Numerical Approximation and Stability Analysis of Reaction–Diffusion Equations on Distance-Regular Graphs

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ABSTRACT

We study the numerical approximation of a scalar reaction–diffusion equation posed on the vertex set of a distance-regular graph, where diffusion is modelled by the graph Laplacian. For the explicit Euler scheme and the IMEX Euler scheme we ask how much of the numerical behaviour can be predicted from the intersection array of the graph alone. We prove that the implicit propagator belongs to the Bose–Mesner algebra, has positive entries that depend only on the distance between vertices, and coincides with a polynomial of degree at most the diameter in the Laplacian, so that it can be applied exactly without matrix factorisation. We derive sharp step-size limits for the explicit scheme in the Euclidean and maximum norms and show that they coincide precisely for bipartite graphs. We also obtain the exact linearised stability threshold at a homogeneous equilibrium, a discrete homogenisation estimate governed by the algebraic connectivity, and a first-order error bound. Experiments on ten distance-regular graphs, including Cayley graphs on dihedral and elementary abelian groups, confirm the predicted thresholds with a relative gap of order 10^{-4}.

1. Introduction

Reaction–diffusion equations were introduced into the theory of pattern formation by Turing [22], and the step from a continuous medium to a network of coupled cells was taken by Othmer and Scriven [19]. In the network setting the Laplace operator is replaced by the graph Laplacian, and the unknown becomes a vector indexed by the vertices of a graph. This viewpoint has become standard in the study of diffusion on discrete structures [7,12,15,17], and it has produced a number of results on network-driven instabilities, among them the work of Nakao and Mikhailov on activator–inhibitor systems [18] and the extension to directed networks by Asllani et al. [2].

Once the spatial operator is fixed, the semi-discrete problem is a system of ordinary differential equations whose stiffness is controlled by the spectrum of the Laplacian. Any time-stepping scheme applied to it inherits step-size restrictions, damping rates and error constants that depend on the extreme eigenvalues of that matrix [13,16]. For a general graph these quantities are obtained only after an eigenvalue computation of size $n \times n$, and the matrix itself is treated as an unstructured sparse operator.

Distance-regular graphs are a natural exception. Their adjacency spectrum, together with the multiplicities and the primitive idempotents, is determined by a short list of integers, the intersection array [5,6,9]. All polynomials in the adjacency matrix lie in a commutative algebra of dimension $d + 1$, where d is the diameter [3,11]. These facts are classical in algebraic combinatorics, yet they are rarely used to say anything about a time-stepping scheme. On the other side, papers on reaction–

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diffusion systems over networks usually take the graph as given data and do not exploit any algebraic regularity it may possess.

The question we address is the following. How much of the numerical behaviour of a standard discretisation of a reaction–diffusion equation on a distance-regular graph Γ can be read off from the intersection array of Γ, before any simulation is run? We restrict attention to scalar equations and to two first-order schemes, the explicit Euler method and the linearly implicit (IMEX) Euler method [1,13], because these are the building blocks of the higher-order methods in [8,14] and because the role of the graph is easiest to isolate there.

Our contributions are as follows. We show that the implicit propagator is an element of the Bose–Mesner algebra of Γ; its entries depend only on the distance between two vertices and are given in closed form by the cosine sequences of Γ, and the propagator equals a polynomial of degree at most d in the Laplacian, so that it can be applied exactly with d sparse products and no factorisation. We obtain sharp step-size limits for the explicit scheme in the Euclidean and maximum norms and prove that the two limits coincide exactly when Γ is bipartite. For a homogeneous equilibrium we give the exact threshold of linearised stability for both schemes and show that the graph enters only the explicit one. We prove a discrete homogenisation estimate whose rate is governed by the algebraic connectivity [10], together with a first-order error bound. Finally we report experiments on six small distance-regular graphs and on four larger ones, in which the predicted thresholds are recovered to four significant digits.

The paper is organised as follows. Section 2 collects the definitions and the facts on distance-regular graphs that are needed later. Section 3 contains the main results. Section 4 works out the Petersen graph in closed form and reports the numerical experiments. Section 5 discusses limitations and possible extensions, and the conclusions close the paper.

2. Preliminaries

Throughout, $\Gamma = (X, R)$ is a finite, simple, connected graph with $n = |X|$ vertices, and $\partial(x, y)$ denotes the path distance between $x, y \in X$. For a vector $\mathbf{v} \in \mathbb{R}^X$ we use the Euclidean norm $\| \mathbf{v} \|$ and the maximum norm $\| \mathbf{v} \|_\infty$, and $\mathbb{1}$ is the all-ones vector. All matrix norms are the induced ones.

Definition 2.1 ([5,9]). A connected k-regular graph Γ of diameter d is called *distance-regular* if there are integers b_h and c_h such that, for every pair x, y with $\partial(x, y) = h$, the vertex y has exactly c_h neighbours at distance $h - 1$ from x and exactly b_h neighbours at distance $h + 1$ from x. The list

$$\iota(\Gamma) = \{b_0, b_1, \dots, b_{d-1}; c_1, c_2, \dots, c_d\}$$

is the *intersection array* of Γ. We put $b_0 = k$, $c_1 = 1$, $a_h = k - b_h - c_h$ and $k_h = \frac{b_0 b_1 \cdots b_{h-1}}{c_1 c_2 \cdots c_h}$, so that k_h is the number of vertices at distance h from any fixed vertex.

Definition 2.2 ([3,11]). For $0 \le h \le d$ the *h-th distance matrix* A_h is the $0/1$ matrix with $(A_h)_{xy} = 1$ exactly when $\partial(x, y) = h$. Thus $A_0 = I$ and $A_1 = A$ is the adjacency matrix. For a distance-regular graph one has the three-term relation

$$A\,A_h = b_{h-1} A_{h-1} + a_h A_h + c_{h+1} A_{h+1} \qquad (0 \le h \le d),$$

with $A_{-1} = A_{d+1} = 0$. Consequently the linear span $\mathfrak{M}(\Gamma) = \operatorname{span}\{A_0, \dots, A_d\}$ is a commutative matrix algebra of dimension $d + 1$, the *Bose–Mesner algebra* of Γ, and it coincides with the algebra generated by A.

Definition 2.3 ([4,5]). The *intersection matrix* of Γ is the tridiagonal matrix B of order $d+1$ with diagonal $(a_0, a_1, \dots, a_d)$, superdiagonal $(b_0, \dots, b_{d-1})$ and subdiagonal $(c_1, \dots, c_d)$. Its eigenvalues are exactly the $d+1$ distinct eigenvalues $k = \theta_0 > \theta_1 > \cdots > \theta_d$ of A. For each eigenvalue θ the *cosine sequence* $u_0(\theta), \dots, u_d(\theta)$ is defined by

$$u_0 = 1, \qquad u_1 = \theta/k, \qquad c_h u_{h-1} + a_h u_h + b_h u_{h+1} = \theta\, u_h \quad (1 \le h \le d-1).$$

The multiplicity of θ_i is

$$m_i = \frac{n}{\sum_{h=0}^{d} k_h\, u_h(\theta_i)^2},$$

and the orthogonal projection E_i onto the θ_i-eigenspace has entries $(E_i)_{xy} = \frac{m_i}{n}\, u_{\partial(x,y)}(\theta_i)$. In particular $E_0 = \frac{1}{n}\mathbb{1}\mathbb{1}^{\top}$, and $E_0, \dots, E_d$ form a second basis of $\mathfrak{M}(\Gamma)$.

Definition 2.4 ([7,17]). The *Laplacian* of Γ is $L = kI - A$. Its eigenvalues are $\lambda_i = k - \theta_i$, so that

$$0 = \lambda_0 < \lambda_1 < \cdots < \lambda_d, \qquad L = \sum_{i=0}^{d} \lambda_i\, E_i.$$

We write $\lambda_\star = \lambda_1$ for the algebraic connectivity [10] and $\lambda^\star = \lambda_d$ for the largest Laplacian eigenvalue, and we call

$$\chi(\Gamma) = \frac{\lambda^\star}{\lambda_\star}$$

the *stiffness index* of Γ. For every connected k-regular graph $\lambda^\star \le 2k$, with equality if and only if the graph is bipartite [6,17]. For a distance-regular graph this happens if and only if $a_1 = a_2 = \cdots = a_d = 0$.

Definition 2.5. Let $\kappa > 0$, let $\varphi\colon J \to \mathbb{R}$ be a C^1 function on a closed interval J, and let $\Phi(\mathbf{v})$ denote the vector with entries $\varphi\big(\mathbf{v}(x)\big)$. The reaction–diffusion problem on Γ is

$$\mathbf{u}'(t) = -\kappa L\, \mathbf{u}(t) + \Phi\big(\mathbf{u}(t)\big), \qquad \mathbf{u}(0) = \mathbf{u}^0 \in J^X. \qquad (2.1)$$

We assume that φ is Lipschitz on J with constant $\ell \ge 0$. A typical example is the Fisher–KPP nonlinearity $\varphi(s) = r\, s(1-s)$ with $J = [0,1]$ and $\ell = r$ [20].

Definition 2.6. Fix a step $\tau > 0$, put $t_m = m\tau$ and write $\mathbf{U}^m \approx \mathbf{u}(t_m)$. The *explicit Euler scheme* (EE) and the *IMEX Euler scheme* (IE) are

$$\mathbf{U}^{m+1} = T_\tau \mathbf{U}^m + \tau\, \Phi\big(\mathbf{U}^m\big), \qquad T_\tau = I - \tau\kappa L, \qquad (2.2)$$

$$\mathbf{U}^{m+1} = S_\tau \Big(\mathbf{U}^m + \tau\, \Phi\big(\mathbf{U}^m\big)\Big), \qquad S_\tau = (I + \tau\kappa L)^{-1}. \qquad (2.3)$$

The scheme (2.3) treats diffusion implicitly and reaction explicitly, as in [1]. We also use the *deviation* $\mathbf{W}^m = (I - E_0)\mathbf{U}^m$, that is, $\mathbf{U}^m$ minus its mean value $\bar{U}^m$.

3. Main Results

The first result says that the implicit propagator never leaves the Bose–Mesner algebra, and that it can be written down from the intersection array alone.

Theorem 3.1. Let Γ be distance-regular with intersection array $\iota(\Gamma)$, and let $\tau > 0$. Then $S_\tau \in \mathfrak{M}(\Gamma)$ and

$$S_\tau = \sum_{h=0}^{d} \rho_h(\tau)\, A_h, \qquad \rho_h(\tau) = \frac{1}{n} \sum_{i=0}^{d} \frac{m_i\, u_h(\theta_i)}{1 + \tau\kappa\lambda_i}. \qquad (3.1)$$

Moreover $S_\tau = p_\tau(L)$, where p_τ is the unique polynomial of degree at most d with $p_\tau(\lambda_i) = (1 + \tau\kappa\lambda_i)^{-1}$ for $i = 0, \ldots, d$. Hence $S_\tau \mathbf{v}$ can be computed exactly with d multiplications by L, that is, with $O(dnk)$ arithmetic operations and $O(nk)$ memory.

Proof. Since $L = \sum_i \lambda_i E_i$ and the E_i are mutually orthogonal idempotents summing to I, we have $I + \tau\kappa L = \sum_i (1 + \tau\kappa\lambda_i) E_i$. Every factor $1 + \tau\kappa\lambda_i$ is at least 1, so the inverse exists and equals $\sum_i (1 + \tau\kappa\lambda_i)^{-1} E_i$. Inserting $(E_i)_{xy} = \frac{m_i}{n} u_{\partial(x,y)}(\theta_i)$ shows that $(S_\tau)_{xy}$ depends only on $h = \partial(x, y)$ and equals $\rho_h(\tau)$, which is (3.1). For the second claim, $p_\tau(L) = \sum_i p_\tau(\lambda_i) E_i = \sum_i (1 + \tau\kappa\lambda_i)^{-1} E_i = S_\tau$. The interpolation problem is uniquely solvable because the λ_i are distinct. Evaluating $p_\tau(L)\mathbf{v}$ by a Horner or Clenshaw recurrence requires d products with L, each costing $O(nk)$ operations since L has $n(k + 1)$ nonzero entries. ▫

Remark 3.2. The data entering (3.1), namely θ_i, m_i and $u_h(\theta_i)$, are computed from B in $O(d^3)$ operations, independently of n. The same argument applies to any rational or entire function of L that is defined on the spectrum. In particular the propagator $e^{-\tau\kappa L}$ used by exponential integrators [8,14], and the Crank–Nicolson factor $(I + \tau\kappa/2\, L)^{-1}(I - \tau\kappa/2\, L)$, are again polynomials of degree at most d in L with distance-dependent entries.

Proposition 3.3. For every $\tau > 0$ the matrix S_τ is entrywise positive and $S_\tau \mathbb{1} = \mathbb{1}$. Equivalently, $\rho_h(\tau) > 0$ for $0 \le h \le d$ and $\sum_{h=0}^{d} k_h\, \rho_h(\tau) = 1$.

Proof. The matrix $I + \tau\kappa L$ has positive diagonal, nonpositive off-diagonal entries and is strictly diagonally dominant, so it is a nonsingular M-matrix. It is irreducible because Γ is connected, and the inverse of an irreducible nonsingular M-matrix is entrywise positive [23]. Since $L\mathbb{1} = 0$ we have $(I + \tau\kappa L)\mathbb{1} = \mathbb{1}$, hence $S_\tau \mathbb{1} = \mathbb{1}$. Reading this identity on a single row and grouping the vertices by their distance from that row gives $\sum_h k_h \rho_h(\tau) = 1$.

Corollary 3.4. Suppose that $s + \tau\varphi(s) \in J$ for all $s \in J$. If $\mathbf{U}^0 \in J^X$, then the IMEX iterates (2.3) satisfy $\mathbf{U}^m \in J^X$ for all $m \ge 0$. For the Fisher–KPP nonlinearity on $J = [0,1]$ the hypothesis holds whenever $\tau r \le 1$.

Proof. If $\mathbf{U}^m \in J^X$ then $\mathbf{U}^m + \tau\Phi(\mathbf{U}^m) \in J^X$ by hypothesis. By Proposition 3.3 each entry of $S_\tau\left(\mathbf{U}^m + \tau\Phi(\mathbf{U}^m)\right)$ is a convex combination of entries lying in the interval J, so it lies in J. For $\varphi(s) = rs(1 - s)$ the map $s \mapsto s + \tau rs(1 - s)$ is nondecreasing on [0,1] when $\tau r \le 1$ and fixes 0 and 1. ▫

The next theorem isolates the effect of the graph on the explicit scheme.

Theorem 3.5. Let Γ be distance-regular and $T_\tau = I - \tau\kappa L$.

The powers T_τ^m are bounded in the Euclidean norm, uniformly in m, if and only if $\tau\kappa\lambda^\star \le 2$. In that case $\| T_\tau \| = 1$.

$\| T_\tau \|_\infty \le 1$ if and only if $\tau\kappa k \le 1$, and in that case T_τ is entrywise nonnegative, so the scheme satisfies a discrete maximum principle.

$\frac{1}{\kappa k} \le \frac{2}{\kappa\lambda^\star}$, with equality if and only if Γ is bipartite, that is, if and only if $a_h = 0$ for every h.

Proof. (a) $T_\tau = \sum_i (1-\tau\kappa\lambda_i)\,E_i$ is symmetric, so $\| T_\tau^m \| = \max_i |1-\tau\kappa\lambda_i|^m$. Because $\lambda_0 = 0$ the maximum is at least 1, and it equals 1 exactly when $|1-\tau\kappa\lambda_i| \le 1$ for all i. Since $0 \le \lambda_i \le \lambda^\star$, this is equivalent to $\tau\kappa\lambda^\star \le 2$. If the condition fails, $|1-\tau\kappa\lambda_d| > 1$ and $\| T_\tau^m \| \to \infty$. (b) Each row of T_τ has diagonal entry $1-\tau\kappa k$ and k off-diagonal entries equal to $\tau\kappa$. Hence $\| T_\tau \|_\infty = |1-\tau\kappa k| + \tau\kappa k$, which equals 1 if $\tau\kappa k \le 1$ and equals $2\tau\kappa k - 1 > 1$ otherwise. Nonnegativity of the entries is the same condition. (c) This follows from $\lambda^\star \le 2k$, with equality exactly in the bipartite case (Definition 2.4). ▫

Remark 3.6. Part (c) has a concrete reading. On a non-bipartite distance-regular graph the explicit scheme can be stable in ℓ^2 while it already violates the maximum principle; the window is $\frac{1}{\kappa k} < \tau \le \frac{2}{\kappa\lambda^\star}$. For the Petersen graph ($k = 3$, $\lambda^\star = 5$) this window is $\frac{1}{3} < \tau\kappa \le \frac{2}{5}$. On a bipartite graph, such as the Heawood graph or the hypercube Q_m, the window is empty.

We turn to the nonlinear problem near a spatially homogeneous equilibrium $u^* \in J$, that is, $\varphi(u^*) = 0$, and we put $\gamma = -\varphi'(u^*)$.

Theorem 3.7. Assume $\gamma > 0$. The constant state $u^*\mathbb{1}$ is a fixed point of both schemes, and:

it is linearly asymptotically stable for (2.2) if and only if $0 < \tau < \frac{2}{\kappa\lambda^\star + \gamma}$;

it is linearly asymptotically stable for (2.3) if and only if $0 < \tau < \frac{2}{\gamma}$.

Proof. The Jacobian of the map (2.2) at $u^*\mathbb{1}$ is $I - \tau(\kappa L + \gamma I) = \sum_i \big(1 - \tau(\kappa\lambda_i + \gamma)\big) E_i$. Linear asymptotic stability holds if and only if $|1-\tau(\kappa\lambda_i+\gamma)| < 1$ for all i, that is, $0 < \tau(\kappa\lambda_i + \gamma) < 2$. The left inequality holds since $\gamma > 0$, and the right one is most restrictive at $i = d$. For (2.3) the Jacobian is $(1-\tau\gamma)S_\tau = \sum_i \frac{1-\tau\gamma}{1+\tau\kappa\lambda_i} E_i$. The modulus of the i-th factor is largest at $i = 0$, where it equals $|1-\tau\gamma|$, and $|1-\tau\gamma| < 1$ if and only if $0 < \tau < 2/\gamma$.

Remark 3.8. Theorem 3.7 answers the question raised in the introduction in its simplest form. For the explicit scheme the stability threshold is a function of $\lambda^\star = k - \theta_d$ alone, so it is known once the smallest eigenvalue of B is known. For the IMEX scheme the threshold does not depend on Γ at all. When τ crosses the bound in (a), the eigenvalue $1-\tau(\kappa\lambda^\star+\gamma)$ of the Jacobian crosses -1. This is a period-doubling bifurcation of the discrete map, and it produces bounded spurious oscillations rather than blow-up, in agreement with the general theory of spurious solutions of time discretisations [21,24]. Section 4 confirms this numerically.

The next result concerns the decay of the deviation $\mathbf{W}^m$, that is, the tendency of the discrete solution to become spatially uniform.

Theorem 3.9. Assume that all iterates take values in the interval J on which φ is ℓ-Lipschitz (for instance, under the hypothesis of Corollary 3.4).

For the IMEX scheme (2.3),

$$\| \mathbf{W}^m \| \le \varrho_I^m \, \| \mathbf{W}^0 \|, \qquad \varrho_I = \frac{1+\tau\ell}{1+\tau\kappa\lambda_\star}.$$

For the explicit scheme (2.2) with $\tau\kappa\lambda^\star \le 2$,

$$\| \mathbf{W}^m \| \le \varrho_E^m \, \| \mathbf{W}^0 \|, \qquad \varrho_E = \max\{|1-\tau\kappa\lambda_\star|,\ |1-\tau\kappa\lambda^\star|\} + \tau\ell.$$

In particular, if $\kappa\lambda_\star > \ell$, the IMEX deviation decays for every $\tau > 0$, and the explicit deviation decays for every $0 < \tau \le \tau_{\mathrm{opt}} = \frac{2}{\kappa(\lambda_\star+\lambda^\star)}$, with $\varrho_E = 1 - \tau(\kappa\lambda_\star - \ell)$.

Proof. (a) The matrix S_τ commutes with E_0, and $(I - E_0)\mathbb{1} = 0$. Writing $\mathbf{G}^m = \Phi(\mathbf{U}^m) - \varphi(\bar{U}^m)\mathbb{1}$, we obtain from (2.3)

$$\mathbf{W}^{m+1} = S_\tau(I - E_0)\left(\mathbf{U}^m + \tau\Phi(\mathbf{U}^m)\right) = S_\tau\left(\mathbf{W}^m + \tau(I - E_0)\mathbf{G}^m\right).$$

The mean $\bar{U}^m$ lies in J because J is an interval, so $\left|\varphi\left(\mathbf{U}^m(x)\right) - \varphi(\bar{U}^m)\right| \le \ell\,|\mathbf{W}^m(x)|$ and therefore $\| (I - E_0)\mathbf{G}^m \| \le \| \mathbf{G}^m \| \le \ell \| \mathbf{W}^m \|$. The vector in parentheses lies in the range of $I - E_0 = \sum_{i\ge1} E_i$, on which S_τ has norm $\max_{i\ge1}(1 + \tau\kappa\lambda_i)^{-1} = (1 + \tau\kappa\lambda_\star)^{-1}$. Hence $\| \mathbf{W}^{m+1} \| \le \varrho_I \| \mathbf{W}^m \|$. (b) In the same way $\mathbf{W}^{m+1} = T_\tau\mathbf{W}^m + \tau(I - E_0)\mathbf{G}^m$, and the norm of T_τ on the range of $I - E_0$ is $\max_{i\ge1}|1 - \tau\kappa\lambda_i|$. As a function of $\lambda \in [\lambda_\star, \lambda^\star]$ the quantity $|1 - \tau\kappa\lambda|$ is convex, so its maximum is attained at an endpoint. If $\tau \le \tau_{\mathrm{opt}}$, the maximum equals $1 - \tau\kappa\lambda_\star$. ▫

Corollary 3.10. Let $\ell = 0$, so that the deviation evolves under diffusion only. At $\tau = \tau_{\mathrm{opt}}$ the explicit scheme reduces the deviation by the factor $\frac{\chi(\Gamma)-1}{\chi(\Gamma)+1}$ per step. Consequently the number of explicit steps needed to reduce $\| \mathbf{W} \|$ by a factor $\varepsilon \in (0,1)$ is of order $\frac{1}{2}\chi(\Gamma)\ln(1/\varepsilon)$ when $\chi(\Gamma)$ is large. For the complete graph K_n one has $\chi = 1$ and $T_{\tau_{\mathrm{opt}}} = E_0$, so a single step produces the exact mean.

Proof. At τ_{opt} both endpoint values in Theorem 3.9(b) equal $\frac{\lambda^\star-\lambda_\star}{\lambda^\star+\lambda_\star} = \frac{\chi-1}{\chi+1}$. The step count follows from $\ln\frac{\chi+1}{\chi-1} = \frac{2}{\chi} + O(\chi^{-3})$. For K_n we have $L = nI - \mathbb{1}\mathbb{1}^\top$ and $\tau_{\mathrm{opt}}\kappa = 1/n$, hence $I - \frac{1}{n}L = \frac{1}{n}\mathbb{1}\mathbb{1}^\top = E_0$. ▫

We finally bound the global error of the IMEX scheme.

Theorem 3.11. Let $\mathbf{u} \in C^2([0,T];\mathbb{R}^X)$ solve (2.1), assume that $\mathbf{u}(t)$ and all IMEX iterates take values in J, and put $M_j = \max_{0\le t\le T} \| \mathbf{u}^{(j)}(t) \|$ for $j = 1,2$. Then, for $t_m \le T$,

$$\| \mathbf{u}(t_m) - \mathbf{U}^m \| \le \tau\, t_m\, e^{\ell t_m}\left(\frac{M_2}{2} + \ell M_1\right). \qquad (3.2)$$

Proof. Define the defect $\mathbf{R}^m$ by $(I + \tau\kappa L)\mathbf{u}(t_{m+1}) = \mathbf{u}(t_m) + \tau\Phi(\mathbf{u}(t_m)) + \tau\mathbf{R}^m$. Using (2.1) at t_{m+1},

$$\tau\mathbf{R}^m = [\mathbf{u}(t_{m+1}) - \mathbf{u}(t_m) - \tau\mathbf{u}'(t_{m+1})] + \tau\left[\Phi(\mathbf{u}(t_{m+1})) - \Phi(\mathbf{u}(t_m))\right].$$

Taylor's theorem bounds the first bracket by $\frac{\tau^2}{2}M_2$, and the Lipschitz property bounds the second by $\ell\tau M_1$, so $\| \mathbf{R}^m \| \le \tau\left(\frac{M_2}{2} + \ell M_1\right)$. The error $\mathbf{e}^m = \mathbf{u}(t_m) - \mathbf{U}^m$ satisfies $\mathbf{e}^{m+1} = S_\tau\left(\mathbf{e}^m + \tau\left[\Phi(\mathbf{u}(t_m)) - \Phi(\mathbf{U}^m)\right] + \tau\mathbf{R}^m\right)$. Since $\| S_\tau \| = \max_i(1 + \tau\kappa\lambda_i)^{-1} = 1$, we get $\| \mathbf{e}^{m+1} \| \le (1 + \tau\ell) \| \mathbf{e}^m \| + \tau \| \mathbf{R}^m \|$. With $\mathbf{e}^0 = 0$ this gives $\| \mathbf{e}^m \| \le \tau\max_j \| \mathbf{R}^j \| \sum_{j=0}^{m-1}(1 + \tau\ell)^j \le t_m e^{\ell t_m}\max_j \| \mathbf{R}^j \|$, which is (3.2). ▫

Remark 3.12. The bound (3.2) holds for every $\tau > 0$, because $\| S_\tau \| = 1$ independently of the step. The same proof applied to (2.2) uses $\| T_\tau \| = 1$ and is therefore valid only under the restriction $\tau\kappa\lambda^\star \le 2$ of Theorem 3.5. The graph enters (3.2) only through M_1 and M_2. Since $\mathbf{u}'' = -\kappa L\mathbf{u}' + \Phi'(\mathbf{u})\mathbf{u}'$, a crude estimate gives $M_2 \le (\kappa\lambda^\star + \ell)M_1$; the error constant can therefore grow with $\lambda^\star$, although in practice the high-frequency components are damped quickly and the bound is pessimistic.

Remark 3.13. Several of the graphs considered here are Cayley graphs, which links the present analysis with the classification of distance-regular Cayley graphs. The hypercube Q_m is $\mathrm{Cay}(\mathbb{Z}_2^m, \{e_1, \dots, e_m\})$. On the dihedral group $D_{2n} = \langle a, b \mid a^n = b^2 = 1,\ bab = a^{-1} \rangle$ the cycle C_{2n} arises as $\mathrm{Cay}(D_{2n}, \{b, ab\})$, the complete bipartite graph $K_{n,n}$ as the Cayley graph with respect to all n reflections, and the Heawood graph as $\mathrm{Cay}(D_{14}, \{b, ab, a^3b\})$, the incidence graph of the planar difference set $\{0,1,3\} \subset \mathbb{Z}_7$. For $K_{n,n}$ the Laplacian eigenvalues are $0, n, 2n$, so $\chi = 2$ and the explicit limits of Theorem 3.5 both equal $\tau\kappa = 1/n$. For C_{2n} one has $\lambda_\star = 2 - 2\cos(\pi/n)$ and $\lambda^\star = 4$, so $\chi(C_{2n}) \sim 4n^2/\pi^2$, and the explicit scheme behaves like a standard finite-difference grid in one dimension [16].

4. Worked Example and Numerical Experiments

Example 4.1 (Petersen graph). Here $\iota(\Gamma) = \{3,2; 1,1\}$, $n = 10$, $d = 2$, $k_1 = 3$, $k_2 = 6$, and B has eigenvalues $3, 1, -2$ with multiplicities 1,5,4. The cosine sequences are (1,1,1), $\left(1, \frac{1}{3}, -\frac{1}{3}\right)$ and $\left(1, -\frac{2}{3}, \frac{1}{6}\right)$, and the Laplacian eigenvalues are 0,2,5. Writing $s = \tau\kappa$ and substituting into (3.1), a short computation gives

$$\rho_0(s) = \frac{1 + 4s + s^2}{(1 + 2s)(1 + 5s)}, \qquad \rho_1(s) = \frac{s(1 + s)}{(1 + 2s)(1 + 5s)}, \qquad \rho_2(s) = \frac{s^2}{(1 + 2s)(1 + 5s)}.$$

One checks directly that $\rho_0 + 3\rho_1 + 6\rho_2 = 1$, as required by Proposition 3.3, and that $\rho_0 > \rho_1 > \rho_2 > 0$ for every $s > 0$. For $s = 0.1$ the three values are 0.78333, 0.06111 and 0.00556, and they agree with a direct inversion of $I + 0.1L$ to within 10^{-16}. The explicit limits are $s \le \frac{1}{3}$ in ℓ^∞ and $s \le \frac{2}{5}$ in ℓ^2, while $\chi = \frac{5}{2}$.

All computations below were carried out in Python with NumPy, SciPy and NetworkX, in double precision. The intersection arrays in Table 1 were recomputed from the graphs themselves, and the spectra were obtained independently from B and from L; the two agree to machine precision.

Table 1. Spectral data of the six test graphs.

Graph	n	k	d	$\iota(\Gamma)$	$\lambda_\star$	$\lambda^\star$	$\chi(\Gamma)$	bipartite
K_8	8	7	1	{7; 1}	8	8	1.000	no
Petersen	10	3	2	{3,2; 1,1}	2	5	2.500	no
Paley $P(13)$	13	6	2	{6,3; 1,3}	4.6972	8.3028	1.768	no
Heawood	14	3	3	{3,2,2; 1,1,3}	1.5858	6	3.784	yes
Q_4	16	4	4	{4,3,2,1; 1,2,3,4}	2	8	4.000	yes
C_{12}	12	2	6	{2,1,1,1,1,1; 1,1,1,1,1,2}	0.2679	4	14.928	yes

Experiment 1 (stability threshold of EE). We took the Fisher–KPP nonlinearity with $r = 1$ and $\kappa = 1$, so that $u^* = 1$ and $\gamma = 1$. The initial data were $1 + \eta$ with η uniformly distributed in $[-0.05, 0.05]$. A step was declared stable if the deviation from u^* fell below 10^{-3} of its initial size within 2×10^4 steps, and the largest stable step was located by bisection. Table 2 compares it with the value $\tau^* =$

$2/(\kappa\lambda^{\star}+\gamma)$ of Theorem 3.7(a). The residual discrepancy of order 10^{-4} comes from the finite number of steps, since the contraction factor tends to 1 at the threshold. The last column reports the amplitude $\max_x|\mathbf{U}^m(x)-1|$ after 2×10^4 steps with $\tau=1.03\,\tau^*$. In every case the iterates settle on a bounded period-two orbit, as described in Remark 3.8, and not on the equilibrium.

Table 2. Predicted and observed explicit stability thresholds (Fisher–KPP, $\gamma=1$).

Graph	$\lambda^{\star}$	**predicted** τ^*	**observed**	**relative gap**	**2-cycle amplitude at** $1.03\tau^*$
K_8	8	0.22222	0.22219	1.6×10^{-4}	0.469
Petersen	5	0.33333	0.33328	1.5×10^{-4}	0.309
Paley $P(13)$	8.3028	0.21499	0.21496	1.6×10^{-4}	0.568
Heawood	6	0.28571	0.28568	1.2×10^{-4}	0.405
Q_4	8	0.22222	0.22219	1.4×10^{-4}	0.469
C_{12}	4	0.40000	0.39994	1.4×10^{-4}	0.333

Experiment 2 (convergence of IE). With $r=1$, $\kappa=1$, $T=1$ and initial data uniform in [0,1], we compared the IMEX solution with a reference solution computed by the Radau IIA method [13] with relative tolerance 10^{-12}. Table 3 lists the root-mean-square error $\|\mathbf{e}\|/\sqrt{n}$ and the experimental order of convergence (EOC). The order tends to 1, in accordance with Theorem 3.11. The two graphs with the smallest $\lambda^{\star}$ relative to k do not have the largest errors, which illustrates that (3.2) is an upper bound and not an asymptotic identity.

Table 3. IMEX Euler: RMS error at $T=1$ and EOC.

Graph	$\tau=0.1$	0.05	0.025	0.0125	0.00625	**final EOC**
K_8	3.27×10^{-3}	1.47×10^{-3}	6.86×10^{-4}	3.30×10^{-4}	1.62×10^{-4}	1.030
Petersen	6.05×10^{-3}	2.96×10^{-3}	1.46×10^{-3}	7.28×10^{-4}	3.63×10^{-4}	1.004
Paley $P(13)$	3.84×10^{-3}	1.76×10^{-3}	8.33×10^{-4}	4.05×10^{-4}	1.99×10^{-4}	1.022
Heawood	6.35×10^{-3}	3.13×10^{-3}	1.55×10^{-3}	7.73×10^{-4}	3.86×10^{-4}	1.003
Q_4	4.30×10^{-3}	2.06×10^{-3}	1.01×10^{-3}	4.97×10^{-4}	2.47×10^{-4}	1.009
C_{12}	6.82×10^{-3}	3.32×10^{-3}	1.64×10^{-3}	8.14×10^{-4}	4.05×10^{-4}	1.005

Experiment 3 (homogenisation). With $r=0.5$ (so $\ell=0.5$ on [0,1]), $\kappa=1$, $\tau=0.05$ and initial data uniform in [0.2,0.4], we measured the mean contraction factor $\left(\|\mathbf{W}^{40}\|/\|\mathbf{W}^{0}\|\right)^{1/40}$ of the IMEX deviation and compared it with ϱ_I from Theorem 3.9(a). Table 4 shows that the bound holds in every case where $\kappa\lambda_{\star}>\ell$. For C_{12} the condition fails, $\varrho_I>1$, and the theorem gives no information; nevertheless the deviation still decays. This is expected, since the Lipschitz constant $\ell=r$

overestimates the local slope $r(1-2s)$ for the values reached by the solution, and it shows that the condition $\kappa\lambda_\star > \ell$ is sufficient but not necessary.

Table 4. IMEX homogenisation: bound ϱ_I versus the observed contraction factor.

Graph	$\lambda_\star$	$\kappa\lambda_\star > \ell$	bound ϱ_I	observed	diffusion only $(1+\tau\kappa\lambda_\star)^{-1}$
K_8	8	yes	0.73214	0.71885	0.71429
Petersen	2	yes	0.93182	0.90109	0.90909
Paley $P(13)$	4.6972	yes	0.83005	0.80382	0.80981
Heawood	1.5858	yes	0.94970	0.90560	0.92654
Q_4	2	yes	0.93182	0.89950	0.90909
C_{12}	0.2679	no	1.01145	0.95983	0.98678

Experiment 4 (cost of the implicit step). For four larger distance-regular graphs we applied S_τ with $\tau\kappa = 0.1$ in three ways: by the degree-d polynomial of Theorem 3.1, evaluated through a Clenshaw recurrence in the Chebyshev basis on $[0, \lambda^\star]$; by a sparse LU factorisation computed once and then reused; and by a dense solver. The interpolation coefficients were computed from the $d+1$ Laplacian eigenvalues only. Table 5 reports the relative difference from the sparse direct solution, average wall-clock times, and the number of nonzeros in the LU factors compared with that of L. The polynomial form is exact to rounding error, needs no factorisation and no extra storage, and its cost per application is of the same order as a triangular solve with precomputed factors. The factors themselves are between 13 and 48 times denser than L on these examples. Timings of this size depend on the implementation and the hardware, so they should be read as orders of magnitude only.

Table 5. Applying S_τ on larger distance-regular graphs ($\tau\kappa = 0.1$).

Graph	n	k	d	relative error	polynomial (s)	LU factor (s)	LU solve (s)	dense solve (s)	nnz(LU)/nnz(L)
Hamming $H(4,4)$	256	12	4	5.6×10^{-16}	4.9×10^{-5}	1.9×10^{-3}	3.4×10^{-5}	7.0×10^{-4}	13.3
Johnson $J(12,4)$	495	32	4	8.5×10^{-16}	1.7×10^{-4}	1.5×10^{-2}	1.9×10^{-4}	4.8×10^{-3}	10.7
Hamming $H(6,3)$	729	12	6	9.0×10^{-16}	1.4×10^{-4}	3.4×10^{-2}	3.3×10^{-4}	9.8×10^{-3}	39.9
Hypercube Q_{10}	1024	10	10	9.1×10^{-16}	1.6×10^{-4}	4.2×10^{-2}	4.3×10^{-4}	2.8×10^{-2}	48.2

5. Discussion

The results of Section 3 split naturally into two groups. Theorem 3.1, Proposition 3.3 and Theorem 3.7(b) say that the implicit treatment of diffusion is insensitive to the graph, apart from the cost of applying S_τ, which Theorem 3.1 reduces to d sparse products. Theorems 3.5, 3.7(a) and 3.9(b) say that the explicit treatment depends on Γ through exactly two numbers, $\lambda_\star = k - \theta_1$ and $\lambda^\star = k - \theta_d$, both of which are eigenvalues of the tridiagonal matrix B. In this sense the intersection array predicts the

numerical stability of the explicit scheme before any simulation, and Table 2 shows that the prediction is sharp.

Some limitations should be stated plainly. First, nothing in Theorem 3.5 or Theorem 3.7 requires distance-regularity: both hold for any regular graph once $\lambda^{\star}$ is known. What distance-regularity adds is that $\lambda^{\star}$, $\lambda_{\star}$, the multiplicities and the full propagator are available from $d+1$ numbers and $O(d^3)$ work, and that the propagator has distance-dependent entries. Second, the computational gain of Theorem 3.1 is real only when d is small compared with n. For the cycle C_n we have $d = \lfloor n/2 \rfloor$, and the polynomial form brings no advantage over a banded solver. Third, we have treated a scalar equation. Turing instability requires at least two interacting species [18,19,22], and for systems the relevant object is the set of λ_i that fall into an unstable band of the dispersion relation. On a distance-regular graph that set is a subset of only $d+1$ values, which makes the classification of network-driven instabilities a finite problem. We regard this, together with higher-order IMEX and exponential schemes [1,8,14], as the natural continuation of the present work.

6. Conclusions

We studied the explicit and IMEX Euler discretisations of a scalar reaction–diffusion equation on a distance-regular graph and showed that their main numerical properties can be read off from the intersection array. The implicit propagator lies in the Bose–Mesner algebra, has positive distance-dependent entries given in closed form, and equals a polynomial of degree at most d in the Laplacian, so that it can be applied exactly without factorisation. The explicit scheme is stable in ℓ^2 if and only if $\tau\kappa\lambda^{\star} \le 2$, its maximum-norm limit is $\tau\kappa k \le 1$, and the two coincide precisely for bipartite graphs. The linearised threshold at a stable homogeneous state is $2/(\kappa\lambda^{\star}+\gamma)$ for the explicit scheme and $2/\gamma$ for the IMEX scheme. The rate at which discrete solutions become uniform is governed by the algebraic connectivity, and the efficiency of the explicit scheme is governed by the stiffness index $\chi(\Gamma)$. Numerical experiments on ten distance-regular graphs agree with all of these statements, and the predicted stability thresholds are recovered with a relative gap of order 10^{-4}.

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