OPENMODELICA FOR OPTIMIZATION

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OUTLINE

- Modelica and Optimization
- Theoretical Background
  - multiple shooting method
  - total collocation
  - handling
- Current status & Outlook

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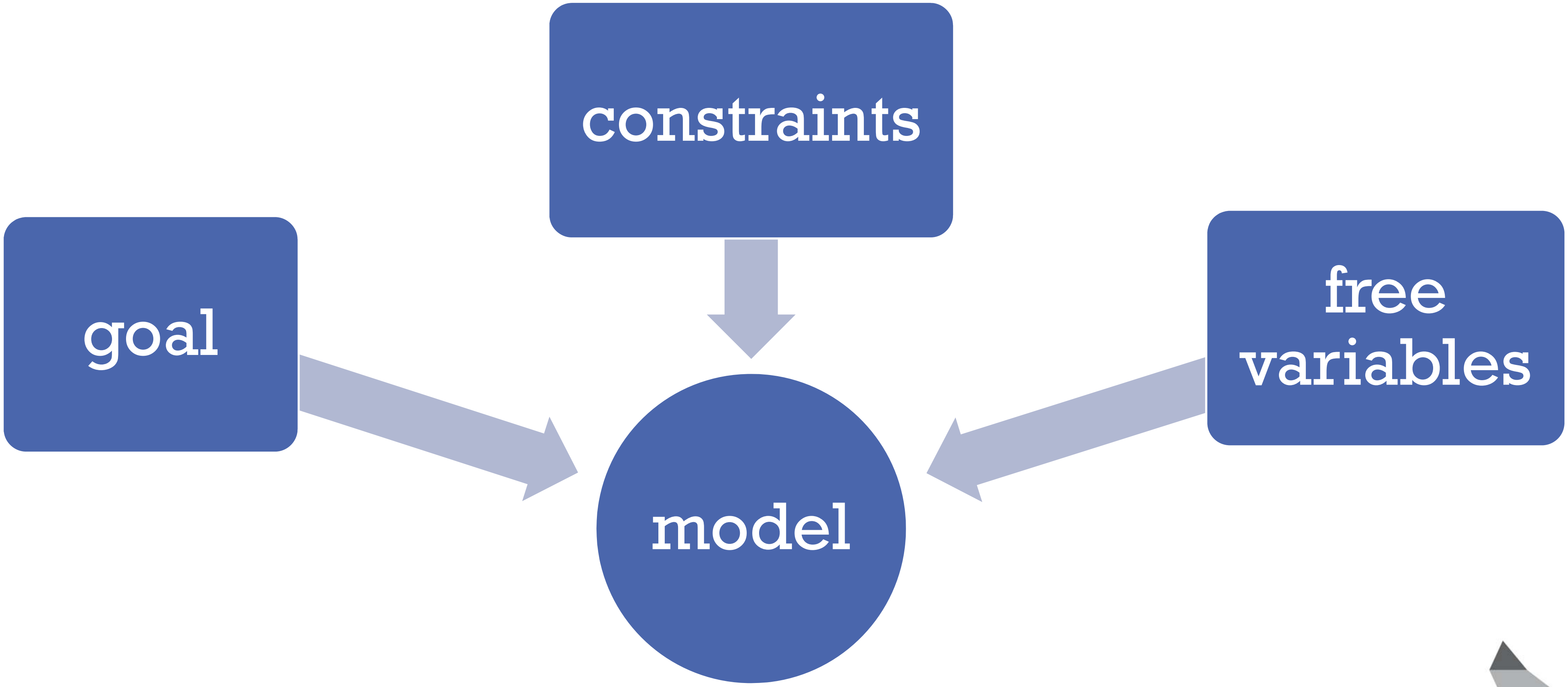
MODELICA AND OPTIMIZATION



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EXAMPLE CHEMICAL BATCH REACTOR

- model

$$\dot{x}_1(t) = -\left(u(t) + \frac{u^2(t)}{2}\right) \cdot x_1(t)$$
$$\dot{x}_2(t) = u(t) \cdot x_1(t)$$

- goal → Maximize the yield of x_2 after one hour of operation

$$\min_{u(t)} \; -x_2(1)$$

- constraints

$$0 \leq x_1(t), x_2(t) \leq 1$$
$$0 \leq u(t) \leq 5$$

- free input → the reaction temperature → $u(t)$

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OPTIMICA LANGUAGE EXTENSION

- Objective function
  - Mayer term
  - Lagrange term
- Path constrains
- New attribute *free*
- *…*

- A part of the MODRIO-Project

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OPTIMICA LANGUAGE EXTENSION

```
optimization modelName(
objective=....,
objectiveIntegrand=....)
    -> Modelica model;
constraints
    ...
end modelName
```

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THEORETICAL BACKGROUND

- objective function

$$\min_{u(t)} \underbrace{M\left(x(t_f)\right)}_{\text{Mayer term}} + \underbrace{\int_{t_0}^{t_f} L(x(t), u(t), t)\, dt}_{\text{Lagrange term}}$$

- subject to
  - model equations
  - path constraints

MULTIPLE SHOOTING

- Mayer term

$$M\left(x(t_f)\right)$$

- requirements for the endpoint → boundary value problem

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MULTIPLE SHOOTING

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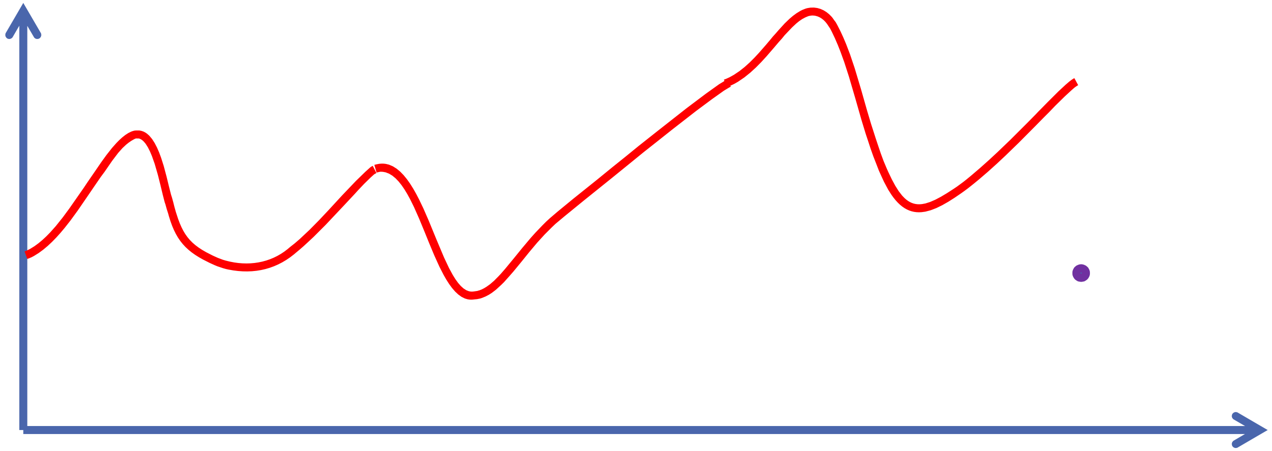

MULTIPLE SHOOTING

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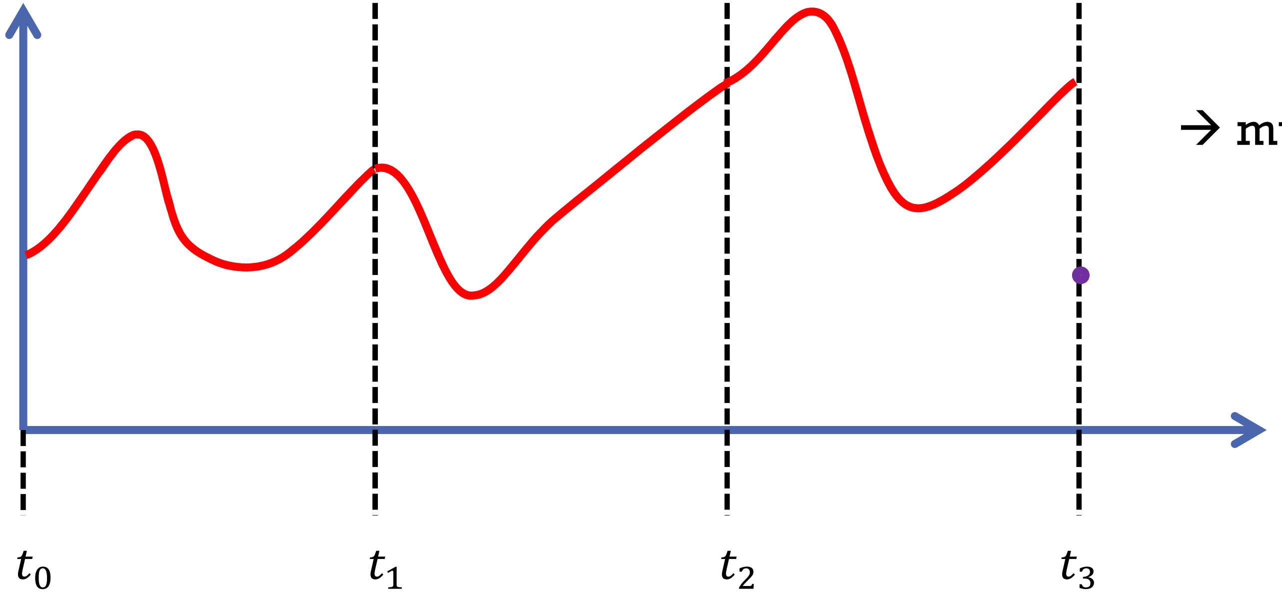

→ multiple shooting method principle

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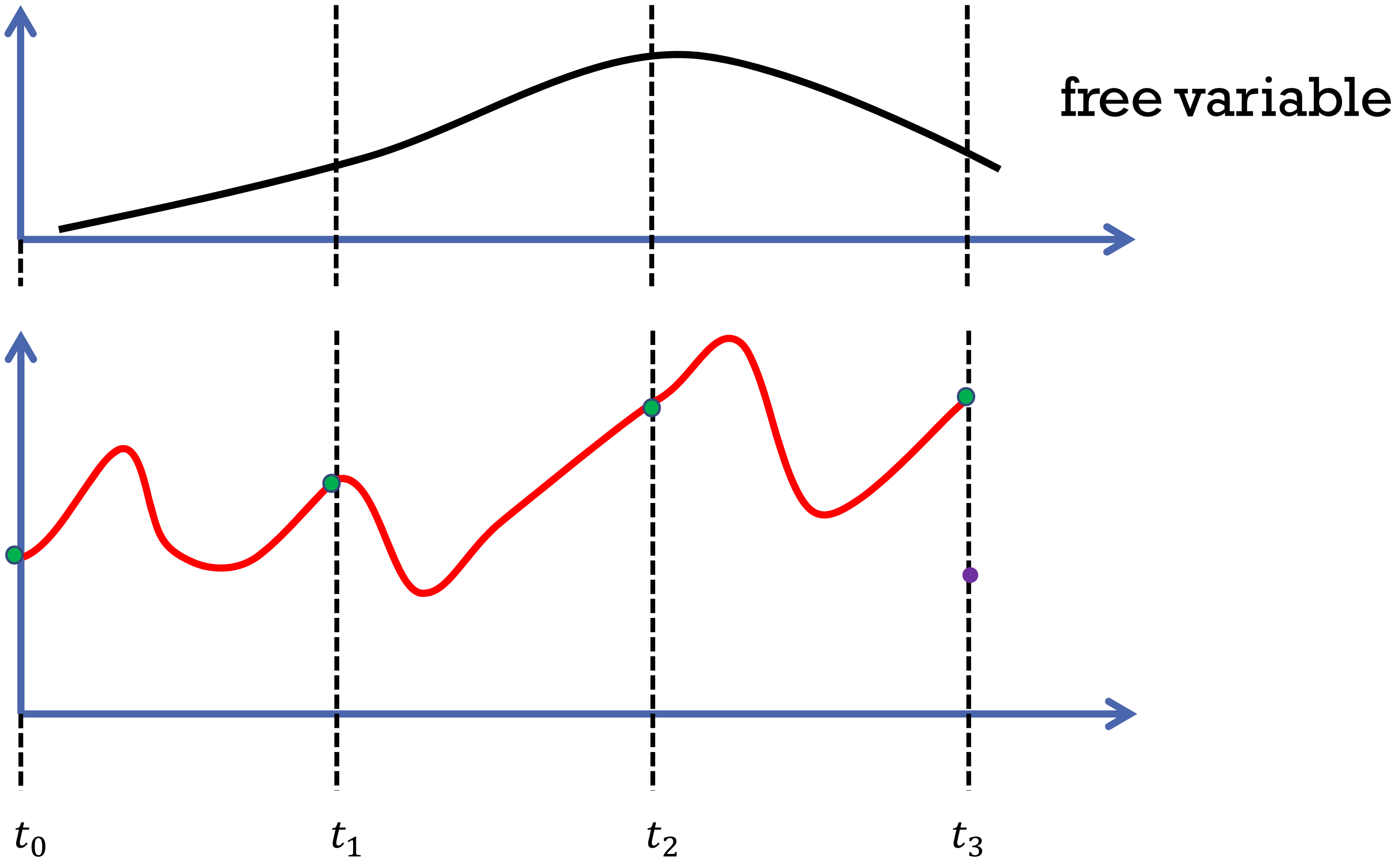
MULTIPLE SHOOTING



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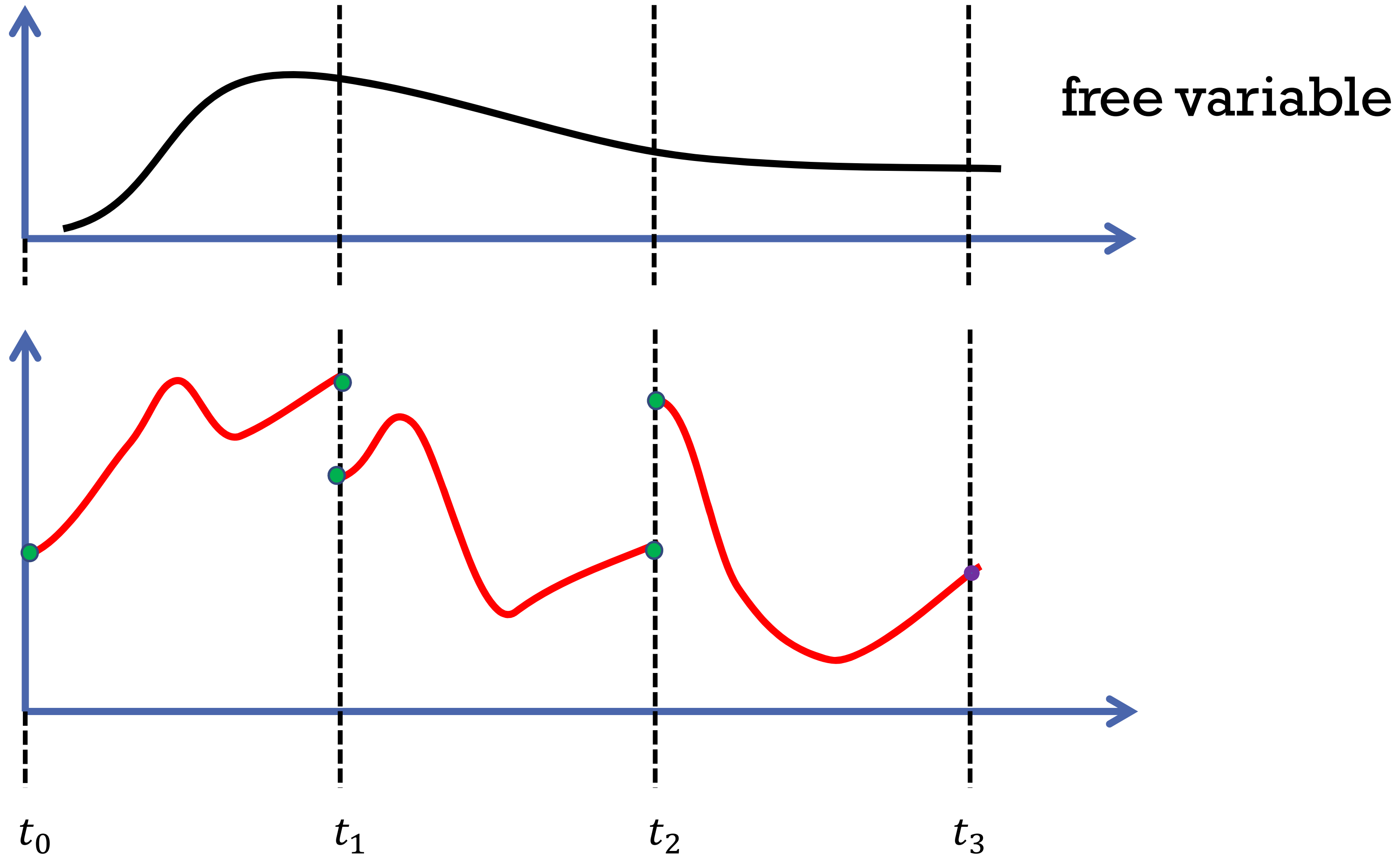
MULTIPLE SHOOTING



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MULTIPLE SHOOTING

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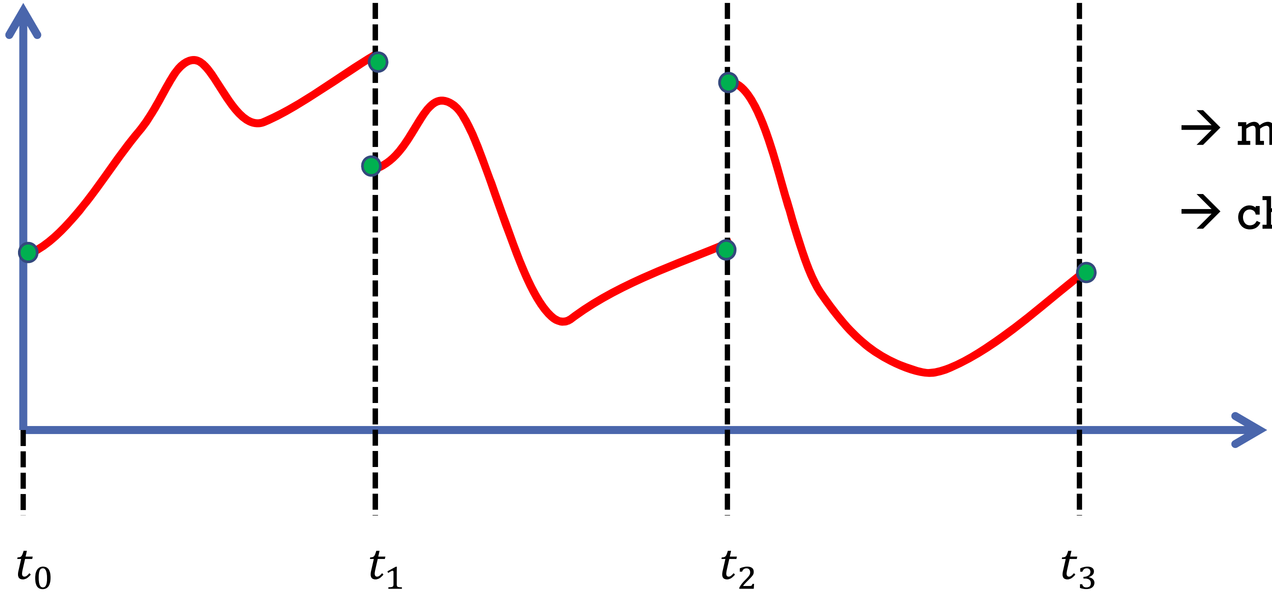

→ multiple shooting method principle

→ change of the free variable

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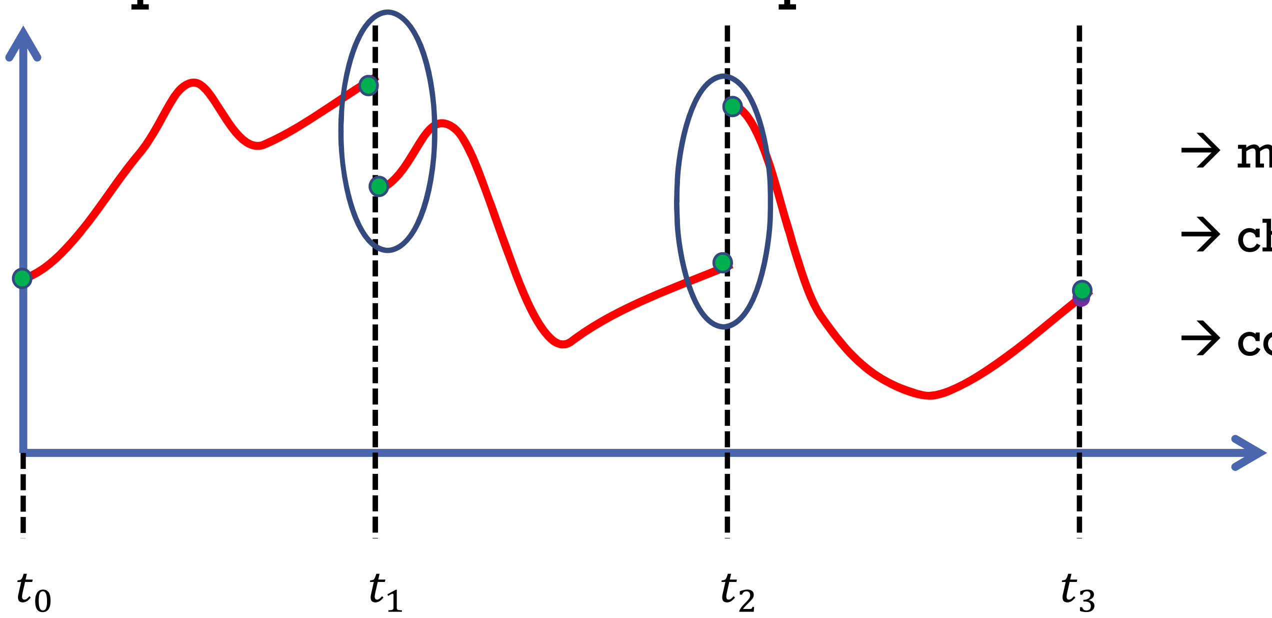
MULTIPLE SHOOTING

- Mayer term

$$M\left(x(t_f)\right)$$

- requirements for the endpoint → boundary value problem



→ multiple shooting method principle

→ change of the free variable

→ continuity conditions

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MULTIPLE SHOOTING

- Mayer term

$$M\left(x(t_f)\right)$$

- requirements for the endpoint → boundary value problem
  → multiple shooting method principle
  → change of the free variable
  → continuity conditions

TOTAL COLLOCATION

- Lagrange term

$$\int_{t_0}^{t_f} L(x(t), u(t), t)\, dt \approx \Delta t \cdot \sum_{j=1}^{m} w_j \sum_{i=0}^{n-1} L\left(x\left(t_{i,j}\right), u\left(t_{i,j}\right), t_{\mathrm{i,j}}\right)$$

- quadrature formula with m abscissas
  - Legendre
  - Radau
  - Lobatto
- $w_j, t_{i,j}$ is given by the quadrature formula

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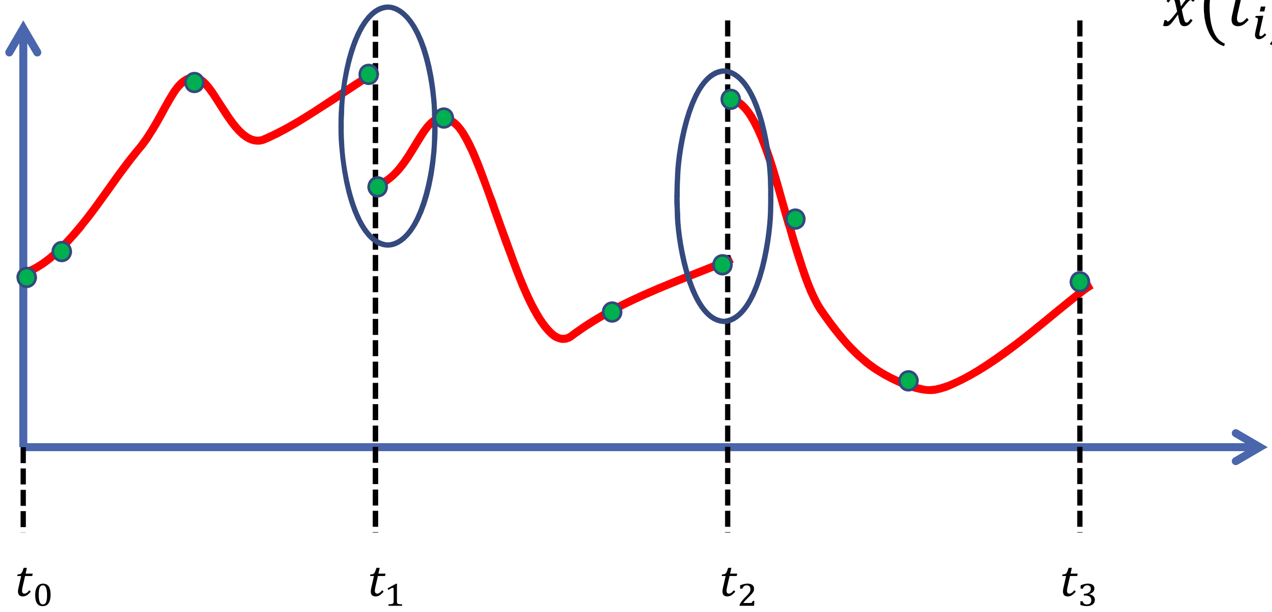
TOTAL COLLOCATION

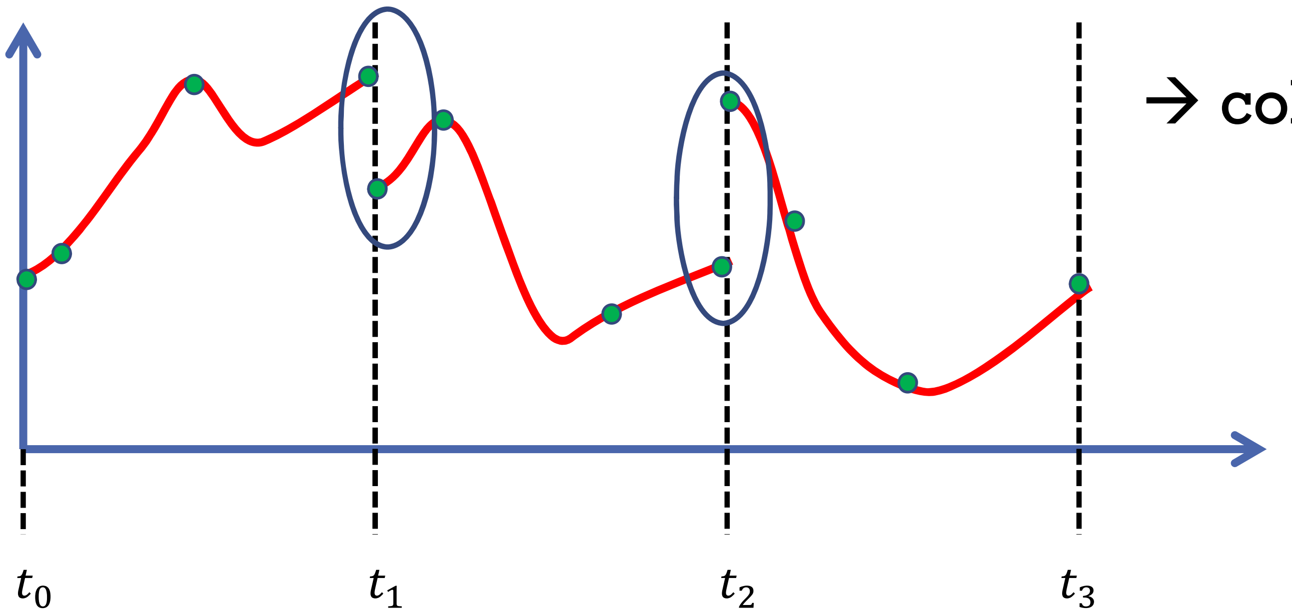
$$\Delta t \cdot \sum_{j=1}^{m} w_j \sum_{i=0}^{n-1} L\left(x\left(t_{i,j}\right), u\left(t_{i,j}\right), t_{\mathrm{i,j}}\right)$$

$x\left(t_{i,j}\right), u\left(t_{i,j}\right)$ are needed



TOTAL COLLOCATION

$$\Delta t \cdot \sum_{j=1}^{m} w_j \sum_{i=0}^{n-1} L\left(x\left(t_{i,j}\right), u\left(t_{i,j}\right), t_{\mathrm{i,j}}\right)$$



→ collocation method

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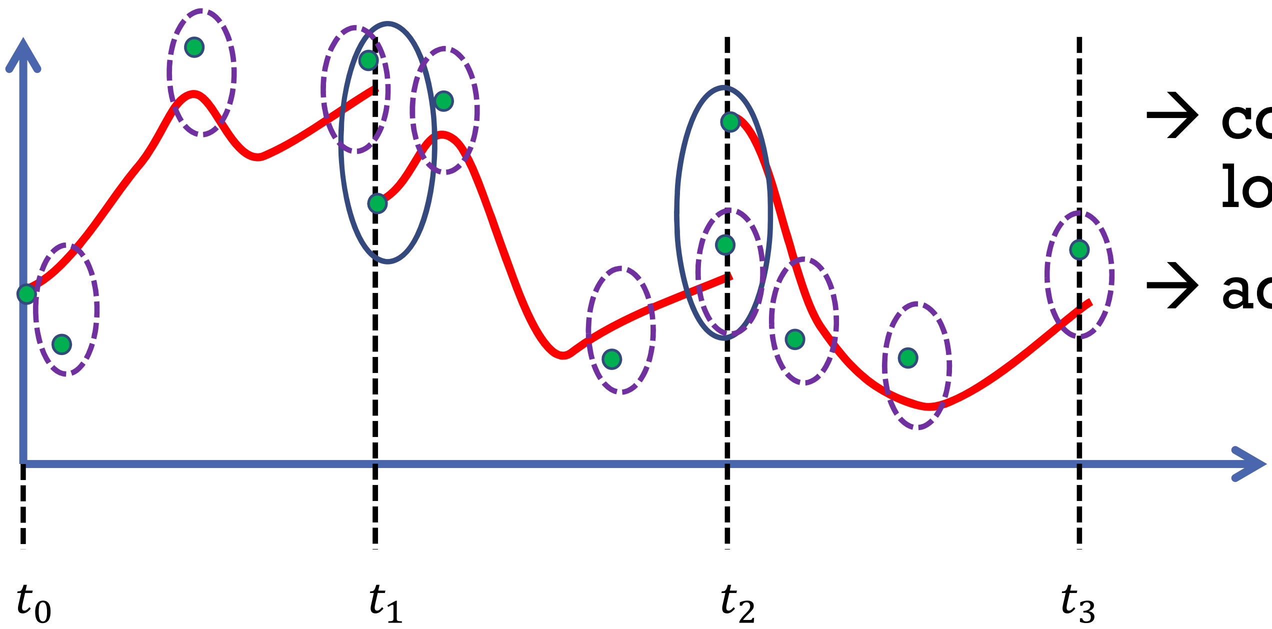
TOTAL COLLOCATION

$$\Delta t \cdot \sum_{j=1}^{m} w_j \sum_{i=0}^{n-1} L\big(x(t_{i,j}), u(t_{i,j}), t_{i,j}\big)$$



→ collocation method in the loop

→ add collocation conditions

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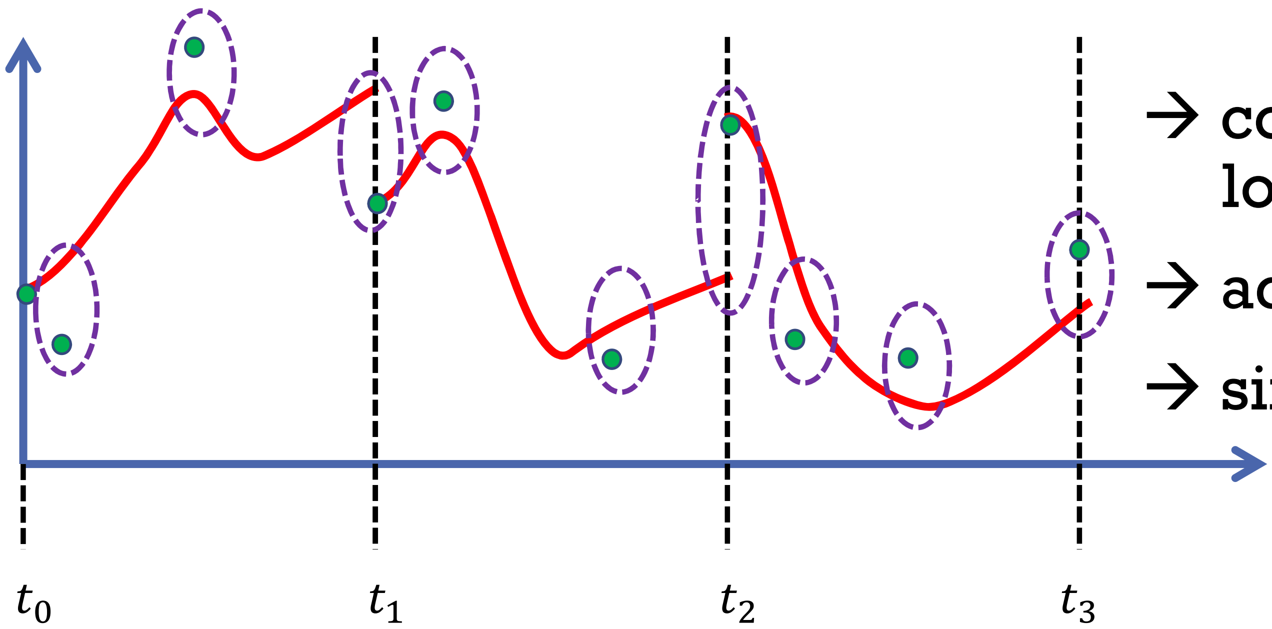
TOTAL COLLOCATION

$$\Delta t \cdot \sum_{j=1}^{m} w_j \sum_{i=0}^{n-1} L\left(x\left(t_{i,j}\right), u\left(t_{i,j}\right), t_{\mathrm{i,j}}\right)$$



→ collocation method in the loop

→ add collocation conditions

→ simplify → Radau IIA or Lobatto IIIA

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HANDLING

- Collocation method and Jacobian structure

$$x_0 + \Delta t \cdot A \cdot f = x$$

- Example

$$res := \begin{pmatrix} x_0 \\ x_0 \\ x_0 \end{pmatrix} + \Delta t \cdot \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \cdot \begin{pmatrix} f(x_1, u_1) \\ f(x_2, u_2) \\ f(x_3, u_3) \end{pmatrix} - \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \overset{!}{=} 0$$

$$\frac{\partial res}{\partial \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}} = \Delta t \cdot \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \cdot \begin{pmatrix} * & 0 & 0 \\ 0 & * & 0 \\ 0 & 0 & * \end{pmatrix} = \begin{pmatrix} * & * & * \\ * & * & * \\ * & * & * \end{pmatrix}$$

HANDLING

- Collocation method and Jacobian structure

$$x_0 + \Delta t \cdot A \cdot f = x \rightarrow \Delta t \cdot f = A^{-1} \cdot (x - x_0)$$

- Example

$$res := \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}^{-1} \cdot \left(\begin{pmatrix} x_0 \\ x_0 \\ x_0 \end{pmatrix} - \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \right) + \Delta t \cdot \begin{pmatrix} f(x_1, u_1) \\ f(x_2, u_2) \\ f(x_3, u_3) \end{pmatrix} \stackrel{!}{=} 0$$

$$\frac{\partial res}{\partial \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}} = \begin{pmatrix} * & 0 & 0 \\ 0 & * & 0 \\ 0 & 0 & * \end{pmatrix}$$

HANDLING

Lagrange-term

- Example Radau quadrature

$$\frac{3}{4}\cdot L\left(x\left(t_i+\frac{1}{3}\Delta t\right),u\left(t_i+\frac{1}{3}\Delta t\right),\mathrm{t_i}+\frac{1}{3}\Delta t\right)+\frac{1}{4}\cdot L(x(t_i+1\cdot\Delta t),u(t_i+1\cdot\Delta t),\mathrm{t_i}+1\cdot\Delta t)$$

- $u(t_0)$ not included in the objective function!
- Lobatto IIIA for the first subinterval

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HANDLING

- Differences between Radau IIA and Lobatto IIIA
  - Radau IIA
    - more sparse structure
    - a high stability
  - Lobatto IIIA
    - continuously differentiable continuation

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HANDLING

- Differences between multiple shooting and total collocation
  - multiple shooting
    - more sparse structure
    - reduced search space
  - total collocation
    - no need to solve nonlinear system in optimization step
    - easier to generate Jacobian, gradient,… for optimizer

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THEORETICAL BACKGROUND

- path constraints
  - evaluate on the collocation points
  - evaluate on the multiple shooting points

CURRENT STATE & OUTLOOK

- Current Status
  - Optimica+Modelica parser and AST building already works
  - C-Code generation for Lagrange- ,Mayer term and path constraints exist
  - numerical differentiation partially automated for the problem

- Outlook
  - generate the equations in Compilier
    - symbolic preprocessing
    - symbolic differentiation

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THANK YOU
QUESTIONS?

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