Chair of Scientific Computing in Computer Science
Univ.-Prof. Dr. Hans-Joachim Bungartz

Technische Universität München

IDP Project Final Presentation

Proliferating Cell Collectives: A Comparison of Hard and Soft Collision Models

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Outline

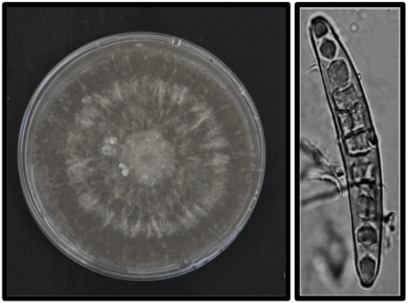
Computational Biology

Why simulate Bacteria?

- Local rules $\rightarrow$ emergent behavior
- Test hypotheses in silico
- Beautiful visualizations

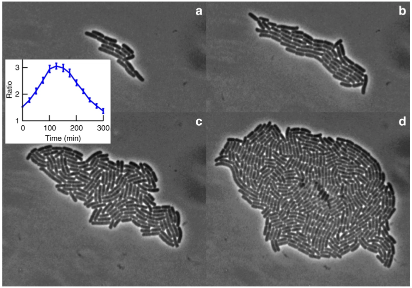
Computational challenge:

- Large system sizes (10^6 cells)
- Complex interactions
- Long timescales

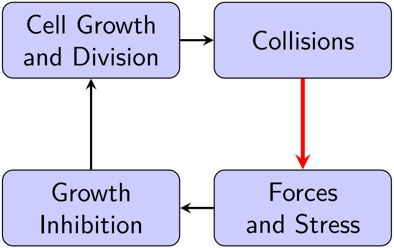


Real fungal colony showing macroscopic ring patterns [Bankole et al., 2023].

Small-scale: Simulating individual Bacteria

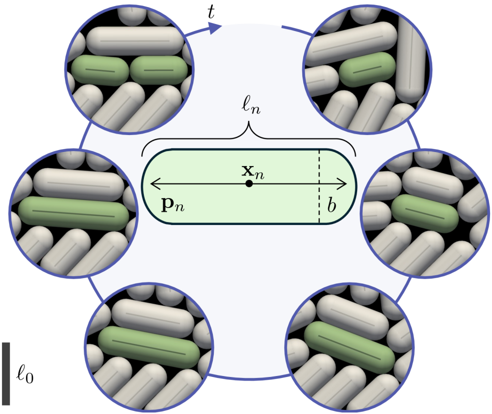


E. coli colony [Dell'Arciprete et al., 2018]



Outline

Cell Representation: Rigid Spherocylinders

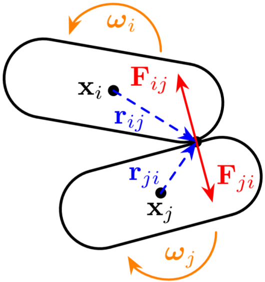


Spherocylindrical cell model [Weady et al., 2024].

Cell Dynamics

Overdamped dynamics:

- Collision cause forces
- Inertia negligible
- Cells "swim in honey"



Equations of motion:

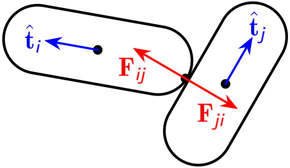
Translation: $$\mathbf{u}_i = \frac{1}{\zeta \ell_i} \sum_{j \neq i} \mathbf{F}_{ij}$$

Rotation: $$\boldsymbol{\omega}_i = \frac{12}{\zeta \ell_i^3} \sum_{j \neq i} \mathbf{r}_{ij} \times \mathbf{F}_{ij}$$

Cell Growth

Stress-dependent growth:

- Exponential growth
- Inhibited by longitudinal stress



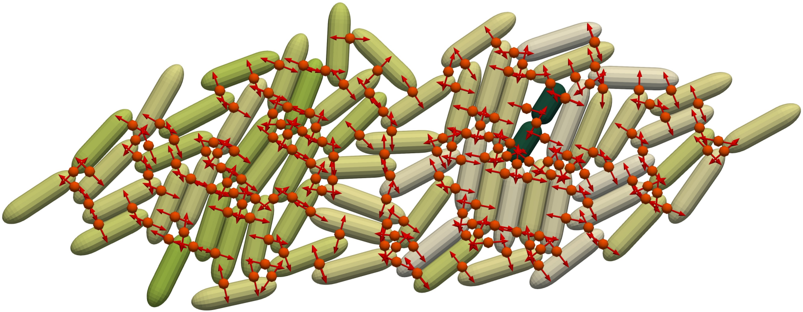
Growth rate:

Growth rate: $\dot{\ell}_i = \frac{\ell_i}{\tau} e^{-\lambda \sigma_i}$

Cell stress: $\sigma_i = \sum_{j \neq i} \frac{1}{2} \left| \hat{\mathbf{t}}_i \cdot \mathbf{F}_{ij} \right|$

Outline

Collision Resolution



- We consider two collision models
- Models only differ in how they calculate force magnitudes

Two Paradigms

Soft Model

Potential-based

- Local pairwise forces
- Allows overlap
- Numerically stiff
- Similar to MD simulations

$$\mathbf{F}_{ij} = k\delta^{3/2}\hat{\mathbf{n}}$$

Hard Model [Weady et al., 2024]

Constraint-based

- Global optimization problem
- Strict non-overlap
- Single-step solution
- Similar to DEM simulations

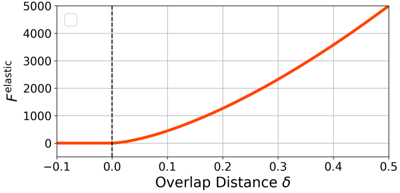
$$\mathbf{F}_{ij} = \gamma_{ij}\hat{\mathbf{n}}$$
$$\text{s.t. } \mathbf{0} \leq \boldsymbol{\gamma} \perp \boldsymbol{\Phi} \geq \mathbf{0}$$

Soft Model: Hertzian Contact

$$\mathbf{F}_{ij} = k_{cc}\sqrt{d}\,\delta^{3/2}\,\hat{\mathbf{n}}$$

Characteristics:

+ Embarrassingly parallel
+ Simple implementation
– Numerically stiff
– Tiny timesteps needed
– Allows overlap



Force increases with overlap

Hard Model: Prevent overlap via optimization

- Define signed distance between cells:

$$\boldsymbol{\Phi}_{ij} = \begin{cases} > 0 & \text{no contact} \\ = 0 & \text{contact} \\ < 0 & \text{overlap} \end{cases}$$

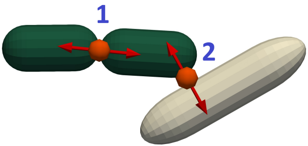
- Find contact forces γ s.t.

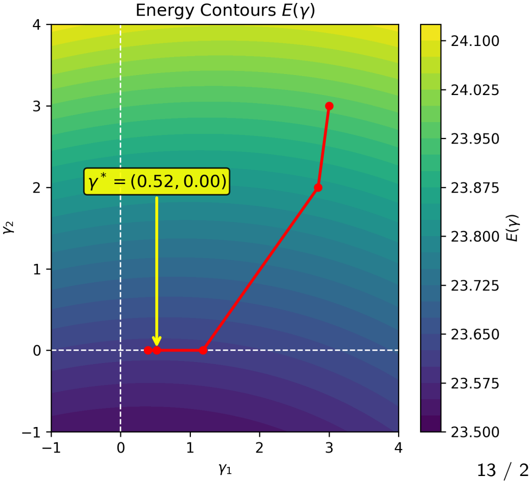
$$\mathbf{0} \leq \boldsymbol{\gamma} \perp \boldsymbol{\Phi}^{k+1} \geq \mathbf{0}$$

- Approximate how individual forces γ_i affect $\boldsymbol{\Phi}^{k+1}$
- Solve convex optimization problem:

$$\min_{\boldsymbol{\gamma} \geq 0} E(\boldsymbol{\gamma}) = \boldsymbol{\gamma}^\top \boldsymbol{\Phi}^k + \frac{\Delta t}{2} \boldsymbol{\gamma}^\top \boldsymbol{\mathcal{D}}^\top \boldsymbol{\mathcal{M}}^k \boldsymbol{\mathcal{D}} \boldsymbol{\gamma} + \mathbf{1}^\top \frac{\Delta t}{\lambda} \left(\frac{\boldsymbol{\ell}}{\tau} \odot e^{-\lambda \boldsymbol{\mathcal{L}} \boldsymbol{\gamma}} \right)$$

Example: Hard Model

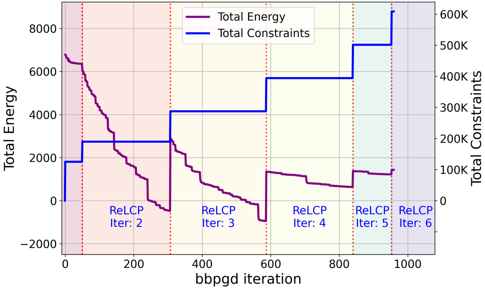




Hard Model: Performance

Characteristics:

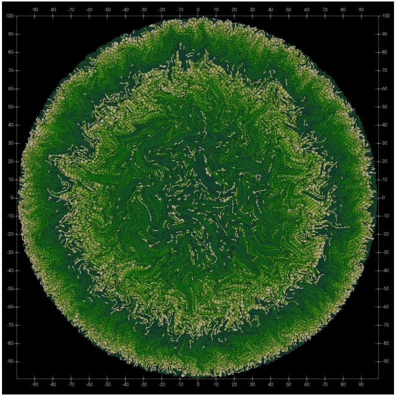
+ Less numerical stiffness
+ Larger timesteps possible
+ Strict non-overlap
– High per-step cost
– Complex implementation
– Requires multiple passes



Outline

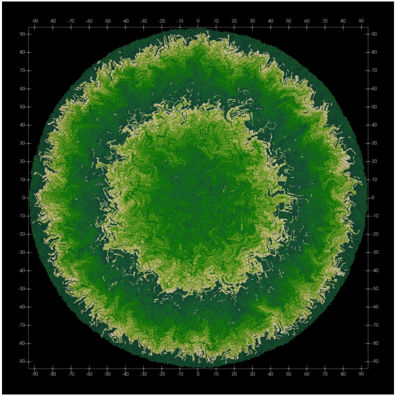
Concentric Ring Formation

Hard Model



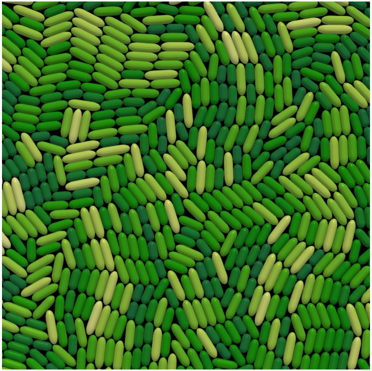
View video

Soft Model

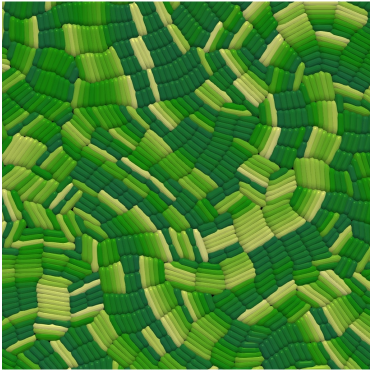


View video

Critical Difference: Packing Density

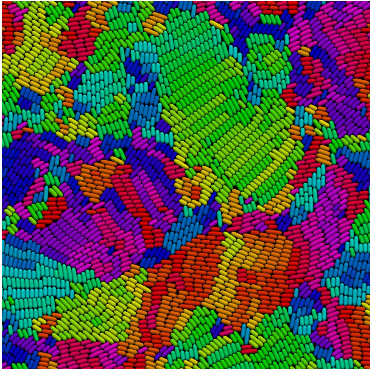


Hard Model

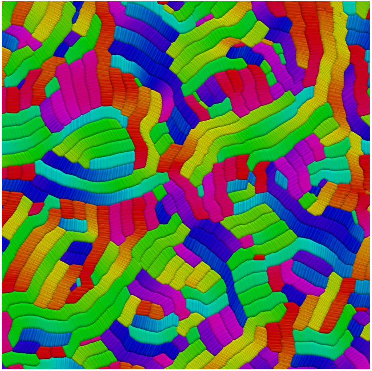


Soft Model

Critical Difference: Microdomain Structure



Hard: realistic patches



Soft: elongated bundles

Outline

CFL Condition

Adaptive timestepping:

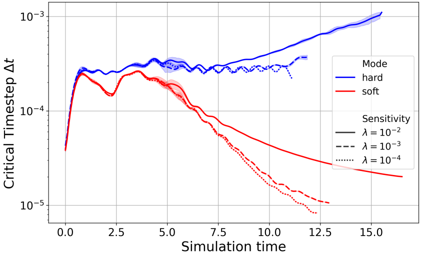
$$\Delta t = \frac{0.5\,\varepsilon}{u_m}$$

where u_m = median velocity,

ε = overlap tolerance

Key observations:

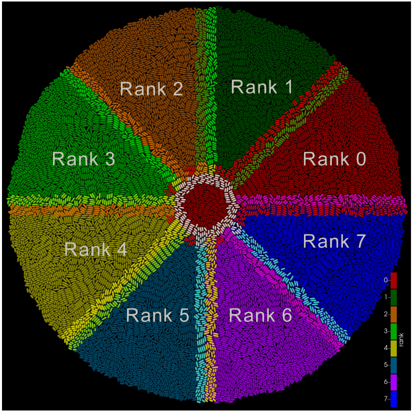
- Hard: stable $\Delta t \sim 3 \cdot 10^{-4}$
- Soft: drops $\Delta t \sim 10^{-5}$
- $30\times$ larger timesteps!



Parallel Architecture

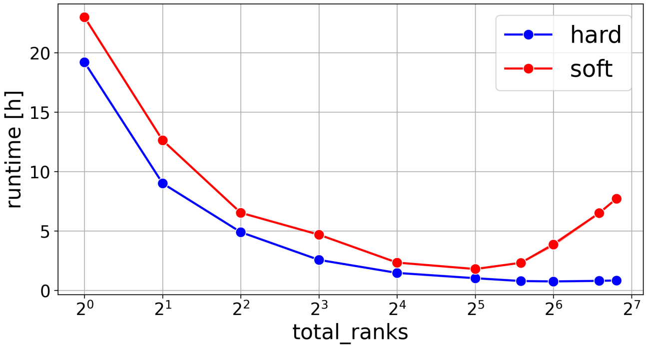
Implementation:

- MPI + PETSc framework
- Distributed vectors/matrices
- Angular sector decomposition
- Ghost particle exchange



Domain decomposition with 8 MPI ranks

Strong Scaling: Runtime to reach $R = 100$



- Hard model is always faster!
- Huge communication overhead (Especially for small Δt)

Outline

When to use each Model?

Soft Model

Use when:

- Exploring small Colonies
- Macroscopic effects matter

Advantages:

- Simple implementation
- Can model "squishy" bacteria

Disadvantages:

- Slow simulations
- Causes Artefacts

Hard Model

Use when:

- Exploring large Colonies
- Cell-scale phenomena matter

Advantages:

- Faster simulations
- Physical accuracy

Disadvantages:

- Complex implementation

Outline

Future Work

1. **Hard Model Solver Improvements**
   - Leverage PETSc GPU support
   - Warm-start BBPGD with previous solution
2. **Soft Model Enhancements**
   - Consider overlap, in adaptive timestepping.
   - Consider alternatives that prevent overlap
   - Slow down cell growth (globally) on overlap?
3. **More Biological Applications**
   - Other cell shapes (soft bodies?)
   - More complex models (Nutrient fields?, Outside forces?)
   - Utilize 3D capabilities

Thank you for your attention!

Questions?

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Code: https://github.com/manuellerchner/MicrobeGrowthSim-IDP

Supplementary materials: https://home.cit.tum.de/~ler/bacteria/

References I

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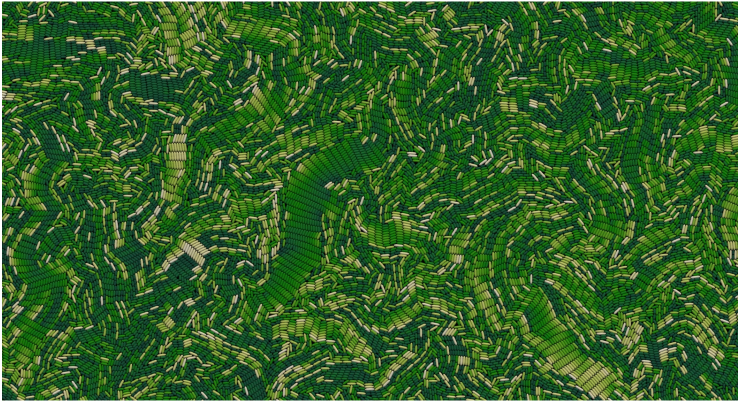
Largest Colony: R = 260, 301k cells, 24h@112 cores



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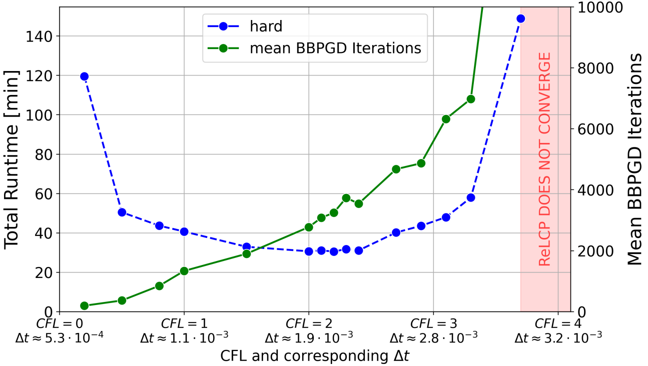
Backup: CFL vs. Runtime and Constraints



Backup: BBPGD Iterations vs. Number of Particles