

A reduced space simultaneous approach for optimization of nonlinear index-1 differential algebraic equations

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This work describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

Prototype implementation is completed; trials are underway

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A semi-explicit index-1 DAE has the form:

$$\begin{aligned}\dot{x} &= f(x, y, u) \\ 0 &= g(x, y, u), \det(\nabla_y g) \neq 0\end{aligned}\quad (1)$$

Our implicit function implementation handles systems:

$$\begin{aligned}F(z, y) &= 0 \\ G(z, y) &= 0, \dim(G) = \dim(y)\end{aligned}\quad (2)$$

First and second derivatives are via the implicit function theorem:

$$\begin{aligned}\nabla_z y &= -\nabla_y G^{-1} \nabla_z G \\ \nabla_{zz}^2 y &= -\nabla_y G^{-1} \left(\nabla_{zz}^2 G + \left(\nabla_{zy}^2 G^T \nabla_z y + \nabla_z y^T \nabla_{zy}^2 G \right) + \nabla_z y^T \nabla_{yy}^2 G \nabla_z y \right)\end{aligned}\quad (3)$$

Application: Chemical looping combustion (CLC) reactor
Algebraic equations are:

- ▶ Highly nonlinear
- ▶ Highly decomposable

Figure: Algebraic Jacobian, $\nabla_y g$, of CLC reactor model

