Active Brownian particles can mimic the pattern of the substrate

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\textbf{ABSTRACT}
Active Brownian particles (ABPs) have been identified as a successful way of modeling the moving microorganism on the substrate. In recent studies, it is shown that such organisms can sense the characteristics of the substrate. Motivated by such work, we studied the dynamics and the steady state of ABP moving on a substrate with space-dependent activity. On the substrate, some regions are marked as high in activity, and other regions are such that particles behave as passive Brownian particles. The system is studied in two dimensions with step, sigmoid, Gaussian, and cone shape distribution of activity profile on the substrate. The whole interface of the activity profile is symmetrically divided into two regions. This led to the flow of particles from the active region to the passive region. The final steady state of particle density profile, polarization and flux very much follows the structure of the inhomogeneous activity, and the density in high activity region is lower, maximum at the interface and nearly constant with mean density in the passive region. Further, the steady state density profile for various shapes and designs on two-dimensional substrates is studied. Hence, the collection of ABPs on an inhomogeneous substrate can mimic the inhomogeneity of the substrate.

\textbf{Introduction}
Active systems\textsuperscript{1,2} have been a frontier area of research in the last two decades because of their unusual properties as compared to the systems in thermal equilibrium. The rapidly growing discipline of active matter\textsuperscript{3–9} seeks to understand and regulate the material characteristics of assemblages of interacting energy-consuming\textsuperscript{10} components on a microscopic level. Examples of motile active matter may be found everywhere in nature, from flocks of birds\textsuperscript{11} to family of fish\textsuperscript{12} to bacterium colonies like Escherichia coli.\textsuperscript{13} Many laboratory investigations of artificial active fluids of suspended lifeless microswimmers have been prompted by the abundance of natural occurrences observed. Simple colloidal particles driven by self-phoresis\textsuperscript{14–21} are frequently used in these “active-particle systems.”\textsuperscript{22} The individual constituents of these systems transduce their internal energy into motion, i.e., they exhibit self-propulsion characteristics, and therefore, they are also called self-propelled particles (SPPs). On the level of a single or a few active particles,\textsuperscript{16,23–28} several intriguing characteristics have been identified, opening up a wide range of possible applications. Microswimmers also have a diverse range of collective dynamics, ranging from mesoscopic turbulence\textsuperscript{29} to macroscopic motility-induced phase separation (MIPS).\textsuperscript{30–37} In addition to the extensive study of these systems in clean environments,\textsuperscript{38–45} recently people have started to look for their bulk properties in heterogeneous medium.\textsuperscript{46–54}

Inhomogeneity can exist at all scales of active matter. The active matter community has only lately concentrated its attention on a detailed examination of typical patterns in local density and polarization in the homogeneous conditions.\textsuperscript{55,56} In recent study,\textsuperscript{57,58} it is shown that the microswimmers can sense the geometry of the substrate and hence can be used as biosensor.

Also, the recent experiment\textsuperscript{59} and simulation\textsuperscript{60} consider the motion of the active Brownian particles (ABPs) moving on the top of a two-dimensional periodic surface. It is found that the ABPs experience competition between hindered and enhanced diffusion due to the pattern of the surface. In these studies, the inhomogeneity is introduced as different surface morphology. Here our aim is to examine whether the inhomogeneity in activity profile will affect the collective properties of ABPs. In this work, we focus on studying the behavior of collection of ABP’s moving on inhomogeneous substrate of various distributions of activity profile. We studied the various distributions using the coarse-grained as well as microscopic simulations of ABPs.\textsuperscript{2}

The response of real microswimmers to the local profile of activity can be experimentally designed by

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introducing different thermal gradient, light-induced activity profile, or field-induced.\textsuperscript{[61–66]} Also it can be naturally present in the systems where bacteria are moving in the background polymer network as discussed in a review work.\textsuperscript{[37]} The above works show the strong dependence of steady-state density of microswimmers in response to the activity profile. In addition to that, in our present work, we also show that the current and density of particles very much depend on the gradient of the activity profile.

In this study, we consider a collection of ABPs\textsuperscript{[34,40,67–69]} moving on a two-dimensional inhomogeneous substrate. The substrate is designed such that the particle experiences high activity in some regions and no or small activity at other places. We have considered varied distributions of activity for the substrate. They are of type; Step function, Sigmoid, Gaussian, Cone and random shape distributions. Our main result is that the particle density can mimic the underneath substrate structure.

The rest of the article is divided in the following manner. In the next section III, we discuss the model in detail and finally discuss the results in section IV. In section V we discuss the steady state density profile for various miscellaneous shapes.

Model

We consider a collection of ABPs moving on a two-dimensional inhomogeneous substrate. The substrate is designed such that there are regions where particle experiences high activity and regions where it behave as passive particle. Hence, particles move on a substrate with inhomogeneous activity profile. The dynamics of ABPs is given by the following update equations for the particles position on the two-dimensional substrate;

\begin{align}
\partial_t x &= v(x, y) \cos \theta + \sqrt{2D_x \xi_x} \\
\partial_t y &= v(x, y) \sin \theta + \sqrt{2D_y \xi_y} \\
\partial_t \theta &= \sqrt{2D_\theta \xi_\theta}
\end{align}

The first term on the right-hand side of Eqs. (1) and (2) incorporates the inhomogeneous activity with space dependence of self-propulsion speed $v(x, y)$. The $\xi_i$’s are due to the thermal noise (translational and rotational). The transitional and rotational diffusion coefficients $D_x$ and $D_\theta$, respectively, measure intensities of independent, unit variance, and Gaussian white noises $\xi_{x,y,\theta}(t)$.

In the following section, we utilize the framework of ref.\textsuperscript{[55]} to derive approximate differential equations for the density $\rho(r, t)$ and local polarisation $\mathbf{p}(r, t)$ at position $r$ and time $t$. The collection of ABPs governed by Eqs. (1)–(3) is called as microscopic (MIC) model. Later, we also write the coarse-grained coupled equations for local density $\rho(r, t)$ and polarisation $\mathbf{p}(r, t)$.

**Moment Equations**

The dynamic probability density function $f(r, \hat{n}, t)$ for finding the particle at time $t$ at position $r$ with the orientation $\hat{n} = (\cos \theta, \sin \theta)$, corresponding to the system of stochastic differential Eqs. (1)–(3), obeys the Fokker Planck equation.\textsuperscript{[69–71]}

\[
\frac{\partial f}{\partial t} = D V f + D_\theta \frac{\partial^2 f}{\partial \theta^2} - \nabla \cdot [\mathbf{f}(r) \hat{n}] \tag{4}
\]

where $\frac{\partial}{\partial \theta}$, $\nabla$, and $\frac{\partial^2}{\partial \theta^2}$ represents differential operators with respect to time $t$, space $r$, angle $\theta$, respectively. The exact moment expansion of $f$ in terms of $\hat{n}\textsuperscript{[70–72]}$ truncated after the second term leads

\[
f(r, \hat{n}, t) = \frac{1}{2\pi} [V(r, t) + 2\mathbf{p}(r, t) \cdot \hat{n}] \tag{5}
\]

where

\[
\rho(r, t) = \int d\hat{n} f(r, \hat{n}, t), \tag{6}
\]

\[
\mathbf{p}(r, t) = \int d\hat{n} \hat{n} f(r, \hat{n}, t) \tag{7}
\]

denote density and polarization, respectively. Multiplying Eq. (4) by 1 or $\hat{n}$, integrating over orientational degrees of freedom, and using the definitions 6 and 7, we obtain the moment equation.\textsuperscript{[71,73]}

\[
\partial_t \rho(r, t) = -\nabla \cdot \mathbf{J}(r, t), \tag{8}
\]

\[
\partial_t \mathbf{p}(r, t) = -D_\theta \mathbf{p}(r, t) - \nabla \cdot \mathbf{M}(r, t) \tag{9}
\]

Here, we introduced the (orientation averaged) flux\textsuperscript{[74]}

\[
\mathbf{J}(r, t) = -D \nabla \rho(r, t) + \nabla (r) \mathbf{p}(r, t) \tag{10}
\]

and the matrix flux

\[
\mathbf{M}(r, t) = -D \nabla \mathbf{p}(r, t) + \frac{\mathbf{r}}{2} \rho(r, t) \mathbf{I} \tag{11}
\]

with the unit matrix $\mathbf{I}$. The set of equations given by Eqs. (8)–(11) is named as coarse-grained (CG) model.

**Numerical Details** : We have performed numerical integration of CG model using Euler’s numerical integration method to solve Eqs. (8)–(11). We randomly initialized density $\rho$ and polarization $\mathbf{p}$ and calculated the
orientation averaged flux $J$ as given in Eq. (10) and matrix flux $M$ as given in Eq. (11). Then, the density $\rho$ is updated by inserting $J$ into Eq. (8) and similarly the polarization $p$ is updated by inserting $M$ into Eq. (9). We define the smallest length scale as $l = \frac{\rho_0}{\tau}$ and time scale $\tau = D_{r,1}^{-1}$.

All the lengths and times are measured in multiple of them. The step size we considered are $dx = dy = 1.0l$ and $dt = 0.01\tau$. All the results are also checked for smaller step size $dx = dy = 0.5$, and we found the same results. Hence, there is no ambiguity with respect to step size of integration and discontinuity of the inhomogeneous profile. We started with mean value of density $\rho_0 = 0.5$, and it remains constant throughout the simulation. The system is studied in two dimensions. We first give the details of parameter for CG model. We considered the length of the system $L = 512l$. The total simulation time is $2 \times 10^5\tau$. The periodic boundary conditions (PBC) are used in both directions. The inhomogeneous activity on the substrate is introduced through following four symmetric shapes of activity on the substrate with the maximum intensity, $v_o$ of the distribution:

(i) **Step Function Shape**: We first introduced the step function distribution of activity on the substrate such that

$$
\nu(x, y) = \begin{cases} 
    v_o & \sqrt{(x - \mu)^2 + (y - \mu)^2} \leq r_o \\
    0 & \sqrt{(x - \mu)^2 + (y - \mu)^2} > r_o 
\end{cases}
$$

(ii) **Sigmoid Shape**: The two-dimensional sigmoid function is defined as follows:

$$
\nu(x, y) = v_o \times \frac{1}{1 + e^{-k \sqrt{(x - \mu)^2 + (y - \mu)^2}}}
$$

where $\mu$ is the center parameter and $k$ is the steepness parameter that controls the shape of the sigmoid function. We fix $k = 50$ throughout the simulation. This is same as the step distribution. The only difference is, rapid, continuous fall in activity at the boundary.

(iii) **Gaussian Shape**: Gaussian distribution with parameters $\mu, \sigma, v_0$. \cite{75}

$$
\nu(x, y) = v_o \times \frac{1}{2\pi\sigma^2} \exp\left(-\frac{1}{2} \left[\frac{(x - \mu)^2}{\sigma^2} + \frac{(y - \mu)^2}{\sigma^2}\right]\right)
$$

$\mu$ is the center of the system. $\sigma = \frac{1}{4} L$ represents variance in both directions. $x$ and $y$ in Eq. (14), represent $x$ and $y$ coordinates in the system.

(iv) **Cone Shape**: We introduce the cone shape distribution of activity on the substrate such that

$$
\nu(x, y) = v_o \times (1 - \sqrt{(x - \mu)^2 + (y - \mu)^2})
$$

where $\mu = L/2$ is at the center of the box. In Eq. (15), the activity falls linearly away from the center of the substrate and finally becomes zero.

Furthermore, we also perform microscopic simulation of Eqs. (1)–(3) for the step and Gaussian profile of activity on a two-dimensional substrate of size $L = 128l$ with the number of ABPs $N = 8692$ and their radii $R = 0.6l$. The dynamics of the ABPs are governed by a discrete time step, $dt$, set to $0.01\tau$ units. At each time step, the particles undergo self-propulsion with a speed denoted by $v_o$. The total simulation time set to $5 \times 10^4\tau$ units. The repulsive force acting between two particles is modeled using a soft-core spring potential

$$
F_{rep}(r_{ij}) = -K \cdot (2R - r_{ij}) \cdot \hat{r}_{ij}
$$

where $r_{ij}$ is the distance between particles $i$ and $j$, $K$ is a positive constant that determines the strength of the repulsive force and it is taken as unit in the simulation, and $\hat{r}_{ij}$ is the vector pointing from particle $i$ to $j$. The force is zero when the distance between particles exceed the sum of their radii, and it increases as particles get closer. The last term in Eqs. (1) and (2) is the translational noise, which is present due to thermal fluctuations. The angular noise in Eq. (3) affects the rotational diffusion of particles and is responsible for the random changes in their orientations. The strengths of translations and rotational diffusion constants are fixed to 1.0 for both.

The system is studied for $v_o = 1.0$ in both CG-grained and MIC simulations and the rest of other parameters are given in each activity profiles. The dimensionless maximum *Peclet number* $\text{Pe} = \frac{l}{\lambda} = 1.33$.

**Results**

In this section, we discuss our results in detail. We divide our study in two parts. In the first part, we show the results of four different shapes of activity profile given in previous section using the CG simulations of Eq. (8)–(11). We also discuss the time evolution of system toward the steady state for one shape of activity profile, i.e., Gaussian shape function. In the second part, we show the time evolution of the system studied using the MIC model introduced in Eq. (1)–(3).
**Coarse-Grained Model (CG)**

We analyze the density $\rho$, polarization $\mathbf{p}$, and flux $\mathbf{J}$ (as given in Eq. (8)–(10), respectively) of the particles observed for various shapes of speed distribution (activity profile) including step, sigmoid, Gaussian, and cone shape in Fig. 1.

For the time at $t = 200000$ and for system size $L = 512$, we find that the density is least in the highly active region and reaches its maximum at the interface between the high and low active regions. We can see in Fig. 1 that the distribution of density depends on the local gradient of activity profile. Since the shape of step distribution of speed has very high gradient at the interface of active and passive region but zero gradient in the rest of the area, we find that there is a sharp change from low density inside the active region to high density at the interface. When we introduce other activity profiles in the model, we observe that there is a region of intermediate density between high and low density. This intermediate density is equal to the average density taken in the system. As we go from sharp to gradual (smooth) decay of gradient of activity profiles such as sigmoid to Gaussian and finally to cone shape, the size of the intermediate region with high density is increasing. The differences in the density profiles for different shapes highlight the influence of the activity profile on the system's behavior. Three-dimensional representation of activity profile and corresponding density distribution are shown in Fig. 2. We observe depletion of the particle density from the active region and the area

![Figure 1](image)

**Figure 1.** The figure shows the activity profiles in the first row for different shapes of distributions of activity of ABPs. Each subplot in the columns represents a different shape of distribution: step function shape, sigmoid function shape, Gaussian function shape, and cone shape from left to right, respectively. The activity profiles are represented by color intensity with warmer colors indicating higher activity levels and cooler colors indicating lower activity levels. In the second, third, and fourth rows, the density $\rho(r, t)$, polarization $\mathbf{p}(r, t)$, and flux/current $\mathbf{J}(r, t)$ of the ABPs are displayed from top to bottom, respectively. The color intensity in the second row represents the density levels, with red indicating higher densities and blue indicating lower densities. In the third and fourth rows, the color intensity represents the magnitude of polarization and flux, with warmer colors indicating higher magnitudes and cooler colors indicating lower magnitudes. The stream of arrows in the third and fourth columns illustrate the direction of polarization and flux, respectively. The rest of the system parameters are given in the main text.
of the depleted region is approximately equal to the area of region where velocity is non-zero.

The corresponding polarization $\mathbf{p}$ in Eq. (9) and current/flux $\mathbf{J}$ in Eq. (10) in the steady state is shown in the third and fourth row in Fig. 1, indicating the magnitude and direction represented by color map and stream of arrows, respectively. These two observables $\mathbf{p}$ and $\mathbf{J}$ are essential in understanding the overall dynamics in the system and how particles move and interact within the active region. The polarization is symmetric and points away from the centre of the substrate. Magnitude of polarization is maximum at the interface, but the maximum value decreases for smooth activity profiles as shown in Fig. 1 (Polarisation).

The current $\mathbf{J}$ is plotted in Fig. 1 (Current). We observe particles flow from high density (maximum current) region at interface to the low density regions both inward (high activity region) and outward (low activity region), but due to high activity, they leave the active region in opposite directions. The value of maximum current at the interface decreases for smooth activity profiles as represented by color bars. The presence of angular dependence of current is solely due to the PBC in the system.

We show time evolution of density, polarization, and current for Gaussian shape of activity profile in Fig. 3. We plot the color snapshots of particle density at different time steps from left to right $t_1 = 1$, $t_2 = 1000$, $t_3 = 40000$, and $t_4 = 200000$. Density pattern evolves with time, and we observed the depletion of particle density inside the active region. In the middle, i.e., the area where the activity of the particles is maximum, we observe the lowest density of the particles, and going from center to the boundary of the active and passive regions, we observe the density of the particles gradually increase. At the initial times, we observe the depletion of the particles getting bigger, but the depletion reaches a saturation state with time.

In the second row of Fig. 3, we observe the polarization snapshots of $\mathbf{p}$ with its magnitude represented by color map and direction with stream arrows. We observe that, at early times, the particles are at random motion and orientation. Along with the time, we observe the polarization of particles increases in the active region. Except at the center of the system, we observe lower polarization. At later time, there is not much change in the profile with time. At early stages, there is no ordering of the polarization, i.e., random direction of the polarization. With time we observe the formation of high polarization regions near the interface inside the high activity region. At the center of the box, where the activity is the highest, we observe low polarization.

From the current plot in the third row of Fig. 3, we can see the current snapshots in the model. The color map represents the magnitude of the current and direction shown by stream arrows. In this model, at early times, we observe that the particles are at random motion and orientation. With time, we see high current in the active region. At later times, as the system evolves, i.e., we don’t observe major change in the density, polarization, and current profiles with time.
**Microscopic (MIC) Model**

Now, we discuss the results of microscopic model (MIC) introduced by Eqs. (1)–(3). We focus on the time evolution of local density of particles $\rho(r, t)$, where $\rho(r, t)$ is obtained by counting number of particles in unit square box, such that the whole system is divided in $L^2$ boxes of unit size. Here, we only focus on the density profile of particles in the system for two activity profiles: (i) step function and (ii) Gaussian. Figure 4 shows the time evolution of local density at times $t_1 = 15000$, $t_2 = 30000$, $t_3 = 40000$, and $t_4 = 50000$. The system is started with random position and orientation of particles in whole substrate. With time density, $\rho(r, t)$ evolves such that inside the activity region less number of particles hence the lower density and outside or in the passive region almost mean density. At the interface, we observe highest density of particles. The color bar in Fig. 4 shows the magnitude of local density, and note that at the interface region, density is high. For step distribution, the width of the high density interface is much sharper than that of the Gaussian case as shown in Fig. 4.

Figure 3. Time evolution snapshots of the model with Gaussian shape distribution of speed at time steps $t_1 = 1$, $t_2 = 1000$, $t_3 = 40000$, and $t_4 = 200000$ are shown from left to right. Density, polarisation, and flux are shown in the first, second, and third rows of the figure, respectively at the given times. The color bars represent the value of the density, polarisation, and flux of the particles from low at bottom to high at the top. The stream of arrows represents the direction of polarisation and flux in the model.

Figure 4. The figure illustrates the time-evolution of particle densities on substrates for the microscopic model (MIC) for two different types of activity profiles, i.e., step and Gaussian shape, represented in the top and bottom rows, respectively. Each column corresponds to a specific time point ($t_1 = 15000$, $t_2 = 30000$, $t_3 = 40000$, and $t_4 = 50000$). The particle density is visualized using color maps, with colors ranging from red to blue, indicating low to high density, respectively.
We demonstrate the remarkable capability of the microscopic (MIC) model in capturing essential features of the system’s behavior when compared to the coarse-grained (CG) model. In Fig. 5, we present radial density profiles as a function of radial distance from the center, with a specific focus on the activity profile of the step function. The radial density profile \( \rho(r) \) is calculated by averaging local density over all directions. The main plot illustrates the behavior of the density profile in the CG model, with a system size of \( L = 512l \) and its center located at coordinates \((256, 256)\). In this configuration, the interface of the activity profile is positioned at a radius \( r = 32 \). Furthermore, the inset plot in Fig. 5 highlights the corresponding density profile in the MIC model, configured with a system size of \( L = 128l \), and a center at coordinates \((64l, 64l)\). In this scenario, the interface of the activity profile also lies at radius \( r = 32 \). This representation reveals the striking similarity in the radial variation of density between the CG and MIC models, particularly with respect to the step function activity profile. We observe for both cases that density profile shows a jump at interface and gradually decreases to global mean density of the system. For MIC model, packing fraction is 0.6, and for CG model, mean density is 0.5.

**Miscellaneous Shapes**

In the previous two cases, we have learnt that the particles deplete from the active region. The particles density can mimic the distributions underneath them. We ask the question of whether the above mechanism be recreated for some miscellaneous shapes without any symmetry. This is the motivation to consider miscellaneous shapes. The aim is to check whether the particles follow the pattern of the substrate as we had observed with various activity profiles such as step, sigmoid, Gaussian, and cone-shaped distribution. All the results of miscellaneous shapes are performed with step size \( dx = dy = 1.0 \), since we have checked the results for \( dx = dy = 0.5 \) for step profile, we believe that results of miscellaneous shapes will also remain unchanged for small step size.

The various other distributions we looked are:

1. English Alphabets
2. Hindi Alphabets
3. Telugu Alphabets
4. Flower Shape

In Fig. 6, we observe four different shaped potentials. We actually had considered various other type potentials in these categories. In English Alphabets, we have considered Alphabets E, (A, M, J, P (data not shown)) Fig. 6(a). In Hindi Alphabets, we have considered Alphabets VA, (PA, NA (data not shown) Fig. 6(b). In Telugu Alphabets, we have considered LA Fig. 6(c) and flower shape Fig. 6(d). In these figures, the yellow color part is the active region and purple color part is the passive region. In the following section, we are attaching the steady state snapshots at time \( t = 100000 \) of particles’ density distribution for different distributions.

We find that the steady state snapshots of particle density Fig. 7 looks very much similar to the original velocity distribution we started with. Hence, we say that the collection of ABPs can mimic the substrate information.

**Figure 5.** Radial density as a function of distance from the center for the activity profile of step function, illustrating the behaviour of density profile in CG model (main plot) and the MIC model (inset plot).
Discussion

In this work, we studied the collection of ABPs using coarse-grained and microscopic simulation on a two-dimensional inhomogeneous substrate. The inhomogeneity is introduced as different pattern of activity particle experiences on the substrate. We looked for different activity profiles: (i) Step function; (ii) Sigmoid; (iii) Gaussian; and (iv) cone, and finally we also studied the system with various asymmetric profiles: we studied the system with shapes of different alphabets. We observed the patterns of local density, polarization, and current along with the activity profile. We find that for all four distributions, the whole interface is symmetrically divided

Figure 6. This figure shows the various distributions we have considered: (a) E-shaped potential, (b) VA-shaped potential, (c) LA-shaped potential, and (d) flower-shaped potential.

Figure 7. Steady state snapshot of the particles density distribution for different potentials. (a) English Alphabet ‘E’. (b) English Alphabet ‘T’. (c) English Alphabet ‘U’. (d) English Alphabet ‘J’. (e) Telugu Alphabet77 ‘la’. (f) random shape ‘flower’. (g) Hindi Alphabet ‘pa’. (h) Hindi Alphabet ‘na’. (i) Hindi Alphabet ‘va.’ The red region represents low density and blue region represents high density of particles. All the snapshots are taken at an activity of 2.0 and at time \( t = 50000 \). The box size is 128 \times 128.
into four different quadrants. Steady state is defined by such pattern of current. The conclusion is same for all four shapes. Interestingly, density distributions are the mirror image of the activity profile. Starting from homogeneous density, in the steady state density achieves the lowest value in the high active region and then follows the pattern of the activity with sign reversed. We also performed the microscopic study and found that steady state density profile matches from the same as obtained by coarse-grained model. To check the same, we replicate many miscellaneous shapes of activity for different alphabets of English, Hindi, and Telugu. We find that for all the cases in the steady state, density follows the pattern of the activity.

Hence, our results show the response of ABPs on the substrate with inhomogeneous activity. Our results can be checked by the similar experiments as suggested in a recent study.\cite{78} The results can be used to detect the pattern of the substrate as well as have applications in printing using biological species or synthetic active particles.

**Author Contributions**

The problem was designed by S.M. and numerically investigated by P.K.M. and A.K. All authors analyzed and interpreted the results. The manuscript was prepared by contribution of each author. All the authors approved the final version of the manuscript.

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