Numerical Simulation of Dynamic Systems XVIII

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Differential Algebraic Equations

As we have meanwhile understood, a model described by *state equations* is not the normal form, in which a model of a dynamical system presents itself initially.

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As the derivatives show up in the DAE model implicitly, we shall need to *iterate over the model equations* during each function evaluation.
The Three Iteration Loops

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- On the next higher level, we need to iterate over each integration step, as we are using an implicit DAE solver for the simulation.

- On the highest level, it may happen that an entire integration step is rejected and needs to be repeated, because the estimation of the local integration error indicates that we are using either a step size that is too large or an order that is too low.
The Three Iteration Loops II

- Numerical integration algorithm
- Step size and order control
- Newton iteration
- State equations
- Model containing algebraic loops

*Error controlled simulation*

*Fixed step/order simulation*
The Three Iteration Loops III

Are these three separate iteration loops really necessary?
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- Do processes that require iterations, really exist in the physical world? Isn’t the physical world *causal*, i.e., isn’t it true that each event has one or several causes, and that a strictly sequential ordering is possible between causes and effects? Don’t iterations defy the principle of strict causality?
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- Mutual causal dependencies do indeed exist in physics and are rather common. The relationship between voltage and current in a resistor is non-causal. It is not true that the potential difference at the two ends of the resistor makes current flow, or that the current flowing through the resistor causes a voltage drop. These are simply two different facets of one and the same physical phenomenon.
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- Yet “causal loops” do not truly exist in the physical world. If we place two resistors in series, this will create an algebraic loop in our model. The idea of a loop implies a sequence of execution, i.e., *a* causes *b*, which in turn causes *c*, which is responsible for *a*. Physics doesn’t understand the concept of a “sequence of execution.” *Physics is by its very nature completely non-causal.*
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All phenomena observed are byproducts of the big balance equations that we call the conservation principles: conservation of energy, conservation of mass, and conservation of momentum.
Let us simulate the model:

\[ f(x, \dot{x}, u, t) = 0.0 \]

using the BDF3 algorithm:

\[ x_{k+1} = \frac{6}{11} h \cdot \dot{x}_{k+1} + \frac{18}{11} x_k - \frac{9}{11} x_{k-1} + \frac{2}{11} x_{k-2} \]
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We can solve the solver equation for the derivative vector:

\[ \dot{x}_{k+1} = \frac{1}{h} \left[ \frac{11}{6} \cdot x_{k+1} - 3x_k + \frac{3}{2} x_{k-1} - \frac{1}{3} x_{k-2} \right] \]
Simulation of Implicit DAEs Using Implicit DAE Solvers

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\]

We substitute the solver equation in its derivative form into the model equations:

\[
\mathcal{F}(x_{k+1}) = f(x_{k+1}, \frac{1}{h} \left[ \frac{11}{6} \cdot x_{k+1} - 3x_k + \frac{3}{2} x_{k-1} - \frac{1}{3} x_{k-2} \right], u_{k+1}, t_{k+1}) = 0.0
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Newton iteration can evidently be applied directly, fusing the two innermost iteration loops.
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- In the context of explicit ODE solvers, this separation comes quite naturally. The state-space model computes \( \dot{x}(t_k) \) out of \( x(t_k) \), and the integration algorithm in turn computes \( x(t_{k+1}) \) out of \( x(t_k) \) and \( \dot{x}(t_k) \) – a meaningful and clean separation of duties.
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- By the time implicit integration algorithms were introduced, this separation was no longer as clean and crisp and beautiful. We now had to deal with causal loops anyway, since the state-space model and the ODE solver now operated on the same time instant, i.e., they had to co-operate to find simultaneously $x(t_{k+1})$ and $\dot{x}(t_{k+1})$. 
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- However, tradition had imprinted this separation so deeply into the brains of the simulation practitioners of that epoch that no one bothered to raise the question whether this separation was still useful, or whether it might not even be detrimental to our task.
By combining the *solver equations* and the *model equations*, i.e., by substituting the solver equations into the model equations, we were able to amalgamate the two innermost iteration loops into a single loop. This often pays off in terms of computational efficiency.
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As a by-product, we were able to throw out \( n \) equations and unknowns from our model, where \( n \) denotes the order of our model, i.e., the number of individual integrators, as we eliminated all of the derivatives from the model. They are no longer computed.
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We shall explore this fruitful idea some more in the context of *inline integration*. 
BDF Algorithms

A numerical integration algorithm that is applied directly to an implicit model description is called *numerical differential algebraic equation solver* or shorter *numerical DAE solver*. 
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To this end, we start with the linear implicit DAE model:

$$A \cdot x + B \cdot \dot{x} = 0$$
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Let us insert the *BDF3 algorithm* in its differential form:

$$A \cdot x_{k+1} + \frac{11B}{6h} \cdot \left( x_{k+1} - \frac{18}{11} x_k + \frac{9}{11} x_{k-1} - \frac{2}{11} x_{k-2} \right) = 0.0$$
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\]

Thus:

\[
x_{k+1} = \left( -B - \frac{6Ah}{11} \right)^{-1} \cdot \left( -\frac{18B}{11} x_k + \frac{9B}{11} x_{k-1} - \frac{2B}{11} x_{k-2} \right)
\]
Let us first discuss the simplest case:

\[ B = -I^{(n)} \]
BDF Algorithms II

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\[ \mathbf{B} = -\mathbf{I}^{(n)} \]

In this case, the linear implicit DAE model degenerates to the explicit linear ODE model:

\[ \dot{\mathbf{x}} = \mathbf{A} \cdot \mathbf{x} \]

and the equation used to compute \( \mathbf{x}_{k+1} \) degenerates to:

\[ \mathbf{x}_{k+1} = \left( \mathbf{I}^{(n)} - \frac{6\mathbf{A}h}{11} \right)^{-1} \cdot \left( \frac{18}{11} \mathbf{x}_k - \frac{9}{11} \mathbf{x}_{k-1} + \frac{2}{11} \mathbf{x}_{k-2} \right) \]

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which is identical to the equation that had been used earlier to determine the stability domain of the BDF3 numerical ODE solver.

- At least in this most simple situation, the stability domain is not at all affected by the DAE formulation.
Let us assume next that $B$ is a non-singular matrix. In this case, the implicit DAE model can be made explicit:

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**Does the inversion of $B$ have an effect on the stability domain?**
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**Does the inversion of $B$ have an effect on the stability domain?**

We can determine the stability domain of the method in the following way. We choose the eigenvalues of $-B^{-1} \cdot A$ along the unit circle of the complex plane, then apply the so found $A$- and $B$-matrices to the $F$-matrix:

$$F = \begin{pmatrix}
O^{(n)} & I^{(n)} & O^{(n)} \\
O^{(n)} & O^{(n)} & I^{(n)} \\
\frac{2}{11} (B + \frac{6}{11}Ah)^{-1} B & -\frac{9}{11} (B + \frac{6}{11}Ah)^{-1} B & \frac{18}{11} (B + \frac{6}{11}Ah)^{-1} B
\end{pmatrix}$$

and determine $h$ such that the dominant eigenvalues of $F$ are on the unit circle.
We arbitrarily chose several different non-singular $B$-matrices of dimensions $2 \times 2$, and computed the corresponding $A$-matrices using:

$$A = -B \cdot \begin{pmatrix} 0 & 1 \\ -1 & 2\cos(\alpha) \end{pmatrix}$$
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In every single case, the stability domain was exactly the same as that of the corresponding numerical ODE solver.

Non-singular $B$-matrices do not influence the numerical stability properties of the method in any way.
Higher Index Models

With a *singular* $B$ *matrix*, the DAE model cannot be reformulated in an explicit form that easily.
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We begin by a *singular value decomposition of the $B$ matrix*:

$$B = U \cdot \Sigma \cdot V^*$$

with:

$$\text{rank}(U) = \text{rank}(V) = n$$

$$\text{rank}(\Sigma) = \text{rank}(B) = r < n$$

$U$ and $V$ are *unitary matrices*, whereas $\Sigma$ is a *diagonal matrix*.

$V^*$ is the *Hermitian transpose of $V$*. 
Therefore:

\[ A \cdot x + U \cdot \Sigma \cdot V^* \cdot \dot{x} = 0.0 \]

\[ \Rightarrow U^* \cdot A \cdot x + \Sigma \cdot V^* \cdot \dot{x} = 0.0 \]
Higher Index Models II

Therefore:

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and with:

\[ z = \mathbf{V}^* \cdot \mathbf{x} \]

we obtain:

\[ \mathbf{U}^* \cdot \mathbf{A} \cdot \mathbf{V} \cdot z + \mathbf{\Sigma} \cdot \dot{z} = 0.0 \]
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and with:

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we obtain:

\[ U^* \cdot A \cdot V \cdot z + \Sigma \cdot \dot{z} = 0.0 \]

or:

\[ \tilde{A} \cdot z + \Sigma \cdot \dot{z} = 0.0 \]
Higher Index Models III

\[
\dot{z}_1 + \sigma_1 \cdot \dot{z}_1 = 0.0
\]

\[
\tilde{A}_{11} \cdot \dot{z}_1 + \tilde{A}_{12} \cdot \dot{z}_2 + \Sigma_{11} \cdot \dot{z}_1 = 0.0
\]

\[
\dot{z}_2 = 0.0
\]
If the matrix $\tilde{A}_{22}$ is singular, the model is poorly defined.
Higher Index Models III

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On the other hand, if the matrix $\tilde{A}_{22}$ is non-singular, we can write:

$$z_2 = -\tilde{A}_{22}^{-1} \cdot \tilde{A}_{21} \cdot z_1$$

and consequently:

$$\dot{z}_1 = \Sigma_{11}^{-1} \cdot (\tilde{A}_{12} \cdot \tilde{A}_{22}^{-1} \cdot \tilde{A}_{21} - \tilde{A}_{11}) \cdot z_1$$
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Such a model is called a \textit{higher index model}.

We have already learnt that there exist \textit{symbolic algorithms} for \textit{automatic index reduction}. One of these algorithms is the \textit{Pantelides algorithm} that was discussed extensively in the previous two presentations.
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The Pantelides algorithm is an algorithm of *linear computational complexity*. Thus, it is very efficient.
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Dealing with higher index models directly, i.e., numerically, without prior index reduction is never worth it. It is always better to first reduce the perturbation index symbolically down to at least index-1 as part of the model compilation.
Higher Index Models IV

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▶ Consequently, the case of singular B matrices is irrelevant.
Let us analyze now what happens when we implement a DAE algorithm of the AM class.
AM Algorithms

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Let us start with the AM3 algorithm:

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AM Algorithms

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\]

We can solve the solver equation for the derivative vector:

\[
\dot{x}(t_{k+1}) = f_{k+1} = \frac{12}{5h} (x(t_{k+1}) - x(t_k)) - \frac{8}{5} f_k + \frac{1}{5} f_{k-1}
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\[ \dot{x}(t_{k+1}) = f_{k+1} = 12 \frac{h}{5} (x(t_{k+1}) - x(t_k)) - 8 \frac{f_k}{5} + \frac{1}{5} f_{k-1} \]

We can substitute that equation into the DAE model:

\[ f(x, \dot{x}, u, t) = 0.0 \]

thereby eliminating the derivative \( \dot{x}_{k+1} \).
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\textbullet\hspace{1em} Numerical linear multi-step (ODE or DAE) solvers that make use of only a single derivative in their formulae are called \textit{one-legged algorithms}. 
Unfortunately, the “known” quantities $f_k$ and $f_{k-1}$ are left in the equation. Yet, we don’t have these values available as we just *eliminated the computation of the derivative vector from the model*.

This didn’t happen in the case of the BDF algorithm, because those solvers don’t make use of the derivatives of the past in their computation.

▶ Numerical linear multi-step (ODE or DAE) solvers that make use of only a single derivative in their formulae are called *one-legged algorithms*.

▶ The BDF algorithms are thus one-legged algorithms. In contrast, the AM algorithms are not.
One way to resolve the problem is to *introduce a second Newton iteration*:

\[
\mathcal{F}_1 (x(t_{k+1})) = \mathbf{f} \left( x(t_{k+1}), \frac{12}{5h} x(t_{k+1}) - \frac{12}{5h} x(t_k) - \frac{8}{5} w(t_k) \right.
\]
\[
+ \frac{1}{5} w(t_{k-1}), u(t_{k+1}), t_{k+1} \right) = 0.0
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- The upper equation determines \( x(t_{k+1}) \). In this iteration, \( u(t_{k+1}), x(t_k), w(t_k) \), and \( w(t_{k-1}) \) are assumed known.

- The lower equation then evaluates \( w(t_{k+1}) \). During that iteration, \( x(t_{k+1}) \) can be assumed known as well. Clearly, \( w \) is just another name for \( \dot{x} \).
Let us now find the \textit{numerical stability domain for the AM3 algorithm} when used in its DAE form.
Let us now find the *numerical stability domain for the AM3 algorithm* when used in its DAE form.

Substituting the AM3 formula in its differentiated form into the linear DAE model, we obtain:

\[
\begin{align*}
    x(t_{k+1}) &= \left( B + \frac{5}{12} Ah \right)^{-1} \cdot \left( Bx(t_k) + \frac{2}{3} Bhw(t_k) - \frac{1}{12} Bhw(t_{k-1}) \right) \\
    w(t_{k+1}) &= - B^{-1} Ax(t_{k+1})
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\]

With the state vector:

\[
z_k = \begin{pmatrix} x_k \\ w_{k-1} \\ w_k \end{pmatrix}
\]

we find the \( F \)-matrix:

\[
F = \begin{pmatrix}
\left( B + \frac{5}{12} Ah \right)^{-1} B & -\frac{1}{12} \left( B + \frac{5}{12} Ah \right)^{-1} Bh & \frac{2}{3} \left( B + \frac{5}{12} Ah \right)^{-1} Bh \\
O^{(n)} & O^{(n)} & I^{(n)} \\
-B^{-1} A \left( B + \frac{5}{12} Ah \right)^{-1} B & \frac{1}{12} B^{-1} A \left( B + \frac{5}{12} Ah \right)^{-1} Bh & -\frac{2}{3} B^{-1} A \left( B + \frac{5}{12} Ah \right)^{-1} Bh
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However, $w(t_{k+1})$ is linear in $x(t_{k+1})$, and consequently, the $F$-matrix is singular. We simply added a few eigenvalues at the origin. These eigenvalues do not influence the numerical stability domain.
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It has become evident that the numerical stability domain of an implicit (index-1) DAE solver is exactly the same as that of the corresponding ODE solver.
AB Algorithms

Let us discuss next what happens if we try to convert an explicit solver to DAE form.
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We start with the AB3 algorithm:

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We solve that equation for the derivative vector:

$$\dot{x}(t_{k+1}) = \frac{12}{23h} (x(t_{k+2}) - x(t_{k+1})) + \frac{16}{23} f_k - \frac{5}{23} f_{k-1}$$
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Unfortunately, *explicit integration formulae* are converted to *over-implicit differentiation formulae*.

*These formulae are useless, as they result in a gigantic iteration over the entire simulation rather than being limited to a single integration step.*
Over-implicit Numerical Integration Algorithms

This brings us to another idea. How if we were to convert *over-implicit integration algorithms* that, until now, had been totally useless to DAE form?
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The over-implicit $3^{rd}$-order Adams formula:

$$x(t_{k+1}) = x(t_k) + \frac{h}{12} (-f(t_{k+2}) + 8f(t_{k+1}) + 5f(t_k))$$

can be converted to the explicit derivative form:

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Let us now consider over-implicit algorithms of the BDF class.
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The over-implicit 3\textsuperscript{rd}-order BDF algorithm:

\[ x(t_{k+1}) = \frac{57}{26}x(t_k) - \frac{21}{13}x(t_{k-1}) + \frac{11}{26}x(t_{k-2}) + \frac{6h}{26}f(t_{k+2}) \]

can be converted to the explicit derivative form:

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Unfortunately, also this over-implicit integration algorithm is unstable. Consequently, also the explicit differentiation formula is unstable.
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The numerical stability properties of a linear multi-step algorithm do not change at all when converted from integral to differential form or vice-versa.
Accuracy Properties

We should also investigate the *accuracy properties* of the *DAE algorithms*. 
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- We know from our earlier discussions that BDF$i$ formulae are inefficient for use in non-stiff ODEs due to their poor accuracy properties. This was documented when we compared the efficiency of different ODE solvers when simulating the wave equation.
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- The problem evidently hasn't vanished by reformulating the model in a DAE format. Thus, we may suspect that the AM$i$ formulae will still work better than the BDF$i$ formulae also in non-stiff DAE simulation. However, whether this is true or not will depend on the relative cost to be paid for the second Newton iteration.
I simulated once more the wave equation using BDF3 and AM3, this time using the DAE formulation of these algorithms:

<table>
<thead>
<tr>
<th>$h$</th>
<th>BDF3</th>
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<tbody>
<tr>
<td>0.1</td>
<td>garbage</td>
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<tr>
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<td>unstable</td>
</tr>
<tr>
<td>0.02</td>
<td>garbage</td>
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<tr>
<td>0.005</td>
<td>0.9469e-2</td>
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- The entries in the above table, displaying the step sizes used, look exactly the same as the corresponding entries in the table shown earlier.
- This is not surprising, as the DAE formulation doesn't change the numerical properties of the methods.
Yet the cost of the AM3 algorithm in terms of the *number of function evaluations* may be higher in the DAE formulation than in the ODE formulation due to the need for a second Newton iteration.
Accuracy Properties III

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The DAE formulation of the AM3 algorithm turned out to be indeed a bit more expensive than the ODE formulation.
In this presentation, we looked at the DAE formulation of linear multi-step integration algorithms, and have reached a number of interesting conclusions:
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Conclusions

In this presentation, we looked at the DAE formulation of linear multi-step integration algorithms, and have reached a number of interesting conclusions:

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▶ It never pays off to simulate a higher-index problem directly. A problem with a perturbation index higher than 1 should always undergo symbolic index reduction first, e.g. using the Pantelides algorithm.

▶ Whether it pays off to transform an index-1 DAE to explicit ODE form, as we proposed in the previous few presentations, is not evident. It may, in some cases, be more efficient to simulate the index-1 DAE problem directly. We shall talk more about this issue later.
Conclusions II

We have learnt earlier that linear multi-step algorithms are mostly used for the simulation of stiff ODE problems, as indeed, implementations of BDF algorithms are to this day among the most widely used stiff system solvers on the market.
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A DAE formulation of explicit linear multi-step methods makes no sense whatsoever.
Conclusions IV

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- Thus, whereas the AM algorithms are definitely not competitive for the simulation of non-stiff index-0 problems, they may become competitive for the simulation of non-stiff index-1 problems, especially in their DAE formulation.
References