Position-based Dynamics

for ODEs with inequality constraints

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PDE Afternoon

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WWTF
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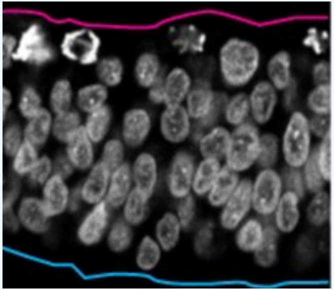
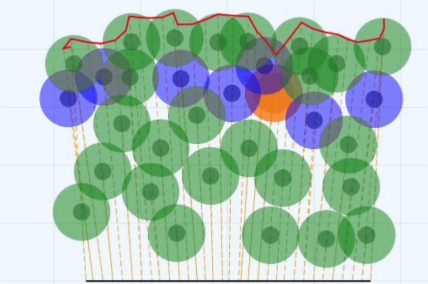
Motivation

Simulation of epithelial cells





What I want to do ☺

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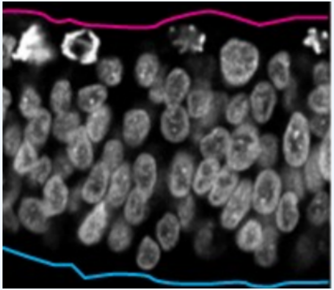

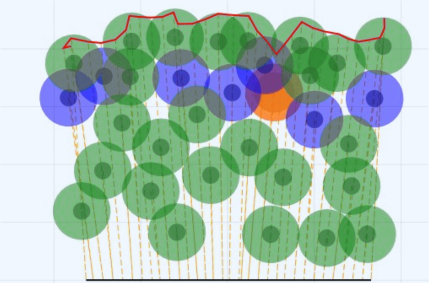

But: There are inequality constraints in the model:

- **non-overlapping constraints** between nuclei cores,
- black line is a **chain of links** with fixed maximal length.

What I have to do ☹

1. Solve an ODE

$$\dot{x} = f(x) + \dots$$

with (many) inequality constraints

$$g_k(x(t)) \geq 0 \quad \text{for all } k.$$

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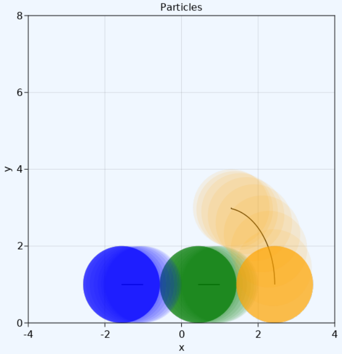
2. Do it fast...



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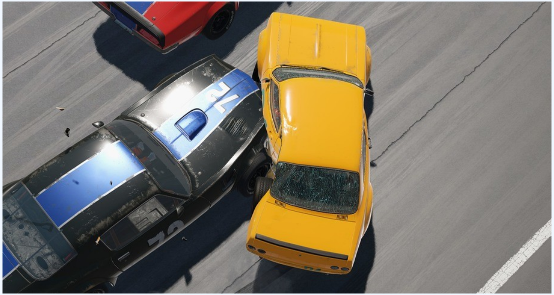

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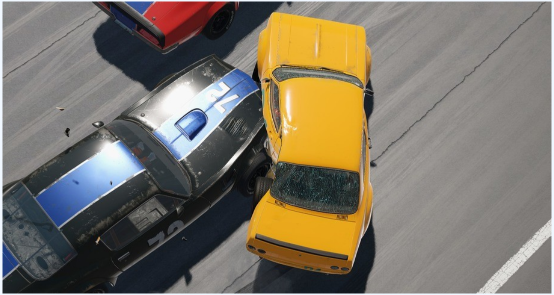
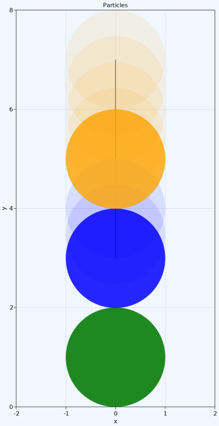


Computer graphics uses **Position-based Dynamics (PBD)**. Let's try that!

Good news: PBD is very stable!

It has not problems to simulate a stack of objects, like this...



...many mathematically more rigorous methods would lead to jittering and a colapsing stack!

Video of PBD

(embedding videos in LaTeX is annoying)

Position-based Dynamics (PBD) **is not a convergent** method.

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The End.

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Goal (work in progress):
Find rigorous mathematical arguments to justify use of Position-based Dynamics (PBD).

Overview of this talk

1. Position-based Dynamics for first order systems,
2. Filippov ODEs and numerical integration,
3. ...attempts to get error bounds.

Position-based Dynamics for first order systems

The toy model: First order hard-sphere model

We consider N particles (in 2D) with radius $R = 1$ and with positions $\boldsymbol{X} = (X_1, \ldots, X_N) \in \mathbb{R}^{2N}$.

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We consider N particles (in 2D) with radius $R = 1$ and with positions $\boldsymbol{X} = (X_1, \ldots, X_N) \in \mathbb{R}^{2N}$. We consider this **complementarity system**

$$\begin{cases} \dot{X}_i = f_i(\boldsymbol{X}) + \sum_{k=1}^{m} \lambda_k \nabla g_k(\boldsymbol{X}) & \text{for all } i = 1, \ldots, N, \\ g_k \geq 0, \quad \lambda_k \geq 0 \quad \text{and} \quad g_k \lambda_k = 0 & \text{for all } k = 1, \ldots, m, \\ X_i(0) = X_i^{\text{init}} & \text{for all } i = 1, \ldots, N \end{cases}$$

where

$$g_k(\boldsymbol{X}) := \|X_i - X_j\| - 2$$

are the $m = \binom{2}{N}$ constraints for non-overlapping spheres. [1]

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Incredients of Position-based Dynamics

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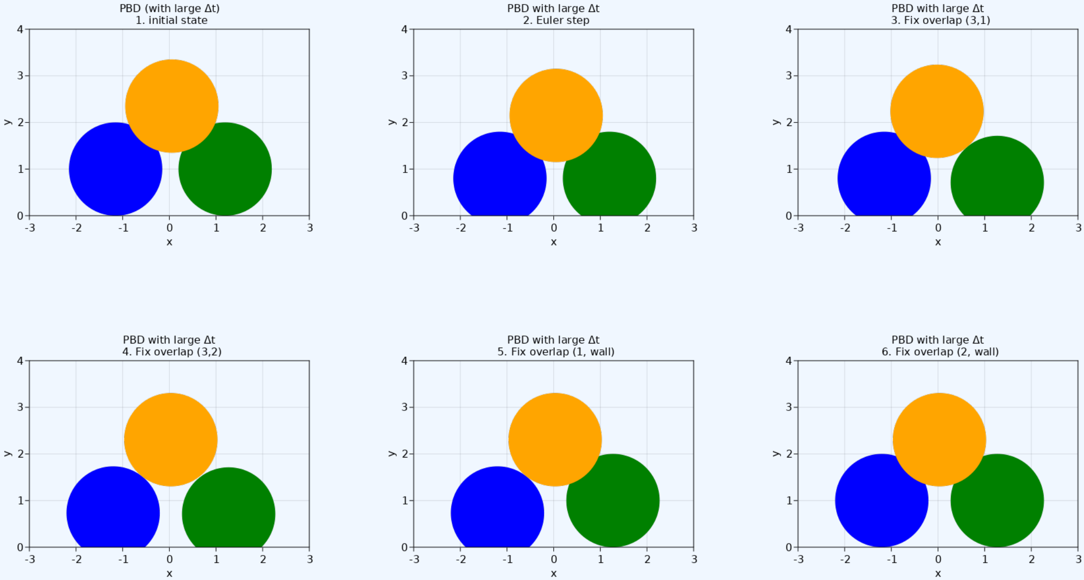
Numerical flow map of PBD

$$\Phi_h^{\text{PBD}}(\boldsymbol{X}) = \text{prox}^{g_m} \circ \cdots \circ \text{prox}^{g_1} \circ \Phi_h^f(\boldsymbol{X})$$

Hence, numerical solution is

$$\boldsymbol{X}^{n+1} = \Phi_h^{\text{PBD}}(\boldsymbol{X}^n)$$


PBD (with large Δt)
1. initial state
PBD with large Δt
2. Euler step
PBD with large Δt
3. Fix overlap (3,1)
PBD with large Δt
4. Fix overlap (3,2)
PBD with large Δt
5. Fix overlap (1, wall)
PBD with large Δt
6. Fix overlap (2, wall)
x
y
-3
-2
-1
0
1
2
3
4

Computational budget

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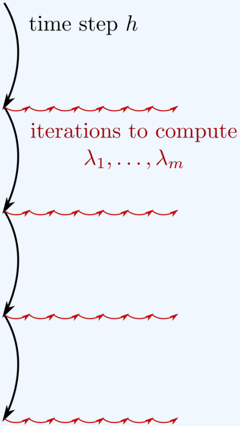
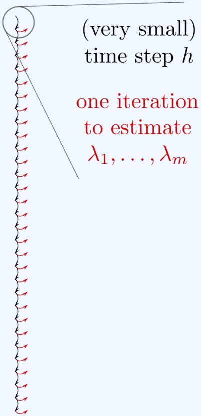
Time-stepping with internal LCP solver



Position-based Dynamics



Filippov ODEs and numerical integration

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$\varphi_t(x) = e^t x$.

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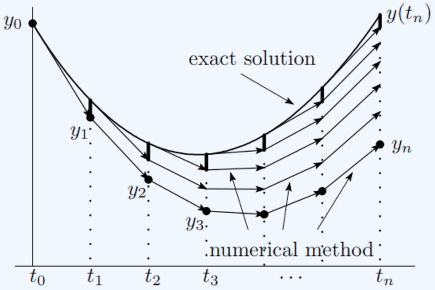

Figure 3: Lady Windermere's fan.

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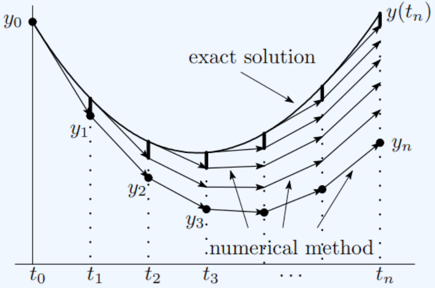

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A typical result is **consistency + stability ⇒ convergence.**

In which sense do exact solutions even exists?

Example:

$$\begin{aligned} \dot{y} &= -1 + \lambda, \\ g(y) &= y \geq 0, \quad \lambda \geq 0, \quad y\lambda = 0. \end{aligned}$$

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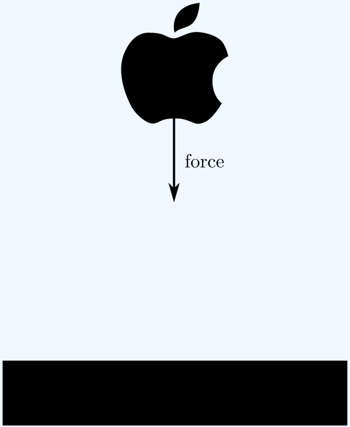

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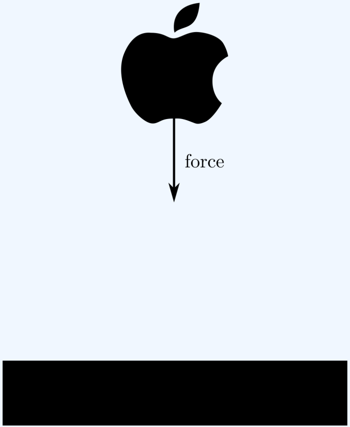
$$\lambda = \begin{cases} 0 & \text{before impact,} \\ 1 & \text{after impact.} \end{cases}$$



On the ground, the complementary condition implies (if $\dot{y}$ exists):

$$\begin{aligned} 0 &= \dot{y}\lambda + y\dot{\lambda} \\ &= (-1 + \lambda)\lambda. \end{aligned}$$

Discontinious right-hand sides

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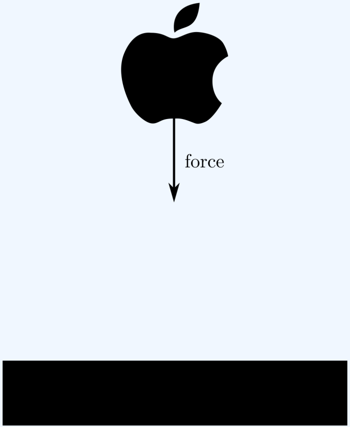

...or as Filippov ODE:

$$\dot{y} \in \begin{cases} \{-1\} & y > 0 \\ [-1, 0] & y = 0 \\ \{0\} & y < 0 \end{cases}$$

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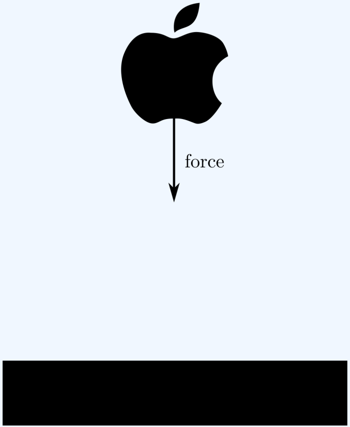

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- Existence theory,
- allows extension of ODE to infeasible positions.

Does numerical integration work for such systems?

Example: Sliding case

$$f^+ := \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad f^- := \begin{pmatrix} 2 \\ 1 \end{pmatrix}$$

$$\dot{x} \in \begin{cases} f^+ & x_2 > 0 \\ \overline{\text{co}}(\{f^+, f^-\}) & x_2 = 0 \\ f^- & x_2 < 0 \end{cases}$$

$\overline{\text{co}}\{\dots\}$ is the closure of the convex hull.

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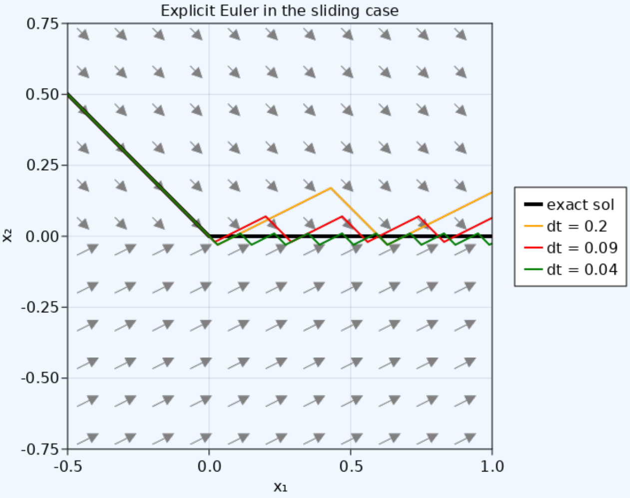
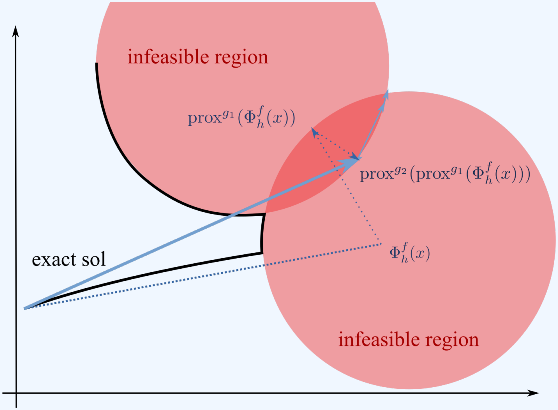
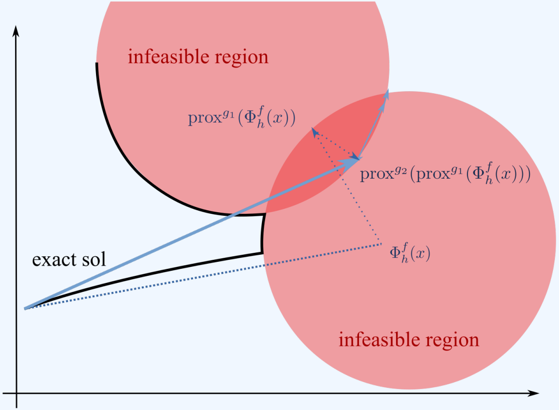


…towards error bounds for PBD

Challenge in the numerical analysis

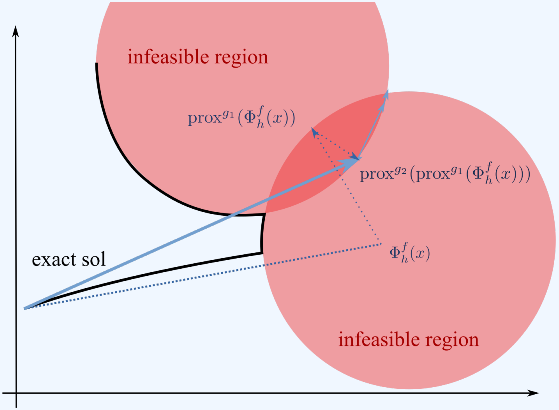


- How fast do we enter the infeasible regions?



- How fast do we enter the infeasible regions?
- What are the chain reactions of

  $P(X) := \text{prox}^{g_m} \circ \cdots \circ \text{prox}^{g_1}(X).$



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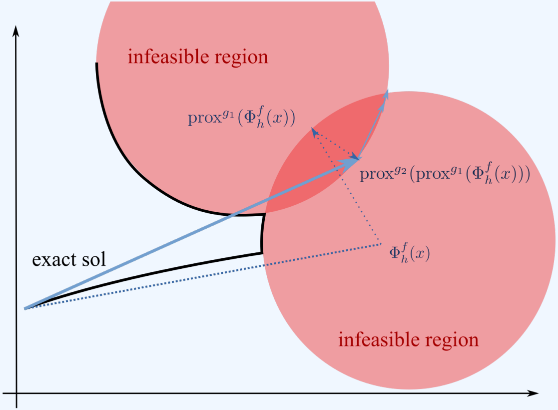
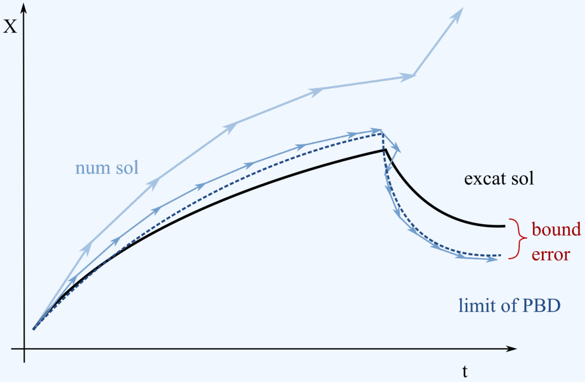
- How likely are bad cases?



- I want to find a global error bound.



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we consider the graph

$$\begin{aligned} G &= (V, E) \quad \text{with} \\ V &= \{1, \dots, N\}, \\ E &= \{(i, j) \mid \text{if } \|X_i - X_j\| < 2R\}. \end{aligned}$$

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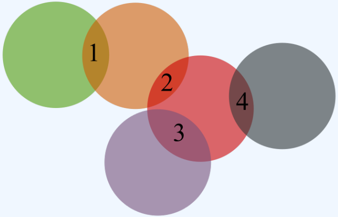
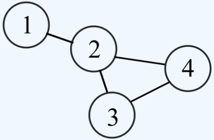
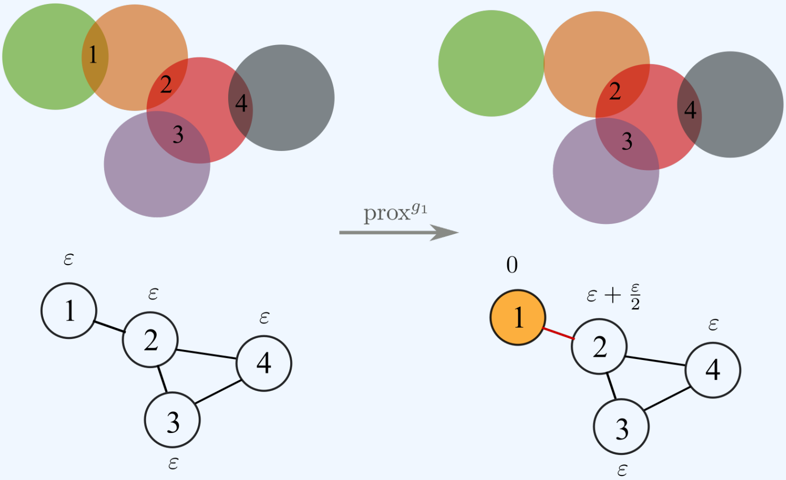
enumerated contacts



dual of unit disc graph



Worst-case violation of constraints



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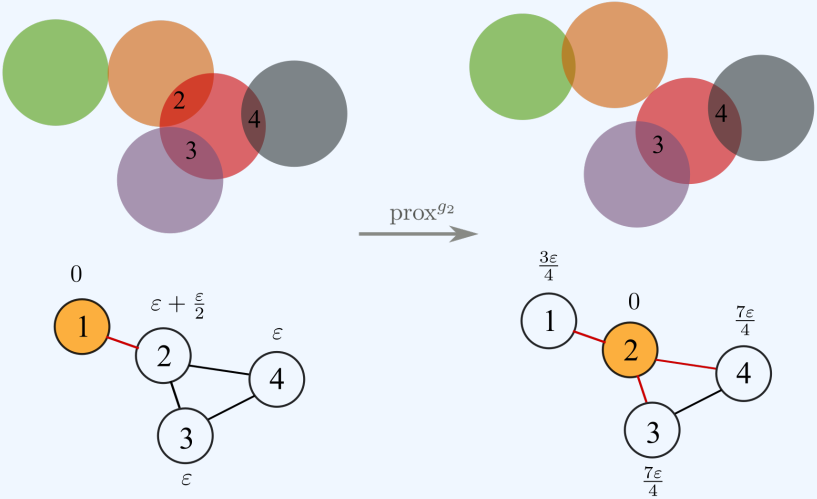

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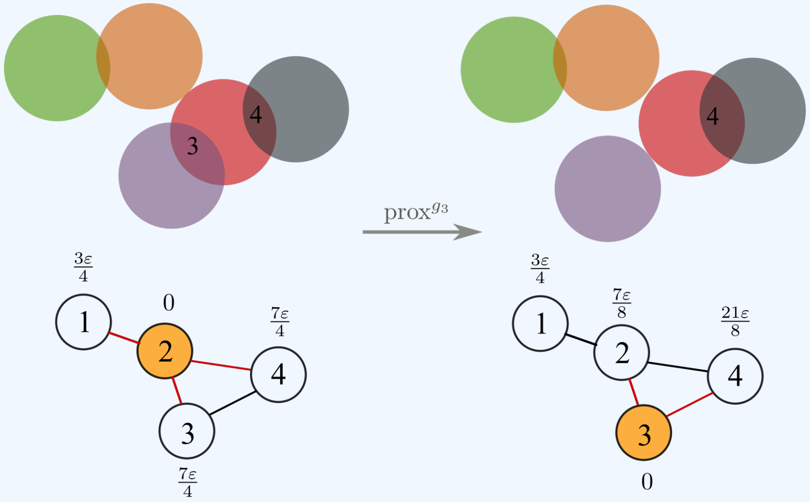

Worst-case bounds

Lemma

Given a state $\boldsymbol{X} \in \mathbb{R}^{2N}$ such that

$$g_k(\boldsymbol{X}) \geq 0 - \varepsilon \quad \text{for all } k$$

then

$$g_k(P(\boldsymbol{X})) \geq 0 - C\varepsilon \quad \text{for all } k$$

where the constant C depends on properties of the unit disk graph.

Lemma

Given a state $\boldsymbol{X} \in \mathbb{R}^{2N}$ such that

$$g_k(\boldsymbol{X}) \geq 0 - \frac{R}{4} \quad \text{for all } k$$

$$\sum_k \max(-g_k(\boldsymbol{X}), 0) \geq C \sum_k \max(-g_k(P(\boldsymbol{X})), 0)$$

where the constant C depends on properties of the unit disk graph.

(But I have no satisfying bound for C yet.)

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- **Proving stability in this sense is possible:**

$$\|\Phi_h(x) - \Phi_h(y)\| \leq (1 + \tilde{C}Lh)\|x - y\|.$$

- **Maybe I can only get this kind of convergence:** For fixed $T > 0$,

$$\|\varphi_{nh}(x) - \Phi_h^n(x)\| \leq \mathbf{C} + Mh \quad \text{for all } n, h \text{ with } nh < T.$$

References I

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Differential Equations with Discontinuous Righthand Sides, volume 18 of *Mathematics and Its Applications*.
Springer Netherlands, Dordrecht, 1988.

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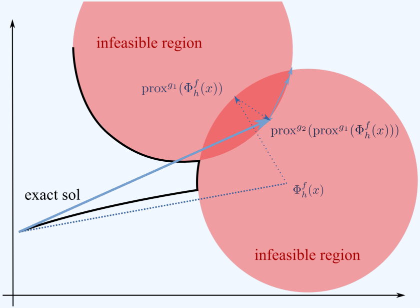
Thank you for your attention!



Alternatives

- **Non-smooth contact dynamics:**
  Solve a nonlinear optimisation problem in each time-step...
- **Smoothening, Repulsive potentials, Penalty method, Discrete Element method, ...**
  Replace non-smooth right-hand side with a smooth approximation or use alternative model.
  $\longrightarrow$ Might be more physical, but also leads to very stiff systems.
- **Implicit methods:**
  Use large time-steps but a nonlinear solve which usually also predicts the collision response.
- **Event time methods:**
  Predict time of collision and compute correct response exactly.

It is very hard to be faster and simpler than PBD, but these methods above are more rigorous and backed by decades of experience.

Discontinious right-hand sides

Example:

$$\dot{y} = -1 + \lambda,$$
$$g(y) = y \geq 0, \quad \lambda \geq 0, \quad y\lambda = 0.$$

Consider a state $y(t^*) = 0$.

Then, the complementary condition implies (if $\dot{y}$ exists):

$$\begin{aligned} 0 &= \dot{y}\lambda + y\dot{\lambda} \\ &= (-1 + \lambda)\lambda. \end{aligned}$$

Hence,

$$\lambda(t^*) = 1.$$