Supplementary Materials for

**Boundary lubrication of heterogeneous surfaces and the onset of cavitation in frictional contacts**

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Other Supplementary Material for this manuscript includes the following:
(available at advances.sciencemag.org/cgi/content/full/2/3/e1501585/DC1)

- Movie S1 (.avi format). Formation of a cavitation bubble under shearing.
Discussion S1. Analytical solution of the Reynolds equation with slip and cavitated zone

The dimensional Reynolds equation with slip on the lower surface is:

$$\frac{\partial}{\partial x} \left( \frac{h^3}{12\eta} \left( \frac{h+4b}{h+b} \right) \frac{\partial P}{\partial x} + \frac{u_2 h}{2} \left( \frac{h}{h+b} \right) \right) = 0 \quad (1)$$

Here, $P$ is the pressure, $h$ the film thickness, $b$ the slip length, $u_2$ the imposed velocity of the upper surface, and $\eta$ the fluid viscosity. Integrating once along the shearing ($x$-) direction gives:

$$\frac{\partial P}{\partial x} = \frac{6\eta u_2}{h^2} \left[ \frac{C(h+b)-h}{h+4b} \right] \quad (2)$$

with $C$ an integration constant. The system, of overall length $L$, can be divided into three domains: a sticking region of length $\lambda_1$ where $P > 0$, a slipping region of length $\lambda_2$ where $P > 0$, and in-between a cavitated domain of length $\lambda_{cav}$ where $P \leq 0$ (see Fig. 4). Periodic boundary conditions $P(x = 0) = P(x = L)$ can be written as:

$$\int_0^L \frac{\partial P}{\partial x} dx = \int_{\lambda_1} \frac{\partial P}{\partial x} \, dx + \int_{\lambda_{cav}} \frac{\partial P}{\partial x} \, dx + \int_{\lambda_2} \frac{\partial P}{\partial x} \, dx = 0 \quad (3)$$

The second term vanishes since the pressures at the beginning and end of the cavitated zone are both zero. Note that this also applies if no cavitation occurs, the system length is simply $L = \lambda_1 + \lambda_2$ and the pressure must equal at the boundary from $\lambda_1$ to $\lambda_2$. The integration constant $C$ can be then obtained by considering $b = 0$ on the sticking domain $\lambda_1$, and a constant slip length of value $b = b_s$ on the slipping domain $\lambda_2$:

$$C = \frac{\int_{\lambda_1} dx + \frac{h}{h+4b_s} \int_{\lambda_2} dx}{\int_{\lambda_1} dx + \frac{h}{h+4b_s} \int_{\lambda_2} dx} = \frac{\lambda_1(h+b_s)+\lambda_2}{\lambda_1 h+4b_s + \lambda_2 h+4b_s} \quad (4)$$

Replacing $C$ into the integrated Reynolds equation gives the pressure gradient along the shearing direction in the sticking and slipping domains:

$$\frac{\partial P}{\partial x} = \begin{cases} \frac{-6\eta u_2}{h^2} \left[ \frac{b_2\lambda_2}{\lambda_1 h+4b_s + \lambda_2 h+4b_s} \right] & \text{(sticking domain)} \\ \frac{6\eta u_2}{h^2} \left[ \frac{b_1\lambda_1}{\lambda_1 h+4b_s + \lambda_2 h+4b_s} \right] & \text{(slipping domain)} \end{cases} \quad (5)$$
In presence of domains of equal length $\lambda$, one obtains:

$$\frac{\partial p}{\partial x} = \pm \frac{6\eta u}{\hbar^2} \left[ \frac{h}{2h + 5b_s} \right]$$

(6)

**Discussion S2. Pressure excursion for random alternations of slip**

In presence of a random sequence of slip/no-slip, across which the pressure jumps by a discrete value $\delta P$, the value of the pressure constitutes a simple random walk along the channel $x$. At a step $N$ its excursion is distributed according to a binomial distribution, which approaches a Gaussian of width $\delta P\sqrt{N}$ in the limit of large $N$. In our case, $N = L/\lambda$ is the total number of patches.

Since the Molecular Dynamics and continuum calculations are periodic, we need to enforce periodic boundary conditions on the random walk. The resulting process is the Brownian bridge which ensures that the walker returns to its origin after $N$ steps. Given two normalized positions $s = x/L$ and $t = y/L$ along the channel length, the Brownian bridge has the covariance [34]

$$\text{cov}(X_t, X_s) = \langle X_t X_s \rangle = \min(s, t) - st$$

(1)

between the random variables $X_s = P_s/\delta P$ and $X_t = P_t/\delta P$ representing the normalized pressures at $s$ and $t$, respectively. The variance $\text{var}(X_t) = \text{cov}(X_t, X_t)$ is zero at $t = 0$ (beginning of channel) and $t = 1$ (end of channel) because the value of the random process is fixed to constant zero at these points, i.e. $X_0 = 0$ and $X_1 = 0$.

In our case, since the average pressure on the channel is constant, we need to fix the average value $\bar{X}$ of the Brownian bridge rather than requiring $X_0 = 0$ and $X_1 = 0$. The mean value of the bridge

$$\bar{X} = \int dt \, X_t$$

(2)

has expectation value of $\langle \bar{X} \rangle = 0$ and variance

$$\text{var}(\bar{X}) = \langle \bar{X}^2 \rangle = \int_0^1 dt \int_0^1 ds \, \text{cov}(X_t, X_s) = \frac{1}{12}$$

(3)

We note that fixing the mean value of this random process makes it translationally invariant, i.e. we can no longer make out the two endpoints at 0 and 1. This implies that the pressure at each channel position fluctuates with standard deviation $\delta P\sqrt{N/12}$ from realization to realization. This is the origin of the factor $\sqrt{N/12}$ found in the main text.
Figure S1. Pressure excursion for two-dimensional slip patterns

Numerical solution of the Reynolds equation for two-dimensional slip patterns. The figure shows the slip length distribution in the simulation domain (left column), the dimensionless pressure in the simulation domain (middle column) and the pressure along the center line y=0 (right column) for several two-dimensional slip patterns. a) Square patches with 25\% coverage of the area; b) Circular
patches with 20% coverage; c) Checkerboard pattern with 50% coverage; d) Hexagonal pattern with 23% coverage.

**Movie S1. Formation of a cavitation bubble under shearing**

System parameters are $u_2 = 10 \text{ m/s}$, $h = 5.5 \text{ nm}$, $L = 143.9 \text{ nm}$, and $P_{\text{ext}} = 1\text{ MPa}$. At this pressure the fluid (n-decane) has viscosity $\eta = 0.30 \text{ mPas}$.