A striking shape was recently observed for the endoplasmic reticulum, a cellular organelle consisting of stacked sheets connected by helical ramps [Terasaki et al., Cell 154, 285 (2013)]. This shape is interesting both for its biological function, to synthesize proteins using an increased surface area for ribosome factories, and its geometric properties that may be insensitive to details of the microscopic interactions. In the present work, we find very similar shapes in our molecular dynamics simulations of the nuclear pasta phases of dense nuclear matter that are expected deep in the crust of neutron stars. There are dramatic differences between nuclear pasta and terrestrial cell biology. Nuclear pasta is 14 orders of magnitude denser than the aqueous environs of the cell nucleus and involves strong interactions between protons and neutrons, while cellular-scale biology is dominated by the entropy of water and complex assemblies of biomolecules. Nonetheless, the very similar geometry suggests both systems may have similar coarse-grained dynamics and that the shapes are indeed determined by geometrical considerations, independent of microscopic details. Many of our simulations self-assemble into flat sheets connected by helical ramps. These ramps may impact the thermal and electrical conductivities, viscosity, shear modulus, and breaking strain of neutron star crust. The interaction we use, with Coulomb frustration, may provide a simple model system that reproduces many biologically important shapes.

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systems. Our justification for also discussing nuclear pasta shapes with the help of Eq. (2) is determined only after the fact. This equation predicts spiral ramp shapes and their arrangements, very similar to what we find in our MD simulations; see below.

One relatively low-energy solution for Eq. (2) is lasagne with flat surfaces where \( C_1 = C_2 = 0 \). This gives \( H_0 = 0 \). Another solution involves spiral ramps with \( C_1 = -C_2 \); here the mean curvature is still zero, but the Gaussian curvature is negative so that \( H_0 < 0 \). Thus the Gaussian curvature term may stabilize spiral ramp configurations in both biological membranes, see below, and nuclear pasta. This term may also stabilize configurations that have additional holes such as the “nuclear waffle” shapes found in Ref. [15]. These shapes consist of flat sheets with a two-dimensional array of holes. Alternatively there may be torus or donut-shaped superheavy nuclei [16], where the donut shape both reduces the large Coulomb energy and is further stabilized by the Gaussian-curvature term.

In this paper we study the self-assembly of these spiral ramp configurations with molecular dynamics simulations of a simple (semi)classical model of nuclear matter. Our simulations are for nuclear pasta, but they may also have implications for phospholipid bilayer membranes.

Our MD formalism is the same as that used by Horowitz and co-workers in previous works [3,17–21] and is briefly reviewed here. It is very similar to a model used by others [22,23]. Our simulation volume is a cubic box with periodic boundary conditions which contains pointlike protons and neutrons with mass \( M \). The positions are uniformly randomly distributed in the simulation volume with a Boltzmann velocity distribution. Figure 1 shows the configuration of a 40,000 particle simulation at times from 40,000 to 2,000,000 fm/c. The proton density \( n_p \) is shown where the opacity of the color scale is 0 for \( n_p = 0.00 \) to 0.02 fm\(^{-3} \) and then increases linearly to 1 at \( n_p = 0.04 \) fm\(^{-3} \). A light cream color corresponds to high-density sheets, while lower-density surfaces are shown in brown. This system undergoes the following self-assembly steps: (1) The low-density system collapses locally to form higher-density filaments that meet in junctions; see Fig. 1(a). This includes the formation of a number of topological holes. (2) Next, the filaments start to grow to form curved sheets, Figs. 1(b) and 1(c). (3) These sheets then start to straighten out over longer length scales; Fig. 1(d). (4) Boundaries between “domains” of sheets with different orientation form four left-handed and four right-handed helical ramps; see Table I. The sheets straighten out over the full simulation volume; see Figs. 1(e) and 1(f), and the ramps move together to form the dipole pattern shown in Fig. 2(a). This pattern
has four left-handed ramps to the left and four right-handed ramps to the right. For this dipole pattern, the ramps are seen in Fig. 2(c) to make about a 45° angle with the flat sheets. We find this final configuration to be stable for times of at least 10 000 000 fm/c.

To study the dependence on boundary conditions, we perform simulations with different numbers of particles and correspondingly different sized simulation volumes; see Table I. The smallest simulation, with only 20 000 particles, forms uniform flat sheets without any spiral ramps (not shown). A 50 000 particle simulation forms four left-handed and four right-handed ramps as shown in Fig. 2(e). This is also a dipole pattern with the left-handed ramps to the left and the right-handed ramps to the right. As a result the ramps make a 45° angle with the sheets; see Fig. 2(f). Finally a 75 000 particle simulation forms four ramps in a quadrupole pattern where one left-handed and one right-handed ramp are to the left as shown in Fig. 2(h). For a quadrupole pattern the ramps are observed to make a 90° angle with the sheets; see Fig. 2(i) and Table I.

The arrangement of the helical ramps shown in Figs. 2(a), 2(e), and 2(h) agrees very well with theoretical predictions in Refs. [13,14] that are based on Eq. (2). Guven et al. argue that tension in the sheets leads to an effective long-range attraction between two ramps of opposite chirality that draws them together until a short-range repulsive bending force stabilizes the pair of ramps at a characteristic distance. Some features of our simulations that are in agreement with

Guven et al. are (1) we find an equal number of left-handed (L) and right-handed (R) ramps, (2) the ramps are all relatively close together with a similar characteristic spacing, and (3) ramps in a quadrupole pattern make a 90° angle with respect to the sheets, while ramps in a dipole pattern make an approximately 45° angle with the sheets. These common features suggest, after the fact, that Eq. (2) may also apply to our nuclear pasta model system.

Most of our simulations form flat sheets connected by helical ramps. However, we are able to obtain only flat sheets, without any ramps, if we add a small one-body potential to the system for early times that biases the formation of only flat sheets, or start a simulation in a smaller box at high densities where the system is nearly uniform and then very slowly expand the box during the simulation until the system reaches the same final density of $n = 0.05 \, \text{fm}^{-3}$.

We compare our results to biological observations. Reconstructing the three-dimensional (3D) geometry of ER sheets from two-dimensional serial sections reveals that the continuity of parallel sheets comes about through the helical winding of the “exposed” sheet edge through space, i.e., the Terasaki ramp; see Fig. 3. The core of the ramp (cytosolic side of the membrane) has a highly negative Gaussian curvature, but potentially small mean curvature, given the opposite signs of the two principal radii of curvature. No considerations seem to set a preferred handedness to the ramps, and the observations at hand, though statistically small, are consistent with right- and left-handed ramps in equal numbers throughout the organelle.
If the sheet edges are treated as effectively one-dimensional defects (thought to be stabilized by membrane proteins on the cytosolic side), then it is sufficient to treat the rest of the membrane by the Helfrich–Canham Hamiltonian. A class of solutions minimizing that functional are minimal surfaces, which have zero mean curvature and locally minimize area. One consequence of the analysis in Ref. [14] is that whereas a single Terasaki ramp has a logarithmically diverging energy, a left–right dipole pair has a finite energy, and a double pair of left–right–left–right ramps (a quadrupole) minimizes it further. The existence of ramp dipoles is natural in the biological context, though convincing evidence for tightly correlated left–right pairs, or for pairs of pairs, is currently lacking. As previously discussed, we find both left–right pairs and pairs of pairs in our MD simulations of nuclear pasta.

In conclusion, we have performed molecular dynamics simulations using a simple classical model of nuclear pasta. Many of our systems spontaneously self-assemble to form flat sheets connected by helical ramps. This geometry is very similar to that observed in the three-dimensional structure of the sheetlike endoplasmic reticulum. Seeing the same helical shapes in the extraordinarily different systems of nuclear pasta in neutron stars and in the membranes of eukaryotic cells strongly suggests that these shapes follow naturally from common geometric considerations and may be independent of details of the microscopic interactions.

The curvature energy could help stabilize these helical ramps, suggesting that they may be common in nuclear pasta. If that is true, electron scattering from the ramps could reduce the electrical and thermal conductivity of neutron-star crust. This may impact crust cooling [3] and possibly lead to the decay of magnetic fields [5]. Alternatively, the helical ramps that connect flat sheets may allow paired protons to percolate throughout the system and make it superconducting. In addition, the ramps may restrict how the sheets can move past each other. This could lead to complex viscoelastic behavior for nuclear pasta that could dampen $r$-mode oscillations in rapidly rotating neutron stars; see for example [25]. Furthermore, the helical ramps likely will increase the shear modulus of neutron-star crust and the frequencies of crust oscillation modes. These modes may have been observed as quasiperiodic oscillations during magnetar giant flares [26]. Finally, the ramps likely increase the breaking strain, or mechanical strength, of neutron-star crust. As a result the crust can support larger mountains that, on a rapidly rotating neutron star, efficiently radiate gravitational waves [27].

One can study soft condensed-matter analogs of nuclear pasta in the laboratory even if direct experiments on nuclear pasta are not feasible. This could provide unique insights. For example, it may be very difficult to predict the actual density of ramps in nuclear pasta using only first-principle simulations. Instead one can observe the actual density and pattern of Terasaki ramps in analog laboratory systems.

Our simple interaction has Coulomb frustration with short-ranged attraction and long-ranged repulsion. This seems to provide a simple model system that reproduces many biologically important shapes. One reason is the fluid nature of bilayer membranes: interactions between phospholipid molecules are determined to a large extent by the repulsive term.

Computational advances have made and will make very large-scale MD simulations for such systems “easy”, and these simulations will likely exhibit very rich varieties of shapes and phases. Uncovering similarities between disparate physical systems allows connections to be made at the deeper level of symmetry, excitations, and the geometry of topological defects.

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