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Time-asymptotic convergence rates towards the discrete evolutionary stable distribution

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This paper is concerned with the discrete dynamics of an integro-differential model that describes the evolution of a population structured with respect to a continuous trait. Various time-asymptotic convergence rates towards the discrete evolutionary stable distribution (ESD) are established. For some special ESD satisfying a strict sign condition, the exponential convergence rates are obtained for both semi-discrete and fully discrete schemes. Towards the general ESD, the algebraic convergence rate that we find is consistent with the known result for the continuous model.

Keywords: Selection dynamics; evolutionary stable distribution; relative entropy; convergence rates.

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1. Introduction

This paper is a continuation of the work in Ref. 14 investigating an entropy satisfying finite volume method for a direct competitive selection model. The

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mathematical problem is given by

$$\partial_t f(t,x) = \left(a(x) - \int_X b(x,y) f(t,y) dy \right) f(t,x), \quad \text{for } t > 0, \ x \in X, \tag{1.1a}$$

$$f(0,x) = f_0(x), \quad x \in X. \tag{1.1b}$$

Equation (1.1a) is an integro-differential model that describes the evolution of a population of density $f(t,x)$ structured with respect to a continuous trait x. The space of traits X can be fairly general in the sense that it is typically a subset of $\mathbb{R}^d$ but not necessarily a regular one (see p. 497 in Ref. 13). Considering (1.1) alone, we naturally take a smooth domain of $\mathbb{R}^d$. In this model, a is the reproduction rate for an individual alone (without competition with other individuals); and $b > 0$ corresponds to the interaction between individuals which we assume here to be only competitive. The total reproduction rate of each individual is thus determined by its trait and the environment through the selective pressure $a(x) - \int_X b(x,y) f(t,y) dy$, leading therefore to selection.

Existence and stability of regular or measure-valued solutions for Eq. (1.1) are known, provided that the coefficients have enough regularity (see Refs. 9, 13 and 20). Together with variants, it has been investigated much in the literature; see e.g. Refs. 2, 4, 11, 12 and 21. In addition, Eq. (1.1a) (with an additive mutation term) can be derived from stochastic models of finite population (see Refs. 5, 6 and 10), and there is a vast literature (see e.g. Refs. 1, 3, 7, 8 and 15–19) on the study of the combining effects of both selection and mutation on the population dynamics. The singular steady-state solutions of the selection model correspond to highly concentrated population densities of the form of well-separated Dirac masses, which have been shown to happen asymptotically in the model with mutation (see e.g. Refs. 3, 7 and 15–19). More complex models are certainly more realistic such as random environments, spatial effects, noncompetitive interactions, which should lead to quite different asymptotic behavior.

The mathematical problem (1.1) is interesting from the point of view of large-time behavior. Natural questions appear, such as does the population really converge to an equilibrium? Is this equilibrium an evolutionarily stable strategy or distribution (ESS or ESD)? Does this limit depend on the initial population distribution? A definite answer to these questions has been provided in Ref. 13 under additional assumptions on b,

$$\forall\, g \in L^1(X)\backslash\{0\}, \quad \iint b(x,y) g(x) g(y) dx dy > 0, \tag{1.2}$$

and b is assumed to satisfy some symmetry, for instance,

$$\forall\, x, y \in X, \quad b(x,y) = b(y,x), \tag{1.3}$$

so that solutions of (1.1) then converge to the unique ESD at rate $O(\log t/t)$ for some proper initial data. Note that the symmetry assumption (1.3) means that the competition $b(x, y)$ between an individual with trait y and an individual with trait x is the same as the competition $b(y, x)$ between x and y. This assumption together with (1.2) is directly connected to the stability of the ESD. It is not strictly satisfied for some biological systems.

We recall the notion of ESD as used for instance in Ref. 13: the measure $\tilde{f}$ is called an ESD for model (1.1a) if

$$\forall\, x \in \operatorname{supp} \tilde{f}, \quad 0 = a(x) - \int_X b(x, y)\tilde{f}(y)dy, \tag{1.4a}$$

$$\forall\, x \in X, \quad 0 \geq a(x) - \int_X b(x, y)\tilde{f}(y)dy. \tag{1.4b}$$

The proof of global convergence to the ESD in Ref. 13 relies on a Lyapunov functional which has been proved to exist under the condition of positivity of a certain operator. The functional has the following form

$$F(t) = \int_X \left[\tilde{f}(x) \log \frac{\tilde{f}(x)}{f(t, x)} + f(t, x) - \tilde{f}(x)\right] dx, \tag{1.5}$$

is consequently dissipating in time and serves as a relative entropy. The particular sign property (1.4) featured by the ESD is essential for the global convergence.

For different combinations of model parameters, one can expect to see a uniform trait distribution or patterns produced from the selection dynamics. It is usually difficult to predict between these two alternatives. Hence numerical methods are useful tools to evaluate the ESD predicted by the model.

The finite volume scheme investigated in Ref. 14 is shown to produce numerical solutions with satisfying long-time selection dynamics. This is achieved through a proper discretization, so that the numerical solution

$$f_\alpha^n \sim \frac{1}{h^d} \int_{I_\alpha} f(n\Delta t, x)dx,$$

approximates $f(t_n, x)$ over the cell I_α indexed by $\alpha \in \Lambda \subset \mathbb{Z}^d$, and the discrete relative entropy

$$F^n = \sum_\alpha \left(\tilde{f}_\alpha \log\left(\frac{\tilde{f}_\alpha}{f_\alpha^n}\right) + f_\alpha^n - \tilde{f}_\alpha\right) h^d,$$

satisfies the entropy dissipation inequality

$$F^{n+1} - F^n \leq -\frac{1}{2}\Delta t\|f^n - \tilde{f}\|_b^2.$$

This implies the convergence of f^n toward the discrete ESD. One may wonder what would be the time-asymptotic convergence rate, such an inquiry motivates therefore the present work.

1.1. *Assumptions and main results*

For simplicity, we only consider the one-dimensional case with $X = [-1, 1]$. We partition X into subcells $I_j = [x_{j-1/2}, x_{j+1/2}]$, $j = 1, \ldots, N$, for a uniform mesh of size $h = 2/N$ so that $x_{j-1/2} = x_{1/2} + (j-1)h$ with $x_{1/2} = -1$, $x_{N+1/2} = 1$. We consider the following semi-discrete scheme

$$\frac{d}{dt} f_j = f_j \left(\bar{a}_j - h \sum_{i=1}^{N} \bar{b}_{ji} f_i \right), \quad j = 1, \ldots, N, \tag{1.6}$$

where

$$\bar{a}_j = \frac{1}{h} \int_{I_j} a(x) dx, \quad \bar{b}_{ji} = \frac{1}{h^2} \int_{I_i} \int_{I_j} b(x, y) dx dy, \tag{1.7}$$

and the numerical solution $f_j(t)$ approximates the cell average of the exact solution f,

$$\bar{f}_j(t) = \frac{1}{h} \int_{I_j} f(t, x) dx.$$

Set

$$s_j[f] = \bar{a}_j - h \sum_{i=1}^{N} \bar{b}_{ji} f_i,$$

then the nonlinear dynamical system Eq. (1.6) admits many steady states satisfying

$$\tilde{f}_j s_j[\tilde{f}] = 0, \quad j = 1, \ldots, N.$$

Of special interest is the discrete ESD $\tilde{f} = \{\tilde{f}_j\}$, which is defined as:

$$\forall\, j \in \{1 \le i \le N, \tilde{f}_i \ne 0\}, \quad s_j[\tilde{f}] = 0, \tag{1.8a}$$

$$\forall\, j \in \{1 \le i \le N, \tilde{f}_i = 0\}, \quad s_j[\tilde{f}] \le 0, \tag{1.8b}$$

and is conjectured to be the limit of the solution provided the initial data $f_j(0) > 0$ for all $j = 1, 2, \ldots, N$.

From the basic assumptions at the continuous level one may derive similar assumptions at the discrete level (see Ref. 14):

$$|\bar{a}_j| \le \|a\|_{L^\infty}, \quad \{1 \le j \le N, \bar{a}_j > 0\} \ne \emptyset; \tag{1.9a}$$

$$0 < b_f \le \bar{b}_{ji} \le \|b\|_{L^\infty} \quad \text{and} \quad \bar{b}_{ji} = \bar{b}_{ij}, \quad \text{for } 1 \le i, \ \ j \le N; \tag{1.9b}$$

$$\sum_{j=1}^{N} \sum_{i=1}^{N} \bar{b}_{ji} g_i g_j > 0 \quad \text{for any } g_j \text{ such that} \quad \sum_{j=1}^{N} |g_j|^2 \ne 0. \tag{1.9c}$$

It is shown that these assumptions ensure the existence and uniqueness of the ESD, as defined by (1.8), in Ref. 14.

Given the positivity assumption, $\bar{b}_{ij}$ induces a discrete weighted norm denoted by $\|\cdot\|_b$:

$$\|g\|_b = \left(h^2 \sum_{i,j=1}^{N} \bar{b}_{ji} g_j g_i \right)^{\frac{1}{2}}. \tag{1.10}$$

We also use the discrete l^p-norm

$$\|g\|_p = \left(\sum_{j=1}^{N} |g_j|^p h \right)^{1/p}.$$

Those norms are related through

$$\sqrt{h\lambda_{\min}} \|g\|_2 \le \|g\|_b \le \sqrt{h\lambda_{\max}} \|g\|_2, \tag{1.11}$$

where $\lambda_{\min}$ ($\lambda_{\max}$) denotes the smallest (largest) eigenvalue of $B = (\bar{b}_{ji})_{N\times N}$ and $\|B\|_2 = \lambda_{\max}$.

Lemma 1.1. *One has*

$$2b_f \le h\lambda_{\max} \le 2\|b\|_{L^\infty}, \quad \lambda_{\max} \ge \lambda_{\min} > 0.$$

Proof. By the positivity of the matrix B, the upper bound can be obtained through the trace of B,

$$\lambda_{\max} \le \mathrm{Tr}(B) = \sum_{i=1}^{N} \bar{b}_{ii} \le N\|b\|_{L^\infty} = \frac{2}{h}\|b\|_{L^\infty}.$$

As for the lower bound, we use

$$\lambda_{\max} = h^{-1} \sup_{\{\|g\|_2 = 1\}} \|g\|_b^2 \ge \frac{h}{2} \sum_{i,j} \bar{b}_{ij} \ge \frac{h}{2} N^2 b_f = 2h^{-1} b_f,$$

by choosing $g = (1/\sqrt{2}, \ldots, 1/\sqrt{2})$.

Finally as B is strictly positive then $\lambda_{\min} > 0$. □

Remark 1.1. The size of $h\lambda_{\max}$ is bounded from above and below, but $h\lambda_{\min}$ can be much smaller as the mesh size vanishes.

We call the ESD a strict ESD if it also satisfies the following strict sign condition,

$$s_j[\tilde{f}] < 0 \quad \text{for } j \in \{i : \tilde{f}_i = 0\}. \tag{1.12}$$

We shall prove that the strict ESD is both linearly and nonlinearly stable, with perturbations decaying to zero exponentially in time. To precisely state the main results, we use the following notation,

$$I = \{j \mid \tilde{f}_j = 0 \text{ and } s_j < 0\}, \quad I^c = \{j, 1 \le j \le N\} - I, \tag{1.13}$$

and

$$s = \min_{j \in I}(-s_j[\tilde{f}]) > 0, \quad f_m = \min_{j \in I^c} \tilde{f}_j > 0.$$

In the sequel we also use

$$\mu = h f_m \lambda_{\min}, \quad r = \min\{s, \mu\},$$

to quantify the exponential decay of the perturbations.

The result for the semi-discrete scheme is summarized in the following.

Theorem 1.1. *Assume* (1.9) *holds. Let* $f_j(t)$ *be the solution to the semi-discrete scheme* (1.6), *associated with the strict ESD. Then there exists* $\delta^* > 0$ *such that for any* $\delta \in (0, \delta^*)$ *if*

$$\|f(0) - \tilde{f}\|_2 \le \delta,$$

then

$$\|f(t) - \tilde{f}\|_p \le C(1+t)^{\xi} e^{-rt}, \quad \xi = 1_{\{s=\mu\}},$$

where $1 \le p \le 2$,

$$\delta^* = \frac{\alpha^2 \min\{1, \sqrt{f_m}\}}{\sqrt{2}\max\{1, \alpha\}}, \quad \alpha = \sqrt{\frac{r}{\|b\|_{L^\infty}} + \frac{\|\tilde{f}\|_1}{2}} - \sqrt{\frac{\|\tilde{f}\|_1}{2}},$$

and C *may depend on the parameters and the norms of the initial data but not explicitly on* N *or* h.

Remark 1.2. While none of the constants in the previous result depend explicitly on the mesh size, most of them depend on it implicitly. For instance s is not in general bounded from below uniformly in h and in most cases one can actually prove that $s \to 0$ as $h \to 0$. This is because the limit $\tilde{f}$ should be an ESD for the continuous model, therefore $s[\tilde{f}]$ is a smooth function of x. The extension of I is now the set of x where the measure $\tilde{f}$ vanishes, that is the complement of the support of $\tilde{f}$. But the function $s[\tilde{f}]$ vanishes on the support of $\tilde{f}$, which is a closed set, and therefore cannot be bounded from below on the complement. The same argument applies to f_m.

As a consequence the exponential convergence is not uniform in h and actually degenerates as $h \to 0$. The same is true for all the exponential convergence results presented here. Only the algebraic rate, Theorem 1.3, is uniform in h.

For the fully discrete scheme

$$\frac{f_j^{n+1} - f_j^n}{\Delta t} = f_j^{n+1}\left(\bar{a}_j - h\sum_{i=1}^{N} \bar{b}_{ji} f_i^n\right), \tag{1.14}$$

the exponential convergence rate toward the strict ESD can still be obtained under some restriction on the time step.

Theorem 1.2. *Assume* (1.9) *holds. Let* f_j^n *be the numerical solution to* (1.14), *associated with the strict ESD*, $\tilde{f} = \{\tilde{f}_j\}$. *If* Δt *satisfies*

$$\Delta t \leq \frac{\min\{s, \mu/2\}}{\|b\|_{L^\infty}^2 \|\tilde{f}\|_1^2},$$

then there exists $\delta^* > 0$ *such that for any* $\delta \in (0, \delta^*)$ *if*

$$\|f^0 - \tilde{f}\|_2 \leq \delta,$$

then for $1 \leq p \leq 2$,

$$\|f^n - \tilde{f}\|_p \leq C(1 + n\Delta t)^\xi \max\{K_s, K_*\}^n, \quad \xi = 1_{\{K_s = K_*\}},$$

where

$$K_s = \frac{1}{\sqrt{1 + 2s\Delta t}}, \quad K_* = \frac{1}{\sqrt{1 + 2\mu\Delta t}} \left(1 + \frac{2\Delta t^2 \|b\|_{L^\infty}^2 \|\tilde{f}\|_1^2}{\sqrt{1 + 2\mu\Delta t}}\right) < 1,$$

and C *may depend on the parameters but not explicitly on* N *or* h.

Remark 1.3. In the above two theorems, r or μ may well approach zero when N tends to ∞. Hence, exponential convergence for the continuous model cannot be deduced from these results and is in fact not expected.

Another objective of this work is to establish an algebraic convergence rate but with parameters uniform in N or h, thus extending the rates known at the limit.

Theorem 1.3. *Assume* (1.9) *with* $b_f = 0$ *holds. Let* f_j^n *be the numerical solution generated from scheme* (1.14) *with positive initial data* $f_j^0 > 0$ *for all* $j = 1, \ldots, N$, *with* $\tilde{f} = \{\tilde{f}_j\}$ *as its associated ESD. If*

$$F^0 := \sum_{j=1}^N \left(\tilde{f}_j \log\left(\frac{\tilde{f}_j}{f_j^0}\right) + f_j^0 - \tilde{f}_j\right) h < +\infty,$$

then

$$\|f^n - \tilde{f}\|_b^2 \leq \frac{2F^0}{n\Delta t},$$

provided that

$$\Delta t \leq \min\left\{\frac{\lambda_{\min}}{\lambda_{\max}[2(\|a\|_{L^\infty} + \|b\|_{L^\infty}\|\tilde{f}\|_1) + 2\lambda_{\max}S(F^0) + \lambda_{\min}S(F^0)]}, \frac{h}{\|b\|_{L^\infty}S(F^0)}\right\},$$

where S *is an explicit nondecreasing, positive function, which we specify in the proof.*

Remark 1.4. When $0 < b_f \leq \bar{b}_{ji}$ is satisfied, the same convergence rate can be obtained under a weaker time step restriction; see Theorem 3.2.

Several techniques are introduced and developed in the proofs of these results.

In the proof of Theorems 1.1 and 1.2 on the exponential convergence, we start with a symmetrization of the system with weight depending on the strict ESD, and then obtain exponential decay of the perturbations using a Lyapunov functional approach, subject to a parameter tuned to allow for the largest possible initial perturbations. Finally the optimal convergence rate is obtained by a refined estimate. In the proof of Theorem 1.3 on the algebraic convergence, we first establish the dissipation inequality of relative entropy, and further show the decreasing property of the dissipation rate, these together ensure the algebraic convergence rate towards the general ESD.

To summarize here, several time-asymptotic convergence rates towards the discrete evolutionary stable distribution (ESD) are established through the following results:

- For the discrete ESD satisfying a strict sign condition, we establish the exponential convergence rate of numerical solutions towards such a strict ESD for both the semi-discrete scheme and the fully discrete scheme. However, the convergence rate is typically mesh-dependent, as a similar result is not expected for the continuous model.
- For general discrete ESD, we prove that numerical solutions of the fully discrete scheme converge towards the discrete ESD at a rate $1/n$, which is faster than the rate $O(\log t/t)$ obtained in Ref. 13 for the continuous model.

Finally, we should point out that the results and the proofs for one dimension can be generalized to a regular domain in arbitrary dimensions. To be more precise, consider $X = [-1,1]^d$, with a structured partition by $I_\alpha = I_{\alpha_1} \times I_{\alpha_2} \times \cdots \times I_{\alpha_d}$, where the definition of every I_{α_i} $(i = 1, 2, \ldots, d)$ is the same as in one-dimensional case, and α denotes the multiple index, which runs over the following index set

$$\Lambda := \{\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_d),\ 1 \leq \alpha_i \leq N,\ i = 1, \ldots, d\}. \tag{1.15}$$

Choose a way to reorder the index set Λ into the natural order from 1 to N^d, in an entirely same way, the results and the proofs for one dimension can be generalized for any dimension. More generally, it is true when X is compact.

The rest of this paper is organized as follows. In Sec. 2, we present linear and nonlinear asymptotic stability of the strict ESD for the semi-discrete scheme. Section 3 is devoted to the fully discrete scheme, including the exponential convergence towards the strict ESD, and the algebraic convergence towards the general ESD.

2. Exponential Convergence Towards the ESD for the Semi-Discrete Scheme

In this section, we show that the strict ESD that satisfies the sign condition (1.12) is both linearly and nonlinearly stable, with perturbations decaying exponentially in time.

2.1. *Linear stability*

We first investigate the linear stability of the strict ESD satisfying (1.12). To do so, we consider the linearized equation

$$\frac{d}{dt}g_j = s_j g_j - \tilde{f}_j h \sum_{i=1}^{N} \bar{b}_{ji} g_i, \quad j = 1, \ldots, N. \tag{2.1}$$

For the strict ESD, we define the weighted l^2-norm by

$$\|g\|_{\tilde{f}} = \left(\sum_{j \in I} g_j^2 h + \sum_{j \in I^c} \frac{g_j^2}{\tilde{f}_j} h \right)^{1/2}.$$

Theorem 2.1. *Assume* (1.9) *holds. Let* $\tilde{f} = \{\tilde{f}_j\}$ *be the strict ESD satisfying* (1.12), *and* $g_j(t)$ *be the solution to the linearized scheme* (2.1) *subject to initial data* $g_j(0)$. *If* $\|g(0)\|_{\tilde{f}} < \infty$, *then*

$$\|g(t)\|_{\tilde{f}} \leq C(1+t)^{\xi} e^{-rt}, \quad \xi = 1_{\{\mu = s\}}, \tag{2.2}$$

for some C *depending on* μ, s, $\|b\|_{L^\infty}$, $\|\tilde{f}\|_1$ *and* $\|g(0)\|_{\tilde{f}}$.

Proof. For the strict ESD considered, and $j \in I$, one has $\frac{d}{dt}g_j = s_j g_j$ and so

$$g_j(t) = g_j(0) e^{s_j t}, \tag{2.3}$$

hence by the definition of s:

$$\left(\sum_{j \in I} g_j^2 h \right)^{1/2} \leq \left(\sum_{j \in I} |g_j(0)|^2 h \right)^{1/2} e^{-st}.$$

For $j \in I^c$, $s_j = 0$, and we have

$$\frac{dg_j}{dt} = -\tilde{f}_j h \sum_{i \in I^c} \bar{b}_{ji} g_i - \tilde{f}_j h \sum_{i \in I} \bar{b}_{ji} g_i.$$

Therefore

$$\begin{aligned} \frac{d}{dt}\left(\sum_{j \in I^c} \frac{g_j^2}{\tilde{f}_j} h \right) &= -2h^2 \sum_{j,i \in I^c} \bar{b}_{ji} g_i g_j - 2h^2 \sum_{j \in I^c} g_j \sum_{i \in I} \bar{b}_{ji} g_i \\ &\leq -2h^2 f_m \lambda_{\min} \sum_{j \in I^c} \frac{g_j^2}{\tilde{f}_j} + 2h^2 e^{-st} \sum_{j \in I^c} \left(|g_j| \sum_{i \in I} \bar{b}_{ji} |g_i(0)| \right) \\ &\leq -2\mu \sum_{j \in I^c} \frac{g_j^2}{\tilde{f}_j} h + 2h^{\frac{3}{2}} e^{-st} \left(\sum_{j \in I^c} \frac{g_j^2}{\tilde{f}_j} h \right)^{1/2} \end{aligned}$$

$$\times \left[\sum_{j\in I^c} \tilde{f}_j \left(\sum_{i\in I} \bar{b}_{ji}|g_i(0)|\right)^2\right]^{1/2}$$

$$\leq -2\mu \sum_{j\in I^c} \frac{g_j^2}{\tilde{f}_j} h + 2C_1 e^{-st} \left(\sum_{j\in I^c} \frac{g_j^2}{\tilde{f}_j} h\right)^{1/2},$$

where $C_1 = \sqrt{2}\|b\|_{L^\infty} |\tilde{f}|_1^{\frac{1}{2}} \|g(0)\|_{L^2(I)}$. Calling $A(t) = \left(\sum_{j\in I^c} \frac{g_j^2}{\tilde{f}_j} h\right)^{1/2}$, we have

$$\frac{dA}{dt} \leq -\mu A + C_1 e^{-st},$$

which upon integration gives

$$A \leq \begin{cases} \left(A(0) - \dfrac{C_1}{\mu - s}\right) e^{-\mu t} + \dfrac{C_1}{\mu - s} e^{-st}, & \mu - s \neq 0, \\ (A(0) + C_1 t) e^{-st}, & \mu - s = 0. \end{cases}$$

Therefore, one has

$$A \leq C(1+t)^\xi e^{-rt},$$

with $\xi = 1_{\{\mu = s\}}$, and

$$C = A(0) + C_1 |\mu - s|^{-1} 1_{\{\mu \neq s\}} + C_1 1_{\{\mu = s\}}.$$

Then

$$\|g(t)\|_{\tilde{f}} \leq \left(\sum_{j\in I} |g_j(0)|^2 h\right)^{1/2} e^{-st} + A(t)$$

$$\leq (\|g(0)\|_{\tilde{f}} + C_1 |\mu - s|^{-1} 1_{\{\mu \neq s\}} + C_1 1_{\{\mu = s\}})(1+t)^\xi e^{-rt}.$$

This ensures claimed estimate (2.2). □

2.2. *Nonlinear stability*

We now turn to the nonlinear stability of the ESD under assumption (1.12).

Theorem 2.2. *Assume* (1.9) *holds. Let $f_j(t)$ be the solution to* (1.6), *associated with the strict ESD $\tilde{f} = \{\tilde{f}_j\}$. Then there exists $\delta^* > 0$ such that for any $\delta \in (0, \delta^*)$ if*

$$\|f(0) - \tilde{f}\|_{\tilde{f}} \leq \delta,$$

then

$$\|f(t) - \tilde{f}\|_{\tilde{f}} \leq C(1+t)^\xi e^{-rt}, \quad \xi = 1_{\{\mu = s\}}, \tag{2.4}$$

for some C depending on μ, s, $\|b\|_\infty$, $\|\tilde{f}\|_1$ and the norm of the initial data.

Proof. (1) Symmetrization with weight depending on $\tilde{f}$. For the strict ESD considered, we substitute $f_j = \tilde{f}_j + g_j$ into (1.6) so that

$$\frac{d}{dt} g_j = s_j g_j - \tilde{f}_j h \sum_{i=1}^N \bar{b}_{ji} g_i - g_j h \sum_{i=1}^N \bar{b}_{ji} g_i, \quad j = 1, \ldots, N.$$

For $j \in I$, $\frac{d}{dt} g_j = s_j g_j - g_j h \sum_{i=1}^N \bar{b}_{ji} g_i$, and thus

$$\begin{aligned} \frac{d}{dt} \sum_{j \in I} g_j^2 h &= 2h \sum_{j \in I} s_j g_j^2 - 2h^2 \sum_{j \in I} g_j^2 \sum_{i=1}^N \bar{b}_{ji} g_i \\ &\leq -2s \sum_{j \in I} g_j^2 h + 2\|b\|_\infty \|g\|_1 \sum_{j \in I} g_j^2 h. \end{aligned}$$

For $j \in I^c$, $s_j = 0$, and we have

$$\frac{d}{dt} g_j = -\tilde{f}_j h \sum_{i \in I^c} \bar{b}_{ji} g_i - \tilde{f}_j h \sum_{i \in I} \bar{b}_{ji} g_i - g_j h \sum_{i=1}^N \bar{b}_{ji} g_i,$$

so that

$$\begin{aligned} \frac{d}{dt} \left(\sum_{j \in I^c} \frac{g_j^2}{\tilde{f}_j} h \right) &= -2h^2 \sum_{j,i \in I^c} \bar{b}_{ji} g_i g_j - 2h^2 \sum_{j \in I^c} \left(g_j \sum_{i \in I} \bar{b}_{ji} g_i \right) \\ &\quad - 2h^2 \sum_{j \in I^c} \left(\frac{g_j^2}{\tilde{f}_j} \sum_{i=1}^N \bar{b}_{ji} g_i \right) \\ &\leq -2\mu \sum_{j \in I^c} \frac{g_j^2}{\tilde{f}_j} h + 2\|\tilde{f}\|_1^{1/2} \|b\|_{L^\infty} \left(\sum_{j \in I} |g_j| h \right) \left(\sum_{j \in I^c} \frac{g_j^2}{\tilde{f}} h \right)^{1/2} \\ &\quad + 2\|b\|_{L^\infty} \|g\|_1 \left(\sum_{j \in I^c} \frac{g_j^2}{\tilde{f}} h \right). \end{aligned}$$

Here we have used the Cauchy–Schwarz inequality in bounding the second term.

(2) Coupling the two quantities.

Let

$$A_1 = \left(\sum_{j \in I} g_j^2 h \right)^{1/2}, \quad A_2 = \left(\sum_{j \in I^c} \frac{g_j^2}{\tilde{f}_j} h \right)^{1/2},$$

then

$$\begin{cases} \dfrac{dA_1}{dt} \leq -sA_1 + \|b\|_\infty \|g\|_1 A_1, \\ \dfrac{dA_2}{dt} \leq -\mu A_2 + \|b\|_{L^\infty} \|g\|_1 A_2 + \|b\|_{L^\infty} \|\tilde{f}\|_1^{1/2} \left(\displaystyle\sum_{j \in I} |g_j| h \right). \end{cases}$$

Further simplification by using $\sum_{j\in I}|g_j|h \leq \sqrt{2}A_1$ and setting $C_2 = \|b\|_{L^\infty}\left(\frac{\|\tilde{f}\|_1}{2}\right)^{1/2}$ leads to:

$$\frac{dA_1}{dt} \leq (-s + \|b\|_\infty \|g\|_1)A_1, \tag{2.5a}$$

$$\frac{dA_2}{dt} \leq (-\mu + \|b\|_{L^\infty}\|g\|_1)A_2 + 2C_2A_1. \tag{2.5b}$$

(3) Decay estimates using a Lyapunov functional.

Set

$$L := A_1^2 + \alpha^2 A_2^2,$$

so that

$$2\alpha A_1 A_2 \leq L. \tag{2.6}$$

Here α is to be determined, so that the exponential decay of L is ensured, yet with largest possible initial data.

A direct calculation gives

$$\begin{aligned}\dot{L} &= 2A_1\dot{A}_1 + 2\alpha^2 A_2\dot{A}_2 \\ &\leq -2sA_1^2 - 2\mu\alpha^2 A_2^2 + 4C_2\alpha^2 A_1A_2 + 2\|b\|_{L^\infty}\|g\|_1(A_1^2 + \alpha^2 A_2^2).\end{aligned}$$

Proceeding with (2.6) and

$$\|g\|_1 \leq \sqrt{2}A_1 + |\tilde{f}|_1^{1/2}A_2 \leq (\sqrt{2} + \alpha^{-1}\|\tilde{f}\|_1^{1/2})\sqrt{L}, \tag{2.7}$$

we see that

$$\dot{L} \leq -[2r - 2C_2\alpha - 2\|b\|_{L^\infty}(\sqrt{2} + \alpha^{-1}\|\tilde{f}\|_1^{1/2})\sqrt{L}]L.$$

This implies that for any $\alpha \in (0, r/C_2)$, if

$$\sqrt{L(0)} < k(\alpha) := \frac{r - C_2\alpha}{(\sqrt{2} + \alpha^{-1}\|\tilde{f}\|_1^{1/2})\|b\|_{L^\infty}}, \tag{2.8}$$

then L is decreasing in time, and its decay rate is governed by the linear part as

$$L \leq C_3 e^{-2(r - C_2\alpha)t}, \tag{2.9}$$

where C_3 is given by

$$C_3 = \sup_{t\geq 0}\frac{L(0)}{[1 + \sqrt{L(0)}/k(\alpha)(e^{-(r-C_2\alpha)t} - 1)]^2} = \frac{L(0)}{[1 - \sqrt{L(0)}/k(\alpha)]^2}.$$

It suffices to select α such that $k(\alpha)$ achieves its maximum. One can verify that

$$\frac{(k_1 - x)x}{x + k_2} \leq (\sqrt{k_1 + k_2} - \sqrt{k_2})^2,$$

and this maximum is achieved at $x = \sqrt{k_2^2 + k_1 k_2} - k_2$. This when applied to $k(\alpha)$ with $k_1 = r/C_2$ and $k_2 = (\|\tilde{f}\|_1/2)^{1/2}$ leads to

$$\begin{aligned}\max k(\alpha) &= k(\alpha^*)\\ &= \frac{C_2}{\sqrt{2}\|b\|_{L^\infty}}\left(\sqrt{r/C_2 + (\|\tilde{f}\|_1/2)^{1/2}} - \sqrt{(\|\tilde{f}\|_1/2)^{1/2}}\right)^2, \end{aligned} \tag{2.10}$$

where

$$\alpha^* = \sqrt{\|\tilde{f}\|_1/2 + r/C_2(\|\tilde{f}\|_1/2)^{1/2}} - (\|\tilde{f}\|_1/2)^{1/2}.$$

Recall that $C_2 = \|b\|_{L^\infty}\big(\frac{\|\tilde{f}\|_1}{2}\big)^{1/2}$, and

$$\sqrt{L(0)} \le \max\{1,\alpha\}\|f(0) - \tilde{f}\|_{\tilde{f}} \le \delta \max\{1,\alpha\}.$$

Hence (2.8) is ensured to hold if we choose δ^* such that:

$$\begin{aligned}\delta^* &= \frac{k(\alpha^*)}{\max\{1,\alpha^*\}} = \frac{(\alpha^*)^2}{\sqrt{2}\max\{1,\alpha^*\}},\\ \alpha^* &= \sqrt{\frac{r}{\|b\|_{L^\infty}} + \frac{\|\tilde{f}\|_1}{2}} - \sqrt{\frac{\|\tilde{f}\|_1}{2}}.\end{aligned} \tag{2.11}$$

This value of α is indeed less than $r/C_2 = \sqrt{2}r/(\|b\|_{L^\infty}\|\tilde{f}\|_1^{1/2})$, as required.

(4) Optimal decay rates.

We use C to denote different constants from line-to-line. Equation (2.5a), combining with (2.7) and (2.9), leads to

$$\frac{dA_1}{dt} \le -sA_1 + Ce^{-kt}A_1, \quad k = r - C_2\alpha^* > 0. \tag{2.12}$$

Integration of (2.12) gives

$$A_1(t) \le A_1(0)e^{C\frac{1}{k}(1-e^{-kt})}e^{-st} \le Ce^{-st}.$$

Substitution of this into (2.5b) yields

$$\frac{dA_2}{dt} \le -\mu A_2 + Ce^{-kt}A_2 + Ce^{-st}.$$

This upon rewriting gives

$$\frac{d}{dt}[A_2 e^{\mu t + C(e^{-kt}-1)/k}] \le Ce^{C(e^{-kt}-1)/k}e^{(\mu-s)t} \le Ce^{(\mu-s)t}.$$

Hence,

$$A_2(t) \le \begin{cases} Ce^{-rt}, & \mu - s \ne 0,\\ C(1+t)e^{-st}, & \mu - s = 0.\end{cases}$$

These when combined with $\|f - \tilde{f}\|_{\tilde{f}}^2 = A_1^2 + A_2^2$ lead to the estimate (2.4). □

3. Convergence Rate for the Fully Discrete Scheme

For the fully discrete scheme

$$\frac{f_j^{n+1} - f_j^n}{\Delta t} = f_j^{n+1}\left(\bar{a}_j - h\sum_{i=1}^{N}\bar{b}_{ji}f_i^n\right), \quad j = 1, \ldots, N, \tag{3.1}$$

we establish the exponential convergence towards the strict ESD and algebraic convergence towards the general ESD for Δt suitably small.

3.1. *Exponential convergence*

Theorem 3.1. *Assume* (1.9) *holds. Let f_j^n be the numerical solution to* (3.1), *associated with the strict ESD $\tilde{f} = \{\tilde{f}_j\}$. If Δt satisfies*

$$\Delta t \le \frac{\min\{s, \mu/2\}}{\|b\|_{L^\infty}^2 \|\tilde{f}\|_1^2}, \tag{3.2}$$

then there exists $\delta^* > 0$ such that for any $\delta \in (0, \delta^*)$ if

$$\|f^0 - \tilde{f}\|_{\tilde{f}} \le \delta,$$

then

$$\|f^n - \tilde{f}\|_{\tilde{f}} \le C(1 + n\Delta t)^\xi \max\{K_s, K_*\}^n, \quad \xi = 1_{\{K_s = K_*\}}, \tag{3.3}$$

where

$$K_s = \frac{1}{\sqrt{1 + 2s\Delta t}}, \quad K_* = \frac{1}{\sqrt{1 + 2\mu\Delta t}}\left(1 + \frac{2\Delta t^2 \|b\|_{L^\infty}^2 \|\tilde{f}\|_1^2}{\sqrt{1 + 2\mu\Delta t}}\right) < 1,$$

and C depends on μ, s, $\|b\|_\infty$, $\|\tilde{f}\|_1$ and the norm of the initial data.

Proof. The proof follows steps similar to the semi-discrete case.

(1) Symmetrization with weight depending on $\tilde{f}$.

For the strict ESD considered, we substitute $f_j^n = \tilde{f}_j + g_j^n$ into (3.1) so that

$$\frac{g_j^{n+1} - g_j^n}{\Delta t} = s_j g_j^{n+1} - \tilde{f}_j h\sum_{i=1}^{N}\bar{b}_{ji}g_i^n - g_j^{n+1}h\sum_{i=1}^{N}\bar{b}_{ji}g_i^n, \quad j = 1, \ldots, N.$$

Then

$$\frac{g_j^{n+1} - g_j^n}{\Delta t} = s_j g_j^{n+1} - g_j^{n+1}h\sum_{i=1}^{N}\bar{b}_{ji}g_i^n, \quad j \in I.$$

Multiplying $g_j^{n+1}h$ on both sides and summing over $j \in I$, we have

$$h\sum_{j\in I}\frac{(g_j^{n+1})^2 - g_j^{n+1}g_j^n}{\Delta t} = h\sum_{j\in I}s_j(g_j^{n+1})^2 - h^2\sum_{j\in I}\left((g_j^{n+1})^2\sum_{i=1}^{N}\bar{b}_{ji}g_i^n\right). \tag{3.4}$$

The left-hand side of (3.4) may be written as

$$h\sum_{j\in I}\left[\frac{(g_j^{n+1})^2-(g_j^n)^2}{2\Delta t}+\frac{(g_j^{n+1}-g_j^n)^2}{2\Delta t}\right], \tag{3.5}$$

and the right-hand side of (3.4) is bounded from above by

$$-s\sum_{j\in I}(g_j^{n+1})^2h+\|b\|_{L^\infty}\|g^n\|_1\sum_{j\in I}(g_j^{n+1})^2h.$$

Hence

$$h\sum_{j\in I}\frac{(g_j^{n+1})^2-(g_j^n)^2}{2\Delta t}\le -s\sum_{j\in I}(g_j^{n+1})^2h+\|b\|_{L^\infty}\|g^n\|_1\sum_{j\in I}(g_j^{n+1})^2h. \tag{3.6}$$

For $j\in I^c$, $s_j=0$, and

$$\frac{g_j^{n+1}-g_j^n}{\Delta t}=-\tilde{f}_jh\sum_{i=1}^N\bar{b}_{ji}g_i^n-g_j^{n+1}h\sum_{i=1}^N\bar{b}_{ji}g_i^n.$$

Against $\frac{g_j^{n+1}h}{\tilde{f}_j}$ on both sides, summation over $j\in I^c$ gives

$$h\sum_{j\in I^c}\frac{(g_j^{n+1})^2-g_j^{n+1}g_j^n}{\tilde{f}_j\Delta t}=-h^2\sum_{j\in I^c}\left(g_j^{n+1}\sum_{i=1}^N\bar{b}_{ji}g_i^n\right)$$
$$-h^2\sum_{j\in I^c}\left[\frac{(g_j^{n+1})^2}{\tilde{f}_j}\sum_{i=1}^N\bar{b}_{ji}g_i^n\right]. \tag{3.7}$$

The term on the left-hand side is treated same way as in (3.5), and the last term on the right is bounded by

$$\|b\|_{L^\infty}\|g^n\|_1\sum_{j\in I^c}\frac{(g_j^{n+1})^2}{\tilde{f}_j}h.$$

We focus on the estimate of the first term on the right-hand side of (3.7), which can be estimated by

$$\begin{aligned}
&\le -h^2\sum_{j\in I^c}\left(g_j^{n+1}\sum_{i\in I^c}\bar{b}_{ji}g_i^{n+1}\right)+h^2\sum_{j\in I^c}\left[g_j^{n+1}\sum_{i\in I^c}\bar{b}_{ji}(g_i^{n+1}-g_i^n)\right]\\
&\quad -h^2\sum_{j\in I^c}\left(g_j^{n+1}\sum_{i\in I}\bar{b}_{ji}g_i^n\right)\\
&\le -\mu\sum_{j\in I^c}\frac{(g_j^{n+1})^2}{\tilde{f}_j}h-\Delta t h^3\sum_{j\in I^c}\left[g_j^{n+1}\sum_{i\in I^c}\bar{b}_{ji}(\tilde{f}_i+g_i^{n+1})\sum_{k=1}^N\bar{b}_{ik}g_k^n\right]\\
&\quad +\|b\|_{L^\infty}\left(\sum_{i\in I}|g_i^n|h\right)\|\tilde{f}\|_1^{1/2}\left[\sum_{j\in I^c}\frac{(g_j^{n+1})^2}{\tilde{f}}h\right]^{1/2}.
\end{aligned}$$

Applying the Cauchy–Schwarz inequality to estimate the second term above gives

$$
\begin{aligned}
&-\Delta t h^3 \sum_{j\in I^c}\left[g_j^{n+1}\sum_{i\in I^c}\bar b_{ji}\Delta t(\tilde f_i+g_i^{n+1})\sum_{k=1}^N \bar b_{ik}g_k^n\right]\\
&\quad\le \Delta t h^2\left[\sum_{j\in I^c}\frac{(g_j^{n+1})^2}{\tilde f}h\right]^{1/2}\left\{\sum_{j\in I^c}\tilde f_j h\left[\sum_{i\in I^c}\bar b_{ji}(\tilde f_i+g_i^{n+1})\sum_{k=1}^N\bar b_{ik}g_k^n\right]^2\right\}^{1/2}\\
&\quad\le \Delta t h^2\|b\|_{L^\infty}\|\tilde f\|_1^{1/2}\sum_{i\in I^c}\left[(\tilde f_i+|g_i^{n+1}|)\left|\sum_{k=1}^N\bar b_{ik}g_k^n\right|\right]\left[\sum_{j\in I^c}\frac{(g_j^{n+1})^2}{\tilde f}h\right]^{1/2}\\
&\quad\le \Delta t\|b\|_{L^\infty}^2\|\tilde f\|_1^{1/2}\|g^n\|_1\left\{\|\tilde f\|_1+\|\tilde f\|_1^{1/2}\left[\sum_{j\in I^c}\frac{(g_j^{n+1})^2}{\tilde f}h\right]^{1/2}\right\}\\
&\qquad\times\left[\sum_{j\in I^c}\frac{(g_j^{n+1})^2}{\tilde f}h\right]^{1/2}.
\end{aligned}
$$

(2) Coupling the two quantities.

We set

$$
A_1^n=\sum_{j\in I}(g_j^n)^2h,\quad A_2^n=\sum_{j\in I^c}\frac{(g_j^n)^2}{\tilde f_j}h,
$$

so that the above estimates may be written as

$$
\frac{A_1^{n+1}-A_1^n}{2\Delta t}\le -sA_1^{n+1}+\|b\|_\infty\|g^n\|_1A_1^{n+1}, \tag{3.8a}
$$

$$
\begin{aligned}
\frac{A_2^{n+1}-A_2^n}{2\Delta t}&\le -\mu A_2^{n+1}+\|b\|_{L^\infty}\|g^n\|_1A_2^{n+1}\\
&\quad+\|b\|_{L^\infty}\|\tilde f\|_1^{1/2}\left(\sum_{i\in I}|g_i^n|h\right)\sqrt{A_2^{n+1}}\\
&\quad+\Delta t\|b\|_{L^\infty}^2\|\tilde f\|_1\|g^n\|_1A_2^{n+1}\\
&\quad+\Delta t\|b\|_{L^\infty}^2\|\tilde f\|_1^{3/2}\|g^n\|_1\sqrt{A_2^{n+1}}.
\end{aligned} \tag{3.8b}
$$

(3) Decay estimates using a Lyapunov functional.

Set

$$
L^n:=A_1^n+\alpha^2A_2^n. \tag{3.9}
$$

Next we determine the range of the initial data so that L^n decays in n, with proper choices of α and Δt.

Note that

$$\sum_{i\in I} |g_i^n| h \leq \sqrt{2A_1^n},$$

with which, (3.8) and (3.9), it follows that

$$\frac{L^{n+1}-L^n}{2\Delta t} \leq -rL^{n+1} + \|b\|_{L^\infty}\|g^n\|_1 L^{n+1} + \sqrt{2}\alpha^2\|b\|_{L^\infty}|\tilde f\|_1^{1/2}\sqrt{A_1^n A_2^{n+1}}$$
$$+ \Delta t\|b\|_{L^\infty}^2\|\tilde f\|_1\|g^n\|_1 L^{n+1} + \Delta t\alpha\|b\|_{L^\infty}^2\|\tilde f\|_1^{3/2}\|g^n\|_1\sqrt{L^{n+1}}.$$

Proceeding with

$$\|g^n\|_1 \leq \sqrt{2A_1^n} + \sqrt{\|\tilde f\|_1 A_2^n} \leq (\sqrt{2} + \alpha^{-1}\|\tilde f\|_1^{1/2})\sqrt{L^n}, \tag{3.10}$$

we see that

$$\frac{L^{n+1}-L^n}{2\Delta t} \leq -rL^{n+1} + c_1\sqrt{L^n}L^{n+1} + c_2\sqrt{L^nL^{n+1}}, \tag{3.11}$$

where

$$c_1 = \|b\|_{L^\infty}(1+\Delta t\|b\|_{L^\infty}\|\tilde f\|_1)(\sqrt{2}+\alpha^{-1}\|\tilde f\|_1^{1/2}),$$
$$c_2 = \sqrt{2}\alpha\|b\|_{L^\infty}\|\tilde f\|_1^{1/2} + \Delta t\alpha\|b\|_{L^\infty}^2\|\tilde f\|_1^{3/2}(\sqrt{2}+\alpha^{-1}\|\tilde f\|_1^{1/2}).$$

Using $\sqrt{L^nL^{n+1}} \leq L^n/2 + L^{n+1}/2$ in (3.11) we obtain

$$L^{n+1}(1+2r\Delta t - 2c_1\Delta t\sqrt{L^n} - c_2\Delta t) \leq (1+c_2\Delta t)L^n.$$

Note that if the time step is taken as

$$0 < \Delta t < \frac{r-\sqrt{2}\alpha\|b\|_{L^\infty}\|\tilde f\|_1^{1/2}}{\|b\|_{L^\infty}^2\|\tilde f\|_1^{3/2}(\sqrt{2}\alpha + \|\tilde f\|_1^{1/2})}, \tag{3.12}$$

then $c_2 < r$. Therefore, $L^{n+1} < L^n$ provided

$$c_2 < r - c_1\sqrt{L^0} \leq r - c_1\sqrt{L^n}.$$

This implies that if

$$\sqrt{L^0} < k(\alpha) := \frac{r-c_2}{c_1}, \tag{3.13}$$

then L^n is strictly decreasing in n, and

$$L^{n+1} \leq KL^n, \quad K := \frac{(1+c_2\Delta t)}{1+2r\Delta t - 2c_1\Delta t\sqrt{L^0} - c_2\Delta t} < 1.$$

Therefore exponential decay holds

$$L^n \le K^n L^0. \tag{3.14}$$

We now check how to choose α so that $k(\alpha)$, defined in (3.13), is maximized for each fixed Δt satisfying

$$\Delta t < \frac{r}{\|b\|_{L^\infty}^2 \|\tilde{f}\|_1^2}.$$

Note that (3.12) is equivalent to the following requirement

$$\alpha < \beta(\Delta t) := \frac{r - \Delta t \|b\|_{L^\infty}^2 \|\tilde{f}\|_1^2}{\sqrt{2\|\tilde{f}\|_1}\|b\|_{L^\infty}(1 + \Delta t\|b\|_{L^\infty}\|\tilde{f}\|_1)}. \tag{3.15}$$

Rewriting $k(\alpha)$ as

$$k(\alpha) = \frac{\alpha(\beta(\Delta t) - \alpha)}{\alpha + \sqrt{\|\tilde{f}\|_1/2}} \cdot \sqrt{\|\tilde{f}\|_1}. \tag{3.16}$$

The maximum of this function is achieved at α^*, with

$$\begin{aligned}\alpha^* &= \sqrt{\|\tilde{f}\|_1/2 + (\|\tilde{f}\|_1/2)^{1/2}\beta(\Delta t)} - (\|\tilde{f}\|_1/2)^{1/2} \\ &= \frac{\beta(\Delta t)}{1 + \sqrt{1 + (2/\|\tilde{f}\|_1)^{1/2}\beta(\Delta t)}}.\end{aligned}$$

Such an α^* clearly satisfies (3.15). Moreover,

$$k(\alpha^*) = \sqrt{\|\tilde{f}\|_1}\left(\sqrt{\beta(\Delta t) + (\|\tilde{f}\|_1/2)^{1/2}} - \sqrt{(\|\tilde{f}\|_1/2)^{1/2}}\right)^2 = \sqrt{2}(\alpha^*)^2.$$

Furthermore,

$$\sqrt{L^0} \le \max\{1, \alpha\}\|f^0 - \tilde{f}\|_{\tilde{f}} \le \delta \max\{1, \alpha\}.$$

Hence (3.13) is ensured to hold if we choose δ^* such that

$$\delta^* = \frac{k(\alpha^*)}{\max\{1, \alpha^*\}} = \frac{\sqrt{2}(\alpha^*)^2}{\max\{1, \alpha^*\}}. \tag{3.17}$$

(4) Optimal decay rates.

In the estimate to follow, we use C to denote different constants from line-to-line if applicable. From (3.8a), combining with (3.10) and (3.14), it follows

$$\frac{A_1^{n+1} - A_1^n}{2\Delta t} \le -(s - \gamma K^{n/2})A_1^{n+1},$$

for $\gamma = \|b\|_{L^\infty}(\sqrt{2} + \alpha^{-1}\|\tilde{f}\|_1^{1/2})\sqrt{L^0} < s$ which can be obtained from (3.16). Then

$$A_1^n \le \frac{A_1^{n-1}}{1 + 2s\Delta t - 2\gamma\Delta t K^{(n-1)/2}}$$

$$\le \frac{A_1^0}{(1+2s\Delta t)^n} \prod_{i=0}^{n-1} \frac{1 + 2s\Delta t}{1 + 2s\Delta t - 2\gamma\Delta t K^{i/2}}$$

$$\le C_\gamma A_1^0 K_s^{2n}, \tag{3.18}$$

where $K_s = \frac{1}{\sqrt{1+2s\Delta t}}$. In fact, the product may be estimated as follows:

$$\le \prod_{i=0}^{n-1}(1 + 2\gamma\Delta t K^{i/2})$$

$$\le \exp\left(\sum_{i=0}^{n-1} \log(1 + 2\gamma\Delta t K^{i/2})\right)$$

$$\le \exp\left(2\gamma\Delta t \sum_{i=0}^{n-1}(\sqrt{K})^i\right) \le \exp\left(\frac{2\gamma\Delta t}{1-\sqrt{K}}\right),$$

leading to the claimed bound in (3.18).

We now estimate the decay rate of A_2^n. Substitution of (3.10), (3.14) and (3.18) into (3.8b) yields

$$\frac{A_2^{n+1} - A_2^n}{2\Delta t} \le -\mu A_2^{n+1} + c_1\sqrt{L^0}K^{n/2}A_2^{n+1} + \sqrt{2}\|b\|_{L^\infty}\|\tilde{f}\|_1^{1/2}\sqrt{A_1^n}\sqrt{A_2^{n+1}}$$

$$+ \Delta t\|b\|_{L^\infty}^2\|\tilde{f}\|_1^{3/2}\left(\sqrt{2A_1^n} + \sqrt{\|\tilde{f}\|_1 A_2^n}\right)\sqrt{A_2^{n+1}}$$

$$\le -\mu A_2^{n+1} + c_1\sqrt{L^0}K^{n/2}A_2^{n+1} + C_1K_s^n\sqrt{A_2^{n+1}}$$

$$+ \Delta t\|b\|_{L^\infty}^2\|\tilde{f}\|_1^2\sqrt{A_2^n A_2^{n+1}},$$

where $C_1 = \sqrt{2}\|b\|_{L^\infty}\|\tilde{f}\|_1^{1/2}(1 + \|b\|_{L^\infty}\|\tilde{f}\|_1\Delta t)\sqrt{C_\gamma A_1^0}$. Hence

$$A_2^{n+1} - 2e_n d_n^2\sqrt{A_2^{n+1}} - d_n^2 A_2^n \le 0,$$

where

$$d_n = \frac{1}{[1 + 2\Delta t(\mu - c_1\sqrt{L^0}K^{n/2})]^{1/2}},$$

$$e_n = C_1\Delta t K_s^n + \Delta t^2\|b\|_{L^\infty}^2\|\tilde{f}\|_1^2\sqrt{A_2^n}.$$

This gives

$$\sqrt{A_2^{n+1}} \le e_n d_n^2 + \sqrt{e_n^2 d_n^4 + d_n^2 A_2^n}$$

$$\le 2e_n d_n^2 + d_n\sqrt{A_2^n}$$

$$\le 2C_1\Delta t K_s^n d_n^2 + \tilde{d}_n\sqrt{A_2^n}, \quad \tilde{d}_n := d_n(1 + 2\Delta t^2\|b\|_{L^\infty}^2\|\tilde{f}\|_1^2 d_n).$$

By induction,

$$\sqrt{A_2^n} \le \left(\prod_{i=0}^{n-1} \tilde{d}_i\right) \sqrt{A_2^0} + 2C_1 \Delta t \sum_{i=0}^{n-1} \left(K_s^i d_i^2 \prod_{j=i+1}^{n-1} \tilde{d}_j\right).$$

For fixed Δt, $d_\infty := K_\mu = \frac{1}{\sqrt{1+2\mu\Delta t}} \le d_j \le 1$, a similar estimate as in (3.18) gives

$$\begin{aligned}
\prod_{j=i}^{n-1} \tilde{d}_j &= (\tilde{d}_\infty)^{n-i} \prod_{j=i}^{n-1} \frac{d_j}{d_\infty} \cdot \prod_{j=i}^{n-1} \frac{1 + 2\Delta t^2 \|b\|_{L^\infty}^2 \|\tilde{f}\|_1^2 d_j}{1 + 2\Delta t^2 \|b\|_{L^\infty}^2 \|\tilde{f}\|_1^2 d_\infty} \\
&\le (\tilde{d}_\infty)^{n-i} \prod_{j=i}^{n-1} \frac{d_j}{d_\infty} \cdot \prod_{j=i}^{n-1} \frac{d_j}{d_\infty} \\
&\le \exp\left(\frac{2c_1\sqrt{L_0}\Delta t}{1-\sqrt{K}}\right) (K_*)^{(n-i)}, \quad \text{for } i = 0, 1, 2, \ldots, n-1,
\end{aligned}$$

where

$$K_* := \tilde{d}_\infty = K_\mu (1 + 2\Delta t^2 \|b\|_{L^\infty}^2 \|\tilde{f}\|_1^2 K_\mu),$$

which is strictly less than one provided (3.2) is satisfied. In fact, from (3.2) it follows that

$$\begin{aligned}
\Delta t \frac{\|b\|_{L^\infty}^2 \|\tilde{f}\|_1^2}{\mu} &\le \frac{1}{2} < 1 - \frac{1}{1 + \sqrt{1 + 2\mu\Delta t}} \\
&= \frac{\sqrt{1+2\mu\Delta t}(\sqrt{1+2\mu\Delta t} - 1)}{2\mu\Delta t},
\end{aligned}$$

which yields

$$K_* = K_\mu + 2\Delta t^2 \|b\|_{L^\infty}^2 \|\tilde{f}\|_1^2 K_\mu^2 < 1.$$

Furthermore,

$$\begin{aligned}
2C_1 \Delta t \sum_{i=0}^{n-1} \left(K_s^i d_i^2 \prod_{j=i+1}^{n-1} \tilde{d}_j\right) &\le 2C_1 \Delta t \sum_{i=0}^{n-1} \left(K_s^i d_i \prod_{j=i}^{n-1} \tilde{d}_j\right) \\
&\le C \Delta t K_*^n \sum_{i=0}^{n-1} \left(\frac{K_s}{K_*}\right)^i.
\end{aligned}$$

This is bounded by $CK_s^n n\Delta t$ if $K_* = K_s$, and if $K_* \ne K_s$,

$$\Delta t K_* \frac{K_*^n - K_s^n}{K_* - K_s} \le \frac{K_* \Delta t}{|K_* - K_s|} \max\{K_s, K_*\}^n \le C \max\{K_s, K_*\}^n.$$

The consistency of this bound with the semi-discrete case can be seen from the fact that

$$\lim_{\Delta t \to 0} \frac{K_* \Delta t}{|K_* - K_s|} = \frac{1}{|s - \mu|}.$$

In summary, we have

$$\sqrt{A_2^n} \le C \begin{cases} \max\{K_s, K_*\}^n, & K_* \neq K_s, \\ K_s^n n\Delta t, & K_* = K_s. \end{cases}$$

These when combined with $\|f - \tilde{f}\|_{\tilde{f}} \le \sqrt{A_1^n} + \sqrt{A_2^n}$ lead to the estimate (3.3). □

3.2. *Algebraic convergence*

It was shown in Ref. 14 that the numerical solution of (3.1) converges to the ESD in weighted norm $\|\cdot\|_b$. In this section we investigate the convergence rate of the numerical solution toward the ESD in this norm.

Define the relative entropy

$$F^n = \sum_{j=1}^{N} \left(\tilde{f}_j \log\left(\frac{\tilde{f}_j}{f_j^n}\right) + f_j^n - \tilde{f}_j \right) h, \tag{3.19}$$

and a nonlinear function

$$H(f) = \frac{f^{\mathrm{T}} B f}{2} h^2 - a^{\mathrm{T}} f h,$$

with $f = (f_1, f_2, \ldots, f_N)^{\mathrm{T}}$ and $a = (\bar{a}_1, \bar{a}_2, \ldots, \bar{a}_N)^{\mathrm{T}}$.

For later use, we present a uniform l^1-bound of the numerical solution when $b \ge b_f > 0$.

Lemma 3.1. *Assume* (1.9) *holds. Let* f_j^n *be the numerical solution generated from scheme* (3.1) *with non-negative initial data* $f_j^0 \ge 0$ *for all* $j = 1, \ldots, N$, *and* $\|f^0\|_1 < \infty$. *Then for any* $n > 0$,

$$\|f^n\|_1 \le \max\left\{ \|f^0\|_1, \frac{\|a\|_{L^\infty}}{b_f} \right\}, \tag{3.20}$$

provided

$$\Delta t \le \frac{1}{\|a\|_{L^\infty}}. \tag{3.21}$$

Proof. From (3.1) it follows that if $f_j^n \ge 0$ and (3.21) holds, then $f_j^{n+1} \ge 0$, hence the numerical solution remains non-negative at all time steps.

Let $M^n = h \sum_{j=1}^N f_j^n = \|f^n\|_1$ and $\gamma = \frac{\|a\|_{L^\infty}}{b_f}$. From scheme (3.1) it follows:

$$\begin{aligned} M^{n+1} - M^n &= \Delta t \left(h \sum_{j=1}^{N} f_j^{n+1} \bar{a}_j - h \sum_{j=1}^{N} f_j^{n+1} h \sum_{i=1}^{N} \bar{b}_{ji} f_i^n \right) \\ &\le \Delta t (\|a\|_{L^\infty} M^{n+1} - b_f M^{n+1} M^n) \\ &= -\Delta t b_f M^{n+1} (M^n - \gamma). \end{aligned}$$

There are two cases to distinguish:

(i) if $M^n \geq \gamma$, then $M^{n+1} \leq M^n$;
(ii) if $M^n < \gamma$, we rewrite

$$M^{n+1} - \gamma = (M^n - \gamma)(1 - \Delta t M^{n+1} b_f).$$

According to (3.21), we have

$$M^{n+1} - \gamma \leq (M^n - \gamma)\left(1 - \frac{M^{n+1}}{\gamma}\right),$$

which leads to $M^{n+1} \leq \gamma$. Hence,

$$M^{n+1} \leq \max\{M^n, \gamma\} \leq \cdots \leq \max\{M^0, \gamma\},$$

which is as desired. □

Lemma 3.2. (See Theorem 3.1 in Ref. 14) *Assume* (1.9) *holds. Let* f_j^n *be the numerical solution generated from scheme* (3.1) *with positive initial data* $f_j^0 > 0$ *for all* $j = 1, \ldots, N$. *Then*

$$F^{n+1} - F^n \leq -\frac{1}{2}\Delta t \|f^n - \tilde{f}\|_b^2,$$

provided time step Δt *is suitably small.*

This implies the following assertions:

$$\lim_{n\to\infty} F^n = 0, \quad \lim_{n\to\infty} \|f^n - \tilde{f}\|_b = 0. \tag{3.22}$$

The main aim here is to obtain the convergence rate toward the ESD.

Theorem 3.2. *Assume* (1.9) *holds, and* $F^0 < +\infty$. *Let* f_j^n *be the numerical solution generated from scheme* (3.1) *with positive initial data* $f_j^0 > 0$ *for all* $j = 1, \ldots, N$, $\tilde{f} = \{\tilde{f}_j\}$ *is the discrete ESD. Then*

$$\|f^n - \tilde{f}\|_b^2 \leq \frac{2F^0}{\Delta t n}, \tag{3.23}$$

provided $\Delta t \leq \tau$, *where*

$$\tau = \min\left\{\frac{\lambda_{\min}}{\lambda_{\max}(2C_1 + 2C_2\lambda_{\max} + C_2\lambda_{\min})}, \frac{2}{C_2\|b\|_{L^\infty}}\right\}, \tag{3.24}$$

where $C_1 = \|a\|_{L^\infty} + \|b\|_{L^\infty}\|\tilde{f}\|_1$ *and* $C_2 = \max\{\|f^0\|_1, \frac{\|a\|_{L^\infty}}{b_f}\}$.

Proof. We proceed in two steps:

(i) we first establish for the relative entropy F^n the dissipation inequality of the form

$$F^{n+1} - F^n \leq -\Delta t[H(f^{n+1}) - H(\tilde{f})]; \tag{3.25}$$

(ii) we then show that $H(f^n)$ is decreasing in n, i.e.

$$H(f^{n+1}) - H(f^n) \leq 0. \tag{3.26}$$

We postpone the proof of these two inequalities, while we now use them to prove estimate (3.23). The summation of (3.25) in n gives

$$\Delta t \sum_{i=0}^{+\infty} [H(f^{i+1}) - H(\tilde{f})] \leq F^0 - F^\infty = F^0. \tag{3.27}$$

On the other hand, for any large number n,

$$\begin{aligned}\Delta t \sum_{i=0}^{+\infty} [H(f^{i+1}) - H(\tilde{f})] &\geq \Delta t \sum_{i=0}^{n-1} [H(f^{i+1}) - H(\tilde{f})] \\ &\geq n\Delta t [H(f^n) - H(\tilde{f})], \end{aligned} \tag{3.28}$$

where we have used (3.26). Combining (3.27) and (3.28), we have

$$0 \leq H(f^n) - H(\tilde{f}) \leq \frac{F^0}{n\Delta t},$$

which when combined with

$$H(f^n) - H(\tilde{f}) = \frac{1}{2}\|f^n - \tilde{f}\|_b^2 - h\sum_{j=1}^{N} s_j[\tilde{f}] f_j^n \geq \frac{1}{2}\|f^n - \tilde{f}\|_b^2,$$

gives the desired estimate (3.23).

Finally we specify the restrictions on the time step for both (3.25) and (3.26) to hold true. Denote $\|\cdot\|$ the usual Euclidean norm of a vector.

Scheme (3.1) can be written as

$$f_j^{n+1} = \frac{f_j^n}{1 - \Delta t \bar{a}_j + h\Delta t (Bf^n)_j}, \tag{3.29}$$

if Δt is suitably small, for example, for

$$\Delta t < \|a\|_{L^\infty}^{-1}, \tag{3.30}$$

we have $f_j^{n+1} > 0$ for $f_j^n > 0$. This positivity property will be used below.

We now prove (3.25). Using $\log x \leq x - 1$ for any $x > 0$ and the scheme (3.1), we obtain

$$\begin{aligned} F^{n+1} - F^n &= h\sum_{j=1}^{N}\left(\tilde{f}_j \log\frac{f_j^n}{f_j^{n+1}} + f_j^{n+1} - f_j^n\right) \\ &\leq h\sum_{j=1}^{N}\left(\tilde{f}_j \frac{f_j^n - f_j^{n+1}}{f_j^{n+1}} + f_j^{n+1} - f_j^n\right) \\ &= \Delta t h \sum_{j=1}^{N}\left(\bar{a}_j - h\sum_{i=1}^{N}\bar{b}_{ji} f_i^n\right)(f_j^{n+1} - \tilde{f}_j). \end{aligned}$$

Proceeding with $g^n := f^n - \tilde{f}$, we have

$$\begin{aligned} F^{n+1} - F^n &\le -\Delta t h^2 g^n \cdot B g^{n+1} + \Delta t h \sum_{j=1}^N \left(\bar{a}_j - h \sum_{i=1}^N \bar{b}_{ji} \tilde{f}_i \right) g_j^{n+1} \\ &= -\Delta t h^2 g^{n+1} \cdot B g^{n+1} + \Delta t h^2 (g^{n+1} - g^n) \cdot B g^{n+1} \\ &\quad + \Delta t h \sum_{j=1}^N s_j[\tilde{f}] f_j^{n+1} \\ &\le -\Delta t h^2 g^{n+1} \cdot B g^{n+1} + \Delta t h^2 \|B\|_2 \|g^{n+1} - g^n\| \|g^{n+1}\| \\ &\quad + \Delta t h \sum_{j=1}^N s_j[\tilde{f}] f_j^{n+1}. \end{aligned} \tag{3.31}$$

Next, we show there exists C^*, which may depend on Δt, such that

$$\|g^{n+1} - g^n\| \le C^* \Delta t \|g^{n+1}\|. \tag{3.32}$$

Using the fact that $\tilde{f}_j(\bar{a}_j - h \sum_{i=1}^N \bar{b}_{ji} \tilde{f}_i) = 0$, we have

$$\begin{aligned} (g^{n+1} - g^n)_j &= \Delta t f_j^{n+1} \left[\bar{a}_j - h \sum_{i=1}^N \bar{b}_{ji} (g_i^n + \tilde{f}_i) \right] \\ &= \Delta t \left[(f_j^{n+1} - \tilde{f}_j) \left(\bar{a}_j - h \sum_{i=1}^N \bar{b}_{ji} \tilde{f}_i \right) - h f_j^{n+1} \sum_{i=1}^N \bar{b}_{ji} g_i^n \right]. \end{aligned}$$

Hence,

$$\begin{aligned} \|g^{n+1} - g^n\| &\le \Delta t \|s[\tilde{f}]\|_{L^\infty} \|g^{n+1}\| + \Delta t h \|f^{n+1}\|_\infty \|B\|_2 \|g^n\| \\ &\le \Delta t (\|s[\tilde{f}]\|_{L^\infty} + \|f^{n+1}\|_1 \|B\|_2) \|g^{n+1}\| \\ &\quad + \Delta t \|f^{n+1}\|_1 \|B\|_2 \|g^{n+1} - g^n\| \\ &\le c_1 \Delta t \|g^{n+1}\| + c_2 \Delta t \|g^{n+1} - g^n\|, \end{aligned}$$

where in virtue of Lemma 3.1,

$$c_2 = \max\left\{ \|f^0\|_1, \frac{\|a\|_{L^\infty}}{b_f} \right\} \|B\|_2, \quad c_1 = \|a\|_{L^\infty} + \|b\|_{L^\infty} \|\tilde{f}\|_1 + c_2. \tag{3.33}$$

This has proved (3.32) with

$$C^* = \frac{c_1}{1 - c_2 \Delta t},$$

for

$$\Delta t < \frac{1}{c_2}. \tag{3.34}$$

Substituting (3.32) into (3.31) and using $\lambda_{\min}\|g^{n+1}\|^2 \leq g^{n+1} \cdot Bg^{n+1}$, we have

$$\begin{aligned} F^{n+1} - F^n &\leq -\Delta th^2[g^{n+1} \cdot Bg^{n+1} - \Delta tC^*\|B\|_2\|g^{n+1}\|^2] \\ &\quad + \Delta th \sum_{j=1}^{N} s_j[\tilde{f}]f_j^{n+1} \\ &\leq -\frac{1}{2}\Delta th^2 g^{n+1} \cdot Bg^{n+1} + \Delta th \sum_{j=1}^{N} s_j[\tilde{f}]f_j^{n+1}, \end{aligned}$$

as long as $\Delta t \leq \frac{\lambda_{\min}}{2C^*\|B\|_2} = \frac{\lambda_{\min}}{2C^*\lambda_{\max}}$, that is

$$\Delta t \leq \frac{\lambda_{\min}}{2c_1\lambda_{\max} + c_2\lambda_{\min}}. \tag{3.35}$$

We proceed

$$\begin{aligned} F^{n+1} - F^n &\leq -\Delta th \left(\frac{f^{n+1} \cdot Bf^{n+1}}{2}h - f^{n+1} \cdot B\tilde{f}h \right. \\ &\quad \left. + \frac{\tilde{f} \cdot B\tilde{f}}{2}h - a \cdot f^{n+1} + f^{n+1} \cdot B\tilde{f}h \right) \\ &= -\Delta t[H(f^{n+1}) - H(\tilde{f})]. \end{aligned} \tag{3.36}$$

We next prove (3.26). Using the fact that B is symmetric and scheme (3.1), we calculate:

$$\begin{aligned} H(f^{n+1}) - H(f^n) &= \left[\frac{1}{2}(f^{n+1} - f^n)^{\mathrm{T}}B(f^{n+1} + f^n)h^2 - a^{\mathrm{T}}(f^{n+1} - f^n)h\right] \\ &= -\sum_{j=1}^{N}\left[(f_j^{n+1} - f_j^n)\left(\bar{a}_j - h\sum_{i=1}^{N}\bar{b}_{ji}\frac{f_i^{n+1} + f_i^n}{2}\right)\right]h \\ &= -\Delta th\sum_{j=1}^{N} f_j^{n+1}\left(\bar{a}_j - h\sum_{i=1}^{N}\bar{b}_{ji}f_i^n\right)^2 \\ &\quad + \Delta th^2\sum_{j=1}^{N}\left[f_j^{n+1}\left(\bar{a}_j - h\sum_{i=1}^{N}\bar{b}_{ji}f_i^n\right)\sum_{k=1}^{N}\bar{b}_{jk}\frac{f_k^{n+1} - f_k^n}{2}\right] \\ &=: -T_1 + T_2. \end{aligned}$$

Since $T_1 \geq 0$, we only need to show $T_2 \leq C\Delta t T_1$ for suitably small Δt. Using scheme (3.1), we obtain

$$\begin{aligned} T_2 &= \frac{(\Delta t)^2 h^2}{2} \sum_{j,k=1}^{N} \bar{b}_{jk} f_k^{n+1} f_j^{n+1} \left(\bar{a}_j - h\sum_{i=1}^{N} \bar{b}_{ji} f_i^n\right)\left(\bar{a}_k - h\sum_{i=1}^{N} \bar{b}_{ki} f_i^n\right) \\ &\leq \frac{(\Delta t)^2 h^2}{2} \sum_{j,k=1}^{N} \bar{b}_{jk} f_k^{n+1} f_j^{n+1} \left(\bar{a}_j - h\sum_{i=1}^{N} \bar{b}_{ji} f_i^n\right)^2 \\ &\leq \frac{(\Delta t)^2 h^2}{2} \left(\max_j \sum_{k=1}^{N} \bar{b}_{jk} f_k^{n+1}\right) \sum_{j=1}^{N} f_j^{n+1} \left(\bar{a}_j - h\sum_{i=1}^{N} \bar{b}_{ji} f_i^n\right)^2, \end{aligned} \tag{3.37}$$

where we have used the symmetry of B in the second inequality. Note that

$$h \max_j \sum_{k=1}^{N} \bar{b}_{jk} f_k^{n+1} \leq \|b\|_{L^\infty} \|f^{n+1}\|_1. \tag{3.38}$$

Then

$$T_2 \leq \frac{\Delta t}{2} \|b\|_{L^\infty} \|f^{n+1}\|_1 T_1.$$

The above estimates lead to

$$H(f^{(n+1)}) - H(f^n) \leq -\left(1 - \frac{\Delta t}{2}\|b\|_{L^\infty}\|f^{n+1}\|_1\right) T_1 \leq 0,$$

if

$$\Delta t \leq \frac{2\|B\|_2}{c_2 \|b\|_{L^\infty}}. \tag{3.39}$$

Hence we obtain (3.26) for $\Delta t \leq \tau$ as defined in (3.24). □

Remark 3.1. When $0 < b_f \leq \bar{b}_{ji}$ in (1.9) is weakened to $\bar{b}_{ji} \geq 0$, we are still able to show the same convergence rate, but with a different time step restriction.

A more precise statement is as follows.

Theorem 3.3. *Let $\bar{b}_{ji} \geq 0$ and other assumptions remain the same as those in Theorem* 3.2. *Then*

$$\|f^n - \tilde{f}\|_b^2 \leq \frac{2F^0}{n\Delta t}, \tag{3.40}$$

provided that

$$\Delta t \leq \min\left\{\frac{\lambda_{\min}}{\lambda_{\max}(2C_1 + 2\lambda_{\max}S(F^0) + \lambda_{\min}S(F^0))}, \frac{h}{\|b\|_{L^\infty}S(F^0)}\right\}. \tag{3.41}$$

Proof. We use the fact (refer to the proof in Theorem 3.1 of Ref. 14) that there exists a nondecreasing, positive function S such that

$$h\|f^n\|_\infty \le S(F^n), \tag{3.42}$$

and F^n is decreasing in n. Thus, $c_2 = S(F^0)\|B\|_2$ in (3.33). Combining this with estimate

$$h \max_j \sum_{k=1}^{N} \bar{b}_{jk} f_k^{n+1} \le 2\|b\|_{L^\infty}\|f^n\|_\infty \le 2\|b\|_{L^\infty} h^{-1} S(F^0),$$

instead of (3.38). The remaining proof follows the same strategy as in the proof of Theorem 3.2, then (3.40) is established if condition (3.41) holds. □

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