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Abstract

Numerical approximation of one-dimensional kinetic models for directed motion of bacterial populations in response to a chemical gradient, usually called *chemotaxis*, is considered in the framework of well-balanced (WB) schemes. The validity of one-dimensional models have been shown to be relevant for the simulation of more general situations with symmetry in all but one direction along which appears the chemical attractant gradient. Two main categories are considered depending on whether or not the kinetic equation with specular boundary conditions admits non-constant macroscopic densities for large times. The WB schemes are endowed with the property of having zero artificial viscosity at steady-state; in particular they furnish numerical solutions for which the macroscopic flux vanishes, a feature that more conventional discretizations can miss. A class of equations which admit constant asymptotic states can be treated by a slight variation of the method of Case's elementary solutions originally developed for radiative transfer problems. More involved models which can display concentrations are handled through a different, but closely related, treatment of the tumbling term at the computational grid's interfaces. Both types of WB algorithms can be implemented efficiently relying on the Sherman-Morrison formula for computing interface values. Transient and stationary numerical results are displayed for several test-cases.

Key words: Chemotaxis "run and tumble" models, Case's elementary solutions, One-dimensional kinetic equations, Slab geometry, Rank-one perturbation and Sherman-Morrison formula, Stabilization in large times, Well-balanced schemes.
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1 Introduction

Chemotaxis describes the directed movement of a large population of micro-organisms (cells, bacteria, ...) in response to a gradient of a chemical substance, usually referred to as the chemo-attractant. Indeed the swimming displacement of certain flagellated bacteria can be described by straight-line "runs" suddenly interrupted by "tumbles" of very short duration (see realistic time-scale measures in [19], Table 1.1, and [43]). Usually, cell velocities are of the order of 10/20 μm/sec, run lengths can be of 10/20 cell diameters and tumbling lasts at most 0.1 sec. In the absence of chemo-attractant, their motion would be a random walk; however, its presence results in a decrease of tumbling frequency when cells move in the direction of increasing concentration, a process called *chemokinesis* which tends to increase run lengths in the favorable direction.

1.1 One-dimensional reduction of Alt-Stroock's model

The most general kinetic model for directed movement of bacterial populations is probably the "run and tumble" equation proposed by Alt [2], which reads

$$\partial_t f(t,\mathbf{x},\mathbf{v},\tau) + \partial_\tau f + \mathbf{v}\cdot\nabla_{\mathbf{x}} f + \gamma(t,\mathbf{x},\mathbf{v},\tau) f = 0, \qquad \tau > 0,$$

in case the mean velocity of organisms is assumed to be constant in $\mathbf{x} \in \mathbb{R}^3$. When $\tau = 0$,

$$f(t,\mathbf{x},\mathbf{v},0) = \int_0^\infty \int_{\mathbb{R}^3} \gamma(t,\mathbf{x},\mathbf{v}',\tau') f(t,\mathbf{x},\mathbf{v}',\tau') k(t;\mathbf{x},\mathbf{v}',\mathbf{v}) d\mathbf{v}' d\tau'.$$

The variables $t > 0$, $\mathbf{x} \in \mathbb{R}^3$, $\mathbf{v} \in \mathbb{R}^3$, $\tau \geq 0$ stand for the time, spatial position, velocity and run time. The kinetic density $f \geq 0$ represents the statistical repartition of cells at time t, with velocity $\mathbf{v}$ at the position $\mathbf{x}$ with a run time τ. The function $\gamma(t,\mathbf{x},\mathbf{v},\tau)$ is the probability per unit time that a cell moving in direction $\mathbf{v}$ located at $\mathbf{x}$ at time t with run time τ (counted starting from the beginning of the run) tumbles instantaneously; in such a case, the probability that this cell chooses the particular direction $\bar{\mathbf{v}}$ afterwards is given by $k(t;\mathbf{x},\mathbf{v},\bar{\mathbf{v}})$. The first equation quantifies the rate of change in the population in $t,\mathbf{x},\mathbf{v}$ with run time τ by means of a convection term rendering the net motion of cells in the vicinity of $\mathbf{x}$ and a loss term due to tumbling process (with probability γ). The second equation states that the only initial (meaning that the run time τ is zero) distribution of cells moving in the direction $\mathbf{v}$ comes from the other cells which were moving with velocity $\mathbf{v}'$ and tumbled at time t for any run time τ'.

It can be considered reasonable, as a first set of simplifying hypotheses, to assume that γ is independent of τ and that the chemo-attractant presence doesn't affect turning probabilities, thus k becomes a function of $\mathbf{v},\mathbf{v}'$ only [39]. The resulting model is still generally too involved and a second simplification can be made by eliminating the dependence on the run time τ of the organisms. By defining the probability per unit time $p(t;\mathbf{x},\mathbf{v}',\mathbf{v})$ that a cell with velocity $\mathbf{v}'$ tumbles in $t,\mathbf{x} \in \mathbb{R}^+ \times \mathbb{R}^3$ and changes direction to $\mathbf{v}$, a more tractable kinetic equation is derived for a reduced kinetic density (still denoted by f):

$$\partial_t f(t,\mathbf{x},\mathbf{v}) + \mathbf{v}\cdot\nabla_{\mathbf{x}} f = \int_{\mathbb{R}^3} p(t;\mathbf{x},\mathbf{v}',\mathbf{v}) f(t,\mathbf{x},\mathbf{v}') d\mathbf{v}' - f\int_{\mathbb{R}^3} p(t;\mathbf{x},\mathbf{v},\mathbf{v}') d\mathbf{v}'. \qquad (1)$$

This equation is referred to as the Stroock's model [48] (it appears also in [16,18,43,42]), see also (36) without birth/death term in [41]; it can be deduced from Alt's model by assuming that the run times τ follow a Poisson distribution [23]. This type of motion belongs to the class of *velocity-jump processes* because individuals run in given directions, but at random instants, they stop in order to choose a new velocity, and the time spent in the latter stage is small compared to the run length, thus this tumbling step can be considered instantaneous.

As the three-dimensional framework can be still considered too heavy for the development of efficient numerical strategies, a reduction to a more convenient one-dimensional setting can be performed following some computations in [23] while maintaining some realistic features. Basically, the one-dimensional models we intend to study hereafter correspond to particular solutions of (1) which display rotational symmetry with respect to one axis (this is reminiscent to 1-D models studied in [30] being invariant by translation in 2 directions) and for which chemo-attractant gradients appear along the corresponding direction only. Denoting $\mathbf{x} = (x, y, z) \in \mathbb{R}^3$ and assuming that velocities are of unit length, $\mathbf{v} = (v_x, v_y, v_z) \in \mathbb{S}^2$, this peculiar direction can be chosen as z and spherical coordinates yield in standard notation:

$$\mathbf{v} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta).$$

Symmetry about the z coordinate means that $\mathbf{v}$ is independent of ϕ thus by integrating the kinetic density in x, y and $\phi \in (0, 2\pi)$, one obtains a so–called "reduced distribution" (still denoted by f) depending on $t, z, \cos\theta$. Computations displayed in pages 1436/1437 of [23] show that this reduced kinetic density is solution of

$$\partial_t f(t, z, \cos\theta) + \cos\theta\partial_z f = \int_0^\pi \gamma(t, z, \theta')K(\theta, \theta')f(t, z, \cos\theta')\sin\theta' d\theta' - \gamma(t, z, \theta)f,$$

with γ depending on a reduced set of coordinates and K a reduced turning probability,

$$K(\theta, \theta') = \frac{1}{2\pi}\int_0^{2\pi}\int_0^{2\pi} k(\mathbf{v}', \mathbf{v})d\phi' d\phi.$$

It remains to let the one-dimensional velocity in the z direction $v \in [-1, 1]$ stand for $\cos\theta$ in order to derive the linear equation which is the main topic of this paper:

$$\partial_t f(t, z, v) + v\partial_z f = \int_{-1}^1 \gamma(t, z, v')K(v, v')f(t, z, v')dv' - \gamma(t, z, v)f. \tag{2}$$

Two representative cases of (2), already studied in [42,10], will be scrutinized in detail in the forthcoming sections. Numerical approximations will be derived and their large-time behavior will be studied. The kinetic equation (2) can be completed by another one governing the time evolution of the chemo-attractant substance: let $S(t, z)$ stand for its concentration. Creation, adsorption and diffusion can be rendered through

$$\partial_t S = D\partial_{zz}S + \alpha\rho - \beta S, \qquad \rho(t, z) = \int_{-1}^1 f(t, z, v)dv, \ (D, \alpha, \beta) \in (\mathbb{R}^+)^3. \tag{3}$$

Of course, since γ generally depends on t, z through $\partial_z S$ the coupling of (3) with (2) leads to a weakly nonlinear one-dimensional problem; see also [27,28,40].

1.2 Well-balanced techniques for 1-D linear kinetic equations

Now it becomes necessary to quickly recall the main topics about the so–called *well-balanced* numerical approximations of linear kinetic equations of the type (2), sometimes referred to as of Barbashin type [4]. Such methods have already been used in the context of solving radiative transfer problems [26] and closely follow the classic method of Case's elementary solutions [1,12,13,37], further developed by Siewert and co-workers [6,7,46]. Another area of application is the treatment of linearized Boltzmann models [29]: in this case, one follows early papers of Cercignani [14,15].

Let's consider a uniform Cartesian computational grid determined by the positive parameters Δz, Δt such that $z_j = j\Delta z$ for $j \in \mathbb{Z}$ with a generic cell $C_j = [z_{j-\frac{1}{2}}, z_{j+\frac{1}{2}}]$. The Cauchy

problem for the simple time-dependent kinetic equation reads:

$$\partial_t f + v\partial_z f = \frac{1}{2}\int_{-1}^{1} f(t,x,v')dv' - f, \qquad x \in \mathbb{R}, v \in [-1,1], t > 0 \tag{4}$$

with initial data $f(t=0) = f_0$. Denoting the macroscopic density $\rho(t,x) = \int_{-1}^{1} f(t,x,v)dv$, the main idea for deriving a well-balanced numerical scheme for (4) is to set up a classical Godunov scheme for the "localized" equation:

$$\partial_t f + v\partial_z f = \Delta z \sum_{j\in\mathbb{Z}} \left(\frac{\rho}{2} - f\right)\delta(z - z_{j-\frac{1}{2}}), \tag{5}$$

where δ stands for the Dirac mass in $z = 0$. Consistency has been investigated for nonlinear problems in [3]; formally, it is a consequence of the easy formula $\Delta z \sum_{j\in\mathbb{Z}} \delta(z - z_{j-\frac{1}{2}}) \rightharpoonup 1$ when $\Delta z \to 0$. Considering (5) instead of (4) allows to keep elementary Riemann problems homogeneous, hence self-similar, at the price of introducing a term on the right-hand side which can become ambiguous if f is discontinuous at locations $z = z_{j-\frac{1}{2}}$. However, such a *non-conservative product* [38] can be rigorously defined within the theory of distributions; the resulting non-conservative Riemann problem contains one supplementary static wave (called "zero-wave" in [3] and "standing wave" in [35]) which renders the effects of the relaxation term concentrated on the discrete lattice. It has been shown (see *e.g.* [32]) that the correct jump relation across this "zero-wave" is obtained through solving the forward-backward problem [8,9] for the stationary equation of (4):

$$v\partial_z \bar{f} = \frac{1}{2}\int_{-1}^{1} \bar{f}(x,v')dv' - \bar{f}, \qquad x \in [0,\Delta z], v \in [-1,1], \tag{6}$$

with inflow boundary conditions,

$$\bar{f}(0, v > 0) = f_{left}(v), \qquad \bar{f}(\Delta z, v < 0) = f_{right}(v).$$

We emphasize that this construction is very similar to the extension of the classical I'lin scheme for parabolic equations presented in [20]. From this perspective, well-balanced schemes are by no means restricted to hyperbolic of kinetic problems, but exist for nonlinear parabolic ones as well with the same type of building block, that is to say, the stationary equation. There are also deep connections with so–called *Asymptotic-Preserving* schemes as explained in [26,31,32].

An essential feature for WB schemes for (4) is therefore that the boundary-value problem for (6) admits an explicit, or at least easily computable, solution. This is indeed the case, (as shown by Case and co-workers [1,12,13,36] and then by Cercignani [14,15]) because such a solution can be expressed by means of *elementary solutions*. Namely, under mild regularity assumptions the solution of (6) is derived by separation of variables [8,24]:

$$\bar{f}(z,v) = \alpha + \beta(z - v) + \int_{-1}^{1} A(\nu)\varphi_\nu(v)\exp(-z/\nu)d\nu, \tag{7}$$

where ν are the proper modes satisfying of the equation [12,37],

$$1 - \frac{\nu}{2}\log\frac{\nu+1}{\nu-1} = 0, \qquad \nu \in (-1,1), \tag{8}$$

φ_ν are the "generalized eigenfunctions", α, β and $A(\nu)$ are determined by boundary conditions (see also [4,24,34,37]). Later, this technique has been adapted to numerical computations by Siewert and co-workers who introduced the so–called *Analytical Discrete-Ordinate* (ADO) method [6,7,46]. Roughly speaking, it consists in discretizing the velocity variable v

according to a Gaussian quadrature rule in order to be able to compute astutely a vector of normal modes $\vec{\nu}$ to be used for computing approximately the integral term in (7). Altogether, these elements allow to build an efficient Riemann solver for (5) and thus a WB scheme for (4): it has been shown in [26,29] that this type of discretizations are feasible and moreover endowed with interesting stability properties.

1.3 Outline of the paper

This paper is organized as follows. Section 2 deals with the simplest kinetic model rendering "run and tumble" dynamics, as explained in [42] (see §4.1), for which it is rather easy to adapt the formalism of Case's elementary solutions. This unusual spectral technique allows for solving the forward-backward problem at each interface of the computational grid thus providing a reliable expression of well-balanced numerical fluxes. These fluxes, derived in §2.2 through the so–called *Analytical Discrete Ordinates* method [6,7,46], are endowed with the property that the free transport step and the relaxation process are **not separated**, thus allowing for improved performances when it comes to stabilization in large times (see also [47]). The resulting time-marching scheme is also less viscous than more conventional time-splitting schemes (see §2.3). A more challenging kinetic model from [41], which has been studied theoretically in [10], is tackled in Section 3. It did not result possible to adapt Case's formalism to this problem hence the forward-backward integro-differential equation is discretized in such a way that the interface values which are needed to set up the well-balanced scheme can be obtained by solving a linear system derived in §3.1. Another advantage of this formulation is that the matrices involved are rank-one perturbations of diagonal matrices, thus allowing for the use of the Sherman-Morrison formula (see [33] and §3.2). In §3.3, a challenging test-case is studied in some detail and the comparison between the new WB scheme and a more classical time-splitting algorithm is briefly displayed, for which it is interesting to notice that the same type of erroneous behavior than the one reported in [40] is still observed here (enormous macroscopic flow close to the border of the domain and stalling of residues). Finally some concluding remarks are given in §4.

Numerical simulation of mathematical models rendering chemotaxis dynamics is a topic attracting substantial interest from the research community. Let us quote first results dealing with the parabolic Patlak-Keller-Segel model [45]: a very general convergence framework has been obtained by Filbet [21]. However, the parabolic formulation has the drawback of inducing an infinite propagation speed of information, which can be fairly considered unphysical. Hyperbolic models eliminate this undesirable feature, see [18,22,43]; discrete velocity kinetic models can be handled by means of similar techniques [27,28,40]. Advances in numerical analysis allow to simulate efficiently much more detailed kinetic models [2,16,23,41,42,48]: consult for instance [11,50]. Finally, we stress again the similarity between this class of distinguished numerical schemes and the ones derived for the nonlinear parabolic equations by extending the ideas of the classic Scharfetter-Gummel scheme [44] for which numerical fluxes are computed by solving a Dirichlet problem for the stationary equations, see [20].

2 Othmer-Hillen model: flat asymptotic regimes

The simplest model which is proposed in [42] (see also [16]) in order to model a biased velocity redistribution resulting from the presence of a chemical attractant consists in rewriting (1) with $p(t;\mathbf{x},\mathbf{v}',\mathbf{v}) \equiv T(\mathbf{v},\mathbf{v}')$ and in multiplying the right-hand side by $\lambda \geq 0$. The quantity $T(\mathbf{v},\mathbf{v}')$ gives the probability of a velocity jump from $\mathbf{v}'$ to $\mathbf{v}$ and is supposed to satisfy: $T \geq 0$, $\int T(\mathbf{v},\mathbf{v}')d\mathbf{v} = \int T(\mathbf{v},\mathbf{v}')d\mathbf{v}' = 1$, $T \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$. One way to obtain this framework is to take $\gamma \equiv \lambda \in \mathbb{R}^+$ and $k \equiv T$ in the original Alt's equations; the case of order-one perturbations of the turning kernel (§4.1 in [42]) corresponds to

$$T(\mathbf{v},\mathbf{v}') = T_0(\mathbf{v},\mathbf{v}') + T_1(\mathbf{v},\mathbf{v}',S), \qquad T_1(\mathbf{v},\mathbf{v}',S) = \mathbf{v}\cdot M(\nabla S)\mathbf{v}',$$

with M a 3×3 matrix-valued function of ∇S. Taking now into account for the fact that only $\partial_z S \neq 0$ and picking for M the diagonal matrix whose entries are precisely the components of ∇S allows for carrying out the one-dimensional reduction of [23]. Suppose that T_0 stands for a uniform redistribution of velocities, the 1-D model (2) with $\lambda = 1$ reads:

$$\partial_t f(t,z,v) + v\partial_z f = \int_{-1}^{1} \left[\frac{1}{2} + v(\partial_z S.v')\right] f(t,z,v')dv' - f. \tag{9}$$

In order to keep the positivity property $T \geq 0$, one has to assume a **sub-characteristic property**: $\frac{1}{2} + v(\partial_z S.v') \geq 0$, which is precisely the condition $(T_1 1)$ on page 1233 of [42]. Such a condition has been extensively used in order to prove stability results in the simpler context of a discrete 2-velocity model in [27] in both hyperbolic and diffusive scalings.

2.1 Case's elementary solutions for biased velocity redistribution

The sub-characteristic property has already been encountered in [27] in a simpler form corresponding to the case where $v \in \{-1, 1\}$ only, that is to say, a 2×2 velocity model. In this section, it will be shown that the construction of [27] can be extended to (9) in roughly the same manner than the numerical schemes of [32] extend to those of [26], *i.e.* by means of Case's elementary solutions.

Under the assumption that $\partial_z S$ remains small enough to keep $T \geq 0$ (which means that ρ, α are small and D, β are relatively big) the first step in building a well-balanced scheme for (9) is to compute the solution of the time-independent problem:

$$v\partial_z \bar{f}(z,v) = \int_{-1}^{1} \left[\frac{1}{2} + v(\sigma v')\right] \bar{f}(z,v')dv' - \bar{f} \qquad z \in (0, \Delta z),\ \sigma \in \mathbb{R}, \tag{10}$$

with inflow boundary conditions. A simple way to ensure the sub-characteristic condition is to replace the term 2σ by $\tanh(\sigma) \in [-1, 1]$ for instance.

Lemma 1 *Assume that the forward-backward problem for (6) admits a complete set of Case's generalized eigenfunctions depending on normal modes ν which are solutions of (8),*

$$1,\ z - v,\ \exp(-z/\nu)\varphi_\nu(v),$$

then for $\sigma \neq 0$, a complete set of eigenfunctions for the equation (10) is:

$$1,\ \left(\frac{2}{3}\sigma - 1\right) z - v,\ \exp(-z/\nu)\varphi_\nu(v),$$

where ν denotes the same normal modes.

The conclusion of the Lemma is that the biasing term in (10) involving a constant σ induces only a velocity shift in the *linear diffusion solution* (as it is called in [24]).

Proof: The proof is divided in several steps for the sake of clarity:

- The first step is to establish that the macroscopic flux $J = \int_{-1}^{1} v'\bar{f}(z,v')dv'$ in (10) is actually a constant. By integrating the equation in $v \in [-1, 1]$, it comes:

$$\partial_z \int_{-1}^{1} v\bar{f}(z,v)dv = \int_{-1}^{1} \left(\int_{-1}^{1} \bar{f}(z,v')dv'\right) \frac{dv}{2} + \sigma \int_{-1}^{1} v \left(\int_{-1}^{1} v'\bar{f}(z,v')dv'\right) dv - \int_{-1}^{1} \bar{f}(z,v)dv.$$

The term $\int_{-1}^{1} v\left(\int_{-1}^{1} v'\bar{f}(z,v')dv'\right)dv$ vanishes because v is an odd function on $[-1,1]$. Moreover, $\int_{-1}^{1}\left(\int_{-1}^{1}\bar{f}(z,v')dv'\right)\frac{dv}{2} - \int_{-1}^{1}\bar{f}(z,v)dv = 0$ too. Thus $\partial_z\int_{-1}^{1} v\bar{f}(z,v)dv = 0$ and (10) rewrites as:

$$v\partial_z\bar{f}(z,v) = \frac{1}{2}\int_{-1}^{1}\bar{f}(z,v')dv' + \sigma vJ - \bar{f}.$$

If the set of generalized eigenfunctions $1, z-v, \exp(-z/\nu)\varphi_\nu(v)$ is complete for $\sigma = 0$, then one will get a complete set for (10) by adding a linear function in v and keeping the same normal modes (computed in [12]).

- By plugging the function $az - v$, $a \in \mathbb{R}$, in (10), one can find the correct value of a in order to obtain a particular solution:

$$v\partial_z(az-v) = -av = az + \sigma v\int_{-1}^{1} v'(az+v')dv' - az + v = -\sigma v\int_{-1}^{1}(v')^2dv' + v.$$

This simplifies into:

$$\int_{-1}^{1}(v')^2dv' = \frac{2}{3}, \qquad a = \frac{2}{3}\sigma - 1, \qquad v \neq 0,$$

which matches the conclusion of the Lemma. The general form of sufficiently smooth solutions of (10) with inflow boundary conditions is given by the full-range expansion:

$$\bar{f}(z,v) = \alpha + \beta\left[\left(\frac{2}{3}\sigma - 1\right)z - v\right] + \int_{-1}^{1} A(\nu)\varphi_\nu(v)\exp(-z/\nu)d\nu \qquad \square \qquad (11)$$

Theorem I in [12] states that generalized eigenfunctions are orthogonal in the sense:

$$\int_{-1}^{1} v\varphi_\nu(v)\varphi_{\nu'}(v).dv = N_\nu\delta_{\nu,\nu'},$$

where N_ν is an explicit function of the proper mode ν.

Lemma 2 *Generalized eigenfunctions for (10) $\varphi_\nu(v)$ with ν the set of proper modes satisfy:*

$$\int_{-1}^{1} v\varphi_\nu(v).dv = 0.$$

Proof: It suffices to integrate the equation on φ_ν in the v variable and divide by 2. Inserting the separated variables ansatz $\exp(-x/\nu)\varphi_\nu(v)$ into (10) leads to

$$\left(1 - \frac{v}{\nu}\right)\varphi_\nu(v) = \frac{1}{2}\int_{-1}^{1}\varphi_\nu(v').dv' + \sigma vJ, \qquad (12)$$

which can be integrated in v in order to make the σvJ term disappear. This yields:

$$-\frac{1}{2}\int_{-1}^{1}\frac{v}{\nu}\varphi_\nu(v).dv = \frac{1}{2}\int_{-1}^{1}\varphi_\nu(v').dv' - \frac{1}{2}\int_{-1}^{1}\varphi_\nu(v).dv = 0.$$

$\square$

Theorem 1 *Let $\bar{f}(x,v)$ be a smooth solution to the forward-backward boundary-value problem (10) written in the form (11); its macroscopic flux satisfies:*

$$\int_{-1}^{1} v\bar{f}(x,v)dv = -\frac{2}{3}\beta,$$

with β the coefficient of the so–called "linear diffusion solution" $(\frac{2}{3}\sigma - 1)z - v$ in (11).

Proof: Existence, uniqueness and regularity results for this type of forward-backward problems have been given in [9]. From Lemma 2 one deduces that the eigenfunctions $1, \varphi_\nu(v)$ have no contribution to the (constant) macroscopic flux induced by $\bar{f}(x,v)$. Moreover, Lemma 1 gives the explicit expression of the remaining eigenfunction, the *linear diffusion solution*. Multiplying (7) by v and integrating leads to the conclusion. □.

The terminology *linear diffusion solution* is taken from [24] where it is introduced in the context of steady Fokker-Planck equations. It is shown there that this particular solution (with variables separated in a sum instead of a product) emanates from the degeneracy of the 0-eigenvalue (corresponding here to $\nu \to \infty$). Results about this degeneracy in the context of BGK-type mass-preserving equations are given in [13,49].

2.2 Derivation of the corresponding well-balanced scheme

Based on the representation (11), there are only small algorithmic changes to conduct with respect to [26]. The first task is to derive the normal modes ν, but since the presence of σ has no effect on them, the procedure will follow the results by Siewert and co-authors published in [6,7,46] under the name "Analytical Discrete-Ordinate method".

It consists in first, introducing a $2N$-point Gaussian quadrature on $(-1,1)$, zero is excluded, which is assumed to meet at least with the following requirements:

$$\sum_{\ell=1}^{2N} \omega_\ell v_\ell^k = \begin{cases} 2 \text{ for } k=0, \\ \frac{2}{3} \text{ for } k=2. \end{cases}$$

By symmetry, it is more convenient to work with its restriction to the positive interval $(0,1)$, given by the N points and weights,

$$\mathcal{V} := (v_1, v_2, ..., v_N) \in (0,1)^N, \qquad \omega := (\omega_1, ..., \omega_N) \in \mathbb{R}^+, \tag{13}$$

and obtained by retaining only the N last values in the original $2N$ quadrature. Then, it computes a vector of eigen-modes $\nu \in (\mathbb{R}^+)^N$ which is an approximation of the proper modes. Last, it determines the coefficients of the generalized eigenfunctions out of the given inflow boundary conditions. Let us consider (12) for $\sigma = 0$: its approximation by means of the aforementioned quadrature rule reads,

$$\left(1 \mp \frac{v_k}{\nu_k}\right) \varphi(\nu, \pm v_k) = \frac{1}{2} \sum_{\ell=1}^{N} \omega_\ell \Big(\varphi(\nu, v_\ell) + \varphi(\nu, -v_\ell)\Big), \qquad k \in \{1, ..., N\}.$$

At this level, a trick can be used in order to reduce the cost of this eigenvalue problem: let us denote $\Phi_\pm(\nu) = (\varphi_\nu(\pm v_k))_{k\in\{1,...,N\}}$ and Id the identity matrix of $\mathbb{R}^N$. By using the same notation for a vector in $\mathbb{R}^N$ and its corresponding $N \times N$ diagonal matrix, it comes:

$$\pm\frac{1}{\nu}\mathcal{V}\Phi_\pm(\nu) = \left(Id - \frac{\omega}{2}\right)\Phi_\pm(\nu) - \frac{\omega}{2}\Phi_\mp(\nu) \tag{14}$$

Barichello, Siewert and Wright [7,46] define $S(\nu) = \mathcal{V}(\Phi_+(\nu) + \Phi_-(\nu)) \in \mathbb{R}^N$ in order to reduce (14) into: $\mathcal{V}^{-1}(Id - \omega)\mathcal{V}^{-1}S(\nu) = \frac{1}{\nu^2}S(\nu)$. By multiplying by the diagonal $N \times N$ matrix $T = diag(\sqrt{\omega_k})$, this eigenvalue problem boils down to:

$$\left(\mathcal{V}^{-2} - ww^T\right) X(\nu) = \frac{1}{\nu^2}X(\nu), \qquad w = diag\left(\frac{\sqrt{\omega_k}}{v_k}\right) = \sqrt{\omega}\mathcal{V}^{-1},\ X(\nu) = TS(\nu). \quad (15)$$

The eigenvalue problem is known to possess numerous "good properties" [46]; in particular, since the components of w never vanish, the interlacing repartition holds,

$$0 < v_1 < \nu_1 < v_2 < \nu_2 < ... < v_N < \nu_N \notin (0, 1].$$

The biggest value ν_N stands for the discrete part of the spectrum [12] and since equation (10) is mass-preserving, it displays a degeneracy at infinity which leads to the particular solutions 1 and $z - v$ of (10). Finally, the usual normalization of the N eigenvectors is:

$$\sum_{\ell=1}^{N} \omega_\ell \Big(\varphi(\nu_k, v_\ell) + \varphi(\nu_k, -v_\ell)\Big) = 1, \qquad k \in \{1, ..., N\}. \quad (16)$$

The last step is to derive the WB Godunov scheme for the "localized problem" (5); this proceeds according to the roadmap presented in [26,29]. Such a scheme aims at computing a piecewise-constant approximation of $f(t, z, v)$, solution of the Cauchy problem for (9):

$$\forall j, n \in \mathbb{Z} \times \mathbb{N}, \qquad f_j^n(\pm v_k) \simeq f(t^n = n\Delta t, z_j = j\Delta z, \pm v_k),\ v_k \in \mathcal{V}.$$

The standard finite-volume approach [20] proceeds by integrating the localized equation (5) on $C_j \times [t^n, t^{n+1}]$ and invoke the divergence theorem: the method is completely determined once the numerical flux function is known. In the Godunov setting, the numerical flux consists in computing the exact solution of elementary Riemann problems located at each interface separating adjacent control cells C_j and C_{j+1}: see Figure 3 in [29].

Following again [26], one derives the 2 matrices which allow to compute the interface values to be inserted in the upwind discretization. The main difference with the preceding setting is that these "transfer matrices" now depend on position and time through the piecewise approximation of $\partial_z S$. Define a piecewise constant approximation of $S(t, z)$ solution of (3),

$$\forall j, n \in \mathbb{Z} \times \mathbb{N}, \qquad S_j^n \simeq S(t^n = n\Delta t, z_j = j\Delta z),$$

the natural piecewise constant approximation of $\partial_z S$ is defined on the staggered grid:

$$\forall j, n \in \mathbb{Z} \times \mathbb{N}, \qquad (\partial_z S)_{j+\frac{1}{2}}^n := \frac{1}{\Delta z}(S_{j+1}^n - S_j^n) \simeq \partial_z S(t^n, z_{j+\frac{1}{2}}).$$

Clearly, the value $(\partial_z S)_{j+\frac{1}{2}}^n$ is to be inserted in place of σ at each interface where a forward-backward problem for (10) must be solved in order to compute the WB interface values: the following notation is therefore convenient,

$$\forall j, n \in \mathbb{Z} \times \mathbb{N}, \qquad \sigma_{j+\frac{1}{2}}^n = \frac{1}{\Delta z}(S_{j+1}^n - S_j^n) = (\partial_z S)_{j+\frac{1}{2}}^n, \quad (17)$$

and one is led to compute transfer matrices which depend on $\sigma_{j+\frac{1}{2}}^n$ at each interface. The representation (11) suggests the following approximation of $\bar{f}$ denoted by $\tilde{f}$, for $z \in [0, \Delta z]$:

$$\forall k \in \{1, ..., N\}, \qquad \tilde{f}(z, \pm v_k) \simeq \alpha + \beta\left((\frac{2}{3}\sigma - 1)z \mp v_k\right) + E(z, \pm v_k, \nu),$$

where E stand for a finite superposition of the exponentially damped modes,

$$E(z,v,\nu)=\sum_{\ell=1}^{N-1}\left(A_\ell\frac{\exp(-z/\nu_\ell)}{1-v/\nu_\ell}+B_\ell\frac{\exp(z/\nu_\ell)}{1+v/\nu_\ell}\right). \tag{18}$$

Since the convection terms are linear, the Godunov scheme for (9) reads:

$$\left\{\begin{array}{l} f_j^{n+1}(v_k)=f_j^n(v_k)-v_k\dfrac{\Delta t}{\Delta z}\left(f_j^n(v_k)-\tilde f_{R,j-\frac12}(v_k)\right),\\ f_j^{n+1}(-v_k)=f_j^n(-v_k)+v_k\dfrac{\Delta t}{\Delta z}\left(\tilde f_{L,j+\frac12}(-v_k)-f_j^n(-v_k)\right),\end{array}\right. \tag{19}$$

where the left/right states $\tilde f_{L,j+\frac12}(-\mathcal{V})/\tilde f_{R,j-\frac12}(\mathcal{V})$ are deduced from the previous numerical approximation of the steady-state curves (10). For the left-side state located at $z_{j+\frac12}$,

$$\tilde f_{L,j+\frac12}(-v_k)=\alpha+\beta v_k+E(0,-v_k,\nu),$$

with the corresponding set of coefficients α, β, $\mathbf{A}=\{A_1,A_2,...A_{N-1}\}$ and $\mathbf{B}=\{B_1,B_2,...B_{N-1}\}$ as written in (18) computed at $z_{j+\frac12}$, and the right-side state located at $z_{j-\frac12}$,

$$\tilde f_{R,j-\frac12}(v_k)=\alpha+\beta\left((\frac23\sigma-1)\Delta z-v_k\right)+E(\Delta z,v_k,\nu).$$

In order not to have to treat with a matrix containing both $\exp(\Delta z/\nu_\ell)>1$ and $\exp(-\Delta z/\nu_\ell)<1$ terms, the $N-1$ coefficients $\mathbf{B}$ are rescaled like: $B_\ell\to B_\ell\exp(\Delta z/\nu_\ell)$. This leads to:

$$M_{j+\frac12}^n\begin{pmatrix}\boldsymbol{A}\\ \alpha\\ \boldsymbol{B}\\ \beta\end{pmatrix}=\begin{pmatrix}f_j^n(\mathcal{V})\\ f_{j+1}^n(-\mathcal{V})\end{pmatrix}\in\mathbb{R}^{2N}, \tag{20}$$

where the $2N\times 2N$ matrix $M_{j+\frac12}^n$ reads for $\nu:=\{\nu_1,\nu_2,...,\nu_{N-1}\}\in(0,1)^{N-1}$,

$$M_{j+\frac12}^n=\begin{pmatrix}\left(1-\mathcal{V}\otimes\nu^{-1}\right)^{-1} & 1_{\mathbb{R}^N} & \left(1+\mathcal{V}\otimes\nu^{-1}\right)^{-1}\exp(-\frac{\Delta z}{\nu}) & -\mathcal{V}\\ \left(1+\mathcal{V}\otimes\nu^{-1}\right)^{-1}\exp(-\frac{\Delta z}{\nu}) & 1_{\mathbb{R}^N} & \left(1-\mathcal{V}\otimes\nu^{-1}\right)^{-1} & (\frac23\sigma_{j+\frac12}^n-1)\Delta z+\mathcal{V}\end{pmatrix}.$$

Completeness properties established at the continuous level [8,12,14,37] suggest that each matrix $M_{j+\frac12}^n$ is invertible. By defining the complementary matrix,

$$\tilde M_{j+\frac12}^n=\begin{pmatrix}\left(1-\mathcal{V}\otimes\nu^{-1}\right)^{-1}\exp(-\frac{\Delta z}{\nu}) & 1_{\mathbb{R}^N} & \left(1+\mathcal{V}\otimes\nu^{-1}\right)^{-1} & (\frac23\sigma_{j+\frac12}^n-1)\Delta z-\mathcal{V}\\ \left(1+\mathcal{V}\otimes\nu^{-1}\right)^{-1} & 1_{\mathbb{R}^N} & \left(1-\mathcal{V}\otimes\nu^{-1}\right)^{-1}\exp(-\frac{\Delta z}{\nu}) & \mathcal{V}\end{pmatrix},$$

one observes that, for any $j\in\mathbb{Z}$, the interface values in (19) are given by:

$$\begin{pmatrix}\tilde f_{R,j+\frac12}(\mathcal{V})\\ \tilde f_{L,j+\frac12}(-\mathcal{V})\end{pmatrix}=\tilde M_{j+\frac12}^n\ (M_{j+\frac12}^n)^{-1}\begin{pmatrix}f_j^n(\mathcal{V})\\ f_{j+1}^n(-\mathcal{V})\end{pmatrix}. \tag{21}$$

A big difference with the schemes formerly studied in [26,29] lies in the fact that here, both matrices $M_{j+\frac12}^n$ and $\tilde M_{j+\frac12}^n$ depend on space and time through the value of $(\partial_z S)_{j+\frac12}^n$ (see

[27,28] for the analogous situation in the special case where $v \in \{-1,1\}$ only). Consequently, it isn't possible to compute the product $\tilde{M}^n_{j+\frac{1}{2}}\ (M^n_{j+\frac{1}{2}})^{-1}$ once for all as a pre-processing step before starting the time-marching iterations. The easiest way out is to invert a linear system (20) at each interface in order to obtain the set of coefficients $(\alpha, \mathbf{A}, \beta, \mathbf{B}) \in \mathbb{R}^{2N}$. However, there exists a cheap way of computing each inverse matrix $(M^n_{j+\frac{1}{2}})^{-1}$, based on the *Sherman-Morrison formula* [33]: see especially Remark 3 in the forthcoming §3.2.

Remark 1 *(well-balanced boundary conditions) Usually the kinetic model (9) is set in a bounded domain, say $z \in [0,L]$, with specular boundary boundary conditions on each border of the computational interval. Therefore, in a well-balanced framework, one must implement both the specular reflexion and the localized source term on these boundaries: see Figure 2.1 in [28] for an illustration in the simpler context of a 2×2 discrete model. However, since the parabolic equation governing the chemo-attractant concentration (3) is supplemented by Neumann conditions $\partial_z S = 0$ in $z = 0$, $z = L$, the implementation of boundary data is somewhat simplified. Let's compute the left boundary condition in $z = 0$: at each time step t^n, one is given outcoming kinetic densities $f^n_{j=1}(-\mathcal{V})$ by means of the upwind/Godunov scheme (19); from these N values, one deduces the specularly reflected ones denoted by $f^n_{j=0}(\mathcal{V}) = f^n_{j=1}(-\mathcal{V})$. Observe that, in order to take fully into account for the source term located in $j = \frac{1}{2}$, one has to use the modified vector $\tilde{f}^n_{R,j=\frac{1}{2}}(\mathcal{V})$ which satisfies:*

$$\begin{pmatrix} \tilde{f}_{R,\frac{1}{2}}(\mathcal{V}) \\ \tilde{f}_{L,\frac{1}{2}}(-\mathcal{V}) \end{pmatrix} = \tilde{M}^n_{j+\frac{1}{2}}\ (M^n_{j+\frac{1}{2}})^{-1} \begin{pmatrix} f^n_0(\mathcal{V}) \\ f^n_1(-\mathcal{V}) \end{pmatrix} = \tilde{M}\ M^{-1} \begin{pmatrix} f^n_1(-\mathcal{V}) \\ f^n_1(-\mathcal{V}) \end{pmatrix}.$$

To pass from the first to the second equality, one should use the specular reflexion on f and the Neumann condition on S: this last property makes both matrices M and $\tilde{M}$ independent of space and time because $\partial_z S$ vanishes identically on the borders $z = 0$ and $z = L$. The product $\tilde{M}\ M^{-1}$ can still be computed as a pre-processing step. The values $\tilde{f}_{L,\frac{1}{2}}(-\mathcal{V})$ are useless. Numerically, there is no net flux through the boundary:

$$\forall n > 0, \qquad \sum_{\ell=1}^{N} \omega_\ell \Big(f^n_1(\mathcal{V}) - f^n_1(-\mathcal{V}) \Big) = 0.$$

2.3 Numerical results: comparison with time-splitting

In order to test the new algorithm (19), (21), the standard time-splitting scheme is now quickly recalled: it consists in implementing a differently localized equation, (see [25])

$$\partial_t f(t,z,v) + v\partial_z f = \Delta t \sum_{n\in\mathbb{N}} \left(\int_{-1}^{1} \left[\frac{1}{2} + v(\partial_z S.v') \right] f(t,z,v')dv' - f \right) \delta(t - t^n).$$

Since the source term is ignited only at discrete instants $t^n = n\Delta t$, this "time-localization" yields the well-known algorithm:

$$\begin{cases} f_j^{n+\frac{1}{2}}(v_k) = f_j^n(v_k) - v_k \dfrac{\Delta t}{\Delta z} \left(f_j^n(v_k) - f_{j-1}(v_k) \right), \\ f_j^{n+\frac{1}{2}}(-v_k) = f_j^n(-v_k) + v_k \dfrac{\Delta t}{\Delta z} \left(f_{j+1}(-v_k) - f_j^n(-v_k) \right), \end{cases}$$

for the transport step and, with obvious notation,

$$f_j^{n+1}(\pm\mathcal{V}) = \exp(-\Delta t) f_j^{n+\frac{1}{2}}(\pm\mathcal{V}) + (1 - \exp(-\Delta t)) \left(\frac{\rho_j^{n+\frac{1}{2}}}{2} \pm \mathcal{V}(\partial_z S)^n_j J_j^{n+\frac{1}{2}} \right),$$

for the tumbling step. Observe that one weakness of such a method is that, in the present context, there is no natural definition of the centered approximation $(\partial_z S)_j^n$: one choice can be to work with a mean value of $\sigma_{j\pm\frac{1}{2}}^n$ (see [47] for other issues with time-splitting algorithms). The second step is exact in case $\partial_z S \equiv 0$ by mass conservation. The numerical test consists in evolving in time an initial kinetic density of the following form:

$$f^0(z,v) = 10\exp\left(-30(v \pm 0.25)^2 - 10(z \mp 0.65)^2\right), \qquad (z,v) \in (-1,1)^2. \qquad (22)$$

The grid parameters have been chosen as $N = 15$ for the Gaussian quadrature (so as to have 30 points in the velocity variable) and 2^6 points in the z variable. The time-step is deduced by the standard CFL condition, that is $0.95\Delta t \leq \Delta z$. Numerical results at time $t = 2.95$ are displayed on Fig. 1 for macroscopic quantities and on Fig. 2 for a precise comparison between kinetic densities obtained by means of (19) and by the standard time-splitting method. The WB scheme (19) is clearly less viscous that the more conventional algorithm; its computational cost is higher too. According to Remark 4.2 in [42], there is no *taxis* (*i.e*

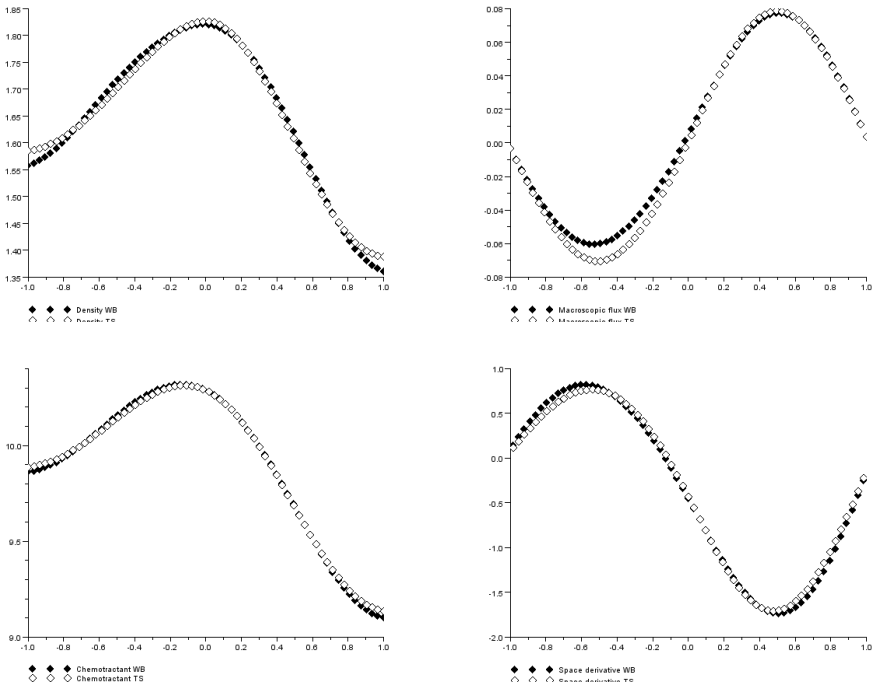

Fig. 1. Comparison of well-balanced (black squares) and time-splitting (white ones) schemes: macroscopic density (top, left), flux (top, right), chemo-attractant (bottom, left), space derivative of chemo-attractant (bottom, right) at time $t = 2.95$).

drift) component in the diffusion approximation of (9). Hence only constant solutions should remain asymptoticly in time when specifying Neumann boundary conditions in complement of (3) and no aggregation phenomenon can occur. From Theorem 1, one deduces that $\beta = 0$ at each interface of the computational grid when numerical steady-state is reached.

Remark 2 *(stabilization in time) The time-splitting scheme stabilizes when the 2 steps are stationary, that is to say, for piecewise-constant kinetic densities for which both the free transport and the tumbling steps are invariant. Clearly, this requirement asks for a density which is constant in z for the first step and constant in v for the relaxation. This is precisely the kind of asymptotic states one expects for (9) according to Remark 4.2 in [42] and this is the reason why few differences appear between both numerical methods. In particular, they admit very similar time-asymptotic (constant) states, see also [18].*

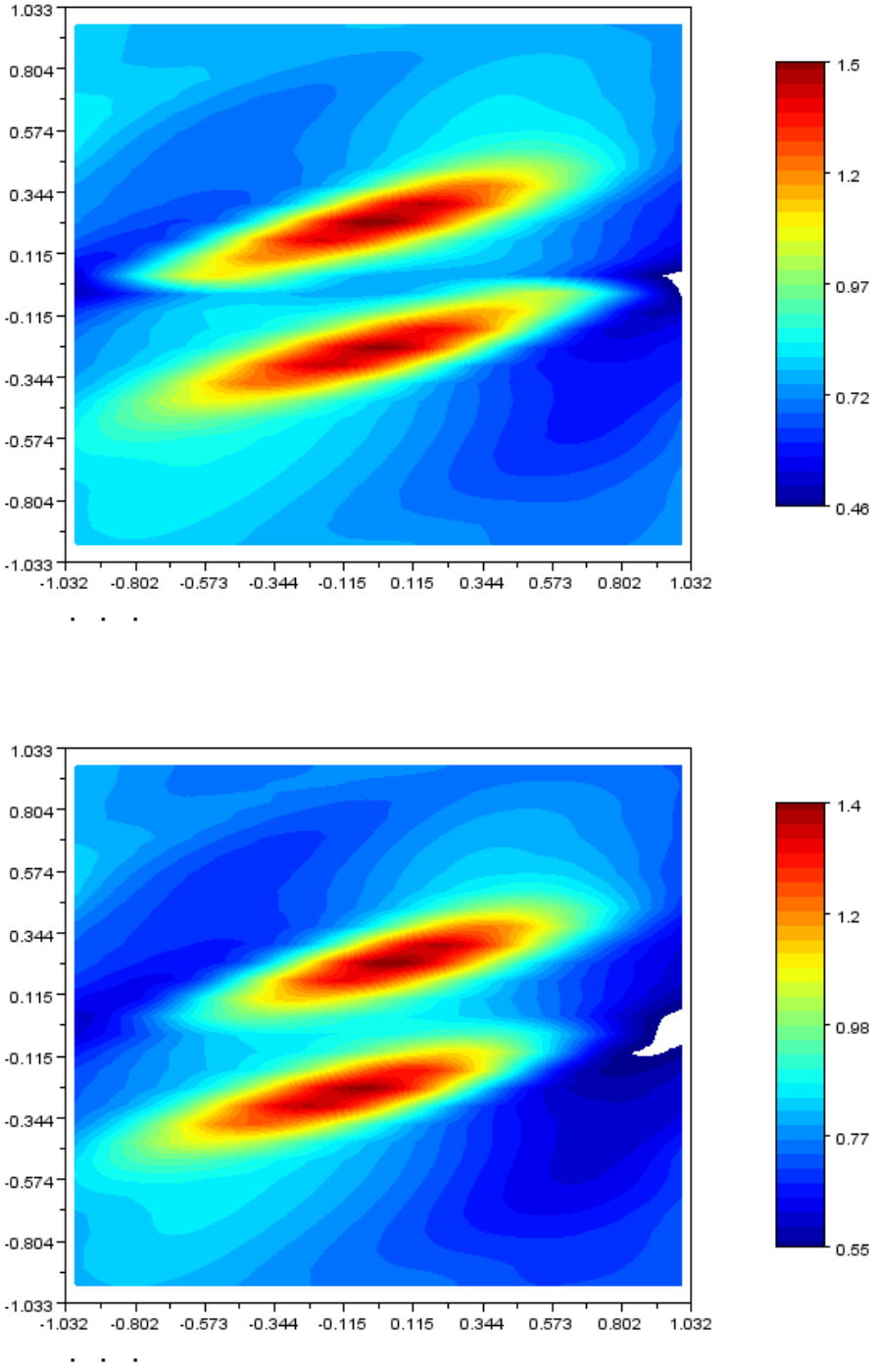

Fig. 2. Kinetic densities for well-balanced (top) and time-splitting (bottom) schemes.

3 Bournaveas-Calvez model: possible concentrations

Since there is no strong gain in setting up well-balanced methods in case the kinetic model stabilizes asymptoticly onto constant states, this section will deal with different equations

leading to more involved (non-constant) asymptotic regimes. Similar studies for simpler 2×2 discrete velocities models have been conducted in *e.g.* [28,40] (see also [11,50]).

3.1 Approximation of a local forward-backward stationary equation

The scope of this section will therefore be the construction of a well-balanced scheme of the type (19) for the mass-conservative model studied in [10], which is of the form originally introduced by Othmer-Dunbar-Alt [41],

$$\partial_t f(t,z,v) + v\partial_z f = \chi(v\partial_z S)\int_{-1}^{1} f(t,z,v')dv' - f\int_{-1}^{1}\chi(v'\partial_z S)dv', \tag{23}$$

and corresponds to the turning probability $p(t,\mathbf{x},\mathbf{v}',\mathbf{v}) = \chi(\mathbf{v}\cdot\nabla S(t,\mathbf{x}))$ in (1). The equation (23) is again obtained by assuming that only $\partial_z S \neq 0$ and following the Ford-Cummings reduction [23] (recalled in the introduction). In [10], there holds $\chi(x) = \Theta(x)$, the Heaviside function; however, here a smooth χ can be preferred,

$$\chi(x) = \frac{1}{2}(1+\tanh(10x)) \in [0,1].$$

The equation on the chemo-attractant substance is again (3) supplemented with Neumann boundary conditions; similarly (23) is endowed with specular reflexion conditions too.

It is possible to adapt the construction of Case's elementary solutions to one-dimensional kinetic models with a velocity-dependent frequency [1,15]; however, in these calculations, it is customary to assume that the collision frequency is even in the v variable. This requirement is generally not met by the model (23) thus another method is proposed hereafter.

Following what has been formerly done in §2.2, the same Gaussian quadrature is used on the interval $v \in (-1,1)$ together with the notation (13). In order to solve the local forward-backward stationary problem for (23) without the Case's "generalized eigenfunctions",

$$v\partial_z \bar{f} = \chi(v\partial_z S)\int_{-1}^{1}\bar{f}(z,v')dv' - \bar{f}\int_{-1}^{1}\chi(v'\partial_z S)dv', \qquad z \in (0,\Delta z),$$

with inflow boundary conditions, a second-order approximation can be considered as follows:

$$\begin{aligned} v_k\frac{\tilde{f}(\Delta z,v_k)-\tilde{f}(0,v_k)}{\Delta z} &= \chi(v_k\sigma)\sum_{\ell=1}^{N}\omega_\ell\left(\frac{\tilde{f}(\Delta z,v_\ell)+\tilde{f}(0,v_\ell)+\tilde{f}(\Delta z,-v_\ell)+\tilde{f}(0,-v_\ell)}{2}\right)\\ &\quad-\left(\frac{\tilde{f}(\Delta z,v_k)+\tilde{f}(0,v_k)}{2}\right)\sum_{\ell=1}^{N}\omega_\ell\Big[\chi(v_\ell\sigma)+\chi(-v_\ell\sigma)\Big]. \end{aligned}$$

For the set of values $0 < v_k \in \mathcal{V}$, a linear system has to be solved at each interface $z_{j+\frac{1}{2}}$:

$$P^n_{j+\frac{1}{2}}\begin{pmatrix}\tilde{f}(0,-\mathcal{V})\\ \tilde{f}(\Delta z,\mathcal{V})\end{pmatrix} = \tilde{P}^n_{j+\frac{1}{2}}\begin{pmatrix}f^n_{j+1}(-\mathcal{V})\\ f^n_j(\mathcal{V})\end{pmatrix}. \tag{24}$$

Introducing the notation $\mathbf{\Omega},\mathcal{W} \in \mathbb{R}^{2N}_+ \times (-1,1)^{2N}$ as the set of weights and points of the Gaussian quadrature introduced at the beginning of §2.2,

$$\mathbf{\Omega} = \{\omega_N,\omega_{N-1},\dots,\omega_2,\omega_1,\omega_1,\omega_2,\dots,\omega_N\},$$

with a similar expression for $\mathcal{W}$ simplifies the expression of the matrices $P^n_{j+\frac{1}{2}}, \tilde{P}^n_{j+\frac{1}{2}}$:

$$P^n_{j+\frac{1}{2}} = \frac{\Delta z}{2}\left(diag(\frac{2|\mathcal{W}|}{\Delta z} + \bar{\chi}) - \chi(\sigma^n_{j+\frac{1}{2}}\mathcal{W}) \otimes \mathbf{\Omega}\right), \quad \bar{\chi} = \sum_{\ell=1}^{N} \omega_\ell \Big[\chi(v_\ell \sigma) + \chi(-v_\ell \sigma)\Big].$$

and:

$$\tilde{P}^n_{j+\frac{1}{2}} = \frac{\Delta z}{2}\left(diag(\frac{2|\mathcal{W}|}{\Delta z} - \bar{\chi}) + \chi(\sigma^n_{j+\frac{1}{2}}\mathcal{W}) \otimes \mathbf{\Omega}\right), \qquad \sigma^n_{j+\frac{1}{2}} = \frac{1}{\Delta z}(S^n_{j+1} - S^n_j).$$

The well-balanced Godunov scheme for (23) is therefore made of the upwind discretization (19) supplemented by (24) with the inflow boundary data $\tilde{f}(0, \mathcal{V}) = f^n_j(\mathcal{V})$, $\tilde{f}(\Delta z, -\mathcal{V}) = f^n_{j+1}(-\mathcal{V})$ at each interface $z_{j+\frac{1}{2}}$. Of course, one can also set up the same kind of numerical method involving a second-order approximation of the local stationary problem for the model (9) studied in the preceding section by means of Case's elementary solutions.

3.2 Rank-one perturbations and Sherman-Morrison formula

The first result states that matrices $P^n_{j+\frac{1}{2}}$ are invertible under a mild condition on Δz:

Lemma 3 *Let $TV(\chi)$ stand for the total variation of χ on $\mathbb{R}$: under the restriction,*

$$v_1 > TV(\chi)\Delta z, \tag{25}$$

the matrix $P^n_{j+\frac{1}{2}}$ is strictly diagonal-dominant and invertible.

This is somewhat a non-resonance condition [3,35] for the semilinear hyperbolic system obtained by approximating by means of the Discrete-Ordinates method a kinetic equation endowed with a continuous velocity variable; roughly speaking (25) forbids the inclusion in the Gaussian quadrature of particles with too small velocities [5].

Proof: It consists in proving the positivity for any $k \in \{1, .., N\}$ of the expression:

$$\left|2\frac{|v_k|}{\Delta z} + \bar{\chi} - \omega_k \chi(\sigma^n_{j+\frac{1}{2}} v_k)\right| - (2 - \omega_k)|\chi(\sigma^n_{j+\frac{1}{2}} v_k)|, \qquad \sigma^n_{j+\frac{1}{2}} = (\partial_z S)^n_{j+\frac{1}{2}}.$$

One sees easily that, since $\chi \geq 0$:

$$\bar{\chi} - \omega_k \chi(\sigma^n_{j+\frac{1}{2}} v_k) = \sum_{\mathbf{\Omega}\setminus\omega_k} \omega_\ell \chi(\sigma^n_{j+\frac{1}{2}} v_\ell) \geq 0.$$

This allows to remove the moduli in the former expression:

$$\begin{aligned} 2\frac{|v_k|}{\Delta z} + \sum_{\mathbf{\Omega}} \omega_\ell \chi(\sigma^n_{j+\frac{1}{2}} v_\ell) - 2\chi(\sigma^n_{j+\frac{1}{2}} v_k) &= 2\frac{|v_k|}{\Delta z} + \sum_{\mathbf{\Omega}} \omega_\ell \left[\chi(\sigma^n_{j+\frac{1}{2}} v_\ell) - \chi(\sigma^n_{j+\frac{1}{2}} v_k)\right] \\ &= 2\frac{|v_k|}{\Delta z} + \sum_{\mathbf{\Omega}} \omega_\ell \int_{\sigma^n_{j+\frac{1}{2}} v_\ell}^{\sigma^n_{j+\frac{1}{2}} v_k} \chi'(s) ds \\ &\geq 2\left(\tfrac{|v_k|}{\Delta z} - TV(\chi)\right). \end{aligned}$$

By the Hadamard Lemma, a strictly diagonal-dominant real matrix is invertible. □

Theorem 2 *Under the non-resonance restriction (25) and with the shorthand notation* $D_\pm = diag(\frac{2|\mathcal{W}|}{\Delta z} \pm \bar{\chi})$*, the matrix product* $(P^n_{j+\frac{1}{2}})^{-1}\tilde{P}^n_{j+\frac{1}{2}}$ *has the explicit expression:*

$$(P^n_{j+\frac{1}{2}})^{-1}\tilde{P}^n_{j+\frac{1}{2}} = \left(D_+^{-1} + \frac{D_+^{-1}[\chi(\sigma^n_{j+\frac{1}{2}}\mathcal{W})\otimes\mathbf{\Omega}]D_+^{-1}}{1-\mathbf{\Omega}\cdot D_+^{-1}\chi(\sigma^n_{j+\frac{1}{2}}\mathcal{W})} \right)\Big(D_- + \chi(\sigma^n_{j+\frac{1}{2}}\mathcal{W})\otimes\mathbf{\Omega}\Big) \qquad (26)$$

Proof: By Lemma 3, (25) ensures invertibility of $P^n_{j+\frac{1}{2}}$; the classical "determinant lemma" yields that:

$$det(D_+ - \chi(\sigma^n_{j+\frac{1}{2}}\mathcal{W})\otimes\mathbf{\Omega}) = det(D_+)[1-\mathbf{\Omega}\cdot D_+^{-1}\chi(\sigma^n_{j+\frac{1}{2}}\mathcal{W})] \neq 0.$$

Since $v_k \neq 0$ for any $k \in \{1,2,\dots,N\}$ and $\chi \geq 0$, the determinant of the diagonal matrix $det(D_+) \neq 0$. By the same calculations, one has the scalar product $\mathbf{\Omega}\cdot D_+^{-1}\chi(\sigma^n_{j+\frac{1}{2}}\mathcal{W}) \neq 1$. One can therefore apply the well-known Sherman-Morrison formula [33] for the explicit computation of the inverse of a rank-one perturbation of any diagonal matrix D:

$$(D+\mathbf{u}\otimes\mathbf{v})^{-1} = D^{-1} - \frac{D^{-1}\mathbf{u}\otimes\mathbf{v}D^{-1}}{1+\mathbf{v}\cdot D^{-1}\mathbf{u}}. \qquad (27)$$

The conclusion of the theorem is reached by inserting $D = D_+$, $\mathbf{u} = -\chi(\sigma^n_{j+\frac{1}{2}}\mathcal{W})$, $\mathbf{v} = \mathbf{\Omega}$ in the Sherman-Morrison expression (27) and then writing $\tilde{P}^n_{j+\frac{1}{2}} = D_- + \chi(\sigma^n_{j+\frac{1}{2}}\mathcal{W})\otimes\mathbf{\Omega}$ as another rank-one perturbation of the diagonal matrix D_-. □

Theorem 2 allows for a sensible reduction of the computational cost for the well-balanced scheme (19), (24). Indeed, the computation of the interface values (24) asks only for a matrix product, and not for an inversion of a linear system.

Remark 3 *One can take advantage of the Sherman-Morrison formula (27) when setting up the well-balanced Godunov scheme (19), (21) involving Case's elementary solutions for the Othmer-Hillen model (9) too. Indeed, by observing that:*

$$M^n_{j+\frac{1}{2}} = \begin{pmatrix} \left(1-\mathcal{V}\otimes\nu^{-1}\right)^{-1} & 1_{\mathbb{R}^N} & \left(1+\mathcal{V}\otimes\nu^{-1}\right)^{-1}\exp(-\frac{\Delta z}{\nu}) & -\mathcal{V} \\ \left(1+\mathcal{V}\otimes\nu^{-1}\right)^{-1}\exp(-\frac{\Delta z}{\nu}) & 1_{\mathbb{R}^N} & \left(1-\mathcal{V}\otimes\nu^{-1}\right)^{-1} & -\Delta z+\mathcal{V} \end{pmatrix} + \frac{2}{3}\Delta z\sigma^n_{j+\frac{1}{2}}\mathbf{a}\otimes\mathbf{b},$$

with $\mathbf{a} = (0,0,...,0,1) \in \mathbb{R}^{2N}$ *and* $\mathbf{b} = (0,...0,1_{\mathbb{R}^N}) \in \mathbb{R}^{2N}$*. Hence* $M^n_{j+\frac{1}{2}}$ *is a rank-one perturbation of the M matrix written in [26] (p. 1999): thus assuming that the inverse* M^{-1} *can be computed before starting the time-marching scheme (19), the formula (27) yields,*

$$(M^n_{j+\frac{1}{2}})^{-1} = M^{-1} - \frac{M^{-1}\mathbf{a}\otimes\mathbf{b}M^{-1}}{\frac{3}{2\Delta z\sigma^n_{j+\frac{1}{2}}} - \mathbf{b}\cdot M^{-1}\mathbf{a}},$$

and then it remains only to multiply by $\tilde{M}^n_{j+\frac{1}{2}}$ *in order to be able to compute efficiently the interface values (21) without inverting any* $2N\times 2N$ *linear system.*

Obviously, the treatment of the specular boundary conditions still follows Remark 1: the effects of the localized tumble term have to be included in the interfaces on both the borders of the computational domain. Indeed, thanks to Neumann conditions $\partial_z S(t,z=0) = 0$, there holds $\chi(v\partial_z S) = \frac{1}{2}$ on the borders and there is no biasing mechanism involved.

In this section, the WB scheme (19), (24) will be tested on the equation (23) posed in $z, v \in (-1,1)^2$ with specular reflexion on the borders, similar initial data than (22),

$$f^0(z,v) = 5\exp(-20(v \pm 0.45)^2 - 10(z \mp 0.65)^2),$$

and an identical computational grid than in §2.3. However it is possible to select a set of coefficients α, β, D in (3) in order to make such a problem very delicate to stabilize in time, thus illustrating the richness of behaviors which can be described by such a kinetic model. By selecting $\alpha = 30$, $\beta = 3$, $D = 15$ and $N = 20$ (40 points in the velocity variable), one

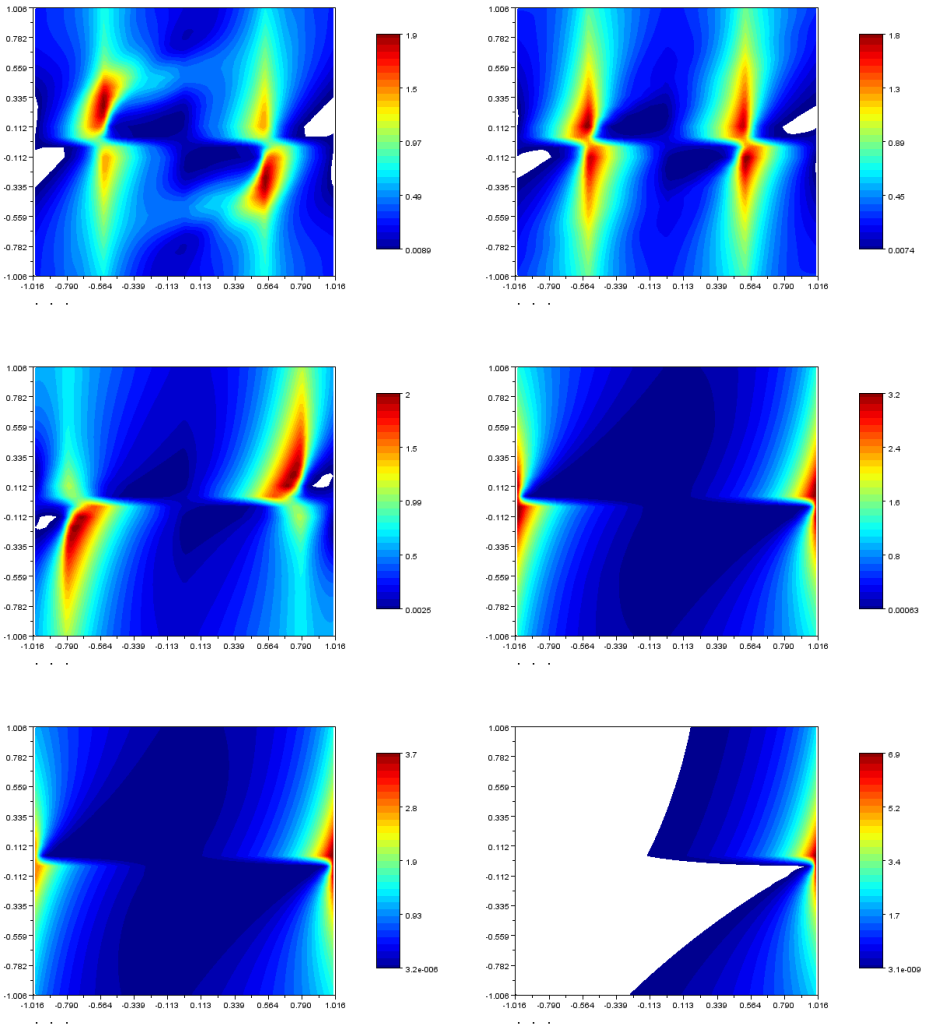

Fig. 3. Kinetic densities in the plane z, v at times $t = 1, 2, 6, 9, 252, 310$.

can set up the time-marching scheme (19), (24). The computational grid is determined by 2^7 points griding uniformly $z \in (-1,1)$ and the time-step is given by the CFL number, here 0.95. It will prove interesting to study the residues r^n, $n \in \mathbb{N}$, which are defined by:

$$r^n := \left\| \sum_{\mathbf{\Omega}} \omega_k |f_j^{n+1}(v_k) - f_j^n(v_k)| \right\|_{\ell^2}.$$

Numerical results for the numerical approximation of the kinetic density $f(t,z,v)$ generated by the WB Godunov scheme (19), (24) are shown on Fig. 3. One can see that the time evolution of the system is quite interesting because it reveals 4 clearly different steps:

(1) a first concentration of cells in $z = \pm\frac{1}{2}$, close to the centers of the initial Gaussian repartitions, makes the residues decay in a monotonic manner (up to time $t \simeq 2$).
(2) this first aggregation is unstable, residues grow and cells move to accumulate on both the borders $z = \pm 1$ of the computational domain. This process seems to be more stable as residues decayed very strongly (up to time $t \simeq 16$).
(3) surprisingly, residues start to increase again albeit very slowly despite the changes in the kinetic density are nearly invisible. However, the important quantity to be scrutinized during this phase is the macroscopic flow, which has a positive sign despite its smallness.
(4) residues grew up again to values of the order of those around $t \simeq 2$; the positive macroscopic flow pushed all the cells onto the right border ($z = 1$) of the computational domain (at time $t \simeq 280$). The system has finally reached steady-state around $t \simeq 320$ and the residues are now stalling at a global minimum level. The macroscopic flow oscillates very close to the zero-machine level without having a definite sign (contrary to the former step).

This type of evolution, suggesting that the time-dependent problem seeks to equilibrate the differential and integral terms in the kinetic equation with vanishing macroscopic flow, is quite reminiscent of what has been found in [28] (see Section 5.3) for a simpler Greenberg-Alt discrete velocity model: the well-balanced scheme seeks possible stationary regimes, more and more distant from the initial kinetic density f^0, which make the macroscopic flux decrease. Clearly, conventional time-splitting schemes cannot stabilize correctly in long time on such delicate problems because of their excessive numerical viscosity. On Fig. 4,

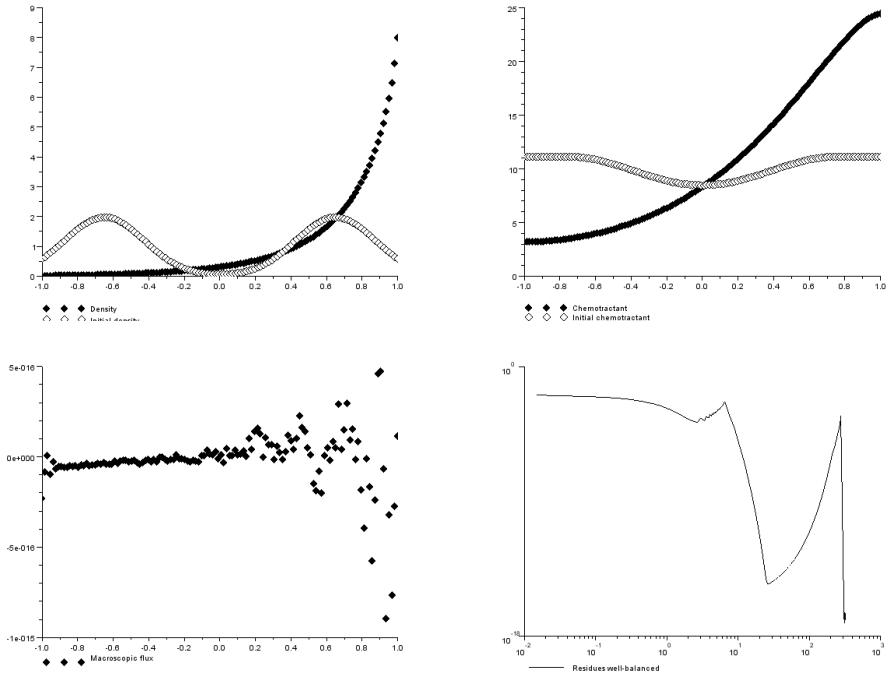

Fig. 4. Macroscopic density (top, left), chemo-attractant (top, right), flux (bottom, left) and residues (bottom, right) at time $t = 320$) for the WB scheme (19), (24).

the stationary numerical macroscopic quantities ρ and J are displayed. It is actually challenging to reach a steady-state with such a big space derivative on the first moment ρ while maintaining the second moment J this close to the zero-machine level after so many itera-

tions in time. Hence it is necessary to be very careful when seeking to compute stationary aggregation patterns for chemotaxis kinetic models by iterating conventional schemes up to convergence. A similar conclusion has been reached independently by Natalini and Ribot [40] when trying to stabilize in large time a 2-velocity kinetic model. For completeness, a comparison between the results of the new WB scheme and the ones generated by means of a classical time-splitting scheme at time $t = 10$ are shown on Fig. 5: cells accumulate on the wrong side of the domain, the macroscopic flux is quite big with a shape similar to what has been reported earlier in [40] and residues stall. The WB scheme shows a neat superiority.

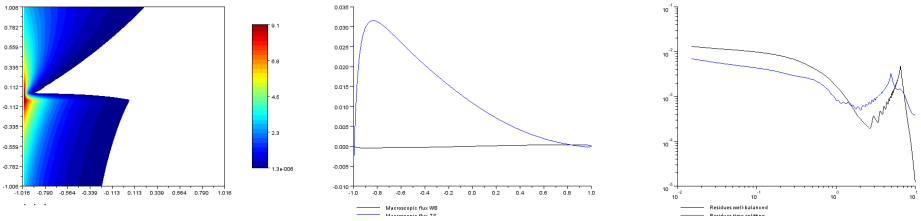

Fig. 5. Kinetic density (left), macroscopic flux (middle) and residues (bottom, right) at time $t \simeq 10$ for the time-splitting scheme (blue curves, WB scheme is in black).

4 Conclusion and outlook

A general methodology for the construction of well-balanced schemes for the numerical approximation of one-dimensional kinetic models of chemotaxis dynamics has been presented. It relies either on the formalism of Case's elementary solutions (especially the simplest models presented in [42]), or on a second-order approximation of the forward-backward problem for the steady-state equation (for more sophisticated models like for instance the ones in [10,41]). Both approaches can be implemented efficiently (*e.g.* without inverting matrices inside the time-marching process) by taking advantage of the classical Sherman-Morrison formula which gives an analytic expression of the inverse of a rank-one perturbation.

This method can be extended in a direct manner at least in 2 directions:

(1) General kinetic models of chemotaxis [16,18]: another widely used mass-preserving model, different from (23), reads

$$\partial_t f(t,z,v) + v\partial_z f = \int_{-1}^{1} \phi(v'\partial_z S) f(t,z,v')dv' - 2\phi(v\partial_z S)f,$$

with ϕ a smooth function related to γ in (2). By following carefully the calculation in §3.1, one arrives to a $2N \times 2N$ transfer matrix of the type,

$$Q^n_{j+\frac{1}{2}} = \frac{\Delta z}{2}\left(diag(\frac{2|\mathcal{W}|}{\Delta z} + 2\phi(\mathcal{W}\sigma^n_{j+\frac{1}{2}})) - (\mathbf{\Omega}\phi(\sigma^n_{j+\frac{1}{2}}\mathcal{W})) \otimes \mathbf{1}_{\mathbb{R}^{2N}} \right),$$

which is still a rank-one perturbation of an easily invertible diagonal matrix. Observe that a rescaling of the "tumbling term" by a factor $\frac{1}{\epsilon}$ reduces to a multiplication of ϕ by the same factor thus the invertibility of $Q^n_{j+\frac{1}{2}}$ asks for a more restrictive condition on ϵv_1 instead of (25). In this case, the Sherman-Morrison formula [33] will provide again a result like Theorem 2. The general models studied in [16,43] read:

$$\partial_t f(t,z,v) + v\partial_z f(t,z,v) = \int_{-\frac{1}{2}}^{\frac{1}{2}} T(v,v')f(t,z,v') - T(v',v)f(t,z,v)dv'. \qquad (28)$$

They don't lead to transfer matrices which are rank-one perturbations; however, their inverse may be computed by means of the *Woodbury formula* (see again [33]).

(2) Inclusion of the time-derivative $\partial_t S$: it can be considered interesting to include inside the kinetic model an information about the time-evolution of the chemo-attractant substance at the location z. This is explained for instance on pages 1241/1243 of [42], where the following expression of the turning rate in (2) is studied:

$$\gamma(t,x,v) = \exp\left(-\frac{ab}{(b+S)^2}(\partial_t S + v\partial_z S)\right), \qquad a,b \in \mathbb{R}^+.$$

The equality $\exp(a+b) = \exp(a)\exp(b)$ allows to separate the effects of the time and space derivative of $S(t,z)$. Hence, it is possible to factorize the term $\exp(-\frac{ab\partial_t S}{(b+S)^2})$ in front of a right-hand side written like the one in (28), to which the method of §3 can be applied. The exponential term related to $\partial_t S$ is therefore a *stiffness coefficient* which can be handled exactly like the variable opacity coefficient in §3.3 of [26] (see also the variable Knudsen numbers in [29]). However, one real issue is that there is no natural definition of the numerical approximation of $\partial_t S$ at the interfaces $z_{j+\frac{1}{2}}$ of the computational grid thus only mean values can be used.

Lastly, the extension to a multi-dimensional framework can be performed by following the guidelines already used for nonlinear parabolic equations in [20] (see also the conclusion in [29]) because a finite volumes scheme stems on the computation of *one-dimensional numerical fluxes* in the normal directions of the borders of each computational cell.

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