Numerical Optimal Control with DAEs
Lecture 10: DAE Models

Sébastien Gros

AWESCO PhD course

Objectives of the Lecture

- What is a Differential-Algebraic Equation (DAE), why they are used
- DAEs in mechanical applications: why and how to build them
- Introduction to Lagrange mechanics, and DAEs from Lagrange
- Some first remarks on solving DAEs

Outline

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The second equation is algebraic ! Observe that $\dot{\mathbf{x}}_2$ is not in $\mathbf{F}$ in the first place !

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The notion of DAE can be "deceptive". In these lectures, we will focus on "clear-cut" cases.

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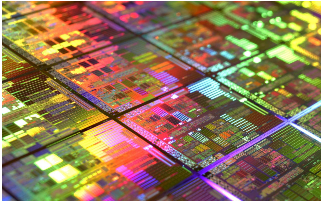

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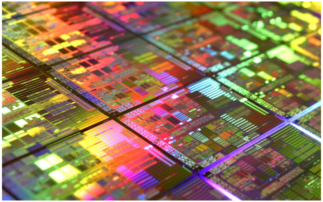

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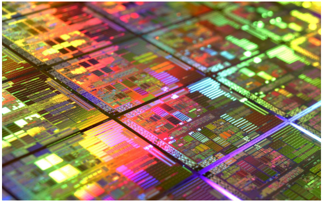

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Most often one can make an explicit distinction between differential and algebraic variables. Some DAEs can be ambiguous on that distinction though (c.f. "DAE freak show")

Some examples of DAEs - CSTR system

Isothermal CSTR:

$$A \leftrightharpoons B \rightarrow C$$

has the model equation:

$$\begin{aligned}
\dot{V} &= F_a - F \\
\dot{C}_A &= \frac{F_a}{V}\left(C_{A_0} - C_A\right) - R_1 \\
\dot{C}_B &= -\frac{F_a}{V} C_B + R_1 - R_2 \\
\dot{C}_C &= -\frac{F_a}{V} C_C + R_2 \\
0 &= C_A - \frac{C_B}{K_{eq}} \\
0 &= R_2 - k_2 C_B
\end{aligned}$$

Variables:

- F_a: feed rate of A
- C_{A_0}: feed concentration of A
- $R_{1,2}$: rates of the reactions
- F: product withdrawal rate
- $C_{A,B,C}$: concentration of species

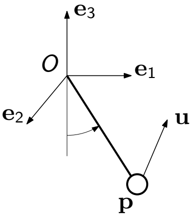
Note that:

- F and F_a are inputs
- V and $C_{A,B,C}$ are **differential** variables
- $R_{1,2}$ are **algebraic** variables

Some examples of DAEs - 3D pendulum

Position given by $\mathbf{p} \in \mathbb{R}^3$, dynamics:

$$m\ddot{\mathbf{p}} = \mathbf{u} - mg\mathbf{e}_3$$



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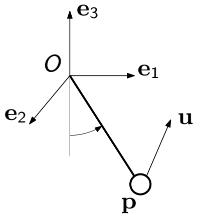

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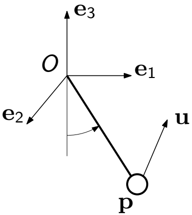

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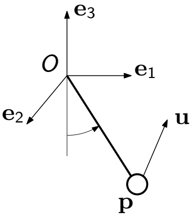

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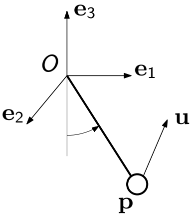

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Position given by $\mathbf{p} \in \mathbb{R}^3$, dynamics:

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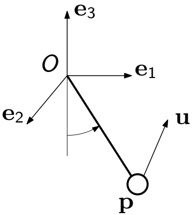

Force in the cable: direction given by $-\mathbf{p}$, amplitude given by algebraic variable $z \in \mathbb{R}_+$

Then z must be chosen such that:

$$c(\mathbf{p}) = \mathbf{p}^\top \mathbf{p} - L^2 = 0$$

holds at all time.

Using $\mathbf{v} = \dot{\mathbf{p}}$, the **DAE** reads as:

$$\begin{aligned} \dot{\mathbf{p}} &= \mathbf{v} \\ \dot{\mathbf{v}} &= \frac{\mathbf{u}}{m} - g\mathbf{e}_3 - \frac{z}{m}\mathbf{p} \\ 0 &= \mathbf{p}^\top \mathbf{p} - L^2 \end{aligned}$$

What kind of DAE is that ?!?

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{F}(\mathbf{x}, \mathbf{u}, z) \\ 0 &= \mathbf{G}(\mathbf{x}) \end{aligned}$$

Semi-explicit with $\mathbf{G}$ independent of z...

Outline

Lagrange Mechanics - Key idea

Generalised coordinates:

- A given $\mathbf{q}$ provides a "snapshot" of the configuration of the system, often simply "positions"

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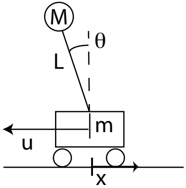

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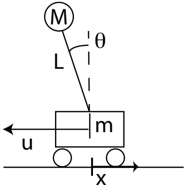

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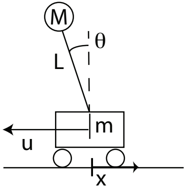
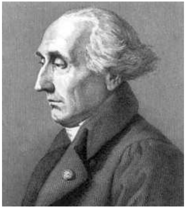


Lagrange (1788) function:

$$\mathcal{L}(\mathbf{q}, \dot{\mathbf{q}}) = \underbrace{T(\mathbf{q}, \dot{\mathbf{q}})}_{\text{kinetic energy}} - \underbrace{V(\mathbf{q})}_{\text{potential energy}}$$



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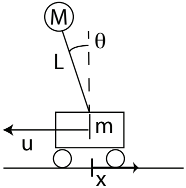

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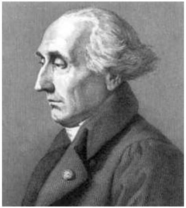
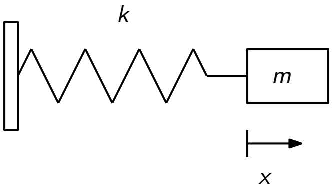
then the integral action:

$$\mathcal{I} = \int_{t_0}^{t_\mathrm{f}} \mathcal{L}(\mathbf{q}, \dot{\mathbf{q}})\, \mathrm{d}t$$

is minimised by the systems (free) trajectory.

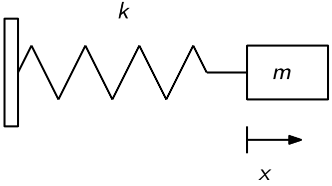


Lagrange Mechanics - A silly example



Lagrange Mechanics - A silly example

Generalized coordinates $\mathbf{q} = x$



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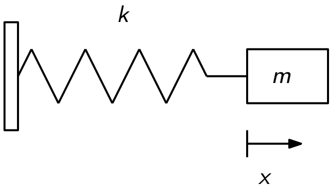

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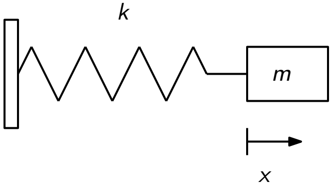

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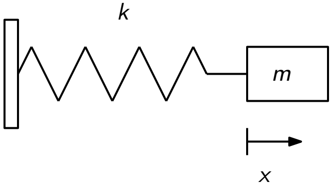

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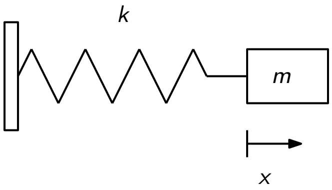

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From *variational calculus*, the free trajectories satisfy (Euler-Lagrange equation):

$$\frac{\mathrm{d}}{\mathrm{d}} \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}} - \frac{\partial \mathcal{L}}{\partial \mathbf{q}} = 0$$

Lagrange Mechanics - A silly example

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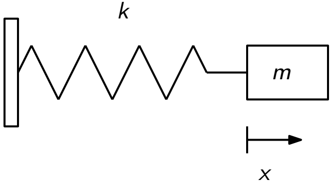

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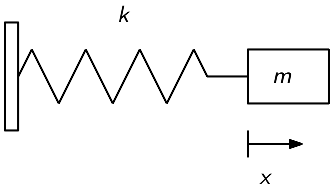

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$$\frac{\mathrm{d}}{\mathrm{d}} \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}} = m\ddot{x}$$

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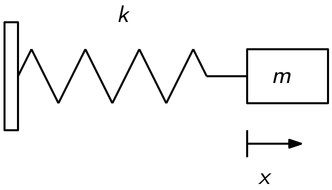

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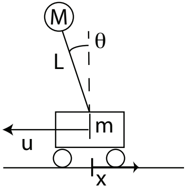
Yield the ODE:

$$m\ddot{x} + kx = 0$$

Lagrange Mechanics - Example

Generalized coordinates $\mathbf{q} = \begin{bmatrix} \theta \\ x \end{bmatrix}$

$$\begin{aligned} \text{Kinetic energy:} \quad & T(\mathbf{q}, \dot{\mathbf{q}}) = \frac{1}{2}(m+M)\dot{x}^2 + \frac{1}{2}ML^2\dot{\theta}^2 - LM\dot{\theta}\dot{x}\sin\theta \\ \text{Potential energy:} \quad & V(\mathbf{q}) = MgL\cos\theta \\ \text{Lagrange function:} \quad & \mathcal{L}(\mathbf{q}, \dot{\mathbf{q}}) = T(\mathbf{q}, \dot{\mathbf{q}}) - V(\mathbf{q}) \end{aligned}$$



From *variational calculus*, the free trajectories satisfy:

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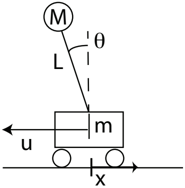

$$\text{Kinetic energy:} \quad T(\mathbf{q},\dot{\mathbf{q}}) = \frac{1}{2}(m+M)\dot{x}^2 + \frac{1}{2}ML^2\dot{\theta}^2 - LM\dot{\theta}\dot{x}\sin\theta$$

$$\text{Potential energy:} \quad V(\mathbf{q}) = MgL\cos\theta$$

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From *variational calculus*, the free trajectories satisfy:

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Yields the free trajectory:

$$\frac{\partial\mathcal{L}}{\partial\dot{\mathbf{q}}}^\top = \begin{bmatrix} (M+m)\dot{x} - ML\dot{\theta}\sin(\theta) \\ ML^2\dot{\theta} - ML\dot{x}\sin(\theta) \end{bmatrix}, \quad \frac{\partial\mathcal{L}}{\partial\mathbf{q}}^\top = \begin{bmatrix} 0 \\ MgL\sin(\theta) - ML\dot{\theta}\dot{x}\cos(\theta) \end{bmatrix}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial\dot{\mathbf{q}}}^\top = \begin{bmatrix} -ML\cos(\theta)\dot{\theta}^2 + \ddot{x}(M+m) - ML\ddot{\theta}\sin(\theta), \\ -ML\ddot{x}\sin(\theta) + ML^2\ddot{\theta} - ML\dot{\theta}\dot{x}\cos(\theta)) \end{bmatrix}$$

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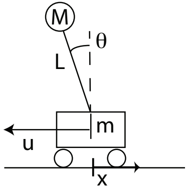

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$$\begin{bmatrix} M+m & -ML\sin(\theta) \\ -ML\sin(\theta) & ML^2 \end{bmatrix}\begin{bmatrix} \ddot{x} \\ \ddot{\theta} \end{bmatrix} = \begin{bmatrix} ML\dot{\theta}^2\cos(\theta) \\ MgL\sin(\theta) \end{bmatrix}$$

Useful tip: the whole procedure can be easily coded in a CAS.

Lagrange Mechanics - External Forces

Consider a system described by the **generalized coordinates** $\mathbf{q}$ with:

$$\begin{aligned} \text{Kinetic energy:} \quad & T(\mathbf{q}, \dot{\mathbf{q}}) \\ \text{Potential energy:} \quad & V(\mathbf{q}) \end{aligned}$$

Define the **Lagrange function**: $\mathcal{L}(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{z}) = T - V$.

Then the free dynamics are given by

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$$\frac{\mathrm{d}}{\mathrm{d}} \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}} - \frac{\partial \mathcal{L}}{\partial \mathbf{q}} = 0$$

... and the *forced* dynamics are given by

$$\frac{\mathrm{d}}{\mathrm{d}} \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}} - \frac{\partial \mathcal{L}}{\partial \mathbf{q}} = \mathbf{F}_{\mathrm{g}}$$

where $\mathbf{F}_{\mathrm{g}}$ are the **generalized forces**

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$$\underbrace{\delta W}_{\textit{work}} = \langle \mathbf{F}_{\mathrm{g}}, \, \delta \mathbf{q} \rangle$$

is satisfied for all compatible displacement $\delta \mathbf{q}$.

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DAE modeling using Lagrange Mechanics

Consider a system described by the **generalized coordinates** $\mathbf{q}$ with:

$$\begin{aligned} \text{Kinetic energy:} \quad & T\left(\mathbf{q}, \dot{\mathbf{q}}\right) \\ \text{Potential energy:} \quad & V\left(\mathbf{q}\right) \end{aligned}$$

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Define the **Lagrange function**:

$$\mathcal{L}\left(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{z}\right) = T\left(\mathbf{q}, \dot{\mathbf{q}}\right) - V\left(\mathbf{q}\right) - \mathbf{z}^\top \mathbf{c}\left(\mathbf{q}\right)$$

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$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}} \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}} - \frac{\partial \mathcal{L}}{\partial \mathbf{q}} &= \mathbf{F}_{\mathrm{g}} \\ \mathbf{c}(\mathbf{q}) &= 0 \end{aligned}$$

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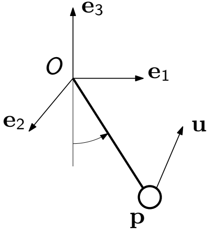
The "force" keeping the system on $\mathbf{c}(\mathbf{q}) = 0$ is in the space spanned by $\nabla_\mathbf{q} \mathbf{c}_i$

3D pendulum in Lagrange Mechanics

Generalized coordinates: $\mathbf{q} \equiv \mathbf{p}$, and:



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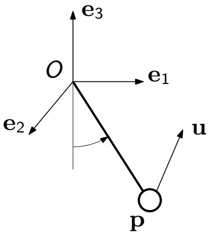

Lagrange function: $\mathcal{L} = \frac{1}{2} m \dot{\mathbf{p}}^\top \dot{\mathbf{p}} - mg\mathbf{e}_3^\top \mathbf{p} - \frac{1}{2} z \left(\mathbf{p}^\top \mathbf{p} - L^2\right)$ yields:

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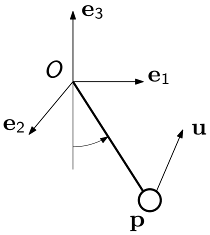

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Using $\frac{\mathrm{d}}{\mathrm{d}} \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}} - \frac{\partial \mathcal{L}}{\partial \mathbf{q}} = \mathbf{u}$ the dynamics read as

$$m\ddot{\mathbf{p}} + mg\mathbf{e}_3 + z\mathbf{p} = \mathbf{u}$$
$$\frac{1}{2}\left(\mathbf{p}^\top \mathbf{p} - L^2\right) = 0$$

Delta robot in Lagrange Mechanics

L: length "long" arms
l: length "small" arms
d: distance center-motors

- Position of the nacelle $\mathbf{p} \in \mathbb{R}^3$.

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$$\mathbf{p}_k^{\mathrm{R}} = \begin{bmatrix} \cos\gamma_k & -\sin\gamma_k & 0 \\ \sin\gamma_k & \cos\gamma_k & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} d + l\cos\alpha_k \\ 0 \\ -l\sin\alpha_k \end{bmatrix}$$

where $\gamma_{1,2,3} = \left\{0, \frac{2\pi}{3}, \frac{4\pi}{3}\right\}$.

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Outline

1. Introduction
2. Lagrange Mechanics in a Nutshell
3. A first view on approaching DAEs numerically

Handling semi-explicit DAEs

Semi-explicit DAE:

$$\dot{\mathbf{x}} = \mathbf{F}(\mathbf{x}, \mathbf{z}, \mathbf{u})$$
$$0 = \mathbf{G}(\mathbf{x}, \mathbf{z}, \mathbf{u})$$

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of $\mathbf{G}(\mathbf{x}, \mathbf{z}, \mathbf{u}) = 0$, i.e.

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- Function $\boldsymbol{\xi}$ may not exist explicitly or may have a very high symbolic complexity...
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Does $\boldsymbol{\xi}(\mathbf{x}, \mathbf{u})$ necessarily exist ?!? Only if $\nabla_{\mathbf{z}}\mathbf{G}$ is full rank (Implicit Function Theorem) !!

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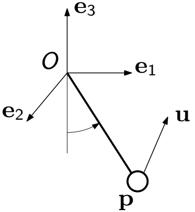
Position given by $\mathbf{p} \in \mathbb{R}^3$, dynamics:

$$m\ddot{\mathbf{p}} = \mathbf{u} - mg\mathbf{e}_3 - z\mathbf{p}$$



Force in the cable: direction given by $-\mathbf{p}$, amplitude given by algebraic variable z

Algebraic variable z must be chosen such that:

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holds at all time.

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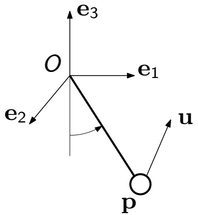

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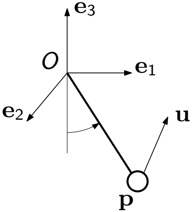

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with $\mathbf{x} = \begin{bmatrix} \mathbf{p} \\ \mathbf{v} \end{bmatrix}$

Does $\mathbf{z} = \boldsymbol{\xi}(\mathbf{x}, \mathbf{u})$ necessarily exist ?!? Only if $\nabla_{\mathbf{z}} \mathbf{G}$ is full rank !!

Semi-explicit DAE

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{F}(\mathbf{x}, \mathbf{u}, z) \\ 0 &= \mathbf{G}(\mathbf{x}) \end{aligned}$$

with $\mathbf{G}$ independent of z !! Then $\nabla_{\mathbf{z}} \mathbf{G}(\mathbf{x}) = 0$... not full rank !!

Handling fully-implicit DAEs

Fully implicit DAE:

$$\mathbf{F}\left(\dot{\mathbf{x}}, \mathbf{z}, \mathbf{x}, \mathbf{u}\right) = 0$$

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of $\mathbf{F}\left(\dot{\mathbf{x}}, \mathbf{z}, \mathbf{x}, \mathbf{u}\right) = 0$, i.e.

$$\mathbf{F}\left(\boldsymbol{\xi}_1\left(\mathbf{x}, \mathbf{u}\right), \boldsymbol{\xi}_2\left(\mathbf{x}, \mathbf{u}\right), \mathbf{x}, \mathbf{u}\right) = 0$$

holds for all $\mathbf{x}, \mathbf{u}$.

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Then one can write the ODE:

$$\dot{\mathbf{x}} = \boldsymbol{\xi}_1\left(\mathbf{x}, \mathbf{u}\right)$$

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$$\mathbf{F}\left(\dot{\mathbf{x}}, \mathbf{z}, \mathbf{x}, \mathbf{u}\right) = 0$$

E.g.

$$M\left(\mathbf{x}\right)\left[\begin{array}{c}\dot{\mathbf{x}}\\ \mathbf{z}\end{array}\right] = \mathbf{f}$$

with $z \in \mathbb{R}^m$ and $\mathbf{x} \in \mathbb{R}^n$.

Find solution:

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DAE can be solved as:

$$\begin{bmatrix} \dot{\mathbf{x}} \\ \mathbf{z} \end{bmatrix} = M(\mathbf{x})^{-1} \mathbf{f}$$

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holds for all $\mathbf{x}, \mathbf{u}$.

Then one can write the ODE:

$$\dot{\mathbf{x}} = \boldsymbol{\xi}_1(\mathbf{x}, \mathbf{u})$$

- Symbolic inverse of $M(\mathbf{x})$ can be very complex for n large
- Can be inverted numerically "on-the-fly" to generate $\dot{\mathbf{x}}$ (and $\mathbf{z}$ as a by-product), and then use an ODE integrator.
- Functions $\boldsymbol{\xi}_1$ and $\boldsymbol{\xi}_2$ exist only if $\nabla_{\dot{\mathbf{x}},\mathbf{z}}\mathbf{F}$ is full rank !!

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Implicit integration for semi-explicit DAEs - A first view

Semi-explicit DAE:

$$\begin{aligned}\dot{\mathbf{x}} &= \mathbf{F}\left(\mathbf{x},\mathbf{z},\mathbf{u}\right)\\ 0 &= \mathbf{G}\left(\mathbf{x},\mathbf{z},\mathbf{u}\right)\end{aligned}$$

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BDF method (m-steps, size Δt)

$$\begin{aligned} \mathbf{x}_{k+1} &= -\sum_{j=1}^{m} a_j \mathbf{x}_{k+1-j} + \Delta t b_m \mathbf{F}\left(\mathbf{x}_{k+1}, \mathbf{z}_{k+1}, \mathbf{u}\right) \\ 0 &= \mathbf{G}\left(\mathbf{x}_{k+1}, \mathbf{z}_{k+1}, \mathbf{u}\right) \end{aligned}$$

where a_j and b_m are given by the Butcher tableau.

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Special case - Implicit Euler

$$\begin{aligned} \mathbf{x}_{k+1} &= \mathbf{x}_k + \Delta t \mathbf{F}\left(\mathbf{x}_{k+1}, \mathbf{z}_{k+1}, \mathbf{u}\right) \\ 0 &= \mathbf{G}\left(\mathbf{x}_{k+1}, \mathbf{z}_{k+1}, \mathbf{u}\right) \end{aligned}$$

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Residual:

$$\mathbf{r}\left(\mathbf{x}_{k+1}, \mathbf{z}_{k+1}, \mathbf{x}_k, \mathbf{u}\right) = \left[\begin{array}{c} \mathbf{x}_{k+1} - \mathbf{x}_k - \Delta t \mathbf{F}\left(\mathbf{x}_{k+1}, \mathbf{z}_{k+1}, \mathbf{u}\right) \\ \mathbf{G}\left(\mathbf{x}_{k+1}, \mathbf{z}_{k+1}, \mathbf{u}\right) \end{array}\right] = 0$$

to solve for $\mathbf{x}_{k+1}$, $\mathbf{z}_{k+1}$

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to solve for $\mathbf{x}_{k+1}$, $\mathbf{z}_{k+1}$ using Newton based on:

$$\nabla_{\mathbf{x}_{k+1}, \mathbf{z}_{k+1}} \mathbf{r}\left(\mathbf{x}_{k+1}, \mathbf{z}_{k+1}, \mathbf{x}_k, \mathbf{u}\right) = \left[\begin{array}{cc} I - \Delta t \nabla_{\mathbf{x}_{k+1}} \mathbf{F} & \nabla_{\mathbf{x}_{k+1}} \mathbf{G} \\ -\Delta t \nabla_{\mathbf{z}_{k+1}} \mathbf{F} & \nabla_{\mathbf{z}_{k+1}} \mathbf{G} \end{array} \right]$$

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Note that this requires (among other things) $\nabla_{\mathbf{z}_{k+1}} \mathbf{G}$ to have a correct rank.

DAEs are not "just" ODEs with an algebraic extension

Fully-implicit linear DAE:

$$E\dot{\mathbf{x}} = A\mathbf{x} + B\mathbf{u}$$

with $E = \frac{\partial \mathbf{F}}{\partial \dot{\mathbf{x}}}$ rank deficient. E.g.

$$E = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}, \quad A = I, \quad B = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

reads as:

$$\begin{aligned} \dot{\mathbf{x}}_2 &= \mathbf{x}_1 \\ \dot{\mathbf{x}}_3 &= \mathbf{x}_2 \\ \mathbf{x}_3 &= -\mathbf{u} \end{aligned}$$

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$$\frac{1}{h}E\left(\mathbf{x}_+ - \mathbf{x}(t)\right) = A\mathbf{x}_+ + B\mathbf{u}_+$$

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$$E\left[\frac{1}{h}\left(\mathbf{x}\left(t+h\right) - \mathbf{x}\left(t\right)\right) + \frac{h}{2}\ddot{\mathbf{x}}\left(\xi\right)\right] = A\mathbf{x}\left(t+h\right) + B\mathbf{u}\left(t+h\right)$$

for some $\xi \in [t,\ t+h]$.

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for some $\xi \in [t,\, t+h]$. Integration error is:

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- E full rank (ODE), the error is of $\mathcal{O}\left(h^2\right)$ (error for implicit Euler)
- E rank deficient, then $E - Ah$ tends to a singular matrix for $h \to 0$. The error **can be** of order $\mathcal{O}\left(h\right)$ or even $\mathcal{O}\left(1\right)$!!