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EXPLOSIVE BEHAVIOR IN SPATIALLY DISCRETE REACTION-DIFFUSION SYSTEMS

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Abstract. Explosive instabilities in spatially discrete reaction-diffusion systems are studied. We identify classes of initial data developing singularities in finite time and obtain predictions of the blow-up times, whose accuracy is checked by comparison with numerical solutions. We present averaged and local blow-up estimates. Local blow-up results show that it is possible to have blow-up after blow-up. Conditions excluding or implying blow-up at space infinity are discussed.

1. **Introduction.** Continuous reaction-diffusion models which exhibit explosive instabilities have important applications in plasma physics [1], chemical reactor design, combustion theory [2, 3], quantum and fluid mechanics [4], biology [5]. Such instabilities often represent an important change in the properties of the model, such as the ignition of a heated gas mixture, the formation of shocks or the origin of a spore in the chemotaxis of cellular aggregates. Detailed descriptions of of the structure of singularities in continuous models and analytical evidence of selfsimilar behavior can be found in [5, 6]. Rigorous blow-up predictions are available for nonlinear heat equations with sources, see [7, 8, 9] for instance. Considerable work has been done in understanding relevant analytical solutions and designing adaptive numerical schemes which fit the expected qualitative behavior [10, 11]. Since computation on fixed meshes may entirely miss blow-up or qualitatively change the blow-up region and structure, most efforts in the numerical solution of continuous reaction-diffusion systems are centered in the design of multiscale meshes to capture changes on increasingly small length scales as the singularities develop, see the review [12].

Continuum limits often fail to reproduce phenomena taking place at atomic or cellular scales in physical and biological systems comprising interacting smaller components such as atoms, quantum wells, cells... In this paper, we study explosive

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instabilities in spatially discrete reaction-diffusion systems formulated on a fixed spatial lattice that is determined by the underlying molecular or cellular structure. Theoretical results are needed to distinguish unbounded growth from finite time blow-up in numerical tests. Typical contexts in which spatial discreteness becomes important are related to pattern formation in cellular lattices [13], growth of cellular aggregates [14], the lifetime of molecular aggregates [15], nucleation [16], crystal growth and interface motion [17], motion of domain walls in semiconductor superlattices [18] and so on. Many elementary models take the forms

$$u_n' = d(u_n)(u_{n+1} - 2u_n + u_{n-1}) + v(u_n)(u_{n-1} - u_n) + f(u_n), \quad (1)$$
$$u_n' = d_n(u_{n+1} - 2u_n + u_{n-1}) + v_n(u_{n-1} - u_n) + f(u_n), \quad (2)$$
$$u_n' = g(u_{n+1} - u_n) - g(u_n - u_{n-1}) + f(u_n), \quad (3)$$

where $f(u)$ represents a reactive source, $d(u), d_n$ diffusion coefficients, $v(u), v_n$ transport coefficients and g the derivative of some potential acting as nonlinear diffusion. Problems with a similar structure but particular scaling relationships between parameters may arise in the context of the method of lines with first order $u_{n+1} - u_n$ and second order differences $u_{n+1} - 2u_n + u_{n-1}$ replaced by $\frac{u_{n+1}-u_n}{h}$ and $\frac{u_{n+1}-2u_n+u_{n-1}}{h^2}$, $h \to 0$ being the lattice constant. This method constructs numerical approximations to the solutions of partial differential equations by first discretizing the spatial derivatives to replace the original model by a large system of ordinary differential equations. Conditions for semidiscretized semilinear heat equations to explode like its continuous counterparts have been given in [10, 19, 20, 21].

For models (1)-(3), a stable evolution is expected when the initial state is small enough for the spreading effect of diffusion and convection to act, see Figure 1. Whenever the initial state is large enough in one or several regions, explosive instabilities develop. We investigate the impact of discreteness on the spatial structure of the instabilities and find a number of conditions on the data and the parameters involved ensuring blow-up in finite time. Blow-up solutions are found by constructing a lower bound of the solution which tends to infinity at a finite time. From this lower bound of the solution an upper bound of the blow-up time can be estimated. Blow-up may occur at isolated components or at all of them. Selfsimilar patterns are lost, except when taking continuum limits. Local blow-up results show that it is possible to have a blow-up after a blow-up, see Figure 6. Explosions may develop at the same or different times in different regions. Most local results are intrinsically discrete, being lost when taking continuum limits.

The paper is organized as follows. In Section 2, we obtain blow-up results for positive solutions. These results are local, and hold for a large class of models, including nonlinear diffusion or convection terms, in bounded or unbounded domains, as long as they satisfy a maximum principle. In Section 3, we establish blow-up conditions without sign restrictions by energy arguments. Section 4 discusses blow-up at space infinity. In Section 5, we carry out several numerical experiments to test our predictions. Section 6 contains our conclusions.

2. **Explosive behavior of positive solutions.**

In this section, we focus on positive solutions of (1)-(3). The functions $f(u)$, $d(u)$, $v(u)$, $g(u)$ are assumed to be differentiable. Typical choices for the reactive source are $f(u) = u^p$, $p > 1$, or $f(u) = e^u$. The discrete spatial variable varies over a set I, that may be infinite $I = \mathbb{Z}$ or finite $I = \{1, ..., N\}$. When I is finite, we must specify boundary conditions

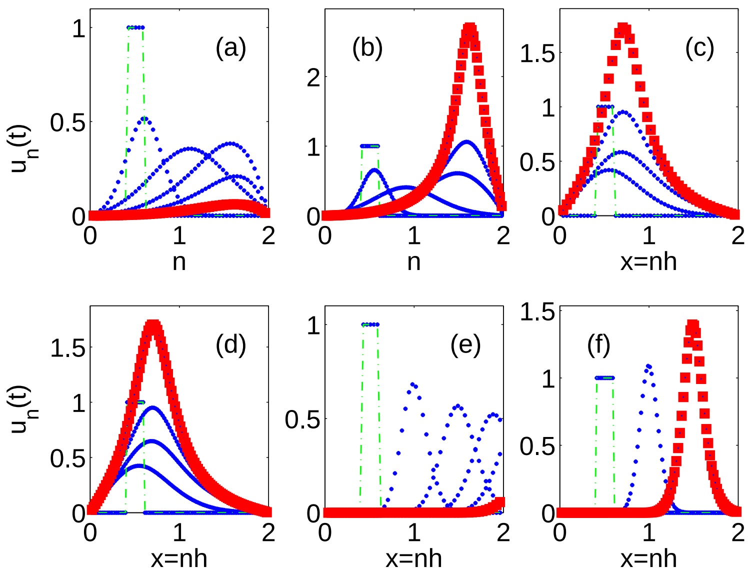

FIGURE 1. Time evolution computed with (37) for $u_n^0 = u_0(nh)$, $u_0(x) = \chi_{[0.4,0.6]}$, $u_0(t) = u_{N+1}(t) = 0$ and $h = \frac{2}{N+1}$, $d = \frac{\mu}{h^2}$, $v = \frac{\nu}{h}$: (a) $N = 50$, $\mu = 0.02$ and $\nu = 0.1$, (b) same with $N = 100$, blow-up at $T = 12.0781$, (c) $N = 50$, $\mu = 0.02$ and $\nu = 0$, blow-up at $T = 14.1935$, (d) same with $N = 100$, blow-up at $T = 13.7000$, (e) $N = 50$, $\mu = 0$ and $\nu = 1$, (f) same with $N = 100$, blow-up at $T = 1.3732$.

at the ends. For simplicity, we will choose non negative Dirichlet boundary conditions for u_0 and u_{N+1}. The choice of boundary conditions affects the blowing-up patterns.

Local in time existence of solutions $u_n(t)$ for initial value problems on a time interval $[0, T)$ is straightforward by rewriting (1)-(3) as differential equations with a locally Lipschitz right hand side, in $\mathbb{R}^N$ (when I is finite) or in spaces of sequences as $l^\infty(I)$ or $l^2(I)$ (when I is unbounded). Positive solutions are found when a maximum principle holds. This is guaranteed if $d(u) > 0, d(u) + v(u) > 0$ for $u > 0$ in (1), $d_n > 0, d_n + v_n > 0$ in (2) or g is increasing in (3). Under these hypotheses the three systems under study are 'cooperative'. This means that they share the general structure:

$$u_n' = h(t, u_{n+1}, u_n, u_{n-1}), \quad \frac{\partial h}{\partial u_{n+1}} > 0, \frac{\partial h}{\partial u_{n-1}} > 0, \tag{4}$$

where $h(t, x, y, z)$ is at least globally continuous with respect to all its variables and locally Lipschitz continuous with respect to (x, y, z). For such systems, when the initial data $u_n(0)$ and the boundary conditions $u_0(t)$, $u_{N+1}(t)$ (if any) are positive, the solution $u_n(t)$ remains positive. This is a consequence of the following comparison principle, see [22, 23, 24]:

Comparison principle. *Let $v_n(t)$ and $u_n(t)$ satisfy*

$$u_n' - h(t, u_{n+1}, u_n, u_{n-1}) \le v_n' - h(t, v_{n+1}, v_n, v_{n-1}), \quad 0 \le t < T, \tag{5}$$

for $n \in L$, where L may be any of the following sets: $\mathbb{Z}$, $\{n \le n_0\}$, $\{n \ge n_1\}$ or $\{n_0 \le n \le n_1\}$. In the latter cases, (5) holds at the extremes n_0 or n_1 with a slight modification: $u_{n_0-1} \le v_{n_0-1}$ or $u_{n_1+1} \le v_{n_1+1}$ are fixed. We assume that h is given by either (1),(2) or (3) and satisfies (4). Then, $u_n(0) \le v_n(0)$ for $n \in L$ implies $u_n(t) \le v_n(t)$ for $n \in L$ and $0 < t < T$, T being the maximal existence time.

Blow-up in finite time is established by using positivity to compare the solutions of (1)-(3) with solutions of explosive differential inequalities. We state below two local results. The first one applies to single components whereas the second one holds for a finite collection of them.

Theorem 2.1. *Let $u_n(t)$ be a non negative solution of (1), (2) or (3) with non negative initial data and a strong reactive source f such that $f(u) > Cu^p$ for large $u > 0$, with $p > 1$, $C > 0$.*

In (1), we set $a(u) = -(2d(u)+v(u))u+f(u)$ and assume that $d(u), d(u)+v(u) > 0$ grow slower than u^p for u large. For any component k such that $a(u_k(0)) > 0$ and $a'(u) > 0$ when $u > u_k(0)$

$$u_k(t) \to \infty \quad \text{as} \quad t \to T \le T_b = \int_{u_k(0)}^{\infty} \frac{ds}{a(s)} < \infty. \tag{6}$$

In (2), we assume $d_n > 0, d_n + v_n > 0$ for all n. For each k fixed, set $a(u) = -(2d_k + v_k)u + f(u)$. If $a(u_k(0)) > 0$ and $f'(u) > 2d_k + v_k$ when $u > u_k(0)$, then (6) holds. In particular, when $f(u) = u^p$, $p > 1$, and $u_k(0) > (2d_k + v_k)^{\frac{1}{p-1}}$

$$T_b = \frac{1}{\lambda(1-p)} \log(1 - \lambda u_k(0)^{1-p}), \quad \lambda = 2d_k + v_k. \tag{7}$$

In (3), we set $a(u) = g(-u) - g(u) + f(u)$ and assume that g is increasing. For any component k such that $a(u_k(0)) > 0$ and $a'(u) > 0$ when $u > u_k(0)$, (6) holds.

Proof. In all cases, the comparison principle ensures the positivity of $u_n(t)$ everywhere.

Using $u_{k+1}, u_{k-1} \ge 0$, we obtain the differential inequality $u_k'(t) \ge a(u_k)$. By hypothesis, $a(u) > a(u_k(0)) > 0$ for $u \ge u_k(0)$. Then $u_k(t)$ is increasing and it is bounded from below by the solution $y(t)$ of $y'(t) = a(y)$, $y(0) = u_k(0)$, which is given implicitly by:

$$t = \int_{u_k(0)}^{y(t)} \frac{ds}{a(s)}. \tag{8}$$

The integral $\int_{u_k(0)}^{\infty} \frac{ds}{a(s)} < \infty$ due to the growth condition $a(s) >> s^p$, $p > 1$, for s large. When $t \to T_b = \int_{u_k(0)}^{\infty} \frac{ds}{a(s)} < \infty$, $y(t) \to \infty$.

An analogous computation can be reproduced for (2). When $f(u) = u^p$, choosing $u_k(0) > (2d_k + v_k)^{\frac{1}{p-1}}$ ensures $a(u) > 0$ for $u \ge u_k(0)$. Then, $y(t)$ can be computed explicitly:

$$y(t) = e^{-\lambda t}\Big(\frac{1}{\lambda} e^{\lambda(1-p)t} - \frac{1}{\lambda} + u_k(0)^{1-p}\Big)^{\frac{1}{1-p}} \tag{9}$$

with $\lambda = 2d_k + v_k$ and $T_b = \frac{1}{\lambda(1-p)} \log(1 - \lambda u_k(0)^{1-p})$.

For (3), $g(u_{n+1} - u_n) \ge g(-u_n)$ and $g(u_n - u_{n-1}) \le g(u_n)$. Then, $u_k'(t) \ge a(u_k)$ and (6) follows as before. $\square$

Theorem 2.1 is a pointwise result ensuring blow-up of single components $u_k(t)$ for large $u_k(0)$. The condition on the size of the initial data can be relaxed for the semilinear problem (2) at the expense of increasing the amount of initial points k where $u_k(0)$ is large. Theorem 2.2 below proves local blow-up in a region $L = \{n_0, ..., n_1\}$ provided $u_{n_0}, ..., u_{n_1}$ are large enough. Single components within the region explode.

Let A_{dv} and A_d be the $M \times M$ matrices

$$A_{dv} = \begin{pmatrix} 2d_{n_0}+v_{n_0} & -d_{n_0+1}-v_{n_0+1} & 0 & 0 & ... & 0 \\ -d_{n_0} & 2d_{n_0+1}+v_{n_0+1} & -d_{n_0+2}-v_{n_0+2} & 0 & ... & 0 \\ & ... & ... & ... & ... & \\ 0 & ... & 0 & 0 & -d_{n_1-1} & 2d_{n_1}+v_{n_1} \end{pmatrix} \tag{10}$$

$$A_d = \begin{pmatrix} 2d_{n_0} & -d_{n_0+1} & 0 & 0 & 0 & ... & 0 \\ -d_{n_0} & 2d_{n_0+1} & -d_{n_0+2} & 0 & 0 & ... & 0 \\ 0 & -d_{n_0+1} & 2d_{n_0+2} & -d_{n_0+3} & 0 & ... & 0 \\ & ... & ... & ... & ... & ... & \\ 0 & 0 & ... & 0 & -d_{n_1-2} & 2d_{n_1-1} & -d_{n_1} \\ 0 & 0 & ... & 0 & 0 & -d_{n_1-1} & 2d_{n_1} \end{pmatrix} \tag{11}$$

with $M = n_1 - n_0 + 1 \le N$. Their k-th order leading principal minors δ_k satisfy the recurrences:

$$\delta_k = (2d_{n_0+k-1} + v_{n_0+k-1})\delta_{k-1} - d_{n_0+k-2}(d_{n_0+k-1} + v_{n_0+k-1})\delta_{k-2}, \tag{12}$$

$$\delta_k = 2d_{n_0+k-1}\delta_{k-1} - d_{n_0+k-2}d_{n_0+k-1}\delta_{k-2}, \tag{13}$$

respectively. Assuming $d_n > 0, d_n + v_n > 0$ and using recurrences (12) and (13), $\delta_k > d_{n_0+k-1}\delta_{k-1} > 0$ follows by induction since $\delta_1 > d_{n_0}\delta_0$ and $\delta_0 = 1 > 0$. Both matrices are definite positive and their eigenvalues are positive.

When $d_k = d$, A_d is also symmetric. Its smallest eigenvalue is $\lambda_1 = 2d(1 - \cos(\frac{\pi}{M+1}))$, with a normalized associated eigenvector $\phi_n = c\sin(\frac{n\pi}{M+1}) > 0$, $n = 1, ..., M$, where $c = \big(\sum_{n=1}^{M} \sin(\frac{n\pi}{M+1})\big)^{-1}$. For non symmetric A_{dv} and A_d, ϕ might fail to be positive, but it remains so if they are close to symmetric matrices.

Theorem 2.2. *Let $u_n(t)$ be a non negative solution of (2) with non negative initial data. The coefficients d_n+v_n and d_n are assumed to be positive for all n. The source $f(u)$ is positive and convex when $u > 0$, and satisfies $f(u) > Cu^p$ for u large, with $p > 1$, $C > 0$. We set $L = \{n_0, ..., n_1\} \subset I$ and define the positive definite matrices A_{dv}, A_d by (10) and (11).*

In any of the following two cases:

- *$\lambda_{dv,1} > 0$ is the smallest eigenvalue of A_{dv} and ϕ_i, $i = 1, ..., M$, an associated normalized eigenvector,*
- *$0 < v_n < v$ for $n \in L$, $\lambda_{d,1} > 0$ is the smallest eigenvalue of A_d and ϕ_i, $i = 1, ..., M$, an associated normalized eigenvector,*

we extend ϕ_i by $\phi_0 = \phi_{M+1} = 0$ and define $w(t) = \sum_{n\in L} u_n(t)\phi_{n-n_0+1}$. Let us set $\lambda = \lambda_{dv,1}$ in the first case and $\lambda = \lambda_{d,1} + v$ in the second one.

If ϕ is positive, $f'(u) > \lambda$ when $u > w(0)$ and $f(w(0)) > \lambda w(0)$, then $w(t) \to \infty$ as $t \to T \le T_b$, where

$$T_b = \int_{w(0)}^{\infty} \frac{ds}{-\lambda s + f(s)} < \infty. \tag{14}$$

In particular, when $f(u) = u^p$, $p > 1$, *and* $w(0) \geq \lambda^{\frac{1}{p-1}}$,

$$T_b = \frac{1}{\lambda(1-p)} \log\left(1 - \lambda w(0)^{1-p}\right). \tag{15}$$

Proof. The assumptions on the coefficients guarantee that u_n inherits the non negativity of the initial data.

For each $n \in L$, we multiply (2) by the corresponding component of the first eigenvector ϕ_{n-n_0+1} of A_{dv} and sum over L:

$$w'(t) = \sum_{n\in L}(d_n u_{n+1} - (2d_n + v_n)u_n + (d_n + v_n)u_{n-1})\phi_{n-n_0+1} + \sum_{n\in L} f(u_n)\phi_{n-n_0+1}.$$

The first sum can be rewritten as follows:

$$\begin{aligned}
&\sum_{n\in L}(d_n u_{n+1} - (2d_n + v_n)u_n + (d_n + v_n)u_{n-1})\phi_{n-n_0+1} \\
&= \sum_{n\in L}((d_{n+1} + v_{n+1})\phi_{n-n_0+2} - (2d_n + v_n)\phi_{n-n_0+1} + d_{n-1}\phi_{n-n_0})u_n \\
&\quad + (d_{n_0} + v_{n_0})\phi_1 u_{n_0-1} + d_{n_1}\phi_M u_{n_1+1} \geq -\lambda_{dv,1}\sum_{n\in L}\phi_{n-n_0+1}u_i.
\end{aligned}$$

For $u > 0$, f is convex, thus $\sum_{n\in L} f(u_n)\phi_{n-n_0+1} \geq f(\sum_{n\in L} u_n\phi_{n-n_0+1})$ and

$$w'(t) \geq -\lambda_{dv,1}w(t) + \sum_{n\in L} f(u_n(t))\phi_{n-n_0+1} \geq -\lambda_{dv,1}w(t) + f(w(t)).$$

The blow-up times (14) and (15) with $\lambda = \lambda_{d,1}$ are found as in Theorem 2.1.

Reproducing the same steps with the eigenvector of A_d we get

$$w' \geq \sum_{n\in L}(d_{n+1}\phi_{n-n_0+2} - 2d_n\phi_{n-n_0+1} + d_{n-1}\phi_{n-n_0})u_n - vw + \sum_{i\in L} f(u_n)\phi_{n-n_0+1}.$$

Thus,

$$w' \geq -(\lambda_{d,1} + v)w + \sum_{n\in L} f(u_n)\phi_{n-n_0+1} \geq -(\lambda_{d,1} + v)w + f(w)$$

and (14), (15) with $\lambda = \lambda_{d,1} + v$ follow. □

Theorem 2.1 and Theorem 2.2 hold for variable diffusion and convection. Theorem 2.1 is intrinsically discrete and it is lost in the continuum limit $h = \frac{1}{N+1}$, $d_n = \frac{d(nh)}{h^2}$, $v_n = \frac{v(nh)}{h}$. An example showing blow-up after a blow-up based on Theorem 2.2 will be given later in Section 5. Theorem 2.2 is intrinsically discrete for non vanishing convection.

Blow-up results for positive solutions of

$$\begin{array}{ll}
u_t = u_{xx} + f(u), & x \in (0,1),\ t > 0, \\
u(x,0) = u_0(x), & x \in (0,1), \\
u(0,t) = u(1,t) = 0, & t > 0,
\end{array} \tag{16}$$

using positive eigenfunctions were established in [7]. When $u_0(x) \in C([0,1])$ satisfies $f(\overline{w}(0)) > \pi^2\overline{w}(0)$, with $\overline{w}(0) = \int_0^1 \overline{\phi}(s)u_0(s)ds$ and $\overline{\phi} = \sin(\pi x)(\int_0^1 \sin(\pi s)ds)^{-1}$, the solution of (16) blows up at time $T \leq \overline{T}_b$:

$$\overline{T}_b = \int_{\overline{w}(0)}^{\infty} \frac{ds}{-\pi^2 s + f(s)}.$$

If we set $L = I = \{1, ..., N\}$ in Theorem 2.2 and add a superscript h to denote the dependence on h we see that

$$\lambda_1^h = 2(N+1)^2(1-\cos(\pi h)) \to \overline{\lambda}_1 = \pi^2$$

as $h \to 0$. For h small, $f(w^h(0)) > \lambda_1^h w^h(0)$ and Theorem 2.2 predicts blow-up at time $T_b^h = \int_{w^h(0)}^\infty (-\lambda_1^h s + f(s))^{-1} ds$, where $w^h(0) = \sum_{n=1}^N \phi_n^h u_0(nh)$. As $h \to 0$, the predicted blow-up times converge: $T_b^h \to \overline{T}_b$. From a numerical point of view, $f(w^h(0)) > \lambda_1^h w^h(0)$ provides a condition on the spatial step size h which ensures explosive behavior for both the heat equation and its spatial approximations. A rigorous proof of the convergence of the blow-up times in semidiscretized heat equations has been given in [21].

3. **Explosive behavior for negative potential energies.** For solutions changing sign, instability results can be obtained by energy methods. The restriction on the sign is removed at the expense of power like growth conditions on the reactive source and restrictions on the structure of the difference operator. For simplicity, we shall restrict our study here to problems of the form (3), in particular,

$$u_n' = d(u_{n+1} - 2u_n + u_{n-1}) + f(u_n). \tag{17}$$

Their solutions blow-up in finite time when the potential energy becomes negative. For positive solutions, the predictions found in Section 2 are usually sharper.

We consider (17) with a reactive source $f(u)$ deriving from a potential $F(u)$, $f(u) = -\frac{\partial F(u)}{\partial u}$. Potentials are defined up to an additive constant. We fix $F(u) = -\int_0^u f(s)ds$. For a finite chain $n = 1, ..., N$ with zero Dirichlet boundary conditions $u_0(t) = u_{N+1}(t) = 0$, $t > 0$, we define the potential energy:

$$E(u_n(t)) = \frac{1}{2}\mathbf{u}^t A\mathbf{u} + \sum_{n=1}^N F(u_n(t)), \tag{18}$$

where A is the matrix defined in (11) with $d_n = d$ and $\mathbf{u} = (u_1, ..., u_N)$. Since A is symmetric and positive definite:

$$\mathbf{u}^t A\mathbf{u} \geq \lambda_1 \mathbf{u}^t\mathbf{u} > 0 \qquad \text{when } \mathbf{u} \neq 0, \tag{19}$$

$$\mathbf{v}^t A\mathbf{u} = \mathbf{u}^t A\mathbf{v}, \tag{20}$$

$$\frac{d\mathbf{u}^t}{dt} A\mathbf{u} = \frac{1}{2}\frac{d}{dt}(\mathbf{u}^t A\mathbf{u}). \tag{21}$$

Any other boundary conditions producing symmetric matrices are handled in the same way. For infinite systems, the energy reads:

$$E(u_n(t)) = \frac{d}{2}\sum_n (u_{n+1}(t) - u_n(t))^2 + \sum_n F(u_n(t)) \tag{22}$$

and we must work with initial data u_n^0 having finite energy. Existence of local in time solutions with finite energy is discussed in Section 4. We multiply (17) by u_n' and sum over n to get:

$$\frac{d}{dt}E(u_n(t)) = -\sum_{n=1}^N |u_n'(t)|^2. \tag{23}$$

The energy is decreasing, therefore $E(u_n(t)) \leq E(u_n(0))$ for $t > 0$. The energy identity (23) provides a bound on the energy ensuring the existence of globally bounded solutions when the energy functional is positive, or at least bounded from below. Such is the case when the potential $F(u)$ satisfies $F(u) > 0$ for $|u|$ large. For reactive potentials like $F(u) = -|u|^{p+1}$ the energy functional (18) may take on negative values and it is not bounded from below. That is the reason why explosive instabilities may develop.

In (3), $g(u)$ derives from a potential $G(u)$, $g(u) = \frac{\partial G(u)}{\partial u}$. We select $G(u) = \int_0^u g(s)ds$. The energy reads:

$$E(u_n(t)) = \sum_n G(u_{n+1}(t) - u_n(t)) + \sum_n F(u_n(t)). \tag{24}$$

The right hand side of (3) is then $-\frac{\partial E(u_n)}{\partial u_n}$. The finite lattice is recovered setting $u_n = 0$ for $n \leq 0$ and $n \geq N+1$.

Blow-up results are obtained by establishing differential inequalities for modified energy functionals whose solutions blow up in finite time. Simple inequalities of the form $Q' \geq cQ^{1+\delta}$, $\delta, c > 0$, can be established for the L^2 norm. Theorem 3.1 below supplies a first estimate of the blow-up time for negative energies. Notice that this estimate does not depend on d, but it does depend on N and the nonlinearities.

Theorem 3.1. *Let $u_n(t)$ be a solution of (3) with a strong reactive potential $F(u) = -\frac{r}{p+1}|u|^{p+1}$ and nonlinear diffusion given by $G(u) = \frac{d}{q+1}|u|^{q+1}$, $d, r, q > 0$ and $p > q \geq 1$. We consider a finite chain of length N with Dirichlet boundary conditions. If the initial potential energy (24) is negative, then $\sum_{n=1}^N |u_n|^2(t)$ blows up at time $T \leq T_b$, with*

$$T_b = \frac{(p+1)}{4r}\frac{p-1}{p-q}\Big(\sum_{n=1}^N |u_n|^2(0)\Big)^{\frac{-(p-1)}{2}} N^{\frac{(p-1)}{2}}. \tag{25}$$

Proof. Multiplying (3) by u_n and summing over n, we get:

$$\frac{1}{2}\frac{d}{dt}\sum_{n=1}^N u_n^2 = \sum_{n=1}^N [g(u_{n+1} - u_n)u_n - g(u_n - u_{n-1})u_n] + \sum_{n=1}^N f(u_n)u_n,$$

which can be rewritten as:

$$\frac{1}{2}\frac{d}{dt}\sum_{n=1}^N u_n(t)^2 = -(q+1)E(u_n(t)) + (p-q)\frac{r}{p+1}\sum_{n=1}^N |u_n|^{p+1}.$$

Let us set $Q(t) = \sum_{n=1}^N |u_n|^2(t)$. Using $Q(t) \leq (\sum_{n=1}^N |u_n|^{p+1})^{\frac{2}{(p+1)}} N^{\frac{p-1}{p+1}}$ and $-E(u_n(t)) \geq -E(u_n(0)) \geq 0$ we get:

$$Q'(t) \geq cQ(t)^{\frac{p+1}{2}}, \quad c = \frac{2(p-q)r}{p+1}\frac{1}{N^{(p-1)/2}}.$$

Solving this differential inequality we obtain $Q(t)^{\frac{p-1}{2}} \geq \big(Q(0)^{\frac{-(p-1)}{2}} - \frac{2ct}{p-1}\big)^{-1}$ and estimate on the blow-up time follows. $\square$

Theorem 3.1 is restricted to finite domains because we use inequalities to relate $\sum_{n=1}^N |u_n|^2$ and $\sum_{n=1}^N |u_n|^{p+1}$, with constants depending on N, as in [8]. By establishing differential inequalities for more refined functionals $Q(t)$ we may obtain blow-up predictions which are not restricted to finite domains and reflect the impact of the coupling G, d through the initial energy. Instead of looking for inequalities of the form $Q' \geq cQ^{1+\delta}$, $\delta, c > 0$, we resort to other explosive inequalities, such as $(Q^{-\alpha})'' \leq 0$, $\alpha > 0$. This technique, known as 'concavity method', was already exploited in [9] for semilinear parabolic equations.

The growth hypothesis on G and F can be somewhat relaxed. We assume that F satisfies the following growth condition:

$$2(\alpha+1)F(u) + uf(u) \geq 0 \tag{26}$$

for some $\alpha > 0$. This includes $F(u) = -\frac{|u|^{p+1}}{p+1}$, for $p > 1$, with $\alpha = \frac{p-1}{2} > 0$. Then, the following blow-up result holds. We restrict to (17) not to encumber the proof.

Theorem 3.2. *Let $u_n(t)$ be a solution of (17) with finite energy for a source f satisfying (26). The chain may be infinite or finite. In finite chains we impose zero Dirichlet boundary conditions at the boundary. If the initial energy $E(0) < 0$, then $\sum_{n\in I} |u_n|^2(t)$ blows up at time $T \leq T_b$ with*

$$T_b = -\frac{(2\alpha+1)\sum_{n\in I} |u_n|^2(0)}{2\alpha^2(\alpha+1)E(0)}, \tag{27}$$

where $I = \{1, ..., N\}$ for a finite chain and $I = \mathbb{Z}$ when the chain is infinite.

Proof. Let us consider first a finite chain governed by (17). A new functional is constructed modifying the L^2 norm (following [9]):

$$Q(t) = \int_0^t \sum_{n=1}^N u_n(s)^2 ds + (\sigma - t)\sum_{n=1}^N u_n(0)^2 + \beta(t+\tau)^2.$$

The parameters $\sigma > 0$, $\tau > 0$ and $\beta > 0$ must be chosen in such a way that $(Q^{-\alpha})'' = -\alpha Q^{-\alpha-2}(Q''Q - (\alpha+1)(Q')^2) \leq 0$. Then, $Q(t) > 0$ for $t \in [0, \sigma]$, $Q'(0) = 2\beta\tau > 0$ and an explosive lower bound is found

$$Q(t) \geq Q^{1+\frac{1}{\alpha}}(0)\big(Q(0) - \alpha t Q'(0)\big)^{\frac{-1}{\alpha}}.$$

This implies blow-up at time

$$T \leq T_b(\beta,\tau) = \frac{Q(0)}{\alpha Q'(0)} = (2\alpha\beta\tau)^{-1}\Big(\sigma\sum_{n=1}^N u_n(0)^2 + \beta\tau^2\Big).$$

We set $\sigma = T_b(\beta, \tau)$. Let us show how to select β and τ. We first compute the derivatives:

$$Q' = \sum_{n=1}^N u_n(t)^2 - \sum_{n=1}^N u_n(0)^2 + 2\beta(t+\tau) = 2\Big(\int_0^t \sum_{n=1}^N u_n(s)u_n'(s)ds + \beta(t+\tau)\Big),$$

$$Q'' = 2\sum_{n=1}^N u_n(t)u_n'(t) + 2\beta = 2\Big(\int_0^t \sum_{n=1}^N \big(u_n(s)u_n'(s)\big)' ds + \sum_{n=1}^N u_n(0)u_n'(0) + \beta\Big).$$

Adding and subtracting $4(\alpha+1)\big(\int_0^t \sum_{n=1}^N u_n'(s)^2 ds + \beta\big)$ in Q'' we can rearrange terms to obtain:

$$QQ'' - (\alpha+1)(Q')^2 = 4(\alpha+1)S + 2QH$$

with $S \geq 0$,

$$S = \Big(\beta(t+\tau)^2 + \int_0^t \sum_{n=1}^N u_n^2\Big)\Big(\beta + \int_0^t \sum_{n=1}^N (u_n')^2\Big) - \Big(\beta(t+\tau) + \int_0^t \sum_{n=1}^N u_n u_n'\Big)^2,$$

and $H = H_1 + H_2 + H_3 + H_4$ estimated below. Set $\mathbf{u} = (u_1, ..., u_N)$. Then,

$$\begin{aligned} H_1 &= \int_0^t \Big((-\mathbf{u}^t A\mathbf{u})' + 2(\alpha+1)\mathbf{u}'^t A\mathbf{u} \Big) \\ &= \alpha\Big(\mathbf{u}^t A\mathbf{u}(t) - \mathbf{u}^t A\mathbf{u}(0) \Big) \geq -\alpha \mathbf{u}^t A\mathbf{u}(0), \end{aligned} \tag{28}$$

thanks to (21) and (19). Now, H_2 is bounded from below using (26):

$$\begin{aligned} H_2 &= \int_0^t \sum_{n=1}^N \Big((u_n f(u_n))' - 2(\alpha+1)u_n' f(u_n) \Big) \\ &\geq -\sum_{n=1}^N \Big(u_n(0) f(u_n(0)) + 2(\alpha+1)F(u_n(0)) \Big). \end{aligned} \tag{29}$$

The term H_3 is positive:

$$H_3 = 4(\alpha+1)(\sigma - t)\Big(\sum_{n=1}^N u_n(0)^2 \Big)\Big(\int_0^t \sum_{n=1}^N (u_n')^2 + \beta \Big) \geq 0,$$

and H_4 is rewritten using (17):

$$\begin{aligned} H_4 &= \sum_{n=1}^N u_n'(0)u_n(0) - (2\alpha+1)\beta \\ &= -\mathbf{u}^t A\mathbf{u}(0) + \sum_{n=1}^N u_n(0) f(u_n(0)) - (2\alpha+1)\beta. \end{aligned} \tag{30}$$

Adding all these lower estimates for S and H, we find the desired inequality

$$QQ'' - (\alpha+1)(Q')^2 \geq 4(\alpha+1)Q\Big(-E(0) - \frac{(2\alpha+1)\beta}{2(\alpha+1)} \Big) \geq 0,$$

for β small enough. We select $\beta = \beta_0 = -\frac{2(\alpha+1)}{2\alpha+1}E(0)$. Then, the blow-up time is $T(\beta_0, \tau) = \beta_0 \tau^2 \big(2\alpha\tau\beta_0 - \sum_{n=1}^N u_n(0)^2 \big)^{-1} = \sigma$. It remains to select a value $\tau > (2\beta_0\alpha)^{-1} \sum_{n=1}^N u_n(0)^2$. In this range, $T(\beta_0, \tau)$ attains a minimum value at $\tau = \tau_0 = (\beta_0\alpha)^{-1} \sum_{n=1}^N u_n(0)^2$ and $T(\beta_0, \tau_0) = (\alpha^2\beta_0)^{-1} \sum_{n=1}^N u_n(0)^2$. Notice that we take for β_0 the largest available value, so that $T(\beta_0, \tau_0)$ is as small as possible.

For infinite lattices, a similar argument works substituting $\sum_{n=1}^N$ with $\sum_{n=-\infty}^\infty$. The energy is defined in (22). $\mathbf{u}^t A\mathbf{u}$, $\mathbf{u}'^t A\mathbf{u}$ are replaced by $\frac{d}{2}\sum_n (u_{n+1} - u_n)^2$ and $-\frac{d}{2}\sum_n (u_{n+1} - 2u_n + u_{n-1})u_n' = d\sum_n (u_{n+1} - u_n)(u_{n+1}' - u_n')$, respectively. $\square$

In the continuum limit, $d = \frac{1}{h^2}$, $h = 1/(N+1)$, the corresponding solutions $u_n^h(t)$ of (17) with zero boundary conditions and initial datum $u_n^0 = u_0(nh)$ are expected to converge to the solution of the nonlinear heat equation (16). Let us assume that $u_0(x) \in C([(0,1])$. We define the continuous energy as:

$$E(u(x,t)) = \frac{1}{2}\int_0^1 |u_x(s,t)|^2 ds + \int_0^1 F(u(s,t)) ds. \tag{31}$$

If $E(u_0(x)) < 0$, $E^h(u_0(nh)) < 0$ for h small and blow-up is expected in both the heat equation and its discrete approximations. We keep the notations of Theorems

3.1 and 3.2, but adding a superscript h to stress dependence on h. The predictions for the blow-up times T_b^h provided by Theorem 3.1 tend as $h \to 0$ to:

$$\overline{T}_b = \frac{p+1}{4}\Big(\int_0^1 |u_0(s)|^2 ds\Big)^{\frac{-(p-1)}{2}}. \tag{32}$$

By [8], we know that $u(x,t)$ blows up before time $\overline{T}_b$. Similarly, the predictions T_b^h found in Theorem 3.2 tend as $h \to 0$ to:

$$\overline{T}'_b = -\frac{(2\alpha+1)\int_0^1 u_0^2(s)ds}{2\alpha^2(\alpha+1)E(0)}. \tag{33}$$

By [9], we know that $u(x,t)$ blows up before time $\overline{T}'_b$.

4. **Infinite chains.** Local in time existence for (1)-(2) and (17) in infinite chains is guaranteed using the existence theory for systems of ordinary equations in infinite dimensional Banach spaces B [25]. We may rewrite the original systems as $\mathbf{u}' = A\mathbf{u} + H(\mathbf{u})$, where A is a linear and continous operator in $B = l^2(\mathbb{Z})$ or $B = l^\infty(\mathbb{Z})$ and H is a locally Lipschitz perturbation in B provided f is a locally Lipschitz function. Whenever $(u_n(0))_{n\in\mathbb{Z}} \in B$, local in time existence of a solution $\mathbf{u}(t) = (u_n(t))_{n\in\mathbb{Z}} \in B$ up to a maximal time T follows. Notice that, for sequences, $l^2(\mathbb{Z}) \subset l^{p+1}(\mathbb{Z})$ when $p > 1$ and $l^2(\mathbb{Z}) \subset l^\infty(\mathbb{Z})$. To ensure that a solution $u_n(t) \in l^2(\mathbb{Z})$ has finite energy we set $F(u) = -\frac{|u|^{p+1}}{p+1}$ and $f(u) = |u|^{p-1}u$ for $p > 1$ thoughout this section.

The space-localized blow-up results for positive solutions established in Section 2 apply for either finite or infinite chains. In the l^2 setting, we may also apply Theorem 3.2 regardless of the sign of the solutions. For infinite chains, the question arises of whether blow-up in the l^2 norm is induced by the behavior of $u_n(t)$ as $|n| \to \infty$ before any component becomes infinite. Below, we show that blow-up at space infinity cannot occur when we work with nonnegative initial data vanishing at infinity. The results are obtained using solutions of spatially discrete heat equations to control the behavior of the tails as $|n|$ grows. The solutions of

$$u'_n = d(u_{n+1} - 2u_n + u_{n-1}), \quad n \in \mathbb{Z}, t > 0, \tag{34}$$

are given by

$$u_n(t) = \sum_{m\in\mathbb{Z}} G_{n-m}(t) u_m(0), \quad n \in \mathbb{Z}, t > 0, \tag{35}$$

where

$$\begin{aligned} G_k(t) &= \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} e^{-4d\sin^2(\theta/2)t}\cos(k\theta) \\ &= e^{-2dt}\int_{-\pi}^{\pi} \frac{d\theta}{2\pi} e^{2dt\cos(\theta)}\cos(k\theta) = e^{-2dt} I_k(2dt) \end{aligned} \tag{36}$$

is the Green function for the discrete heat equation, $I_k(2Dt)$ being a modified Bessel function of integer order [26, 27]. Notice that $G_k(t) = G_{-k}(t)$ and $|G_k(t)| \le 1$. The Green function solves (34) and takes a Kronecker delta as initial datum: $G_k(0) = \delta_{k,0}$ (equal to 1 when $k = 0$, to zero otherwise). The comparison principle stated in Section 2 implies that $G_k(t) \ge 0$ for all t and k. Integrating the equation we see that $\|G_k(t)\|_1 = 1$. Young's inequality for convolutions implies then:

$$\|u_n(t)\|_{l^p} \le \|G_n(t)\|_{l^1}\|u_n(0)\|_{l^p} \le \|u_n(0)\|_{l^p}, \quad p \ge 1.$$

Expressions (35) and (36) are computed using generating functions (discrete Fourier transforms) to get rid of the difference operators [28]. Setting $p(\theta,t)=\sum_n u_n(t)e^{in\theta}$, (34) becomes

$$p'(\theta,t)+4d\sin^2(\theta/2)p(\theta,t)=0, \quad p(\theta,0)=\sum_k u_k(0)e^{ik\theta}.$$

The solution of this ordinary differential equation is

$$p(\theta,t)=e^{-4d\sin^2(\theta/2)t}\sum_m u_m(0)e^{-im\theta}.$$

Inverting the discrete Fourier transform we recover $u_n(t)$ as

$$\begin{aligned} u_n(t) &= \int_{-\pi}^{\pi}\frac{d\theta}{2\pi}e^{in\theta}p(\theta,t)=\sum_m u_m(0)\int_{-\pi}^{\pi}\frac{d\theta}{2\pi}e^{-4d\sin^2(\theta/2)t}e^{i(n-m)\theta} \\ &= \sum_m u_m(0)\int_{-\pi}^{\pi}\frac{d\theta}{2\pi}e^{-4d\sin^2(\theta/2)t}\cos((n-m)\theta), \end{aligned}$$

which is exactly (35)-(36). The resulting expression is real because $\sin^2(\theta/2)$ is even with respect to θ.

Thanks to the comparison principle stated in Section 2 and the knowledge of solutions of spatially discrete linear heat equations we find the following space-localized blow-up result for radially decreasing symmetric solutions of (17).

Theorem 4.1. *Let $u_n(0)\geq 0$ a sequence which increases for $n\leq 0$, decreases for $n\geq 1$, vanishes at infinity and satisfies $u_{-n}(0)=u_{n+1}(0)$ for $n\geq 1$. Let $u_n(t)$ be the solution of (17) with $f(u)=|u|^{p-1}u$ and initial datum $u_n(0)\in l^2(\mathbb{Z})$. If $E(u_n(0))<0$, $u_n(t)$ blows up in finite time T at $n=0,1$.*

Proof. $u_n(t)$ can be computed by solving (17) for $n\geq 1$ with boundary condition $u_0(t)=u_1(t)$ and then setting $u_{-n}(t)=u_{n+1}(t)$ for $n\geq 1$. Applying the comparison principle to $u_n(t)$ and $u_{n+1}(t)$ for $n\geq 1$ we find $u_n(t)\geq u_{n+1}(t)$ for $n\geq 1$ and $u_{n-1}(t)\leq u_n(t)$ for $n\leq 0$. For each $0<t<T$, $u_{|n|}(t)\to 0$ as $|n|\to\infty$.

Let us assume that u_n does not blow up at the center: $0\leq u_0(t)=u_1(t)<M$ for all $t<T$. Then, $0\leq u_n(t)<M$ for all n and $t<T$. Thus,

$$u_n' = d(u_{n+1}-2u_n+u_{n-1})+f(u_n)<d(u_{n+1}-2u_n+u_{n-1})+M^{p-1}u_n.$$

The equation $w_n'=d(w_{n+1}-2w_n+w_{n-1})+M^{p-1}w_n$ has solutions of the form

$$w_n(t)=e^{M^{p-1}t}\sum_m G_{n-m}(t)u_m(0),$$

where $G_k(t)$ is the Green function of the spatially discrete heat equation. Then, $u_n(t)\leq w_n(t)$ for all $t<T$ and all n. Now, $\sum_n|w_n(t)|^2$ does not blow up because $\|w_n(t)\|_{l^2}\leq e^{M^{p-1}t}\|u_n(0)\|_{l^2}\|G_n(t)\|_{l^1}\leq e^{M^{p-1}t}\|u_n(0)\|_{l^2}$. Therefore, $\|u_n(t)\|_{l^2}$ cannot blow up as $t\to T$, which contradicts Theorem 3.2. Thus, $u_0(t)=u_1(t)$ must blow up at time T. □

A more refined comparison technique allows to exclude blow-up at space infinity for more general data.

Theorem 4.2. *Let $u_n(t)$ be a solution of (17) for $f(u)=|u|^{p-1}u$, $p>1$, with nonnegative initial data $u_n(0)\in l^2(\mathbb{Z})$. Then, u_n cannot blow up at space infinity.*

Proof. We select N_1 such that $0 \le u_n(0) < \varepsilon << 1$ for $|n| \ge N_1$. The same inequality is true for $u_n(t)$ at least up to a time t_1. For $t \le t_1$,

$$u_n' = d(u_{n+1} - 2u_n + u_{n-1}) + f(u_n) < d(u_{n+1} - 2u_n + u_{n-1}) + \varepsilon^{p-1} u_n.$$

Set $v_n(0) = u_{-N_1+n}(0)$ for $n < 0$, $v_n(0) = u_{-N_1-n+1}(0)$ for $n > 1$ and $v_0(0) = v_1(0) = u_{-N_1}(0) + 2\varepsilon$. Then,

$$0 \le u_{-N_1+n}(t) \le v_n(t) = e^{\varepsilon^{p-1} t} \sum_m G_{n-m}(t) v_m(0)$$

for $n \le 0$ and $t \le \tau_1 = \min(t_1, s)$, s being such that $v_0(t) \ge 2\varepsilon e^{\varepsilon^{p-1} t} G_0(t) \ge \varepsilon$ for $t \le s$. Notice that $v_n(t) \ge 2\varepsilon e^{\varepsilon^{p-1} t} G_n(t)$ for all $t \ge 0$ and n. If $t \in [0, \tau_1]$

$$\begin{aligned} \sum_{n \le 0} |u_{-N_1+n}(t)|^2 &\le \sum_{n \le 0} |v_n(t)|^2 = \frac{1}{2} \sum_n |v_n(t)|^2 \le \frac{1}{2} e^{\varepsilon^{p-1} \tau_1} \sum_n |v_n(0)|^2 \\ &= e^{\varepsilon^{p-1} \tau_1} \left(\sum_{n<0} |u_{-N_1+n}(0)|^2 + |u_{-N_1}(0) + 2\varepsilon|^2 \right). \end{aligned}$$

We select $N_2 \ge N_1$ large enough to ensure that

$$\sum_{n<0} |u_{-N_2+n}(\tau_1)|^2 \le \sum_{n<0} |u_{-N_1+n}(0)|^2$$

and $0 \le u_n(\tau_1) < \varepsilon << 1$ when $|n| \ge N_2$. This inequality remains true for $u_n(t)$ up to a time $\tau_1 + t_2$, with $t_2 \le t_1$. Then, we repeat the previous step selecting $u_n(\tau_1)$ and $v_n(0) = u_{-N_2+n}(\tau_1)$ for $n < 0$, $v_n(0) = u_{-N_2-n+1}(\tau_1)$ for $n > 1$ and $v_0(0) = v_1(0) = u_{-N_2}(\tau_1) + 2\varepsilon$ as initial data. In this way we reach a new time $\tau_2 = \min(t_2, s)$ such that for $t \in [\tau_1, \tau_1 + \tau_2]$

$$\begin{aligned} \sum_{n \le 0} |u_{-N_2+n}(t)|^2 &\le e^{\varepsilon^{p-1} \tau_2} \left(\sum_{n<0} |u_{-N_2+n}(\tau_1)|^2 + |u_{-N_2}(\tau_1) + 2\varepsilon|^2 \right) \\ &\le e^{\varepsilon^{p-1} \tau_2} \left(\sum_{n<0} |u_{-N_1+n}(0)|^2 + (3\varepsilon)^2 \right). \end{aligned}$$

We may repeat the procedure and find a sequence τ_k bounded from above such that $\sum_{n \le 0} |u_{-N_k+n}(t)|^2 \le e^{\varepsilon^{p-1} \tau_k} \left(\sum_{n<0} |u_{-N_1+n}(0)|^2 + (3\varepsilon)^2 \right)$ for any $t \in [\tau_{k-1}, \tau_{k-1} + \tau_k]$. We conclude that $\sum_{n \le -N} |u_n(t)|^2$ cannot tend to infinity in finite time as N grows. A similar argument works for the right tail. $\square$

The previous results exclude blow-up at space infinity for discrete semilinear heat equations in spaces of sequences decaying at infinity. For continuum heat equations a similar phenomenon is observed when solutions decay at space infinity, see [29] for a detailed study of local blow-up conditions. However, blow-up at space infinity is possible in nonlinear heat equations for nonconstant bounded initial data behaving at infinity like a constant $M > 0$ and satisfying $u(x, 0) \le M$ everywhere [30]. In our spatially discrete context, choosing similar bounded initial data and $M > (2d)^{\frac{1}{p-1}}$, Theorem 2.1 ensures blow-up at space infinity in a $l^\infty(\mathbb{Z})$ setting.

5. **Numerical results.** We have solved numerically:

$$\begin{aligned} u_n' &= d(u_{n+1} - u_n + u_{n-1}) + v(u_{n-1} - u_n) + u_n^3, \quad n = 1, ..., N,\ t > 0, && (37) \\ u_n' &= d(u_{n+1} - u_n + u_{n-1}) + v(u_{n-1} - u_n) + e^{u_n}, \quad n = 1, ..., N,\ t > 0, && (38) \end{aligned}$$

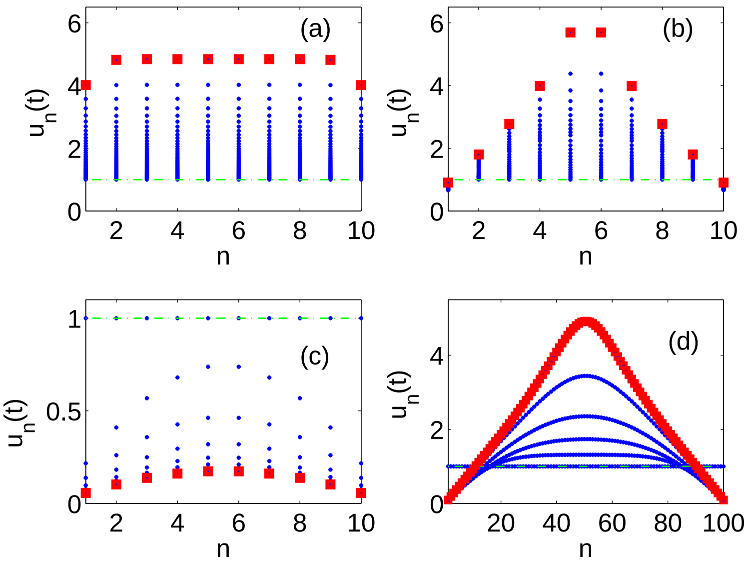

FIGURE 2. Time evolution of (38) for $u_n^0 = 1$, $v = 0$: (a) $N = 10$, $d = 0.1$, (b) $N = 10$, $d = 10$, (c) $N = 10$, $d = 100$, (d) $N = 100$, $d = 100$.

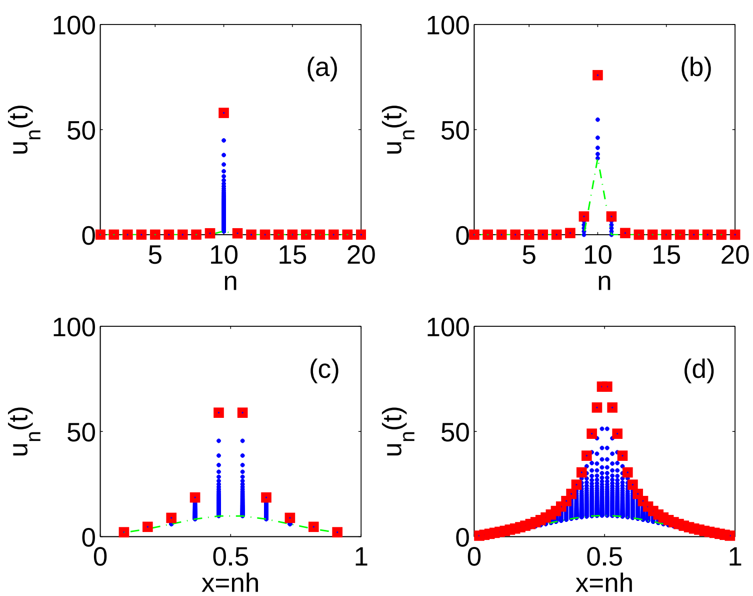

FIGURE 3. Time evolution of (37) for data concentrated at point $n = N/2$, $u_n^0 = \sqrt{3d}\ \delta_{n,N/2}$, and $v = 0$, (a) $N = 20$, $d = 1$, (b) $N = 20$, $d = (N+1)^2$; and for exponentially concentrated data $u_n^0 = u_0(nh)$, $u_0(x) = 10e^{-10(x-0.5)^2}$ in the continuum limit $d = \frac{1}{h^2} = (N+1)^2$: (c) $N = 50$, (d) $N = 100$.

with zero Dirichlet boundary conditions for different choices of the initial data $u_n(0) = u_n^0$, the diffusion and convection coefficients d, v and the size of the lattice N. Instability is expected when the initial states are too large for diffusive or convective effects to compensate the fast growth of the reactive source, see Figure 1. When (37) is seen as a semidiscretization of a continuous equation, Figure 1 illustrates the dramatic changes observed in the solution by just dividing the step size by two: decay to equilibrium in (a),(e) is replaced by blow-up in (b),(f) and blow-up is greatly delayed from (d) to (c).

Let us discuss the impact of the parameters d and N on the evolution of the system. We consider first the influence of d. Theorems 2.1 and 2.2 suggest that weakly coupled systems (d small) are more unstable than strongly coupled systems (d large). As d increases the sets of initial states for which they predict blow-up shrink and the blow-up times grow. A similar remark follows from theorem 3.2. As d grows, the initial energy may become positive. The same effect is observed by increasing the positive convection coefficient v. Let us consider now the effect of N. Theorem 2.2 suggests that large chains are more unstable than short chains. As N grows, the eigenvalue λ_1 tends to zero, the size restriction for blow-up is weaker and the blow-up times become shorter. Figure 2 illustrates this behavior for (38) starting from an initially uniform configuration $u_n^0 = 1$. Figures 2 (a)-(b) show the evolution of the system when $d = 0.1$ and $d = 10$. For small couplings we find almost simultaneous generalized blow-up. For larger couplings, the singularity formation is leaded by the central points and takes place later (see Table I). Above a threshold value of d, the system tends to a stable equilibrium, see Fig. 2 (c) for $d = 100$. Increasing the length of the chain from $N = 10$ to $N = 100$, we enter again the explosive region. The threshold coupling d separating stable and unstable behavior grows with N, as one would expect from the scaling $\lambda_1 \sim \frac{d}{(N+1)^2}$ for large N.

Let us check now the accuracy of the predictions for the blow-up times. For the numerical integration of (37) and (38), we have used variable time step schemes. The size of the time step must be governed by the growth of the solution to handle changes near the blow-up time, which occur on increasingly small time scales [19, 20]. The figures have been computed with Runge-Kutta-Fehlberg methods of orders 4,5, with variable step size and tolerance 10^{-5}. The computation stops when the numerical scheme cannot meet the tolerance required without reducing the step size below 10^{-16}. We use the stopping time as a numerical estimate of the blow-up time. Table I below shows the numerical blow-up times and the predictions provided by the different theorems in Sections 2 and 3 for most of the figures in this paper.

TABLE I: Predicted versus numerically estimated blow-up times

	Num.	*Th.2.1*	*Th.2.2*	*Th.2.2 (opt)*	*Th.3.1*	*Th.3.2*
Fig. 2(a)	0.36788	0.38955	0.3697			
Fig. 2(b)	0.40349		0.4781			
Fig. 2(d)	0.41834		0.5093			
Fig. 3(a)	0.26174	0.27465				
Fig. 3(b)	0.00059	0.00062				
Fig. 3(c)	0.00604		0.0114	0.00839 (3-8)	0.023	0.0612
Fig. 3(d)	0.00600		0.0116	0.00708 (14-36)	0.0247	0.0648
Fig. 4(a)	0.02129				0.04	0.1724
Fig. 4(b)	0.02129				0.04	0.1727
Fig. 4(c)	0.08213					
Fig. 6(a)	0.51230		4.1104	0.58202 (6-10)	4	15
Fig. 6(b)	0.50643		2.4171	0.55720 (6-11)	1.83	9
Fig. 6(c)	0.51721			0.58202 (6-10)		
Fig. 6(d)	0.12507	0.17328	0.2045	0.12938 (1-5)	0.4	1.0273

Figure 3 (a)-(b) illustrates the dynamics of (37) for initial data concentrated at one point $u_n^0 = \sqrt{3d}\, \delta_{n,N/2}$. The component $u_{n,N/2}(t)$ blows up in finite time, as predicted by Theorem 2.1 for small $d = 1$ and large $d = (N+1)^2$. In the continuum limit, an apparently selfsimilar mechanism develops, see Fig. 3 (c)-(d). Notice that the estimate of the blow-up time can be optimized by applying Theorem 2.2 to a selected set of components where the initial data is concentrated. Table 1 compares the numerical estimate with the optimized predictions choosing components $3-8$ and $14-36$, respectively.

Figure 4 reproduces the dynamics of (37) for oscillatory initial data, taking positive and negative values. For a weak coupling $d = 1$, the initial energy is negative and blow-up occurs at the borders. Notice the symmetry effect depending on whether N is even Fig 4 (a) or odd Fig 4 (b). For a stronger coupling $d = 10$, the initial energy is positive and the system is stable: $u_n(t)$ tends to equilibrium as t grows, see Fig 4 (d). Near this value, for $d = 9$, the interior points decay to equilibrium while the boundary points start to blow up, see Fig 4 (c).

Figure 5 shows the evolution of the same oscillatory initial pattern for (38). The source term here is positive and only positive explosions are allowed. Blow-up does not necessarily occur at the border, see Fig. 5 (d)-(e). None of our theorems applies in this example, but the blow-up times are quite close to those obtained by applying Theorem 2.2 to single components regardless of the changes in sign.

Figure 6 illustrates localized blow-up. Explosions may develop almost at the same time in different regions as shown in 6 (c). It is possible to have a blow-up after a blow-up. In (d), the left half blows up earlier. However, Theorem 2.2 also ensures the blow-up of the right half. Examples like this or Figure 5 (d) raise the problem of how to compute the evolution of the other components of the system once blow-up has occurred in a small region.

6. **Conclusions.** We have studied unstable growth in spatially discrete reaction-diffusion systems. For strongly reactive sources, a number of conditions on the initial states ensuring blow-up in finite time have been found: positive data which are large enough in a large enough region or data with negative potential energy lead to explosive behavior of the system. In infinite systems we have given conditions

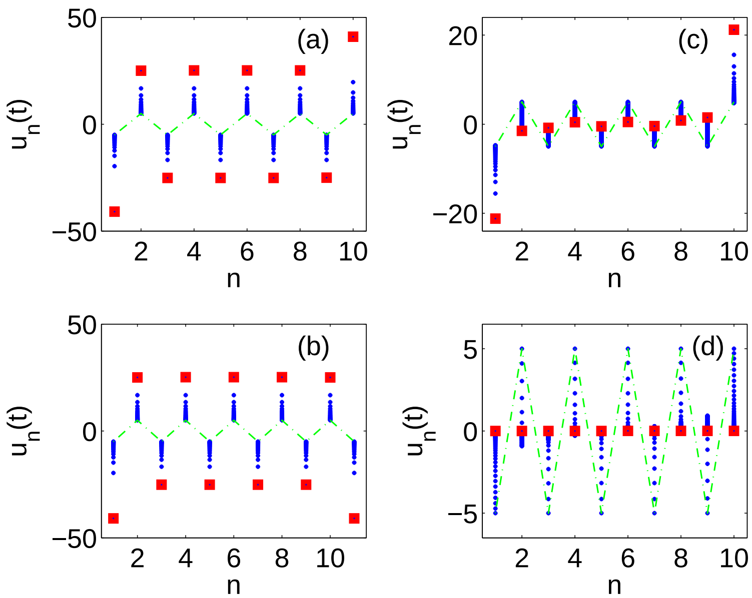

FIGURE 4. Time evolution of (37) for $u_n^0 = 5\cos(\pi n)$ and $v = 0$: (a) $N = 10$, $d = 1$, (b) same with $N = 11$, (c) $N = 10$, $d = 9$, (d) $N = 10$, $d = 10$.

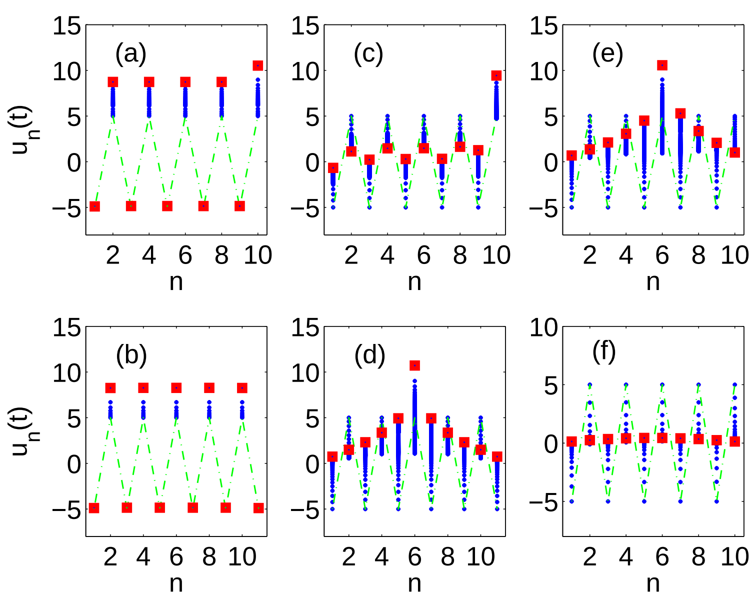

FIGURE 5. Time evolution of (38) for $u_n^0 = 5\cos(\pi n)$ and $v = 0$: (a) $N = 10$, $d = 1$, (b) same with $N = 11$, (c) $N = 10$, $d = 11$, (d) same with $N = 11$, (e) $N = 10$, $d = 12$, (f) $N = 10$, $d = 50$

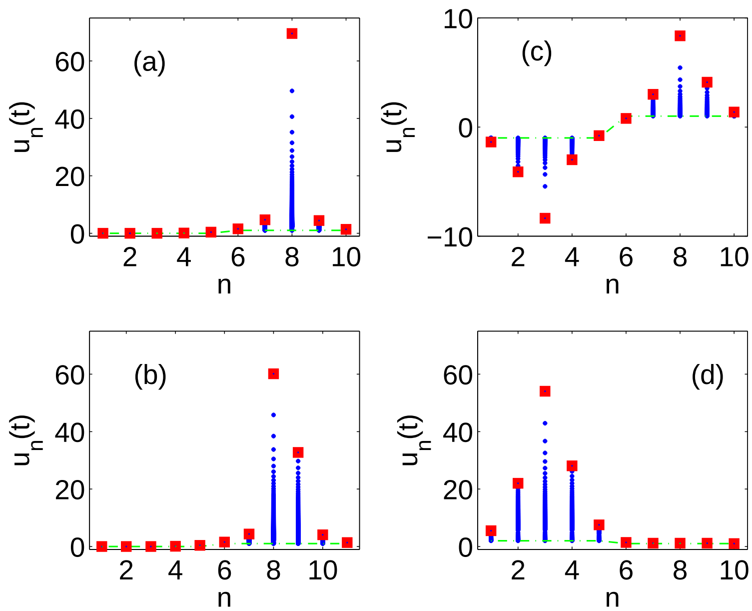

FIGURE 6. Time evolution of (37) with $d = 1$, $v = 0$ and piecewise constant data $u_n^0 = \alpha$ for $N \le 5$, $u_n^0 = \beta$ for $N \ge 6$: (a) $N = 10$, $\alpha = 0$, $\beta = 1$, (b) same with $N = 11$, (c) $N = 10$, $\alpha = -1$, $\beta = 1$, (d) $N = 10$, $\alpha = 2$, $\beta = 1$.

excluding and implying blow-up at space infinity in blow-up solutions. We have obtained estimates of the blow-up times and checked their accuracy numerically. For positive solutions, comparison arguments are more accurate than energy methods. Weakly coupled systems are more unstable than strongly coupled systems in the sense that larger sets of initial states may undergo unstable growth and the blow-up times are shorter.

The main impact of spatial discreteness in such models seems to be related to higher instability and changes in the way explosions occur. Highly discrete systems may blow up at just one component or simultaneously at almost all of them. Our work on local blow-up shows that it is possible to have a blow-up after a blow-up. It is a challenging problem for computational scientists to obtain the solution after the first blow-up to catch the second blow-up. The result showed in the paper would be of some guidance to further numerical development.

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