Simulating Granular Material using Nonsmooth Time Stepping and a Matrixfree Interior Point Method

Workshop on the Intersection of Set-Valued Analysis, Plasticity and Friction
December 1-4, 2020

Jan Kleinert

DLR

Background information

- The work presented here was conducted as part of my PhD thesis from 2012 – 2015
  - ***Fraunhofer Institute for Industrial Mathematics ITWM*** in Kaiserslautern
  - Supervisors:
    - Bernd Simeon (***TU Kaiserslautern/Felix Klein Zentrum für Mathematik***)
    - Alessandro Tasora (***Università di Parma***)
  - The thesis won the best Dissertation award out of 17 Fraunhofer ICT institutes in 2016
- Since then, I have moved on to work on other topics.

Fraunhofer ITWM

TECHNISCHE UNIVERSITÄT KAISERSLAUTERN

FELIX KLEIN ZENTRUM FÜR MATHEMATIK

Disclaimer:
⇒ These are old results, from a field that I am still very interested in, but haven't worked on for a while.

Thank you very Oleg Makarenkov for giving me the opportunity to talk at this workshop!

Motivation: Fatique Assessment of earth moving equipement

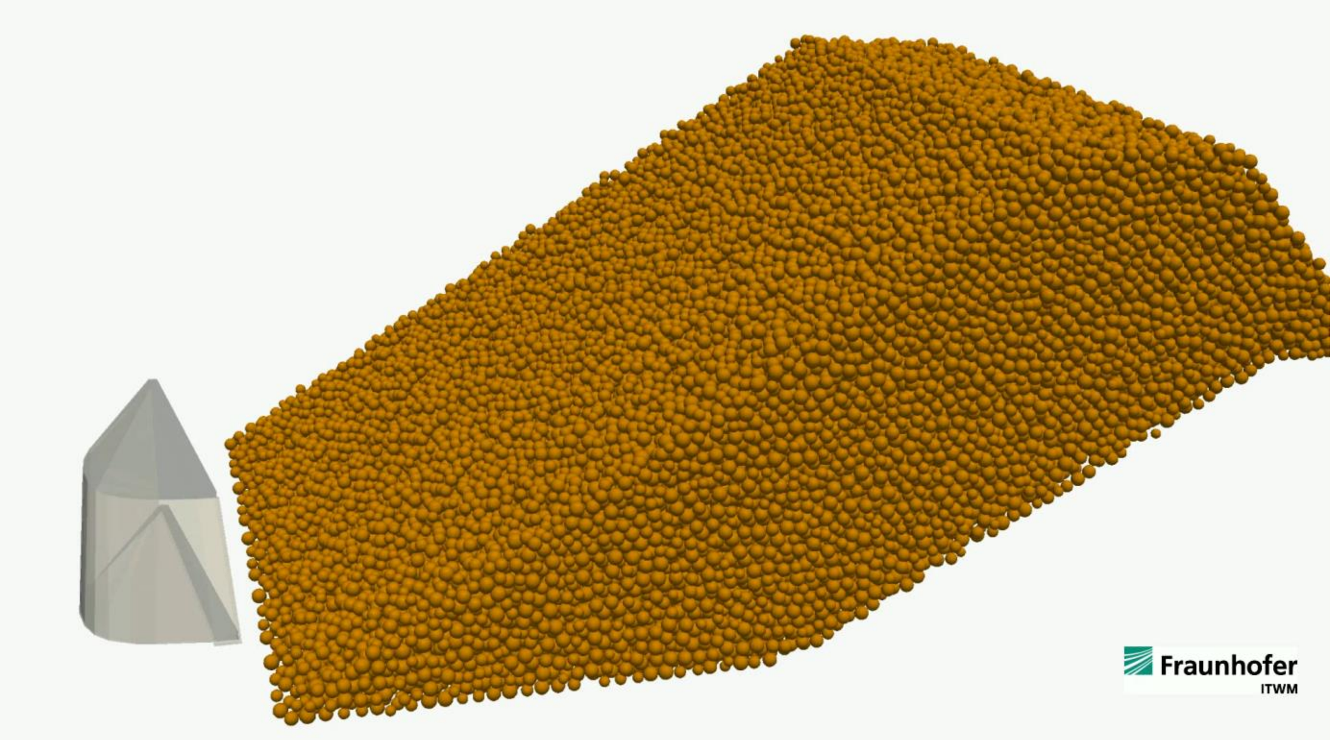
Mechanical loads depend on

1. vehicle
2. driver
3. **soil-tool-interaction**

Motivation: Numerical Model for soil-tool-interaction

Soil model:

Granular material, consisting of a large number of **rigid bodies** subject to **unilateral contact** and **friction**

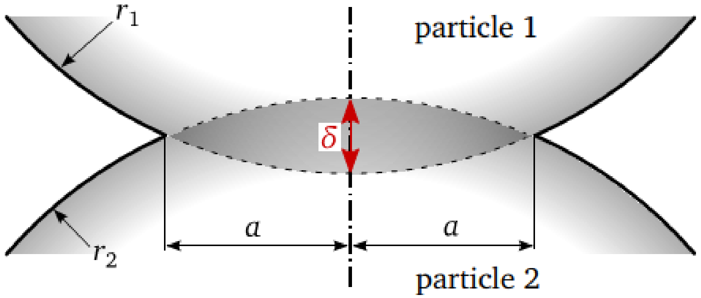


Two paradigms

- **Discrete Element Method** (DEM)
  - *penalty terms*
- **Nonsmooth Contact Dynamics** (NSCD)
  - hard constraints

Discrete Element Method (DEM)

- For every particle: $m\,\ddot{x} = F$
- Particles are allowed to overlap
- Normal contact force **proportional to overlap:**



$$F_N = k_N\delta + d_N\dot{\delta}$$

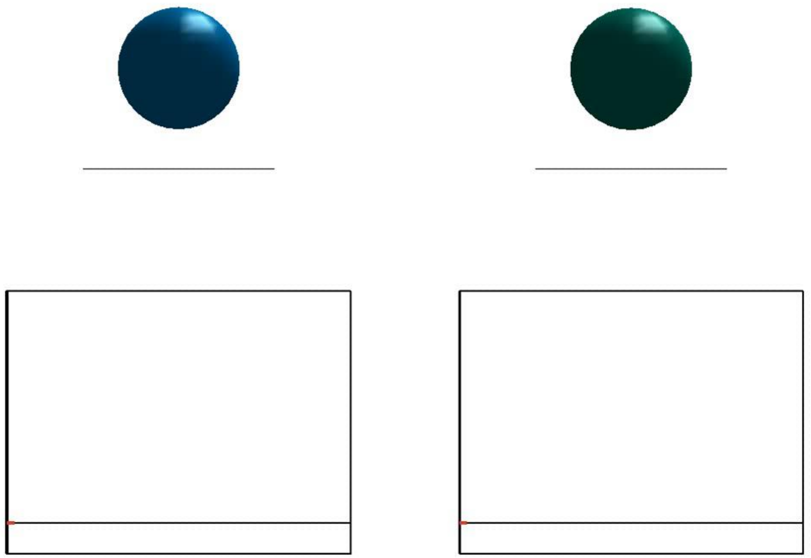
- With proper calibration, DEM is suitable to **reproduce experimental data**

Caveat

- stiffness k_N is typically very large
- DEM is only stable for very small timesteps

Martin Obermayr 2013; Prediction of Load Data for Construction Equipment using the Discrete Element Method

A nonsmooth formulation might help



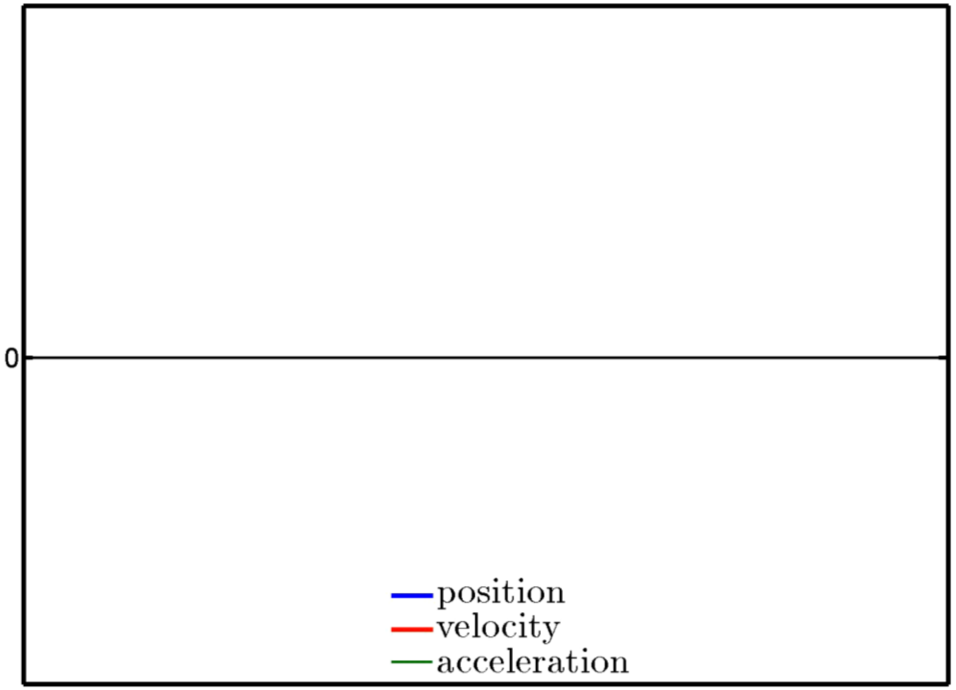
- In DEM small penetrations are used to emulate microscopic deformations of particles
- Simulations run at **uninterestingly small time scales**

Nonsmooth Formulation

From a larger time scale perspective…
- …collisions of rigid bodies seem to be resolved instantaneously
- …trajectories of rigid bodies seem nonsmooth

A nonsmooth timestepping formulation is stable for arbitrary time step sizes

Bouncing Ball: A closer look at the function spaces



- positions q are **absolutely continuous**

$$q(t) = q(0) + \int_0^t v(\tau)d\tau$$

- velocites v are functions of **bounded variation**

$$v(t) = v(0) + \int_0^t dv(t)$$

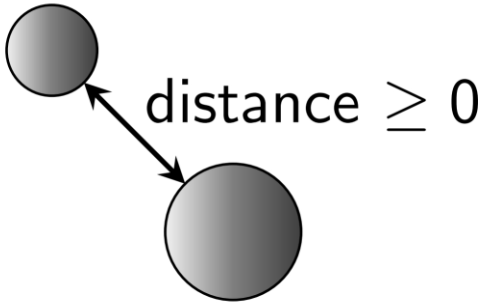
- accelerations dv are **signed Radon measures**

$$\langle dv, \phi \rangle = -\langle v, \dot{\phi} \rangle \quad \textit{for all test functions } \phi$$

Formulation as a constrained dynamical system: Conical inclusions

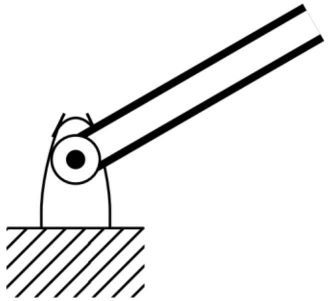
- Inequality constraints on position level:

$$g(q,t) \geq 0 \quad \Leftrightarrow \quad g(q,t) \in K = \mathbb{R}^{+}$$



- Equality constraints on position level:

$$g(q,t) = 0 \quad \Leftrightarrow \quad g(q,t) \in K = \{0\}$$



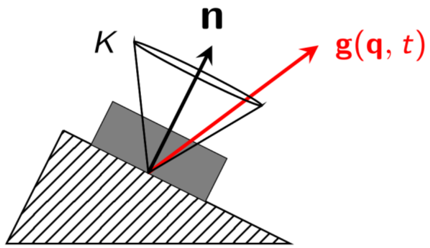
Definition: A subset $K \subset X$ of a vectorspace X is a **convex cone**, iff for all $x, y \in K$ and $\alpha, \beta \geq 0$ it holds

$$\alpha x + \beta y \in K$$

Both $\mathbb{R}^{+}, \{0\}$ are convex cones $\Rightarrow$ ***Let's formulate all constraints as conical inclusions!***

Why?

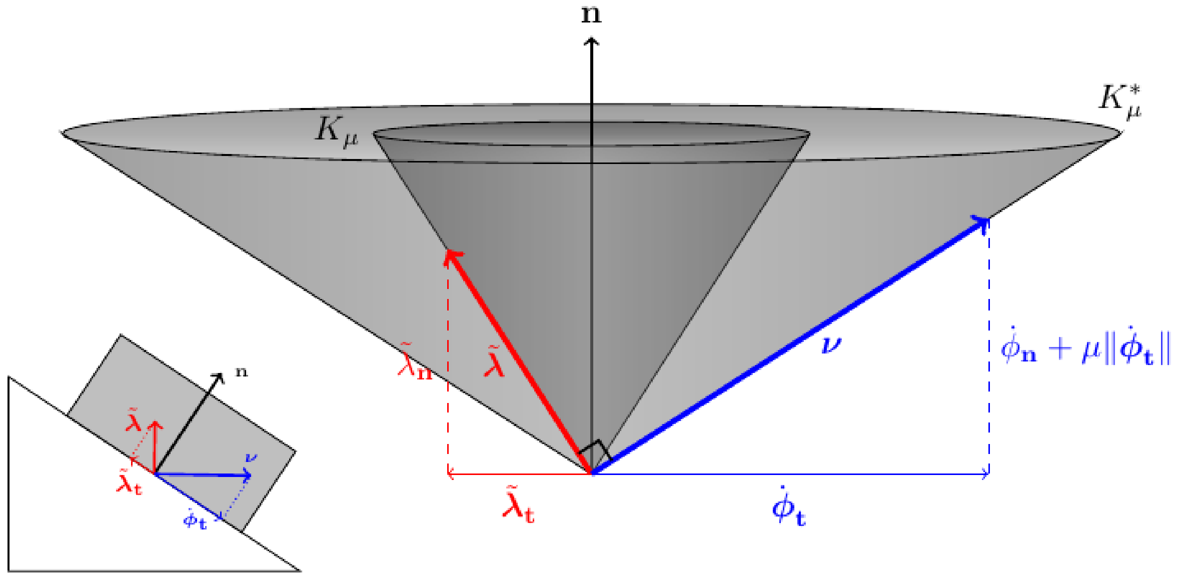
1. Continuous optimization provides **rich theory** on conical constraints, both in a function space settings and for the discretized case
2. We can use the "**dirty friction trick**"



"The dirty friction trick"

Coulomb Friction:

$$\|\tilde{\boldsymbol{\lambda}}_t\| \leq \mu\tilde{\lambda}_n \quad \Leftrightarrow \tilde{\boldsymbol{\lambda}} = \begin{bmatrix} \tilde{\lambda}_n \\ \tilde{\boldsymbol{\lambda}}_t \end{bmatrix} \in K_\mu$$



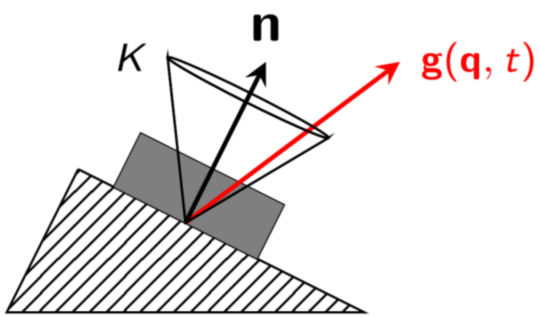
Unilateral contact with Coulomb Friction*(DeSaxcé & Feng)*:

$$K_\mu^* \ni \boldsymbol{\nu} = \begin{bmatrix} \dot{\phi}_n + \mu\|\dot{\boldsymbol{\phi}}_t\| \\ \dot{\boldsymbol{\phi}}_t \end{bmatrix} \perp \tilde{\boldsymbol{\lambda}} = \begin{bmatrix} \tilde{\lambda}_n \\ \tilde{\boldsymbol{\lambda}}_t \end{bmatrix} \in K_\mu$$

$\tilde{\lambda}_n \in \mathbb{R}$	Normal contact force	$\mu \in \mathbb{R}$ Friction coefficient
$\tilde{\boldsymbol{\lambda}}_t \in \mathbb{R}^2$	Tangential contact force	$K_\mu = \left\{ \tilde{\boldsymbol{\lambda}} = \begin{bmatrix} \tilde{\lambda}_n \\ \tilde{\boldsymbol{\lambda}}_t \end{bmatrix} \in \mathbb{R}^3 \middle| \|\tilde{\boldsymbol{\lambda}}_t\| \leq \mu\tilde{\lambda}_n \right\}$ Coulomb friction cone
$\boldsymbol{\phi}_t \in \mathbb{R}^2$	Tangential contact displacement	

- This looks like a complementarity problem associated with a constraint
- *Can we mimic Coulomb friction as a rheonomous conical constraint?*

“The dirty friction trick”



- Can we use $\nu = \begin{bmatrix} \dot{\phi}_n + \mu \|\dot{\boldsymbol{\phi}}_t\| \\ \dot{\boldsymbol{\phi}}_t \end{bmatrix} \in K_\mu^*$ for our mimicking friction constraint?

No:

It translates directly to $\dot{\phi}_n \geq 0$, which is just the unilateral constraint on velocity level

But we can use:

$$g(q,t) = \begin{bmatrix} \phi_n + \mu \int_{t_c}^{t} \|\dot{\boldsymbol{\phi}}_t\| d\tau \\ \boldsymbol{\phi}_t \end{bmatrix} \in K_\mu^*$$

for small time scales $|t - t_c| < \epsilon$ and if $\boldsymbol{\phi}(t_c) = 0$.

It can be shown that

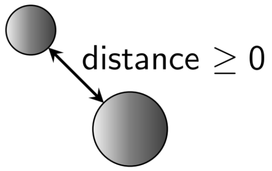
- The introduced error is of order $O(|t - t_c|^2)$, which is lower than order of commonly used numerical integrators
- The error dissappears if the constraint is linearized within one time step

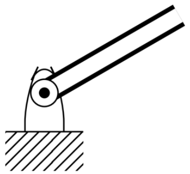
What have we gained by this?

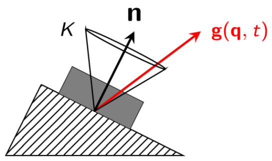
- We can derive the equations of motion using functional analysis and classical mechanics, without having to worry about the devilish intricacies of Coulomb friction

Putting it all together: A nonsmooth version of Hamilton's Principle

- Feasable set of trajectories: $M = \{\ q \text{ abs. cont.} \mid \ \ g(q,t) \in K\ \}$







- Hamilton's principle as a variational inequality *(Leine, Aeberhard, Glocker 2009)*:

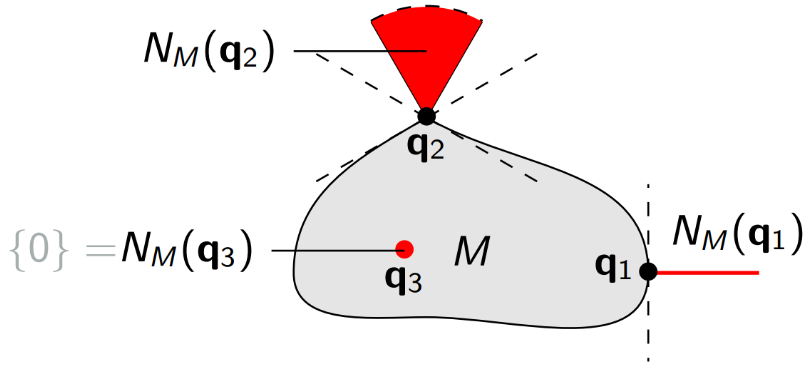
$$\delta \int_0^T L(q,v)dt \in N_M(q)$$

Normal cone of M at q

Notes:

- The normal cone $N_M(q)$ of M at q is a **subset of the dual space of absolutely continuous functions**
- The dual space of absolutely continuous functions can be identified with the **set of signed Radon measures**, and a linear functional from the dual space can be written as

$$\langle \lambda, \phi \rangle = \int_0^T \phi \, d\lambda$$



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Characterization using Lagrange multipliers

$$\delta \int_0^T L(q,v)dt \in N_M(q)$$

$$M = \{\ q \text{ abs. cont.} \mid \ g(q,t) \in K\ \}$$

Theorem: Existence of Lagrange Multipliers *(modified from Kurcyusz 1976)*

Let X, Y be Banach spaces and $\emptyset \neq K \subset Y$ be a closed convex cone. Let $g: X \to Y$ be continuously Fréchet-diff'ble with Fréchet-derivative δg_q at q. Let $q \in M = \{x \mid g(x) \in K\} \subset X$ and $im\ \delta g_q - \text{span}\{g(q)\} \in K$.

Then there exists a $\lambda \in K^*$ for every $f \in N_M(q)$ such that

$$\delta \int_0^T L(q,v)\,dt = f(\delta q) = -\left\langle \lambda, \frac{\partial g}{\partial q}\delta q \right\rangle \quad \forall \delta q \text{ in } X$$

$$\langle \lambda, g(q) \rangle = 0$$

constraint qualification

$$\langle \lambda, \phi \rangle = \int \phi \, d\lambda$$

Characterization using Lagrange multipliers

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$$\int \delta q \left(\frac{\partial L}{\partial q}\right) dt - \int \delta q\, d\left(\frac{\partial L}{\partial v}\right) = \delta \int_0^T L(q,v)dt = -\int_0^T \frac{\partial g}{\partial q} \delta q d\lambda \quad \forall \delta q \ in\ X$$

$$\int_0^T g(q)\, d\lambda = 0$$

DLR

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Then there exists a $\lambda \in K^*$ for every $f \in N_M(q)$ such that

$$\int_0^T \delta q d\left(\frac{\partial L}{\partial v}\right) = \int_0^T \delta q \frac{\partial L}{\partial q} dt + \int_0^T \frac{\partial g}{\partial q} \delta q d\lambda \quad \forall \delta q \text{ in } X$$

$$\int_0^T g(q)\, d\lambda = 0$$

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force

$$d\left(\frac{\partial L}{\partial v}\right) = \frac{\partial L}{\partial q}dt + \frac{\partial g}{\partial q}d\lambda$$

momentum

$$K \ni g(q) \perp d\lambda \in K^*$$

Characterization using Lagrange multipliers

$$\delta \int_0^T L(q,v)dt \in N_M(q)$$

$$M = \{\ q \text{ abs. cont.} \mid \ g(q,t) \in K\ \}$$

Theorem: Equations of motion

$$M dv = f dt + \frac{\partial g}{\partial q} d\lambda$$

Measure differential equation (MDE)

$$K \ni g(q) \perp d\lambda \in K^*$$

Cone Complementarity Problem (CCP)

Time-Discretization: A Petrov-Galerkin Approach

Idea: Satisfy

$$\int_0^T \phi M\, dv = \int_0^T \phi f\, dt + \int_0^T \phi \frac{\partial g}{\partial q} d\lambda \qquad \forall\, abs.cont.\phi$$

$$K \ni g(q,t) \perp d\lambda \in K^*$$

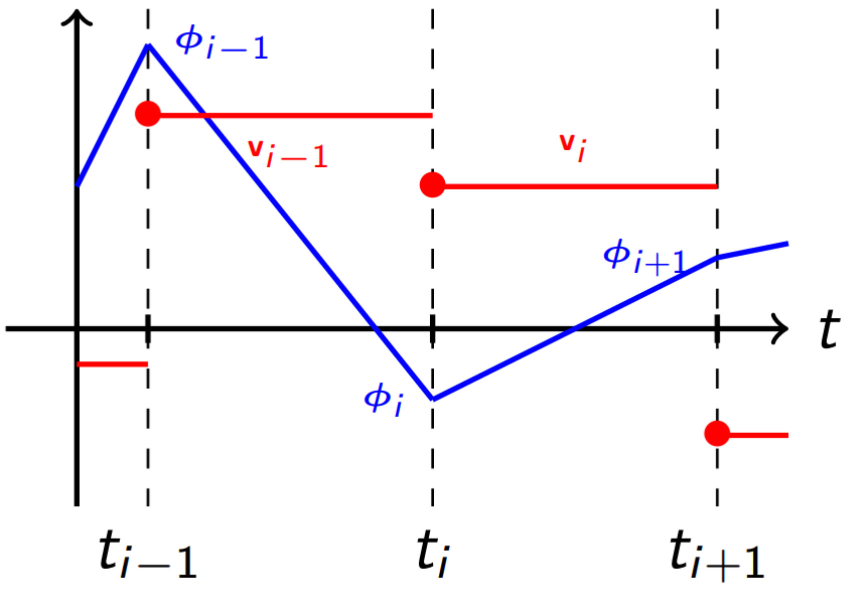
in **finite dimensional subspaces**

- q, ϕ continuous and piecewise linear

  Basis: e.g. hat functions

- v, λ piecewise constant

  Basis: e.g. $f_i(t) = \begin{cases} 1, & if\ t \in [t_i, t_{i+1}) \\ 0, & else \end{cases}$



Equations of Motion in discretized time

The Nonsmooth SHAKE stepper

$$\boldsymbol{q}_{i+1} = \boldsymbol{q}_i + \boldsymbol{v}_{i+1}\Delta t$$

$$\boldsymbol{v}_{i+1} = \boldsymbol{v}_i + M^{-1}\left(\boldsymbol{f}_i\Delta t + \frac{\partial g(q_i)}{\partial q}\boldsymbol{\gamma}_{i+1}\right)$$

$$K \ni \boldsymbol{u}_{i+1} = N_i\boldsymbol{\gamma}_{i+1} + \boldsymbol{r}_i \quad \perp \quad \boldsymbol{\gamma}_{i+1} \in K^*$$

- Constraint has been linearized: Reappears as “stabilized velocity constraint”
- N_i is symmetric, positive **semi**-definite *(in all interesting cases rank-deficient)*
- $\gamma_{i+1} = \int_{t_i}^{t_{i+1}} d\boldsymbol{\lambda}$ appears as new unknown. Can be associated with a net ***impulse***

- We have to solve one **Cone Complementarity Problem (CCP)** per time step.
- But how?

Numerical Methods for CCPs

Cone Complementarity Problem CCP

$$K \ni \boldsymbol{u} = N\boldsymbol{\gamma} + \boldsymbol{r} \quad \perp \quad \boldsymbol{\gamma} \in K^*$$

- Several numerical methods to solve CCPs existed at the time
  - Lemke's pivoting strategy (for LCPs – requires faceting of Friction Cone)
  - IPMs for LCPs
  - Quasi-Newton methods, smoothing Newton methods
  - **Projected Gauß-Jacobi (PGJ)**, Gauß-Seidel (PGS), Successive Overrelaxation (PSOR), Augmented Lagrangian
  - …

- PGJ was dominant in the literature for granular simulations
  - Works for large systems
  - Can be implemented in a matrixfree fashion
  - Can be parallelized
  - Very simple recursion:

Projected Gauß-Jacobi (PGJ)

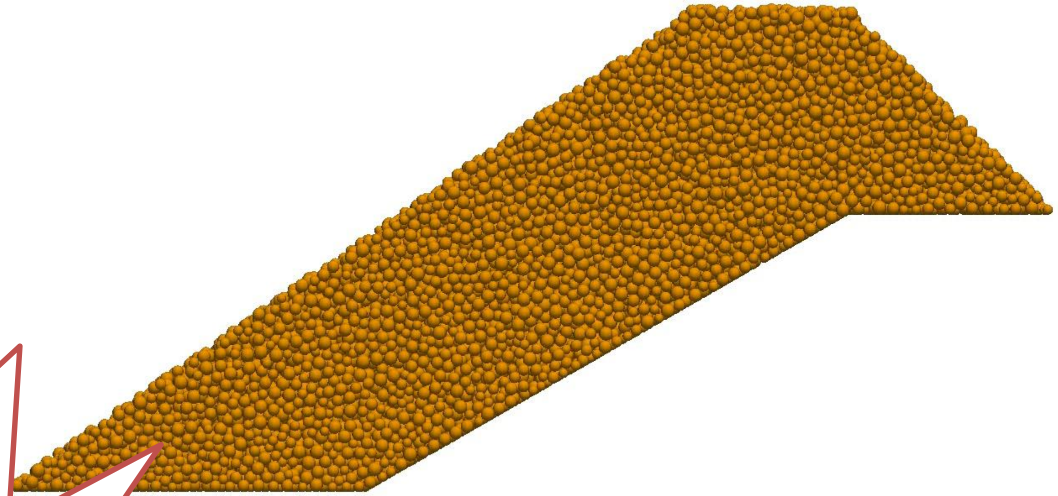
$$\boldsymbol{\gamma}^{(r+1)} = \Pi_{K^*}(\boldsymbol{\gamma}^{(r)} - \omega D^{-1}(N\boldsymbol{\gamma}^{(r)} + \boldsymbol{r}))$$

Projection onto K^*

relaxation factor

Inverse of diagonal part of N

Drawbacks of PGJ



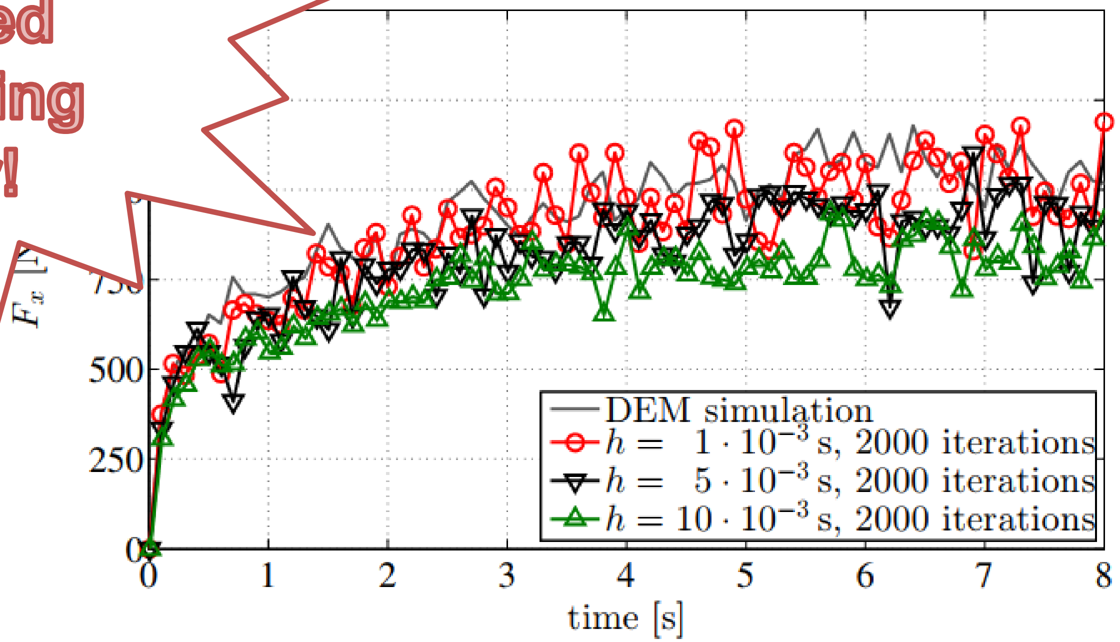
PGJ converges slowly for

- large densely coupled systems
- large mass ratios

As a result, **when stopping the iteration prematurely**:

- draft forces are far from the expected r

We need something faster!



Interior Point Method (Outline)

Frictional contacts ⇒ Solve CCP

$$K_\mu^* \ni \boldsymbol{u}_i = (\bar{N}\boldsymbol{\gamma}_i + \bar{\boldsymbol{r}})_i, \qquad \boldsymbol{\gamma}_i \in K_\mu, \qquad \boldsymbol{u}_i^T \boldsymbol{\gamma}_i = 0$$

for every contact i

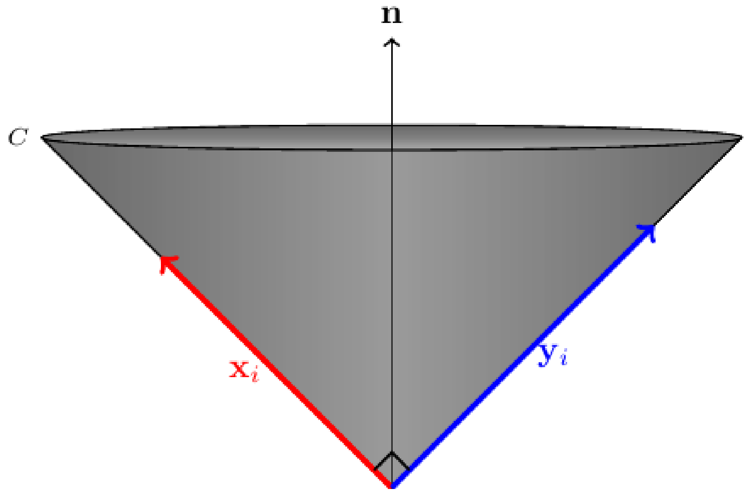
- Linear transform to **symmetric cone** $C = C^*$

C is the **cone of squares**

$$C := \{\, \boldsymbol{x} \circ \boldsymbol{x} \mid \boldsymbol{x} \in \mathbb{R}^3 \,\}$$

with respect to the **Jordan Product**

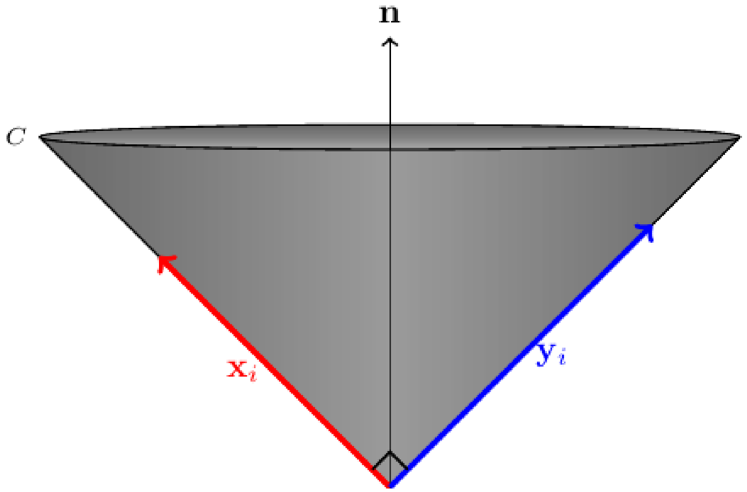
$$\boldsymbol{x} \circ \boldsymbol{y} = \begin{bmatrix} \boldsymbol{x}^T \boldsymbol{y} \\ x_n \boldsymbol{y}_t + y_n \boldsymbol{x}_t \end{bmatrix} \in \mathbb{R} \times \mathbb{R}^2$$



$$C \ni \boldsymbol{y}_i = (N\boldsymbol{x}_i + \boldsymbol{r})_i, \qquad \boldsymbol{x}_i \in C, \qquad \boldsymbol{y}_i^T \boldsymbol{x}_i = 0$$

$$x = \begin{bmatrix} x_n \\ x_t \end{bmatrix}, y = \begin{bmatrix} y_n \\ y_t \end{bmatrix} \in \mathbb{R} \times \mathbb{R}^2$$

Interior Point Method (Outline)

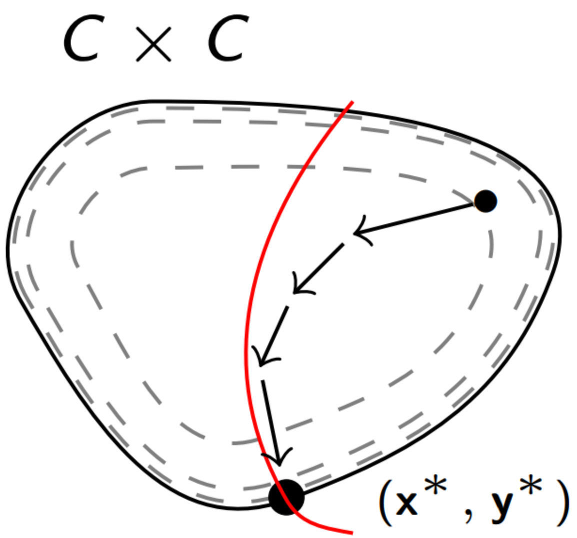


- CCP ⇒ Constrained Optimization Problem:

$$\min \sum_i \boldsymbol{x}_i^T \boldsymbol{y}_i \quad \text{such that} \quad \boldsymbol{x}_i, \boldsymbol{y}_i \in C, \quad \boldsymbol{y} = N\boldsymbol{x} + \boldsymbol{r}$$

- Introduce **logarithmic potential** $P(\boldsymbol{x}_i, \boldsymbol{y}_i)$, pushing $\boldsymbol{x}_i, \boldsymbol{y}_i$ away from boundary of C

$$\min \sum_i \boldsymbol{x}_i^T \boldsymbol{y}_i + P(\boldsymbol{x}_i, \boldsymbol{y}_i) \quad \text{such that} \quad \boldsymbol{x}_i, \boldsymbol{y}_i \in C \backslash \partial C, \quad \boldsymbol{y} = N\boldsymbol{x} + \boldsymbol{r}$$



- **Central Path**: Zero set of P is a smooth curve through the solution

$$S_{cen} = \{ (\boldsymbol{x}, \boldsymbol{y}) \in C \times C \mid \boldsymbol{x} \circ \boldsymbol{y} = \alpha \boldsymbol{e}, \ \alpha \geq 0 \}$$

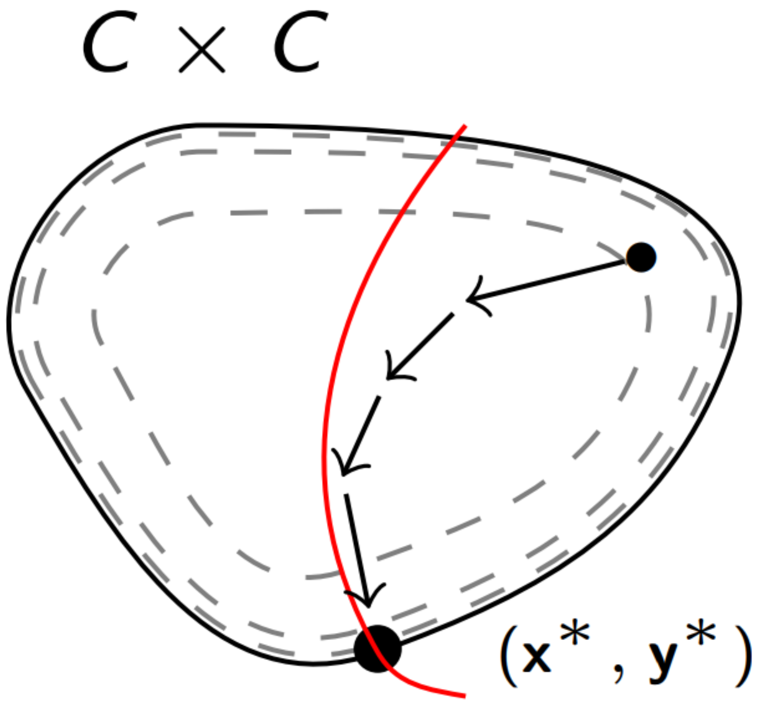
with solution at $\boldsymbol{x} \circ \boldsymbol{y} = \boldsymbol{0}$

IPM = Sequence of Newton steps towards

$$\boldsymbol{x}^{(k)} \circ \boldsymbol{y}^{(k)} - \alpha^{(k)} \boldsymbol{e}, \qquad \boldsymbol{y}^{(k)} = N\boldsymbol{x}^{(k)} + \boldsymbol{r}$$

with $\alpha^{(k)} \to 0$

Interior Point Method: The algorithm



Let $(\boldsymbol{x}^{(k)}, \boldsymbol{y}^{(k)})$ be an interior point (i.e. $\boldsymbol{x}_i^{(\boldsymbol{k})}, \boldsymbol{y}_i^{(k)} \in C \backslash \partial C$).

Until converged do:

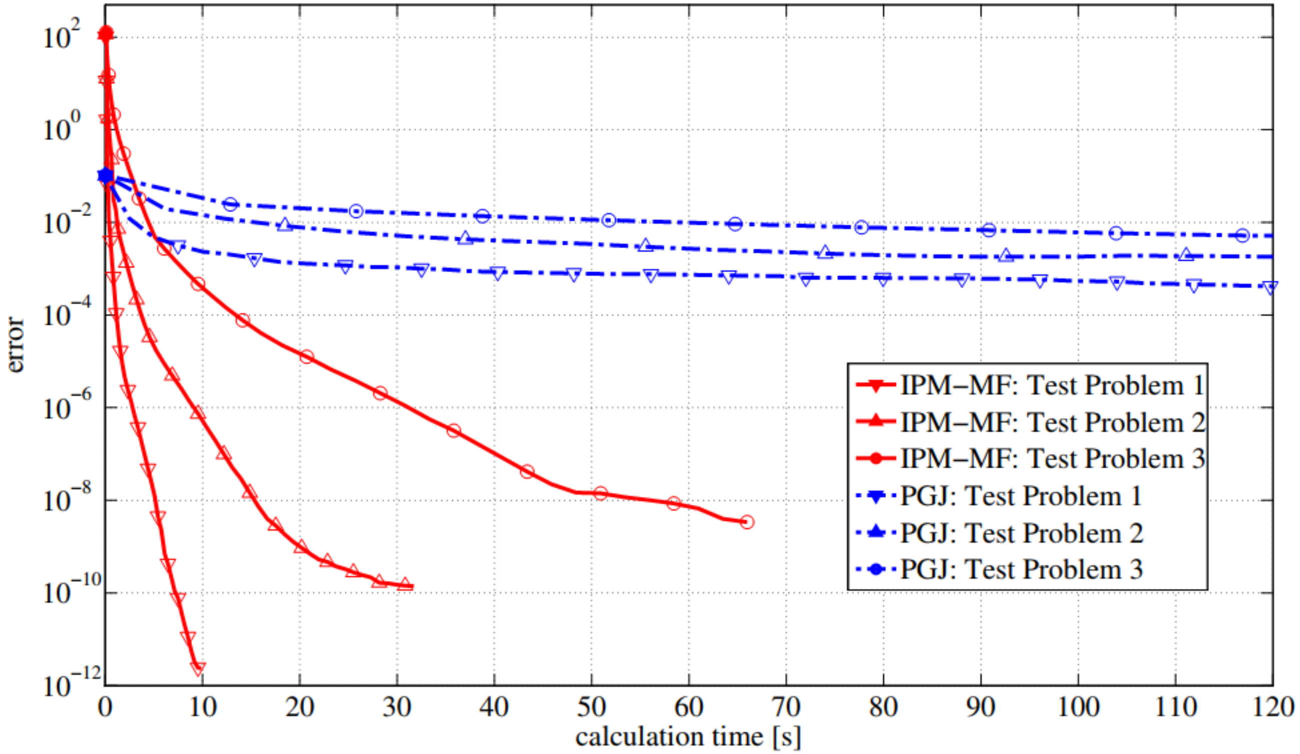
- Choose α
- Calculate **block-diagonal** W_k from $\boldsymbol{x}^{(k)}$and $\boldsymbol{y}^{(k)}$.
- Calculate **right-hand side** $\boldsymbol{b}_k(\alpha)$ from $\boldsymbol{x}^{(k)}$and $\boldsymbol{y}^{(k)}$ and α.
- Perform Newton step to obtain $\left(d\boldsymbol{x}^{(\boldsymbol{k})}, d\boldsymbol{y}^{(k)}\right)$

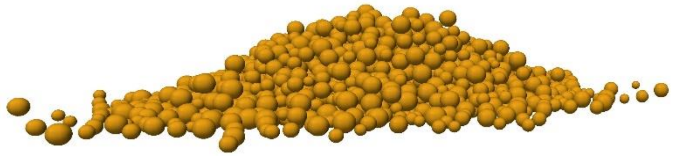
$$\begin{aligned} (W_k + N) d\boldsymbol{x}^{(\boldsymbol{k})} &= \boldsymbol{b}_k(\alpha) \\ d\boldsymbol{y}^{(\boldsymbol{k})} &= N d\boldsymbol{x}^{(\boldsymbol{k})} \end{aligned}$$

use matrixfree Conjugate Gradient (CG) here

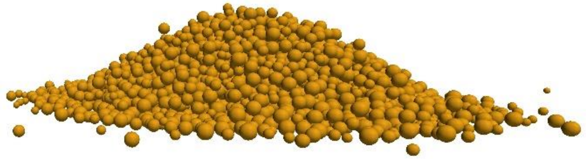
- Calculate step length θ
- $\left(\boldsymbol{x}^{(k+1)}, \boldsymbol{y}^{(k+1)}\right) = \left(\boldsymbol{x}^{(k)}, \boldsymbol{y}^{(k)}\right) + \theta\left(d\boldsymbol{x}^{(\boldsymbol{k})}, d\boldsymbol{y}^{(\boldsymbol{k})}\right)$
- $k \leftarrow k + 1$

PGJ vs IPM

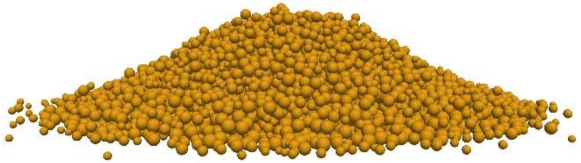




Test Problem 1: 2048 particles

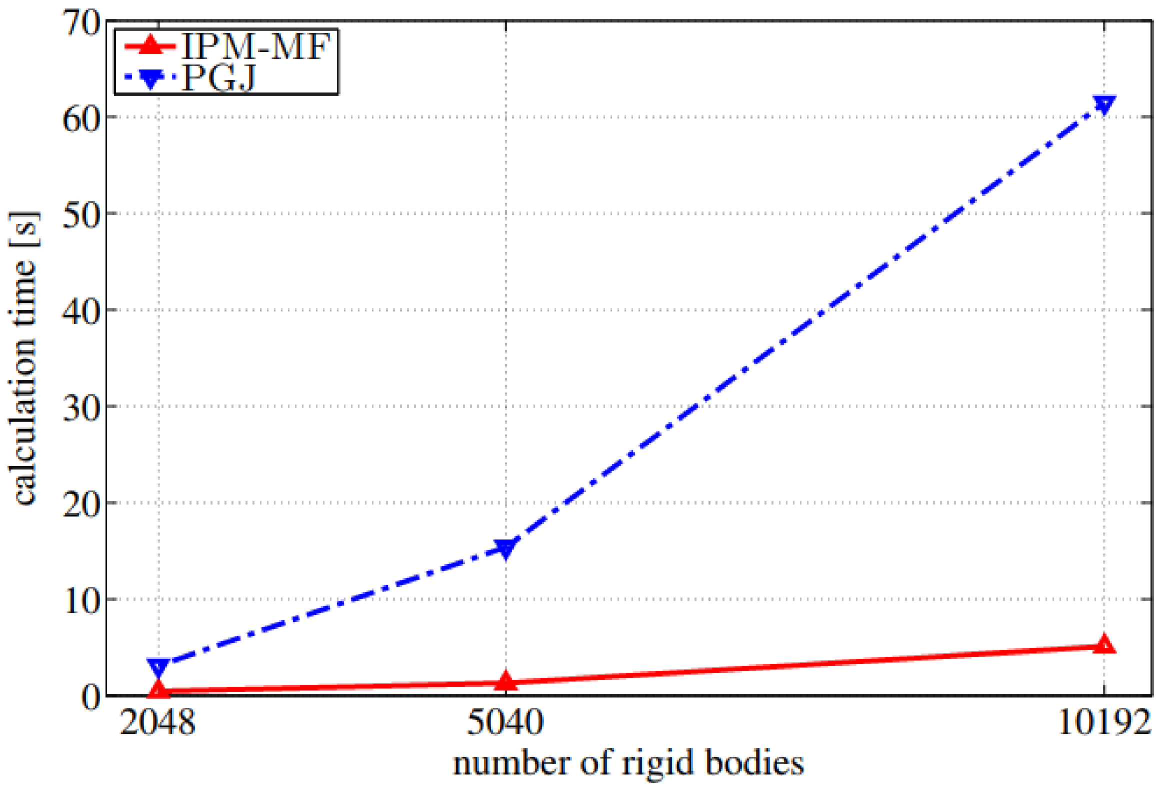


Test Problem 2: 5040 particles



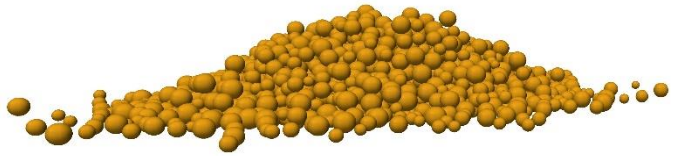
Test Problem 3: 10192 particles

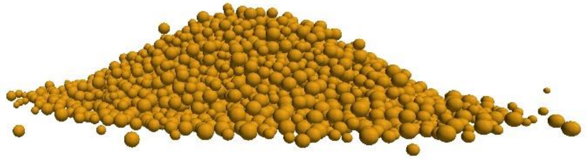
Calculation time for a given tolerance

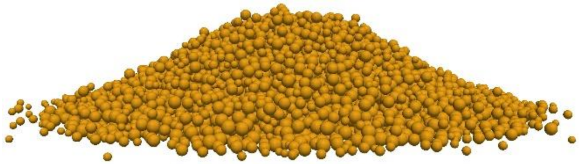


$$tol = 1 \cdot 10^{-2}$$

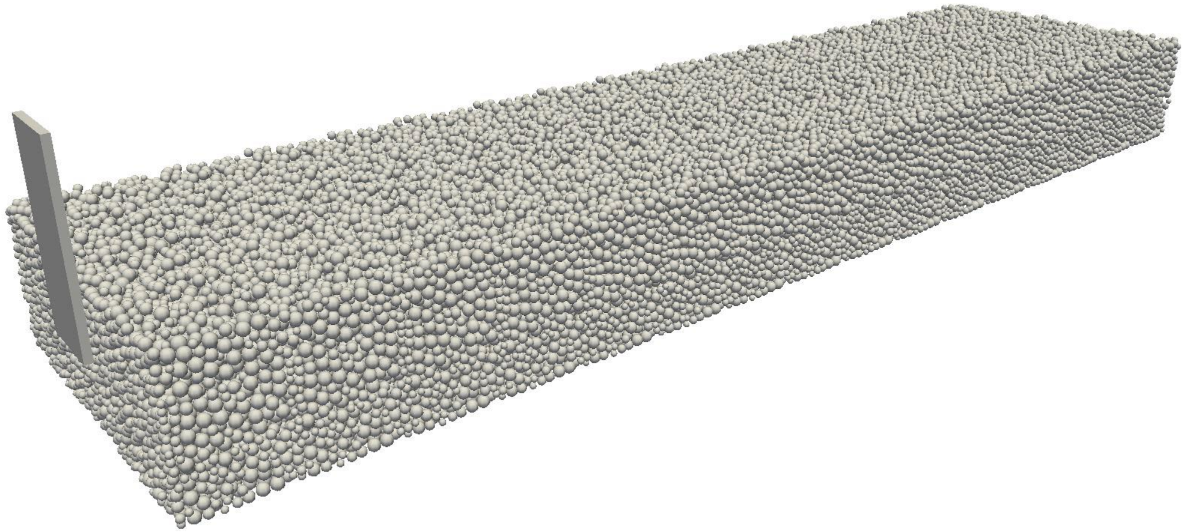
- For $tol = 5 \cdot 10^{-4}$ IPM is **200 times faster** than PGJ

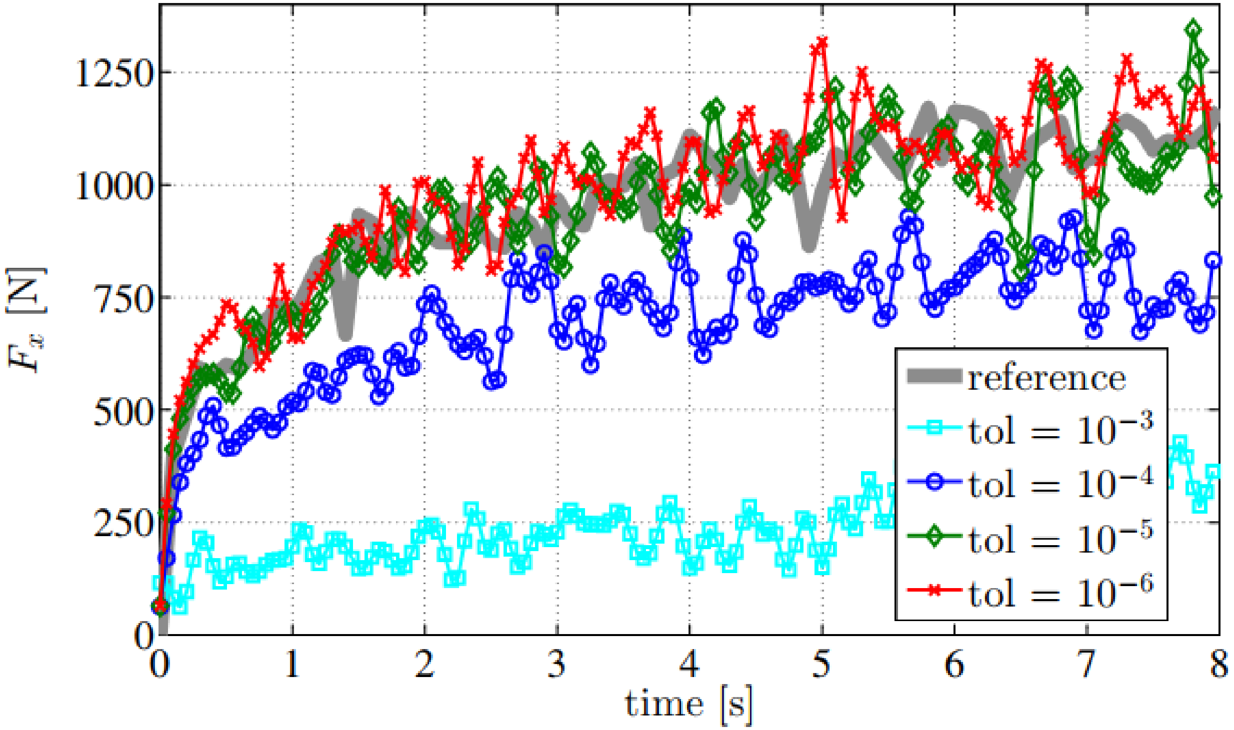

Test Problem 1: 2048 particles


Test Problem 2: 5040 particles


Test Problem 3: 10192 particles

IPM applied to an industrial size problem



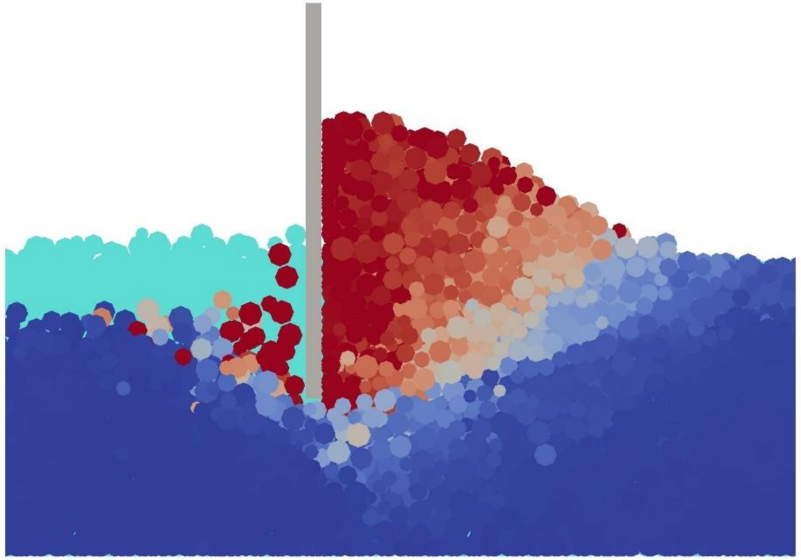


- 105,144 particles
- Ø 1,261,972 unknowns/step
- $\Delta t = 10^{-2}\ s$

At high accuracy requirements *(determination of draft forces)*:

- DEM is still about 12,2% faster
- IPM is more than 10 time faster than PGJ

Summary and Conclusion



Discrete Element Method

- Well suited for the prediction of draft forces, validated against experiment
- Only stable for small time steps ⇒ Computationally expensive

Nonsmooth Contact Dynamics

- Stable for arbitrary time step sizes
- Forces and accelerations are measures
- Need to solve a complementarity problem per time step

- With the new IPM solver, both DEM **and** NSCD can be used to **estimate draft forces**
- IPM has lots of **room for improvement**, on algorithmic level and by parallelization
- Simultaneously and after my PhD, other researchers contributed promising solvers that should be analysed

References

More details

Many references

https://bit.ly/3mcD9QM

Summary paper of my thesis

Kleinert, Simeon, Dreßler 2017

https://bit.ly/2JgDrHX

free copy of my thesis

Kleinert 2015

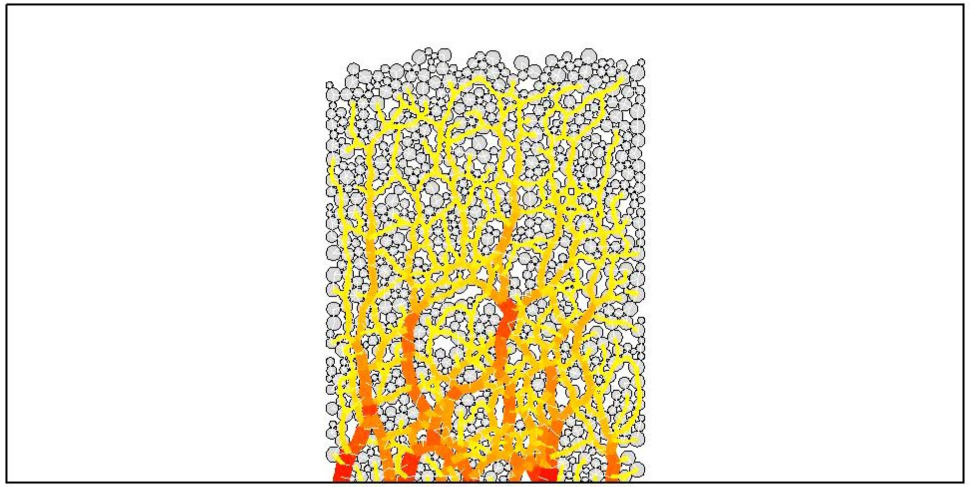
https://bit.ly/3l5vUc0

Overview book chapter on DAEs and nonsmooth dynamical systems

Kleinert, Simeon 2018

Thank you very much for your attention!

Any Questions?



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