A multibody dynamics model of bacterial biofilms

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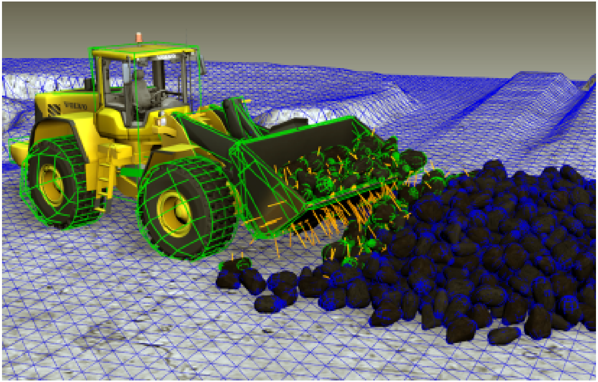
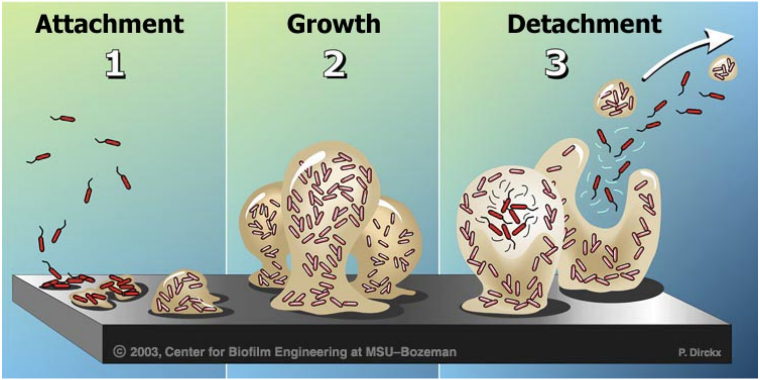
Nonsmooth multidomain dynamics



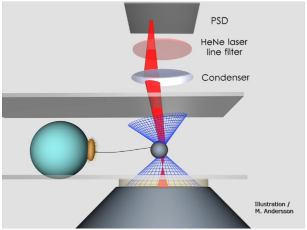
What has this to do with bacterias?

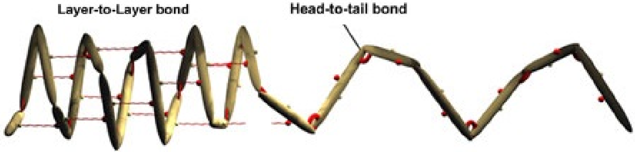
Bacterial biofilms



- aggregate of microorganisms
- attachment, growth and dispersion
- microbial infections, dental plaque, organic waste in pipes

Bacterial adhesion - E. coli

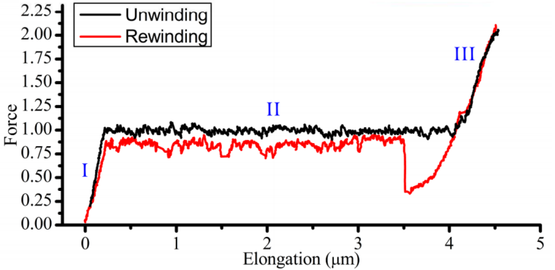




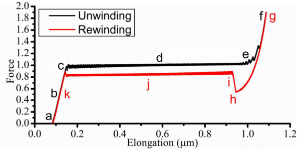
- pili = surface organelles, $\sim 1\mu\text{m}$
- $\gtrsim$ 1k subunit macromolecules in helix structure
- strong and weak bonds

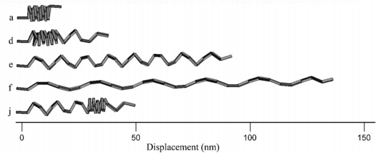
Pili force

Laser tweezer measurement [7]

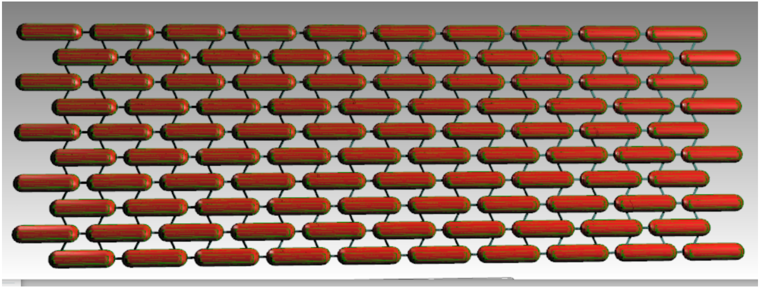


Multibody simulation [2]



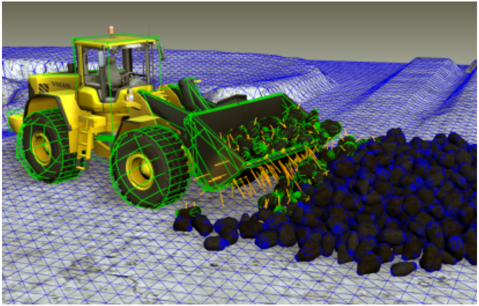


Biofilm model



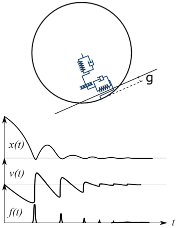
- rigid bacterias
- contact constraints
- pili constraints
- hydrodynamics

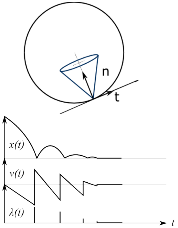
Nonsmooth multidomain dynamics

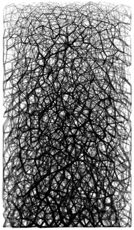


- Heterogeneous multibody dynamics
- Rigid, flexible, fluid, hydraulics, electronics,...
- Nonsmooth contact dynamics - large fixed time-step
- Variational stepper with constraint regularization
- Numerical solvers for heterogeneous subsystems

Smooth versus nonsmooth dynamics







Smooth dynamics	**Nonsmooth dynamics**
smooth trajectories	velocity discontinuities
smooth forces & constraints	+ impulses & inequalities
small time-step	large time-step
linear or nonlinear solver	QP or MLCP solver

Nonsmooth contact dynamics (Moreau [6], Jean [3], Acary [1], Servin [8])

Multibody dynamics

Multibody system $(\mathbf{q}, \dot{\mathbf{q}})$ on descriptor form $(\mathbf{q}, \dot{\mathbf{q}}, \boldsymbol{\lambda}, \bar{\boldsymbol{\lambda}})$

$$\mathbf{M}\ddot{\mathbf{q}} + \dot{\mathbf{M}}\dot{\mathbf{q}} - \mathbf{G}(\mathbf{q})^T\boldsymbol{\lambda} - \bar{\mathbf{G}}(\mathbf{q})^T\bar{\boldsymbol{\lambda}} = \mathbf{f}_e \quad (1)$$

$$\varepsilon\boldsymbol{\lambda} + \mathbf{g}(\mathbf{q}) = 0 \quad (2)$$

$$\gamma\bar{\boldsymbol{\lambda}} + \bar{\mathbf{G}}(\mathbf{q})\dot{\mathbf{q}} = \boldsymbol{w}(t) \quad (3)$$

constrained by $\mathbf{g}(\mathbf{q}) = 0$ and $\bar{\mathbf{G}}(\mathbf{q})\dot{\mathbf{q}} = \boldsymbol{w}(t)$ with compliance ε and damping γ.

Multibody dynamics - numerical solver

Linearized varational time stepper SPOOK (Lacoursière [4, 5])

$$\mathbf{q}_{n+1} = \mathbf{q}_n + h\dot{\mathbf{q}}_{n+1} \tag{4}$$

$$\underbrace{\begin{bmatrix} \mathbf{M} & -\mathbf{G}^T & -\bar{\mathbf{G}}^T \\ \mathbf{G} & \mathbf{\Sigma} & 0 \\ \bar{\mathbf{G}} & 0 & \bar{\mathbf{\Sigma}} \end{bmatrix}}_{\mathbf{H}} \underbrace{\begin{pmatrix} \dot{\mathbf{q}}_{n+1} \\ \boldsymbol{\lambda} \\ \bar{\boldsymbol{\lambda}} \end{pmatrix}}_{\mathbf{z}} = \underbrace{\begin{pmatrix} \mathbf{M}\dot{\mathbf{q}}_n + h\mathbf{f}_n \\ -\frac{4}{h}\Upsilon\mathbf{g} + \Upsilon\mathbf{G}\dot{\mathbf{q}}_n \\ \boldsymbol{\omega}_n \end{pmatrix}}_{-\mathbf{r}} \tag{5}$$

Diagonal regularization and stabilization matrices

$$\mathbf{\Sigma} = \frac{4}{h^2}\,\mathrm{diag}\left(\frac{\varepsilon_i}{1 + 4\frac{\tau_i}{h}}\right)$$

$$\bar{\mathbf{\Sigma}} = \frac{1}{h}\,\mathrm{diag}\left(\gamma_i\right)$$

$$\Upsilon = \mathrm{diag}\left(\frac{1}{1 + 4\frac{\tau_i}{h}}\right)$$

Constraint potential and dissipation

$$U = \tfrac{1}{2}\mathbf{g}^T\varepsilon^{-1}\mathbf{g}$$

$$R = \tfrac{1}{2}(\bar{\mathbf{G}}\boldsymbol{v})^T\gamma^{-1}\bar{\mathbf{G}}\boldsymbol{v}$$

Nonsmooth MBD - numerical solver

Including frictional contacts, impacts, joint ant motor limits lead to limits and complementarity conditions on the solution variables

$$
\begin{aligned}
\mathbf{H}\boldsymbol{z} + \mathbf{r} &= \boldsymbol{w}_+ - \boldsymbol{w}_- \\
0 \leqslant \boldsymbol{w}_+ &\perp \boldsymbol{z} - \mathbf{l} \geqslant 0 \\
0 \leqslant \boldsymbol{w}_- &\perp \mathbf{u} - \boldsymbol{z} \geqslant 0
\end{aligned} \tag{6}
$$

The problem transforms from linear system to a mixed linear complementarity condition (MLCP)

Nonsmooth MBD - numerical solver

Direct MLCP solver

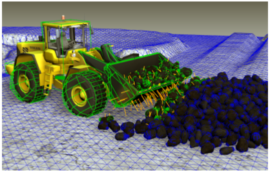
- block pivoting method
- block sparse LDLT factorization
- fill-reducing reordering
- BLAS3 optimized

Iterative MLCP solver

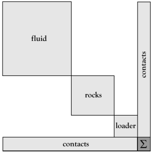
- block sparse projected Gauss-Seidel (PGS)

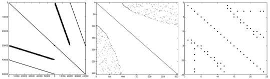
Hybrid direct-iterative split solver

- vehicle vs granular
- normals vs tangents



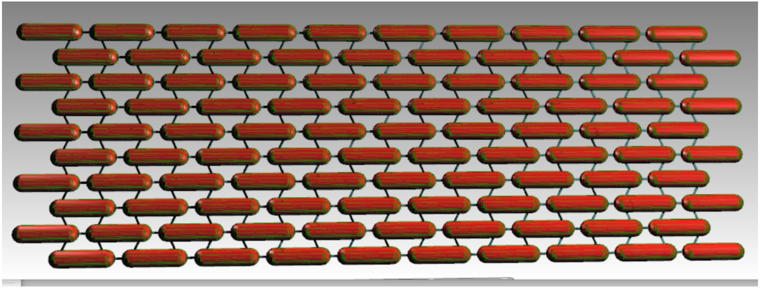
$$\begin{bmatrix} \boldsymbol{M} & -\boldsymbol{G}_A^T & -\boldsymbol{G}_B^T & -\boldsymbol{G}_C^T \\ \boldsymbol{G}_A & \boldsymbol{\Sigma}_A & 0 & 0 \\ \boldsymbol{G}_B & 0 & \boldsymbol{\Sigma}_B & 0 \\ \boldsymbol{G}_C & 0 & 0 & \boldsymbol{\Sigma}_C \end{bmatrix} \begin{pmatrix} \boldsymbol{v} \\ \boldsymbol{\lambda}_A \\ \boldsymbol{\lambda}_B \\ \boldsymbol{\lambda}_C \end{pmatrix} = \begin{pmatrix} \boldsymbol{b}_v \\ \boldsymbol{b}_A \\ \boldsymbol{b}_B \\ \boldsymbol{b}_C \end{pmatrix}$$





Research prototype code and AgX Dynamics [4]

Biofilm model



- rigid bacterias
- contact constraints
- pili constraints
- hydrodynamics

biofilms
Multidomain
Pili constraint
Summary

Pili constraint

Piecewise linear constraint - extension δ - Jacobian $G = \frac{\partial g}{\partial \delta}$

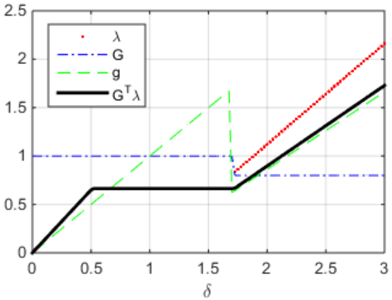
$$g = \delta - k_2 * \max(0, \delta - \delta_2) - \kappa\Theta(\delta - \delta_2) \quad (7)$$

$$G = 1 - k_2\Theta(\delta - \delta_2) \quad (8)$$

Constraint regularization and multiplier limit

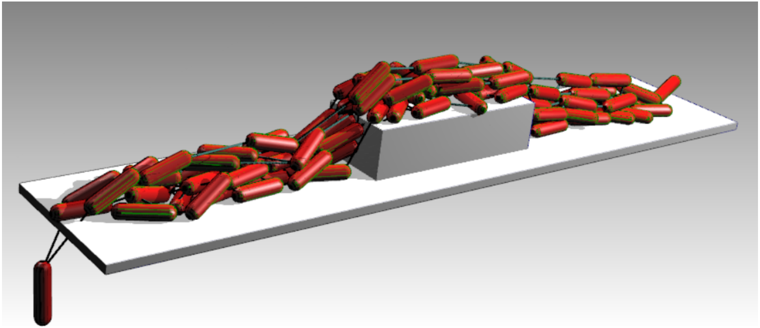
$$\lambda = k_1 g \;, \quad \delta < \delta_1, \; \delta > \delta_2 \quad (9)$$

$$\lambda = \lambda_1 \;, \quad \delta_1 \leqslant \delta \leqslant \delta_2 \quad (10)$$



Biofilm simulation

A first mockup model - with cartoon physics parameters



Summary and conclusions

- Bacterial biofilm as a multibody system
- A piecewise linear pili constraint was introduced

Future work

- Nonsmooth dynamics at discontinuity
- Dynamic generation of pili constraints
- Simple hydrodynamics
- Numerical experiments and validation

biofilms
Multidomain
Pili constraint
Summary

References

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