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Elastohydrodynamics of Roll-to-Plate Nanoimprinting on Non-Flat Substrates

October 25, 2023

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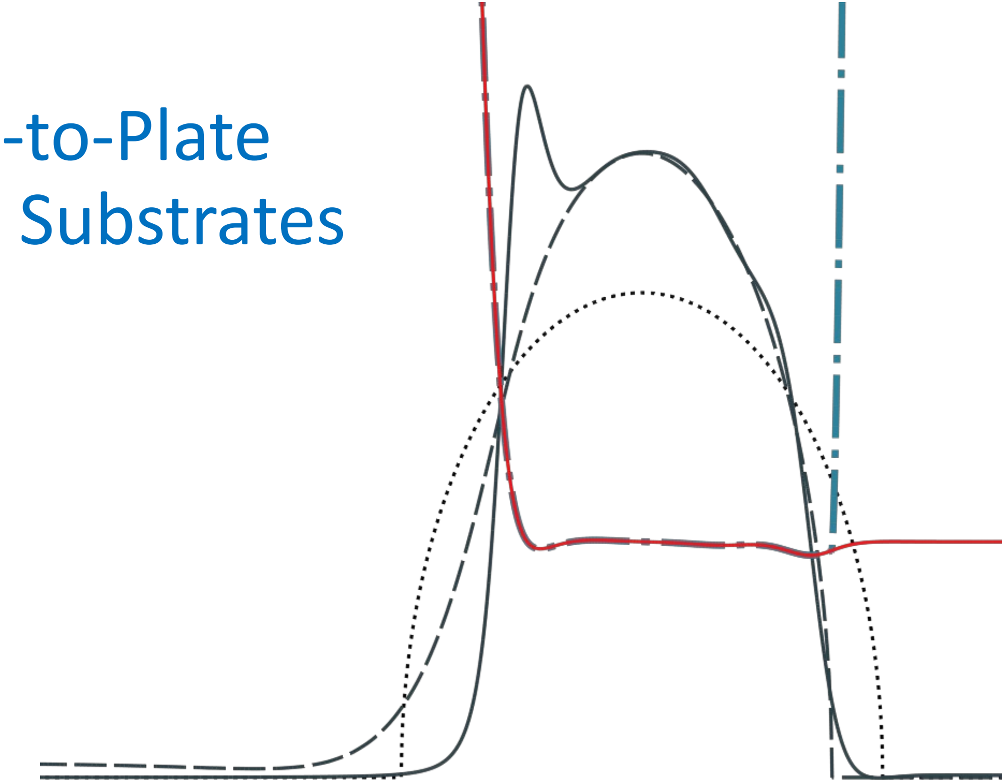
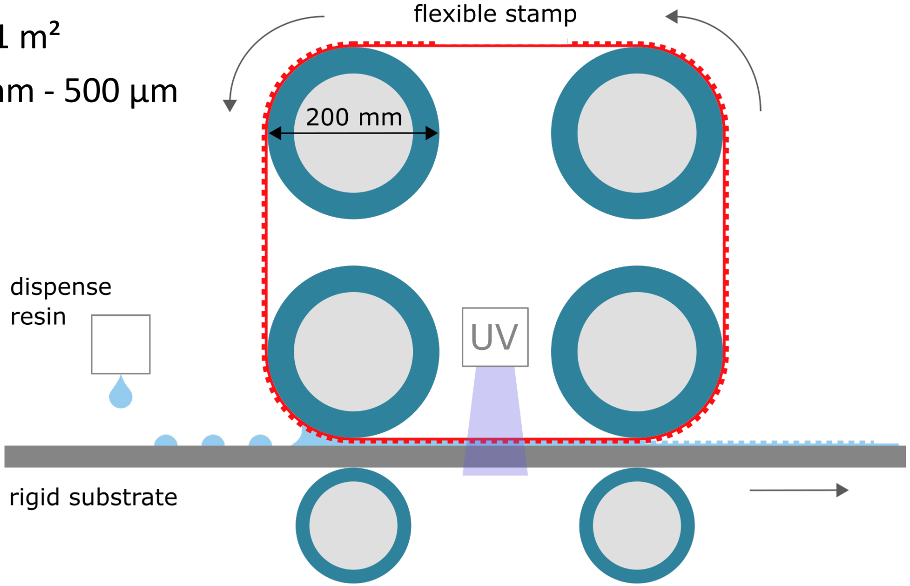
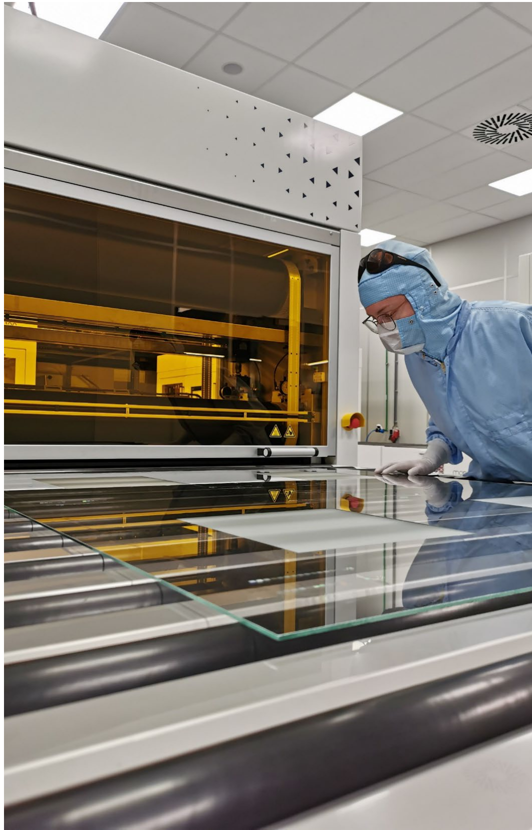


Introduction | roll-to-plate imprinting

- **Technology** – large-area roll-to-plate micro- and nanoimprinting
  - Large-area: >1 m²
  - Textures: 50 nm - 500 µm

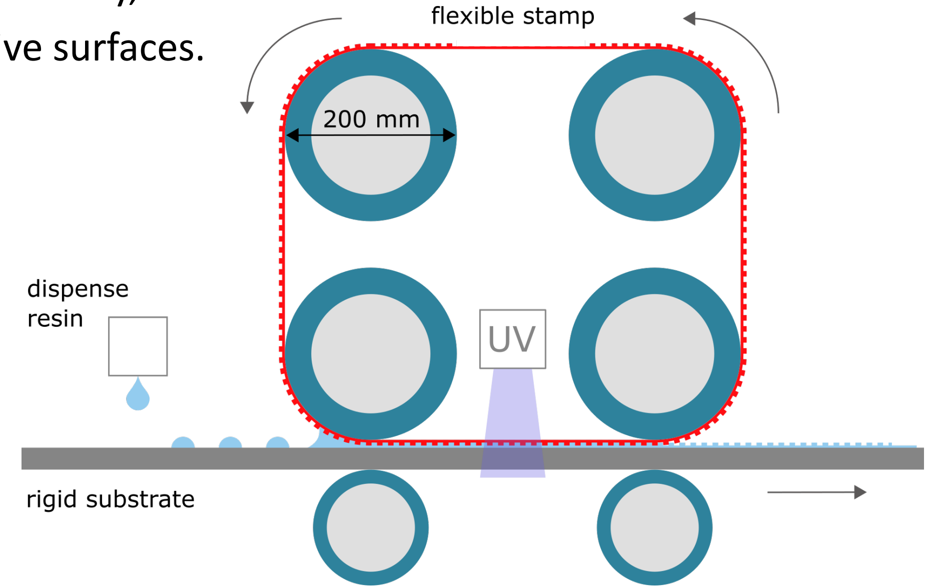




“Morphotonics Nanoimprint Technologies,” Morphotonics. https://www.morphotonics.com (accessed Dec. 13, 2022).

Introduction | roll-to-plate imprinting

- Various applications[1], such as:
  - Augmented reality,
  - Antireflective surfaces.



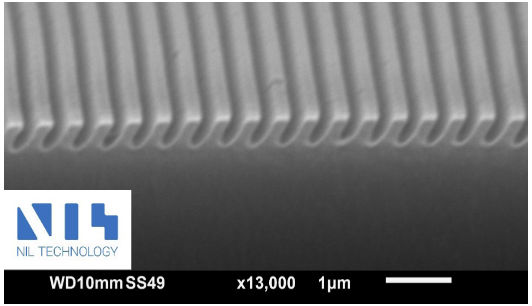
flexible stamp

200 mm

dispense resin

UV

rigid substrate



reflection

no reflection

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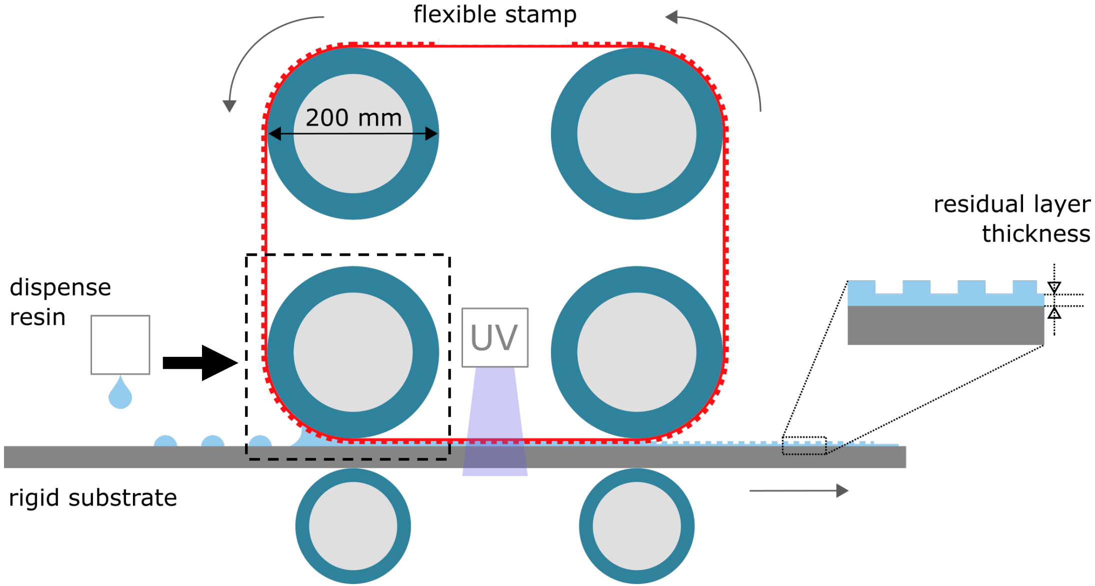
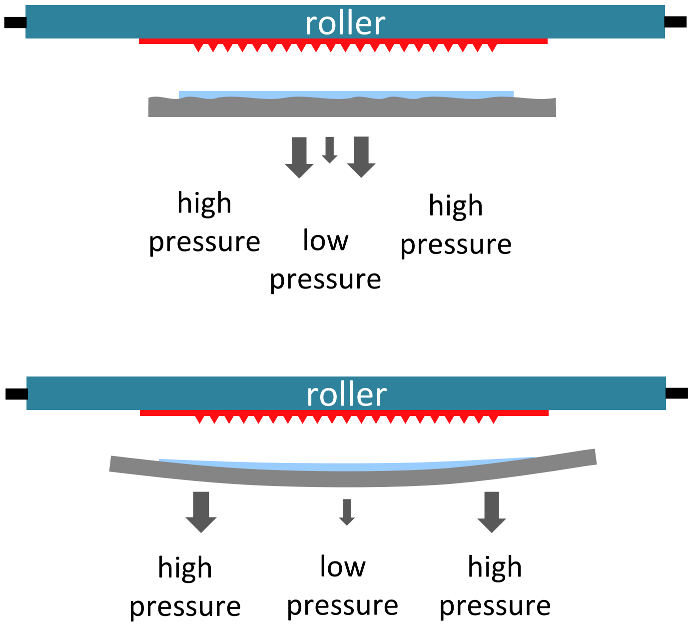
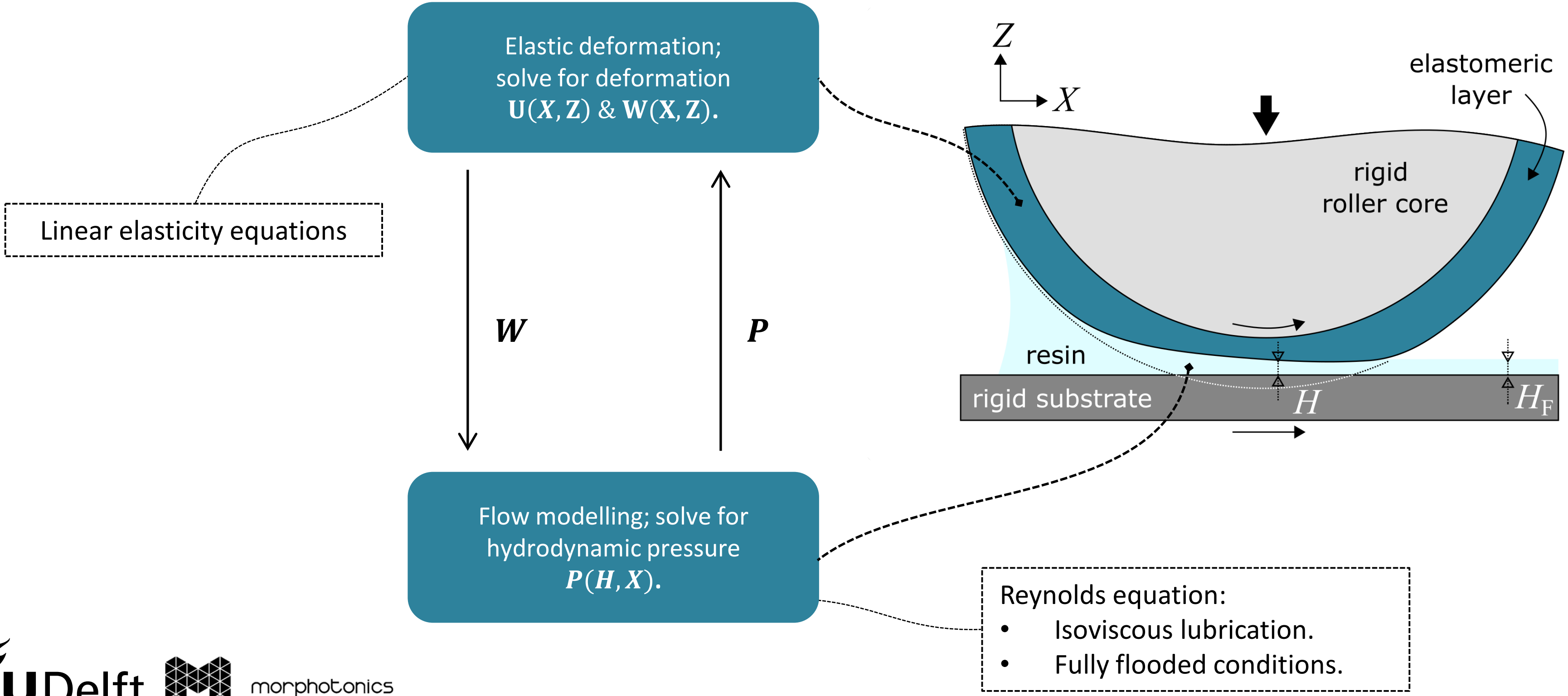
[1] H. Lan, "Large-Area Nanoimprint Lithography and Applications," in Micro/Nanolithography - A Heuristic Aspect on the Enduring Technology, London: IntechOpen, 2018. [Online]. Available: https://doi.org/10.5772/intechopen.72860

Introduction | roll-to-plate imprinting





Model | elastohydrodynamic lubrication (EHL)



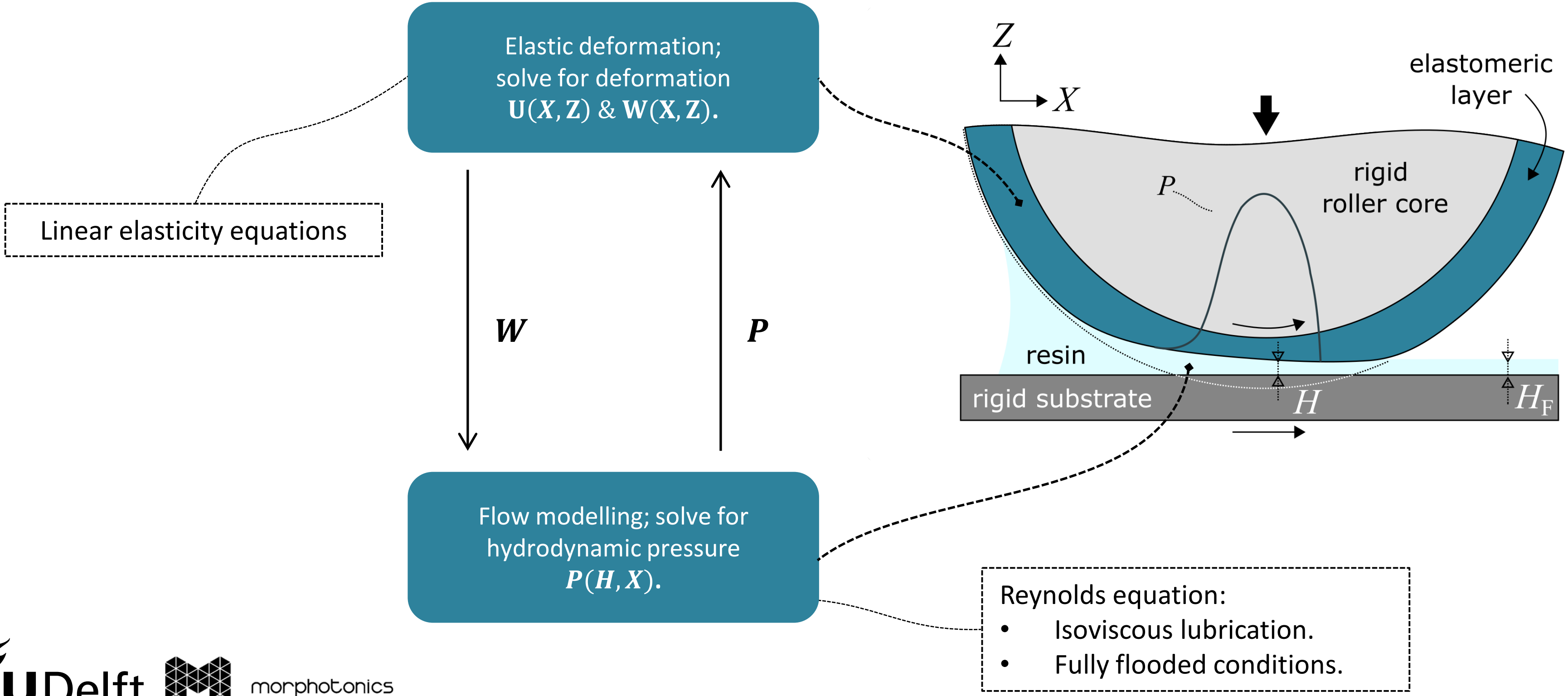
Elastic deformation; solve for deformation $\mathbf{U}(\boldsymbol{X},\mathbf{Z})$ & $\mathbf{W}(\mathbf{X},\mathbf{Z})$.

Linear elasticity equations

Flow modelling; solve for hydrodynamic pressure $\boldsymbol{P}(\boldsymbol{H},\boldsymbol{X})$.

Reynolds equation:
- Isoviscous lubrication.
- Fully flooded conditions.

Model | elastohydrodynamic lubrication (EHL)



Elastic deformation; solve for deformation $\mathbf{U}(\boldsymbol{X},\mathbf{Z})$ & $\mathbf{W}(\mathbf{X},\mathbf{Z})$.

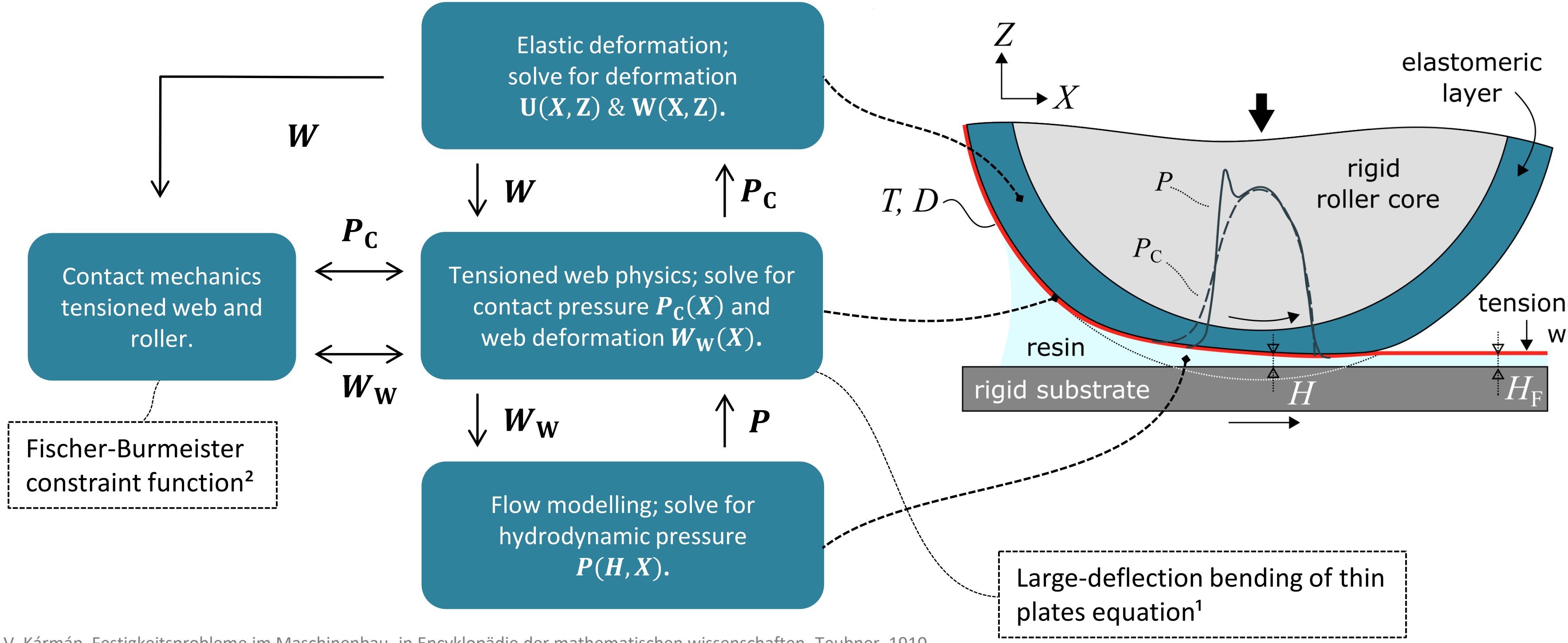
Linear elasticity equations

Flow modelling; solve for hydrodynamic pressure $\boldsymbol{P}(\boldsymbol{H},\boldsymbol{X})$.

Reynolds equation:

- Isoviscous lubrication.
- Fully flooded conditions.

Model | elastohydrodynamic lubrication (EHL) – extension



Elastic deformation; solve for deformation $\mathbf{U}(\boldsymbol{X},\mathbf{Z})$ & $\mathbf{W}(\mathbf{X},\mathbf{Z})$.

Tensioned web physics; solve for contact pressure $\boldsymbol{P}_{\mathbf{C}}(\boldsymbol{X})$ and web deformation $\boldsymbol{W}_{\mathbf{W}}(\boldsymbol{X})$.

Flow modelling; solve for hydrodynamic pressure $\boldsymbol{P}(\boldsymbol{H},\boldsymbol{X})$.

Contact mechanics tensioned web and roller.

Fischer-Burmeister constraint function[2]

Large-deflection bending of thin plates equation[1]

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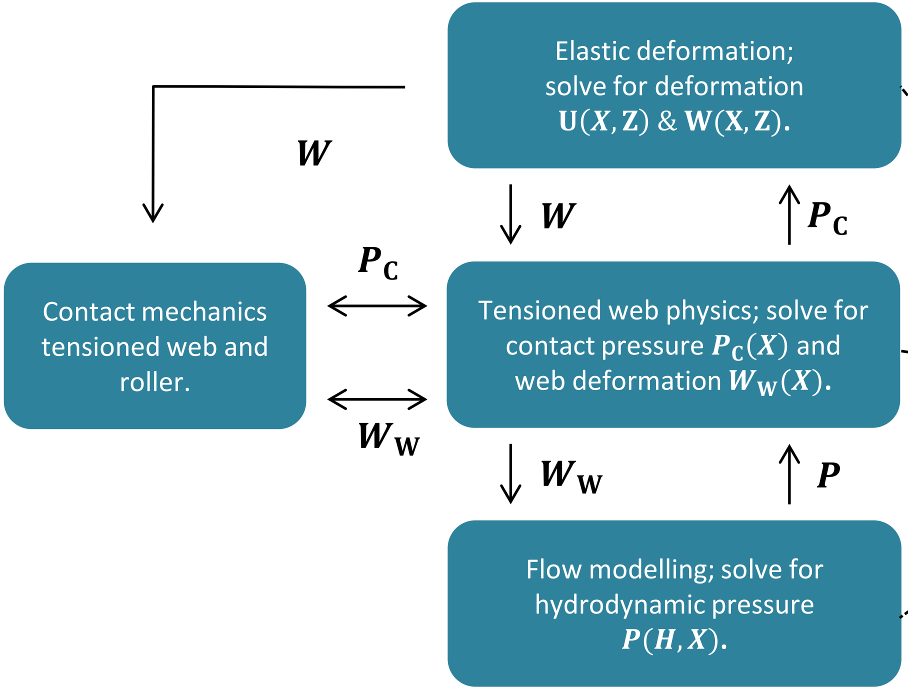
[1] T. V. Kármán, Festigkeitsprobleme im Maschinenbau. in Encyklopädie der mathematischen wissenschaften. Teubner, 1910.

[2] A. Fischer, “A special newton-type optimization method,” *Optimization*, vol. 24, no. 3–4, pp. 269–284, Jan. 1992, doi: 10.1080/02331939208843795.

Model | elastohydrodynamic lubrication (EHL) – extension



Elastic deformation; solve for deformation $\mathbf{U}(X,\mathbf{Z})$ & $\mathbf{W}(\mathbf{X},\mathbf{Z})$.

W

W P_C

Contact mechanics tensioned web and roller.

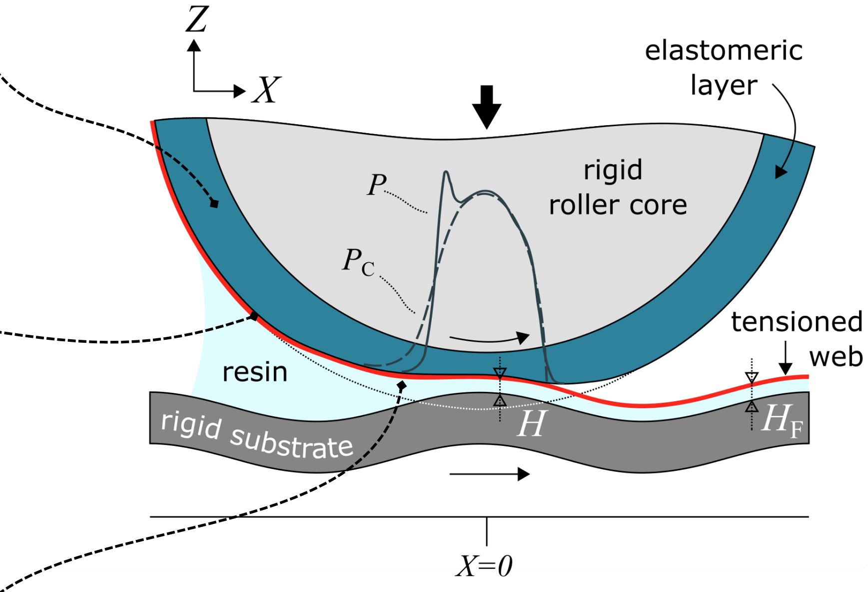
P_C

W_W

Tensioned web physics; solve for contact pressure $P_C(X)$ and web deformation $W_W(X)$.

W_W P

Flow modelling; solve for hydrodynamic pressure $P(H,X)$.

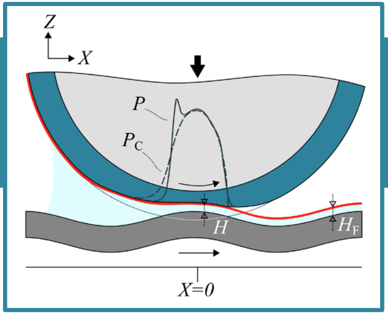


$$\text{waviness} = A\cos\left(\frac{2\pi}{\Lambda}(X-\Phi)\right)$$

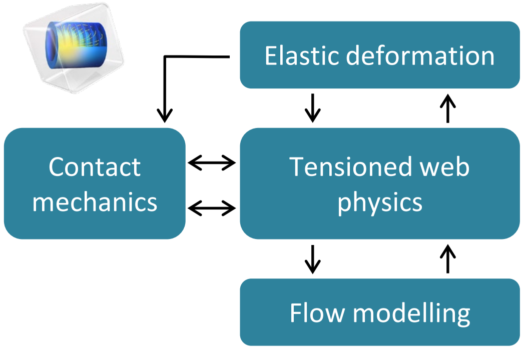
A → amplitude
Λ → wavelength
Φ → phase shift

TU Delft morphotonics

Model | solution procedure



Multiphysics model[1,2]



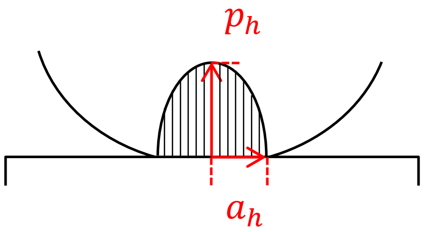
Elastic deformation

Contact mechanics

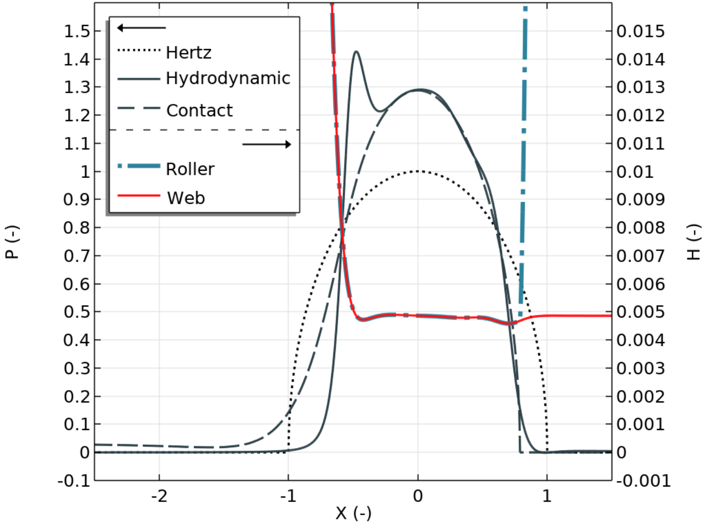
Tensioned web physics

Flow modelling

Hertzian scaling



Solution



Equations implemented via Mathematics module:
- Linear elasticity → Weak Form PDE
- Others → General Form Boundary PDE

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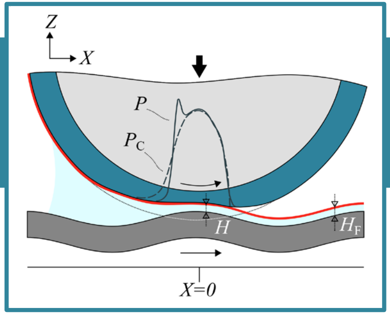
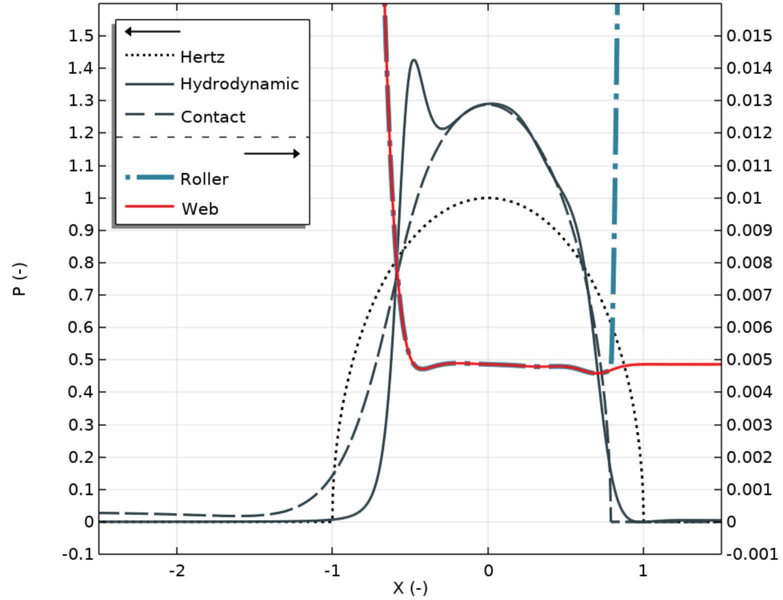
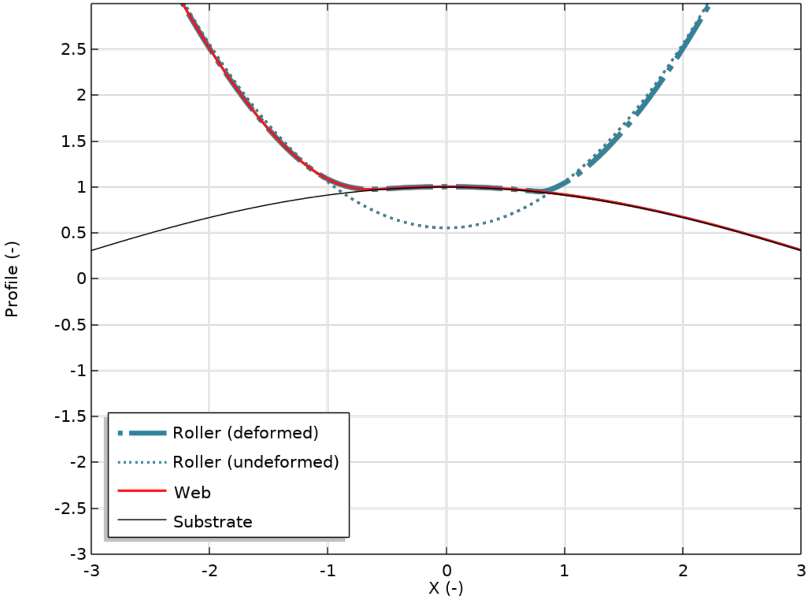
[1] Habchi, W., 2018, *Finite Element Modeling of Elastohydrodynamic Lubrication Problems*, John Wiley & Sons, Hoboken, NJ.

[2] J. Snieder, M. Dielen, and R. A. van Ostayen, “Elastohydrodynamic lubrication of soft-layered rollers and tensioned webs in roll-to-plate nanoimprinting,” Proceedings of the Institution of Mechanical Engineers, Part J: Journal of Engineering Tribology, vol. 237, no. 10, pp. 1871–1884, Oct. 2023, doi: 10.1177/13506501231183860.

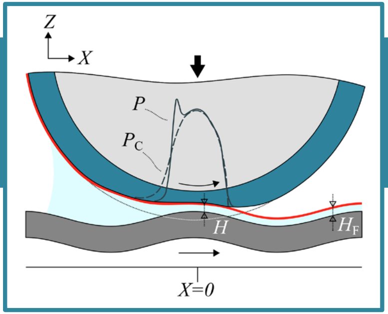
Model results | varying phase shift

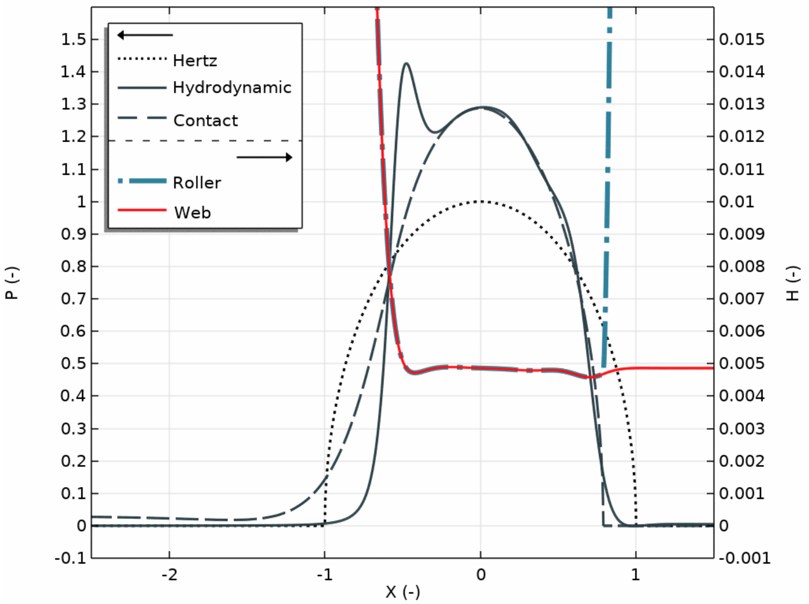


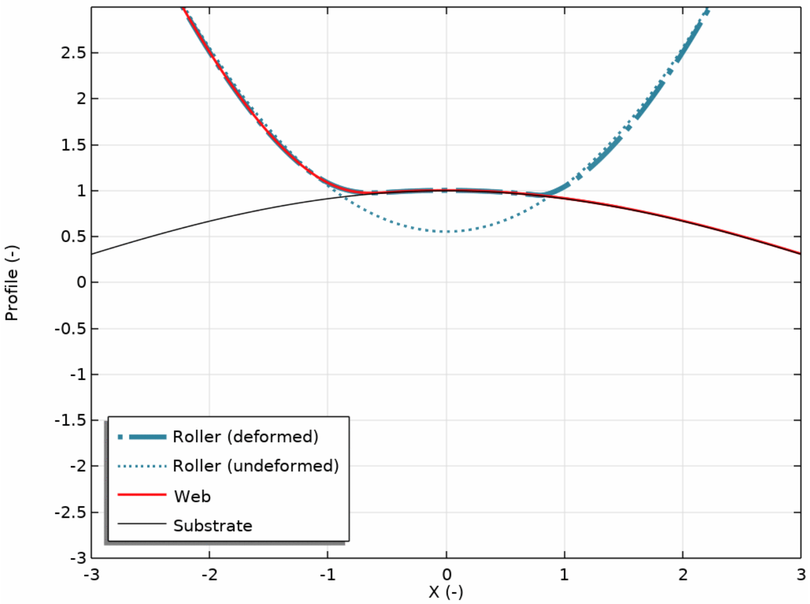




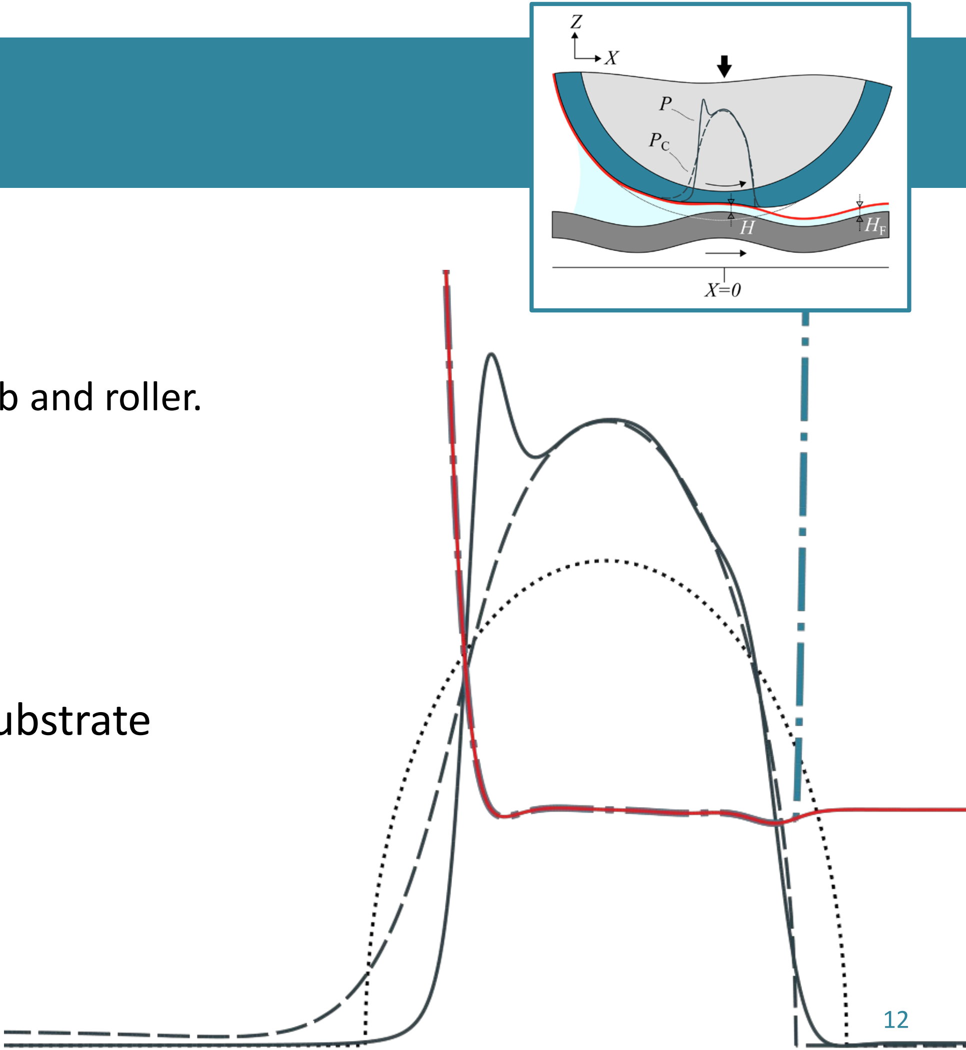
Model results | varying phase shift







Conclusion



- ✓ Development of an extended EHL model.
  - Tensioned web kinematics.
  - Contact mechanics between tensioned web and roller.

- ✓ Useful to predict the layer height in roller-based imprint systems.

- ✓ Design tool to minimize the influence of substrate waviness on the layer height.

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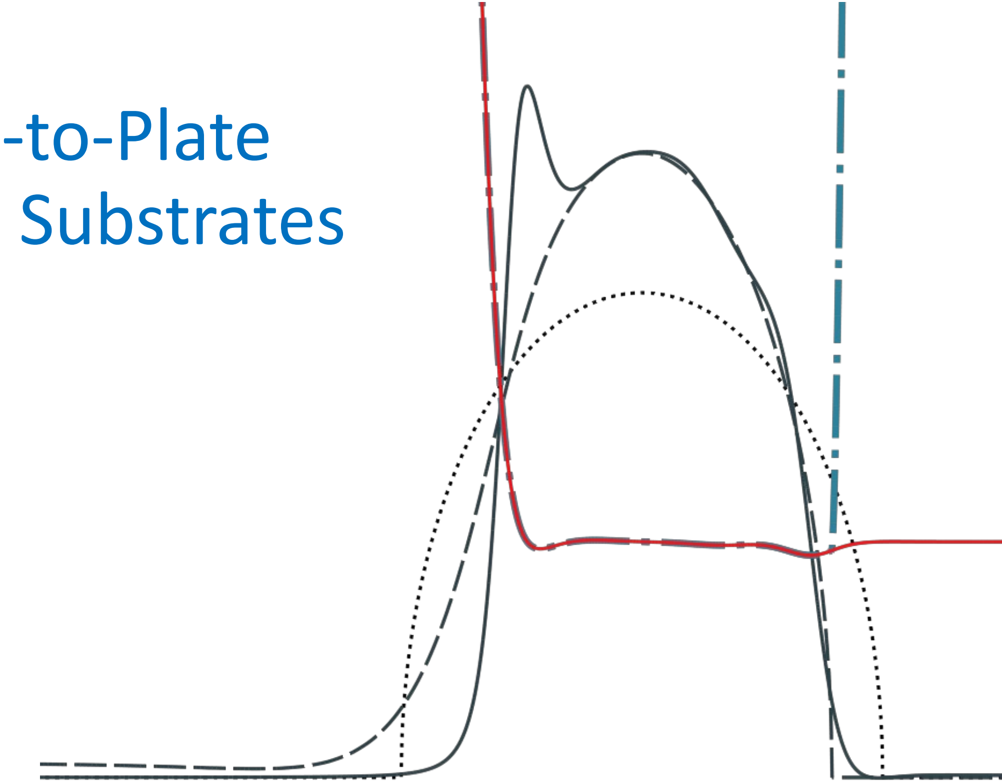

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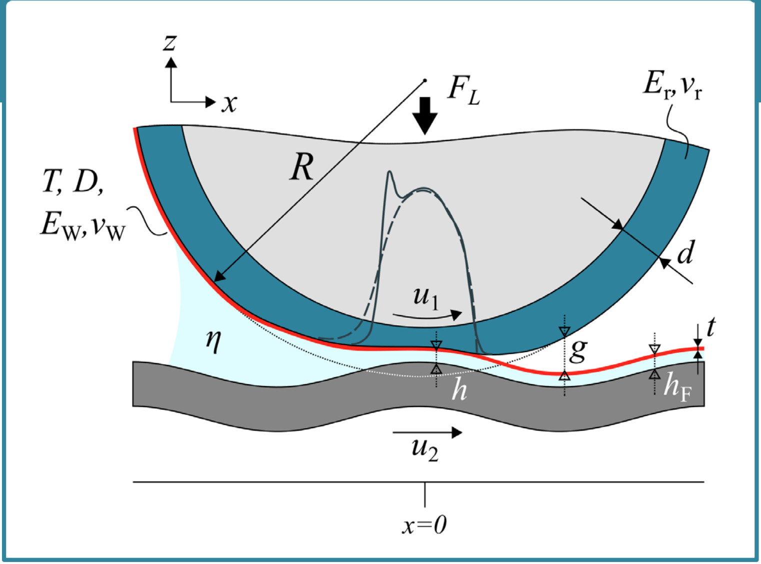
Model | parameters & scaling

- Process variables
  - Load: F_L
  - Velocity: u_1 and u_2
  - Web tension: T
- Material properties
  - Viscosity resin: η
  - Elastic modulus: E_r
  - Poisson ratios: ν_r
  - Bending stiffness: D
- Geometry
  - Roller radius: R
  - Elastomeric layer thickness: d

$$a_{\mathrm{h}} = \sqrt{\frac{8F_{\mathrm{L}}R}{\pi E'}}$$

$$p_{\mathrm{h}} = \frac{2F_{\mathrm{L}}}{\pi a_{\mathrm{h}}}$$

$$\frac{2}{E'} = \frac{1-{\nu_{\mathrm{r}}}^2}{E_{\mathrm{r}}}$$



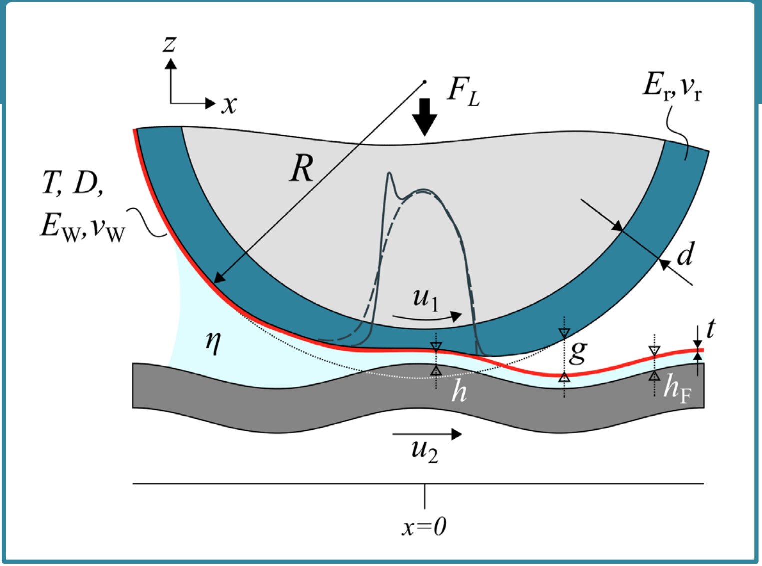
- Scaling of variables

$$P = \frac{p}{p_{\mathrm{h}}}, \quad P_{\mathrm{c}} = \frac{p_{\mathrm{c}}}{p_{\mathrm{h}}} \qquad G = \frac{gR}{a_{\mathrm{h}}^2}, \quad H = \frac{hR}{a_{\mathrm{h}}^2}, \quad K = R\kappa$$

$$U = \frac{uR}{a_{\mathrm{h}}^2}, \quad W = \frac{wR}{a_{\mathrm{h}}^2}, \quad W_{\mathrm{w}} = \frac{w_{\mathrm{w}}R}{a_{\mathrm{h}}^2} \qquad X' = \frac{x'}{a_{\mathrm{h}}}, \quad Z' = \frac{z'}{d}$$

Model | parameters – nominal

- Process variables
  - Load: F_L $= 2000\ \mathrm{N/m}$
  - Velocity: u_1 and u_2 $= 10.6\ \mathrm{mm/s}$
  - Web tension: T $= 464\ \mathrm{N/m}$
- Material properties
  - Viscosity resin: η $= 100\ \mathrm{mPa \cdot s}$
  - Elastic modulus: E_r $= 3\ \mathrm{MPa}$
  - Poisson ratios: ν_r $= 0.45$
  - Bending stiffness: D $= 0.01\ \mathrm{Nm}$
- Geometry
  - Roller radius: R $= 100\ \mathrm{mm}$
  - Elastomeric layer thickness: d $= 9.9\ \mathrm{mm}$

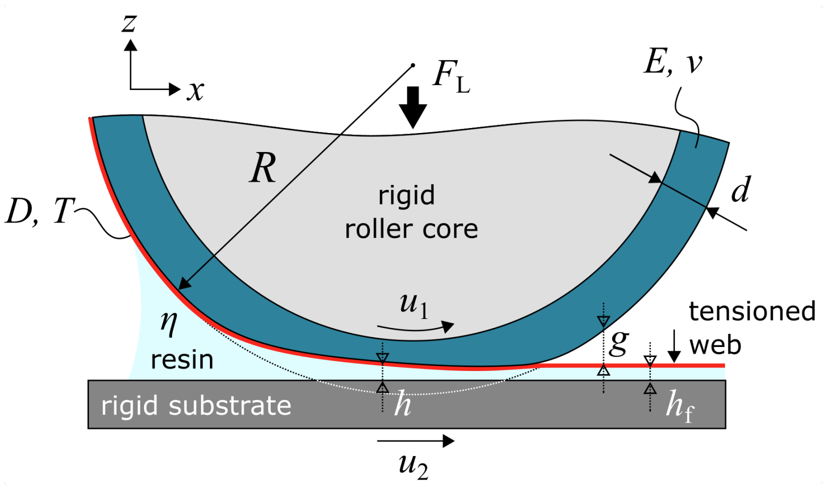


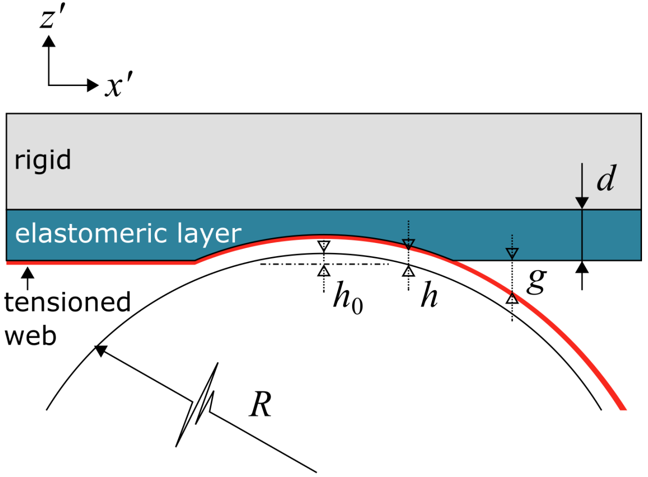
Waviness = $a \cos\left(\frac{2\pi}{\lambda}(x-\varphi)\right)$

- a → amplitude of 0.68 mm
- λ → wavelength of 123 mm
- φ → phase shift 0 mm.

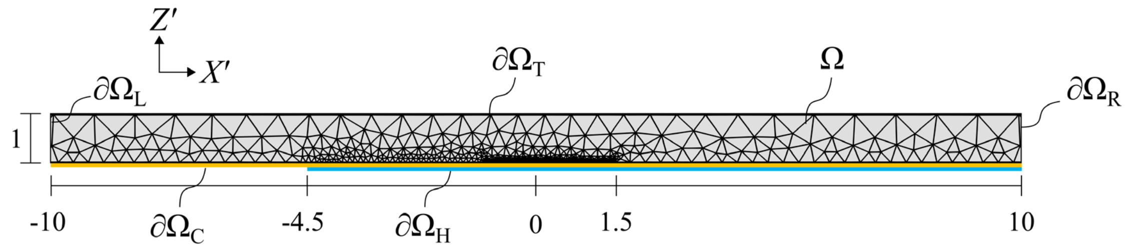
Model | set-up

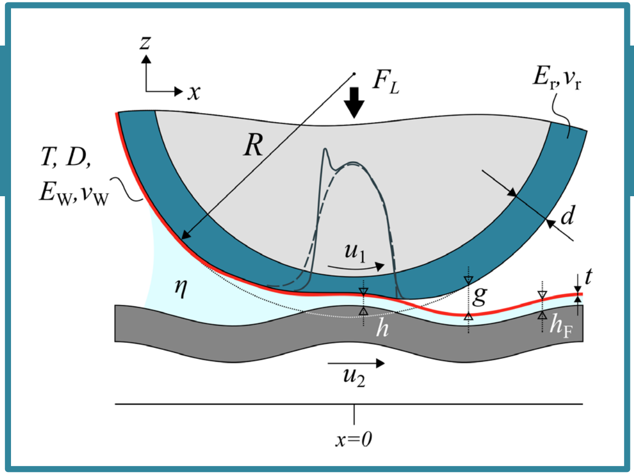
- Unwrapping of the roller





Model | elastic deformation

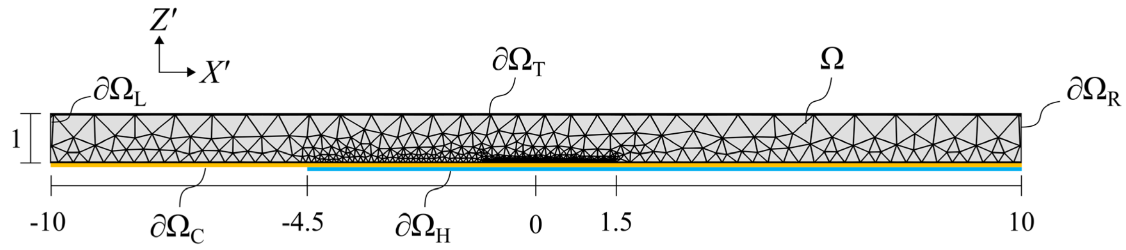


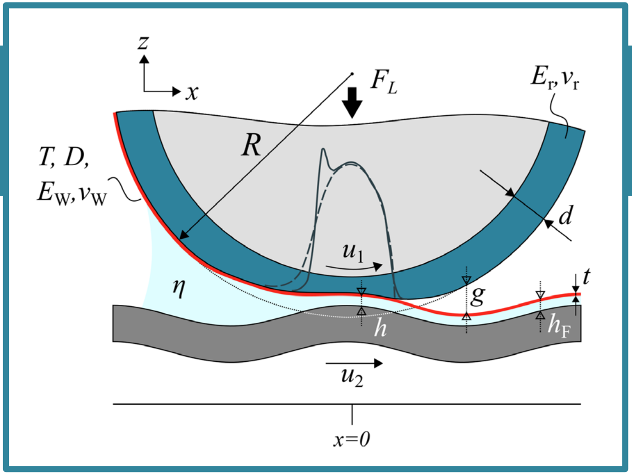


- Applied on domain Ω
- Linear elasticity equations
  - $X': \frac{\partial}{\partial X'}\left[(\lambda+2\mu)\frac{d}{a_h}\frac{\partial U}{\partial X'}+\lambda\frac{\partial W}{\partial Z'}\right]+\frac{\partial}{\partial Z'}\left[\mu\left(\frac{a_h}{d}\frac{\partial U}{\partial Z'}+\frac{\partial W}{\partial X'}\right)\right]$
  - $Z': \frac{\partial}{\partial X'}\left[\mu\left(\frac{\partial U}{\partial Z'}+\frac{d}{a_h}\frac{\partial W}{\partial X'}\right)\right]+\frac{\partial}{\partial Z'}\left[\lambda\frac{\partial U}{\partial X'}+(\lambda+2\mu)\frac{a_h}{d}\frac{\partial W}{\partial Z'}\right]$
- Lamé parameters
  - $\lambda = \frac{\nu E_{eq}}{(1-2\nu)(1+\nu)}$ and $\mu = \frac{E_{eq}}{2(1+\nu)}$ and $E_{eq} = E_r\frac{a_h}{R p_h}$

- Boundary conditions
  - $U = W = 0$ on $\partial\Omega_T$
  - $U = 0$ on $\partial\Omega_L$ and $\partial\Omega_R$
  - $\sigma_n = P_c$ on $\partial\Omega_C$
  - $\sigma_n = \sigma_t = 0$ elsewhere

Model | flow modelling





- Applied on domain boundary $\partial\Omega_{\mathrm{H}}$
- Reynolds equation
  - $\frac{\partial}{\partial X'}\left(-\frac{a_{\mathrm{h}}^3 p_{\mathrm{h}}}{12R^2\eta(u_1+u_2)}H^3\frac{\partial P}{\partial X'}+\frac{H}{2}\right)=0$
  - $H = H_0 + H_{\mathrm{W}} + W_{\mathrm{W}} - H_{\mathrm{sub}}$
- Boundary conditions
  - $P = 0$ on $X' = -4.5$
  - $\frac{\partial P}{\partial X'} = \frac{H}{2}$ on $X' = 10$

H_0: offset (roller engagement)

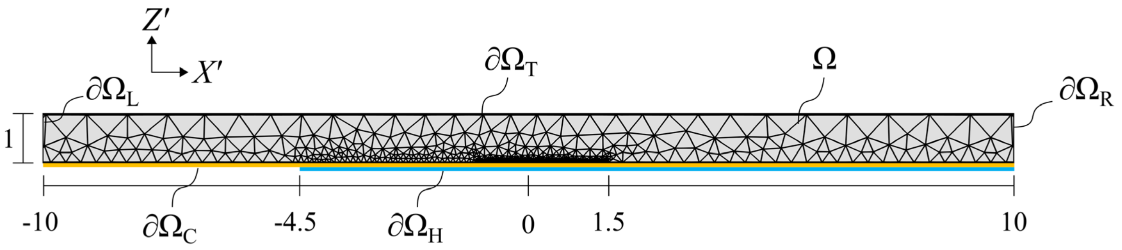
H_{W}: initial shape web
- $\frac{X'^2}{2}$ for $X' \leq 0$
- 0 for $X' > 0$

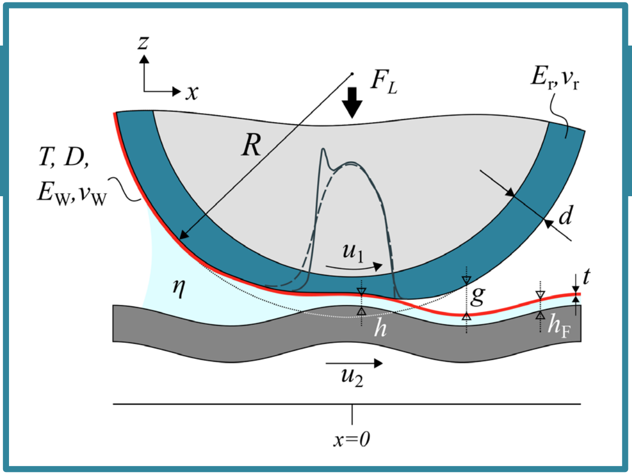
W_{W}: deformation web

H_{sub}: substrate profile / waviness
- $A\cos\left(\frac{2\pi}{\Lambda}(X'-\Phi)\right)$

A → amplitude
Λ → wavelength
Φ → phase shift

Model | tensioned web kinematics



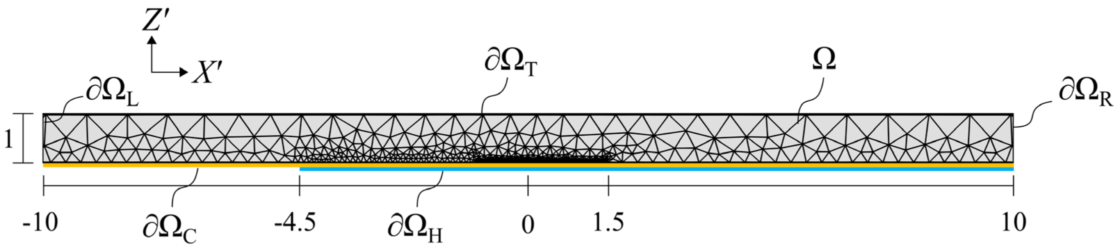


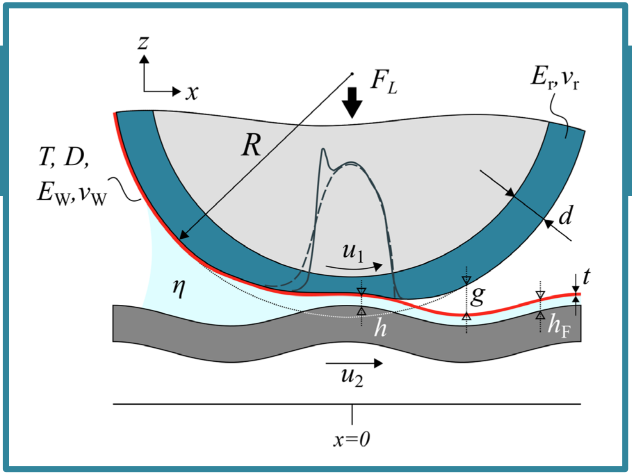
- Applied on domain boundary $\partial\Omega_{\mathrm{C}}$
- Large-deflection bending of thin plates equation:
  - $\left(-\frac{D}{a_{\mathrm{h}}^2 p_{\mathrm{h}} R}\right)\frac{\partial^2 K}{\partial X'^2}+\left(\frac{T}{p_{\mathrm{h}} R}\right)K+P_{\mathrm{n}}=0$
  - Curvature: $\mathrm{K}=\frac{\partial^2}{\partial X'^2}(H_{\mathrm{W}}+W_{\mathrm{W}})=$

$$\begin{cases} 1+\frac{\partial^2 W_{\mathrm{W}}}{\partial X'^2}, & \text{for } X'\leq 0 \\ \frac{\partial^2 W_{\mathrm{W}}}{\partial X'^2}, & \text{for } X'>0 \end{cases}$$

- Boundary conditions → it is assumed the web has the same curvature and direction at the end of the domain ($X'=10$):
  - $\left.\frac{\partial K}{\partial X'}\right|_{X'=10}=\left.\frac{\partial^3 H_{\mathrm{sub}}}{\partial X'^3}\right|_{X'=10}$
  - $\left.\frac{\partial W_{\mathrm{W}}}{\partial X'}\right|_{X'=10}=\left.\frac{\partial H_{\mathrm{sub}}}{\partial X'}\right|_{X'=10}$
- Bending stiffness: $D=\frac{Et^3}{12(1-\nu^2)}$
- Normal stress: $P_{\mathrm{n}}=P-P_{\mathrm{C}}$

Model | load balance & contact mechanics

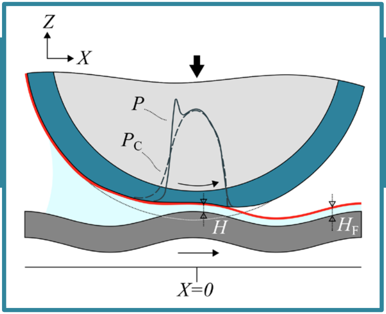




- Ordinary integral equation, which is associated with the unknown constant film thickness gap H_0
- $\int P \, \mathrm{d}X' = F_L$
  - F_L is the effective applied load

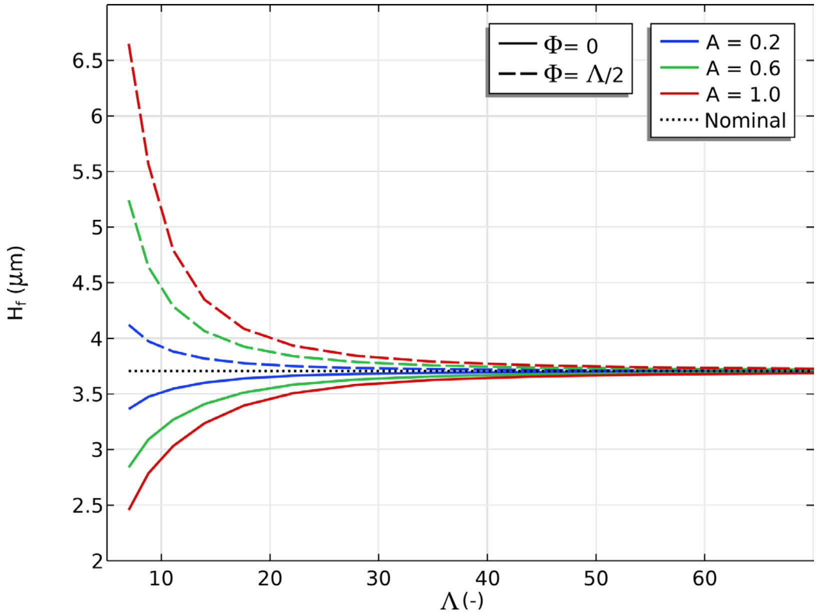
- Fischer-Burmeister complementarity condition to describe contact
  - $P_c + G - \sqrt{P_c^{\,2} + G^2} = 0$
  - $G = G_0 + W - W_W$
  - W_W: deformation web
  - W: deformation roller material
  - $G_0 = \begin{cases} 0, & \text{for } X' \leq 0 \\ \frac{X'^2}{2}, & \text{for } X' > 0 \end{cases}$

Model results | varying waviness



$$\text{waviness} = A\cos\left(\frac{2\pi}{\Lambda}(X-\Phi)\right)$$

A → amplitude
Λ → wavelength
Φ → phase shift



$\Lambda = 15$