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EXTENSIONAL MOTIONS OF SPATIALLY PERIODIC LATTICES

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Abstract—The behavior of microrheological models for multiphase fluids that have spatially periodic structure depends on certain kinematic properties of the unit cell. Anomalous results associated with identical objects approaching too closely during the flow can be reduced if not eliminated by satisfying lattice compatibility conditions. This is straightforward for simple shearing flow but subtle for extensional flows. Using the connection between lattice compatibility and lattice reproducibility (periodic lattice behavior with the flow) we establish sufficient conditions for compatibility of arbitrary lattices in planar extensional flow. Detailed results for square and hexagonal unit cells include: initial orientations for periodic behavior; strain periods; and minimum lattice spacings D. We identify the orientation of a square unit cell that leads to periodic behavior (with the minimum period) and the largest D of any lattice in planar extensional flow. We show that no lattice exhibits periodic behavior in uniaxial extensional flow (or biaxial extensional flow) even though Adler & Brenner have established the existence of compatibility.

Key Words: compatibility, extensional flow, lattice, microrheology, planar extension, periodicity, spatially periodic, unit cell

INTRODUCTION

One familiar approach to developing rheological models for multiphase fluids involves following the detailed evolution of the fluid microstructure with the flow. This deterministic method is often applied to concentrated particulate suspensions (Adler *et al.* 1985; Brady & Bossis 1988), foams and emulsions (Weaire & Fu 1988; Reinelt & Kraynik 1990; Kraynik 1988; Herdtle 1991), granular media (Bashir & Goddard 1991) and other systems. When modeling bulk rheological behavior, as opposed to boundary conditions such as slip at the wall, one often considers idealized situations where unbounded multiphase fluids undergo homogeneous shearing flows. The detailed analysis for specific multiphase fluids usually involves numerical simulation, especially when the dispersed phase is neither dilute nor arranged in a perfectly ordered manner. Practical limitations on ever increasing but finite computational resources are resolved by adopting a spatially periodic description of the fluid microstructure. This focuses attention on structure evolution within a unit cell that changes shape according to the imposed macroscopic flow. The obvious advantages of spatially periodic models include rigorous mathematical formulation and tractability. However, the imposed order can be a serious drawback, especially when the physical systems of interest are inherently disordered or the predictions depend strongly on the choice of unit cell.

Because the rheology of multiphase fluids can be highly nonlinear, behavior in extensional flows can be dramatically different from behavior in simple shearing flow. However, most rheological studies that involve steady flow of spatially periodic systems only consider simple shearing flow. In this well-understood situation, the undisturbed streamlines are straight; the kinematics of a unit cell are easy to visualize; and, it is particularly obvious—if not taken for granted—how to choose a convenient unit cell. By contrast, for isochoric extensional flows, not only are streamlines curved, in general, but "natural" choices of the unit cell lead to serious problems that are discussed below. In this investigation we focus on the formulation of spatially periodic models for extensional flows. We will show that planar extensional flow is particularly convenient to analyze because the shape of certain unit cells evolves periodically in time. More importantly, this periodicity guarantees the existence of a compatibility condition, which is necessary to reduce, if not eliminate, artifacts associated with a spatially periodic formulation.

Figure 1 shows the idealized structure of a two-dimensional, spatially periodic foam with 256 bubbles in the unit cell. We show this example to emphasize that a structure can be spatially periodic on large length scales and still possess significant disorder on smaller length scales. The results of the current analysis for planar extensional flow can be used to prevent the formation of spatially periodic structures with short-range order from systems where the order was originally only long ranged. When modeling disordered systems, it is very important to keep identical objects well separated for all time.

The idealized geometry of a spatially periodic model is specified in terms of a lattice with basis vectors that define the edges of a representative unit cell. For homogeneous macroscopic flows, the motion of the lattice points, the underlying basis vectors, and the shape of the unit cell are completely determined through affine kinematics. As a result, many conditions that must be satisfied for a spatially periodic model of a flowing system to be viable are purely kinematical in nature. For example, to completely avoid overlap of rigid spheres in suspension the minimum separation D of all lattice points, which are occupied by identical image particles, must exceed the maximum particle diameter d, as discussed by Adler & Brenner (1985). By contrast, deformable particles like the bubbles in foam or the drops in concentrated liquid–liquid emulsions, can change shape to prevent image particles from overlapping. However, their shape will be highly exaggerated when $D \ll d$, where d refers to the undisturbed particle diameter. More subtle influences of imposed order on the behavior of a spatially periodic multiphase fluid are expected to diminish when $D \gg d$. Because the minimum lattice spacing D strongly influences the response of a spatially periodic model, it is important to understand how D depends on the lattice and the flow.

Other useful properties of spatially periodic models, which have been described by Adler & Brenner (1985), are easily understood by considering the situation for simple shearing flow that is shown in figure 2. The structure of a suspension of monodisperse, rigid disks is initially specified on a square lattice aligned with the axes of a Cartesian coordinate system. For simple shearing flow parallel to the X-axis, it is easy to determine the instantaneous position and relative separation of the particle centers, which occupy lattice sites. This lattice exhibits *reproducibility* or *strain periodicity* because it repeats itself periodically with deformation. This lattice also exhibits *compatibility* with the flow because particles of finite size never collide or overlap. A square lattice with this particular orientation permits the largest concentration of monodisperse disks without overlap during simple shearing flow; the maximum area fraction is $\Phi^* = \pi/4 \approx 0.7854$. This result

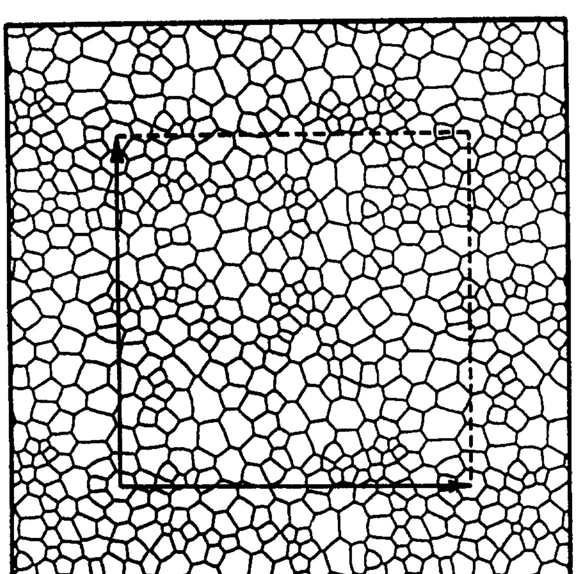

Figure 1. Idealized structure of a two-dimensional, spatially periodic foam with 256 bubbles in a representative unit cell defined by two basis vectors. Even though bubbles associated with the corners of the unit cell are identical, the structure in the vicinity of any bubble lacks obvious order. Adapted with permission from Herdtle (1991).

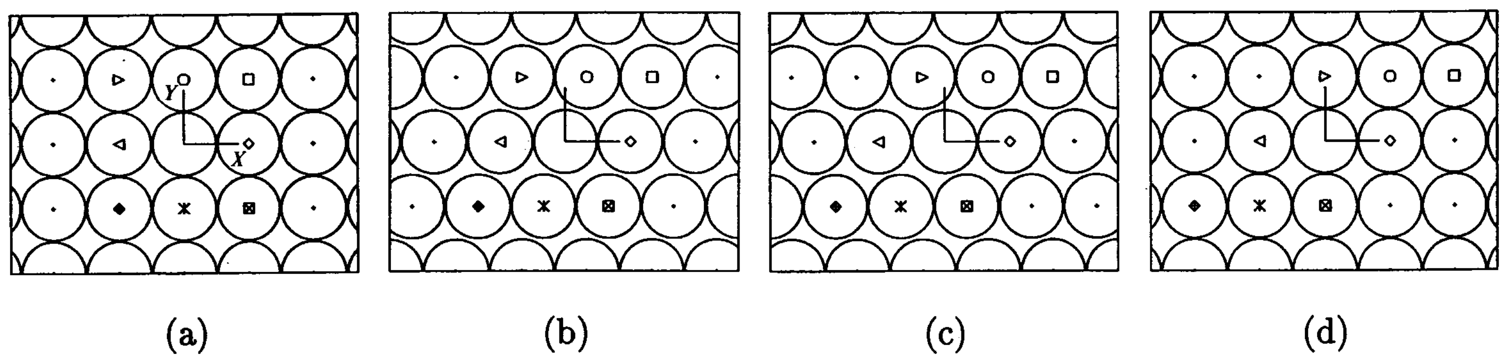

Figure 2. Evolution with shear strain $\gamma = \dot{\gamma}t$ of the structure of a perfectly ordered, spatially periodic suspension of disks in a simple shearing flow. The velocity field is given by $\mathbf{u} = (\dot{\gamma}y, 0)$, where $\dot{\gamma}$ is the shear rate and t is time. (a) When $\gamma = 0$, the disks are confined to a square lattice that is aligned with the axes of a Cartesian coordinate system; (b) $\gamma = 1/3$; (c) $\gamma = 2/3$; (d) when $\gamma = 1$, the structure exhibits reproducibility or strain periodicity by repeating itself. This particular lattice is not only compatible with the flow but gives the maximum area fraction of disks for simple shearing flow $\Phi^* = \pi/4 \approx 0.7854$.

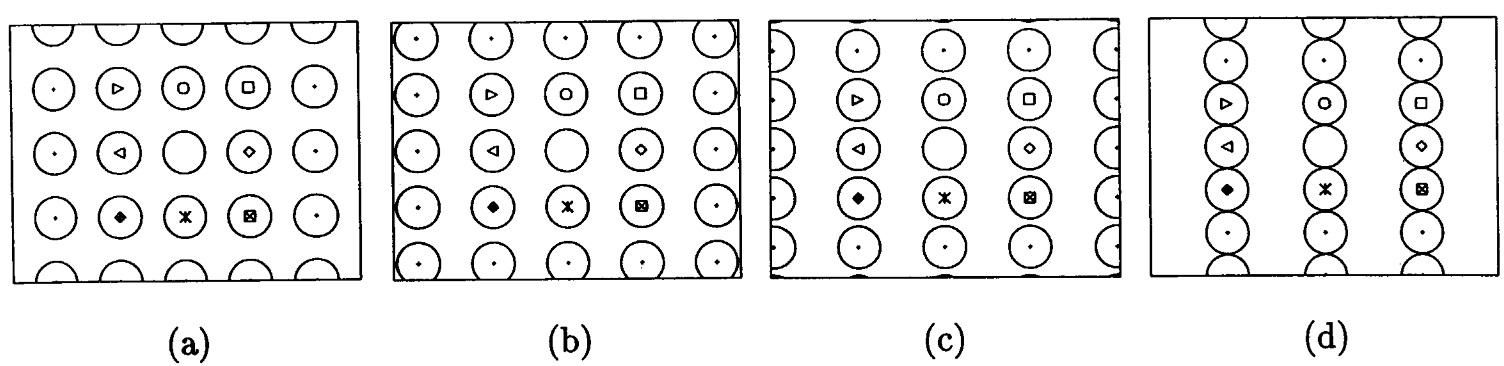

Figure 3. Evolution of the structure of a perfectly ordered, spatially periodic suspension of disks in an isochoric planar extensional flow. The velocity field is given by $\mathbf{u} = (\dot{\epsilon}x, -\dot{\epsilon}y)$, where $\dot{\epsilon}$ is the extension rate and $\epsilon = \dot{\epsilon}t$ is the Hencky strain. The disks are initially associated with a square lattice that is aligned with the stretching directions. The disks follow the unperturbed hyperbolic streamlines of the flow and eventually collide regardless of their size. By contrast with the situation for simple shearing flow shown in figure 1, this structure is neither reproducible nor compatible with the flow.

can be expressed without reference to suspended particles by saying that the minimum lattice spacing D has a maximum value of $D^* = \sqrt{A}$, where A is the area of the unit cell. A lattice is compatible with the flow when $D/\sqrt{A}$ is finite. There are, in fact, an infinite number of lattices that are compatible with simple shearing flow, and, $D/\sqrt{A}$ can be very small. The necessary and sufficient condition for compatibility of a two-dimensional lattice (with arbitrary linearly independent basis vectors) in simple shear is easy to envision: the set of lines that contains all lattice points and is parallel to the flow direction must have a finite spacing. This spacing is uniform and equals D. The same condition also implies reproducibility in simple shearing flow. This strain periodic behavior is extremely convenient when specifying the evolution with flow of the representative basis vectors and the unit cell.

To analyze the behavior of spatially periodic systems in extensional flow, it is necessary to satisfy compatibility conditions. To illustrate the problem, consider an example for isochoric planar extensional flow, which is shown in figure 3 and does not have the desirable attributes of the simple shearing case discussed above. When the particles, no matter how small, are aligned with the stretching direction, they eventually collide so the lattice is incompatible with the flow. Furthermore, a square lattice with this initial orientation is not reproducible. In the following sections, we will show that it is possible to specify unit cells that are both compatible and reproducible in planar extensional flow—this result is not intuitively obvious.

Using theoretical arguments based on the geometry of numbers, Adler & Brenner (1985) investigated compatibility for two-dimensional hyperbolic flows. For the special case of isochoric planar extension, D has a maximum value of $D^*/\sqrt{A} = (4/5)^{1/4} \approx 0.9457$, which is only slightly less than 1—the corresponding value for simple shearing flow. Even though compatibility was established, the existence of reproducibility was overlooked.

While investigating the rheology of perfectly ordered, two-dimensional foams, Kraynik & Hansen (1986) recognized that regular hexagonal lattices can be reproduced in planar extension. That discovery motivated this study of lattice reproducibility for extensional flows. As in the case of simple shearing flow, reproducibility is important because it guarantees compatibility. Reproducibility is also convenient because the time evolution of the basis vectors and the unit cell is simple. In contrast with simple shear, compatibility does not imply reproducibility in planar extension. This is illustrated by counterexample in the appendix provided by Ernest F. Brickell.

In the next section, we investigate existence conditions for reproducibility in general three-dimensional extensional flow, which includes planar extension, uniaxial extension and biaxial extension as special cases. Adler (1984) has established compatibility conditions for uniaxial extensional flow and shown that $D^{*3}/V = \sqrt{27/23}$, where V is the volume of the unit cell. In view of the fact that compatibility has been established, our finding that *no lattice is reproducible in uniaxial extensional flow* is unexpected.

EXISTENCE OF REPRODUCIBILITY FOR EXTENSIONAL FLOWS

To investigate conditions for reproducibility in extensional flow, we construct an arbitrary three-dimensional lattice consisting of all the points

$$\mathbf{R}_\mathbf{n} = n_1\mathbf{b}_1 + n_2\mathbf{b}_2 + n_3\mathbf{b}_3, \tag{1}$$

where $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$ are linearly independent basis vectors and $\mathbf{n} = \{n_1, n_2, n_3\}$ is any set of integers. We consider all homogeneous, isochoric, extensional motions of the lattice. The time evolution of the basis vectors satisfies

$$\frac{\mathrm{d}\mathbf{b}_i}{\mathrm{d}t} = \mathbf{D}\mathbf{b}_i, \tag{2}$$

where $\mathbf{D}$ is a constant diagonal matrix with

$$\operatorname{tr}\mathbf{D} = D_1 + D_2 + D_3 = 0. \tag{3}$$

In terms of the initial basis vectors $\mathbf{b}_i^0$, we get

$$\mathbf{b}_i = \mathbf{\Lambda}\mathbf{b}_i^0, \tag{4}$$

where the matrix $\Lambda = \exp \mathbf{D}t$ and $\det \Lambda = 1$. For a given Λ, a lattice is reproducible if and only if there exist integers N_{ij} such that

$$\Lambda \mathbf{b}_i^0 = N_{i1}\mathbf{b}_1^0 + N_{i2}\mathbf{b}_2^0 + N_{i3}\mathbf{b}_3^0, \qquad [5]$$

for $i = 1, 2, 3$. These vector equations can be rewritten in the form

$$(\mathbf{N} - \lambda_i \mathbf{I})\mathbf{c}_i = 0. \qquad [6]$$

Here, $\mathbf{N}$ is an integer matrix composed of elements N_{ij}, $\mathbf{I}$ is the identity matrix and $\lambda_i = \exp D_i t$. The vector $\mathbf{c}_i$ contains the ith components of the basis vectors $\mathbf{b}_j^0$; equivalently, if $\mathbf{b}_j^0$ are the column vectors of a matrix, then $\mathbf{c}_i$ are the row vectors. The problem has been reduced to an eigenvalue problem for λ_i with corresponding eigenvectors $\mathbf{c}_i$.

Before examining this problem, we note that the matrix $\mathbf{D}$ in [2] can be replaced by any diagonalizable constant matrix $\mathbf{A}$ that has real eigenvalues and $\operatorname{tr}\mathbf{A} = 0$. This matrix can be factored into $\mathbf{A} = \mathbf{SDS}^{-1}$, where the column vectors of $\mathbf{S}$ are the eigenvectors of $\mathbf{A}$ and the diagonal elements of $\mathbf{D}$ are the corresponding eigenvalues. The only difference would be that $\mathbf{b}_i^0$ in [5] would be replaced by $\mathbf{S}^{-1}\mathbf{b}_i^0$; thus, $\mathbf{c}_i$ in [6] would now contain the ith components of these new vectors.

Returning to the eigenvalue problem given in [6], we see that the eigenvalues λ_i are the roots of the characteristic polynomial

$$p(x) = x^3 - kx^2 + mx - 1 = 0, \qquad [7]$$

where

$$\begin{aligned} k &= \lambda_1 + \lambda_2 + \lambda_3 = \operatorname{tr}\mathbf{N} = N_{11} + N_{22} + N_{33}, \\ m &= \frac{1}{\lambda_1} + \frac{1}{\lambda_2} + \frac{1}{\lambda_3} = N_{11}N_{22} - N_{12}N_{21} + N_{22}N_{33} - N_{23}N_{32} + N_{33}N_{11} - N_{31}N_{13}, \\ 1 &= \lambda_1\lambda_2\lambda_3 = \det \mathbf{N}. \end{aligned} \qquad [8]$$

Using the last equation, which follows from our restriction to isochoric deformations, we minimize k and m subject to $\lambda_i > 0$ and find that $k \geqslant 3$ and $m \geqslant 3$. The trivial case when there is no deformation of the lattice corresponds to $k = m = 3$ and $\Lambda = \mathbf{I}$. Excluding the trivial solution, we search for integers k and m for which there exist lattices that are reproducible.

In the planar extension case, the roots of the polynomial are λ, $1/\lambda$, and 1. Substituting these expressions into [8] we find that $k = m$ and

$$\lambda + \frac{1}{\lambda} = k - 1, \qquad [9]$$

where $k = 4, 5, 6, \ldots$. Solving for λ, we get

$$\lambda = \frac{(k-1) + \sqrt{(k-1)^2 - 4}}{2}. \qquad [10]$$

The other root of [9] corresponds to $1/\lambda$.

We have now found a discrete set of strain periods λ for which there exist lattices that exhibit periodic planar extensional flow. No other values of λ will give periodic planar extensional flow. This is very different from simple shearing flow where there exist lattices with arbitrary strain periods. To illustrate this situation, consider a rectangular lattice aligned with the X and Y axes. If the lattice has length d in the X direction and unit length in the Y direction, then the strain period for simple shearing flow parallel to the X axis is just d, which is arbitrary.

In the general extensional flow case, we seek integers k and m such that the three roots of the cubic equation are real and positive. We observe that if λ_1, λ_2, λ_3 is a solution of [8] for a specific k and m, then $1/\lambda_1$, $1/\lambda_2$, $1/\lambda_3$ is also a solution of the same equations when k and m are interchanged. This means that the domain of allowable integers k and m is symmetric across the line $k = m$; thus, we restrict ourselves to the case $k < m$.

Figure 4 is a graph of the cubic equation [7]. We note that $p(0) = -1$ and $p(1) = m - k > 0$ as shown. The curve has a local minimum at

$$x_0 = \frac{k + \sqrt{k^2 - 3m}}{3}. \quad [11]$$

Unless $k^2 > 3m$ and $m^2 > 3k$ (from the symmetry between k and m), the polynomial will be monotone and there will only be one real root. The local minimum value is

$$p(x_0) = \frac{km}{9} - \frac{2}{27}(k^2 - 3m)\left(k + \sqrt{k^2 - 3m}\right) - 1. \quad [12]$$

The cubic polynomial will have three real roots if $p(x_0) \leqslant 0$.

When $p(x_0) = 0$, there is a simple root less than one and a double root greater than one; this corresponds to biaxial extensional flow. We get the opposite case corresponding to uniaxial extensional flow when $m < k$ and the local maximum value equals zero. Asymptotically, we find that m must be proportional to k^2 in order that $p(x_0) \approx 0$. In fact, if we substitute $m = k^2/4$ into [12], we get exactly $p(x_0) = -1$. We describe this solution as near biaxial extensional flow; the roots of the cubic equation are

$$x \sim \frac{4}{k^2} \quad \text{and} \quad x \sim \frac{k}{2} \pm \sqrt{\frac{2}{k}} \quad \text{as } k \to \infty. \quad [13]$$

The roots of [7] corresponding to near uniaxial extensional flow can be found by replacing k by m in [13] and taking the reciprocal of each root.

We now show that the curve $m = k^2/4$ provides an upper bound on a set of allowable integers k and m; from symmetry, the curve $k = m^2/4$ provides the lower bound. By substituting $m = k^2/4 + q$ into [12], we get

$$p(x_0) = \frac{k^3}{36}\left\{\left(1 + \frac{4q}{k^2}\right) - \left(1 - \frac{12q}{k^2}\right)\left[\frac{2}{3} + \frac{1}{3}\sqrt{1 - \frac{12q}{k^2}}\right]\right\} - 1. \quad [14]$$

For m to be an integer, we require that

$$q = \begin{cases} \text{integer} & k \text{ even;} \\ \frac{3}{4} + \text{integer} & k \text{ odd.} \end{cases} \quad [15]$$

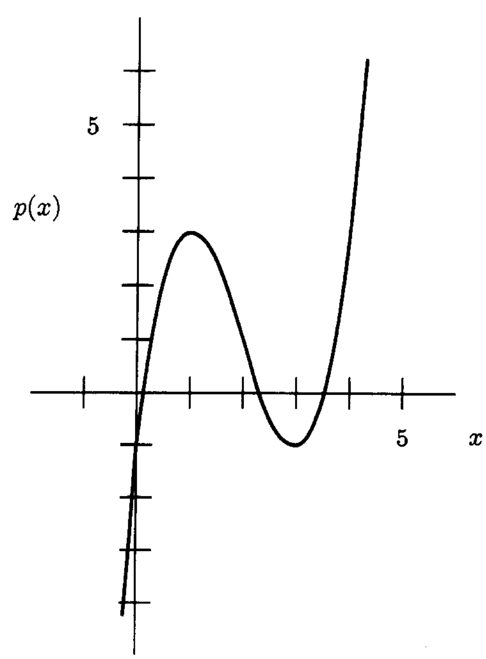

Figure 4. Graph of a typical cubic equation [7] with $k < m$.

We first note that when $q = 0$ in [14], we get $p(x_0) = -1$ as discussed above. When $q < 0$ both terms within the braces decrease; thus, $p(x_0) < -1$ and there are three real roots. When $q > 0$ both terms within the braces increase, which gives $p(x_0) > -1$, but because the term in brackets is always < 1, we have

$$p(x_0) > \frac{k^3}{36}\left\{\left(1 + \frac{4q}{k^2}\right) - \left(1 - \frac{12q}{k^2}\right)\right\} - 1 = \tfrac{4}{9}kq - 1 \geqslant 0. \qquad [16]$$

This last inequality results from $k \geqslant 3$ and $q \geqslant 3/4$, which follows from [15]. Because $p(x_0) > 0$, the cubic equation only has one real root. Therefore, the curve $m = k^2/4$ provides a boundary between integer pairs (k, m) that are allowed and those that are not. We emphasize that *no integer pairs give* $p(x_0) = 0$.

It should also be pointed out that having determined an allowable integer pair and the corresponding roots, we can construct many different integer matrices **N** that satisfy [8]. For example,

$$\mathbf{N} = \begin{pmatrix} 1 & 0 & 1 \\ k - m & 1 & k - m \\ k - 3 & 1 & k - 2 \end{pmatrix}. \qquad [17]$$

The corresponding eigenvectors for this matrix and the basis vectors for the lattice can then be determined; thus, finding an allowable integer pair is a necessary and sufficient condition to insure the existence of a reproducible lattice.

In summary, there exist lattices that are reproducible for each of the extensional flows defined by the integer pairs (k, m) that lie in the region $m \leqslant k^2/4$ and $k \leqslant m^2/4$ (see figure 5). Integer pairs that lie on these curves correspond to near biaxial and near uniaxial extensional flows, respectively. Secondly, it is impossible to find a lattice that is reproducible in biaxial or uniaxial extensional flow.

REPRODUCIBLE LATTICES IN PLANAR EXTENSIONAL FLOW

In the last section, we determined a discrete set of strain periods for which there exist lattices that are periodic in planar extensional flow. We now construct integer matrices **N** that correspond

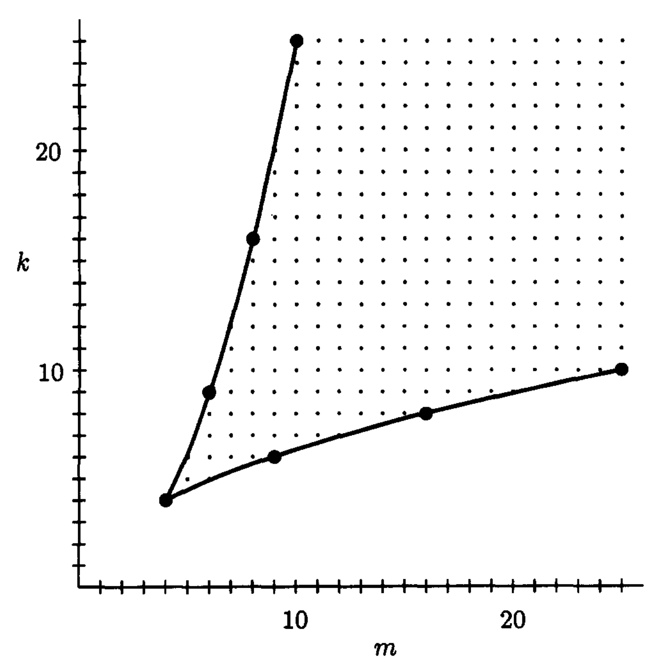

Figure 5. Integer pairs for which there exist lattices that are reproducible (strain periodic) in extensional flow. Solutions that lie on the boundaries of the region correspond to near uniaxial and near biaxial extensional flow.

to a specific lattice and strain period. The two-dimensional lattice is defined in terms of the ratio of lengths of the basis vectors, a, and the angle between the basis vectors ϕ, where $0 < \phi < \pi$. These basis vectors can be written as

$$\mathbf{b}_1 = (\cos\theta, \sin\theta), \qquad \mathbf{b}_2 = a(\cos(\theta+\phi), \sin(\theta+\phi)), \tag{18}$$

where θ is the orientation angle of the lattice. The square and hexagonal lattices that are examined more closely in the next section correspond to $a = 1$ and either $\phi = \pi/2$ or $\phi = \pi/3$, respectively.

As given in [6], the components of the basis vectors must satisfy

$$\begin{bmatrix} N_{11}-\lambda & N_{12} \\ N_{21} & N_{22}-\lambda \end{bmatrix} \begin{bmatrix} \cos\theta \\ a\cos(\theta+\phi) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{19}$$

and

$$\begin{bmatrix} N_{11}-\dfrac{1}{\lambda} & N_{12} \\ N_{21} & N_{22}-\dfrac{1}{\lambda} \end{bmatrix} \begin{bmatrix} \sin\theta \\ a\sin(\theta+\phi) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \tag{20}$$

Since the matrices in the previous two equations are singular, it is sufficient to satisfy the first equation in each linear system; the second equations are redundant. Solving for $\tan\theta$ in these two equations, we not only get an equation for the orientation angle θ, but also get a relationship between a, ϕ and the integer matrix $\mathbf{N}$:

$$\tan\theta = \frac{N_{11}-\lambda+N_{12}a\cos\phi}{N_{12}a\sin\phi} = \frac{-N_{12}a\sin\phi}{N_{11}-\dfrac{1}{\lambda}+N_{12}a\cos\phi}. \tag{21}$$

The last equation simplifies to

$$a^2N_{12}+(N_{11}-N_{22})a\cos\phi - N_{21} = 0, \tag{22}$$

using

$$\det\mathbf{N} = N_{11}N_{22}-N_{12}N_{21} = 1 \tag{23}$$

and

$$\operatorname{tr}\mathbf{N} = N_{11}+N_{22} = k = \lambda + \frac{1}{\lambda}, \tag{24}$$

where $k = 3, 4, 5, \ldots$. We note that when we considered planar extension as a special case of the three-dimensional problem [9], we got $k - 1$ instead of k in the previous equation. Here, we simply used k and have adjusted the integer values of k accordingly.

For a given lattice defined by a and ϕ and a strain period specified by k, the lattice will be reproducible if we can find integers N_{ij} satisfying [22]–[24]. To determine if there are any solutions to this problem for the given parameters, we combine the last three equations into a single equation for N_{11} and N_{12}:

$$\left(N_{11}-\frac{k}{2}\right)^2 + 2a\cos\phi\left(N_{11}-\frac{k}{2}\right)N_{12} + a^2N_{12}^2 = \frac{k^2}{4} - 1. \tag{25}$$

The graph of this equation is an ellipse in the (N_{11}, N_{12}) plane centered at $(k/2, 0)$. The major and minor axes of the ellipse are not aligned with the N_{11} and N_{12} axes unless $\phi = \pi/2$. By determining the points at which the ellipse has a vertical tangent, we can easily find an explicit range for N_{11} in terms of the given parameters. For each integer in this range, we determine N_{12} by solving the quadratic equation [25]. If N_{12} is an integer, we determine N_{22} from [24] and N_{21} from [22]. If N_{21} is also an integer, we have found a solution.

The orientation angle of the strain periodic lattice is determined from [21]. This angle is related to the graph of the ellipse in the following way. First we note that the ellipse intersects the N_{11} axis at $(1/\lambda, 0)$ and $(\lambda, 0)$ and that the ellipse lies in between the two tangent lines passing through these points (see figure 6). These tangent lines give us the following inequalities:

$$N_{11} - 1/\lambda + N_{12}a\cos\phi \geqslant 0 \tag{26}$$

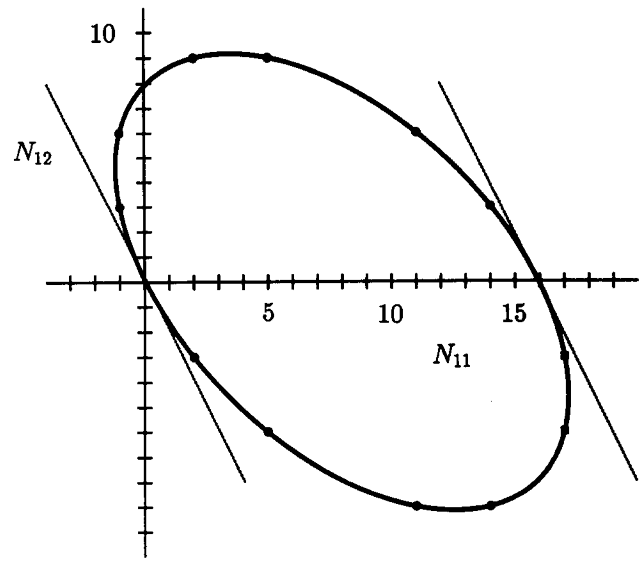

Figure 6. Graph of [30] when $k = 16$. Tangent lines through $(1/\lambda, 0)$ and $(\lambda/0)$ are also shown.

and

$$N_{11} - \lambda + N_{12} a \cos \phi \leqslant 0. \qquad [27]$$

Equality corresponds to the tangent line equations. Second, we note that these exact terms appear in [21] and that the sign of the orientation angle θ is opposite the sign of N_{12}. Furthermore, as we move along the ellipse in the upper half plane corresponding to $N_{12} \geqslant 0$ (see figure 6), the orientation angle θ varies from $-\pi/2$ at $(1/\lambda, 0)$ to 0 at $(\lambda, 0)$. Similarly, in the lower half plane θ varies from 0 at $(\lambda, 0)$ to $\pi/2$ at $(1/\lambda, 0)$. Due to the symmetry of a given lattice, we may only be interested in a certain range of orientation angles; the above information will allow us to further restrict the range of N_{11} values that we need to examine.

SQUARE AND HEXAGONAL LATTICES IN PLANAR EXTENSIONAL FLOW

The square lattice corresponds to $a = 1$ and $\phi = \pi/2$. In this case, [25] reduces an equation for a circle,

$$\left(N_{11} - \frac{k}{2}\right)^2 + N_{12}^2 = \frac{k^2}{4} - 1, \qquad [28]$$

and [22] reduces to $N_{21} = N_{12}$. Due to the symmetry of the lattice, we are only interested in orientation angles satisfying $0 \leqslant \theta \leqslant \pi/4$. These angles correspond to the lower right portion of the circle, where

$$\frac{k}{2} \leqslant N_{11} \leqslant \lambda = \frac{k}{2} + \frac{\sqrt{k^2 - 4}}{2} \quad \text{and} \quad N_{12} \leqslant 0. \qquad [29]$$

For each integer N_{11} in this range, we solve for N_{12} using [28]. If N_{12} is an integer, then we have found an integer solution as both N_{21} and N_{22} will also be integers. The orientation angle is determined from [21]. Table 1 gives the value of k, the Hencky strain $\epsilon = \ln \lambda$, the orientation angle θ and integers N_{ij} for strain periods in the range $0 < \epsilon < 4$. Once an allowable orientation angle and strain period have been determined, there will be other solutions that have the same orientation angle and integer multiples of the strain period. In the range discussed above, there are solutions of this type at $k = 7$, 18, 34 and 47 that are not shown in the table. Even with these additional solutions, there are many values of k for which the square lattice does not have an orientation that is periodic.

Table 1. Strain periodic orientations for a square lattice in planar extensional flow

k	$\epsilon = \ln \lambda$	θ	N_{11}	N_{12}	N_{21}	N_{22}	D^a	Φ
3	0.962424	0.553574	2	−1	−1	1	0.945742	0.702481
6	1.762747	0.392699	5	−2	−2	1	0.840896	0.555360
11	2.389526	0.294001	10	−3	−3	1	0.744782	0.435661
15	2.703576	0.613886	10	−7	−7	5	0.820166	0.528316
15	2.703576	0.368908	13	−5	−5	2	0.820166	0.528316
18	2.887271	0.231824	17	−4	−4	1	0.668740	0.351241
27	3.294462	0.653901	17	−13	−13	10	0.721073	0.408365
27	3.294462	0.273394	25	−7	−7	2	0.721073	0.408365
27	3.294462	0.190253	26	−5	−5	1	0.609418	0.291690
38	3.636893	0.624523	25	−18	−18	13	0.795271	0.496729
38	3.636893	0.160875	37	−6	−6	1	0.562341	0.248365
39	3.662904	0.530602	29	−17	−17	10	0.817034	0.524289
39	3.662904	0.365453	34	−13	−13	5	0.817034	0.524289
43	3.760659	0.679851	26	−21	−21	17	0.647347	0.329128
43	3.760659	0.216204	41	−9	−9	2	0.647347	0.329128
51	3.931441	0.139150	50	−7	−7	1	0.524138	0.215765

[a]These lengths are based on a square lattice with basis vectors of unit length.

The hexagonal lattice corresponds to $a = 1$ and $\phi = \pi/3$. In this case, [25] reduces to

$$\left(N_{11} - \frac{k}{2}\right)^2 + \left(N_{11} - \frac{k}{2}\right)N_{12} + N_{12}^2 = \frac{k^2}{4} - 1. \qquad [30]$$

The major axis of the ellipse is at an angle of $-\pi/4$ with respect to the horizontal N_{11} axis (see figure 6). Due to the symmetry of the hexagonal lattice, we are only interested in orientation angles satisfying $0 \leqslant \theta \leqslant \pi/6$. The portion of the ellipse satisfying these orientation angles is given by

$$\lambda = \frac{k}{2} + \frac{\sqrt{k^2 - 4}}{2} \leqslant N_{11} \leqslant \frac{k}{2} + \frac{\sqrt{k^2 - 4}}{\sqrt{3}}. \qquad [31]$$

The first inequality follows from [21] and $0 \leqslant \theta \leqslant \pi/6$; the second inequality just states that N_{11} is less than or equal to its maximum value which occurs at the point where the graph has a vertical tangent. Even when k is as large as 100, there will only be 8 values of N_{11} that satisfy [30] and need to be examined. In addition, k must be an even integer or N_{21} will not be an integer. This result follows from [22] and [24], which give

$$N_{21} = N_{11} + N_{12} - \frac{k}{2}. \qquad [32]$$

Therefore, for each even integer k, we determine integers N_{11} satisfying [31] and then solve [30] for N_{12}. If N_{12} is an integer, we have found a solution. These solutions occur in pairs and were called periodic pairs by Kraynik & Hansen (1986). We note that if $(N_{11}, N_{12}, N_{21}, N_{22})$ is an integer solution of [22]–[24] for the hexagonal lattice ($a = 1$ and $\phi = \pi/3$), then $(N_{11}, -N_{21}, -N_{12}, N_{22})$ is also a solution. Graphically, they correspond to the two roots of the elliptic equation at a given value of N_{11}. In addition, if θ is the orientation angle of the first solution, then it can be shown that $\pi/6 - \theta$ is the orientation angle of the second solution. These two solutions correspond to the largest value of N_{11}, as shown in figure 6. The solutions outside the range of interest are also shown; they correspond to the above two orientation angles plus integer multiples of $\pi/6$.

Table 2 gives the results for a hexagonal lattice with strain periods in the range, $0 < \epsilon < 5$. Only the first half of the pair is given in the table. The first solution in the table, given by $k = 4$ and $\theta = \pi/12$, is a degenerate solution (both solutions in the pair are identical) and corresponds to the point on the ellipse where the graph has a vertical tangent. There are additional solutions with this same orientation angle at $k = 14$ and 52 that are not shown; they correspond to 2 and 3 times the strain period given.

Table 2. Strain periodic orientations for a hexagonal lattice in planar extensional flow

k	$\epsilon = \ln \lambda$	θ	N_{11}	N_{12}	N_{21}	N_{22}	D[a]	Φ
4	1.316958	0.261799	4	−1	1	0	0.707107	0.453450
16	2.768659	0.166737	17	−3	6	−1	0.572125	0.296853
40	3.688254	0.109256	42	−5	17	−2	0.465594	0.196595
40	3.688254	0.224217	43	−10	13	−3	0.658449	0.393191
50	3.911623	0.140517	53	−8	20	−3	0.526640	0.251529
76	4.330560	0.080136	79	−7	34	−3	0.399482	0.144729
76	4.330560	0.162428	81	−14	29	−5	0.564954	0.289457
110	4.700398	0.095063	115	−12	48	−5	0.434721	0.171388
124	4.820217	0.063032	128	−9	57	−4	0.354584	0.114024
124	4.820217	0.127094	131	−18	51	−7	0.501457	0.228048
146	4.983560	0.220653	157	−36	48	−11	0.653545	0.387356
148	4.997167	0.211032	159	−35	50	−11	0.540928	0.265361

[a]These lengths are based on a hexagonal lattice with basis vectors of unit length.

MINIMUM LATTICE SPACING D DURING PLANAR EXTENSIONAL FLOW

The reproducibility of a lattice guarantees compatibility, the existence of a finite minimum spacing D of all lattice points during flow. In planar extension all lattice points away from the origin follow hyperbolic paths given by

$$xy = x_0 y_0 = \pm\frac{d^2}{2}, \qquad [33]$$

where (x, y) are the coordinates of any lattice point, the subscript 0 refers to initial position and d is the minimum distance from the origin to the hyperbola. Expressing d in terms of the initial lattice parameters defined by [18] and the integer lattice coordinates n_i defined by [1] gives

$$d^2 = 2\,|[n_1 \cos\theta + n_2 a \cos(\theta + \phi)][n_1 \sin\theta + n_2 a \sin(\theta + \phi)]|. \qquad [34]$$

Given a and ϕ, a reproducible lattice must satisfy [22]–[24] for integer k and N_{ij}. Using these integers, the orientation angle θ is obtained from [21]. The minimum lattice spacing D, the smallest value of d for all lattice points, can be expressed as

$$D = \min_{\{n_1, n_2\}} d. \qquad [35]$$

For square lattices,

$$d^2 = |2n_1 n_2 \cos 2\theta + (n_1^2 - n_2^2)\sin 2\theta|, \qquad [36]$$

where θ is given by

$$\tan\theta = \frac{N_{11} - \lambda}{N_{12}}, \qquad [37]$$

the value of λ comes from [29], and $0 \leqslant \theta \leqslant \pi/4$. Because of reproducibility, the minimization in [35] over an infinite set $\{n_1, n_2\}$ reduces to searching a finite number of integer pairs. In table 1 we show D for the reproducible initial lattice orientations θ.

The orientation of a square lattice that maximizes D corresponds to the first entry in table 1 with $\tan\theta$ given by the "golden ratio"

$$\tan\theta = \frac{\sqrt{5} - 1}{2} \qquad [38]$$

and

$$D = \left(\frac{4}{5}\right)^{1/4}. \qquad [39]$$

Adler & Brenner (1985) have shown that this is the largest value of D for planar extensional flow. Because of this, the square lattice with orientation given by [38] is called a *critical lattice*. In figure 7 we show the critical lattice in the initial condition and follow its evolution with Hencky

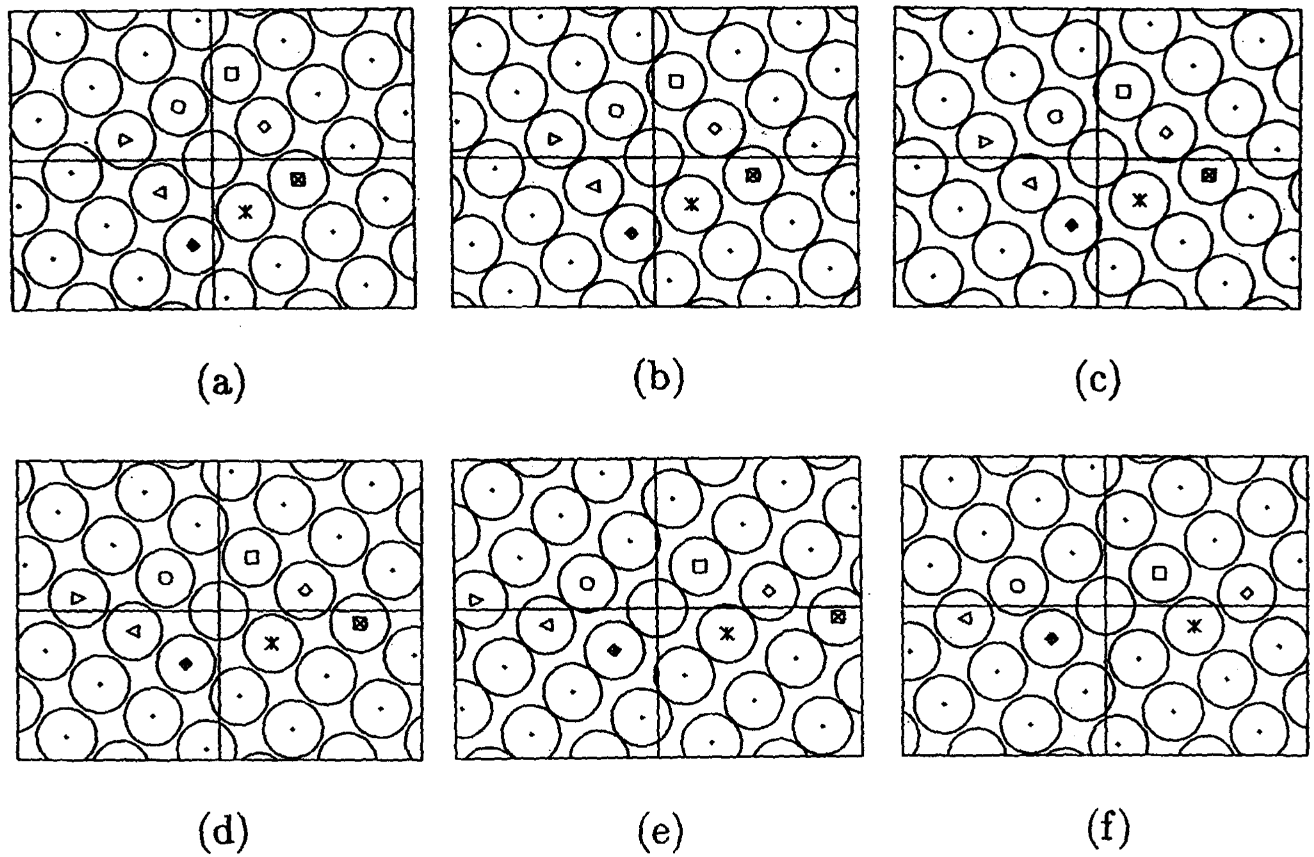

Figure 7. Evolution with Hencky strain ϵ of a square lattice in planar extensional flow. This lattice exhibits both reproducibility and compatibility. The period is $\epsilon_p \approx 0.9624$. A square lattice with this initial orientation has the smallest period and the largest minimum lattice spacing of any lattice in planar extensional flow; the corresponding area fraction of disks is $\Phi^* = \pi\sqrt{5}/10 \approx 0.7025$. (a) When $\epsilon = 0$ the initial lattice orientation angle θ, measured counterclockwise from the X-axis, is related to the golden ratio through $\tan\theta = (\sqrt{5}-1)/2$; (b) $\epsilon = \epsilon_p/8$; (c) when $\epsilon = \epsilon_p/4$, the circles touch; (d) when $\epsilon = \epsilon_p/2$, the points form into a square lattice with a different orientation than $\epsilon = 0$; (e) when $\epsilon = 3\epsilon_p/4$, the circles touch again along lines perpendicular to (c); (f) when $\epsilon = \epsilon_p$ the lattice repeats itself.

strain ϵ over one period. Notice that when the lattice is in the deformed state that determines the minimum spacing, circles of diameter D touch and form parallel chains that are uniformly spaced. The area fraction Φ of these circles is given by

$$\Phi = \frac{\pi D^2}{4A}, \qquad [40]$$

where $A = |\mathbf{b}_1 \times \mathbf{b}_2|$ is the unit cell area. For a square lattice the maximum value of Φ, which corresponds to [38], is

$$\Phi^* = \frac{\pi\sqrt{5}}{10}. \qquad [41]$$

The hexagonal lattice is useful when describing the equilibrium structure of perfectly ordered two-dimensional foams (Kraynik & Hansen 1986; Reinelt & Kraynik 1990). The same procedure as above determines D for regular hexagonal lattices. The minimum lattice spacing is maximized when $\theta = \pi/12$, giving

$$D = \frac{\sqrt{2}}{4} \qquad [42]$$

and

$$\Phi = \frac{\pi\sqrt{3}}{12}. \qquad [43]$$

Values of D and Φ for other strain periodic orientations of the hexagonal lattice are contained in table 2.

CONCLUDING REMARKS

The predictions of microrheological models that are based on a spatially periodic formulation, can depend very strongly on the kinematics of the unit cell in the particular flow of interest. Compatibility of the lattice with the flow guarantees that identical lattice objects with a maximum dimension d that is smaller than the minimum lattice spacing D will *never* overlap. It is important to satisfy a stricter condition, $d \ll D$, when modeling the behavior of disordered systems. In contrast with simple shearing flow, it is not intuitively obvious how to satisfy these conditions for extensional flows.

In this analysis, we have identified compatibility conditions for arbitrary lattices in planar extensional flow by establishing reproducibility, the periodic behavior of the lattice with the flow. Equations [22]–[24] determine reproducibility conditions for an arbitrary lattice. Finding solutions to these equations can involve searching large numbers of integers and be quite tedious. This is in sharp contrast with the situation for simple shearing flow where one can guarantee compatibility and reproducibility by merely aligning either basis vector of the lattice with the flow direction. We have considered two special cases, square and regular hexagonal lattices, and calculated several initial orientation angles and strain periods for planar extension. A square lattice with a particular orientation angle that is related to the golden ratio, $\tan\theta = (\sqrt{5} - 1)/2$, has the smallest period and the largest minimum lattice spacing $D = (4/5)^{1/4} \approx 0.9457$ of any lattice. This value of D is only slightly smaller than the maximum value for simple shearing flow: $D = 1$.

When the physics of the problem does not dictate the geometry of the lattice, a square unit cell oriented according to the golden ratio will usually represent the best choice for planar extension because D is maximized. This choice is not appropriate for a perfectly ordered, two-dimensional foam, which requires a regular hexagonal lattice.

We have shown that no lattice is reproducible in either uniaxial extensional flow or biaxial extensional flow, even though Adler & Brenner (1984) have established the existence of compatibility. Thus, our approach to identifying compatibility conditions does not apply to these flows. The appendix shows by counterexample that compatibility does not imply reproducibility for planar extensional flow, as it does for simple shearing flow.

Reproducibility is convenient when developing a spatially periodic model but certainly not necessary. In its absence, one can, in principle, establish the strict compatibility condition that we have discussed, by other means. However, in the absence of strict compatibility, which refers to the minimum value of D for all time, one can just examine D over finite time intervals. This would provide an assessment of whether or not lattice points approach too closely during a flow of finite but not necessarily small duration. The important thing is to ensure that predictions are not influenced too strongly by the lattice geometry associated with a spatially periodic formulation.

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APPENDIX

This appendix gives an example that shows that compatibility does not imply reproducibility for planar extensional flow. This example is due to Ernest F. Brickell of Sandia National Laboratories.

Let $\theta = (\sqrt{5} - 1)/2$ (the golden ratio).

We will use several facts from number theory that can be found in standard number theory texts. The theorem and page numbers below refer to Hardy & Wright (1979). For $n \geqslant 1$, let p_n/q_n be the rational number that is the nth convergent in the continued fraction expansion of θ. These convergents satisfy:

1. If $n > 1$ and if p and q are integers such that $0 < q \leqslant q_n$ and

$$\frac{p}{q} \neq \frac{p_n}{q_n},$$

then $|p_n - q_n\theta| < |p - q\theta|$. (Theorem 182)

2. $q_n \leqslant 2q_{n-1}$. (p. 163)

3. $|q_n\theta - p_n| \geqslant \dfrac{1}{3q_n}$.

(On p. 163, it is shown that

$$|q_n\theta - p_n| = \frac{1}{q_n\left(1+\theta+\dfrac{q_{n-1}}{q_n}\right)}.$$

But

$$1+\theta+\frac{q_{n-1}}{q_n} < 2+\theta < 3.\Big)$$

Let L be the lattice generated by the vectors $\mathbf{v} = (1, -1)$ and $\mathbf{w} = (6+\theta, 6+\theta)$. The following theorem will show that L is compatible but not periodic since any vector $\mathbf{u}(0) = (x(0), y(0))$ in L will follow a curve $\mathbf{u}(t) = (x(t), y(t))$ in the extensional flow that satisfies $x(t)y(t) = x(0)y(0)$.

Theorem 1

The only vectors (x, y) *in* L *that satisfy* $|xy| \leqslant 1$ *are the vectors* $(0, 0)$, $(1, -1)$ *and* $(-1, 1)$.

Proof. Any vector in L can be written as $(q(6+\theta)+p, q(6+\theta)-p)$ for integers p and q. For $q = 0$, the vector $(p, -p)$ satisfies $p^2 \leqslant 1$ iff $p = 0$, 1 or -1. Suppose now that $q \neq 0$. By symmetry, we can assume that $q > 0$ and $p \geqslant 0$. Let n be the integer such that $q_{n-1} < q \leqslant q_n$. Then

$$\begin{aligned}
|(q(6+\theta)+p)(q(6+\theta)-p)| &\geqslant |(q(6+\theta)+p)||(q(6+\theta)-p)| \\
&\geqslant |(q(6+\theta)+p)||q_n\theta - p_n| \\
&\geqslant |(q(6+\theta)+p)|\,\frac{1}{3q_n} \\
&\geqslant \frac{q}{q_n}\,\frac{6+\theta}{3} \\
&\geqslant \frac{6+\theta}{6} \\
&> 1.
\end{aligned}$$