A new fast method for
determining local properties
of striped patterns

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From the striped coats of zebras to the ripples in windblown sand, the natural
world abounds with locally banded patterns. Such patterns have been of great interest
throughout history, and, in the last twenty years, scientists in a wide variety of fields
have been studying the patterns formed in well-controlled experiments that yield
enormous quantities of high-precision data. These experiments involving phenomena
as diverse as chemical reactions in shallow layers, thermal convection in horizontal
fluid layers, periodically shaken layers of sand, and the growth of slime mold colonies,
often display patterns that appear qualitatively similar. Methods are needed to
characterize in a reasonable amount of time the differences and similarities in patterns
that develop in different systems, as well as in patterns formed in one system for
different experimental conditions. In this Letter, we introduce a novel, fast method for
determining local pattern properties such as wavenumber, orientation, and curvature
as a function of position for locally striped patterns.

Fig. 1 shows a locally striped pattern formed in a simulation of Rayleigh-Bénard convection,
in which a horizontal layer of fluid of lateral extent $L$ is confined between two parallel plates
with separation $d$ and a temperature difference $\Delta T = T_{\text{bottom}} - T_{\text{top}} > 0$. For $\Delta T$ larger than
a critical value $\Delta T_c$, a convective instability develops. In most situations studied experimentally,
this instability leads to the development of a striped convective roll pattern with a horizontal local wavenumber \( k \approx \pi/d \). For systems of large aspect ratio \( \Gamma = L/d \) (i.e., many convective rolls), the patterns formed are often spatially and temporally disordered but are still locally striped as seen in Fig. 1. The development of disordered locally periodic patterns through instabilities is common to a wide variety of large aspect ratio experiments in biological, chemical, optical, and fluid systems.

The use of local pattern properties to describe patterns similar to that in Fig. 1 has already been explored by several researchers. Heutmaker and Gollub\(^6\) determined the wavevector field and statistics such as the “roll bending” and “roll obliqueness” in both stationary and time-dependent patterns in a circular Rayleigh-Bénard convection cell. They studied whether these quantities could be used to understand the stability of convective patterns. More recently, Hu, et al.\(^7\) computed local wavenumbers and curvatures in experimental pictures very similar to the one shown in Fig. 1. Based on these local measurements, they proposed order parameters to describe transitions in spatiotemporal chaos in Rayleigh-Bénard convection. In a numerical study of a model of Rayleigh-Bénard convection rotated about a vertical axis, Cross, et al.\(^8\) computed the local orientation of rolls to characterize domain structure. Ouyang and Swinney\(^1\) also used the local orientation to analyze patterns in a chemical reaction-diffusion system. Gunaratne, et al.\(^9\) have suggested an invariant measure of the disorder of locally striped patterns, and they have demonstrated its use on reaction-diffusion patterns. In a set of recent papers, Newell and coworkers\(^10–12\) have begun to use local wavenumbers to study the behavior of phase-diffusion equations in the presence of defects.

Although these previous studies clearly demonstrated the potential utility of local pattern properties, they were somewhat limited by the large amount of time it took to process each snapshot of a complicated time-dependent behavior. The researchers used a variety of methods including nonlinear least squares fits to small patches of the pattern,\(^6\) automated\(^7\) and semi-automated\(^6\) determination of pattern “skeletons”, and modern wavelet-based procedures.\(^1,8,10–12\) In this Letter we describe a new, fast method for calculating these local properties based on ratios of simple partial derivatives.

For patterns that are locally striped, we can approximate each field point \( u(\vec{x}) \) using:

\[
 u(\vec{x}) = A(\vec{x}) \cos(\phi(\vec{x})). \tag{1}
\]

The local wavevector \( \vec{k} \) is defined as:

\[
 \vec{k}(\vec{x}) \equiv \vec{\nabla} \phi(\vec{x}). \tag{2}
\]
Sufficiently far from defects and grain boundaries, we expect that the variations in $A(\vec{x})$ are small compared to the variations in $\phi(\vec{x})$. In that case, the components of the wavevector $\vec{k}$ can be found using simple partial derivatives. For example,

$$k_x^2 = -\frac{\partial^2 u(\vec{x})}{u(\vec{x})},$$

where $k_x = \vec{k} \cdot \hat{x}$ and $\partial_x^2 \equiv \partial^2 / \partial x^2$. A similar expression can be written for $k_y^2$. However, two problems are immediately apparent. The first is that when $u(\vec{x})$ is close to zero, Eq. (3) will be very sensitive to small uncertainties in $u(\vec{x})$ due to experimental or numerical noise. This problem is easily remedied by taking the ratio of the third partial derivative to the first partial derivative for points where $u(\vec{x})$ is small.

The second problem is more subtle. Eq. (3) and the equivalent equation for $k_y^2$ yield only the magnitudes of the wavevector components $k_x$ and $k_y$. From these magnitudes, the vector can be specified in any of four directions. We note, however, that periodicity in a real field is invariant under rotations by $\pi$, so the wavevector $(k_x, k_y)$ is equivalent to the wavevector $(-k_x, -k_y)$; i.e., the wavevector is actually a director, so we only need to determine the relative signs of $k_x$ and $k_y$. We accomplish this by using combinations of partial derivatives in the $x$-direction and the $y$-direction. For example, if Eq. (3) is used to determine $|k_x|$, the value of $k_y$ with its sign relative to $k_x$ is computed using:

$$k_y = k_x \frac{\partial_{xy} u(\vec{x})}{\partial_{xx}^2 u(\vec{x})}.$$  

If $\partial_{xx}^2 u(\vec{x})$ is close to zero, which occurs when the wavedirector lies in a direction close to the $y$-axis, $k_y$ is determined first and then $k_x$.

Our procedure for determining the values of $k_x$ and $k_y$ at each point of the field $u(\vec{x})$ is summarized as follows. The global mean of the field, $<u(\vec{x})>$, is first subtracted from the field. This result is then normalized so that the largest absolute value of the field is 1. For each point $\vec{x}$, the value of the normalized field $u(\vec{x})$ and its partial derivatives $\partial_x u(\vec{x}), \partial_y u(\vec{x}), \partial_x^2 u(\vec{x}),$ and $\partial_y^2 u(\vec{x})$ are used to choose between the following four cases:

1. $|u(\vec{x})| > \max(|\partial_x u(\vec{x})|, |\partial_y u(\vec{x})|)$ and $|\partial_x^2 u(\vec{x})| > |\partial_y^2 u(\vec{x})|$: 

$$k_x = \sqrt{\left| \frac{\partial_x^2 u(\vec{x})}{u(\vec{x})} \right|}$$  

$$k_y = k_x \frac{\partial_{xy} u(\vec{x})}{\partial_{xx}^2 u(\vec{x})}.$$  

If $\partial_{xx}^2 u(\vec{x})$ is close to zero, which occurs when the wavedirector lies in a direction close to the $y$-axis, $k_y$ is determined first and then $k_x$.
2. \( |u(\vec{x})| > \max(|\partial_x u(\vec{x})|, |\partial_y u(\vec{x})|) \) and \( |\partial_x^2 u(\vec{x})| \leq |\partial_y^2 u(\vec{x})| \):

\[
\begin{align*}
    k_y &= \sqrt{\frac{\partial_y^2 u(\vec{x})}{u(\vec{x})}} \\
    k_x &= k_y \frac{\partial_x^2 u(\vec{x})}{\partial_x u(\vec{x})}
\end{align*}
\] (7)

3. \( |u(\vec{x})| \leq \max(|\partial_x u(\vec{x})|, |\partial_y u(\vec{x})|) \) and \( |\partial_x u(\vec{x})| > |\partial_y u(\vec{x})| \):

\[
\begin{align*}
    k_x &= \sqrt{\frac{\partial_y^2 u(\vec{x})}{\partial_x u(\vec{x})}} \\
    k_y &= k_x \frac{\partial_y^2 u(\vec{x})}{\partial_x u(\vec{x})}
\end{align*}
\] (8)

4. \( |u(\vec{x})| \leq \max(|\partial_x u(\vec{x})|, |\partial_y u(\vec{x})|) \) and \( |\partial_x u(\vec{x})| \leq |\partial_y u(\vec{x})| \):

\[
\begin{align*}
    k_y &= \sqrt{\frac{\partial_x^2 u(\vec{x})}{\partial_y u(\vec{x})}} \\
    k_x &= k_y \frac{\partial_x^2 u(\vec{x})}{\partial_y u(\vec{x})}
\end{align*}
\] (9)

If the value of \( k_x \) is negative, the signs of both \( k_x \) and \( k_y \) are changed to ensure that \( k_x \geq 0 \), while \( k_y \) contains the information about the orientation of the wavedirector.

Because this method is local, the effects of noise, of higher harmonics, and of amplitude variations neglected in Eq. (1) are often noticeable. We reduce these effects by smoothing the \( k_x \) and \( k_y \) fields over small regions. Although more sophisticated smoothing methods are possible, we have successfully employed a simple method in which the \( k_x \) (or \( k_y \)) value is replaced by the average of the \( k_x \) (or \( k_y \)) values within a small square region of the field points. We have generally found it sufficient to smooth over a region of size \( \lambda^2 \), where \( \lambda \) is approximately the average wavelength in the pattern. The particular choice of \( \lambda^2 \) removes most of the contributions from higher harmonics and amplitude variations. Further smoothing can be accomplished by repeating the procedure multiple times as necessary. The size of the smoothing region and the number of smoothings can be easily determined empirically since local higher harmonics will appear as obvious modulations to the wavenumber field.

As we noted above, the wavevector field is actually a director field, so care must be taken when averaging the neighboring \( k_x \) (\( k_y \)) values since \( \vec{k} \) is equivalent to \( -\vec{k} \). To determine whether to include \( \vec{k} \) or \( -\vec{k} \) in the average, we take the dot product of the wavevector at the point of interest,
\( \vec{k}_0 \), and the wavevector of the point to be included in the average, \( \vec{k} \). If \( \vec{k}_0 \cdot \vec{k} \geq 0 \), the angle between \( \vec{k}_0 \) and \( \vec{k} \) is less than \( \pi/2 \) so we average in \( k_x (k_y) \); however, if \( \vec{k}_0 \cdot \vec{k} < 0 \), we average in \( -k_x (-k_y) \).

Since the local wavenumber is undefined at defects and grain boundaries, our procedure yields spurious values of \( k_x \) and \( k_y \) at these points. In the averaging procedure we are careful to exclude values of \( k_x \) and \( k_y \) for which \( k^2 = k_x^2 + k_y^2 \) is far outside the range of expected values. We have found that typically only values within a distance of about 1-2 field points around the defects need to be excluded from the average.

Two other factors need to be considered when analyzing experimentally generated data fields (as opposed to fields generated by simulating partial differential equations). Typically, experimental data have a larger component of large-wavenumber noise than simulational data. The effect of this noise can be lessened by applying a Fourier filter to the entire data field before our procedure is employed. This Fourier filter should only be applied at wavenumbers well outside the expected range of local wavenumbers. Another potential problem is that in some experiments the mean of the picture varies spatially, perhaps due to optical imaging effects. One solution to this problem is to first determine the mean of the field everywhere through averages over large regions and subtract this spatially varying mean from the data field. However, for fields in which the variation of the mean is slow compared to typical local wavelengths, a simpler solution is to replace the ratios \( \partial_x^2 u(\vec{x})/u(\vec{x}) \) and \( \partial_y^2 u(\vec{x})/u(\vec{x}) \) in Eqs. (5) and (7) with \( \partial_x^4 u(\vec{x})/\partial_x^2 u(\vec{x}) \) and \( \partial_y^4 u(\vec{x})/\partial_y^2 u(\vec{x}) \), respectively.

A final consideration in this procedure is the best method for computing the partial derivatives in Eqs. (6)–(12). To obtain high-order derivatives, we perform the differentiation in Fourier space. Alternatively, the partial derivatives could be obtained in coordinate space directly using high-order finite-difference schemes. We note that the calculation of the derivatives only consumes a small fraction of the total time to evaluate a pattern. The computation is heavily dominated by the smoothing procedure and by the choice of what derivatives to use at each field point. If, for a given application (such as locating disclinations), it is not necessary to determine the wavevector field very precisely, little or no smoothing is required and the computation time is reduced drastically.

Once the values of \( k_x \) and \( k_y \) are determined for each point of a data field, local quantities such as the wavenumber, the orientation of the periodicity, and the curvature can be computed. As a sample of the use of our procedure, we present four figures showing these quantities for patterns
generated by simulations of the Boussinesq equations describing Rayleigh-Bénard convection.

The local orientation of the rolls, \( \theta(\bar{x}) = \arctan(k_y(\bar{x})/k_x(\bar{x})) \), at each point of the pattern in Fig. 1 is shown in Fig. 2. This figure emphasizes the large regions of straight rolls often found within the spiral defect chaos state of Rayleigh-Bénard convection. Fig. 3 shows the local wavevector magnitude, \( |\mathbf{k}(\bar{x})| = \sqrt{k_x^2(\bar{x}) + k_y^2(\bar{x})} \), at each point of Fig. 1. The wavenumber is approximately constant across the pattern with a mid-range value (green), but small localized regions of high (red) and low (blue) wavenumber are interspersed throughout. (These data, plus the value of the roll curvature at each point, were obtained in less than 30 seconds on a single RS/6000 POWER2 processor running at 66.7 MHz, and even less time would be required at lower levels of smoothing.)

The region inside the small rectangle in Fig. 1 is shown in greater detail in Fig. 4(a). Fig. 4(b) and (c) show the local roll orientation and local wavevector magnitude, respectively, for this pattern. The rotation of the roll orientation about the centers of each of the two spirals is shown clearly in Fig. 4(b). Also, along the left side and along parts of the top and bottom portions of the figure are regions of almost constant color indicating that the rolls are approximately straight in those regions. In Fig. 4(c), areas with compressed rolls (high wavenumber) are highlighted in red (e.g., the bottom left corner), while defects and regions with low wavenumber are shown as blue.

As an illustration of how these local pattern properties relate to the features of the pattern, Fig. 5(a) shows a simple pattern with a single dislocation moving up the page. Fig. 5(b) and (c) show the magnitude of the wavevector and roll curvature \( C = \mathbf{\nabla} \cdot \mathbf{k} \), respectively, as a function of position for this pattern. The deformation of the pattern caused by the dislocation is clear from this figure. A “wake” of locally high wavenumber follows the defect while small regions of low wavenumber form diagonally in front of the defect. The locality of the majority of the deformation is also evidenced by the small regions of high curvature shown in Fig. 5(c).

We are currently studying the use of statistics based on the quantities described above as order parameters for describing transitions between different spatiotemporal chaotic states. In addition, we are looking at how the spatial and temporal behavior of the local quantities are related to the dynamics of the chaotic states. Of particular interest is the behavior of defects and disclinations, which can be located and classified based on the local wavevector field. These works will be described in future publications.

We have presented a novel, fast, automated method for determining local pattern properties as
a function of spatial position for patterns that are locally striped. Although we have emphasized our method’s utility for characterizing spatiotemporal chaotic states, we stress that our method is simple and general, and it can be applied to locally striped patterns independent of their origin. Because of its speed, this new method may allow for the calculation of new statistics to characterize disordered patterns in a wide variety of scientific disciplines.

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Figures

FIG. 1. The temperature field at the midplane of a simulation of the Boussinesq equations with reduced Rayleigh number $\epsilon = 0.6$ and Prandtl number $\sigma = 1.0$ in a box with square periodic lateral boundaries with aspect ratio $\Gamma = 160 \times 160$ and 512 grid points in each lateral direction. Dark points indicate cold downflow; white points indicate warm upflow.

FIG. 2. The local roll orientation $\theta(\vec{x}) = \arctan(k_y(\vec{x})/k_x(\vec{x}))$ in radians for the field shown in Fig. 1. Two smoothings, each with a radius of 3 field points ($\approx \lambda/2$), are performed.

FIG. 3. The local wavevector magnitude $|\vec{k}(\vec{x})|/k_c$ for the field shown in Fig. 1, where $k_c$ is the magnitude of the wavevector at the onset of convection. Two smoothings, each with a radius of 3 field points ($\approx \lambda/2$), are performed.

FIG. 4. (a) A detailed view of the pattern inside the small rectangle in Fig. 1. (b) its local roll orientation, and (c) its local wavevector magnitude $|\vec{k}(\vec{x})|/k_c$. The color schemes for (b) and (c) are the same as in Fig. 2 and Fig. 3, respectively.

FIG. 5. (a) A small region ($\Gamma = 55 \times 48$) from the temperature field at the midplane of a simulation of the Boussinesq equations with reduced Rayleigh number $\epsilon = 0.55$ and Prandtl number $\sigma = 1.1$ in a box with square periodic lateral boundaries with aspect ratio $\Gamma = 201 \times 201$ and 512 grid points in each lateral direction. Dark points indicate cold downflow; white points indicate warm upflow. (b) The local wavevector magnitude $|\vec{k}(\vec{x})|/k_c$ for the pattern shown in (a). The colors range from blue (1.32) to red (1.49). (c) The local roll curvature $C = \vec{\nabla} \cdot \hat{k}$ for the pattern shown in (a). The colors range from blue ($0.00 \times 10^{-3} k_c$) to red ($7.33 \times 10^{-3} k_c$).
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