Numerical Simulation of Dynamic Systems XVIII

Prof. Dr. François E. Cellier
Department of Computer Science
ETH Zurich

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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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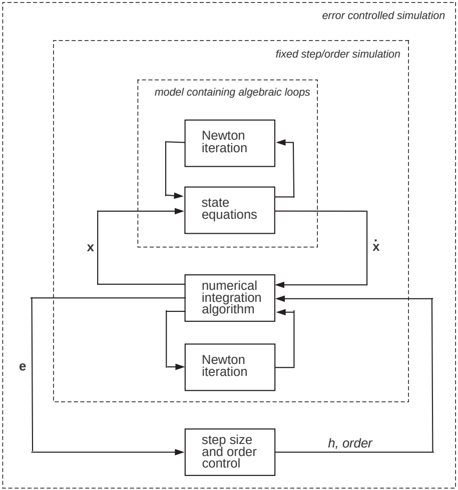
- On the next higher level, we need to iterate over each integration step, as we are using an implicit DAE solver for the simulation.
- On the highest level, it may happen that an entire integration step is rejected and needs to be repeated, because the estimation of the local integration error indicates that we are using either a step size that is too large or an order that is too low.

The Three Iteration Loops II



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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.

Simulation of Implicit DAEs Using Implicit DAE Solvers

Let us simulate the model:

$$\mathbf{f}(\mathbf{x}, \dot{\mathbf{x}}, \mathbf{u}, t) = 0.0$$

using the BDF3 algorithm:

$$\mathbf{x_{k+1}} = \frac{6}{11} h \cdot \dot{\mathbf{x}}_{\mathbf{k+1}} + \frac{18}{11} \mathbf{x_k} - \frac{9}{11} \mathbf{x_{k-1}} + \frac{2}{11} \mathbf{x_{k-2}}$$

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We can solve the solver equation for the derivative vector:

$$\dot{\mathbf{x}}_{\mathbf{k+1}} = \frac{1}{h} \left[\frac{11}{6} \cdot \mathbf{x_{k+1}} - 3\mathbf{x_k} + \frac{3}{2} \mathbf{x_{k-1}} - \frac{1}{3} \mathbf{x_{k-2}} \right]$$

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

$$\mathcal{F}(\mathbf{x_{k+1}}) = \mathbf{f}(\mathbf{x_{k+1}}, \frac{1}{h}\left[\frac{11}{6} \cdot \mathbf{x_{k+1}} - 3\mathbf{x_k} + \frac{3}{2}\mathbf{x_{k-1}} - \frac{1}{3}\mathbf{x_{k-2}}\right], \mathbf{u_{k+1}}, t_{k+1}) = 0.0$$

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Newton iteration can evidently be applied directly, fusing the two innermost iteration loops.

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- It originated with the desire to separate the process of *modeling* (in a simple-minded way of looking at things, the process of generating a state-space model out of physical observations) from that of *simulation* (the process of translating the state-space model into trajectory behavior).

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- In the context of explicit ODE solvers, this separation comes quite naturally. The state-space model computes $\dot{\mathbf{x}}(t_k)$ out of $\mathbf{x}(t_k)$, and the integration algorithm in turn computes $\mathbf{x}(t_{k+1})$ out of $\mathbf{x}(t_k)$ and $\dot{\mathbf{x}}(t_k)$ – 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 $\mathbf{x}(t_{k+1})$ and $\dot{\mathbf{x}}(t_{k+1})$.

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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.

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- We shall explore this fruitful idea some more in the context of *inline integration*.

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Let us insert the *BDF3 algorithm* in its differential form:

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

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Thus:

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

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- At least in this most simple situation, the stability domain is not at all affected by the DAE formulation.

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Let us assume next that $\mathbf{B}$ 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?

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

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

and determine h such that the dominant eigenvalues of **F** are on the unit circle.

BDF Algorithms IV

- We arbitrarily chose several different non-singular **B**-matrices of dimensions 2×2, and computed the corresponding **A**-matrices using:

$$\mathbf{A} = -\mathbf{B} \cdot \begin{pmatrix} 0 & 1 \\ -1 & 2\cos(\alpha) \end{pmatrix}$$

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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

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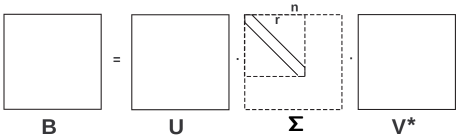
We begin by a *singular value decomposition of the* **B** *matrix*:

$$\mathbf{B} = \mathbf{U} \cdot \boldsymbol{\Sigma} \cdot \mathbf{V}^*$$



with:

$$\text{rank}(\mathbf{U}) = \text{rank}(\mathbf{V}) = n$$
$$\text{rank}(\boldsymbol{\Sigma}) = \text{rank}(\mathbf{B}) = r < n$$

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

$\mathbf{V}^*$ is the *Hermitian transpose* of **V**.

Higher Index Models II

Therefore:

$$\begin{aligned} & \mathbf{A} \cdot \mathbf{x} + \mathbf{U} \cdot \mathbf{\Sigma} \cdot \mathbf{V}^* \cdot \dot{\mathbf{x}} = 0.0 \\ \Rightarrow \quad & \mathbf{U}^* \cdot \mathbf{A} \cdot \mathbf{x} + \mathbf{\Sigma} \cdot \mathbf{V}^* \cdot \dot{\mathbf{x}} = 0.0 \end{aligned}$$

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and with:

$$\mathbf{z} = \mathbf{V}^* \cdot \mathbf{x}$$

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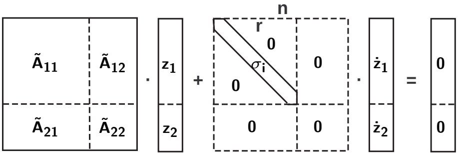
we obtain:

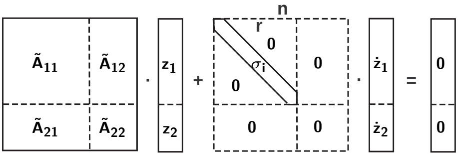
$$\mathbf{U}^* \cdot \mathbf{A} \cdot \mathbf{V} \cdot \mathbf{z} + \mathbf{\Sigma} \cdot \dot{\mathbf{z}} = 0.0$$

or:

$$\tilde{\mathbf{A}} \cdot \mathbf{z} + \mathbf{\Sigma} \cdot \dot{\mathbf{z}} = 0.0$$



Higher Index Models III



$$\tilde{\mathbf{A}}_{11} \cdot \mathbf{z}_1 + \tilde{\mathbf{A}}_{12} \cdot \mathbf{z}_2 + \mathbf{\Sigma}_{11} \cdot \dot{\mathbf{z}}_1 = 0.0$$

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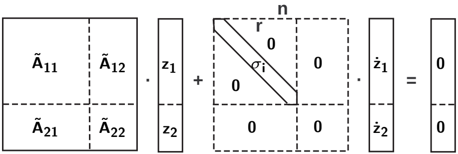

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If the matrix $\tilde{\mathbf{A}}_{22}$ is *singular*, the *model is poorly defined*.

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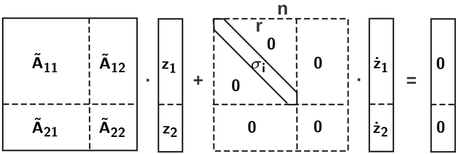

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$$\tilde{\mathbf{A}}_{21} \cdot \mathbf{z}_1 + \tilde{\mathbf{A}}_{22} \cdot \mathbf{z}_2 = 0.0$$

If the matrix $\tilde{\mathbf{A}}_{22}$ is *singular*, the *model is poorly defined*.

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

$$\mathbf{z}_2 = -\tilde{\mathbf{A}}_{22}^{-1} \cdot \tilde{\mathbf{A}}_{21} \cdot \mathbf{z}_1$$

and consequently:

$$\dot{\mathbf{z}}_1 = \mathbf{\Sigma}_{11}{}^{-1} \cdot \left(\tilde{\mathbf{A}}_{12} \cdot \tilde{\mathbf{A}}_{22}^{-1} \cdot \tilde{\mathbf{A}}_{21} - \tilde{\mathbf{A}}_{11} \right) \cdot \mathbf{z}_1$$

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- **Consequently, the case of singular $\mathbf{B}$ matrices is irrelevant.**

AM Algorithms

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We can solve the solver equation for the derivative vector:

$$\dot{\mathbf{x}}(t_{k+1}) = \mathbf{f}_{\mathbf{k+1}} = \frac{12}{5h}\left(\mathbf{x}(t_{k+1}) - \mathbf{x}(t_k)\right) - \frac{8}{5}\mathbf{f}_\mathbf{k} + \frac{1}{5}\mathbf{f}_{\mathbf{k-1}}$$

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We can substitute that equation into the DAE model:

$$\mathbf{f}(\mathbf{x}, \dot{\mathbf{x}}, \mathbf{u}, t) = 0.0$$

thereby eliminating the derivative $\dot{\mathbf{x}}_{\mathbf{k+1}}$.

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Unfortunately, the "known" quantities $\mathbf{f_k}$ and $\mathbf{f_{k-1}}$ 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*.

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- 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.

AM Algorithms III

One way to resolve the problem is to *introduce a second Newton iteration*:

$$\mathcal{F}_1(\mathbf{x}(t_{k+1})) = \mathbf{f}\Big(\mathbf{x}(t_{k+1}), \frac{12}{5h}\mathbf{x}(t_{k+1}) - \frac{12}{5h}\mathbf{x}(t_k) - \frac{8}{5}\mathbf{w}(t_k) + \frac{1}{5}\mathbf{w}(t_{k-1}), \mathbf{u}(t_{k+1}), t_{k+1}\Big) = 0.0$$

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- The upper equation determines $\mathbf{x}(t_{k+1})$. In this iteration, $\mathbf{u}(t_{k+1})$, $\mathbf{x}(t_k)$, $\mathbf{w}(t_k)$, and $\mathbf{w}(t_{k-1})$ are assumed known.

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- The lower equation then evaluates $\mathbf{w}(t_{k+1})$. During that iteration, $\mathbf{x}(t_{k+1})$ can be assumed known as well. Clearly, $\mathbf{w}$ is just another name for $\dot{\mathbf{x}}$.

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

$$\mathbf{x}(t_{k+1}) = \left(\mathbf{B} + \frac{5}{12}\mathbf{A}h\right)^{-1} \cdot \left(\mathbf{B}\mathbf{x}(t_k) + \frac{2}{3}\mathbf{B}h\mathbf{w}(t_k) - \frac{1}{12}\mathbf{B}h\mathbf{w}(t_{k-1})\right)$$

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With the state vector:

$$\mathbf{z_k} = \begin{pmatrix}\mathbf{x_k}\\ \mathbf{w_{k-1}}\\ \mathbf{w_k}\end{pmatrix}$$

we find the **F**-matrix:

$$\mathbf{F} = \begin{pmatrix} \left(\mathbf{B} + \frac{5}{12}\mathbf{A}h\right)^{-1}\mathbf{B} & -\frac{1}{12}\left(\mathbf{B} + \frac{5}{12}\mathbf{A}h\right)^{-1}\mathbf{B}h & \frac{2}{3}\left(\mathbf{B} + \frac{5}{12}\mathbf{A}h\right)^{-1}\mathbf{B}h \\ \mathbf{O}^{(\mathbf{n})} & \mathbf{O}^{(\mathbf{n})} & \mathbf{I}^{(\mathbf{n})} \\ -\mathbf{B}^{-1}\mathbf{A}\left(\mathbf{B} + \frac{5}{12}\mathbf{A}h\right)^{-1}\mathbf{B} & \frac{1}{12}\mathbf{B}^{-1}\mathbf{A}\left(\mathbf{B} + \frac{5}{12}\mathbf{A}h\right)^{-1}\mathbf{B}h & -\frac{2}{3}\mathbf{B}^{-1}\mathbf{A}\left(\mathbf{B} + \frac{5}{12}\mathbf{A}h\right)^{-1}\mathbf{B}h \end{pmatrix}$$

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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.

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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.

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can be converted to the explicit derivative form:

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

can be converted to the explicit derivative form:

$$\dot{\mathbf{x}}(t_{k+1}) = \frac{1}{6h}\left(26\mathbf{x}(t_k) - 57\mathbf{x}(t_{k-1}) + 42\mathbf{x}(t_{k-2}) - 11\mathbf{x}(t_{k-3})\right)$$

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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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- In contrast, implicit differentiation formulae are numerically stable if the corresponding implicit integration formulae are stable as well.
- 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

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- The problem evidently hasn't vanished by reformulating the model in a DAE format. Thus, we may suspect that the AMi formulae will still work better than the BDFi 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.

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I simulated once more the wave equation using BDF3 and AM3, this time using the DAE formulation of these algorithms:

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0.01	garbage	unstable
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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**.

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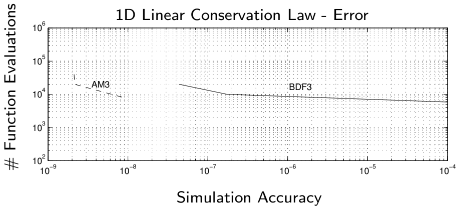

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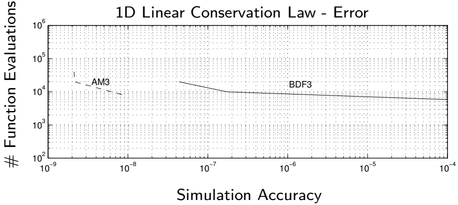

- The DAE formulation of the AM3 algorithm turned out to be indeed a bit more expensive than the ODE formulation.

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- The numerical properties of these algorithms, i.e., their numerical stability and accuracy properties, at least for index-0 and index-1 problems, do not change when switching from an ODE to a DAE formulation.
- 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.

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- We shall introduce DASSL in the next presentation.

Conclusions III

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- **Matlab** makes use of AB3 for the simulation of linear time-invariant systems, which is reasonable.
- A DAE formulation of explicit linear multi-step methods makes no sense whatsoever.

Conclusions IV

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Conclusions IV

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- The situation changes, when we look at index-1 problems. Here, the algebraic loops force us to employ a Newton iteration anyway, and if we do, we might just as well use a DAE formulation to start with.
- 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

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