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# Critical role of pinning defects in scroll-wave breakup in active media

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**Abstract** – The breakup of rotating scroll waves in three-dimensional excitable media has been linked to important biological processes. The known mechanisms for this transition almost exclusively involve the dynamics of the scroll filament, *i.e.*, the line connecting the phase singularities. In this paper, we describe a novel defect-induced route to breakup of a scroll wave pinned by an inexcitable obstacle partially extending through the bulk of the medium. The wave is helically wound around the defect inducing sudden changes in velocity components of the wavefront at the obstacle boundary. This results in breakup far from the filament, eventually giving rise to spatiotemporal chaos. Our results suggest a potentially critical role of pinning obstacles in the onset of life-threatening disturbances of cardiac activity.

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**Introduction.** – Spatiotemporal patterns such as rotating spiral waves are frequently observed in excitable media models that describe the dynamics of a wide range of physical, chemical and biological systems [1–3]. The ubiquity of such waves in numerous natural processes makes it imperative to understand their genesis and the means by which they can be controlled. Patterns in homogeneous active media have been the subject of intense theoretical and experimental investigations for several decades [4–6]. However, most natural systems possess significant inhomogeneities and the dynamics of waves in *disordered* media has come under increasing scrutiny in recent times [7–10]. The heterogeneities considered can be partially or wholly inexcitable obstacles [9–11], gradients of excitation or conduction properties [12] and anisotropy in the speed of propagation [13]. Most such studies have focused on two-dimensional systems and the results show unexpected complexity, such as fractal basins of attraction for different dynamical states corresponding to pinned waves, spatiotemporal chaos and complete termination of activity [14–16]. Nevertheless, these “planar” models do not completely describe real systems which are necessarily three-dimensional. Adding an extra dimension is

equivalent to considering the thickness of the system, so that one can in principle distinguish between phenomena on the surface and that in the bulk. More importantly, three-dimensional disordered media can exhibit novel dynamical phenomena that do not appear in lower dimensions. A frequently occurring pattern of activity in such systems is the scroll wave, which is a higher-dimensional generalization of the spiral wave (fig. 1(a)). It can be visualized as a set of contiguous rotating spirals whose phase singularities describe a continuous line (filament) along the rotation axis perpendicular to the plane of the spirals [17] (fig. 1(c)). Scroll waves have been experimentally observed in many natural systems including chemical waves in the Belusov-Zhabotinsky reaction [18–20], patterns of aggregation during *Dictyostelium* morphogenesis [21,22] and electrical waves in heart muscles [3]. Indeed scroll waves have been implicated in several types of arrhythmia, *i.e.*, disturbances in the natural rhythmic activity of the heart that can be potentially fatal. Under certain conditions these three-dimensional waves can develop instabilities and break up into multiple scroll fragments. The ensuing spatiotemporally chaotic state of excitation is associated with the complete loss of coherent cardiac activity in life-threatening arrhythmia such as ventricular

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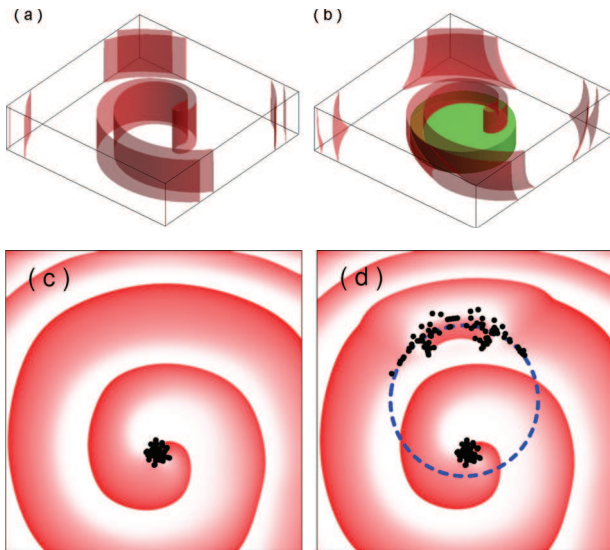


Fig. 1: (Color online) Scroll waves in (a) a homogeneous medium and (b) a medium having an inexcitable cylinder-shaped obstacle that extends only partly through the bulk of the medium. (c), (d): pseudocolor images of spiral waves observed in a cross-sectional plane perpendicular to the axis of rotation, for the systems shown in (a) and (b), respectively. The black dots correspond to the intersection of the plane with the filament at different times, indicating the trajectory of the phase singularity in the plane. In (d), the plane chosen is just above the upper bounding surface of the obstacle whose circumference is indicated using broken lines. The appearance of additional black dots along the broken circle in (d) indicates a wavebreak induced by the obstacle at its boundary, far from the existing scroll filament.

fibrillation [23,24]. Therefore, a deeper understanding of the mechanisms that lead to chaotic activity through breakup of scroll waves is of great practical significance.

At present almost all proposed scenarios for scroll wave breaking involve complex filament dynamics [25]. The question as to whether there can be other mechanisms, especially one involving breakup far from the singularities, is of special significance when considering disordered media [26]. This is because heterogeneities such as inexcitable obstacles can anchor rotating waves and stabilize filament dynamics preventing the usual breakup scenario. While the interaction of scroll waves with inexcitable obstacles has recently been investigated [27–31], the existence of several types of disorder in the systems considered in these studies do not clearly reveal the exact mechanisms for wavebreaks that are involved. By focusing on a simplified situation of a defect with regular geometry we ask whether there can be a purely obstacle-induced breakup mechanism for scroll waves.

In this paper, we have considered an isotropic three-dimensional system with an inexcitable obstacle of uniform cross-section that does not span the entire thickness of the medium (fig. 1(b)). This is motivated by the physiological observation that an inexcitable obstacle may be

located deep in the bulk of heart tissue, where it cannot be detected through electrophysiological imaging of the surface [32,33]. We show a novel dynamical transition that can occur in such a situation which does not appear in the absence of a defect, nor in the effectively two-dimensional situation when the obstacle spans the thickness of the medium. We observe that under certain circumstances, the wave can break near the bounding edge of the obstacle and far from the scroll wave filament (fig. 1(d)). This happens when the wavefront velocity decreases sharply at the edge as a result of sudden change in its curvature (which is related to the “source-sink” relation expressing the balance of electrical currents during wave propagation [34]). The novelty of the mechanism presented in this paper lies in the fact that the breakup does not involve the filament, unlike the previously proposed pathways for the onset of chaos in three-dimensional excitable media. It is especially relevant for disordered media as the transition to chaos is essentially defect induced because the wave is *stable* (*i.e.*, it does not break or result in the generation of additional filaments) in the *absence* of the inexcitable obstacle.

**Models.** – To simulate spatiotemporal activity in three-dimensional excitable tissue, we use models having the generic form

$$\frac{\partial V}{\partial t} = -\frac{I_{ion}(V, g_i)}{C_m} + \nabla \cdot D \nabla V, \quad (1)$$

where  $V$  is the activation variable, typically, the potential difference across a cellular membrane (measured in mV),  $C_m$  ( $= 1 \mu\text{F cm}^{-2}$ ) is the transmembrane capacitance,  $D$  represents the inhomogeneous intracellular coupling,  $I_{ion}$  ( $\mu\text{A cm}^{-2}$ ) is the total current density through ion channels on the cellular membrane, and  $g_i$  describes the dynamics of gating variables of different ion channels. The specific functional form for  $I_{ion}$  varies for different biological systems. For the results reported here we have used the Luo-Rudy I (LR1) model that describes the ionic currents in a ventricular cell [35] with the following modifications. The slow inward  $\text{Ca}^{2+}$  channel conductance  $G_{si}$  is taken to be  $\leq 0.04 \text{ mS cm}^{-2}$  and the maximum  $\text{K}^+$  channel conductance  $G_K$  is increased to  $0.705 \text{ mS cm}^{-2}$  [36]. This reduces the slope of the restitution curve and enables us to study scroll wave dynamics in a stable regime where the waves do not break up spontaneously in the absence of an obstacle [37]<sup>1</sup>.

We have explicitly verified that our results are not sensitively dependent on model-specific details (*e.g.*, description of ion channels) by observing similar effects in the simpler phenomenological model proposed by Panfilov (PV) [38].

**Methods.** – The equations are solved using a forward Euler scheme with time step  $\delta t = 0.01 \text{ ms}$  in a

<sup>1</sup>We have explicitly verified that the scroll wave does not break up in the absence of any obstacle by evolving the system for long durations ( $>10^4 \text{ ms}$ ).



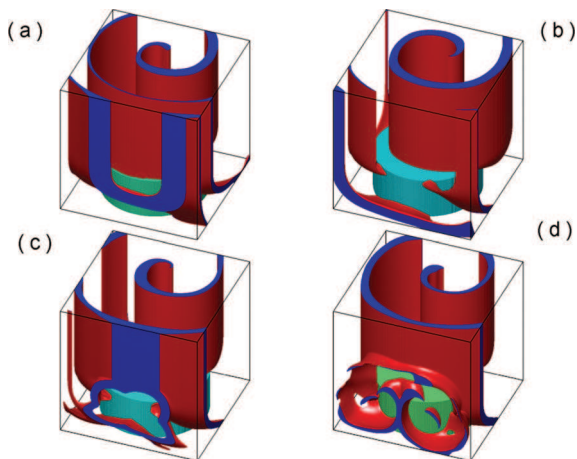


Fig. 2: (Color online) Breakup of a scroll wave induced by a cylindrical obstacle ( $R = 3.4$  cm,  $L_z = 2.7$  cm). (a) By  $T = 275$  ms after the initial wavebreak, the resulting scroll wave has wound itself around the obstacle. (b) A wavefront detaches from the surface of the obstacle, at the boundary of its upper surface, by  $T = 300$  ms. This broken wavefront eventually evolves into new scroll wave filaments ((c), (d)). The period of a free (unpinned) scroll wave in this parameter regime is  $T_{free} = 65.13$  ms.

three-dimensional simulation domain having  $L \times L \times L$  points. Most of the results reported here are for  $L = 400$ , although we have verified their size independence by repeating our simulations with different system sizes up to  $L = 600$ . The space step used is  $\delta x = 0.0225$  cm, with a standard 7-point stencil for the Laplacian describing the spatial coupling [39,40]. No-flux boundary conditions are applied on the boundary planes of the simulation domain. To simulate the electrically non-conducting nature of the inexcitable obstacle, we also impose no-flux boundary conditions along its walls. The coupling  $D$  is set to zero inside the obstacle, while outside it is  $0.001 \text{ cm}^2 \text{ s}^{-1}$ . We have considered obstacles of different shapes, including cylinders and cuboids, and have not observed qualitative differences between them. Obstacles are characterized by their height  $L_z$  (beginning from the base of the simulation domain and ranging between 0 to  $L$ ) and cross-sectional area (*viz.*,  $\pi R^2$  for cylinders where  $R$  is the radius and  $L' \times L'$  for a cuboid). The initial scroll wave, with its filament aligned along the  $L_z$ -axis, is obtained by breaking a three-dimensional planar wavefront. Qualitatively similar results are achieved with waves having curved filaments. Note that the implementation of the non-conducting property of the inexcitable obstacle is important to establish the exclusively three-dimensional feature of the breakup mechanism shown here. This is because wavefronts interacting with heterogeneities that act as electrical sinks (*e.g.*, ref. [41]) may result in conduction block independent of the specific geometry of the setup [9,10].

**Results.** – The most important result obtained from our simulations is that a sufficiently large pinning defect

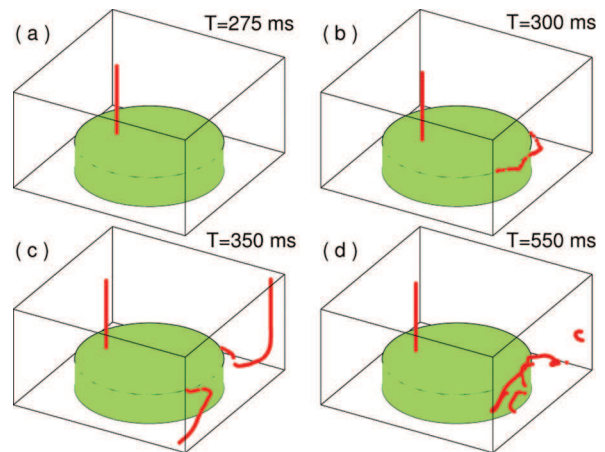


Fig. 3: (Color online) Filament dynamics during obstacle-induced breakup of a scroll wave. (a) At  $T = 275$  ms after the initial wavebreak results in the generation of a scroll wave rotating around the obstacle, there is a single filament (corresponding to the rotating scroll wave) in the system, oriented parallel to the axis of the cylindrical obstacle. (b) By  $T = 300$  ms, another filament has developed away from the original filament (which continues to exist unperturbed by the wavebreak phenomenon occurring at the obstacle boundary). The new filament appears as a result of a “tearing” of the wavefront as it travels past the bounding edge of the inexcitable obstacle. (c) The newly formed filament subsequently collides with the domain boundary, splitting into two separate filaments moving independently of each other. (d) Further interactions between the filaments, the obstacle and the domain boundaries result in the generation of even more filaments over time, eventually leading to spatiotemporal chaos.

can promote wavebreaks in an otherwise stable rotating wave (figs. 2 and 3). At the initial stage, when a broken wave is anchored by the obstacle, the partial extension of the latter through the bulk of the medium produces differential rotation speeds of the scroll wave along the  $L_z$ -axis. Far above the obstacle the period is closer to  $T_{free}$ , that of a free scroll wave unattached to any obstacle, while at the base of the obstacle the period  $T_{pinned} \sim R/c$  is substantially slower depending upon the radius  $R$  of the obstacle ( $c$  being the average propagation speed normal to the wavefront). This results in a helical winding of the scroll wave around the obstacle until a steady state is achieved when the rotation period becomes identical across the domain (fig. 2(a)). The pitch of the wound scroll wave depends on the obstacle size, with larger radius resulting in a tighter winding, *i.e.*, smaller pitch. Note that the filament of the resulting scroll wave, which stretches from the top of the obstacle to the upper boundary of the simulation domain, remains the same as that of a free scroll wave (see figs. 1 and 3(a)). When the wavefront is close to the filament it has velocity components only along the plane perpendicular to the  $L_z$ -axis. However, when the wave crosses the obstacle boundary, it develops a velocity component parallel to the  $L_z$ -axis as the front travels down the vertical sides of the obstacle. Figure 4 shows that

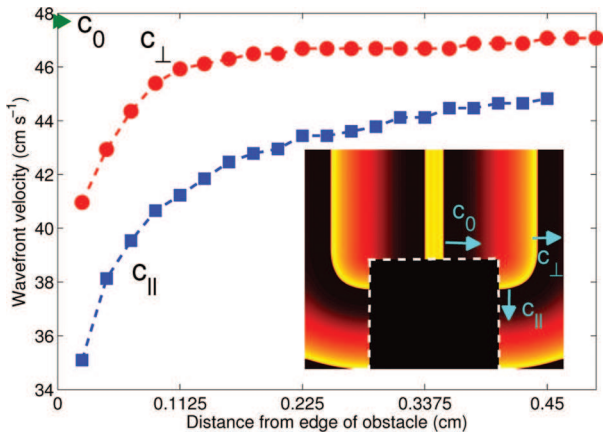


Fig. 4: (Color online) The velocity of the excitation wavefront after it moves past the bounding edge of the obstacle, shown as a function of the increasing distance from the edge. The initial propagation speed of the wave before it crosses the boundary  $c_0$  is indicated. The two velocity components of the front,  $c_\perp$  and  $c_\parallel$ , emerge just after the wavefront traverses the boundary. The large relative change with respect to  $c_0$  very close to the edge indicates a sudden slowing-down of the wave at the obstacle boundary. As the wave propagates away from the obstacle, its velocity increases asymptotically towards  $c_0$ . The inset shows a pseudocolor plot of the transmembrane potential  $V$  for a cross-section of the three-dimensional system along a plane parallel to the  $L_z$ -axis passing through the center of the obstacle. The different velocity components of a traveling excitation front generated by a line electrode parallel to the  $L_z$ -axis are indicated.

both velocity components exhibit a large decrease as the wave crosses the obstacle boundary, with the component parallel to the  $L_z$ -axis having the greater reduction. The magnitude of this change in velocity depends on the pitch of the helical winding, and hence on the circumference of the obstacle, with larger obstacles resulting in greater velocity differences. As seen in fig. 2(b), this sudden change in the velocity components as the front crosses the edge of the obstacle upper surface may result in the detachment of a succeeding wave from the obstacle surface. This is manifested as a “tear” on the wavefront surface as it breaks, generating a new filament (fig. 3(b)). Further evolution of the system produces more complex wave fragments as additional filaments are generated and which interact with each other (figs. 2(c), (d) and 3(c), (d)), eventually leading to spatiotemporal chaos (fig. 5).

To better understand the mechanism by which the pinned scroll wave breaks, we consider the cross-sectional view of the system parallel to the  $L_z$ -axis (fig. 6(a)–(c)). Figure 6(a) indicates the direction of propagation as the waves move first along the upper surface and then down the vertical sides of the obstacle (darkly shaded in the figures). The wave  $W_1$  slows down as it moves past the boundary of the upper surface of the obstacle. This results from a sudden change in the velocity components of the front mentioned earlier and is associated with an

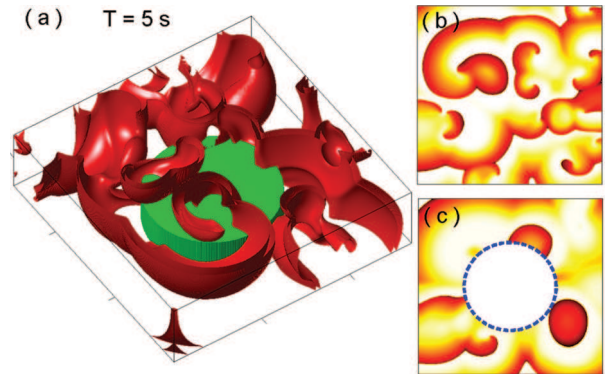


Fig. 5: (Color online) (a) Fully developed spatiotemporal chaos following scroll wave breakup induced by a cylindrical obstacle ( $R = 3.4$  cm,  $L_z = 1.8$  cm) after a duration of  $T = 5$  s following the initiation of the broken wavefront in a rectangular simulation domain having lateral dimensions of 13.5 cm and a height of 3.6 cm. (b), (c): pseudocolor images of the cross-sectional planes perpendicular to the  $L_z$ -axis corresponding to the (b) top ( $z = L$ ) and (c) bottom ( $z = 0$ ) surfaces of the simulation domain. In (c), the perimeter of the obstacle is indicated using broken lines.

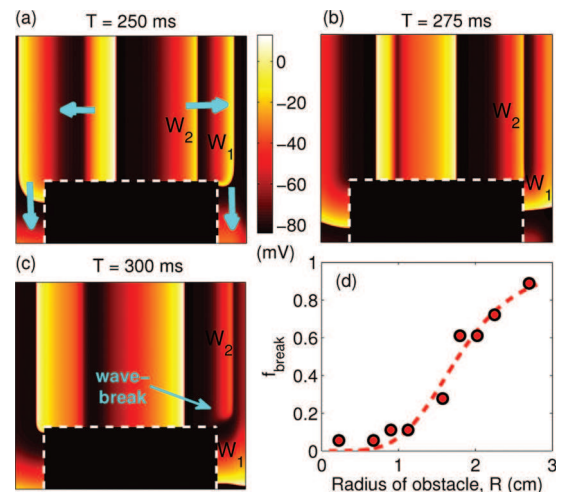


Fig. 6: (Color online) (a)–(c): pseudocolor plots of the transmembrane potential  $V$  for a cross-section of the system shown in fig. 2, along a plane parallel to the  $L_z$ -axis. The boundary of the obstacle (shaded) is marked by broken lines. The arrows in (a) indicate the direction of propagation for wavefronts. The wave  $W_1$  slows down at the boundary of the upper surface of the obstacle. As a result, the wave  $W_2$  closely following  $W_1$  encounters a region that has not fully recovered from its prior excitation by  $W_1$ , leading to (c) the detachment of  $W_2$  from the surface of the obstacle and formation of a singularity. (d) The fraction of initial conditions resulting in scroll wave breakup by  $T = 3$  s,  $f_{breakup}$ , shown as a function of the obstacle size. The fraction for each obstacle size is estimated by using 18 distinct initial scroll wave configurations generated from a three-dimensional planar wavefront and determining the number of cases where new filaments are subsequently formed at the obstacle boundary. The broken line is a sigmoid fit to the data.



increased curvature of the wave [42]. Thus, the wave  $W_2$  closely following  $W_1$  encounters an incompletely recovered region at the edge of the obstacle (fig. 6(b)). The resulting propagation block of  $W_2$  in the direction parallel to the  $L_z$ -axis (immediately adjacent to the obstacle boundary), dislodges the wave from the surface of the obstacle and generates a singularity at the point where the scroll wave breaks (fig. 6(c)). This phenomenon can be further enhanced by filament meandering that results in Doppler-effect-induced changes in the propagation speed of successive waves. As previously mentioned, larger obstacles result in sharper differences in the velocity (and curvature) of the front as it crosses the obstacle, which suggests an increased probability of wavebreak (measured as the fraction of different initial conditions that eventually lead to breakup) with increasing radius  $R$ . This is indeed observed in fig. 6(d) supporting the mechanism outlined above. Note that we have explicitly verified that this increased probability is a function of the increasing obstacle size (and not an artifact of a decreased gap between the obstacle and the system boundary) by making the obstacle bigger while keeping the ratio of its size to that of the system a constant.

**Discussion.** – The significance of the results reported here lies in the fact that almost all previously reported mechanisms by which scroll waves break up leading to spatiotemporal chaos necessarily involve the dynamics of the filament, *e.g.*, negative filament tension in low-excitability regime or filament twist instabilities in the presence of cardiac-fiber rotation [25]. By contrast, the novel transition route to chaos described in this paper is a result of changes in the wavefront velocity components at the edge of a pinning obstacle, far from the existing filament. While there exist a few other mechanisms which can lead to scroll waves breaking, *e.g.*, decreased cell coupling, these are not exclusively three-dimensional phenomena and are known to be involved in two-dimensional spiral wave breakup [25].

We stress that the mechanism described here has no two-dimensional analog. Wavebreaks created through interaction between high-frequency excitation fronts and an inexcitable obstacle, observed in two-dimensional media [7,43], are fundamentally different from the phenomenon described here, as the three-dimensional analog of the former situation would correspond to the obstacle interacting with scroll waves originating from a filament that is *far* from the obstacle (and not pinned by it). Note that, for the geometric setup discussed here, this is not the case. As the filament is attached to the obstacle, the two-dimensional situation corresponding to it will be a source of high-frequency waves contiguous with the obstacle. We have explicitly verified through simulations in two-dimensional media that rapid waves generated by either point or line electrode positioned next to the obstacle do not generate wavebreaks.

The role played by a three-dimensional obstacle in inducing the breakup of an otherwise stable rotating wave

is extremely pertinent for understanding the genesis of certain cardiac arrhythmias as an ageing heart gradually accumulates defects through increased instances of local tissue necrosis [44]. While obstacles in three-dimensional media that do not extend through the entire thickness of the system have been considered earlier, these studies focused on the depinning transition of scroll waves in the presence of drift-inducing parameter gradients [27,28]. In contrast, we show that such defects can give rise to complex dynamics including transition to chaos. The mechanism presented here also provides a qualitative dynamical framework for explaining recent observations in chemical systems of scroll waves wrapping around an inexcitable obstacle [45] and our prediction of obstacle-induced breakup of scroll waves can be directly tested in a similar experimental setup [45].

**Conclusion.** – In conclusion, we have shown that the presence of an inexcitable obstacle in three-dimensional excitable media can result in scroll wave breakup far from the filament through a novel physical mechanism. The helical winding of a wave around a pinning defect causes sudden changes in the velocity components of the wavefront as it crosses the boundary of the obstacle, with an associated increase in the curvature of the wave in the plane parallel to the axis of its rotation. The resulting enhanced interaction between successive waves at the bounding edge of the obstacle increases the probability of a wavefront detaching from the surface of the obstacle giving rise to new filaments. These wavebreaks can eventually lead to spatiotemporal chaos, manifested as fibrillation in the heart. Thus, our results may have consequences for understanding the critical role of defects (such as, inexcitable regions of necrotic tissue) embedded deep inside the bulk of cardiac muscle in the genesis of life-threatening arrhythmia.

\* \* \*

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