

IDP Project Final Presentation

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

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Outline

- 1 Motivation
- 2 Mathematical Framework
- 3 Collision Models
- 4 Pattern Formation Results
- 5 Computational Performance
- 6 Discussion
- 7 Future Directions

Computational Biology

Why simulate Bacteria?

- Local rules → emergent behavior
- Test hypotheses in silico
- Beautiful visualizations

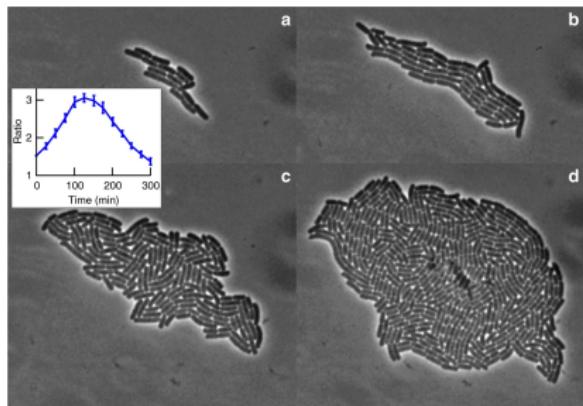
Computational challenge:

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

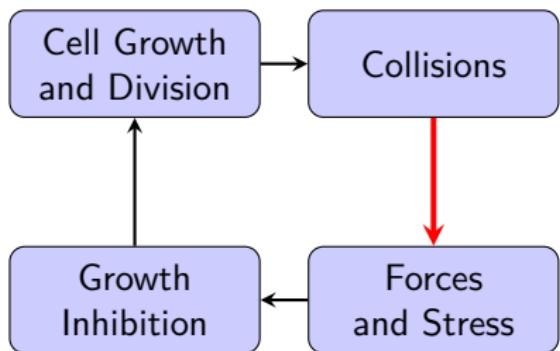


Real fungal colony showing macroscopic ring patterns [Bankole et al., 2023].

Small-scale: Simulating individual Bacteria



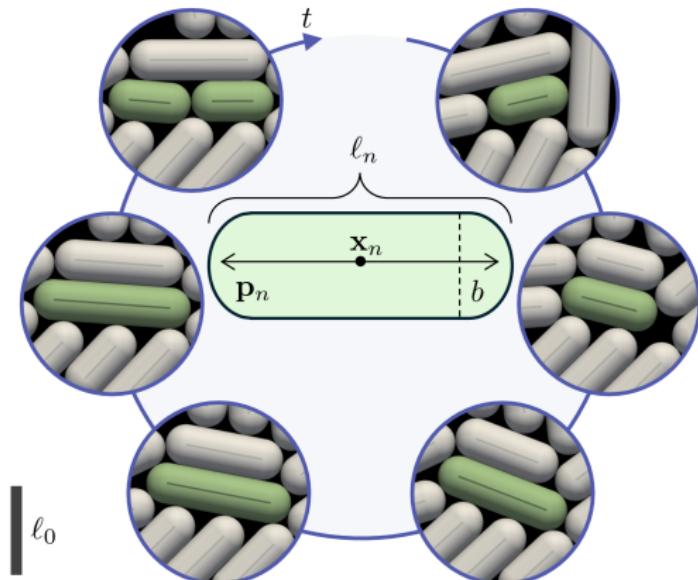
E. coli colony [Dell'Arciprete et al., 2018]



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Cell Representation: Rigid Spherocylinders



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

Cell Dynamics

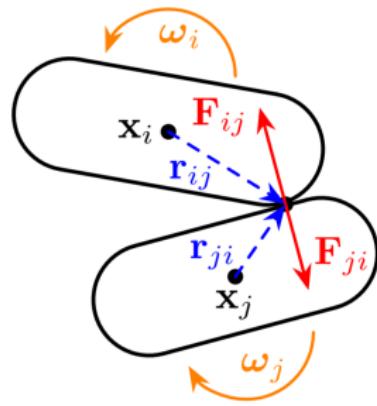
Overdamped dynamics:

- 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

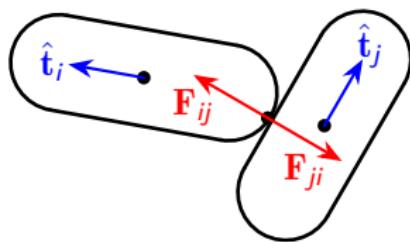
Stress-dependent growth:

- Exponential growth
- Inhibited by longitudinal stress

Growth rate:

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

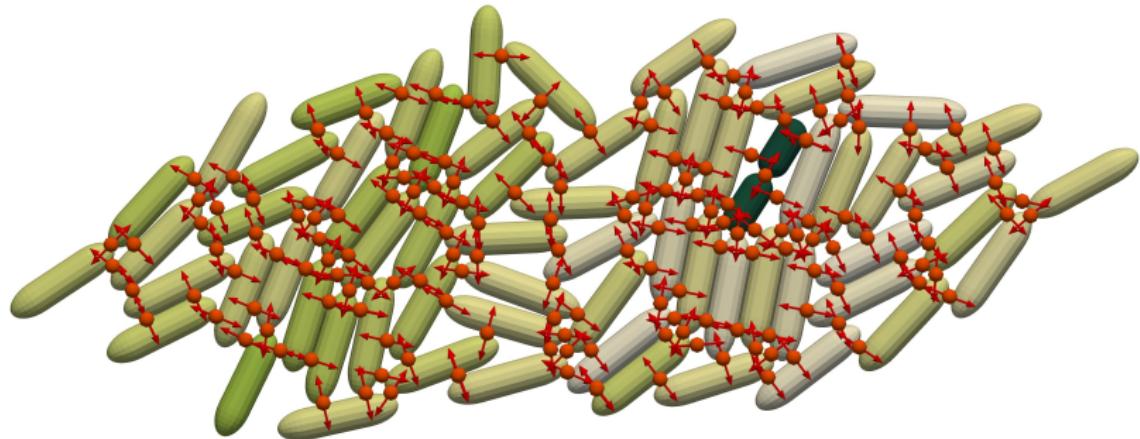
$$\text{Cell stress: } \sigma_i = \sum_{j \neq i} \frac{1}{2} |\hat{\mathbf{t}}_i \cdot \mathbf{F}_{ij}|$$



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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

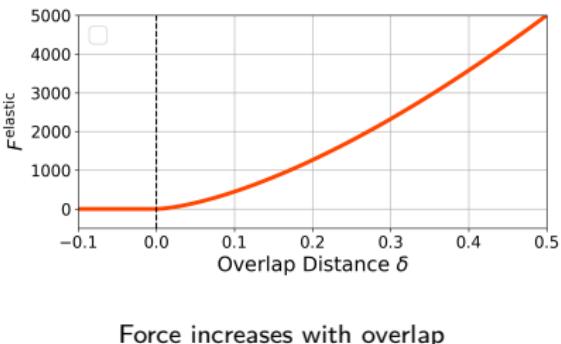
$$\mathbf{F}_{ij} = \gamma_{ij}\hat{\mathbf{n}} \\ \text{s.t. } \mathbf{0} \leq \boldsymbol{\gamma} \perp \boldsymbol{\Phi} \geq \mathbf{0}$$

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



Hard Model: Prevent overlap via optimization

- Define signed distance between cells:

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

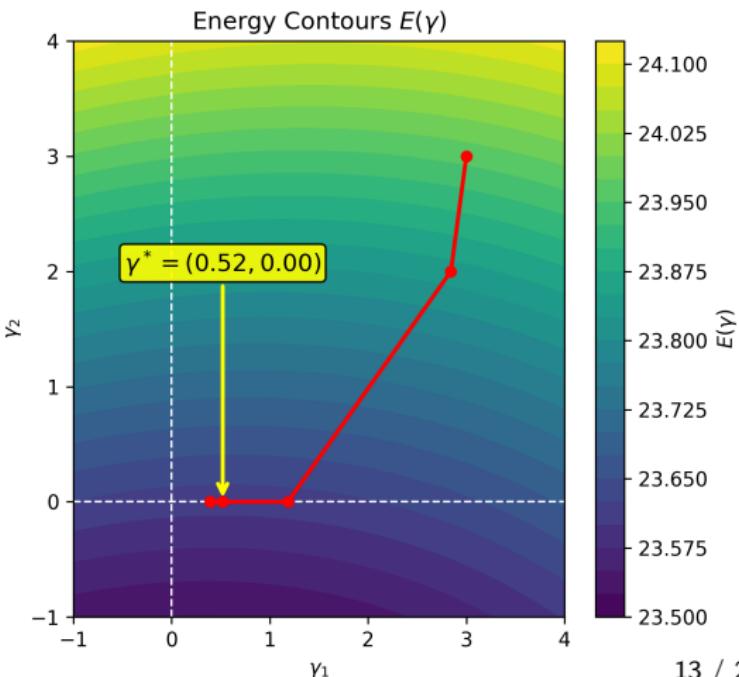
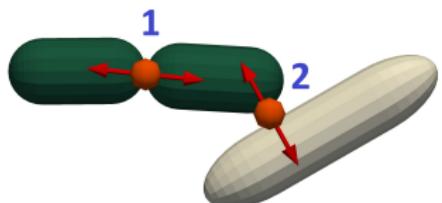
- Find contact forces γ s.t.

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

- Approximate how individual forces γ_i affect Φ^{k+1}
- Solve convex optimization problem:

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

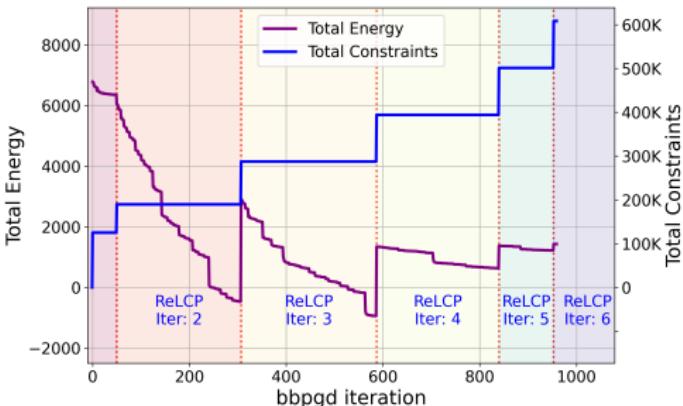
Example: Hard Model



Hard Model: Performance

Characteristics:

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

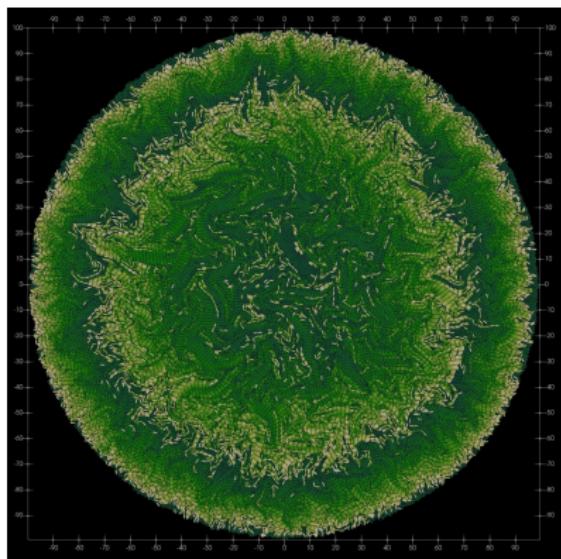


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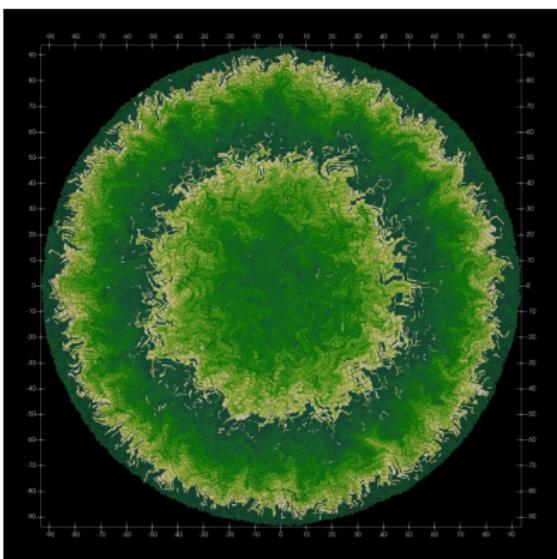
Concentric Ring Formation

Hard Model



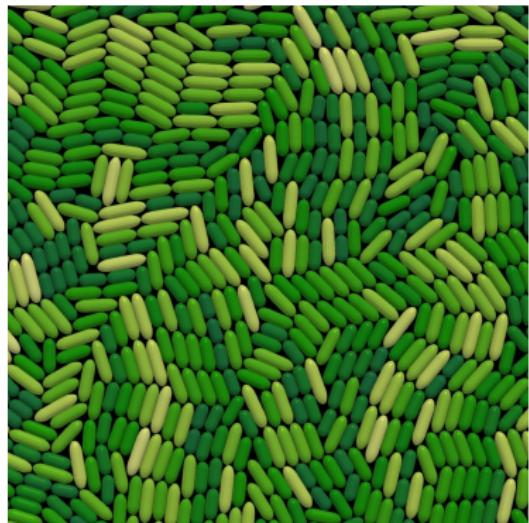
[View video](#)

Soft Model



[View video](#)

Critical Difference: Packing Density

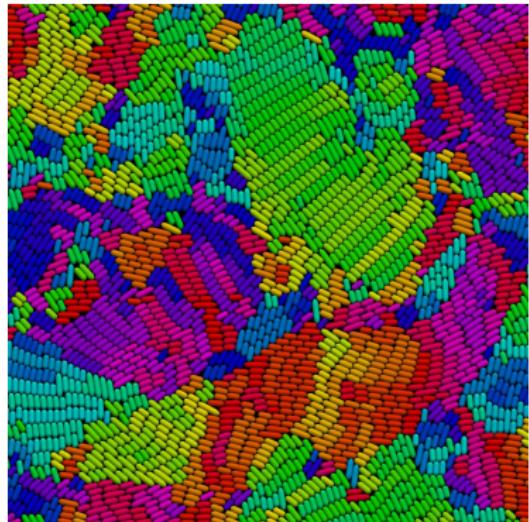


Hard Model

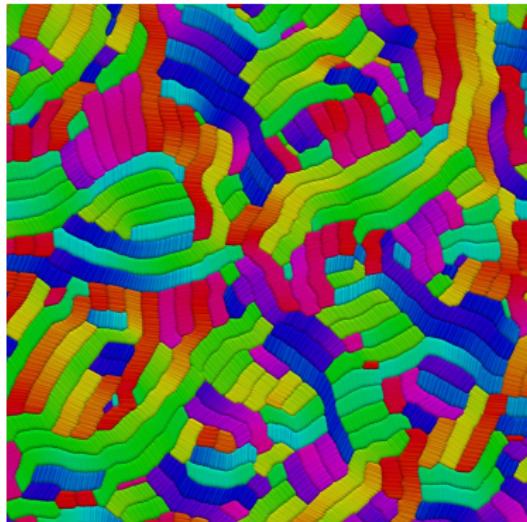


Soft Model

Critical Difference: Microdomain Structure



Hard: realistic patches



Soft: elongated bundles

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CFL Condition

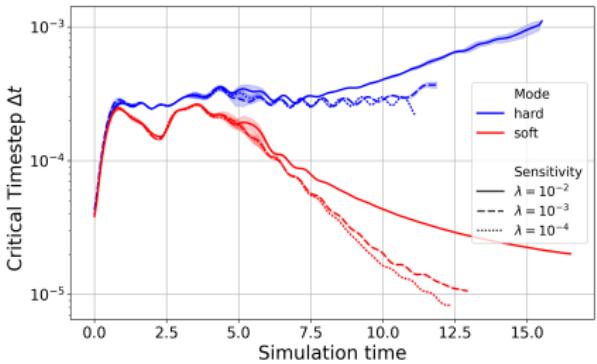
Adaptive timestepping:

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

where u_m = median velocity,
 ε = overlap tolerance

Key observations:

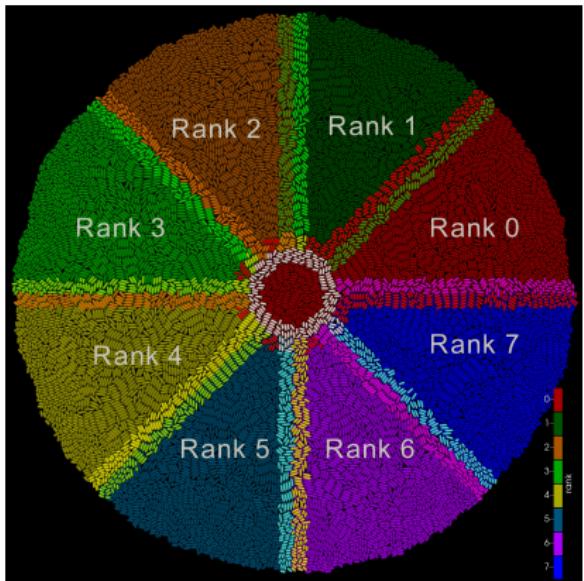
- Hard: stable $\Delta t \sim 3 \cdot 10^{-4}$
- Soft: drops $\Delta t \sim 10^{-5}$
- 30× larger timesteps!



Parallel Architecture

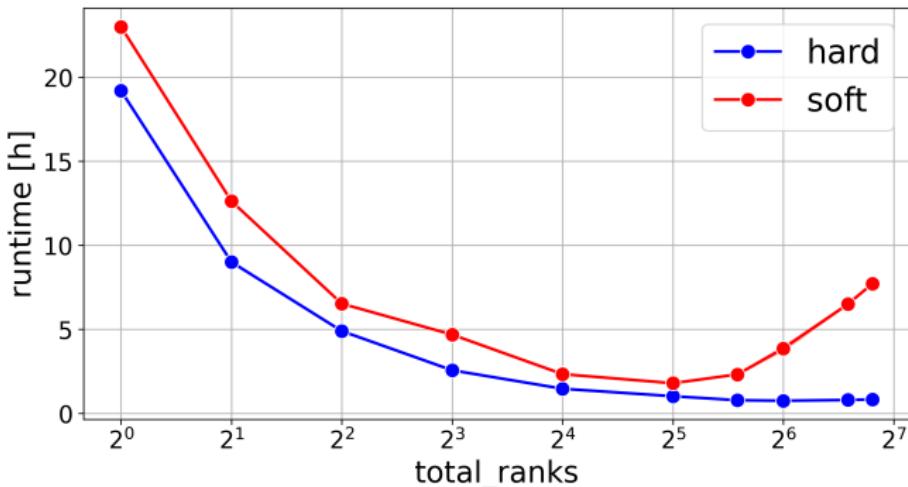
Implementation:

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



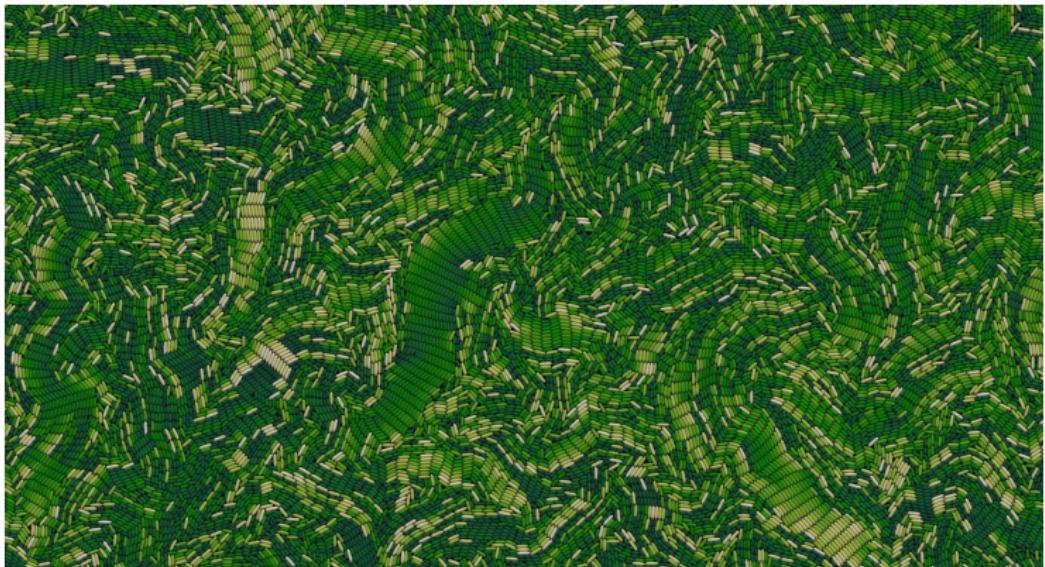
Domain decomposition with 8 MPI ranks

Strong Scaling: Runtime to reach $R = 100$



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

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



[View Full Image](#)

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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

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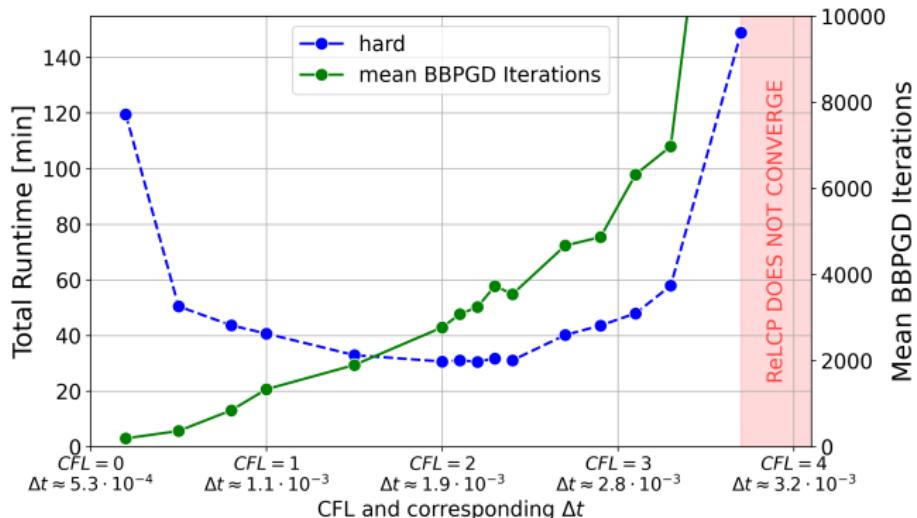
Code: <https://github.com/manuellerchner/MicrobeGrowthSim-IDP>

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

References I

-  Bankole, F. A., Badu-Apraku, B., Salami, A. O., Falade, T. D. O., Bandyopadhyay, R., and Ortega-Beltran, A. (2023). Variation in the morphology and effector profiles of *exserohilum turicum* isolates associated with the northern corn leaf blight of maize in nigeria. *BMC Plant Biology*, 23(1):386.
-  Dell'Arciprete, D., Blow, M. L., Brown, A. T., Farrell, F. D. C., Lintuvuori, J. S., McVey, A. F., Marenduzzo, D., and Poon, W. C. K. (2018). A growing bacterial colony in two dimensions as an active nematic. *Nature Communications*, 9(1):4190.
-  Weady, S., Palmer, B., Lamson, A., Kim, T., Farhadifar, R., and Shelley, M. J. (2024). Mechanics and morphology of proliferating cell collectives with self-inhibiting growth. *Phys. Rev. Lett.*, 133:158402.

Backup: CFL vs. Runtime and Constraints



Backup: BBPGD Iterations vs. Number of Particles

