UNIVERSIDADE DA CORUÑA

Behaviour of augmented Lagrangian algorithms in the simulation of multibody systems with singular configurations

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1. Motivation

- Development of efficient algorithms for multibody system dynamics

- Augmented Lagrangian algorithms
  - Mature (25 years of development by the multibody community)
  - Efficient
    - Successfully used in real-time applications
  - Robust
    - Able to deal with redundant constraints
    - Good performance in systems with singular configurations, impacts, etc.

- Augmented Hamiltonian algorithms
  - A subset of augmented Lagrangian algorithms
  - Relatively less known in the multibody community

1. Motivation

- A relatively large number of augmented Lagrangian algorithms for multibody dynamics currently exists

- Need for benchmarking and guidelines for algorithm selection and parameter tuning

  - Singular configurations
    - Demanding simulation problem
    - Numerical difficulties have been observed with existing algorithms
    - Simple benchmark problems available (e.g. IFToMM benchmark)

  - Identification of sources of numerical difficulties
    - Effect on simulation performance

  - Definition of guidelines for algorithm selection and tuning

2. Augmented Lagrangian algorithms

- First used in multibody system dynamics in the 1980's
- Mechanical system defined by

  n generalized coordinates → $\mathbf{q}$

  m kinematic constraints (holonomic) → $\mathbf{\Phi} = \mathbf{0}$

- Dynamics equations can be expressed as

(1a) $$\mathbf{M}\ddot{\mathbf{q}} + \mathbf{c} = \mathbf{f} + \mathbf{f}_c$$

(1b) $$\mathbf{\Phi} = \mathbf{0}$$

System of *n* + *m* DAE's

- Differentiation of kinematic constraints w.r.t. time

$$\mathbf{\Phi} = \mathbf{0} \xrightarrow{d/dt} \mathbf{\Phi}_{\mathbf{q}}\dot{\mathbf{q}} + \mathbf{\Phi}_{\mathbf{t}} = \mathbf{0} \xrightarrow{d/dt} \mathbf{\Phi}_{\mathbf{q}}\ddot{\mathbf{q}} + \dot{\mathbf{\Phi}}_{\mathbf{q}}\dot{\mathbf{q}} + \dot{\mathbf{\Phi}}_{\mathbf{t}} = \mathbf{0}$$

Configuration level | **Velocity level** | **Acceleration level**

2. Augmented Lagrangian algorithms

- **The Lagrangian approach**

(2a) $$\mathbf{M}\ddot{\mathbf{q}} + \mathbf{c} = \mathbf{f} + \mathbf{\Phi}_{\mathbf{q}}^{\mathrm{T}}\boldsymbol{\lambda}$$

(2b) $$\mathbf{\Phi}_{\mathbf{q}}\ddot{\mathbf{q}} + \dot{\mathbf{\Phi}}_{\mathbf{q}}\dot{\mathbf{q}} + \dot{\mathbf{\Phi}}_{\mathbf{t}} = \mathbf{0}$$

$$\mathbf{f}_c = -\mathbf{\Phi}_{\mathbf{q}}^{\mathrm{T}}\boldsymbol{\lambda}$$

$\boldsymbol{\lambda}$: **Set of *m* Lagrange multipliers**

System of *n* + *m* ODE's, with *n* + *m* unknowns

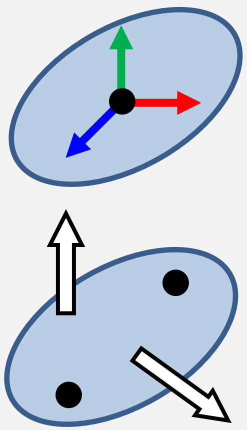
- The system can be expressed as

(3) $$\begin{bmatrix} \mathbf{M} & \mathbf{\Phi}_{\mathbf{q}}^{\mathrm{T}} \\ \mathbf{\Phi}_{\mathbf{q}} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \ddot{\mathbf{q}} \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} \mathbf{f} - \mathbf{c} \\ -\dot{\mathbf{\Phi}}_{\mathbf{q}}\dot{\mathbf{q}} - \dot{\mathbf{\Phi}}_{\mathbf{t}} \end{bmatrix}$$

- Some problems
  - Solution drift ($\mathbf{\Phi} = \mathbf{0}$, $\dot{\mathbf{\Phi}} = \mathbf{0}$ not imposed)
  - The leading matrix is singular if the Jacobian matrix is rank deficient

2. Augmented Lagrangian algorithms

- **A comment on natural coordinates**
  - Natural coordinates were used for the modelling
    - Usually: position and orientation of a reference frame attached to each body
    - Natural coordinates: using reference points and vectors to describe the system



$$\mathbf{q} = \begin{bmatrix} x & y & z & e_0 & e_1 & e_2 & e_3 \end{bmatrix}^{\mathrm{T}}$$

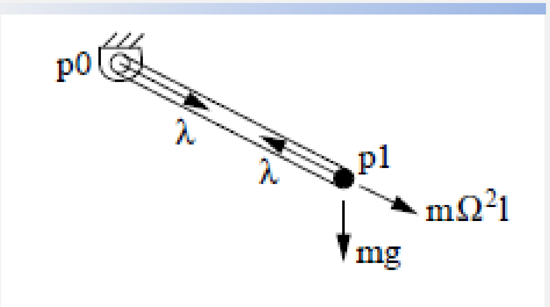
$$\mathbf{q} = \begin{bmatrix} x_1 & y_1 & z_1 & x_2 & y_2 & z_2 & x_{v1} & y_{v1} & z_{v1} & x_{v2} & y_{v2} & z_{v2} \end{bmatrix}^{\mathrm{T}}$$

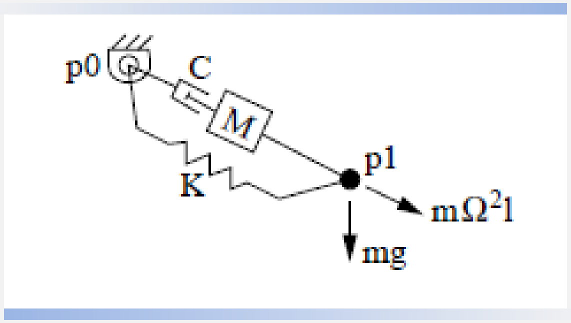
+ rigid body constraint equations

  - Consequences
    - The mass matrix is constant during motion
    - The Coriolis and velocity-dependent forces term vanishes from the equations
    - Generalized velocities are the derivatives w.r.t. time of the generalized coordinates

2. Augmented Lagrangian algorithms

- **Penalty formulation** (Bayo et al., 1988)
  - Starting point for the development of augmented Lagrangian algorithms
  - The kinematic constraints are replaced with mass-spring-damper systems





  - Reactions are made proportional to the violation of kinematic constraints

(4) $$\boldsymbol{\lambda} = \alpha \left(\ddot{\boldsymbol{\Phi}} + 2\xi\omega\dot{\boldsymbol{\Phi}} + \omega^2 \boldsymbol{\Phi} \right)$$

α : **Penalty factor**

$\xi,\ \omega$: **Stabilization parameters (Baumgarte)**

2. Augmented Lagrangian algorithms

- **Penalty formulation** (Bayo et al., 1988)
  - From Eqs. (4) and (2a)

(2a) $$\mathbf{M}\ddot{\mathbf{q}} = \mathbf{f} - \mathbf{\Phi}_{\mathbf{q}}^{\mathrm{T}}\boldsymbol{\lambda}$$

(4) $$\boldsymbol{\lambda} = \alpha\left(\ddot{\mathbf{\Phi}} + 2\xi\omega\dot{\mathbf{\Phi}} + \omega^2\mathbf{\Phi}\right)$$

(5) $$\left(\mathbf{M} + \mathbf{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\mathbf{\Phi}_{\mathbf{q}}\right)\ddot{\mathbf{q}} = \mathbf{f} - \mathbf{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\left(\dot{\mathbf{\Phi}}_{\mathbf{q}}\dot{\mathbf{q}} + \dot{\mathbf{\Phi}}_{\mathbf{t}} + 2\xi\omega\dot{\mathbf{\Phi}} + \omega^2\mathbf{\Phi}\right)$$

  - System of equations with an n x n, SPD lead matrix
  - Solution drift under control
  - Able to deal with rank-deficient Jacobian matrices

  - Kinematic constraints are never perfectly satisfied
  - Choice of penalty factor affects the accuracy of the results

2. Augmented Lagrangian algorithms

- **Augmented Lagrangian algorithm** (Bayo et al., 1988)
  - Starting from the penalty formulation

(6a) $$\left(\mathbf{M}+\boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\boldsymbol{\Phi}_{\mathbf{q}}\right)\ddot{\mathbf{q}}=\mathbf{f}-\boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\left(\dot{\boldsymbol{\Phi}}_{\mathbf{q}}\dot{\mathbf{q}}+\dot{\boldsymbol{\Phi}}_{\mathbf{t}}+2\xi\omega\dot{\boldsymbol{\Phi}}+\omega^{2}\boldsymbol{\Phi}\right)-\boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\boldsymbol{\lambda}^{*}$$

(6b) $$\boldsymbol{\lambda}_{i+1}^{*}=\boldsymbol{\lambda}_{i}^{*}+\alpha\left(\ddot{\boldsymbol{\Phi}}+2\xi\omega\dot{\boldsymbol{\Phi}}+\omega^{2}\boldsymbol{\Phi}\right)$$

  - Lagrange’s multipliers are re-introduced in the dynamics equations
  - Their value is obtained in an iterative way
  - An iterative process is introduced in the solution, but the selection of the penalty factor becomes less critical
  - Mass-orthogonal projections can be used to remove the constraint violations completely at the configuration, velocity, and acceleration levels (Bayo and Ledesma, 1996)

- **Augmented Hamiltonian algorithm** (Bayo and Avello, 1994)
  - Based on Hamilton's canonical equations
  - The canonical momenta are introduced as system variables, together with the generalized coordinates

$$\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{q}}} \longrightarrow H = \mathbf{p}^{\mathrm{T}}\dot{\mathbf{q}} - L$$

Canonical momenta **Hamiltonian**

  - The canonical equations for a constrained system can be expressed as

(7)
$$\dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}}\ ; \qquad -\dot{\mathbf{p}} = \frac{\partial H}{\partial \mathbf{q}} - \mathbf{f}_{nc} + \mathbf{\Phi}_{\mathbf{q}}^{\mathrm{T}}\boldsymbol{\lambda}$$

2. Augmented Lagrangian algorithms

- **Augmented Hamiltonian algorithm** (Bayo and Avello, 1994)
  - Following an approach similar to the one used for the augmented Lagrangian algorithm in Eqs. (6a) and (6b), the time derivatives of the generalized coordinates can be obtained as

(8a) $$\left(\mathbf{M}+\mathbf{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\mathbf{\Phi}_{\mathbf{q}}\right)\dot{\mathbf{q}}=\mathbf{p}-\mathbf{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\left(\mathbf{\Phi}_{\mathbf{t}}+2\xi\omega\mathbf{\Phi}+\omega^{2}\int_{t_0}^{t}\mathbf{\Phi}dt\right)-\mathbf{\Phi}_{\mathbf{q}}^{\mathrm{T}}\boldsymbol{\sigma}$$

(8b) $$\boldsymbol{\sigma}_{i+1}=\boldsymbol{\sigma}_{i}+\alpha\left(\dot{\mathbf{\Phi}}+2\xi\omega\mathbf{\Phi}+\omega^{2}\int_{t_0}^{t}\mathbf{\Phi}dt\right)$$

$\boldsymbol{\sigma}$: Set of m multipliers

$\dot{\boldsymbol{\sigma}}=\boldsymbol{\lambda}$

  - The derivatives with respect to time of the canonical momenta are obtained explicitly from

(8c) $$\dot{\mathbf{p}}=\mathbf{f}+\dot{\mathbf{\Phi}}_{\mathbf{q}}^{\mathrm{T}}\alpha\left(\dot{\mathbf{\Phi}}+2\xi\omega\mathbf{\Phi}+\omega^{2}\int_{t_0}^{t}\mathbf{\Phi}dt\right)+\dot{\mathbf{\Phi}}_{\mathbf{q}}^{\mathrm{T}}\boldsymbol{\sigma}$$

- **Integration formulas**
  - Forward Euler
    - Explicit, single step

(9)
$$\begin{cases} \dot{\mathbf{q}}^{k+1} = \dot{\mathbf{q}}^{k} + h\,\ddot{\mathbf{q}}^{k} \\ \mathbf{q}^{k+1} = \mathbf{q}^{k} + h\,\dot{\mathbf{q}}^{k} \end{cases}$$

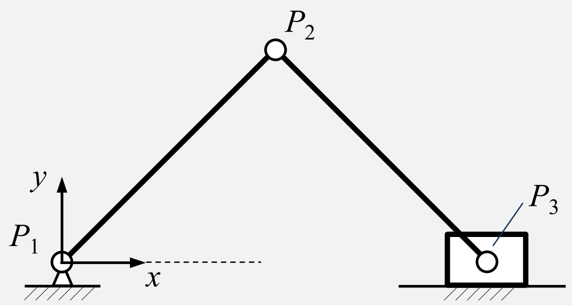
  - Newmark formulas
    - Implicit, single-step

(10)
$$\begin{cases} \dot{\mathbf{q}}^{k+1} = \dot{\mathbf{q}}^{k} + \dfrac{h}{2}\left(\ddot{\mathbf{q}}^{k} + \ddot{\mathbf{q}}^{k+1}\right) \\ \mathbf{q}^{k+1} = \mathbf{q}^{k} + \dfrac{h}{2}\left(\dot{\mathbf{q}}^{k} + \dot{\mathbf{q}}^{k+1}\right) \end{cases}$$

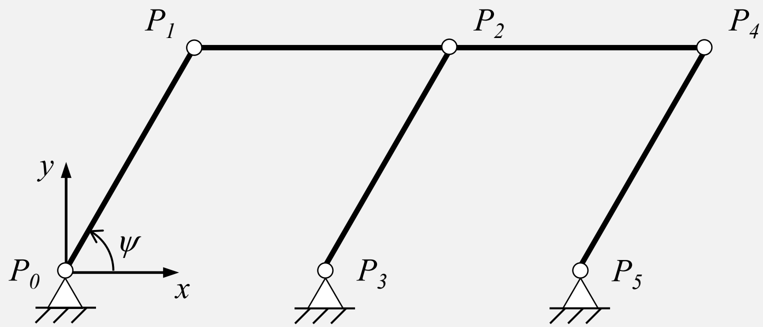
3. Singular configurations

- Benchmark examples (from IFToMM examples library)

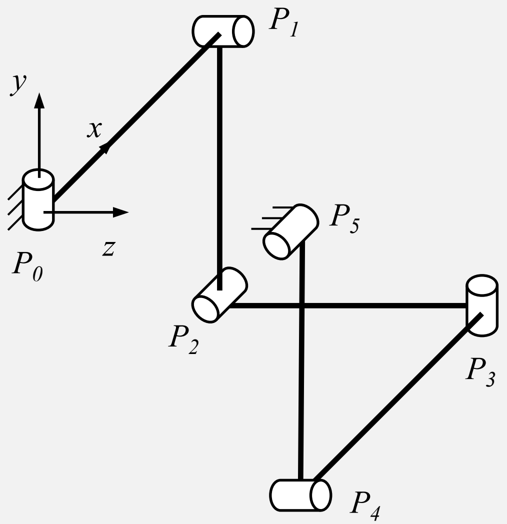
http://iftomm-multibody.org/benchmark/



Slider-crank mechanism



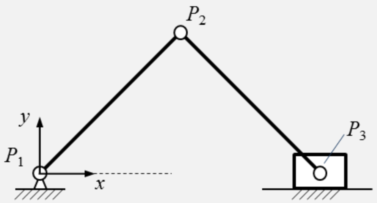
Double four-bar linkage

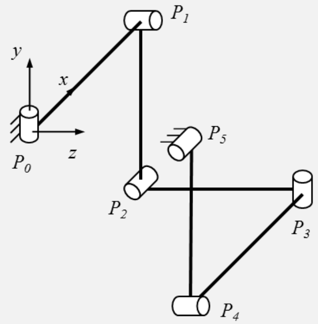


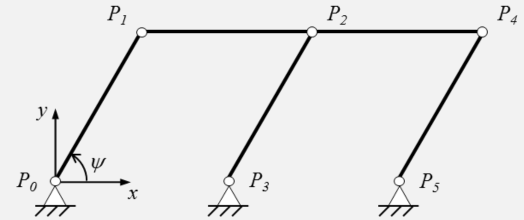
6-link Bricard mechanism

3. Singular configurations

- Benchmark examples (from IFToMM examples library)







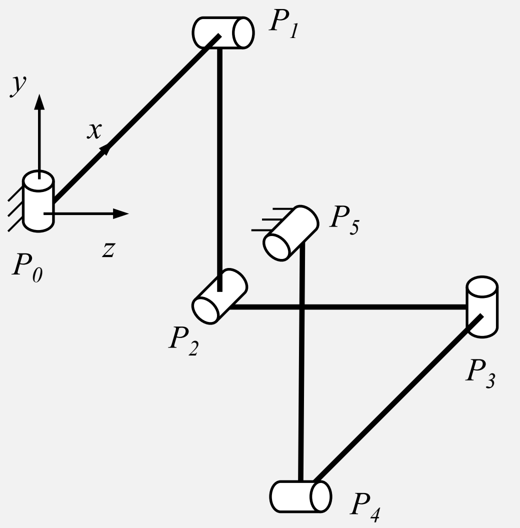
  – These systems result in a rank-deficient Jacobian matrix at some point during the motion

$$\begin{bmatrix} \mathbf{M} & \mathbf{\Phi}_{\mathbf{q}}^{\mathrm{T}} \\ \mathbf{\Phi}_{\mathbf{q}} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \ddot{\mathbf{q}} \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} \mathbf{f} - \mathbf{c} \\ -\dot{\mathbf{\Phi}}_{\mathbf{q}}\dot{\mathbf{q}} - \dot{\mathbf{\Phi}}_{\mathrm{t}} \end{bmatrix}$$

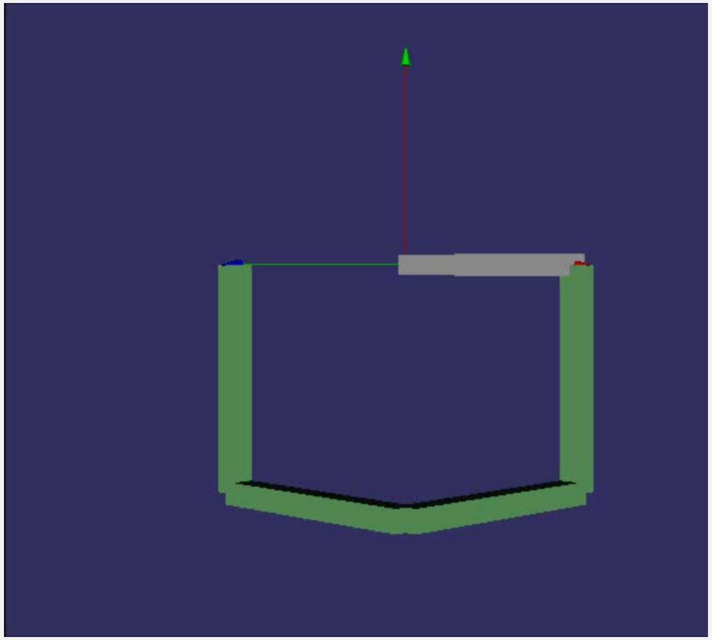
  – The penalty, augmented Lagrangian, and augmented Hamiltonian methods can carry out the numerical simulation in spite of that
    - The simulation can start from a singular configuration

3. Singular configurations

- Benchmark examples (from IFToMM examples library)



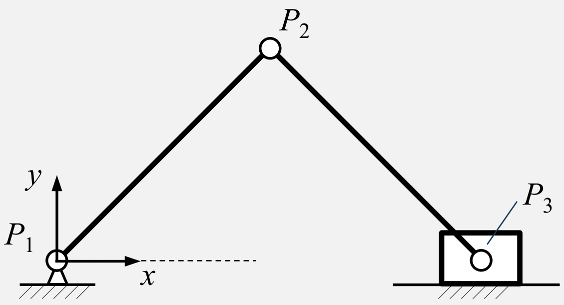
6-link Bricard mechanism



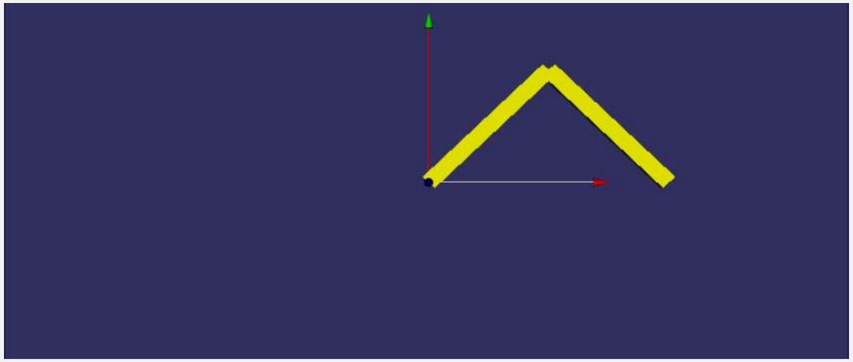
- Rank-deficient Jacobian stemming from redundant constraints, not singular configurations
- The rank of the Jacobian matrix does not change during motion
- All the algorithms were able to simulate its motion correctly

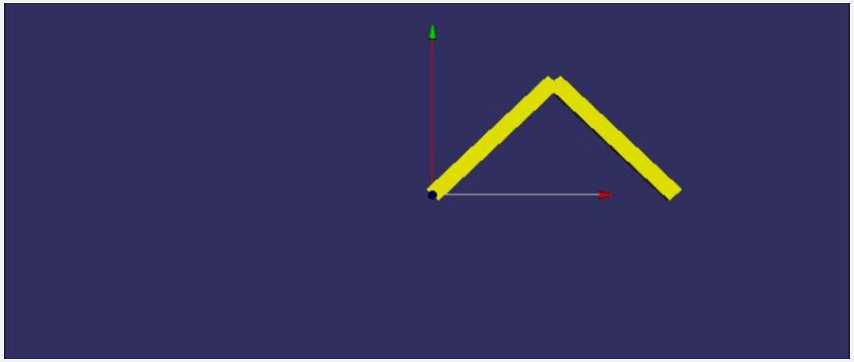
3. Singular configurations

- Benchmark examples (from IFToMM examples library)



Slider-crank mechanism

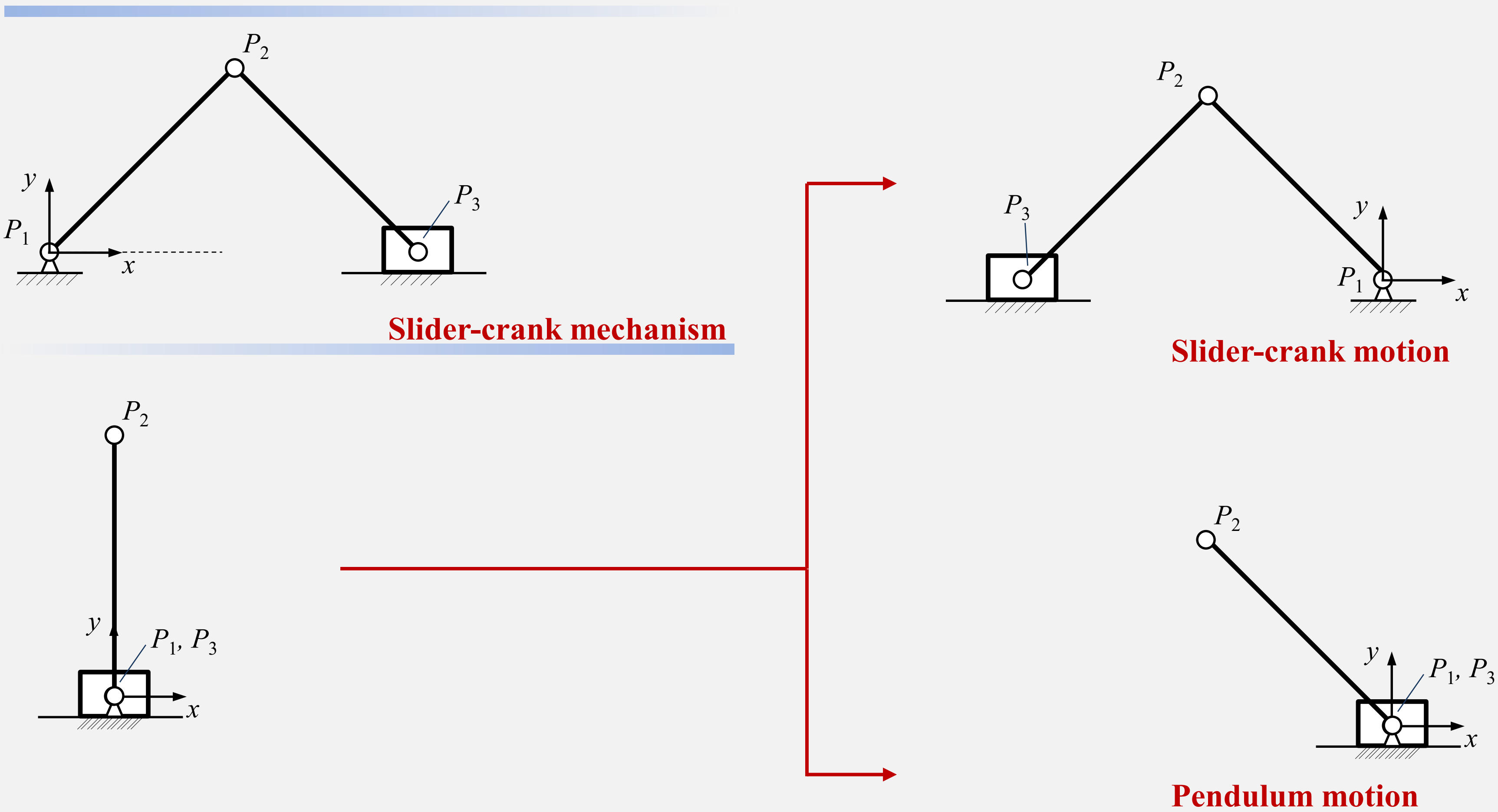




- Singular configuration when rods are aligned on the y-axis
- Jacobian matrix suddenly loses rank
- The system gains one extra d.o.f.
- Singular configuration as bifurcation point
- Numerical problems observed with all the methods, for certain combinations of parameters

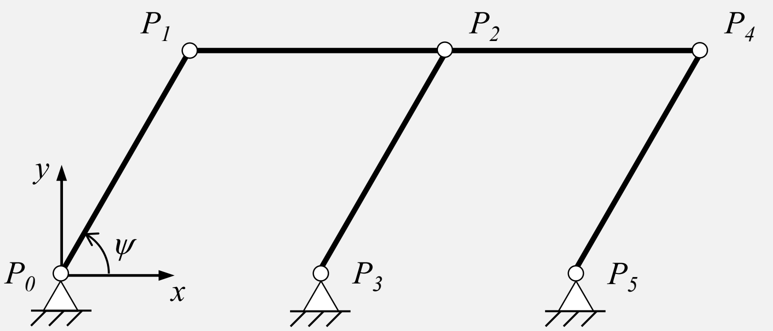
3. Singular configurations

- Benchmark examples (from IFToMM examples library)



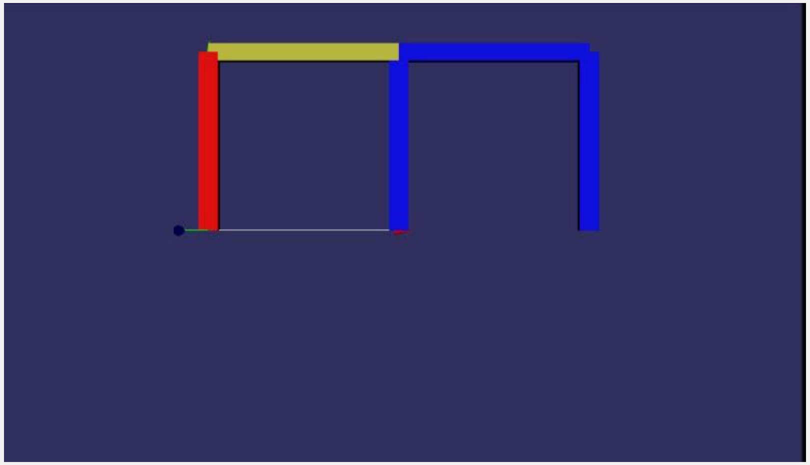
3. Singular configurations

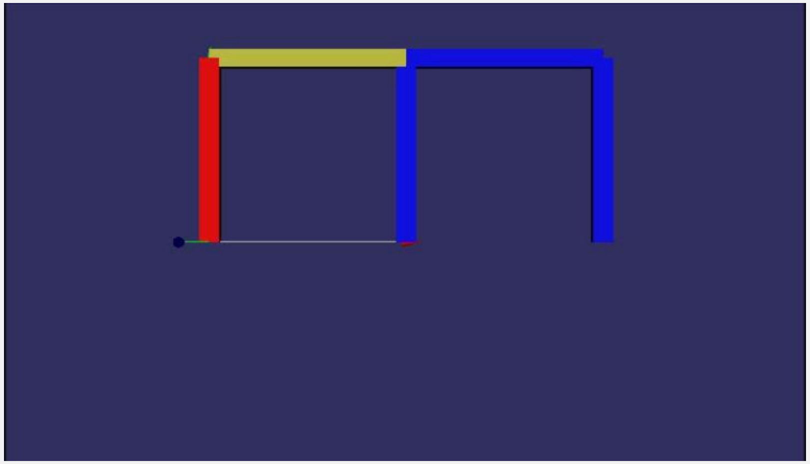
- Benchmark examples (from IFToMM examples library)



Double four-bar linkage

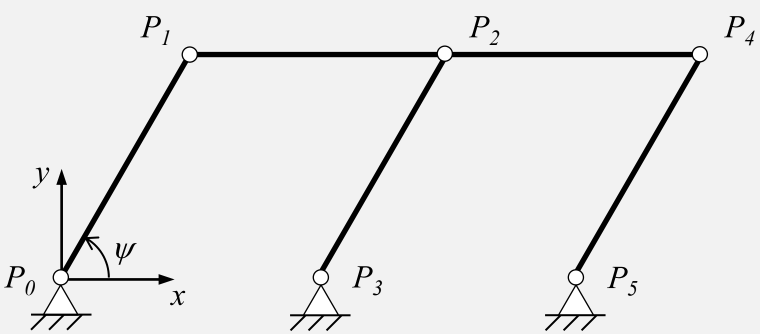
- Singular configuration when rods are aligned on the x-axis
- The system gains two extra d.o.f.



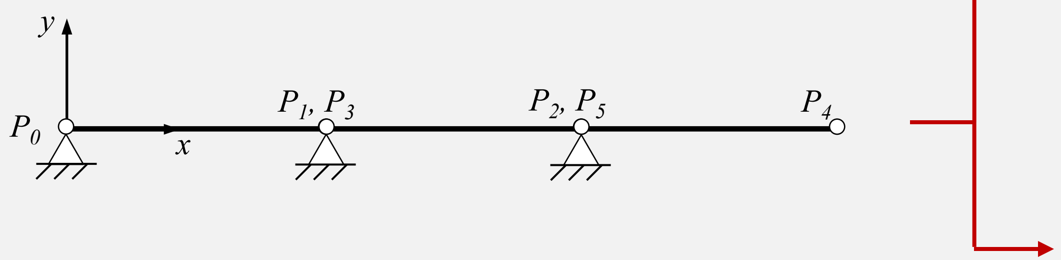


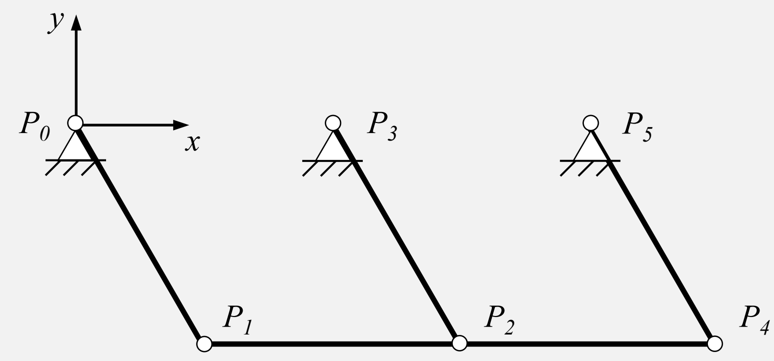
3. Singular configurations

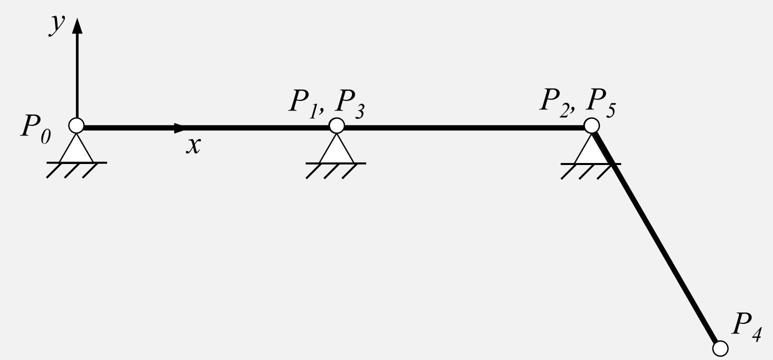
- Benchmark examples (from IFToMM examples library)



Double four-bar linkage

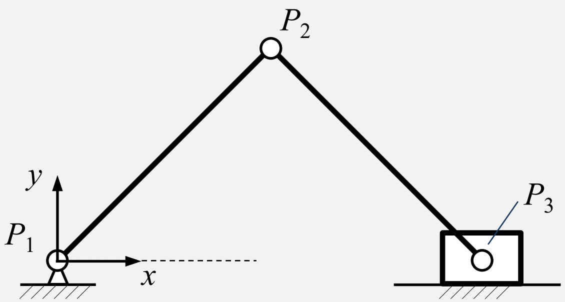






3. Singular configurations

- Enlarged Subspace of Admissible Motion (SAM) at singular configurations



– One-d.o.f. system modelled with three generalized coordinates (x_2, y_2, x_3)

$$x_2^2 + y_2^2 - l^2 = 0$$

$$(x_3 - x_2)^2 + y_2^2 - l^2 = 0$$

– Subspace of constrained motion (SCM) defined by the Jacobian matrix of the constraints

$$\dot{\mathbf{\Phi}}^{sc} = \begin{bmatrix} 2x_2 & 2y_2 & 0 \\ 2(x_2 - x_3) & 2y_2 & 2(x_3 - x_2) \end{bmatrix} \begin{bmatrix} \dot{x}_2 \\ \dot{y}_2 \\ \dot{x}_3 \end{bmatrix} = \mathbf{\Phi}_{\mathbf{q}}^{sc} \dot{\mathbf{q}}^{sc} = \mathbf{0}$$

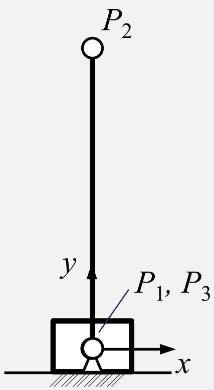
$$\mathbf{\Phi}_{\mathbf{q}} \dot{\mathbf{q}} = \mathbf{u}_c \longrightarrow \dot{\mathbf{q}}_a^{sc} = \eta \begin{bmatrix} 1 \\ -x_2 / y_2 \\ x_3 / (x_3 - x_2) \end{bmatrix}$$

Admissible velocities

SAM has dimension 1

3. Singular configurations

- In a singular configuration the Jacobian suddenly loses rank



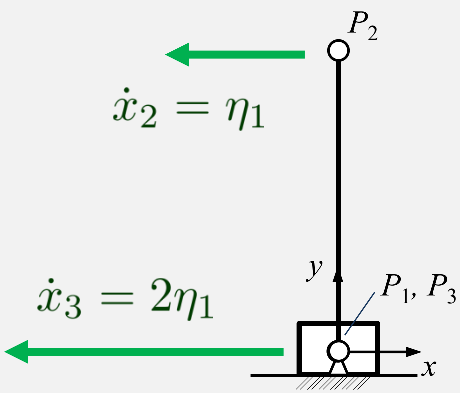
$$x_3 = x_2 = 0 \longrightarrow \left.\mathbf{\Phi}_{\mathbf{q}}^{sc}\right|_{t_s} = \begin{bmatrix} 0 & 2l & 0 \\ 0 & 2l & 0 \end{bmatrix}$$

SAM has dimension 2 now

$$\longrightarrow \left.\dot{\mathbf{q}}_a^{sc}\right|_{t_s} = \eta_1 \begin{bmatrix} 1 \\ 0 \\ 2 \end{bmatrix} + \eta_2 \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = \eta_1 \dot{\mathbf{q}}_{a1}^{sc} + \eta_2 \dot{\mathbf{q}}_{a2}^{sc}$$

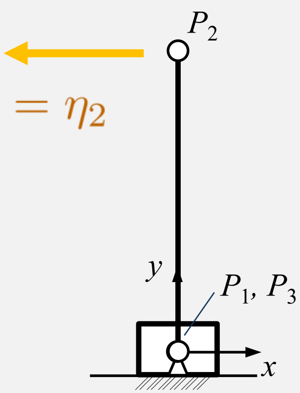
$$\dot{x}_2 = \eta_1$$

$$\dot{x}_3 = 2\eta_1$$



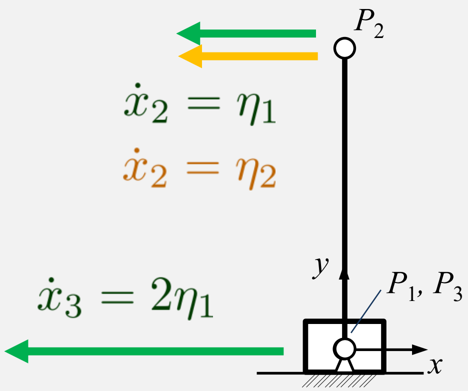
Slider-crank motion

$$\dot{x}_2 = \eta_2$$



Pendulum motion

- Two velocity components can exist simultaneously in the singularity



– Secondary components may be introduced by the numerical integration process

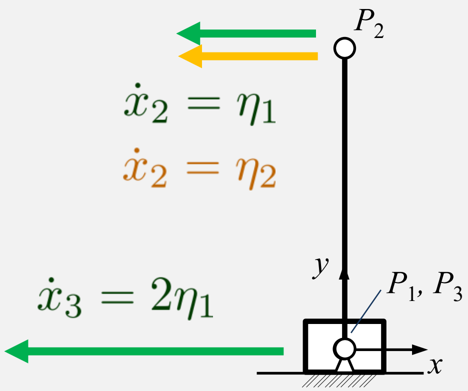
– After the singularity only one can remain, because the Jacobian matrix recovers its original rank

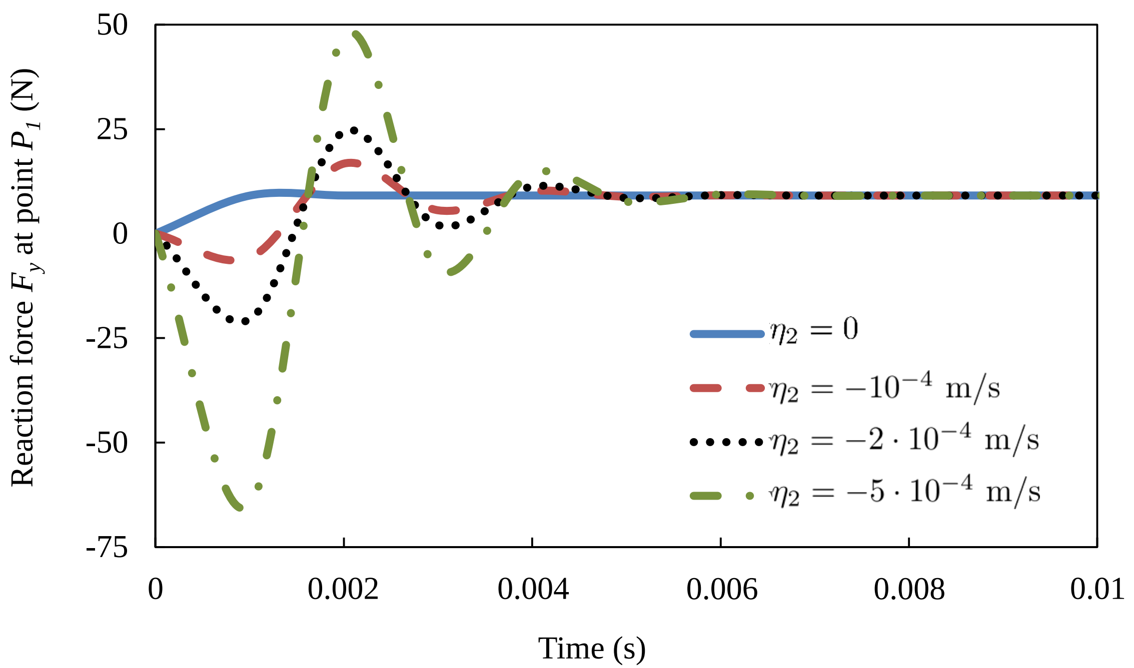
– The other component becomes a violation of the velocity-level constraints
  - Not necessarily a “small” violation of constraints
  - Projections do not remove the secondary component in the singularity: it does not violate the constraints at that point

– Augmented Lagrangian methods transform constraint violations in reactions

$$\boldsymbol{\lambda} = \alpha \left(\ddot{\boldsymbol{\Phi}} + 2\xi\omega\dot{\boldsymbol{\Phi}} + \omega^2\boldsymbol{\Phi} \right) \longrightarrow$$ **Impulsive discontinuities in reactions**

- **Introduction of impulsive discontinuities in reaction forces**

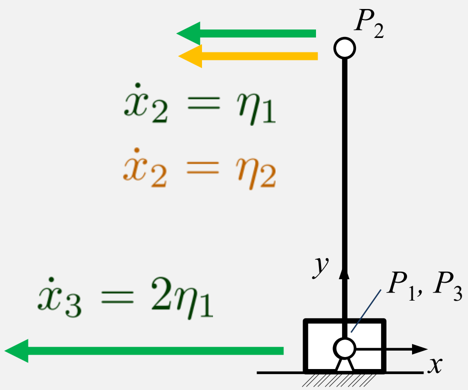


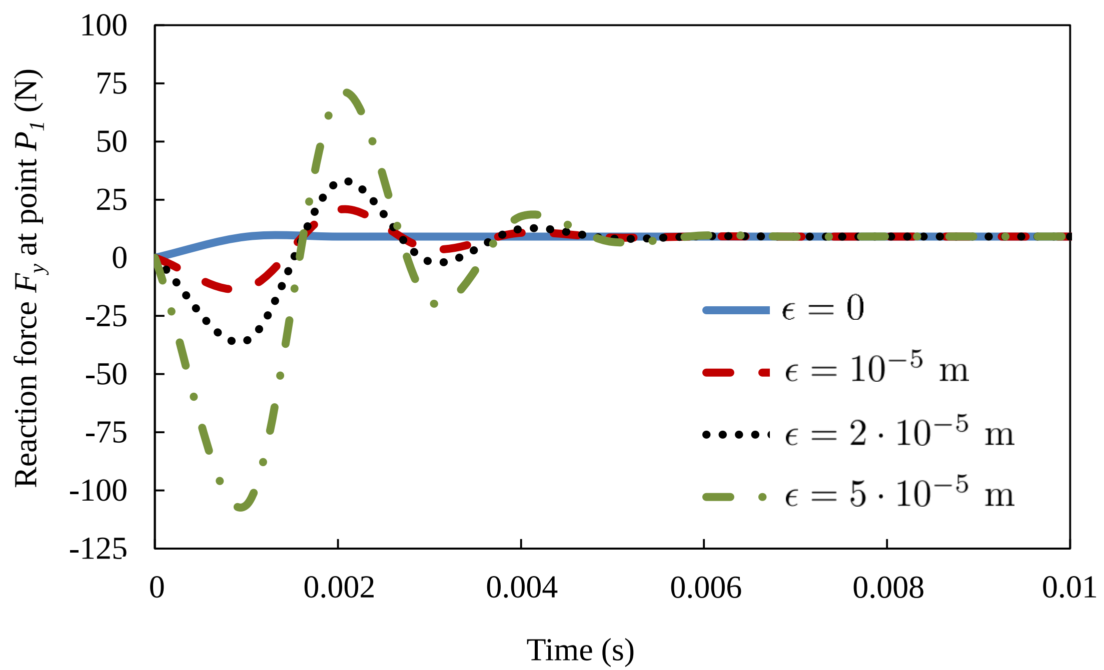


y-reaction at P_1, after starting from the singular configuration; $\eta_1 = 2$ m/s

- **Introduction of impulsive discontinuities in reaction forces**
  - Effect of violation of configuration-level constraints

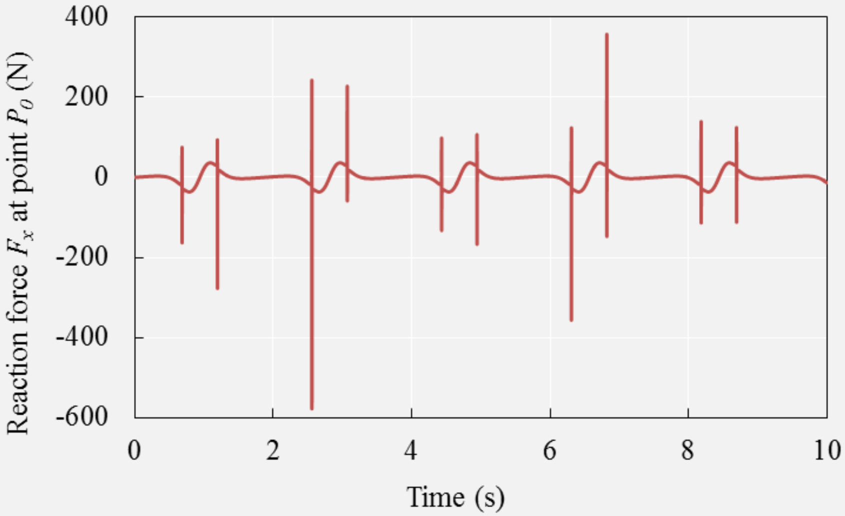
$$\widetilde{\mathbf{\Phi}}_{\mathbf{q}} = \mathbf{\Phi}_{\mathbf{q}}\left(\mathbf{q} + \boldsymbol{\epsilon}\right) \longrightarrow \widetilde{\mathbf{\Phi}}_{\mathbf{q}}\dot{\mathbf{q}} \neq \mathbf{0}$$

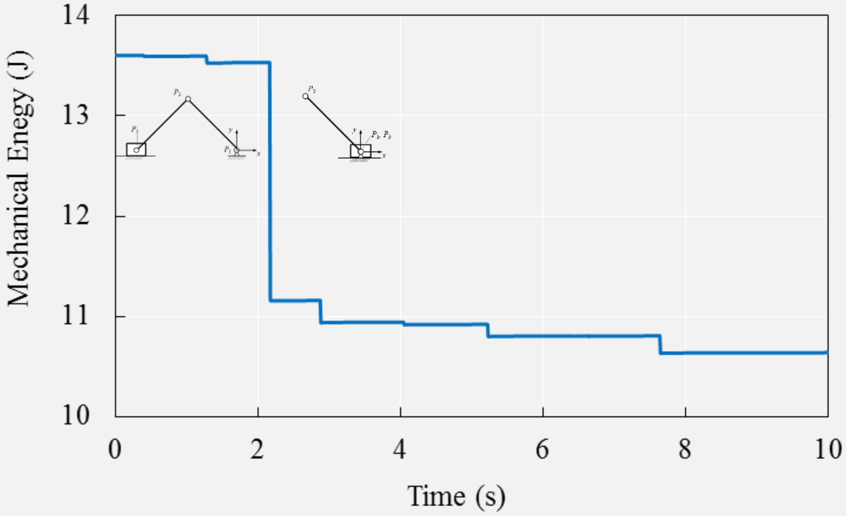




***y*-reaction at P_1, after starting from the singular configuration ($\eta_2 = 0$)**

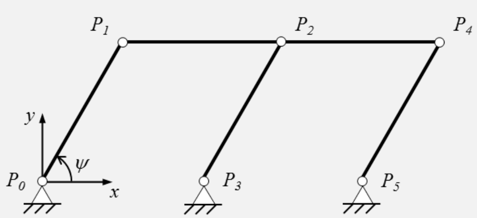
- Effects on simulation

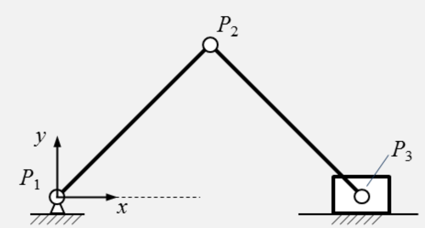




x-reaction at P_0, during motion of the four-bar linkage

Mechanical energy of slider-crank mechanism

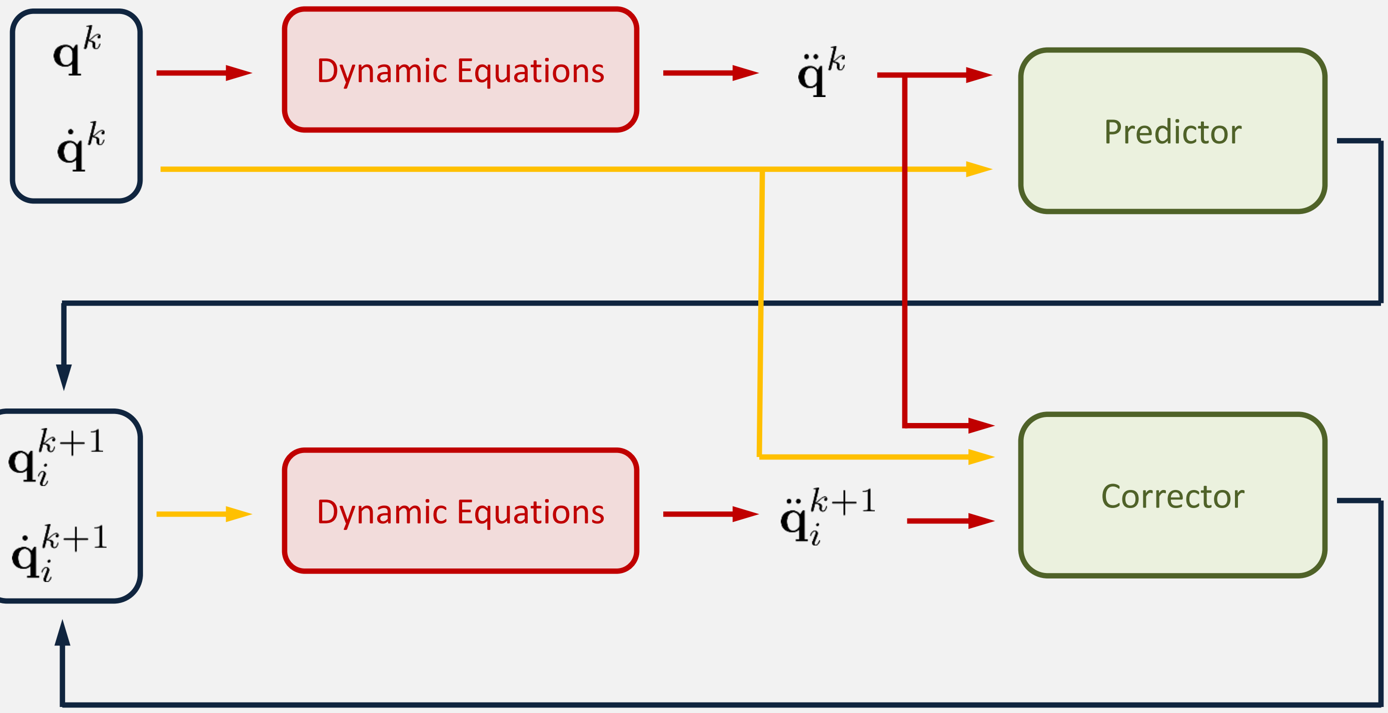




4. Newton-Raphson iterative schemes

- Requirements for the algorithm to meet
  - Able to keep the violation of kinematic constraints under a certain threshold
  - Robust enough to withstand impact forces
- Algorithms with implicit integrators initially implemented in fixed-point iterative scheme
  - They tend to fail near singular configurations
- Implementation in Newton-Raphson iterative scheme
  - Expected to show a more robust behaviour
  - Already done for augmented Lagrangian methods (although not in a general way)
  - New for augmented Hamiltonian algorithms

- **Fixed-point iteration**



4. Newton-Raphson iterative schemes

- **Newton-Raphson iteration**
  - The dynamics equations are combined with the numerical integration formulas to obtain a system of nonlinear equations

(11) $$\mathbf{g}\left(\mathbf{q},\dot{\mathbf{q}}\right)=\mathbf{0}$$

  - The generalized coordinates at the next integration time-step become the system unknowns
  - The system is solved by means of Newton-Raphson iteration

(12a) $$\left[\frac{d\mathbf{g}\left(\mathbf{q},\dot{\mathbf{q}}\right)}{d\mathbf{q}}\right]_i\Delta\mathbf{q}_{i+1}=-\left[\mathbf{g}\left(\mathbf{q},\dot{\mathbf{q}}\right)\right]_i$$

Tangent matrix **RHS (residual)**

(12b) $$\mathbf{q}_{i+1}=\mathbf{q}_i+\Delta\mathbf{q}_{i+1}$$

- **Augmented Lagrangian algorithm in Newton-Raphson form**
  - Proposed in Bayo, 1996 and Cuadrado, 1997
  - General form not published yet

- Numerical integration formulas: Newmark

(13)
$$\begin{cases} \dot{\mathbf{q}}_{k+1} = \dfrac{\gamma}{\beta h}\mathbf{q}_{k+1} - \hat{\dot{\mathbf{q}}}_k \\ \ddot{\mathbf{q}}_{k+1} = \dfrac{1}{\beta h^2}\mathbf{q}_{k+1} - \hat{\ddot{\mathbf{q}}}_k \end{cases}$$

$$\hat{\dot{\mathbf{q}}}_k = \frac{\gamma}{\beta h}\mathbf{q}_k + \left(\frac{\gamma}{\beta} - 1\right)\dot{\mathbf{q}}_k + h\left(\frac{\gamma}{2\beta} - 1\right)\ddot{\mathbf{q}}_k$$

$$\hat{\ddot{\mathbf{q}}}_k = \frac{1}{\beta h^2}\mathbf{q}_k + \frac{1}{\beta h}\dot{\mathbf{q}}_k + \left(\frac{1}{2\beta} - 1\right)\ddot{\mathbf{q}}_k$$

- The integrator formulas are introduced in the augmented Lagrangian expressions (6) and equilibrium is established at time $k+1$

$$\left(\mathbf{M} + \mathbf{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\mathbf{\Phi}_{\mathbf{q}}\right)\ddot{\mathbf{q}} = \mathbf{f} - \mathbf{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\left(\dot{\mathbf{\Phi}}_{\mathbf{q}}\dot{\mathbf{q}} + \dot{\mathbf{\Phi}}_{\mathbf{t}} + 2\xi\omega\dot{\mathbf{\Phi}} + \omega^2\mathbf{\Phi}\right) - \mathbf{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\boldsymbol{\lambda}^*$$

4. Newton-Raphson iterative schemes

- **Augmented Lagrangian algorithm in Newton-Raphson form**
  - We obtain a system of non-linear equations

(14)

$$\mathbf{g}\left(\mathbf{q},\dot{\mathbf{q}}\right) = \left(\mathbf{M}+\boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\boldsymbol{\Phi}_{\mathbf{q}}\right)\left(\frac{1}{\beta h^2}\mathbf{q}_{k+1}-\widehat{\ddot{\mathbf{q}}}_k\right)-\mathbf{f}$$
$$+\boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\left[\dot{\boldsymbol{\Phi}}_{\mathbf{q}}\left(\frac{\gamma}{\beta h}\mathbf{q}_{k+1}-\widehat{\dot{\mathbf{q}}}_k\right)+\dot{\boldsymbol{\Phi}}_{\mathbf{t}}+2\omega\xi\left(\boldsymbol{\Phi}_{\mathbf{q}}\left(\frac{\gamma}{\beta h}\mathbf{q}_{k+1}-\widehat{\dot{\mathbf{q}}}_k\right)+\boldsymbol{\Phi}_{\mathbf{t}}\right)+\omega^2\boldsymbol{\Phi}\right]$$
$$+\boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\boldsymbol{\lambda}_{k+1}^{*}=\mathbf{0}$$

  - With the approximated tangent matrix

(15)

$$\left[\frac{d\mathbf{g}\left(\mathbf{q},\dot{\mathbf{q}}\right)}{d\mathbf{q}}\right]\cong\ \mathbf{M}+\beta h^2\mathbf{K}+\gamma h\mathbf{C}$$
$$+\boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\boldsymbol{\Phi}_{\mathbf{q}}\ \left(1+2\omega\xi\gamma h+\omega^2\beta h^2\right)\ +\boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\dot{\boldsymbol{\Phi}}_{\mathbf{q}}\ \gamma h$$
$$+\boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\left(\beta h^2\left(\dot{\boldsymbol{\Phi}}_{\mathbf{t}}\right)_{\mathbf{q}}+2\omega\xi\beta h^2\left(\boldsymbol{\Phi}_{\mathbf{t}}\right)_{\mathbf{q}}\right)$$

$$\mathbf{C}=-\partial\mathbf{f}/\partial\dot{\mathbf{q}}$$
$$\mathbf{K}=-\partial\mathbf{f}/\partial\mathbf{q}$$

- **Augmented Lagrangian algorithm in Newton-Raphson form**
  - The original expressions can be simplified
  - Augmented Lagrangian of index-3 with projections of velocity and acceleration
    - Projections enforce $\dot{\mathbf{\Phi}} = \mathbf{0}$ and $\ddot{\mathbf{\Phi}} = \mathbf{0}$

(16) $$\mathbf{g}\left(\mathbf{q},\dot{\mathbf{q}}\right) = \mathbf{M}\mathbf{q}_{k+1} + \beta h^2 \mathbf{\Phi}_{\mathbf{q}\,k+1}^{\mathrm{T}} \left(\boldsymbol{\lambda}_{k+1}^{*} + \alpha \mathbf{\Phi}_{k+1}\right) - \beta h^2 \mathbf{f}_{k+1} - \beta h^2 \mathbf{M}\widehat{\ddot{\mathbf{q}}}_k = \mathbf{0}$$

(17) $$\left[\frac{d\mathbf{g}\left(\mathbf{q},\dot{\mathbf{q}}\right)}{d\mathbf{q}}\right] \cong \mathbf{M} + \gamma h \mathbf{C} + \beta h^2 \left(\mathbf{\Phi}_{\mathbf{q}}^{\mathrm{T}} \alpha \mathbf{\Phi}_{\mathbf{q}} + \mathbf{K}\right)$$

  - ALi3 algorithm (Cuadrado et al., 2000)

4. Newton-Raphson iterative schemes

- **Augmented Hamiltonian algorithm in Newton-Raphson form**
  - New development

- Numerical integration formulas: Trapezoidal rule

(18)
$$\begin{cases} \dot{\mathbf{q}}_{k+1} = \frac{2}{h}\mathbf{q}_{k+1} - \hat{\dot{\mathbf{q}}}_k \\ \dot{\mathbf{p}}_{k+1} = \frac{2}{h}\mathbf{p}_{k+1} - \hat{\dot{\mathbf{p}}}_k \end{cases}$$

$$\hat{\dot{\mathbf{q}}}_k = \frac{2}{h}\mathbf{q}_k + \dot{\mathbf{q}}_k$$
$$\hat{\dot{\mathbf{p}}}_k = \frac{2}{h}\mathbf{p}_k + \dot{\mathbf{p}}_k$$

- The integrator formulas are introduced in the augmented Hamiltonian expressions (8) and equilibrium is established at time $k+1$

$$\left(\mathbf{M} + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\boldsymbol{\Phi}_{\mathbf{q}}\right)\dot{\mathbf{q}} = \mathbf{p} - \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\left(\boldsymbol{\Phi}_{\mathbf{t}} + 2\xi\omega\boldsymbol{\Phi} + \omega^2\int_{t_0}^{t}\boldsymbol{\Phi}dt\right) - \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\boldsymbol{\sigma} \longrightarrow \mathbf{g}_1$$

$$\dot{\mathbf{p}} = \mathbf{f} + \dot{\boldsymbol{\Phi}}_{\mathbf{q}}^{\mathrm{T}}\alpha\left(\dot{\boldsymbol{\Phi}} + 2\xi\omega\boldsymbol{\Phi} + \omega^2\int_{t_0}^{t}\boldsymbol{\Phi}dt\right) + \dot{\boldsymbol{\Phi}}_{\mathbf{q}}^{\mathrm{T}}\boldsymbol{\sigma} \longrightarrow \mathbf{g}_2$$

- **Augmented Hamiltonian algorithm in Newton-Raphson form**
  - The system of nonlinear equations has two parts now

(19) $$\mathbf{g}_h(\mathbf{y}) = \begin{bmatrix} \mathbf{g}_1(\mathbf{y}) \\ \mathbf{g}_2(\mathbf{y}) \end{bmatrix} = \mathbf{0} \; ; \quad \text{where} \quad \mathbf{y} = \begin{bmatrix} \mathbf{q} \\ \mathbf{p} \end{bmatrix}$$

  - The tangent matrix is evaluated as follows

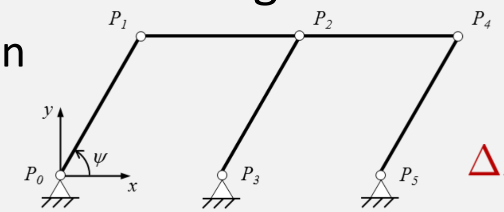
(20) $$\left[\frac{d\mathbf{g}_h(\mathbf{y})}{d\mathbf{y}}\right] = \begin{bmatrix} \dfrac{d\mathbf{g}_1(\mathbf{y})}{d\mathbf{q}} & \dfrac{d\mathbf{g}_1(\mathbf{y})}{d\mathbf{p}} \\ \dfrac{d\mathbf{g}_2(\mathbf{y})}{d\mathbf{q}} & \dfrac{d\mathbf{g}_2(\mathbf{y})}{d\mathbf{p}} \end{bmatrix}$$

5. Numerical simulations

- Summary of tested algorithms
  - Penalty formulation
    - Integration with forward Euler
    - Integration with Newmark
  - Augmented Lagrangian algorithm **(AL)**
    - Integration with forward Euler
    - Integration with Newmark
  - Augmented Hamiltonian algorithm **(AH)**
    - Integrated with forward Euler
    - Integrated with trapezoidal rule
  - Augmented Lagrangian algorithm (Newton-Raphson) **(ALNR)**
    - Integrated with Newmark
  - Augmented Lagrangian algorithm (Newton-Raphson) with projections **(ALi3)**
    - Integrated with Newmark
  - Augmented Hamiltonian algorithm (Newton-Raphson) **(AHNR)**
    - Integrated with trapezoidal rule

5. Numerical simulations

- Simulation of benchmark examples and comparison of algorithms
  - Elapsed time in the simulation of a 10 s motion



$\Delta E < 0.1$ J

- Best results for double four-bar linkage

Method	Integrator	*h* (ms)	α	ω	ξ	Elapsed time (s)
Penalty	FE	0.02	10^7	30	1	2.5
AL	FE	0.005	10^7	10	1	12.21
AH	FE	1	10^9	0.1	1000	0.07
Penalty	TR	5	10^8	25	1	0.04
AL	TR	5	10^8	20	1	0.05
AH	TR	5	10^9	0.1	1000	0.10
ALNR	TR	5	10^7	100	1	0.05
AHNR	TR	5	10^8	1	10000	0.08
ALi3	TR	10	10^9	-	-	0.02

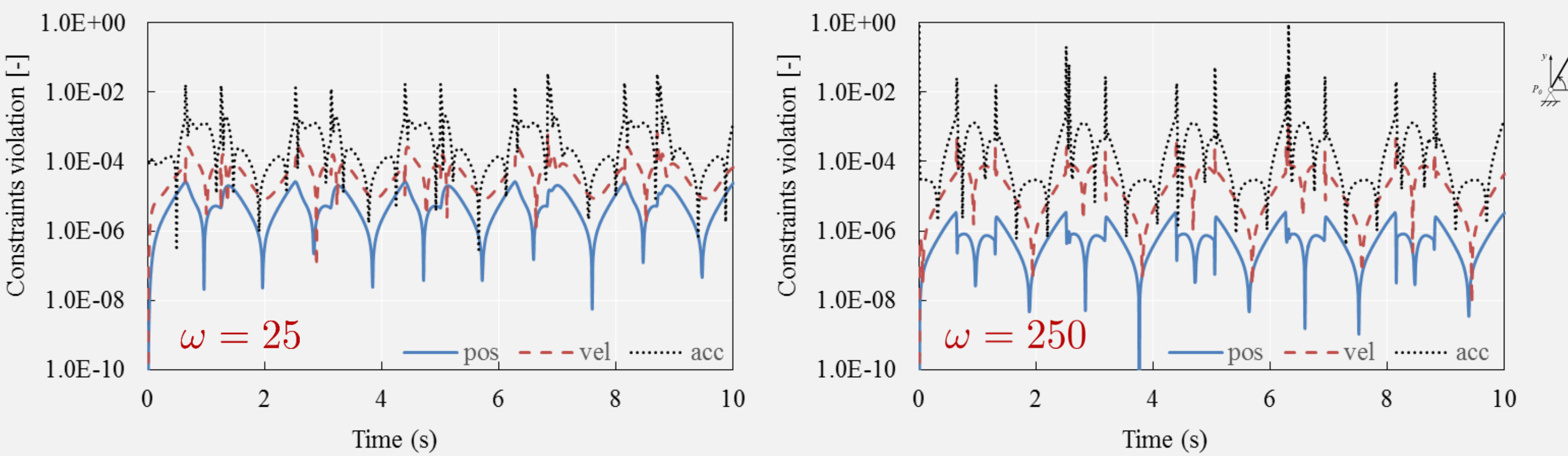
5. Numerical simulations

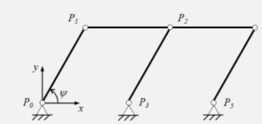
- How to adjust the algorithm parameters?

- Stabilization parameters ω and ξ

$$\boldsymbol{\lambda} = \alpha \left(\ddot{\boldsymbol{\Phi}} + 2\xi\omega\dot{\boldsymbol{\Phi}} + \omega^2\boldsymbol{\Phi} \right) \qquad \boldsymbol{\sigma} = \alpha \left(\dot{\boldsymbol{\Phi}} + 2\xi\omega\boldsymbol{\Phi} + \omega^2 \int_{t_0}^{t} \boldsymbol{\Phi} dt \right)$$

  – Constraint violations should be kept low especially at the configuration level

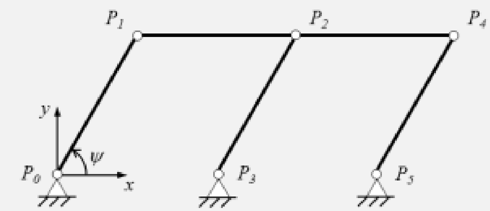




Constraint violations with AL, $\alpha = 10^7$, $\xi = 1$, $h = 1ms$

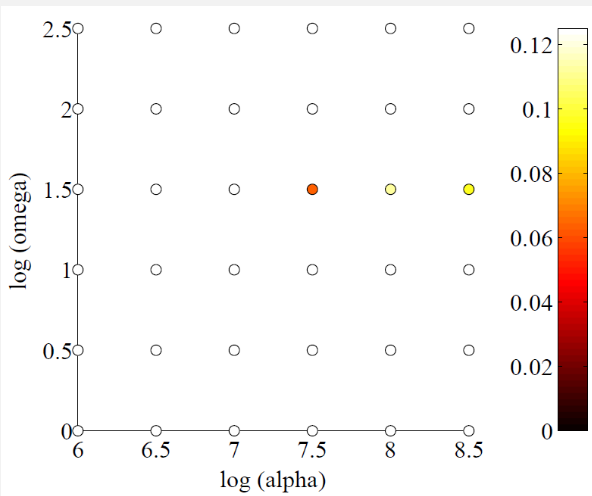
5. Numerical simulations

- How to adjust the algorithm parameters?
- Penalty factor α

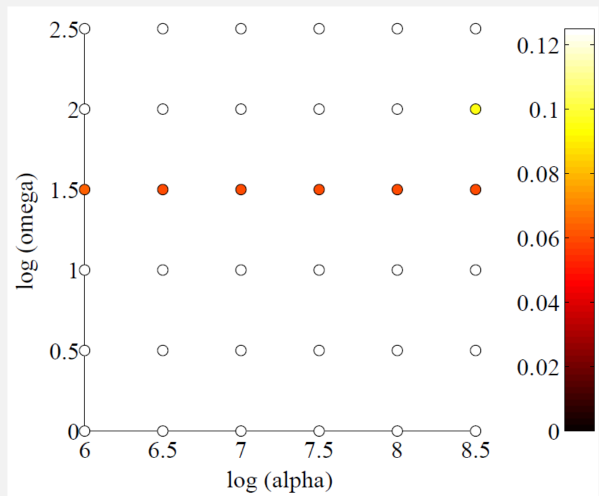


Energy drift with h = 5 ms, ξ = 1 – Lagrangian algorithms

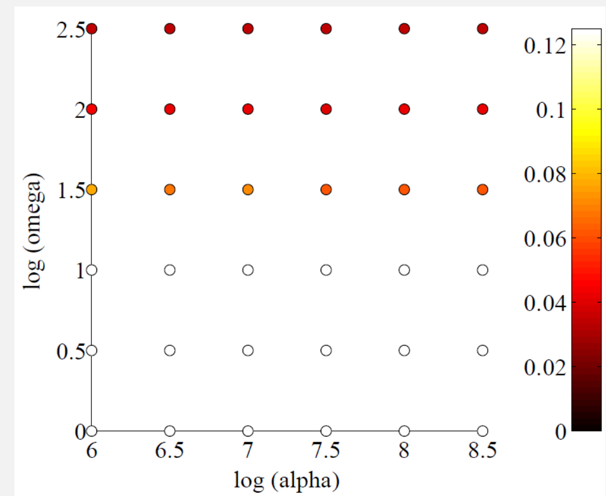
$\Delta E < 0.1$ J



Penalty, trapezoidal rule



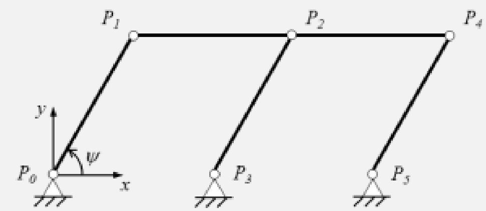
AL, trapezoidal rule



ALNR, trapezoidal rule

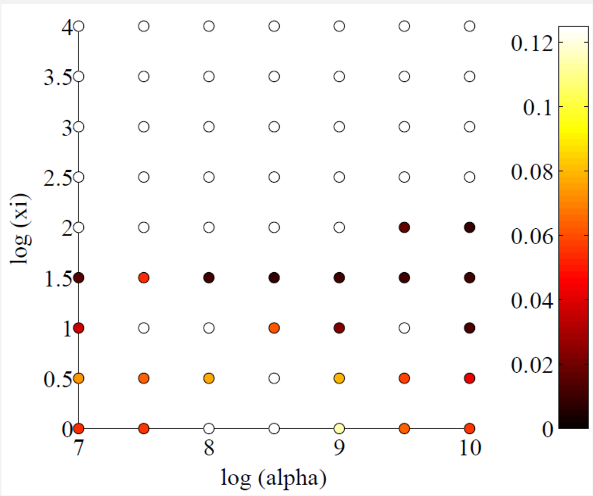
5. Numerical simulations

- How to adjust the algorithm parameters?
- Penalty factor α

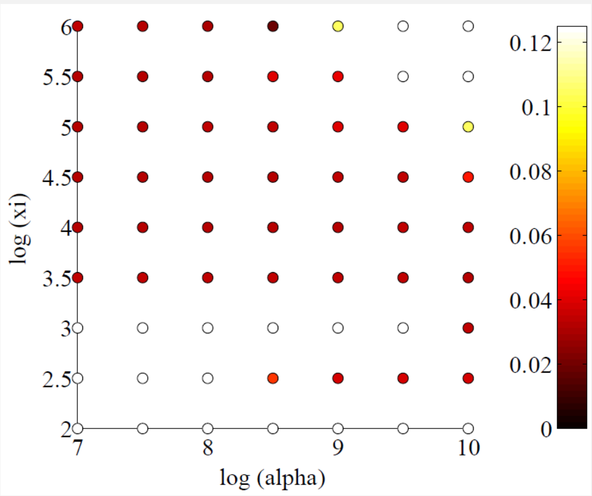


Energy drift with h = 5 ms, $\omega = 1$ – Hamiltonian algorithms

$\Delta E < 0.1$ J



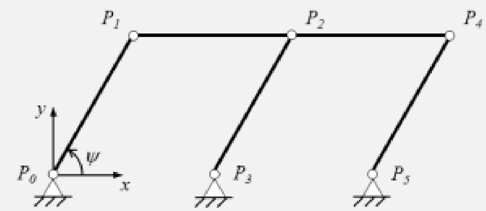
AH, trapezoidal rule



AHNR, trapezoidal rule

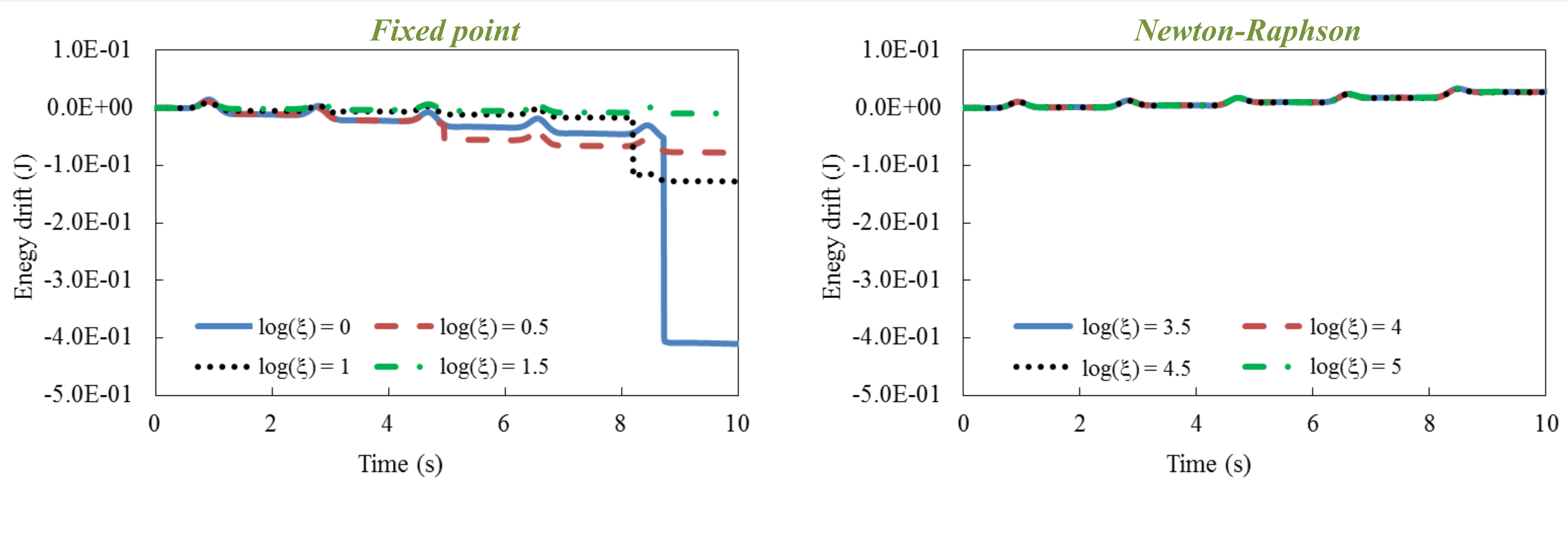
5. Numerical simulations

- How to adjust the algorithm parameters?
- Penalty factor α



Energy drift with h = 5 ms, $\omega = 1$ – Hamiltonian algorithms

$\Delta E < 0.1$ J



Time history of energy drift, $\alpha = 10^8$

6. Conclusions

- Singular configurations cause numerical difficulties in forward-dynamics simulations
  - Sudden enlargement of SAM at singularities
  - With augmented Lagrangian methods this gives rise to
    - Discontinuities in reaction forces and mechanical energy
    - Possible changes of branch and eventual failure of the simulation
  - Augmented Lagrangian methods tested in the simulation benchmark examples
    - Newton-Raphson forms of the algorithms developed and implemented
    - Hamiltonian methods showed good energy-conserving properties with forward Euler integration
  - Guidelines for the tuning of algorithm parameters
    - Dependent on the problem and integrator used
    - Violation of configuration-level constraints should be kept below a threshold
    - Newton-Raphson methods feature a more robust behaviour

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