# RIGOROUS NUMERICS FOR MAPS AND ODEs 

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## Interval arithmetics a cure for round-off errors

Arithmetics on closed intervals. For example:

- $[1,3]\langle+\rangle[3,17]=[4,20]$
- $1\langle/\rangle 3=[0.33333,0.33334]$
$\operatorname{diam}\left[a_{-}, a^{+}\right]=a^{+}-a^{-}, \quad \mathrm{m}\left(\left[a_{-}, a^{+}\right]\right)=\left(a^{+}+a^{-}\right) / 2$
Rigorous interval arithmetics can be realized on the computer i.e. for each arithmetic operator $\diamond \in\{+,-, \cdot, /\}$ the following is true

$$
\left[a_{-}, a^{+}\right] \diamond\left[b_{-}, b_{+}\right] \subset\left[a_{-}, a^{+}\right]\langle\diamond\rangle\left[b_{-}, b_{+}\right]
$$

For any elementary function $f: \mathbf{R}^{n} \rightarrow \mathbf{R}^{s}$ and any set $Z \subset \mathbf{R}^{n}$

$$
f(Z) \subset\langle f\rangle(\langle Z\rangle)
$$

## Interval arithmetics - problems

- wrapping
the result of evaluation of multidimensional map is product of intervals, disastrous results when considering $f^{n}$ for $n$-large, ODEs
- dependency:
for $x=[-1,1]$ holds

$$
x\langle-\rangle x=[-2,2]
$$

Another example:

$$
e^{-x}=\sum_{n=0}^{\infty} \frac{(-1)^{n} x^{n}}{n!}
$$

$$
[1-\sinh (t), \cosh (t)] \subset\left\langle e^{-[0, t]}\right\rangle
$$

$\operatorname{diam}\left(\left\langle e^{-[0, t]}\right\rangle\right) \geq e^{t}-1, \quad \operatorname{diam}\left(e^{-[0, t]}\right)=1-e^{-t}$

## Interval arithmetics - fighting the dependency problem

Let $[X] \subset \mathbf{R}^{n}$ - convex, $x_{0} \in[X], f: \mathbf{R}^{n} \rightarrow \mathbf{R}^{k}$ $C^{1}$-function, then

$$
\begin{equation*}
f([X]) \subset f\left(x_{0}\right)+[d f([X])]_{I} \cdot\left([X]-x_{0}\right) \tag{1}
\end{equation*}
$$

where $[d f([X])]_{I}$ is the interval enclosure of $d f([X])$

$$
\begin{array}{r}
{[d f(Z)]_{I}=\left\{M \in \mathbf{R}^{k \times n},\right.} \\
\left.M_{i j} \in\left[\inf _{z \in Z} \frac{\partial f_{i}}{\partial x_{j}}(z), \sup _{z \in Z} \frac{\partial f_{i}}{\partial x_{j}}(z)\right]\right\}
\end{array}
$$

Mean value form: Let $x_{0}=m\left(\left[X_{0}\right]\right)$, then we set
$\langle f\rangle([X])=\langle f\rangle\left(x_{0}\right)+\left\langle[d f([X])]_{I} \cdot\left([X]-x_{0}\right)\right\rangle$

# Interval arithmetics - fighting the dependency problem, Examples 

- evaluation of $f(x)=x-x$, will give zero
- evaluation of $f(x)=x^{2}-x^{2}$ on $[-1,1]$
$<f([-1,1])>=0+(2 x-2 x)[-1,1]=[-4,4]$ rather bad result
- evaluation of $f(x)=e^{-x}$

$$
\begin{array}{r}
<e^{-[0, t]}>=e^{-t / 2}+\left(-e^{-[0, t]}\right) \cdot\left[-\frac{t}{2}, \frac{t}{2}\right]= \\
e^{-t / 2}+t / 2 \cdot e^{-[0, t]} \cdot[-1,1]= \\
e^{-t / 2}+t \cosh (t) / 2 \cdot[-1,1]
\end{array}
$$

Hence
$\operatorname{diam}\left(<e^{-[0, t]}>\right)=t \cosh t=t+\frac{t^{3}}{2!}+\frac{t^{5}}{4!}+\ldots$,
for small $t$ we have improvement, for $t$ large it is worse.

# Some methods for the reduction of the error growth 

- set division: Let $S_{t}=\varphi(t, S)$. When $S_{t}$ becomes too large, one should divide it into smaller pieces and compute further the evolution of each each piece separately
- Lohner algorithm: in order to avoid wrapping effect one should choose good coordinate frame in each step
- Taylor models (Berz, Makino):


## Interval arithmetics - fighting the dependency problem, Taylor models(Berz, Makino)

All sets represented as image of polynomial maps plus small remainder term (Taylor models) - similar to symbolic computations
application of map to such that such - recomputation of the coefficient in the Taylor model
very general, flexible, virtually no dependency and wrapping problems
very slow and hard to program

One step of the Lohner algorithm
$x^{\prime}=f(x)$ induces $\varphi\left(t, x_{0}\right)$ - $t$-time, $x_{0}$ - initial condition,
$\Phi(h, x)$ - numerical method, Taylor method of order $p$

## Input:

- $t_{k}$ - time, $h_{k}$ - time step
- $\left[x_{k}\right] \subset \mathbf{R}^{n}$, such that $\varphi\left(t_{k},\left[x_{0}\right]\right) \subset\left[x_{k}\right]$


## Output:

- $t_{k+1}=t_{k}+h_{k}$
- $\left[x_{k+1}\right] \subset \mathbf{R}^{n}$, such that $\varphi\left(t_{k+1},\left[x_{0}\right]\right) \subset\left[x_{k+1}\right]$

1. Rough enclosure of $\varphi\left(\left[0, h_{k}\right],\left[x_{k}\right]\right)$
$\left[W_{1}\right] \subset \mathbf{R}^{n}$ compact and convex

$$
\varphi\left(\left[0, h_{k}\right],\left[x_{k}\right]\right) \subset\left[W_{1}\right]
$$

2. $\left[A_{k}\right]=\frac{\partial \Phi}{\partial x}\left(h_{k},\left[x_{k}\right]\right)$
3. $\left[x_{k+1}\right]\left(m\left(\left[x_{k}\right]\right)\right.$ - midpoint of $\left.\left[x_{k}\right]\right)$

$$
\begin{aligned}
{\left[x_{k+1}\right]=} & \Phi\left(h_{k}, m\left(\left[x_{k}\right]\right)\right)+ \\
& {\left[A_{k}\right]\left(\left[x_{k}\right]-m\left(\left[x_{k}\right]\right)\right)+\operatorname{Rem}\left(\left[W_{1}\right]\right) }
\end{aligned}
$$

## Taylor method - for rigorous integration of ODEs

$x^{\prime}=f(x), x(0)=x_{0}$ give rise to $\varphi\left(t, x_{0}\right)$
[ $X$ ], $[Y]$ - interval sets - products of intervals

If $[Y]=[X]+[0, h] f([Z]) \subset \operatorname{int}[Z]$, then $\varphi([0, h],[X]) \subset[Y]$.

Taylor expansion for $\varphi(h, x)$ for $x \in \mathbf{R}^{n}$, with respect to $h$ (below $n=1$ ), can be generted from ODE (automatic differentiation algorithm)

$$
\begin{array}{r}
\frac{\partial}{\partial t} \varphi\left(0, x_{0}\right)=x^{(1)}\left(x_{0}\right)=f\left(x_{0}\right) \\
\frac{\partial^{2}}{\partial t^{2}} \varphi\left(0, x_{0}\right)=x^{(2)}\left(x_{0}\right)=f^{\prime}\left(x_{0}\right) x^{(1)} \\
\frac{\partial^{3}}{\partial t^{3}} \varphi\left(0, x_{0}\right)=x^{(3)}\left(x_{0}\right)=f^{(2)}\left(x_{0}\right)\left(x^{\prime}\right)^{2}+f^{\prime}\left(x_{0}\right) x^{(2)}
\end{array}
$$

Error term ( $r$ - the order of the Taylor method) $\frac{\partial^{r+1}}{\partial t^{r+1}} \varphi\left(\theta h, x_{0}\right)=\frac{\partial^{r+1}}{\partial t^{r+1}} \varphi\left(0, \varphi\left(\theta h, x_{0}\right)\right) \subset x^{r+1}([Y])$.

$$
\begin{aligned}
\varphi\left(h,\left[X_{0}\right]\right) \subset\left[X_{0}\right]+ & \sum_{k=1}^{r} x^{(k)}\left(\left[X_{0}\right]\right) \frac{h^{k}}{k!}+ \\
& x^{r+1}([Y]) \frac{h^{r+1}}{(r+1)!} .
\end{aligned}
$$

## Reduction of the wrapping effect

$$
\left[x_{k}\right]=x_{k}+\left[r_{k}\right], \quad x_{k}=m\left(\left[x_{k}\right]\right),\left[r_{k}\right]=\left[x_{k}\right]-x_{k}
$$

The equation to evaluate:

$$
\left[r_{k+1}\right]=\left[A_{k}\right]\left[r_{k}\right]+\left[z_{k+1}\right]
$$

Eventual reduction of the wrapping effect depends on how we will represent $\left[r_{k}\right]$

- interval set $\left[r_{k}\right]=\Pi I_{j}, I_{j}$-interval
- parallelepiped $\left[r_{k}\right]=B_{k}\left[\tilde{r}_{k}\right], B_{k}$ - matrix, $\tilde{r}_{k}$ -interval set
- cuboid $\left[r_{k}\right]=Q_{k}\left[\tilde{r}_{k}\right], \tilde{r}_{k}$-interval set, $Q_{k}$ orthogonal matrix
- doubleton $\left[r_{k}\right]=C_{k}\left[r_{0}\right]+\left[\tilde{r}_{k}\right], C_{k}$ matrix, $\left[\tilde{r}_{k}\right]$ is either cuboid, parallelepiped or interval set


## using interval sets $==$ wrapping effect

other approaches try to minimize wrapping through choosing good coordinate frame

We choose different coordinate frame: $\left[r_{k}\right]=$ $B_{k}\left[\hat{r}_{k}\right]$,

$$
\begin{array}{r}
{\left[r_{k+1}\right]=\left[A_{k}\right]\left[r_{k}\right]+\left[z_{k+1}\right]=} \\
B_{k+1}\left(B_{k+1}^{-1}\left[A_{k}\right] B_{k}\left[\hat{r}_{k}\right]+B_{k+1}^{-1}\left[z_{k+1}\right]\right)
\end{array}
$$

$$
\begin{gathered}
{\left[r_{0}\right]=\left[B_{0}\right]\left[\widehat{r}_{0}\right], \quad\left[B_{0}\right]=\{I d\}} \\
{\left[\widehat{r}_{k+1}\right]=\left(\left[B_{k+1}^{-1}\right]\left[A_{k}\right]\left[B_{k}\right]\right)\left[\widehat{r}_{k}\right]+\left[B_{k+1}^{-1}\right]\left[z_{k+1}\right]} \\
{\left[r_{k+1}\right]=\left[B_{k+1}\right]\left[\widehat{r}_{k+1}\right]}
\end{gathered}
$$

Usually $B_{k+1}$ is a $Q$-factor from $Q R$ decomposition of $U \in\left[A_{k}\right]\left[B_{k}\right]$, but first we permute columns of $U$, so that their norms are decreasing

## Even better:

$$
\begin{gathered}
{\left[r_{k+1}\right]=C_{k+1}\left[r_{0}\right]+\left[\tilde{r}_{k+1}\right]} \\
{\left[\tilde{r}_{k+1}\right]=\left[A_{k}\right]\left[\tilde{r}_{k}\right]+\left[z_{k+1}\right]+\left(\left[A_{k}\right] C_{k}-C_{k+1}\right)\left[r_{0}\right]} \\
{\left[\tilde{r}_{0}\right]=0} \\
\text { and } C_{0}=I d, \quad C_{k+1} \in\left[A_{k}\right] C_{k}
\end{gathered}
$$

$\left[\tilde{r}_{k}\right]$ is evaluated using previous method

When Lohner algorithm can fail?

Only the first step - the generation of the rough enclosure - is heuristic. It can happen that a solution does not exists on $\left[0, h_{k}\right]$.

## Easy first order rough enclosure

$$
\begin{equation*}
x^{\prime}=f(x), \quad x \in \mathbf{R}^{n}, \quad f \in C^{1} \tag{2}
\end{equation*}
$$

$\varphi(t, x)$ the flow induced by (2)

Theorem: Let $h>0$. Let $X, Z$ be interval sets, $X \subset$ int $Z$. Suppose that

$$
\begin{equation*}
Y:=\text { interval hull }(X+[0, h] f(Z)) \subset \operatorname{int} Z \tag{3}
\end{equation*}
$$

then

$$
\begin{equation*}
\varphi([0, h], X) \subset Y \tag{4}
\end{equation*}
$$

Problem: For $x^{\prime}=-L x$ we have a bound for the time step

$$
h<\frac{1}{L}
$$

Insert here an example for $n=2$ with one dissipative coordinate

## Improved rough enclosure for

 dissipative ODE$$
\begin{equation*}
x_{i}^{\prime}=f_{i}(x)=\lambda_{i} x_{i}+N_{i}(x), \quad i=1, \ldots, n \tag{5}
\end{equation*}
$$

Theorem: $h>0, X \subset Z \subset \mathbf{R}^{n}$ - interval sets. Let $D \subset\{1, \ldots, n\}$ ( dissipative(damped) directions), if $k \in D$, then

$$
\begin{aligned}
\lambda_{k} & <0 \\
\lambda_{k} x_{k}+N_{k}^{-} & <\dot{x}_{k}<\lambda_{k} x_{k}+N_{k}^{+}
\end{aligned}
$$

where $N_{k}(Z) \subset\left(N_{k}^{-}, N_{k}^{+}\right)$.
For $k \in D$ we set

$$
\begin{aligned}
b_{k}^{ \pm} & =\frac{N_{k}^{ \pm}}{-\lambda_{k}} \\
g_{k}^{ \pm} & =\left(X_{k}^{ \pm}-b_{k}^{ \pm}\right) e^{\lambda_{k} h}+b_{k}^{ \pm}
\end{aligned}
$$

Let $Y=\Pi_{i=1}^{n} Y_{i}$ be such that

$$
\begin{aligned}
& Y_{i}=X_{i}+[0, h] f_{i}(Z), \quad i \notin D \\
& Y_{i}=Z_{i}, \quad i \in D .
\end{aligned}
$$

Then

$$
\varphi([0, h], X) \subset Y,
$$

provided the following conditions are satisfied for $i=1, \ldots, n$

1. if $i \notin D$, then

$$
Y_{i} \subset \operatorname{int} Z_{i}
$$

2. upper bounds for $i \in D$
if $Z_{i}^{+}<b_{i}^{+}, \quad$ then $Z_{i}^{+} \geq g_{k}^{+}$
3. lower bounds for $i \in D$
if $Z_{i}^{-}>b_{i}^{-}, \quad$ then $Z_{i}^{-} \leq g_{k}^{-}$

For

$$
x^{\prime}=-L x, \quad L>0
$$

and $X=[-1,1]$ one obtains $Y=[-1,1]$ and no bound on $h>0$.

## Computation of the Poincaré map

- One needs a procedure which gives a rigorous estimates between time steps for $x$-variable for ODE - rough enclosure ok
- we need to come very close to section
-the section error is minimized for sections perpendicular to the flow


## Lohner algorithm

$$
\begin{aligned}
& {\left[x_{k}\right]=x_{k}+\left[r_{k}\right], \text { where }\left[r_{k}\right]=Q_{k}\left[\tilde{r}_{k}\right] \text { or }\left[r_{k}\right]=} \\
& \left.\left.C_{k}\left[r_{0}\right]+Q_{k}\right] \tilde{r}_{k}\right]
\end{aligned}
$$

1. Finding rough enclosure $[W]$ of $\varphi\left(\left[0, h_{k}\right],\left[x_{k}\right]\right)$
2. $\left[A_{k}\right]=\frac{\partial \Phi}{\partial x}\left(h,\left[x_{k}\right]\right)$
3. $x_{k+1}=m\left(\Phi\left(h_{k}, x_{k}\right)\right)$,

$$
\left[z_{k+1}\right]=\operatorname{Rem}([W])+\Phi\left(h_{k}, x_{k}\right)-x_{k+1}
$$

4. $\left[r_{k+1}\right]=\left[A_{k}\right] \cdot\left[r_{k+1}\right]+\left[z_{k+1}\right]$ - the rearangement computations

Step 2 - the most time consuming part (we practically solve variational equation)
$\operatorname{Cost}(S t e p 2) \approx n^{?} \operatorname{Cost}(S t e p 3)$
$\operatorname{Cost}($ Step 3$) \gg \operatorname{Cost}($ Step $1+$ Step 4$)$

Very slow compared to nonrigorous computations by factor of order $10 n$.

## Reasons:

the interval arithmetics is at least two times slower than nonrigorous one

The Lohner algorithm is a $C^{0}$-algorithm, but internally is in fact $C^{1}$

Question: Can one do better with $C^{0}$ algorithm?
$C^{0}$ - algorithm
$\left[x_{k}\right]=x_{k}+B\left(0, r_{k}\right)$, where $r \in \mathbf{R}, B(0, r)$ - the ball of radius $r$. The choice of the good norm is an important parameter of algorithm.

1. Find rough enclosures $\varphi\left(\left[0, h_{k}\right],\left[x_{k}\right]\right) \subset[W]$ of and $\varphi\left(\left[0, h_{k}\right], x_{k}\right) \subset\left[W_{1}\right]$
2. compute $l=l(d f([W]))$
3. $x_{k+1}=m\left(\Phi\left(h_{k}, x_{k}\right)+\operatorname{Rem}\left(\left[W_{1}\right]\right)\right), z_{k+1}=$ $\Phi\left(h_{k}, x_{k}\right)+\operatorname{Rem}\left(\left[W_{1}\right]\right)-x_{k+1}$
4. $r_{k+1}=r_{k} e^{l h_{k}}+\left\|z_{k+1}\right\|$

Question: what is $l(d f([W]))$ ?

# Propagation of errors according to the typical numerical analysis textbook: 

$$
\begin{equation*}
x^{\prime}=f(x) \tag{6}
\end{equation*}
$$

$|f(x)-f(y)| \leq L|x-y|$.
Let $\varphi\left(t, x_{0}\right)$ be a solution of (6) with an initial condition $x(0)=x_{0}$. Then

$$
|\varphi(t, x)-\varphi(t, y)| \leq e^{L t}|x-y|, \quad t \geq 0
$$

This is very bad estimate

## Examples:

- $x^{\prime}=-10 x$, predicts error-growth: $e^{10 t}$
- for the Lorenz attractor (from the proof by Galias and P. Z.), gives an estimate for Lipschitz constant for the Poincare map $L>10^{9}$, while from simulations it is clear that $L \approx 5-6$
- in the proof for Rössler system ( P.Z. ), gives an estimate for the Lipschitz constant of Poincare map $L>5 \cdot 10^{41}$, while from simulations $L \approx$ $2-3$ cosmic computation time


## Logarithmic norms

Logarithmic norm: $Q \in R^{n \times n}$

$$
\mu(Q)=\lim _{h>0, h \rightarrow 0} \frac{\|I+h Q\|-1}{h}
$$

## can be negative !!!

- for Euclidean norm
$\mu(Q)=$ the largest eigenvalue of $1 / 2\left(Q+Q^{T}\right)$.
- for max norm $\|x\|=\max _{k}\left|x_{k}\right|$

$$
\mu(Q)=\max _{k}\left(q_{k k}+\sum_{i \neq k}\left|q_{k i}\right|\right)
$$

- for norm $\|x\|=\sum_{k}\left|x_{k}\right|$

$$
\mu(Q)=\max _{i}\left(q_{i i}+\sum_{k \neq i}\left|q_{k i}\right|\right)
$$

## Logarithmic norms - Fundamental lemma

Lemma: Let $\phi(t, x)$ be a flow induced by

$$
x^{\prime}=f(x) .
$$

Assume that $Z$ is a convex set,

$$
\begin{array}{r}
y([0, T]), \varphi\left([0, T], x_{0}\right) \in Z \\
\mu\left(\frac{\partial f}{\partial x}(\eta)\right) \leq l, \quad \text { for } \eta \in Z \\
\left\|\frac{d y}{d t}(t)-f(y(t))\right\|
\end{array}
$$

Then for $0 \leq t \leq T$ we have
$\left\|\varphi\left(t, x_{0}\right)-y(t)\right\| \leq e^{l t}\left\|y(0)-x_{0}\right\|+\delta \frac{e^{l t}-1}{l}, \quad$ if $l \neq 0$.
For $l=0$ we have

$$
\left\|\varphi\left(t, x_{0}\right)-y(t)\right\| \leq \rho+\delta t .
$$

In particular: $e^{l T}$ is a Lipschitz constant for $\phi(t, \cdot)$ in $Z$ (if $Z$ is forward invariant).

Examples:

- $x^{\prime}=-10 x$, predicts error-growth: $e^{-10 t}$ very good
- in the proof for Rössler system ( P.Z. ) logaritmic norm based on the euclidian norm was used, the estimate for the Lipschitz constant of Poincare map in some region was $L>2 \cdot 10^{4}$, while from simulations $L \approx 2-3$ this is doable. Using Lohner algorithm with cuboids one get Lipschitz constant around 60 and using doubletons something like 6-10.


# Lohner-type algorithm for differential 

 inclusion$$
\begin{equation*}
x^{\prime}(t) \in f(x(t))+[\delta] \tag{7}
\end{equation*}
$$

$x \in \mathbf{R}^{n},[\delta] \subset \mathbf{R}^{n}$
Find a rigorous enclosure for $x(t)$.

We compare the solutions of two ODEs

$$
\begin{align*}
x_{1}^{\prime}= & f\left(x_{1}\right)  \tag{8}\\
x_{2}^{\prime}= & f\left(x_{2}\right)+y(t)  \tag{9}\\
& x_{1}\left(t_{0}\right)=x_{2}\left(t_{0}\right)=x_{0} \tag{10}
\end{align*}
$$

where $y(t) \in[\delta]$ is given (but unknown) function.

## Lohner-type algorithm for differential inclusion - Fundamental Lemma

Lemma: Let:
$\left[W_{1}\right] \subset\left[W_{2}\right] \subset \mathbf{R}^{n}$ - convex and compact. $x_{1}\left(\left[t_{0}, t_{0}+h\right]\right) \subset\left[W_{1}\right], x_{2}\left(\left[t_{0}, t_{0}+h\right]\right) \subset\left[W_{2}\right]$ for any continuous function $y:\left[t_{0}, t_{0}+h\right] \rightarrow[\delta]$.

Then the following inequality holds for $t \in\left[t_{0}, t_{0}+\right.$ $h$ ] and for $i=1, \ldots, n_{1}$

$$
\begin{equation*}
\left|x_{1, i}(t)-x_{2, i}(t)\right| \leq\left(\int_{t_{0}}^{t} e^{J(t-s)} C d s\right)_{i} \tag{11}
\end{equation*}
$$

where

$$
\begin{aligned}
C_{i} & \geq \sup \left|\left[\delta_{i}\right]\right|, \quad i=1, \ldots, n_{1} \\
J_{i j} & \geq \sup \frac{\partial f_{i}}{\partial x_{j}}\left(\left[W_{2}\right]\right) \text { if } i=j, \\
J_{i j} & \geq \sup \left|\frac{\partial f_{i}}{\partial x_{j}}\left(\left[W_{2}\right]\right)\right| \text { if } i \neq j .
\end{aligned}
$$

# Lohner-type algorithm for differential inclusion - one step 

$\varphi\left(t, x_{0},[\delta]\right)$ - a solution of $x^{\prime} \in f(x)+[\delta], x(0)=$ $x_{0}$.
$\bar{\varphi}\left(t, x_{0}\right)$ - a solution of $x^{\prime}=f(x), x(0)=x_{0}$.

Input data:
$t_{k}, h_{k}$ - a time step,
$\left[x_{k}\right] \subset \mathbf{R}^{n}$, such that $\varphi\left(t_{k},\left[x_{0}\right],[\delta]\right) \subset\left[x_{k}\right]$.

Output data:
$t_{k+1}=t_{k}+h_{k}$,
$\left[x_{k+1}\right] \subset \mathbf{R}^{n_{1}}$, such that $\varphi\left(t_{k+1},\left[x_{0}\right],[\delta]\right) \subset\left[x_{k+1}\right]$.

## Lohner-type algorithm for differential inclusion - one step - details

1. Generation of a priori bounds for $\varphi$.

Find a convex and compact set $\left[W_{2}\right] \subset \mathbf{R}^{n}$, such that

$$
\begin{equation*}
\varphi\left(\left[0, h_{k}\right],\left[x_{k}\right],[\delta]\right) \subset\left[W_{2}\right] . \tag{12}
\end{equation*}
$$

2. Computation of $\bar{\varphi}$. We use Lohner algorithm to obtain $\left[\bar{x}_{k+1}\right] \subset \mathbf{R}^{n}$ and a convex and compact set $\left[W_{1}\right] \subset \mathbf{R}^{n}$, such that

$$
\begin{array}{rcc}
\bar{\varphi}\left(h_{k},\left[x_{k}\right]\right) & \left.\subset \bar{x}_{k+1}\right] \\
\bar{\varphi}\left(\left[0, h_{k}\right],\left[x_{k}\right]\right) & \subset\left[W_{1}\right]
\end{array}
$$

# Lohner-type algorithm for differential inclusion - one step - details continued 

3. Computation of perturbation. Using Fundamental Lemma we find a set $[\Delta] \subset \mathbf{R}^{n}$, such that

$$
\begin{equation*}
\varphi\left(t_{k+1},\left[x_{0}\right],[\delta]\right) \subset \bar{\varphi}\left(h_{k},\left[x_{k}\right]\right)+[\Delta] . \tag{13}
\end{equation*}
$$

Hence

$$
\begin{equation*}
\varphi\left(t_{k+1},\left[x_{0}\right],\left[y_{0}\right]\right) \subset\left[x_{k+1}\right]=\left[\bar{x}_{k+1}\right]+[\Delta] \tag{14}
\end{equation*}
$$

## Lohner-type .. - details and comments

Part 3 - details

1. We set

$$
\begin{aligned}
C_{i} & =\operatorname{right}\left(\left|\left[\delta_{i}\right]\right|\right), \quad i=1, \ldots, n_{1} \\
J_{i j} & =\operatorname{right}\left(\frac{\partial f_{i}}{\partial x_{i}}\left(\left[W_{2}\right]\right)\right) \text { if } i=j, \\
J_{i j} & =\operatorname{right}\left(\left|\frac{\partial f_{i}}{\partial x_{j}}\left(\left[W_{2}\right]\right)\right|\right), \text { if } i \neq j .
\end{aligned}
$$

2. $D=\int_{0}^{h} e^{J(h-s)} C d s$
3. $\left[\Delta_{i}\right]=\left[-D_{i}, D_{i}\right]$, for $i=1, \ldots, n_{1}$

$$
\begin{align*}
& \text { Lohner-type .. - Computation of } \\
& \int_{0}^{t} e^{A(t-s)} C d s \\
& \int_{0}^{t} e^{A(t-s)} C d s=t\left(\sum_{n=0}^{\infty} \frac{(A t)^{n}}{(n+1)!}\right) \cdot C . \tag{15}
\end{align*}
$$

We fix any norm $\|\cdot\|$, preferably the $L^{\infty}$-norm, $\left(\|x\|_{\infty}=\max _{i}\left|x_{i}\right|\right)$.

$$
\begin{array}{r}
\tilde{A}=A t, \quad A_{n}=\frac{\tilde{A}^{n}}{(n+1)!}, \\
\sum_{n=0}^{\infty} \frac{(A t)^{n}}{(n+1)!}=\sum_{n=0}^{\infty} A_{n} \\
A_{0}=\mathrm{Id}, \quad A_{n+1}=A_{n} \cdot \frac{\tilde{A}}{n+2}
\end{array}
$$

Remainder: $\left\|A_{N+k}\right\| \leq\left\|A_{N}\right\| \cdot\left\|\frac{\tilde{A}}{N+2}\right\|^{k}$. If $\left\|\frac{\tilde{A}}{N+2}\right\|<$ 1, then

$$
\left\|\sum_{n>N} A_{n}\right\| \leq\left\|A_{N}\right\| \cdot\left\|\frac{\tilde{A}}{N+2}\right\| \cdot\left(1-\left\|\frac{\tilde{A}}{N+2}\right\|\right)^{-1}
$$

Lohner-type .. - Representation of sets and rearrangement.

Lohner's approach.

In part 3:

$$
\begin{equation*}
\left[x_{k+1}\right]=\left[\bar{x}_{k+1}\right]+[\Delta] \tag{16}
\end{equation*}
$$

Evaluations 2 and 3. In this representation

$$
\begin{equation*}
\left[x_{k}\right]=x_{k}+\left[B_{k}\right]\left[\tilde{r}_{k}\right] . \tag{17}
\end{equation*}
$$

In the context of our algorithm in part 3 we obtain

$$
\begin{equation*}
\left[\bar{x}_{k+1}\right]=\bar{x}_{k+1}+\left[B_{k+1}\right]\left[\bar{r}_{k+1}\right] . \tag{18}
\end{equation*}
$$

We set

$$
\begin{aligned}
x_{k+1} & =\mathrm{m}\left(\bar{x}_{k+1}+[\Delta]\right) \\
{\left[\tilde{r}_{k+1}\right] } & =\left[\bar{r}_{k+1}\right]+\left[B_{k+1}^{-1}\right]\left(\bar{x}_{k+1}+[\Delta]-x_{k+1}\right) .
\end{aligned}
$$

## Lohner-type .. - Representation of

 sets and rearrangement IIEvaluation 4. In this representation

$$
\begin{equation*}
\left[x_{k}\right]=x_{k}+C_{k}\left[r_{0}\right]+\left[B_{k}\right]\left[\tilde{r}_{k}\right] . \tag{19}
\end{equation*}
$$

In the context of our algorithm in part 3 we obtain

$$
\left[\bar{x}_{k+1}\right]=\bar{x}_{k+1}+C_{k+1}\left[r_{0}\right]+\left[B_{k+1}\right]\left[\bar{r}_{k+1}\right]
$$

Equation (16) is taken into account exactly in the same way as in previous evaluations, i.e. we use equations (19) and (19).

## Variational equations, $C^{n}$-computations

Let

$$
\begin{aligned}
\frac{\partial \varphi_{i}}{\partial x_{j}}\left(t, x_{0}\right) & =V_{i, j}(t) \\
\frac{\partial^{2} \varphi_{i}}{\partial x_{j} \partial x_{k}}\left(t, x_{0}\right) & =H_{i j k}(t)
\end{aligned}
$$

It is well known that

$$
\begin{align*}
x^{\prime}= & f(x)  \tag{21}\\
\frac{d}{d t} V_{i j}(t)= & \sum_{s=1}^{n} \frac{\partial f_{i}}{\partial x_{s}}(x) V_{s j}(t)  \tag{22}\\
\frac{d}{d t} H_{i j k}(t)= & \sum_{s, r=1}^{n} \frac{\partial^{2} f_{i}}{\partial x_{s} \partial x_{r}}(x) V_{r k}(t) V_{s j}(t)+ \\
& \sum_{s=1}^{n} \frac{\partial f_{i}}{\partial x_{s}}(x) H_{s j k}(x) \tag{23}
\end{align*}
$$

with the initial conditions

$$
\begin{array}{r}
x(0)=x_{0}, \quad V(0)=I d \\
H_{i j k}(0)=0, \quad i, j, k=1, \ldots, n
\end{array}
$$

## An algorithm for $C^{n}$-computations

Simple approach: Apply $C^{0}$-Lohner algorithm to the system of variational equations, this works rather badly

- the control of wrapping effect may for $x$ variables may not work
- computationally ineffective because it totally ignores the structure of the system,

Let $\Phi(h, x)$ be a Taylor expansion for $\varphi(h, x)$ of order $p$, then $V(h, x)=\frac{\partial \Phi}{\partial x}(h, x)+h^{p+1}$

Observe that $\frac{\partial \Phi}{\partial x}(h,[W])$ is already computed in step 2 of $C^{0}$ algorithm

## An effective $C^{n}$-algorithm

-takes into account the structure of the system variational equations

- the rearrangement is done separately which partial derivatives of given order
- implemented in CAPD library, we did some computer assisted proofs involving $C^{5}$ computations for ODE $n=2,3$

