^{(2)} = z^n - \Delta t \tilde{a}_{2,1} \left[ \frac{\partial f}{\partial x}(z^{(1)}) + g(z^{(1)}) \right] + \frac{\Delta t}{\varepsilon} a_{2,1} \underbrace{h(z^{(1)})}_{\equiv 0} + \frac{\Delta t}{\varepsilon} a_{2,2} h(z^{(2)}).$$

Hence the last two components of  $z^{(2)}$  are determined by the stiff terms of the above expression, namely  $h(z^{(1)}) = 0$ . On the other hand, due the form of h(z), there are no stiff terms in the equation for the first component  $u^{(2)}$ , which is then determined by a balance law.

Summarizing, the relaxed scheme yields an alternation of relaxation steps

$$h(z^{(i)}) = 0$$
 i.e.  $w^{(i)} = p(u^{(i)}), v^{(i)} = \frac{\partial w^{(i)}}{\partial x}$ 

and transport steps where we advance for time  $\tilde{a}_{i,k}\Delta t$ 

(5) 
$$\frac{\partial z}{\partial t} + \frac{\partial f(z)}{\partial x} = g(z)$$

with initial data  $z = z^{(i)}$ , retain only the first component and assign it to  $u^{(i+1)}$ . Finally the value of  $u^{n+1}$  is computed as  $u^n + \sum \tilde{b}_i u^{(i)}$ .

# 3.2. Spatial reconstructions

In order to have a fully discrete scheme, we still need to specify the space discretization. We will use discretizations based on finite differences, in order to avoid cell coupling due to the source terms.

Recall that the IMEX technique reduces the integration to a cascade of relaxation and transport steps. The former are the implicit parts of (4) and (2), while the transport steps appear in the evaluation of the explicit terms  $B^{(i)}$  in (3). Since (4) and (2) involve only local operations, the main task of the space discretization is the evaluation of  $\partial_x f$ , where we will exploit the linearity of f in its arguments.

In the one-dimensional case, let us consider a uniform grid on  $[a,b] \subset \mathbb{R}$ ,  $x_j = a - \frac{h}{2} + jh$  for j = 1, ..., m, where h = (b-a)/m is the grid spacing and m the number of cells. We denote with  $z_n^j$  the value of the quantity z at time  $t^n$  at  $x_j$ , the centre of the  $j^{\text{th}}$  computational cell. The fully discrete scheme may be written as

$$z_j^{n+1} = z_j^n - \Delta t \sum_{i=1}^{\nu} \tilde{b}_i \left( F_{j+1/2}^{(i)} - F_{j-1/2}^{(i)} \right) + \frac{\Delta t}{\varepsilon} \sum_{i=1}^{\nu} b_i g(z_j^{(i)}),$$

where  $F_{j+1/2}^{(i)}$  are the numerical fluxes, which are the only item that we still need to specify. It is necessary to write the scheme in conservation form and thus, following, 12 we introduce the function  $\hat{F}$  such that

$$f(z(x,t)) = \frac{1}{h} \int_{x-h/2}^{x+h/2} \hat{F}(s,t) ds$$

and hence

$$\frac{\partial f}{\partial x}(z(x_j,t)) = \frac{1}{h} \left( \hat{F}(x_{j+1/2},t) - \hat{F}(x_{j-1/2},t) \right).$$

The numerical flux function  $F_{j+1/2}$  approximates  $\hat{F}(x_{j+1/2})$ .

In order to compute the numerical fluxes, for each stage value, we reconstruct boundary extrapolated data  $z_{j+1/2}^{(i)\pm}$  with a non-oscillatory interpolation method, starting from the point values  $z_i^{(i)}$  of the variables at the centre of the cells. Next we apply a monotone numerical flux to these boundary extrapolated data.

To minimize numerical viscosity we choose the Godunov flux, which, in the present case of a linear system of equations, reduces to the upwind flux. In order to select the upwind direction we write the linear system with constant coefficients (5) in characteristic form. The characteristic variables relative to the eigenvalues  $\varphi, -\varphi, 0$  are respectively

$$U = \frac{v + \varphi w}{2\varphi}$$
  $V = \frac{\varphi w - v}{2\varphi}$   $W = u - w$ .

Note that u = U + V + W. Therefore the numerical flux in characteristic variables is

 $F_{j+1/2} = (\varphi U_{j+1/2}^-, -\varphi V_{j+1/2}^+, 0).$  The accuracy of the scheme depends on the accuracy of the reconstruction of the boundary extrapolated data. For a first order scheme we use a piecewise constant reconstruction such that  $U_{j+1/2}^- = U_j$  and  $V_{j+1/2}^+ = V_{j+1}$ . For higher order schemes, we use ENO or WENO reconstructions of appropriate accuracy.<sup>12</sup>

Since the transport steps need to be applied only to  $u^{(i)}$ , we have

$$u_j^{(i)} = u_j^n - \lambda \sum_{k=1}^{i-1} \tilde{a}_{i,k} \left[ \varphi \left( U_{j+1/2}^{(k)-} - U_{j-1/2}^{(k)-} - V_{j+1/2}^{(k)+} + V_{j-1/2}^{(k)+} \right) + \Delta t g(u_j^{(k)}) \right]$$

Finally, taking the last stage value and going back to conservative variables,

$$\begin{aligned} u_j^{n+1} &= u_j^n - \frac{\lambda}{2} \sum_{i=1}^{\nu} \tilde{b}_i \left( [v_{j+1/2}^{(i)-} + v_{j+1/2}^{(i)+} - (v_{j-1/2}^{(i)-} + v_{j-1/2}^{(i)+})] \right. \\ &\left. + \varphi [w_{j+1/2}^{(i)-} - w_{j+1/2}^{(i)+} - (w_{j-1/2}^{(i)-} - w_{j-1/2}^{(i)+})] \right) \end{aligned}$$

We wish to emphasize that the scheme reduces to the time advancement of the single variable u. Although the scheme is based on a system of three equations, the construction is used only to select the correct upwinding for the fluxes of the relaxed scheme and the computational cost of each time step is not affected.

#### 3.3. Numerical scheme

Employing a Runge-Kutta IMEX scheme of order p, can give an integration procedure for (1) which is of order up to 2p with respect to h (see<sup>3</sup>), since the CFL restrictions on the time-step are of parabolic type ( $\Delta t \leq Ch^2$ ). We observed that this theoretical convergence rate can be achieved in practice, with careful choice of the approximations of the spatial derivatives.

Summarizing, the relaxed schemes that we propose for the numerical integration of (1)consists of the following steps.

For each Runge-Kutta stage we need to compute the variables  $v^{(i)}$  and  $w^{(i)}$  (relaxation steps). The computation of  $v^{(i)}$  requires the approximation of a spatial gradient operator, for which we choose a central finite difference operator of order at least 2p. Then we need to solve the transport equation by diagonalizing the linear system (5), reconstructing the characteristic variables  $U^{(i)}$  and  $V^{(i)}$  at cell boundaries and computing the fluxes. Again,

we must choose a spatial reconstructions of order at least 2p and, to avoid spurious oscillations, we employ ENO or WENO non-oscillatory procedures. These procedures compare, for each cell, the reconstructions obtained using different stencils and choose the least oscillatory one (ENO) or compute a weighted linear combination of all of them (WENO). For details, see.<sup>12</sup>

#### 4. Numerical results

## 4.1. Travelling waves tests

As a first test, we consider the one-dimensional Fisher-Kolmogoroff equation, namely

(1) 
$$\frac{\partial u}{\partial t} = ku(1-u) + D\frac{\partial^2 u}{\partial x^2}$$

for  $x \in \mathbb{R}$  and t > 0, which was initially proposed for the modelling of spatial spread of populations.<sup>8</sup>

The two uniform steady states of (1) are  $u_0(x) = 0$  and  $u_1(x) = 1$ . A careful analysis of the state space, reveals the existence of travelling wave solutions linking these two states, i.e. of solutions of the form u(x,t) = U(x-ct) such that  $U(-\infty) = 1$  and  $U(\infty) = 0$ . reports the following asymptotic form for such solutions:

(2) 
$$U(z) = \frac{1}{(1+e^{z/c})} + \frac{1}{c^2} \frac{e^{z/c}}{(1+e^{z/c})^2} \log \frac{4e^{z/c}}{(1+e^{z/c})^2} + O\left(\frac{1}{c^4}\right),$$

which is valid when the speed verifies

$$c \ge 2\sqrt{kD}$$
.

Moreover the slope of the inflection point (z = 0) is related to the speed c of the wave by the relation

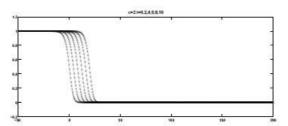
(3) 
$$U'(0) = -\frac{1}{4c} + O\left(\frac{1}{c^5}\right)$$
, for  $c \ge 2$ .

Travelling wave solutions are very important in the modelling of populations, since they represents phenomena like the invasion of a territory by a new species, the expansion of epidemics, etc.

We tested the ability of our integration scheme to reproduce these results. We chose k = D = 1 in (1), set up initial datum u(x,0) = U(x) for  $c = 2,4,\ldots,10$  on  $x \in [-50,200]$  and evolved it with homogeneous Neumann boundary conditions until T = 10. We present the numerical solutions obtained with ENO spatial reconstruction of order 6 and third order Runge-Kutta time integration: they are compared with the asymptotic ones in Figure 1. Moreover we tested the validity of the expansion (3) plotting the maximum of the numerical gradient of the solution, together with the values predicted by the asymptotic analysis. From Figure 2 we clearly see a very accurate agreement, except for the limiting case c = 2, which is however at the boundary of the validity range of (3).

As a second test we consider the following generalization of the Fisher-Kolmogoroff equation (1)

(4) 
$$\frac{\partial u}{\partial t} = u^p (1 - u^q) + \frac{\partial}{\partial x} \left( u^m \frac{\partial u}{\partial x} \right)$$



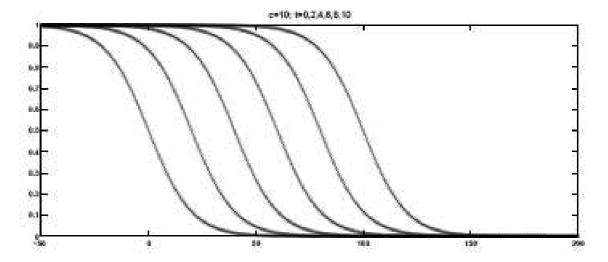


Fig. 1. Travelling waves with c=2 (top) and c=10 (bottom). The crosses represent the numerical solution at t=0,2,4,6,8,10 and the solid lines are the corresponding asymptotic expansions (2).

The existence of travelling waves can be proved for a wide range of parameters p, q, m.<sup>8</sup> The paper<sup>13</sup> gives an expression of such waves for the case p = 1 and q = m. Moreover<sup>13</sup> finds an asymptotic expansion for the case of two merging travelling waves, which is valid for a finite time after the first contact of the two fronts.

Figure 3 shows both the numerical solutions obtained with our method and the asymptotic expansion given in,<sup>13</sup> in the case q = m = 1. The initial data represent two travelling fronts, initially at  $x_0 = -1$  and  $x_1 = 1$ , moving in opposite directions. They first meet at

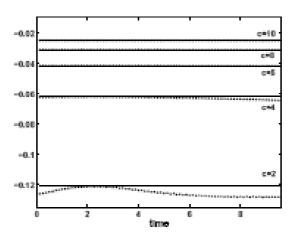


Fig. 2. Comparison of the maximum slope of the numerical solutions (dots) with the value predicted by the asymptotic expansion (3). Time is on the horizontal axis, the values of c are printed on the graph close to each line.

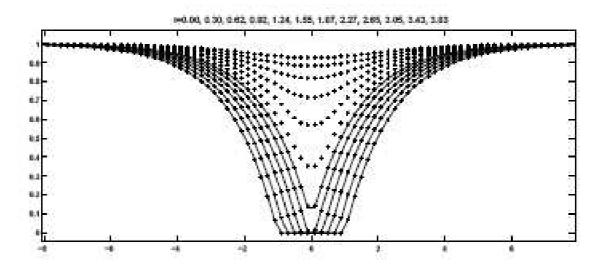


Fig. 3. Comparison of the numerical solutions (dots) of (4) with the asymptotic expansion (solid line). Here p = 1 and q = m. The latter is printed only in the time range where it is valid.

 $t^* \simeq 1.41$  and then the two waves merge. The asymptotic expansion given in <sup>13</sup> is valid for a small time interval after  $t^*$  and it is shown in Figure 3 with solid lines. The numerical solutions (in dots) are shown until the steady state is reached.

## 4.2. Two dimensional tests

We tested the multi-dimensional version of our integration scheme on the equation

(5) 
$$\frac{\partial u}{\partial t} = \Delta(u^m) - cu^p$$

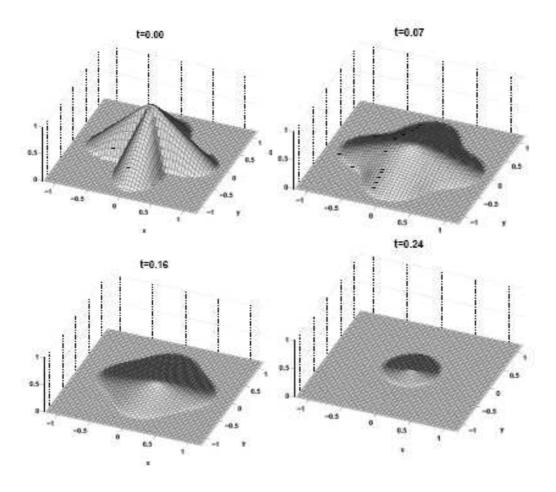


Fig. 4. The numerical solution of (5) with initial data (6) at different times, for  $(x, y) \in [-1.2, 1.2]^2$ .

for  $x \in [-2, 2]^2$  and  $t \ge 0$ . The above equation presents interesting finite-time extinction phenomena, reported in.<sup>7</sup> We take initial data

(6) 
$$u(x,y,0) = \begin{cases} 1, & x = 0, y = 0 \\ \left[1 - \frac{(x^2 + y^2)^2}{\sqrt{x^6 + y^6}}\right]_{\perp}, & \text{otherwise} \end{cases}$$

and evolve it until extinction with equation (5) for c = 5, p = 0.5 and m = 2. The results are presented in Figure 4.

# 5. Conclusions

We have proposed and analyzed relaxed schemes for nonlinear degenerate reaction diffusion equations. By using suitable discretization in space and time, namely ENO/WENO non-oscillatory reconstructions for numerical fluxes and IMEX Runge-Kutta schemes for time integration, we have obtained a class of high order schemes. The theoretical convergence analysis for the semidiscrete scheme and the stability for the fully discrete schemes have been studied by us, for the case of nonlinear diffusion, in.<sup>3</sup>

Here we tested these schemes on travelling waves solutions and in cases where the solution vanishes in finite time. In all cases we observed a very good agreement with known properties of the exact solutions.

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