Guaranteed co-simulation of continuous-time dynamical systems

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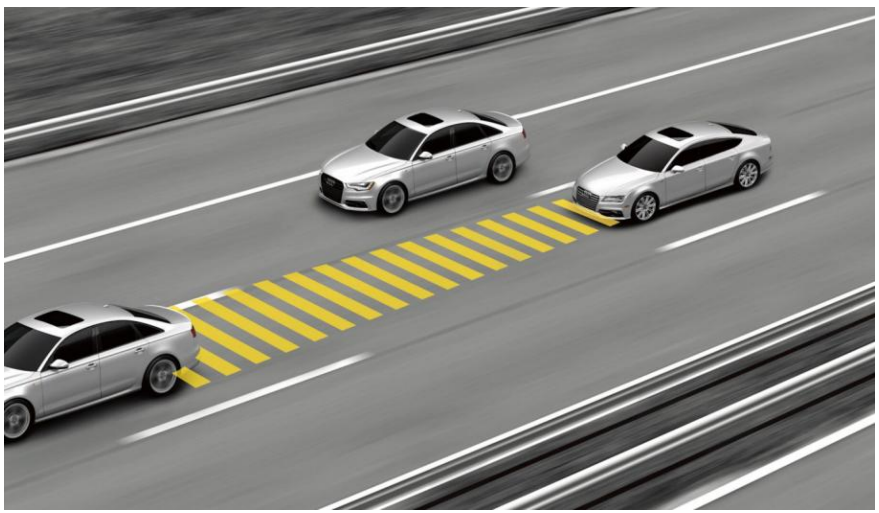
Context : Cyber-Physical Systems



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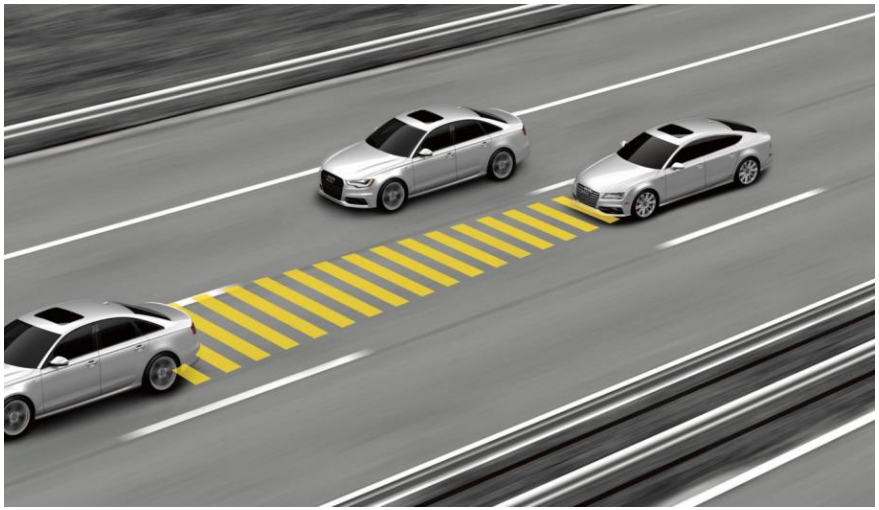

Model-based design of cyber-physical systems :

modeling, analysis, controller synthesis, **simulation**, deployment

Guaranteed Simulation Cyber-Physical Systems

Applications : verification, parameter and/or control synthesis, safety critical systems, **reachability analysis**

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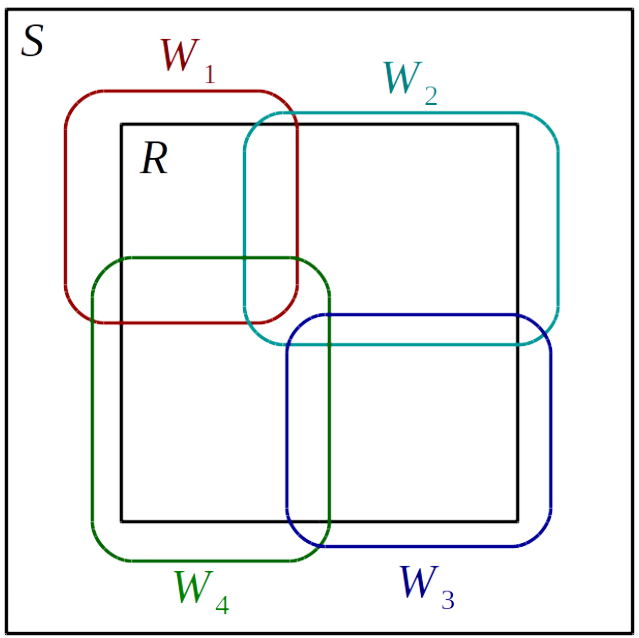
Example of a controller synthesis algorithm for a switched system:

$$\dot{x}(t) = f_{\sigma(t)}(x(t), d(t))$$

Goal: from any $x \in R$, return in R while always staying in S.



Basic idea:

- Generate a covering of R

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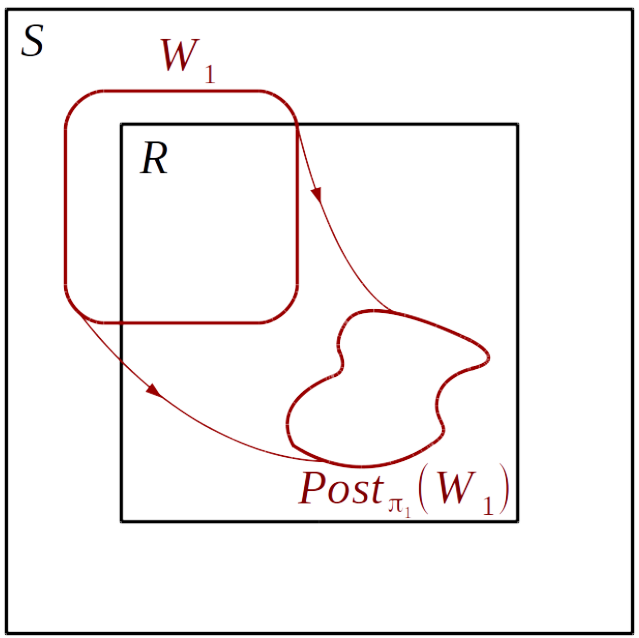

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- Look for patterns (input sequences) mapping the tiles into R while always staying in S

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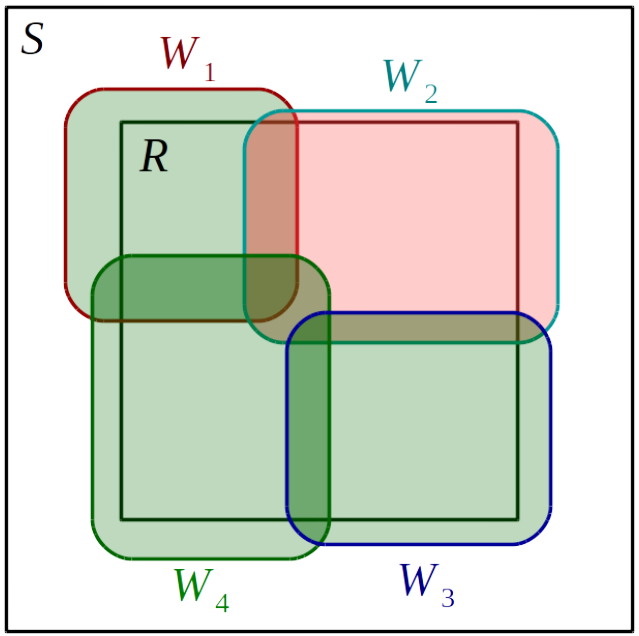

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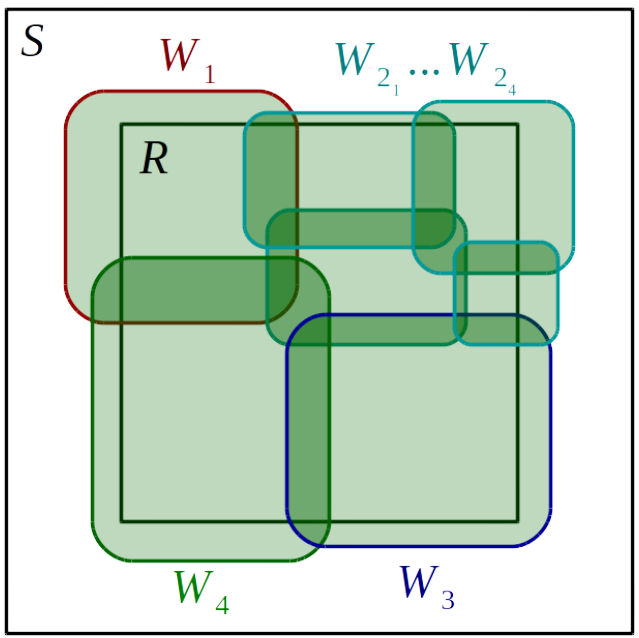

Basic idea:

- Generate a covering of R
- Look for patterns (input sequences) mapping the tiles into R while always staying in S
- If it fails, generate another covering.

Numerical integration, reachability analysis, state-of-the-art

- Classical (non guaranteed) methods: Euler, Runge-Kutta, implicit, explicit schemes...
- Guaranteed reachability analysis: Enclosing solutions, error bounding, additional hypotheses

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  - Monotonicity, ISS, incremental stability [Girard, Sontag, Zamani, Tabuada...]
  - Validated simulation, guaranteed integration [Moore, Lohner, Bertz, Makino, Nedialkov, Jackson, Corliss, Chen, Ábrahám, Sankaranarayanan, Taha, Chapoutot,...]
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  - Sensitivity Analysis [Donzé, Maler...]
- Data structures:
  - Reachability analysis using zonotopes [Dang, Girard, Althoff...]
  - Ellipsoid methods [Kurzhanski, Varaiya, Dang...]

Initial Value Problem of Ordinary Differential Equations

Consider an IVP for ODE, over the time interval $[0, t_{\text{end}}]$

$$\dot{\mathbf{x}} = f(\mathbf{x}, \mathbf{p}) \quad \text{with} \quad \mathbf{x}(0) = \mathbf{x}_0, \ \mathbf{p} \text{ bounded},$$

for a given perturbation $\mathbf{p}(\cdot)$, IVP has a unique solution $\mathbf{x}(t; \mathbf{y}_0, \mathbf{p})$ if $f : \mathbb{R}^n \to \mathbb{R}^n$ is Lipschitz in $\mathbf{y}$ and $f(\cdot, \mathbf{p}(\cdot))$ continuous
but for our purpose we suppose f smooth enough, *i.e.*, of class C^k

Goal of numerical integration

- Compute a sequence of time instants: $t_0 = 0 < t_1 < \cdots < t_n = t_{\text{end}}$
- Compute a sequence of values: $\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_n$ such that

$$\forall \ell \in [0, n], \quad \mathbf{x}_\ell \approx \mathbf{x}(t_\ell; \mathbf{x}_0, \mathbf{p}) \ .$$

- s.t. $\mathbf{x}_{\ell+1} \approx \mathbf{x}(t_\ell + h; \mathbf{x}_\ell, \mathbf{p})$ with an error $\mathcal{O}(h^{p+1})$ where
  - h is the integration **step-size**
  - p is the **order** of the method

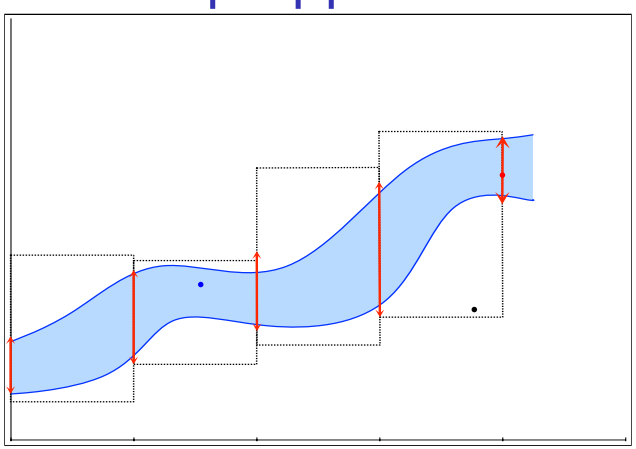
Guaranteed solution of IVP for ODE

Goal of guaranteed numerical integration

- Compute a sequence of time instants: $t_0 = 0 < t_1 < \cdots < t_n = t_{\text{end}}$
- Compute a sequence of values: $[\mathbf{x}_0], [\mathbf{x}_1], \ldots, [\mathbf{x}_n]$ such that

$$\forall \ell \in [0, n], \quad [\mathbf{x}_\ell] \ni \mathbf{x}(t_\ell; \mathbf{x}_{\ell-1}, \mathbf{p}) \ .$$

A two-step approach



- Exact solution of $\dot{\mathbf{x}} = f(\mathbf{x}, \mathbf{p})$ with $\mathbf{x}(0) \in \mathcal{Y}_0$
- Safe approximation at discrete time instants
- Safe approximation between time instants

Taylor Methods, State-of-the-art

Taylor methods

They have been developed since 60's (Moore, Lohner, Makino and Berz, Corliss and Rhim, Neher *et al.*, Jackson and Nedialkov, etc.)

- prove the existence and uniqueness: **high order interval Picard-Lindelöf**
- works very well on various kinds of problems:
  - **non stiff** and **moderately stiff** linear and non-linear systems,
  - with **thin uncertainties on initial conditions**
  - with (a writing process) **thin uncertainties on parameters**
- **very efficient** with automatic differentiation techniques
- **wrapping effect fighting**: interval centered form and QR decomposition
- **many software**: AWA, COSY infinity, VNODE-LP, CAPD, etc.

Some extensions

- Taylor polynomial with Hermite-Obreskov (Jackson and Nedialkov)
- Taylor polynomial in Chebyshev basis (T. Dzetkulic)
- etc.

One question

Why bother to define
new guaranteed numerical integration methods?

An answer: there is no silver bullet

Numerical solutions of IVP for ODEs are produced by

- Adams-Bashworth/Moulton methods
- BDF methods
- Runge-Kutta methods
- etc.

each of these methods is adapted to a particular class of ODEs

Runge-Kutta methods

- have **strong stability** properties for various kinds of problems (A-stable, L-stable, algebraic stability, etc.)
- may **preserve quadratic algebraic invariant** (symplectic methods)
- can produce **continuous output** (polynomial approximation of $\mathbf{x}(t; \mathbf{x}_0)$)

Can we benefit these properties in guaranteed computations?

History on Interval Runge-Kutta methods

- Andrzej Marciniak *et al.* work on this topic since 1999

  "The form of $\psi(t, x(t))$ is very complicated and cannot be written in a general form for an arbitrary p"

  The implementation OOIRK is not freely avalaible.

- Hartmann and Petras, ICIAM 1999
  No more information than an abstract of 5 lines.

- Bouissou and Martel, SCAN 2006 (only RK4 method)
  Implementation GRKLib is not avaliable

- Bouissou, Chapoutot and Djoudi, NFM 2013 (any explicit RK)
  Implementation is not avaliable

- Alexandre dit Sandretto and Chapoutot, 2016 (any explicit and implicit RK)
  implementation DynIBEX is open-source, combine with IBEX

Examples of Runge-Kutta methods

Single-step fixed step-size explicit Runge-Kutta method

e.g. explicit Trapzoidal method (or Heun's method)[1] is defined by:

$$\mathbf{k}_1 = f(t_\ell, \mathbf{x}_\ell) \ , \qquad \mathbf{k}_2 = f(t_\ell + 1h, \mathbf{x}_\ell + h1\mathbf{k}_1)$$

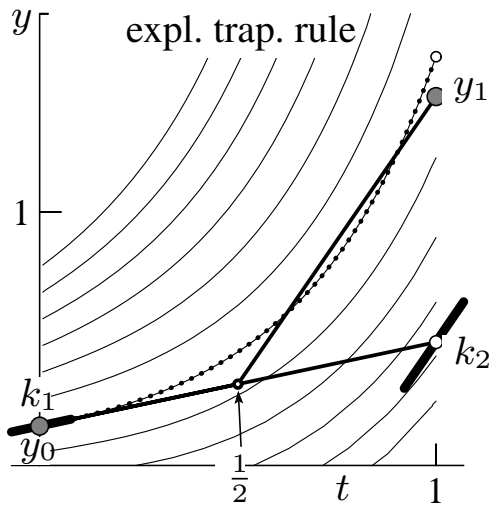
$$\mathbf{x}_{i+1} = \mathbf{x}_\ell + h\left(\frac{1}{2}\mathbf{k}_1 + \frac{1}{2}\mathbf{k}_2\right)$$

$$\begin{array}{c|cc} 0 & & \\ 1 & 1 & \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Intuition

- $\dot{x} = t^2 + x^2$
- $x_0 = 0.46$
- $h = 1.0$

dotted line is the exact solution.



[1] example coming from "Geometric Numerical Integration", Hairer, Lubich and Wanner.

Examples of Runge-Kutta methods

Single-step fixed step-size implicit Runge-Kutta method

e.g. Runge-Kutta Gauss method (order 4) is defined by:

$$\mathbf{k}_1 = f\left(t_\ell + \left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right)h, \quad \mathbf{x}_\ell + h\left(\frac{1}{4}\mathbf{k}_1 + \left(\frac{1}{4} - \frac{\sqrt{3}}{6}\right)\mathbf{k}_2\right)\right)$$

$$\mathbf{k}_2 = f\left(t_\ell + \left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right)h, \quad \mathbf{x}_\ell + h\left(\left(\frac{1}{4} + \frac{\sqrt{3}}{6}\right)\mathbf{k}_1 + \frac{1}{4}\mathbf{k}_2\right)\right)$$

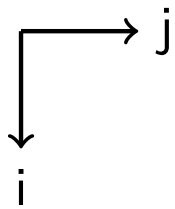
$$\mathbf{x}_{\ell+1} = \mathbf{x}_\ell + h\left(\frac{1}{2}\mathbf{k}_1 + \frac{1}{2}\mathbf{k}_2\right)$$

Remark: A non-linear system of equations must be solved at each step.

Runge-Kutta methods

s-stage Runge-Kutta methods are described by a Butcher tableau

$$\begin{array}{c|ccc|l} c_1 & a_{11} & \cdots & a_{1s} & \\ \vdots & \vdots & & \vdots & \\ c_s & a_{s1} & \cdots & a_{ss} & \\ \hline & b_1 & \cdots & b_s & \\ & b'_1 & \cdots & b'_s & \text{(optional)} \end{array}$$



which induces the following algorithm

$$\mathbf{k}_i = f\left(t_\ell + c_i h_\ell, \quad \mathbf{x}_\ell + h_\ell \sum_{j=1}^{s} a_{ij}\mathbf{k}_j\right), \qquad \mathbf{x}_{\ell+1} = \mathbf{x}_\ell + h_\ell \sum_{i=1}^{s} b_i \mathbf{k}_i$$

- **Explicit** method (ERK) if $a_{ij} = 0$ is $i \leqslant j$
- **Diagonal Implicit** method (DIRK) if $a_{ij} = 0$ is $i \leqslant j$ and at least one $a_{ii} \neq 0$
- **Implicit** method (IRK) otherwise

Guaranteed Runge-Kutta methods

A guaranteed algorithm

$$[\mathbf{x}_{\ell+1}] = [\mathrm{RK}]\,(h, [\mathbf{x}_\ell]) + \mathrm{LTE} \ .$$

Challenges

1. Computing with sets of values taking into account dependency problem and wrapping effect;
2. Bounding the approximation error of Runge-Kutta formula.

Our approach

- **Problem 1** is solved using **affine arithmetic** replacing centered form and QR decomposition
- **Problem 2** is solved by bounding the **Local Truncation Error** (LTE) of Runge-Kutta methods based on **B-series**

We focus on Problem 2 in this talk

Order condition for Runge-Kutta methods

Method order of Runge-Kutta methods and Local Truncation Error (LTE)

$$\mathbf{x}(t_\ell; \mathbf{x}_{\ell-1}) - \mathbf{x}_\ell = C \cdot h^{p+1} \quad \text{with} \quad C \in \mathbb{R}.$$

we want to bound this!

Order condition

This condition states that a method of Runge-Kutta family is of order p **iff**

- the Taylor expansion of the exact solution
- and the Taylor expansion of the numerical methods

have the same $p + 1$ first coefficients.

Consequence

The LTE is the **difference of Lagrange remainders of two Taylor expansions**

. . . but how to compute it?

Example: building an order 2 explicit Runge-Kutta method

Consider, **a scalar IVP**

$$\dot{x}(t) = f(x(t)) \quad \text{with} \quad x(t_0) = x_0$$

Consider **an explicit Runge-Kutta method** of the form

$$\begin{array}{c|cc} 0 & 0 & 0 \\ c_1 & a_{21} & 0 \\ \hline & b_1 & b_2 \end{array}$$

i.e.,

$$x_1 = x_0 + h(b_1 k_1 + b_2 k_2) \quad \text{with} \quad \begin{cases} k_1 = f(x_0) \\ k_2 = f(x_0 + h a_{21} k_1) \end{cases}$$

and **we want to make it of order** 2

Example: building an order 2 explicit Runge-Kutta method

Taylor expansion of the exact solution, *i.e.*,

$$\dot{x}(t) = f(x(t)) \quad \text{with} \quad x(0) = x_0$$

We have, up to order 3

$$\begin{aligned} x(t_0 + h) &= x(t_0) + h\dot{x}(t_0) + \frac{h^2}{2}\ddot{x}(t_0) + \mathcal{O}(h^3) \\ &= x(t_0) + hf(x(t_0)) + \frac{h^2}{2}\frac{\partial f}{\partial x}(x(t_0))f\left(x(t_0)\right) + \mathcal{O}(h^3) \end{aligned}$$

Example: building an order 2 explicit Runge-Kutta method

Taylor expansion of the numerical solution, *i.e.*,

$$x_1 = x_0 + h(b_1 k_1 + b_2 k_2) \quad \text{with} \quad \begin{cases} k_1 = f(x_0) \\ k_2 = f(x_0 + h a_{21} k_1) \end{cases}$$

We have ($h = t - t_0$)

$$\frac{dk_1}{dh} = 0$$

$$\frac{dk_2}{dh} = \left(a_{21} k_1 + h a_{21} \frac{dk_1}{dh} \right) \cdot \frac{\partial f}{\partial x}(x_0 + h a_{21} k_1) \quad = a_{21} f(x_0) \frac{\partial f}{\partial x}(x_0 + h a_{21} f(x_0))$$

so,

$$\frac{dx_1}{dh} = b_1 k_1 + b_2 k_2 + h(b1 \frac{dk_1}{dh} + b_2 \frac{dk_2}{dh})$$

$$= b_1 f(x_0) + b_2 f(x_0 + h a_{21} f(x_0)) + h b_2 a_{21} f(x_0) \frac{\partial f}{\partial x}(x_0 + h a_{21} f(x_0))$$

When $h = 0$, we have

$$\frac{dx_1}{dh} = b_1 f(x_0) + b_2 f(x_0) = (b_1 + b_2) f(x_0)$$

Example: building an order 2 explicit Runge-Kutta method

Taylor expansion of the numerical solution, *i.e.*,

$$x_1 = x_0 + h(b_1 k_1 + b_2 k_2) \quad \text{with} \quad \begin{cases} k_1 = f(x_0) \\ k_2 = f(x_0 + h a_{21} k_1) \end{cases}$$

We can pursue the process at the second order to get

$$\frac{d^2 x_1}{dh^2} = b_2 a_{21} f(x_0) \frac{\partial f}{\partial x}(x_0 + h a_{21} f(x_0)) + (b_2 a_{21} f(x_0)) \frac{\partial f}{\partial x}(x_0 + h a_{21} f(x_0))$$
$$+ h(b_2 a_{21} f(x_0)) a_{21} f(x_0)) \frac{\partial^2 f}{\partial x^2}(x_0 + h a_{21} f(x_0))$$

When $h = 0$, we have

$$\frac{d^2 x_1}{dh^2} = 2 b_2 a_{21} f(x_0) \frac{\partial f}{\partial x}(x_0)$$

Example: building an order 2 explicit Runge-Kutta method

Hence, we get the **Taylor expansion of the numerical solution**

$$x_1 = x_0 + h\,(b_1 + b_2)\,f(x_0) + h^2\,b_2\,a_{21}\,f(x_0)\frac{\partial f}{\partial x}(x_0) + \mathcal{O}(h^3)$$

w.r.t., the **Taylor expansion of the exact solution**

$$x(t+h) = x(t_0) + h1f\,(x(t_0)) + h^2\frac{1}{2}f(x(t_0))\frac{\partial f}{\partial x}(x(t_0)) + \mathcal{O}(h^3)$$

with **localization assumption**, *i.e.*, $x(t_0) = x_0$, we have the constraints

$$\begin{cases} b_1 + b_2 = 1 \\ \quad b_2\,a_{21} = \dfrac{1}{2} \end{cases}$$

Note: there is an infinity set of solutions of order 2 methods. Two notorious

- $b_1 = 0$, $b_2 = 1$ and $a_{21} = \frac{1}{2}$ (Explicit midpoint method)
- $b_1 = \frac{1}{2}$, $b_2 = \frac{1}{2}$ and $a_{21} = 1$ (Heun's method)

A quick view of Runge-Kutta order condition theory[2]

Starting from $\mathbf{x}^{(q)} = (f(\mathbf{x}))^{(q-1)}$ and with the Chain rule, we have

High order derivatives of exact solution x

$$
\begin{aligned}
\dot{\mathbf{x}} &= f(\mathbf{x}) \\
\ddot{\mathbf{x}} &= f'(\mathbf{x})\dot{\mathbf{x}} \\
\mathbf{x}^{(3)} &= f''(\mathbf{x})(\dot{\mathbf{x}},\dot{\mathbf{x}}) + f'(\mathbf{x})\ddot{\mathbf{x}} \\
\mathbf{x}^{(4)} &= f'''(\mathbf{x})(\dot{\mathbf{x}},\dot{\mathbf{x}},\dot{\mathbf{x}}) + 3f''(\mathbf{x})(\ddot{\mathbf{x}},\dot{\mathbf{x}}) + f'(\mathbf{x})\mathbf{x}^{(3)} \\
\mathbf{x}^{(5)} &= f^{(4)}(\mathbf{x})(\dot{\mathbf{x}},\dot{\mathbf{x}},\dot{\mathbf{x}},\dot{\mathbf{x}}) + 6f'''(\mathbf{x})(\ddot{\mathbf{x}},\dot{\mathbf{x}},\dot{\mathbf{x}}) \\
&\quad + 4f''(\mathbf{x})(\mathbf{x}^{(3)},\dot{\mathbf{x}}) + 3f''(\mathbf{x})(\ddot{\mathbf{x}},\ddot{\mathbf{x}}) + f'(\mathbf{x})\mathbf{x}^{(4)} \\
&\vdots
\end{aligned}
$$

$f'(\mathbf{x})$ is a linear map

$f''(\mathbf{x})$ is a bi-linear map

$f'''(\mathbf{x})$ is a tri-linear map

$\vdots$

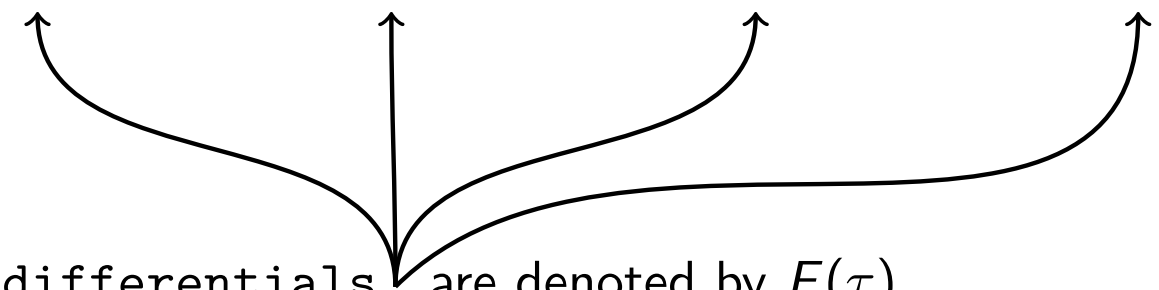
[2] strongly inspired from "Geometric Numerical Integration", Hairer, Lubich and Wanner.

A quick view of Runge-Kutta order condition theory[2]

Inserting the value of $\dot{\mathbf{x}}$, $\ddot{\mathbf{x}}$, ..., we have:

High order derivatives of exact solution x

$$\begin{aligned}
\dot{\mathbf{x}} &= f \\
\ddot{\mathbf{x}} &= f'(f) \\
\mathbf{x}^{(3)} &= f''(f,f) + f'(f'(f)) \\
\mathbf{x}^{(4)} &= f'''(f,f,f) + 3f''(f'f,f) + f'(f''(f,f)) + f'(f'(f'(f))) \\
&\vdots
\end{aligned}$$



- `Elementary differentials`, are denoted by $F(\tau)$

Remark a tree structure is made apparent in these computations

[2] strongly inspired from "Geometric Numerical Integration", Hairer, Lubich and Wanner.

A quick view of Runge-Kutta order condition theory[2]

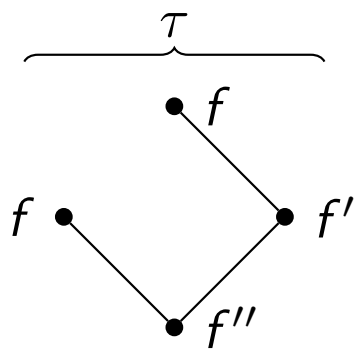
Rooted trees: a combinatorial view of elementary differentials

- f is a leaf
- f' is a tree with one branch, ..., $f^{(k)}$ is a tree with k branches

Example

$$\underbrace{f''(f'f, f)}_{F(\tau)}$$

is associated to



Note: τ is not unique, *e.g.*, symmetry

Consequences

At a given order, an **enumeration of all the trees** is possible $\Rightarrow$ all the elementary differentials are enumerable

Order	1	2	3	4	5	6	7	8	9	10
Number of τ	1	1	2	4	9	20	48	115	286	719

A quick view of Runge-Kutta order condition theory[2]

Theorem 1 (Butcher, 1963)

The qth derivative of the **exact solution** is given by

$$\mathbf{x}^{(q)} = \sum_{r(\tau)=q} \alpha(\tau) F(\tau)(\mathbf{x}_0) \quad \text{with} \quad \begin{array}{l} r(\tau) \text{ the order of } \tau, \textit{ i.e.}, \text{ number of nodes} \\ \alpha(\tau) \text{ a positive integer} \end{array}$$

We can do the same for the numerical solution

Theorem 2 (Butcher, 1963)

The qth derivative of the **numerical solution** is given by

$$\mathbf{x}_1^{(q)} = \sum_{r(\tau)=q} \gamma(\tau)\phi(\tau)\alpha(\tau) F(\tau)(\mathbf{x}_0) \quad \text{with} \quad \begin{array}{l} \gamma(\tau) \text{ a positive integer} \\ \phi(\tau) \text{ depending on a Butcher tableau} \end{array}$$

Theorem 3, order condition (Butcher, 1963)

A Runge-Kutta method has order p iff $\phi(\tau) = \frac{1}{\gamma(\tau)} \quad \forall \tau, r(\tau) \leqslant p$

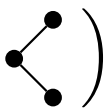
LTE formula for **explicit and implicit** Runge-Kutta

From Theorem 1 and Theorem 2, if a Runge-Kutta has order p then

$$\mathbf{x}(t_1;\mathbf{x}_0) - \mathbf{x}_1 = \frac{h^{p+1}}{(p+1)!} \sum_{r(\tau)=p+1} \alpha(\tau)\big[1-\gamma(\tau)\phi(\tau)\big]F(\tau)(\mathbf{x}(\xi)), \quad \xi \in [t_1, t_0]$$

- $\alpha(\tau)$ and $\gamma(\tau)$ are positive integer (with some combinatorial meaning)
- $\phi(\tau)$ function of the coefficients of the RK method,

Example

$\phi\Big($  $\Big)$ is associated to $\displaystyle\sum_{i,j=1}^{s} b_i a_{ij} c_j$ with $c_j = \displaystyle\sum_{k=1}^{s} a_{jk}$

Remark

Making guaranteed Runge-Kutta is a simpler problem, *i.e.*, for each method the Butcher tableau and the order are already available

Note: $\mathbf{x}(\xi)$ can be enclosed by $[\tilde{\mathbf{x}}]$ using Interval Picard-Lindelöf operator

Implementation of LTE formula

Notations

- n the state-space dimension
- p the order of a Rung-Kutta method

Two ways of computing $F(\tau)$

1. **Symbolic differentiation** : complexity $\mathcal{O}(n^p)$
   - compute all partial derivatives symbolically
   - combine them following the rooted tree structures

2. **Automatic differentiation** : complexity $\mathcal{O}(n3^p)$
   based on the work of Ferenc Bartha and Hans Munthe-Kaas
   "Computing of B-Series by Automatic Differentiation", 2014

A guaranteed numerical integration based on Runge-Kutta

A guaranteed algorithm

$$[\mathbf{x}_{\ell+1}] = [\mathrm{RK}]\,(h, [\mathbf{x}_\ell]) + \mathrm{LTE}\ .$$

Note on the implementation of $[\mathrm{RK}]\,(h, [\mathbf{x}_\ell])$

- If **explicit** method is considered
  [RK] is an **inclusion function**

- If **implicit** method is considered
  [RK] is an **interval contractor operator**

Example: implicit midpoint

$$\mathbf{k}_1 = f\left(t_\ell + \frac{h}{2}, \mathbf{x}_\ell + \frac{h}{2}\mathbf{k}_1\right) \quad \Rightarrow \quad [\mathbf{k}_1] = [\mathbf{k}_1] \cap [f]\left(t_\ell + \frac{h}{2}, [\mathbf{x}_\ell] + \frac{h}{2}[\mathbf{k}_1]\right)$$

$$\mathbf{x}_{\ell+1} = \mathbf{x}_\ell + h\mathbf{k}_1 \qquad [\mathbf{x}_{\ell+1}] = [\mathbf{x}_\ell] + h[\mathbf{k}_1]$$

Starting the contraction with $[\tilde{\mathbf{x}}]$ the result of interval Picard-Lindelöf operator

RK-based of interval Picard-Lindelöf operator

Starting from the expression

$$\mathbf{k}_i(t) = f\left(t_\ell + c_i(t - t_\ell), \mathbf{x}_\ell + (t - t_\ell)\sum_{n=1}^{s} a_{in}\mathbf{k}_n\right), \quad 1 \leqslant i \leqslant s$$

$$\mathbf{x}_{\ell+1}(t, \xi) = \mathbf{x}_\ell + (t - t_\ell)\sum_{i=1}^{s} b_i\mathbf{k}_i(t) + \mathrm{LTE}(t, \mathbf{x}(\xi))$$

We can define an inclusion function with $h = t_{j+1} - t_j$ such that

$$P([t_\ell, t_{\ell+1}], [\tilde{\mathbf{x}}]) := [\mathbf{x}_\ell] + [0, h]\sum_{i=1}^{s} b_i[\mathbf{k}_i]\left([t_\ell, t_{\ell+1}]\right) + \mathrm{LTE}([t_\ell, t_{\ell+1}], [\tilde{\mathbf{x}}])$$

Hence, it is sufficient to have

$$[\tilde{\mathbf{x}}] \supseteq P\left([t_\ell, t_{\ell+1}], [\tilde{\mathbf{x}}]\right)$$

to prove the existence and uniqueness of the solution of IVP ODE.

Interval RK methods summary

Given a RK scheme, guaranteed integration works with a two step approach:

- Prove existence and uniqueness of solution :
  Picard-Lindelöf operator contraction proof
  $\Rightarrow$ Box bounding the state **over** the next time interval
- Apply interval scheme with bounded LTE :
  Computation and evaluation of LTE
  $\Rightarrow$ Box bounding solution **at** next time step

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Complexity comes from :

- Computation of the LTE

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  Computation and evaluation of LTE
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Complexity comes from :

- Computation of the LTE

In practice :

- Dimension limited to ≈ 50

Co-simulation

Let us suppose a **decomposed** dynamics :

$$\begin{aligned}
&\dot{\mathbf{x}}_1 \in f_1(t, \mathbf{x}_1, \mathbf{u}_1) \quad \text{with} \quad \mathbf{x}_1(0) \in [\mathbf{x}_1^0],\ \mathbf{u}_1 \in [\mathbf{u}_1],\\
&\dot{\mathbf{x}}_2 \in f_2(t, \mathbf{x}_2, \mathbf{u}_2) \quad \text{with} \quad \mathbf{x}_2(0) \in [\mathbf{x}_2^0],\ \mathbf{u}_2 \in [\mathbf{u}_2],\\
&\dots\\
&\dot{\mathbf{x}}_m \in f_m(t, \mathbf{x}_m, \mathbf{u}_m) \quad \text{with} \quad \mathbf{x}_m(0) \in [\mathbf{x}_m^0],\ \mathbf{u}_m \in [\mathbf{u}_m],\\
&L(\mathbf{x}_1, \dots, \mathbf{x}_m, \mathbf{u}_1, \dots, \mathbf{u}_m) = 0,
\end{aligned}$$

where the state $\mathbf{x}$ is decomposed in m components $\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_m)$, for all $i \in \{1, \dots, m\}$, $\mathbf{x}_i \in X_i$, $X_1 \times \cdots \times X_m = \mathbb{R}^d$, and L is a coupling function between the components.

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Principle of co-simulation:

- Simulate subsystems in a **distributed** manner
- At some instants, **exchange information** between subsystems

Advantages:

- Faster than simulating the entire system
- Enables large scale systems
- Different solvers can be used (*i.e.* applications to CPS and multi-physics)

Co-simulation, distributed reachability, state-of-the-art

- Co-simulation is widely used (at least 48 industrial applications reported) [survey by C. Gomes et al.]
- Most of the tools developed rely on FMI/FMU standard [M. Arnold, E. Lee]: Modelica, Simulink...
- No guaranteed co-simulation but some work on error bounding [M. Arnold]
- Guaranteed distributed reachability is less common
  - Compositional abstractions based on hybrid automata [Chen, Sankaranarayanan], linear arithmetic relations [Chen, Mover, Sankaranarayanan]
  - Local numerical integration with compositional splitting [Blanes, Casas, Murua]

Co-simulation formalism (Gomes et al.)

Continuous-time simulation unit:

$$
\begin{aligned}
& S_i = \langle X_i, U_i, Y_i, \delta_i, \lambda_i, \mathbf{x}_i(0), \mathbf{\Phi}_{U_I} \rangle, \\
& \delta_i : \mathbb{R} \times X_i \times U_i \to X_i, \\
& \lambda_i : \mathbb{R} \times X_i \times U_i \to Y_i, \text{ or } \mathbb{R} \times X_i \to Y_i, \\
& \mathbf{x}_i(0) \in X_i, \\
& \mathbf{\Phi}_{U_i} : \mathbb{R} \times U_i \times \cdots \times U_I \to U_i,
\end{aligned}
\tag{1}
$$

where

- X_i is the state vector space,
- U_i is the input vector space,
- Y_i is the output vector space,
- $\delta_i(t, \mathbf{x}_i(t), \mathbf{u}_i(t)) = \mathbf{x}_i(t + H)$ advances the simulation (using extrapolation function $\mathbf{\Phi}_{U_i}$)
- $\lambda_i(t, \mathbf{x}_i(t), \mathbf{u}_i(t)) = \mathbf{y}_i(t)$ or $\lambda_i(t, \mathbf{x}_i(t)) = \mathbf{y}_i(t)$ is the output function; and
- $\mathbf{x}_i(0)$ is the initial state.

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$$

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- X_i is the state vector space,
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- Y_i is the output vector space,
- $\delta_i([t, t'], [\mathbf{x}_i], [\mathbf{u}_i]) = ([\mathbf{x}_i]', \{[\mathbf{x}_i^k]'\}_k)$ advances the simulation (using extrapolation function $\mathbf{\Phi}_{U_i}$)
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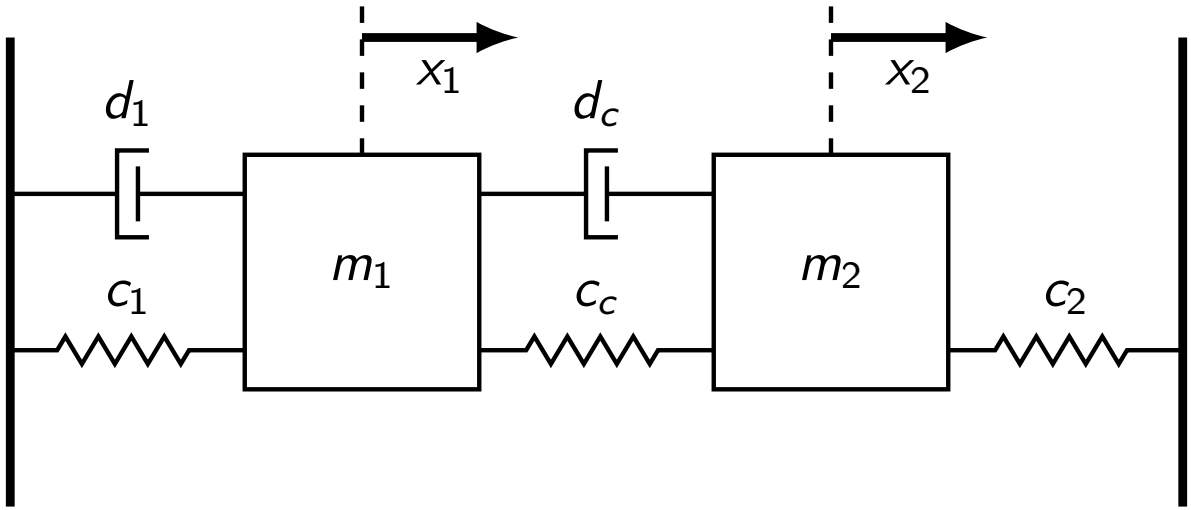
Example of composed system



The dynamics of the system is given by the following system of equations:

$$\begin{cases} \dot{x}_1 = v_1 \\ m_1 \dot{v}_1 = -c_1 x_1 - d_1 v_1 + c_c(x_2 - x_1) + d_c(v_2 - v_1) \\ \dot{x}_2 = v_2 \\ m_2 \dot{v}_2 = -c_c(x_2 - x_1) - c_2 x_2 - d_c(v_2 - v_1) \end{cases}$$

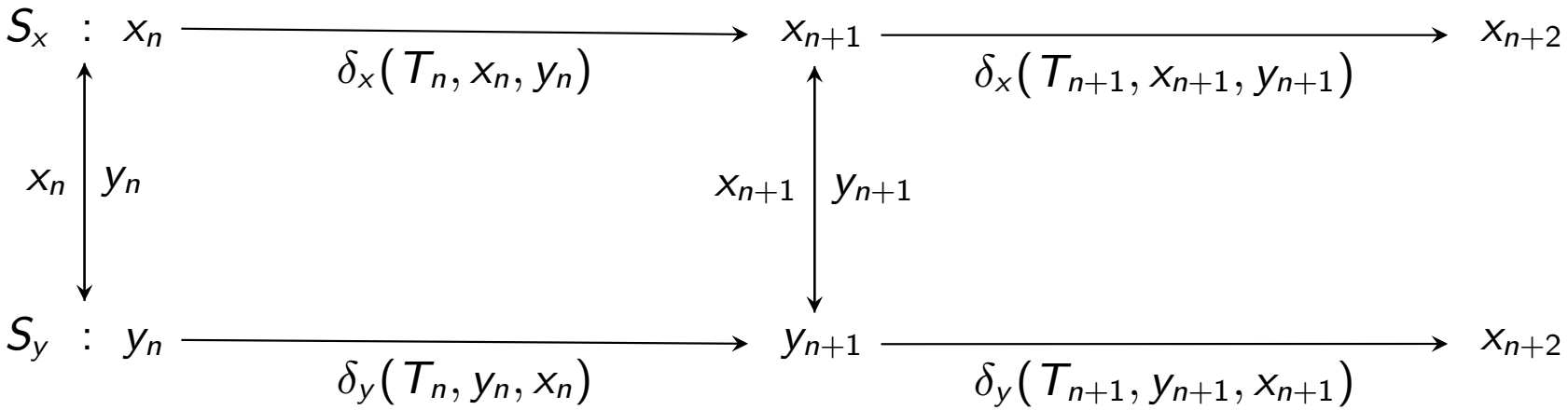
with the initial conditions $x_1(0) = x_2(0) = v_1(0) = v_2(0) = [1, 1]$ (a point interval).

Principle of classical co-simulation

With a simpler dynamics:

$$\dot{x} = f(x, y)$$
$$\dot{y} = g(y, x)$$

where $x(0) \in [x_0]$, $y(0) \in [y_0]$, the principle is :



- on macro-steps, sub-systems advance simulation independently
- at communication times, they exchange output values (x_n and y_n)

Principle guaranteed of co-simulation

With a simpler dynamics:

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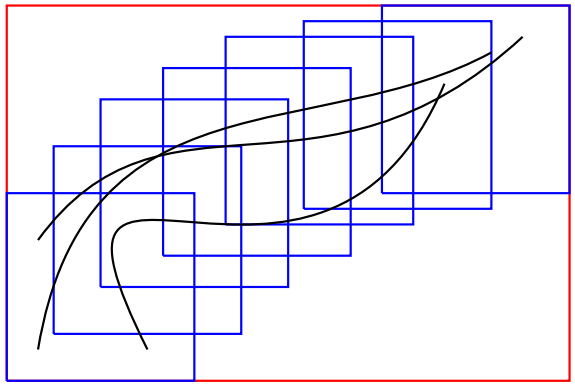
$$\dot{y} = g(y, x)$$



where $x(0) \in [x_0]$, $y(0) \in [y_0]$, the principle is :

$$\begin{array}{ccccccc}
S_x & : & [x_n] & \xrightarrow[\delta_x(T_n, [x_n], [y_n^H])]{} & [x_{n+1}] & \xrightarrow[\delta_x(T_{n+1}, [x_{n+1}], [y_{n+1}^H])]{} & [x_{n+2}] \\
 & & \updownarrow [x_n^H]\ [y_n^H] & & \updownarrow [x_{n+1}^H]\ [y_{n+1}^H] & & \\
S_y & : & [y_n] & \xrightarrow[\delta_y(T_n, [y_n], [x_n^H])]{} & [y_{n+1}] & \xrightarrow[\delta_y(T_{n+1}, [y_{n+1}], [x_{n+1}^H])]{} & [x_{n+2}]
\end{array}$$

with

- $[x_n]$ and $[y_n]$ interval state at communication times
- $[x_n^H]$ and $[y_n^H]$ over-approximation of the state over the next macro-step $[T_n, T_n + H]$

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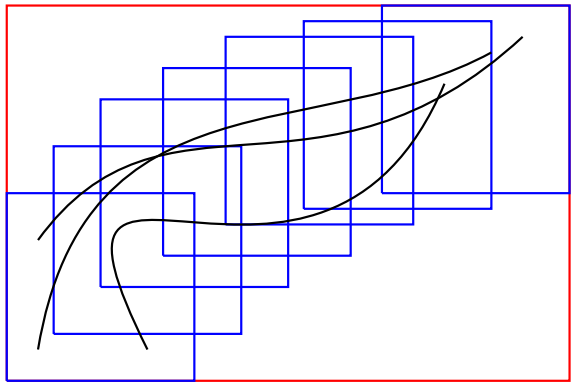

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& \uparrow [x_n^H] \; \downarrow [y_n^H] & & \uparrow [x_{n+1}^H] \; \downarrow [y_{n+1}^H] & & \\
S_y : & [y_n] & \xrightarrow[\delta_y(T_n, [y_n], [x_n^H])]{} & [y_{n+1}] & \xrightarrow[\delta_y(T_{n+1}, [y_{n+1}], [x_{n+1}^H])]{} & [x_{n+2}]
\end{array}$$

with

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- $[x_n^H]$ and $[y_n^H]$ over-approximation of the state over the next macro-step $[T_n, T_n + H]$

Question:
How to compute $[x_n^H]$ and $[y_n^H]$?

The cross-Picard operator

Local Picard-Lindelöf operators on macro-step $[T_n, T_{n+1}]$:

$$P_f([T_n, T_{n+1}], [\tilde{x}], [\tilde{y}]) := [x_n] + \sum_{k=0}^{N} f^{[k]}([x_n], [\tilde{y}])[0, H^k] + f^{[N+1]}([\tilde{x}], [\tilde{y}])[0, H^{N+1}].$$

$$P_g([T_n, T_{n+1}], [\tilde{y}], [\tilde{x}]) := [y_n] + \sum_{k=0}^{N} g^{[k]}([y_n], [\tilde{x}])[0, H^k] + f^{[N+1]}([\tilde{y}], [\tilde{x}])[0, H^{N+1}].$$

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In order to prove that $[x_n^H]$ and $[y_n^H]$ are indeed over-approximating $x(t)$ and $y(t)$ over the next macro-step, the condition to verify is:

$$\mathcal{P}_f([T_n, T_{n+1}], [x_n^H], [y_n^H]) \subset \text{Int}([x_n^H]) \text{ and } \mathcal{P}_g([T_n, T_{n+1}], [y_n^H], [x_n^H]) \subset \text{Int}([y_n^H])$$

The cross-Picard operator

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Procedure: start with an initial guess (heuristics) and contract (fixed point)

The cross-Picard operator

Algorithm 1 Computation of the cross-Picard operator

Data: $cs = \langle \emptyset, Y_{cs}, D = \{1, \ldots, m\}, \{S_i\}_{i \in D}, L, \emptyset \rangle$, a time interval $[t, t + H]$, initial intervals $[x_{i,n}]$ and initial guesses $[r^H_{i,n}]$

Result: $\{[X^H_i]\}_{i=1,\ldots,m}$, a set of boxes over-approximating the global state on $[T_n, T_n + H]$

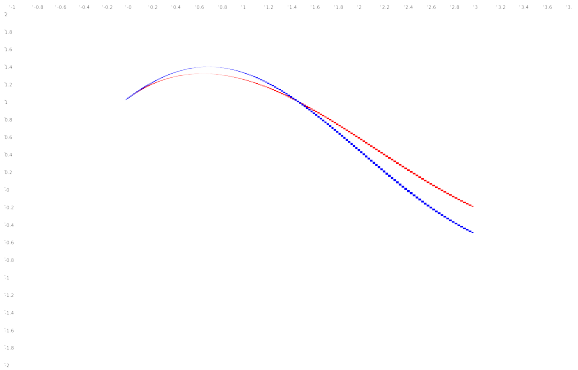
for $i = 1, \ldots, m$ (in parallel) **do**
$[\tilde{X}^H_i] := [r^H_{i,n}]$
$[U^H_i] := K_i([\tilde{X}^H_{1,n}], \ldots, [\tilde{X}^H_{1,n}])$
$[X^H_i] := \mathcal{P}^H_{[x_{i,n}],[U^H_i]}$

while $[X^H_i] \not\subseteq [\tilde{X}^H_i]$ for all i **do**
for $i = 1, \ldots, m$ (in parallel) **do**
$[\tilde{X}^H_i] := [X^H_i]$
$[U^H_i] := K_i([\tilde{X}^H_{1,n}], \ldots, [\tilde{X}^H_{1,n}])$
$[X^H_i] := \mathcal{P}^H_{[x_{i,n}],[U^H_i]}$

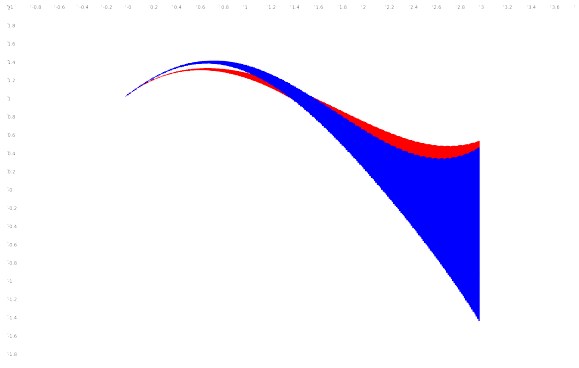
return $[X^H_i]$

Application

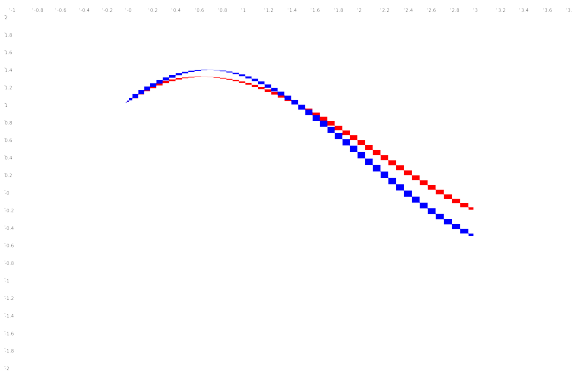
Double mass-spring-damper oscillator



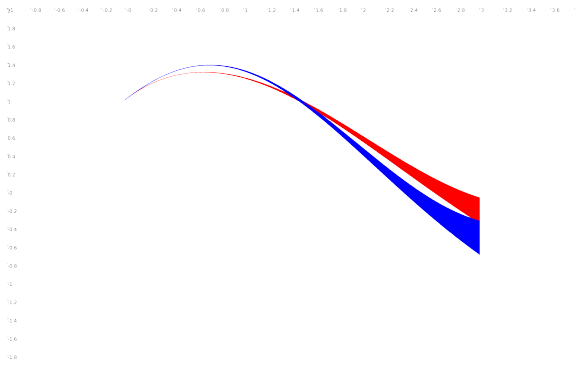
Heun



co-Heun (H=0.05)



RK4



co-RK4 (H=0.01)

More information exchange for more accuracy : guaranteed extrapolation

A simulation unit $S_i = \langle X_i, U_i, Y_i, \delta_i, \lambda_i, \mathbf{x}_i(0), \mathbf{\Phi}_{U_i} \rangle$ can **extrapolate inputs** for the next macro-step based on **previous behavior**:

Classical approach : interpolation polynomials

$$\mathbf{\Phi}_{U_i,n}(t) = \sum_{l=0}^{k} \mathbf{u}_i(T_{n-l}) \prod_{\substack{p=0 \\ p \neq l}}^{k} \frac{t - T_{n-p}}{T_{n-l} - T_{n-p}} = \mathbf{u}_i(t) + O(H^{k+1}) \qquad (2)$$

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Interpolation error :

$$\mathbf{\Phi}_{U_i,n}(t) - \mathbf{u}_i(t) = \frac{1}{(k+1)!} \mathbf{u}_i^{(k+1)}(\xi) \prod_{i=0}^{k} (t - T_{n-k}) \quad \xi \in [T_n, T_{n+1}]$$

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Higher chain formula:

$$\mathbf{u}_i^{(k)}(t) = k! \frac{\partial^{r_1+\cdots+r_m} K_i}{\partial \mathbf{x}_1^{r_1} \ldots \partial \mathbf{x}_m^{r_m}} \prod_{j=1}^{s} \prod_{l=1}^{m} \frac{1}{m_{jl}!} \left[\frac{1}{p_j!} \mathbf{x}_i^{(p_j)} \right]^{m_{jl}}$$

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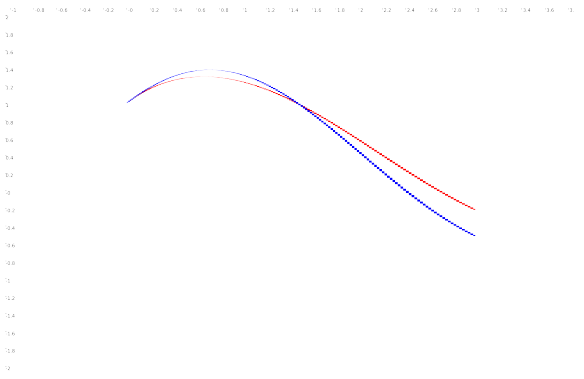
Guaranteed interval extrapolation :

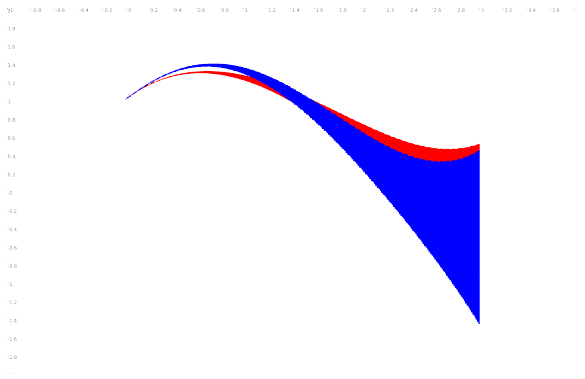
$$[\mathbf{\Phi}_{U_i,n}](t) = \sum_{l=0}^{k} [\mathbf{u}_{i,n-l}] \prod_{\substack{p=0 \\ p \neq l}}^{k} \frac{t - T_{n-p}}{T_{n-l} - T_{n-p}} + \frac{1}{(k+1)!} [\mathbf{u}_{i,n}^{(k),H}] \prod_{i=0}^{k} (t - T_{n-k}) \quad (3)$$

Application

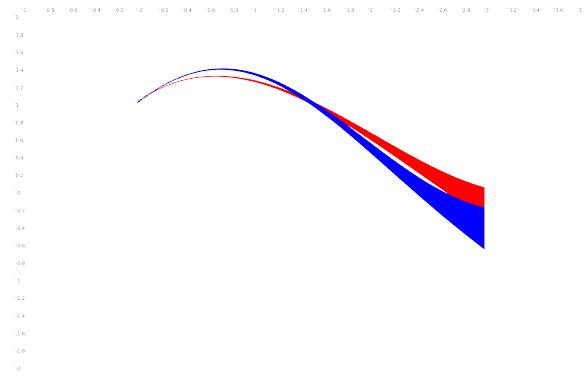
Double mass-spring-damper oscillator



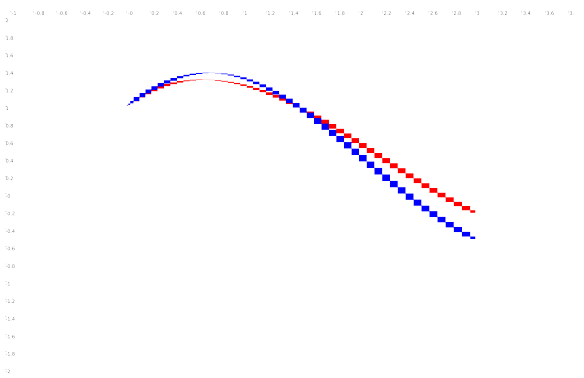
Heun



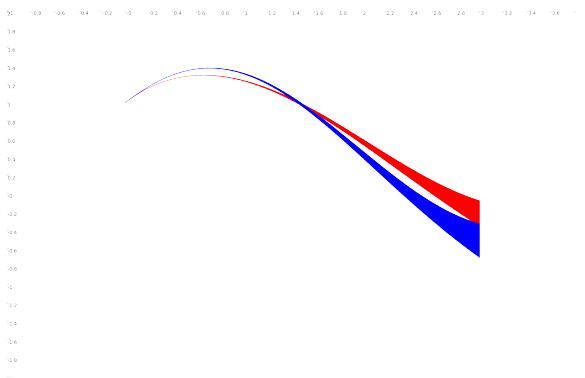
co-Heun (H=0.05)



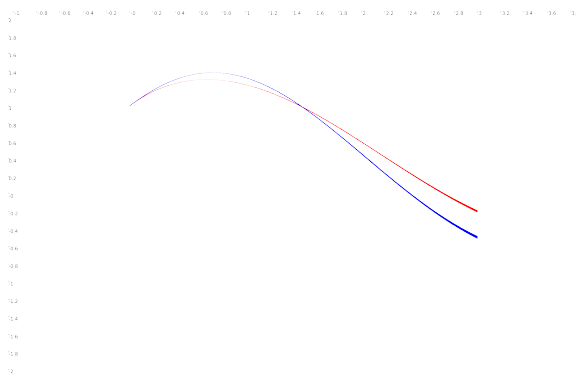
co-Heun-interp (H=0.05)



RK4



co-RK4 (H=0.01)



co-RK4-interp (H=0.01)

Seluxit case study

[K.G. Larsen et al. *Online and Compositional Learning of Controllers with Application to Floor Heating*, TACAS 2016.]

Seluxit case study

[K.G. Larsen et al. *Online and Compositional Learning of Controllers with Application to Floor Heating*, TACAS 2016.]

System dynamics:

$$\frac{d}{dt} T_i(t) = \sum_{j=1}^{n} A^d_{i,j}(T_j(t) - T_i(t)) + B_i(T_{env}(t) - T_i(t)) + H_{i,j}.v_j$$

- System of dimension 11
- 2^{11} combinations of v_j (not all admissible, constraint on the number of open valves)
- Pipes heating a room may influence other rooms
- Doors opening and closing (here: average between open and closed)
- Varying external temperature (here: $T_{env} = 10^\circ C$)
- Measures and switching every 15 minutes

Seluxit case study

[K.G. Larsen et al. *Online and Compositional Learning of Controllers with Application to Floor Heating*, TACAS 2016.]

Simulation over 10 switching times for a given switching sequence

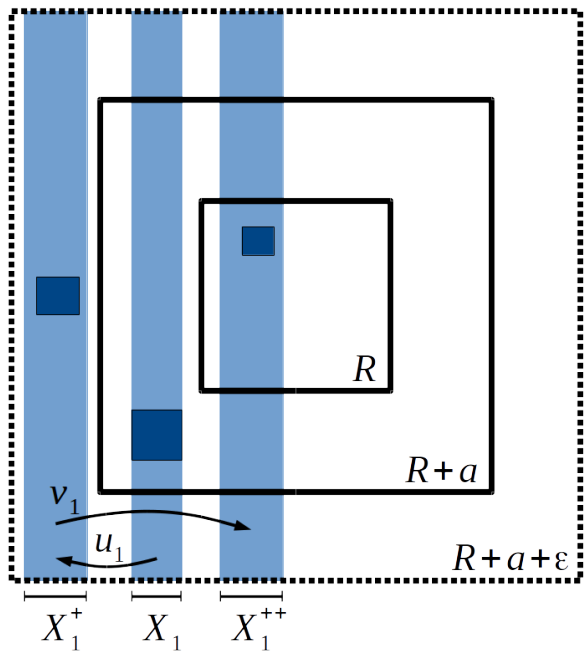
Scheme	Computation time (s)	Final area (m^2)
HEUN	7,96	0.2165
co-HEUN	5,95	0.2407
co-HEUN-interp	27,05	0.2335
RK4	27,60	0.1821
co-RK4	17,87	0.1932
co-RK4-interp	122,17	0.1854

Towards scalable CPS design

Model-based design of cyber-physical systems :

modeling, analysis, **controller synthesis**, **simulation**, deployment

- Progress is being made in scalability of controller synthesis methods
  - **Compositional methods**
    Break exponential complexity in dimension

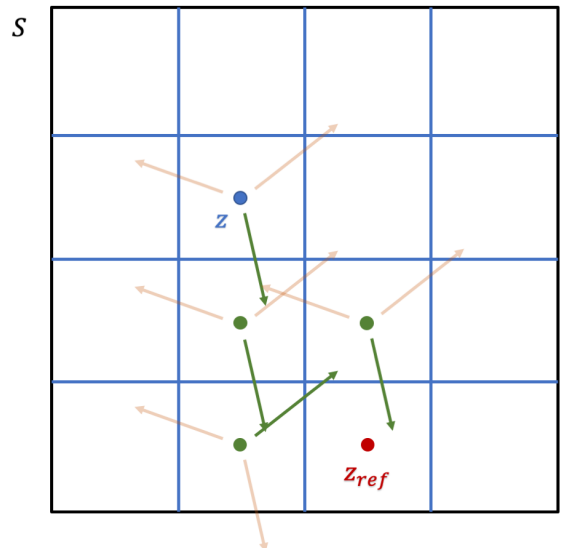


Towards scalable CPS design

Model-based design of cyber-physical systems :

modeling, analysis, **controller synthesis**, **simulation**, deployment

- Progress is being made in scalability of controller synthesis methods
  - **Compositional methods**
    Break exponential complexity in dimension
  - **Optimal control methods**
    From exponential to linear complexity in horizon length



Conclusions and future work

Conclusions:

- Guaranteed RK schemes available for systems with perturbations
- Guaranteed co-simulation possible using only local computations
- Co-simulation provides some significant computation time improvements

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Future work:

- Keep original coupling function formulation with DAE tools
- Parallelize computations and implement in DynIbex
- Test use in control synthesis algorithms
- More case studies (multi-physics)

Bibliography

- **Interval Runge-Kutta methods**
  [Julien Alexandre dit Sandretto and Alexandre Chapoutot. *Validated explicit and implicit runge-kutta methods*, Reliable Computing, 2016]
- **Automatic differentiation**
  [Olivier Mullier, Alexandre Chapoutot, and Julien Alexandre Dit Sandretto, *Validated computation of the local truncation error of runge-kutta methods with automatic differentiation*, Optimization Methods and Software, 2018]
- **Differential Algebraic Equations**
  [Julien Alexandre dit Sandretto and Alexandre Chapoutot. *Validated simulation of differential algebraic equations with runge-kutta methods*, Reliable Computing, 2016]
- **Guaranteed co-simulation**
  [Adrien Le Coënt, Julien Alexandre Dit Sandretto, Alexandre Chapoutot. *Guaranteed cosimulation of Cyber-Physical Systems*, 2020]