Modeling Physics with Differential-Algebraic Equations

Lecture 5

Differential Algebra

COMASIC (M2)

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1. Differential Algebra
2. Multi-Mode DAEs (Structural Analysis)

- Gröbner Bases are central objects in Computer Algebra Systems
- Elimination Theory generalizes Gaussian elimination (BLT Forms)
- Qualitative Analysis of ODE via their algebraic invariant sets

This Lecture

- Differential Algebra (Quick Introduction)
- Hybrid Aspects: Challenges

R denotes a commutative unitary ring.

- $a \in R$ is a zero divisor if and only if there exists $b \in R$, $b \neq 0$ such that $ab = 0$.
- 0 is a trivial zero divisor.
- Domains are rings where the only zero divisor is zero.
- Quotient of a ring R by an ideal I: R/I.
- $\bar{f}$ (or f) is zero in R/I if and only if f is in the ideal I.
- R/I, residue class ring (not necessarily a domain).
- M is a multiplicatively closed subset of R if and only if $m_1 m_2 \in M$ for all m_1, m_2 in M.

The zero divisors of the residue class ring are important.

Prime Ideals

The ideal $\mathfrak{p}$ is said to be *prime* if and only if

- $R/\mathfrak{p}$ is a domain.
- $R/\mathfrak{p}$ does not have nontrivial zero divisors.
- $ab \in \mathfrak{p}$ if and only if either $a \in \mathfrak{p}$ or $b \in \mathfrak{p}$.

Primary Ideals

The ideal $\mathfrak{q}$ is said to be *primary* if and only if

- all zero divisors of $R/\mathfrak{q}$ are nilpotent.
- $ab \in \mathfrak{q}$ if and only if either $a^m \in \mathfrak{q}$ or $b^m \in \mathfrak{q}$ for some positive natural number m.

The radical of a primary ideal, $\sqrt{\mathfrak{q}}$, is a prime ideal.

- Any maximal ideal is prime, the converse is not true.
- For a ring R, (X) is a prime ideal of $R[X]$ but it is not maximal $((X) \subset (X, Y))$.
- Intuition: points of a given affine space are not the only *irreducible* varieties – this will be given a precise meaning later. Lines and circles are also irreducible.

- One constructs the ring R_M (or $M^{-1}R$), the ring R localized at M, with elements of the form $\frac{r}{m}$ where $r \in R$ and $s \in M$.
- For $\frac{r_1}{m_1}$, $\frac{r_2}{m_2}$ in R_M, the "+" composition law is defined by $\frac{m_2 r_1 + m_1 r_2}{m_1 m_2}$.
- Let φ_M denote the ring homomorphism $R \to R_M$, then

$$\varphi_M^{-1}[(\varphi_M(I))] = I : M$$

Let I be an ideal of R and M a multiplicatively closed subset of R. Then

$$I : M \;=\; \{f \in R \mid \exists m \in M \;,\; mf \in I\} \;.$$

is a *Saturation* ideal.

Let $\mathfrak{q}$ be a primary ideal.

- If $M \cap I \neq \emptyset$ then $I : M = R$.
- If $M \cap \mathfrak{q} = \emptyset$ then $\mathfrak{q} : M = \mathfrak{q}$.

Suppose one has a primary decomposition of I: $I = \cap_{i=1}^{s} \mathfrak{q}_i$, then

$$I : M = \bigcap_{\mathfrak{q}_i \cap M = \emptyset} \mathfrak{q}_i$$

- $f = a_d X^d + a_{d-1} X^{d-1} + \cdots + a_1 X + a_0$
- $g = b_e X^e + b_{e-1} X^{e-1} + \cdots + b_1 X + b_0$
- $(d, e) \neq (0, 0)$

The Sylvester Matrix of f and g is the following $(d + e)$ square matrix.

$$S(f,g) = \begin{pmatrix} a_d & 0 & \cdots & 0 & b_e & 0 & \cdots & 0 \\ a_{d-1} & a_d & \cdots & 0 & b_{e-1} & b_e & \cdots & 0 \\ a_{d-2} & a_{d-1} & \ddots & 0 & b_{e-2} & b_{e-1} & \ddots & 0 \\ \vdots & \vdots & \ddots & a_d & \vdots & \vdots & \ddots & b_e \\ \vdots & \vdots & \cdots & a_{d-1} & \vdots & \vdots & \cdots & b_{e-1} \\ a_0 & a_1 & \cdots & a_{d-2} & b_0 & b_1 & \cdots & \vdots \\ 0 & a_0 & \ddots & \vdots & 0 & b_0 & \ddots & \vdots \\ \vdots & \vdots & \ddots & a_1 & \vdots & \vdots & \ddots & b_1 \\ 0 & 0 & \cdots & a_0 & 0 & 0 & \cdots & b_0 \end{pmatrix}$$

$$\begin{aligned} f &= X^2 - X + 1 \\ g &= X - 2 \end{aligned}$$

$$\begin{pmatrix} 1 & 1 & 0 \\ -1 & -2 & 1 \\ 1 & 0 & -2 \end{pmatrix}$$

$$\begin{aligned} f &= X^4 + 3X^3 - 1 \\ g &= -1 \end{aligned}$$

$$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

R is a domain. Let f and g be two polynomials in $R[X]$. The resultant of f and g, $\text{res}(f, g)$, is the determinant of the Sylvester matrix of f and g.

Properties

- f and g have a common root (on an algebraic field extension of R) if and only if $\text{res}(f, g) = 0$.
- $\text{res}(f, g) = (f, g)$. That is, there exists polynomials u and v of respective degrees less that e and d, such that $\text{res}(f, g) = uf + vg$.

Derivation

A *derivation* δ on R is a map $R \to R$ satisfying:

- $\delta(a+b) = \delta(a) + \delta(b)$
- $\delta(ab) = \delta(a)b + a\delta(b)$

- Notation: δa is often used instead of $\delta(a)$.
- δ_1 and δ_2 commute if and only if $\delta_1\delta_2 a = \delta_2\delta_1 a$ for all $a \in R$.
- **High-order** derivatives δ^h are inductively defined as $\delta(\delta^{h-1}a)$.
- **Ordinary** differential ring has a single derivation.
- **Partial** differential ring has a family $\Delta = \{\delta_1, \ldots, \delta_m\}$ of pairwise commuting derivations.
- Same definitions apply for a field k.

$c \in R$ is a **constant** if and only if $\delta c = 0$ for all $\delta \in \Delta$.
If k if a differential field, then the set of constants is a subfield of k.

Differential Ideal

A *differential* ideal $\mathfrak{a}$ of a Δ-ring R is an ideal of R such that

$$\forall \delta \in \Delta,\ \forall a \in \mathfrak{a},\ \delta a \in \mathfrak{a}\ .$$

- The intersection of an arbitrary number of differential ideals is a differential ideal
- The finite sum of differential ideals is also a differential ideal
- $[S]$ denotes the differential ideal generated by $S \subset R$.

Example 1

- $R = \mathbb{Z}[X]$, $\Delta = \left\{ \frac{d}{dX} \right\}$, is a differential ring.
- $\mathfrak{a} = (2, 2X)$ is a differential ideal.
- $[X] = R$ $(\delta X = 1)$

Example 2

- $R = \mathbb{Z}[X, e^X]$, $\Delta = \left\{ \frac{d}{dX} \right\}$, is a differential ring.
- $\mathfrak{a} = (e^X)$ is a differential ideal.
- $[X] = R$ $(\delta X = 1)$

Derivation Order

- Θ: free multiplicative monoid generated by $\Delta = \{\delta_1, \ldots, \delta_m\}$.
- $\theta \in \Theta$ has the form $\delta_1^{e_1} \cdots \delta_m^{e_m}$, $e_i \in \mathbb{N}$.
- **order** of θ is defined as $e_1 + \cdots + e_m$.
- Θ acts on R by $\theta a = \delta_1^{e_1} \cdots \delta_m^{e_m} a$

- Let R be a Δ-ring.
- $\Theta X = \{X_{\theta,j}\}_{1 \leq j \leq n, \theta \in \Theta}$, $n > 0$, family of indeterminates.
- $R[\Theta X]$ has a unique Δ-ring structure extending the Δ-ring structure of R by $\delta X_{\theta,j} = X_{\delta\theta,j}$, for all $\delta \in \Delta$, $\theta \in \Theta$.
- $R[\Theta X]$, equipped with this structure is called **Differential Polynomial Ring**,
- in the differential indeterminates $X_j = X_{1,j}$.
- $R[\Theta X]$ is denoted by $R\{X_1, \ldots, X_n\}$ or simply $R\{X\}$
- We write $X_{\theta,j}$ by θY_j (partial derivative of Y_j)
- The order of θY_j is defined as the order of θ

Differential Polynomial Ring (2/2)

- A **Differential Monomial** is a finite power product of derivatives of the form θY_j
- $\prod_k (\theta_k Y_{j_k})^{e_k}$, the θ_k (and likewise the Y_{j_k}) are not necessarily distinct
- A differential polynomial is a finite sum of terms aM where $a \in R$ and M is a differential monomial
- $R\{X\}$ has a structure of differential ring with $\Delta = \left\{ \frac{\partial}{\partial(\theta Y_j)} \right\}_{1 \leq j \leq n, \theta \in \Theta}$

- $R\{X_1, X_2\}$, $\Delta = \{\delta_1, \delta_2\}$
- $\theta_1 = \delta_1^4 \delta_2^3$
- $\theta_2 = \delta_2^4$
- $\theta_3 = \delta_1^3 \delta_2$
- $(\theta_1 X_1)(\theta_2 X_1)(\theta_3 X_2)^2 X_2$ is a monomial or order 7 and degree 5

The Wronskian determinant of dimension 2:

$$W = \begin{vmatrix} X_1 & X_2 \\ \delta X_1 & \delta X_2 \end{vmatrix}$$

is a differential polynomial in $R\{X_1, X_2\}$.

- $W = X_1 \delta X_2 - X_2 \delta X_1$
- $\delta W = X_1 \delta^2 X_2 - X_2 \delta^2 X_1$
- The partial derivative of W with respect to δX_2 is X_1

- Given a Δ differential ring R, to each element f of $R\{X\}$, one associates a (partial) differential equation $f = 0$.
- Likewise for a finite subset of $S \subset R\{X\}$, one gets a system of partial differential equations.
- The differential ideal $[S]$ is associated with S and contains all the equations derived from S by addition, multiplication by elements of $R\{X\}$ and differentiation.

As seen in the purely algebraic case, one wants to define a weaker notion of triangular forms suitable for the differential case.
We thus need to define *reduction* and hence ordering over differential monomials.

Triangular Form

A system $S \subset R\{X\}$ is in triangular form if its element can be rearranged as $S_1, S_2, \ldots, S_k, \ldots$ such that each S_k involves at least one derivative $\theta_k X_{j_k}$ which does not appear in $S_1, \ldots, S_{k-1}$. In particular $S_1 \notin R$.

Example

$$S := \begin{array}{ll} S_1 : & \delta^2 X_2 + X_2 \\ S_2 : & \delta^2 X_2 + X_2^2 + X_3 \\ S_3 : & \delta^2 X_2 + X_1 \end{array}$$

S is in triangular form with respect to X_2, X_3, X_1 (or $\delta^2 X_2, X_3, X_1$)

There are other definitions of triangular forms.

Definition

A ranking of $X_1, \ldots, X_n$ is a total ordering on ΘX such that for all $u, v \in \Theta X$ and $\delta \in \Delta$, $u \leq \delta u$, and $u \leq v$ implies $\delta u \leq \delta v$.

- A ranking is said to be *orderly* if $\mathrm{ord}(u) \leq \mathrm{ord}(v)$ implies $u \leq v$.
- A ranking is said to be *unmixed* if for every i, j, $X_i \leq X_j$ implies $\theta X_i \leq X_j$ for every $\theta \in \Theta$.

Pure Algebra	Differential Algebra
Monomials	Differential Monomials
Polynomials	Differential Polynomials
Ordering	Ranking
Hilbert Basis Theorem	Ritt-Raudenbush Basis Theorem
Gröbner Bases	Characteristic Sets (Ritt-Kolchin) Coherent Sets (Rosenfeld) Regular Chains (Boulier et al.)

1. Differential Algebra

2. Multi-Mode DAEs (Structural Analysis)

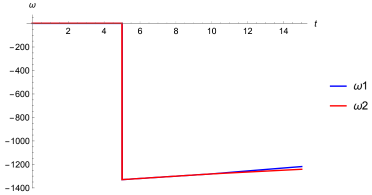
$$\left\{\begin{array}{llll} & & \omega_1' = f_1(\omega_1, \tau_1) & (e_1) \\ & & \omega_2' = f_2(\omega_2, \tau_2) & (e_2) \\ \texttt{when } \gamma & \texttt{do} & \omega_1 - \omega_2 = 0 & (e_3) \\ & \texttt{and} & \tau_1 + \tau_2 = 0 & (e_4) \\ \texttt{when } \neg\gamma & \texttt{do} & \tau_1 = 0 & (e_5) \\ & \texttt{and} & \tau_2 = 0 & (e_6) \end{array}\right.$$

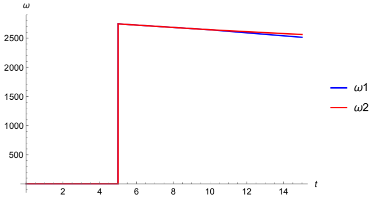
```
model ClutchBasic
  parameter Real w01=1;
  parameter Real w02=1.5;
  parameter Real j1=1;
  parameter Real j2=2;
  parameter Real k1=0.01;
  parameter Real k2=0.0125;
  parameter Real t1=5;
  parameter Real t2=7;
  Real t(start=0, fixed=true);
  Boolean g(start=false);
  Real w1(start = w01, fixed=true);
  Real w2(start = w02, fixed=true);
  Real f1;
  Real f2;
equation
  der(t) = 1;
  g = (t >= t1) and (t <= t2);
  j1*der(w1) = -k1*w1 + f1;
  j2*der(w2) = -k2*w2 + f2;
  0 = if g then w1-w2 else f1;
  f1 + f2 = 0;
end ClutchBasic;
```

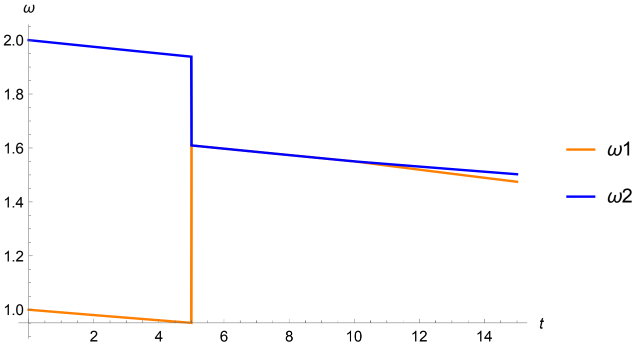
```
The following error was detected at time: 5.002
Error: Singular inconsistent scalar system
for f1 = ((if g then w1-w2 else 0.0))
/(-(if g then 0.0 else 1.0)) = -0.502621/-0
Integration terminated before reaching
"StopTime" at T = 5
```

```
NDSolve[{
    w1'[t] == -0.01 w1[t] + t1[t],
    2 w2'[t] == -0.0125 w2[t] + t2[t],
    t1[t] + t2[t] == 0,
    s[t] (w1[t] - w2[t]) + (1 - s[t]) t1[t] == 0,
    w1[0] == 1.0, w2[0] == 1.5, s[0] == 0,
    WhenEvent[t == 5,
              {s[t] -> 1}
              ]
        },
    {w1, w2, t1, t2,s},
    {t, 0, 7}, DiscreteVariables -> s]
```

Simulation with Mathematica






ω
2.0
1.8
1.6
1.4
1.2
1.0
2
4
6
8
10
12
14
t
ω1
ω2

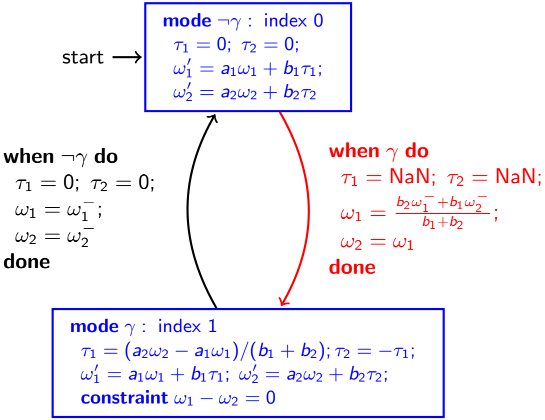
Structural Analysis

- Enforcing a Causality Principle: A guard must be evaluated before its guarded equation
- Extend the definition of the derivative operator for discrete event changes
- Unlocking Overdetermined systems by a "forward shift"
- Call the classical structural index reduction algorithm for underdetermined systems

Resets Computation

- Impulse Analysis
- Standardization (limits computation)

$$
\begin{cases}
 & & \omega_1^{\bullet} = \omega_1 + \partial f_1(\omega_1, \tau_1) & (e_1^{\partial}) \\
 & & \omega_2^{\bullet} = \omega_2 + \partial f_2(\omega_2, \tau_2) & (e_2^{\partial}) \\
\texttt{when } \gamma & \texttt{do} & \omega_1^{\bullet} - \omega_2^{\bullet} = 0 & (e_3^{\bullet}) \\
 & \texttt{and} & \tau_1 + \tau_2 = 0 & (e_4) \\
\texttt{when } \neg\gamma & \texttt{do} & \tau_1 = 0 & (e_5) \\
 & \texttt{and} & \tau_2 = 0 & (e_6)
\end{cases}
$$


start
mode $\neg\gamma$: index 0
$\tau_1 = 0;\ \tau_2 = 0;$
$\omega_1' = a_1\omega_1 + b_1\tau_1;$
$\omega_2' = a_2\omega_2 + b_2\tau_2$
when $\neg\gamma$ **do**
$\tau_1 = 0;\ \tau_2 = 0;$
$\omega_1 = \omega_1^-;$
$\omega_2 = \omega_2^-$
done
when γ **do**
$\tau_1 = \text{NaN};\ \tau_2 = \text{NaN};$
$\omega_1 = \frac{b_2\omega_1^- + b_1\omega_2^-}{b_1 + b_2};$
$\omega_2 = \omega_1$
done
mode γ : index 1
$\tau_1 = (a_2\omega_2 - a_1\omega_1)/(b_1 + b_2); \tau_2 = -\tau_1;$
$\omega_1' = a_1\omega_1 + b_1\tau_1;\ \omega_2' = a_2\omega_2 + b_2\tau_2;$
constraint $\omega_1 - \omega_2 = 0$