Discontinuous Collocation Methods for DAEs in Mechanics

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Outline

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Differential-Algebraic Equations

We consider *overdetermined mixed index 2 and 3 DAEs*:

$$\begin{aligned}
\dot{y} &= v(t, y, z) \\
\dot{z} &= f(t, y, z, \psi) + r(t, y, \lambda) \\
0 &= g(t, y) \\
0 &= g_t(t, y) + g_y(t, y)v(t, y, z) \\
0 &= k(t, y, z)
\end{aligned}$$

The functions

$$\begin{aligned}
v &: \mathbb{R} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_z} \to \mathbb{R}^{n_y} \\
f &: \mathbb{R} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_z} \times \mathbb{R}^{n_k} \to \mathbb{R}^{n_z} \\
r &: \mathbb{R} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_g} \to \mathbb{R}^{n_z} \\
g &: \mathbb{R} \times \mathbb{R}^{n_y} \to \mathbb{R}^{n_g} \\
k &: \mathbb{R} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_z} \to \mathbb{R}^{n_k}
\end{aligned}$$

are assumed to be sufficiently differentiable.

Differential-Algebraic Equations

The two matrices

$$g_y(t,y)v_z(t,y,z)r_\lambda(t,y,\lambda)$$

$$\begin{bmatrix} g_y v_z(t,y,z) \\ k_z(t,y,z) \end{bmatrix} \begin{bmatrix} r_\lambda(t,y,\lambda) & f_\psi(t,y,z) \end{bmatrix}$$

are assumed invertible. These assumptions allow for the system of DAEs to be expressed as ODEs. These are the so called *underlying ODEs*.

Examples from Mechanics

Well-known formulations of classical mechanics are *Hamiltonian Mechanics* and *Lagrangian Mechanics*. If the evolution of the system is constrained, the result is a DAE.

In the context of classical mechanics,

- *Holonomic constraints* are restrictions on the coordinates of a system. For example, the position of a pendulum in Cartesian coordinates is constrained to a circle or sphere.
- *Nonholonomic constraints* are (nonintegrable) restrictions on the velocities of a system. For example, an ice skate is constrained to move in the direction the blade is pointing.

Examples from Mechanics

Lagrangian System

$$\begin{aligned}
\dot{q} &= v \\
\frac{d}{dt}\nabla_v L(t,q,v) &= \nabla_q L(t,q,v) - g_q(t,q)^T\lambda - k_v(t,q,v)^T\psi \\
0 &= g(t,q) \\
0 &= g_t(t,q) + g_q(t,q)v \\
0 &= k(t,q,v)
\end{aligned}$$

Hamiltonian System

$$\begin{aligned}
\dot{q} &= \nabla_p H(t,q,p) \\
\dot{p} &= -\nabla_q H(t,q,p) - g_q(t,q)^T\lambda - k_p(t,q,p)^T\psi \\
0 &= g(t,q) \\
0 &= g_t(t,q) + g_q(t,q)\nabla_p H(t,q,p) \\
0 &= k(t,q,p)
\end{aligned}$$

Outline

Runge-Kutta Type Methods

We introduce two classes of Runge-Kutta type methods for solving overdetermined mixed index 2 and 3 DAEs.

- *Specialized partitioned additive Runge-Kutta (SPARK) methods* were introduced by Jay in 1998, and can be applied to systems with nonholonomic constraints. Methods were developed in 2007 and can be applied to systems with holonomic constraints.
- *Murua's partitioned Runge-Kutta methods* were proposed by Murua in 1996 for index 2 DAEs, and can be applied to systems with nonholonomic constraints.

We consider in this presentation an extension of the SPARK methods for systems of mixed index 2 and 3 DAEs. We consider also the *extended Murua's partitioned Runge-Kutta (EMPRK) methods* to systems of mixed index 2 and 3 DAEs.

An Example Method

(1, 1)-SPARK/EMPRK Midpoint-Trapezoidal Method

$$
\begin{aligned}
Y_1 &= y_0 + \frac{h}{2} v(t_0 + \frac{1}{2}h, Y_1, Z_1) \\
Z_1 &= z_0 + \frac{h}{2} f(t_0 + \frac{1}{2}h, Y_1, Z_1, \Psi_1) + \frac{h}{2} r(t_0, y_0, \Lambda_0) \\
y_1 &= y_0 + h\ v(t_0 + \frac{1}{2}h, Y_1, Z_1) \\
z_1 &= z_0 + h\ f(t_0 + \frac{1}{2}h, Y_1, Z_1, \Psi_1) + \frac{h}{2} r(t_0, y_0, \Lambda_0) + \frac{h}{2} r(t_1, y_1, \Lambda_1) \\
0 &= g(t_1, y_1) \\
0 &= g_t(t_1, y_1) + g_y(t_1, y_1) v(t_1, y_1, z_1) \\
0 &= k(t_1, y_1, z_1)
\end{aligned}
$$

The (s, s)-SPARK/EMPRK Methods

The internal stages

$$Y_i = y_0 + h \sum_{j=1}^{s} a_{ij} v(t_0 + c_j h, Y_j, Z_j), \quad i = 1, \ldots, s$$

$$Z_i = z_0 + h \sum_{j=1}^{s} a_{ij} f(t_0 + c_j h, Y_j, Z_j, \Psi_j) + h \sum_{j=0}^{s} \widetilde{a}_{ij} r(t_0 + \widetilde{c}_j h, \widetilde{Y}_j, \Lambda_j),$$
$$i = 1, \ldots, s$$

$$\widetilde{Y}_i = y_0 + h \sum_{j=1}^{s} \overline{a}_{ij} v(t_0 + c_j h, Y_j, Z_j), \quad i = 0, \ldots, s$$

$$\widetilde{Z}_i = z_0 + h \sum_{j=1}^{s} \overline{a}_{ij} f(t_0 + c_j h, Y_j, Z_j, \Psi_j) + h \sum_{j=0}^{s} \check{a}_{ij} r(t_0 + \widetilde{c}_j h, \widetilde{Y}_j, \Lambda_j),$$
$$i = 0, \ldots, s$$

The (s, s)-SPARK/EMPRK Methods, cont.

The constraints

$$
\begin{aligned}
0 &= g(t_0 + \widetilde{c}_i h, \widetilde{Y}_i), \quad i = 0, \ldots, s \\
0 &= g(t_1, y_1) \\
0 &= g_t(t_1, y_1) + g_y(t_1, y_1) v(t_1, y_1, z_1) \\
0 &= \sum_{j=1}^{s} b_j c_j^{i-1} k(t_0 + c_j h, Y_j, Z_j), \quad i = 1, \ldots, s-1 \\
0 &= k(t_0 + \widetilde{c}_i h, \widetilde{Y}_i, \widetilde{Z}_i), \quad i = 0, \ldots, s \\
0 &= k(t_1, y_1, z_1)
\end{aligned}
$$

The (s, s)-SPARK/EMPRK Methods, cont.

The numerical solution

$$y_1 = y_0 + h \sum_{j=1}^{s} b_j v(t_0 + c_j h, Y_j, Z_j)$$

$$z_1 = z_0 + h \sum_{j=1}^{s} b_j f(t_0 + c_j h, Y_j, Z_j, \Psi_j) + h \sum_{j=0}^{s} \widetilde{b}_j r(t_0 + \widetilde{c}_j h, \widetilde{Y}_j, \Lambda_j)$$

Gauss-Lobatto Coefficients

An example of a class of methods is the (s, s)-Gauss-Lobatto methods.

- Use s-stage Gauss coefficients for the a_{ij}, b_i, c_i
- Use $(s+1)$-stage Lobatto coefficients for the $\widetilde{b}_i$, $\widetilde{c}_i$
- Use $(s+1)$-stage Lobatto-IIIA for $\check{a}_{ij}$
- Define $\overline{a}_{ij}$ and $\widetilde{a}_{ij}$ by

$$\sum_{j=1}^{s} \overline{a}_{ij} c_j^{k-1} = \frac{\widetilde{c}_i^k}{k}, \quad k = 1, \ldots, s$$

$$\overline{a}_{0j} = 0, \quad j = 1, \ldots, s$$

$$\sum_{j=0}^{s} \widetilde{a}_{ij} \widetilde{c}_j^{k-1} = \frac{c_i^k}{k}, \quad k = 1, \ldots, s$$

$$\widetilde{a}_{i0} = \widetilde{b}_0, \quad i = 1, \ldots, s.$$

Existence and Uniqueness

Theorem

Suppose that $y_0 = y_0(h)$, $z_0 = z_0(h)$, $\lambda_0 = \lambda_0(h)$, $\psi_0 = \psi_0(h)$ *satisfy*

$$\begin{aligned}
o(h^2) &= g(t_0, y_0) \\
o(h) &= \frac{d}{dt}(g(t, y))(t_0, y_0, z_0) \\
o(1) &= \frac{d^2}{dt^2}(g(t, y))(t_0, y_0, z_0, \lambda_0, \psi_0) \\
o(h) &= k(t_0, y_0, z_0) \\
o(1) &= \frac{d}{dt}(k(t, y, z))(t_0, y_0, z_0, \lambda_0, \psi_0).
\end{aligned}$$

Then the SPARK and EMPRK methods possess a unique solution for h *sufficiently small.*

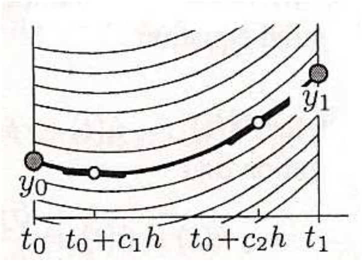
Determining Local Order

- Local order is defined through series expansions of the numerical and exact solutions. However, using series expansions to determine local order is tedious.
- Collocation methods (and discontinuous collocation methods), by contrast, have a much cleaner derivation of their local order.
- We are thus interested in showing the equivalence of the SPARK and EMPRK methods to a class of discontinuous collocation type methods.

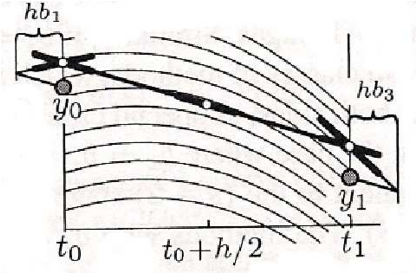
Outline

Collocation and Discontinuous Collocation

Continuous Collocation



Discontinuous Collocation



Hairer, Nørsett, Wanner. *Solving Ordinary Differential Equations I, Nonstiff Problems*. 2000

Discontinuous Collocation Type Methods

Let $c_1, \ldots, c_s$ be distinct real numbers, and $\widetilde{c}_0, \ldots, \widetilde{c}_s$ also be distinct real numbers, with $\widetilde{c}_0 = 0$ and $\widetilde{c}_s = 1$. Assume also that $\widetilde{b}_0$, $\widetilde{b}_s$ are positive real numbers. We then define the s-degree polynomials $Y(t)$, $\Lambda(t)$, $\Psi(t)$, $Z^f(t)$, the $(s+1)$-degree polynomials $Z(t)$, $Z^r(t)$, and the $(s+2)$-degree polynomials $\widetilde{Z}(t)$, $\widetilde{Z}^r(t)$ as the polynomials satisfying the initial conditions

$$
\begin{aligned}
&Y(t_0) = y_0, \\
&Z^f(t_0) = z_0, \quad Z^r(t_0) = -h\widetilde{b}_0\widetilde{\mu}(t_0), \\
&\widetilde{Z}^r(t_0) = 0, \\
&Z(t_0) = Z^f(t_0) + Z^r(t_0) = z_0 - h\widetilde{b}_0\widetilde{\mu}(t_0) \\
&\widetilde{Z}(t_0) = Z^f(t_0) + \widetilde{Z}^r(t_0) = z_0,
\end{aligned}
$$

where

$$\widetilde{\mu}(t) := \dot{Z}^r(t) - r(t, Y(t), \Lambda(t)),$$

Discontinuous Collocation Type Methods

and the conditions

$$
\begin{aligned}
&\dot{Y}(t_0 + c_i h) = v(t_0 + c_i h, Y(t_0 + c_i h), Z(t_0 + c_i h)), \quad i = 1, \dots, s \\
&\dot{Z}^f(t_0 + c_i h) = f(t_0 + c_i h, Y(t_0 + c_i h), Z(t_0 + c_i h), \Psi(t_0 + c_i h)), \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad i = 1, \dots, s \\
&\dot{Z}^r(t_0 + \widetilde{c}_i h) = r(t_0 + \widetilde{c}_i h, Y(t_0 + \widetilde{c}_i h), \Lambda(t_0 + \widetilde{c}_i h)), \quad i = 1, \dots, s-1 \\
&Z(t) = Z^f(t) + Z^r(t) \\
&\dot{\widetilde{Z}}^r(t_0 + \widetilde{c}_i h) = r(t_0 + \widetilde{c}_i h, Y(t_0 + \widetilde{c}_i h), \Lambda(t_0 + \widetilde{c}_i h)), \quad i = 0, \dots, s \\
&\widetilde{Z}(t) = Z^f(t) + \widetilde{Z}^r(t)
\end{aligned}
$$

Discontinuous Collocation Type Methods

$$
\begin{aligned}
0 &= g(t_0 + \widetilde{c}_i h, Y(t_0 + \widetilde{c}_i h)), \quad i = 0, \ldots, s \\
0 &= g_t(t_1, y_1) + g_y(t_1, y_1) v(t_1, y_1, z_1) \\
0 &= k(t_0 + \widetilde{c}_i h, Y(t_0 + \widetilde{c}_i h), \widetilde{Z}(t_0 + \widetilde{c}_i h)), \quad i = 0, \ldots, s \\
0 &= \sum_{j=1}^{s} b_j c_j^{i-1} k(t_0 + c_j h, Y(t_0 + c_j h), Z(t_0 + c_j h)), \quad i = 1, \ldots, s-1 \\
0 &= k(t_1, y_1, z_1).
\end{aligned}
$$

Discontinuous Collocation Type Methods

The numerical solution at $t_1 = t_0 + h$ is taken to be

$$y_1 := Y(t_1)$$
$$z_1 := Z(t_1) - h\widetilde{b}_s\widetilde{\mu}(t_1).$$

These discontinuous collocation type methods can be shown to be equivalent to the Gauss-Lobatto SPARK and EMPRK methods.

Discontinuous Collocation Type Methods

Theorem

A SPARK/EMPRK method with distinct values for c_j and for $\widetilde{c}_j$ is a discontinuous collocation method iff the coefficients satisfy

$$\sum_{j=1}^{s} a_{ij} c_j^{k-1} = \frac{c_i^k}{k}, \qquad \sum_{j=1}^{s} b_j c_j^{k-1} = \frac{1}{k}, \qquad k = 1, \dots, s$$

$$\sum_{j=0}^{s} \widetilde{a}_{ij} \widetilde{c}_j^{k-1} = \frac{c_i^k}{k}, \qquad \sum_{j=0}^{s} \widetilde{b}_j \widetilde{c}_j^{k-1} = \frac{1}{k}, \qquad k = 1, \dots, s-1$$

$$\widetilde{a}_{i0} = \widetilde{b}_0, \qquad \widetilde{a}_{is} = 0$$

$$\sum_{j=1}^{s} \bar{a}_{ij} c_j^{k-1} = \frac{\widetilde{c}_i^k}{k}, \qquad k = 1, \dots, s-1$$

$$\sum_{j=0}^{s} \check{a}_{ij} \widetilde{c}_j^{k-1} = \frac{\widetilde{c}_i^k}{k}, \qquad k = 1, \dots, s+1.$$

Outline

Local Error for Gauss-Lobatto SPARK/EMPRK Methods

Theorem

The (s, s)-Gauss-Lobatto SPARK and EMPRK methods with consistent initial values have local order $2s$, i.e., for $|h| \leq h_0$,

$$y_1 - y(t_1) = \mathcal{O}(h^{2s+1}), \qquad z_1 - z(t_1) = \mathcal{O}(h^{2s+1}).$$

Convergence

Theorem

Consider the (s, s)-Gauss-Lobatto SPARK / EMPRK methods with consistent initial conditions (y_0, z_0) at time t_0. Then the (s, s)-Gauss-Lobatto SPARK / EMPRK methods are convergent of order $2s$, i.e.

$$y_n - y(t_n) = \mathcal{O}(h^{2s}), \quad z_n - z(t_n) = \mathcal{O}(h^{2s}),$$

where y_n and z_n are the numerical solution at time $t_n := t_0 + nh$, for $nh \leq Const$.

Outline

Numerical Example - Simple Pendulum

Consider a simple pendulum of mass m and length ℓ.

$$L(t, q, v) := T - U, \qquad T := \frac{1}{2}m(v_1^2 + v_2^2), \qquad U := -m\gamma q_2,$$

$$0 = g(t, q) = \frac{1}{2}(q_1^2 + q_2^2 - \ell^2).$$

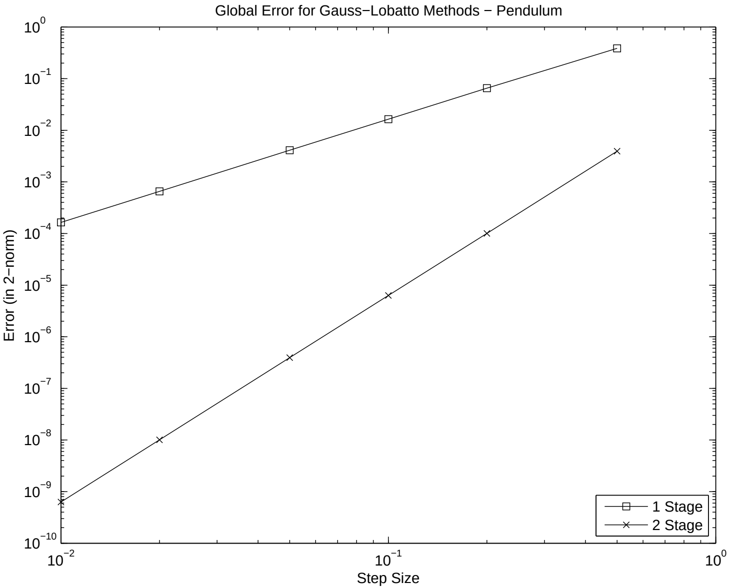
- m is the mass ($m = 1$)
- ℓ is the length of the bob ($\ell = 1$)
- γ is the acceleration due to gravity ($\gamma = 1$)

The initial conditions are

$$q_0 = \begin{pmatrix} 1 & 0 \end{pmatrix}^T, \qquad v_0 = \begin{pmatrix} 0 & 0 \end{pmatrix}^T.$$

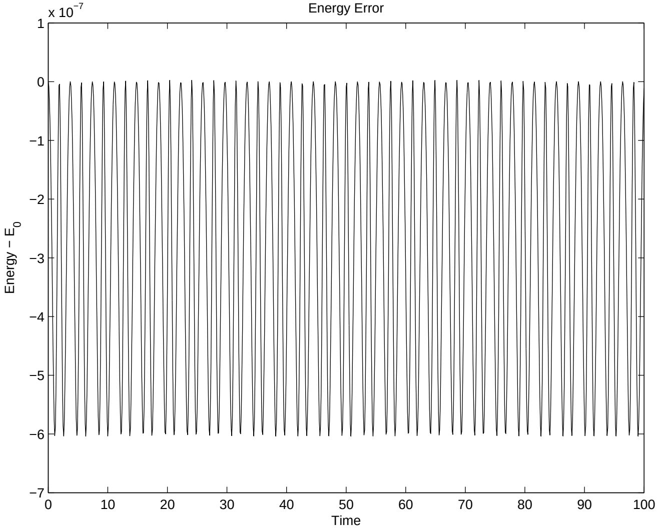
The system is integrated from 0 to 100.

Numerical Example - Simple Pendulum



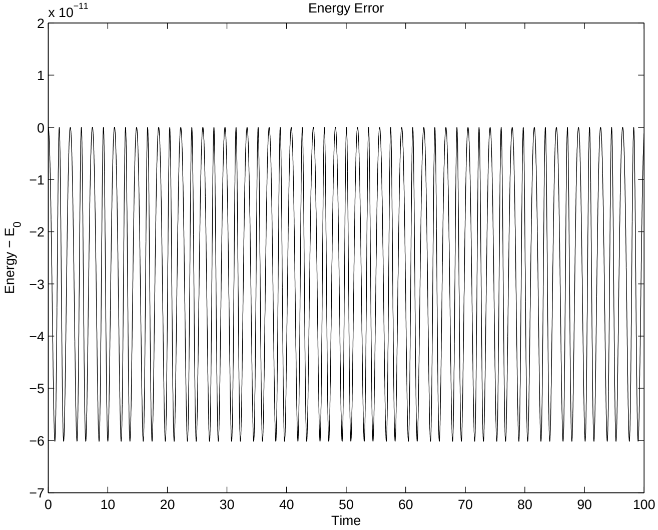
Numerical Example - Simple Pendulum

$(2,2)$–Gauss-Lobatto, $h = .05$



Numerical Example - Simple Pendulum

$(2,2)$–Gauss-Lobatto, $h = .01$



Numerical Example - Skate on an Inclined Plane

Consider a skate sliding on an inclined plane without friction.

$$L(t,q,v) := T - U$$

$$T := \frac{1}{4} m \left(v_1^2 + v_2^2 + v_3^2 + v_4^2\right) \qquad U := -\frac{1}{2} m\gamma \sin(\beta)(q_1 + q_3)$$

$$0 = g(t,q) = \frac{1}{2}\left((q_3 - q_1)^2 + (q_4 - q_2)^2 - \ell^2\right)$$

$$0 = k(t,q,v) = -(q_4 - q_2)(v_1 + v_3) + (q_3 - q_1)(v_2 + v_4)$$

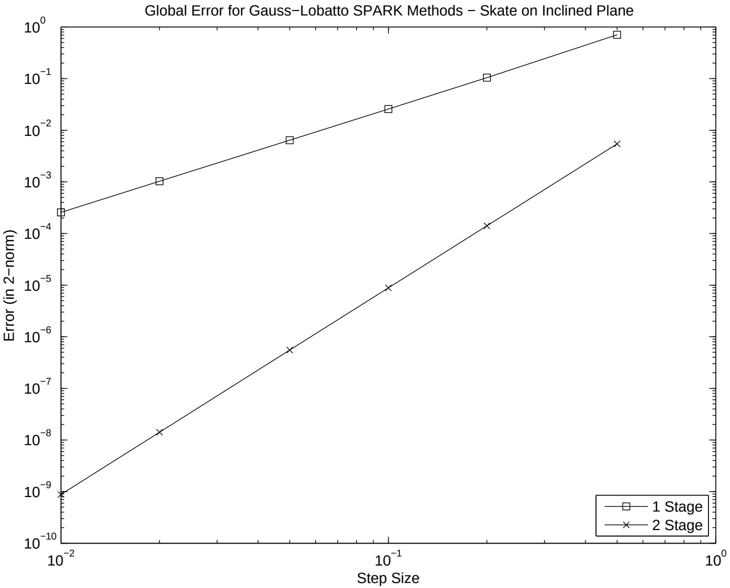
- m is the mass of the skate ($m = 1$)
- ℓ is the length of the skate ($\ell = 2$)
- γ is the acceleration due to gravity, β is the incline of the plane ($\gamma \sin(\beta) = 1$)

The initial conditions are

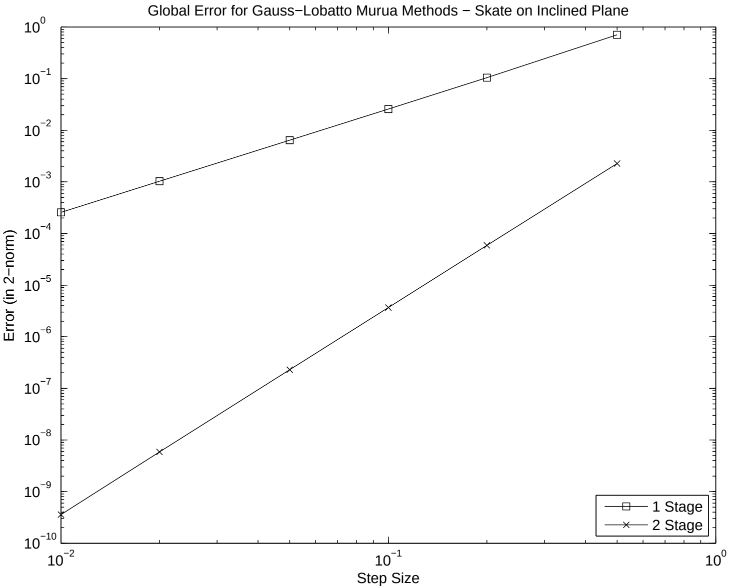
$$q_0 = (-1/2 \quad 0 \quad 1/2 \quad 0)^T \qquad v_0 = (0 \quad -1/2 \quad 0 \quad 1/2)^T.$$

The system is integrated from 0 to 10.

Numerical Example - Skate on an Inclined Plane

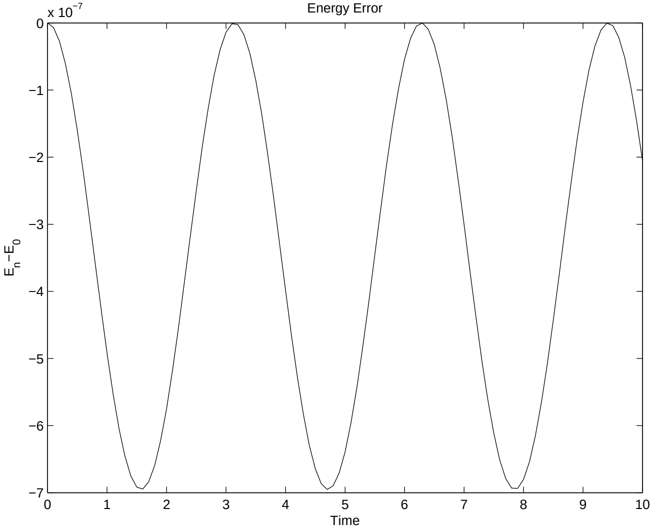


Numerical Example - Skate on an Inclined Plane



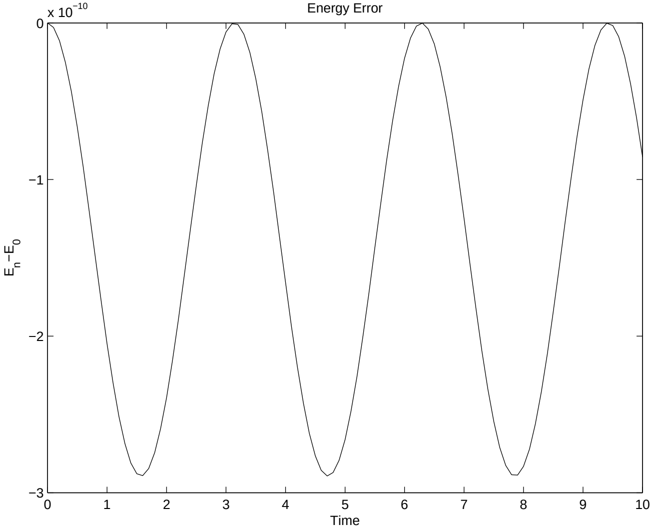
Numerical Example - Skate on an Inclined Plane

$(2,2)$–Gauss-Lobatto SPARK Method, $h = .1$



Numerical Example - Skate on an Inclined Plane

$(2, 2)$–Gauss-Lobatto EMPRK Method, $h = .1$



Outline

Conclusion

- SPARK and EMPRK methods are Runge-Kutta style methods for solving overdetermined mixed index 2 and 3 DAEs.
- These methods have a unique solution.
- These methods can be expressed as discontinuous collocation methods.
- For the Gauss-Lobatto coefficients, the SPARK and EMPRK methods are of order $2s$.