An overview is presented of three different pseudospectral methods based on collocation at Legendre-Gauss (LG), Legendre-Gauss-Radau (LGR), and Legendre-Gauss-Lobatto (LGL) points. For each of the schemes presented here, (1) the state at the final time can be expressed in terms of a quadrature rule associated with the collocation points, (2) the state at the initial time is approximated by interpolation, and (3) the control and the state are approximated at the collocation points. In the corresponding LGL scheme, the state approximation is a polynomial that is one degree lower than the number of collocation points. Each of these schemes can be expressed either as a differential or as an integral formulation. The LG and LGR differentiation and integration matrices are invertible, and the differential and integral versions are equivalent. The LGL differentiation matrix is singular and the equivalence between the differential and integral version is lost. For each scheme, the transformation between the KKT multipliers of the discrete nonlinear programming problem and costates of the continuous optimal control problem is developed. The LGL collocation is the only scheme for which the differentiation matrices for the state and the costate dynamics are the same. Two examples are used to assess the accuracy and features of each collocation scheme.

INTRODUCTION

Over the last decade, pseudospectral methods have risen to prominence in the numerical solution of optimal control problems.\textsuperscript{1–12} Pseudospectral methods are a class of direct collocation where the optimal control problem is transcribed to a nonlinear programming problem (NLP) by parameterizing the state and control using global polynomials and collocating the differential-algebraic equations using nodes obtained from a Gaussian quadrature. It is noted that some researchers prefer the term orthogonal collocation,\textsuperscript{13–15} but the terms pseudospectral and orthogonal collocation have the same meaning.

The three most commonly used sets of collocation points are Legendre-Gauss (LG), Legendre-Gauss-Radau (LGR), and Legendre-Gauss-Lobatto (LGL) points. These three sets of points are obtained from the roots of a Legendre polynomial and/or linear combinations of a Legendre polynomial and its derivatives. All three sets of points are defined on the domain \([-1, 1]\), but differ significantly in that the LG points include neither of the endpoints, the LGR points include one of the endpoints, and the LGL points include both endpoints.
The LG, LGR, and LGL collocation points lie on the open interval $\tau \in (-1, 1)$, the half open interval $\tau \in [-1, 1)$ or $\tau \in (-1, 1]$, and the closed interval $\tau \in [-1, 1]$, respectively. A depiction of these three sets of collocation points is shown in Fig. 1 where it is seen that the LG points contain neither $-1$ or 1, the LGR points contain only one of the points $-1$ or 1 (in this case, the point $-1$), and the LGL points contain both $-1$ and 1. Denoting $N$ as the number of collocation points and $P_N(\tau)$ as the $N^{th}$-degree Legendre polynomial, the LG points are the roots of $P_N(\tau)$, the LGR points are the roots of $P_{N-1}(\tau) + P_N(\tau)$, and the LGL points are the roots of $\tilde{P}_{N-1}(\tau)$ together with the points $-1$ and 1:

- **LG**: Roots obtained from $P_N(\tau)$
- **LGR**: Roots obtained from $P_{N-1}(\tau) + P_N(\tau)$
- **LGL**: Roots obtained from $\tilde{P}_{N-1}(\tau)$ together with the points $-1$ and 1

It is seen from Fig. 1 that the LG and LGL points are symmetric about the origin whereas the LGR points are asymmetric. In addition, the LGR points are not unique in that two sets of points exist (one including the point $-1$ and the other including the point 1). The LGR points that include the terminal endpoint are often called the flipped LGR points. In this paper we use the flipped LGR points, while Ref. 11 uses the standard set of LGR points.

**Notation.** Throughout the paper, we employ the following notation. $A^T$ denotes the transpose of a matrix $A$. Given two matrices $A$ and $B$ of the same dimensions, $\langle A, B \rangle$ is their dot product:

$$\langle A, B \rangle = \text{trace } A^T B.$$  

When $A$ and $B$ are vectors, this is the usual vector inner product. If $f : \mathbb{R}^n \to \mathbb{R}^m$, then $\nabla f$ is the $m$ by $n$ matrix whose $i$-th row is $\nabla f_i$. In particular, the gradient of a scalar-valued function is a row vector. If $\phi : \mathbb{R}^{m \times n} \to \mathbb{R}$ and $X$ is an $m$ by $n$ matrix, then $\nabla \phi$ denotes the $m$ by $n$ matrix whose $(i,j)$ element is

$$\langle \nabla \phi(X) \rangle_{ij} = \frac{\partial \phi(X)}{\partial X_{ij}}.$$  

Generally, a single subscript attached to a matrix denotes a row of the matrix. Thus $X_i$ is the $i$-th row of $X$. The only exception is the differentiation matrix $D$ where subscripts are used to denote columns. We also employ MATLAB submatrix notation: $D_{i,j}$ represents the submatrix of $D$ formed by columns $i$ through $j$. 


Expository Approach  To simplify the exposition, we focus on an unconstrained control problem on the time interval $\tau \in [-1, +1]$ with terminal cost. Note that the time interval can be transformed from $[-1, 1]$ to the time interval $[t_0, t_f]$ via the affine transformation

$$t = \frac{t_f - t_0}{2} \tau + \frac{t_f + t_0}{2}. $$

The goal is to determine the state $x(\tau) \in \mathbb{R}^n$ and the control $u(\tau) \in \mathbb{R}^m$ which minimize the Mayer cost functional

$$\Phi(x(1)), $$

subject to the constraints

$$\frac{dx}{d\tau} = f(x(\tau), u(\tau)), \quad x(-1) = x_0, $$

where $f : \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}^n$, and $x_0$ is the initial condition, which we assume is given.

COLLOCATION AT LG, LGR, AND LGL POINTS

In this section we provide an overview of solving optimal control problems using collocation at Legendre-Gauss (LG), Legendre-Gauss-Radau (LGR), and Legendre-Gauss-Lobatto (LGL) points. In order to provide consistent terminology, $N$ is always the number of collocation points for a particular scheme, and these collocation points are labeled $\tau_1, \ldots, \tau_N$. Using this convention, for LG, neither endpoint $\tau_0 = -1$ or $\tau_{N+1} = +1$ is collocated, for LGR, the initial point $\tau_0 = -1$ is uncollocated, while for LGL, both the initial point $\tau_1 = -1$ and the terminal point $\tau_N = +1$ are collocated. Although both the LG and LGR schemes have noncollocated endpoint(s), we still approximate the state at these endpoints as explained below. The LG and LGR schemes considered in this paper differ from those considered in Ref. 18. For the LG scheme, Ref. 18 imposes the initial condition at the collocation point $\tau_1 > -1$, while the terminal constraint is imposed at $\tau_N < +1$. It is shown in Ref. 18 that these modifications to the boundary conditions lead to a divergent numerical scheme.

Collocation at Legendre-Gauss (LG) Points

Consider collocation at the $N$ LG points. Each component of the state $x$ is approximated by a polynomial of degree at most $N$. Let $L_i(\tau), (i = 0, \ldots, N)$, be a basis of Lagrange polynomials given by

$$L_i(\tau) = \prod_{\substack{j=0 \atop j \neq i}}^{N} \frac{\tau - \tau_j}{\tau_i - \tau_j}, \quad (i = 0, \ldots, N).$$
The $j^{th}$ component of the state is approximated by a series of the form
\[
x_j^N(\tau) = \sum_{i=0}^{N} x_{ij} L_i(\tau). \tag{4}
\]
Notice that this series includes the Lagrange polynomial associated with the point $\tau_0 = -1$, which is not a collocation point. Differentiating the series and evaluating at the $k^{th}$ collocation point, $\tau_k$, gives
\[
\dot{x}_j^N(\tau_k) = \sum_{i=0}^{N} x_{ij} \dot{L}_i(\tau_k) = \sum_{i=0}^{N} D_{ki} x_{ij}, \quad D_{ki} = \dot{L}_i(\tau_k). \tag{5}
\]
The $N \times (N+1)$ non-square matrix $D$ is called the Gauss Pseudospectral differentiation matrix. Let $X$ denote the matrix formed from the coefficients $x_{ij}$ in (4). With this notation, $DX$ is an $N$ by $n$ matrix and (5) can be written
\[
\dot{x}_j^N(\tau_k) = (DX)_{ij}. \tag{6}
\]
Let $X^\text{LG}$ and $U^\text{LG}$ be $N$ by $n$ and $N$ by $m$ matrices respectively with $x_{ij}^\text{LG}$ and $u_{ij}^\text{LG}$ the discrete approximations to the $j^{th}$ component of the state and control, respectively, evaluated at the $i^{th}$ LG point:
\[
x_{ij}^\text{LG} \approx x_{ij}^\text{LG}(\tau_i) \text{ and } u_{ij}^\text{LG} \approx u_{ij}^\text{LG}(\tau_i), \quad 1 \leq i \leq N.
\]
For the matrices $X$, $X^\text{LG}$, and $U^\text{LG}$ (and later for the matrices of Lagrange multipliers) subscripts are used to denote rows of the matrix (e.g., $X_1$ is the $i^{th}$ row of $X$). This row contains the components of the discrete approximation to $x(\tau_i)$. Let $F(X^\text{LG}, U^\text{LG})$ denote an $N$ by $n$ matrix whose $(i, j)$ element is given by
\[
F_{ij}(X, U) = f_j(X_i, U_i), \quad 1 \leq i \leq N, \quad 1 \leq j \leq n. \tag{7}
\]
Collocating the dynamics at the $N$ LG points, we have
\[
DX = F(X^\text{LG}, U^\text{LG}) \tag{8}
\]
Let $X_{N+1}$ be the value of the state approximated at $\tau_{N+1} = +1$:
\[
X_{N+1,j} = x_j^N(1) \tag{1}
\]
By the fundamental theorem of calculus,
\[
X_{N+1,j} = x_j^N(1) = x_j^N(-1) + \int_{-1}^{+1} \dot{x}_j^N(\tau) d\tau. \tag{9}
\]
Let $w_k, 1 \leq k \leq N,$ be the LG quadrature coefficients. Since $x_j^N$ has degree at most $N$, $\dot{x}_j^N$ has degree at most $N - 1$. By (6) and by the exactness of LG quadrature,
\[
\int_{-1}^{+1} \dot{x}_j^N(\tau) d\tau = \sum_{i=0}^{N} w_i \dot{x}_j^N(\tau_i) = \sum_{i=0}^{N} w_i (DX)_{ij}. \tag{10}
\]
Substituting $x_j^N(-1) = X_{0,j}$ in (9) and combining with (8) and (10), we deduce that
\[
X_{N+1} = X_0 + w^T DX = w^T F(X^\text{LG}, U^\text{LG}). \tag{11}
\]
With this background, the discrete nonlinear programming problem (NLP) using LG points is the following:
\[
\begin{align*}
\text{minimize} & \quad \Phi(X_{N+1}) \\
\text{subject to} & \quad DX = F(X^\text{LG}, U^\text{LG}), \\
X_{N+1} & = X_0 + w^T F(X^\text{LG}, U^\text{LG}), \\
X_0 & = x_0,
\end{align*} \tag{12}
\]
where the state initial condition $x_0$ is a row vector. It is seen that the NLP of (12) includes variables for the state $X_i$ at the initial point ($\tau = -1$), the state $X_i$, $1 \leq i \leq N$ at the $N$ LG points, and the state $X_{N+1}$ at the terminal point ($\tau = +1$); the NLP also includes variables for the control $U_i$, $1 \leq i \leq N$, at the $N$ LG points.
We now develop the first-order optimality conditions for (12), also called as the KKT conditions of the NLP. Let \( A_{N+1} \) denote the \( N \times N \) matrix of Lagrange multipliers associated with the system dynamics (8), let \( \Lambda_{N+1} \) denote the \( 1 \times n \) vector of multipliers associated with the equation (11) for \( X_{N+1} \), and let \( \mu \) be the \( 1 \times n \) row vector of Lagrange multipliers associated with the initial condition. The KKT conditions of the NLP of (12) are given as

\[
\begin{align*}
A_{N+1} & = \nabla_X \Phi(X_{N+1}) \\
\mu & = \nabla_X \{A_{N+1}^T + w \Lambda_{N+1} + F(X_{N+1}, U^L)\} \\
A_{N+1} - D_1^T A_{N+1}^L & = 0 \\
\nabla_U \langle A_j, f(X_j, U_j) \rangle + w_j \nabla_U \langle A_{N+1}, f(X_j, U_j) \rangle & = 0 \\
\end{align*}
\]  

(13)

where \( \mathcal{L} \) is the Lagrangian of the NLP of (12), i.e.,

\[
\mathcal{L}(A_{N+1}, \Lambda_{N+1}, \mu, X, X_{N+1}, U^L) = \Phi(X_{N+1}) + \langle A_{N+1}, w^T F(X_{N+1}, U^L) + X_0 - X_{N+1} \rangle + \langle \mu, x_0 - X_0 \rangle.
\]

and \( D_0 \) is the initial column of \( D \). It is noted that the \( N \times N \) matrix \( D_{1:N} \) is nonsingular (see Ref. 19 for details).

**Transformed Adjoint System Using LG Collocation**  
Analogous to Ref. 20, we now reformulate the KKT conditions of the NLP given in (12) so that they become a discretization of the first-order optimality conditions for the continuous control problem (1)–(2). The quadrature weights \( w_i, 1 \leq i \leq N \), associated with the LG points have the property that

\[
\int_{-1}^{1} p(\tau) d\tau = \sum_{i=1}^{N} w_i p(\tau_i)
\]

for all polynomials \( p \) of degree at most \( 2N-1 \). Let \( \lambda \) be an \( N \times N \) matrix with \( i \)-th row

\[
\lambda_i = \frac{\lambda_i}{w_i} + A_{N+1}.
\]

(14)

Furthermore, for use in the discussion that follows, let

\[
\lambda_{N+1} = A_{N+1}.
\]

(15)

Finally, let \( \lambda_0 \) be defined as

\[
\lambda_0 = \lambda_{N+1} - D_{1:N}^T A_{N+1}^L.
\]

(16)

In order to connect the discrete costate equations to the continuous costate equations, we employ an \( N \times N \) matrix \( D^T \), which is a modified version of \( D \), defined as follows:

\[
D^T_{ij} = \begin{cases} 
-\frac{w_j}{w_i} D_{ji}, & (i, j) = 1, \ldots, N, \\
-\sum_{j=1}^{N} D^T_{ij}, & i = 1, \ldots, N
\end{cases}
\]

(17)

(18)

We now develop another equation for \( \lambda_0 \) by manipulating (16). We know that the components of the vector \( D1 \) are the derivatives at the collocation points of the polynomial whose value is 1 at \( \tau_i, 0 \leq i \leq N \). This polynomial is simply the constant 1, whose derivative is 0 everywhere. Hence, we have \( D1 = 0 \), which implies that

\[
D_0 = -\sum_{j=1}^{N} D_j.
\]

(19)

In other words, \( D_0 \) is a linear combination of the columns of \( D_{1:N} \). Returning to the definition of \( \lambda_0 \) in (16), we obtain

\[
\lambda_0 = \lambda_{N+1} - \sum_{i=1}^{N} \lambda_i D_{i0} = \lambda_{N+1} + \sum_{i=1}^{N} \sum_{j=1}^{N} \lambda_i D_{ij}
\]

(20)

\[
= \lambda_{N+1} - \sum_{j=1}^{N} \sum_{i=1}^{N} \lambda_i D^T_{ji} w_j w_i = \lambda_{N+1} - \sum_{i=1}^{N} \sum_{j=1}^{N} w_j (\lambda_i - \lambda_{N+1}) D^T_{ji}
\]

(21)

\[
= \lambda_{N+1} + \sum_{j=1}^{N} w_j \nabla_X \langle \lambda_j, f(X_j, U_j) \rangle.
\]

(22)
In summary, the transformed KKT conditions are the following (see Ref. 19 for details of the derivation):

\[
\lambda_0 = \mu, \quad \lambda_{N+1} = \nabla_X f(X_{N+1}), \quad D_{1:N}^\dagger \lambda + D_{N+1}^\dagger \lambda_{N+1} = -\nabla_X f(X, F(X^{LG}, U^{LG})), \quad \lambda_0 = \lambda_{N+1} + \sum_{j=1}^{N} w_j \nabla_X (\lambda_j, f(X_j, U_j)), \quad 0 = \nabla_U \langle \lambda, F(X^{LG}, U^{LG}) \rangle.
\]

We now compare the transformed KKT conditions for the discrete control problem (the pseudospectral scheme) to the first-order optimality condition for the continuous control problem (1)–(2):

\[
\lambda(-1) = \mu, \quad \lambda(1) = \nabla f(x(1)) \quad \lambda(t) = -\nabla_x (\lambda(t), f(x(t), u(t))) \quad 0 = \nabla_u (\lambda(t), f(x(t), u(t))).
\]

Observe that transformed variables \( \lambda_0 \) and \( \lambda_{N+1} \) satisfy exactly the same conditions as the continuous costate \( \lambda(t) \) evaluated at the endpoints. Also, the discrete and continuous necessary condition for the control have exactly the same structure. In the discrete optimality system, the equation (26) represents a quadrature approximation to the integral over \([-1, 1]\) of the adjoint equation. The connection between the discrete costate dynamics (25) and the continuous costate dynamics is less obvious. It is noted that the system (25) is a pseudospectral scheme for the costate equation (see Ref. 19 for details).

Thus the transformed KKT conditions are related to a pseudospectral discretization of the continuous costate equation. Furthermore, the differentiation matrices of the state and costate discretizations are based on the derivatives of polynomials of degree \( N \). Note that either \( D \) or \( D^\dagger \) operate on polynomial values to give the derivative at the collocation points. However, \( D \) operates on the polynomial values \( p(\tau_i), 0 \leq i \leq N \), while \( D^\dagger \) operates on the polynomial values \( p(\tau_i), 1 \leq i \leq N + 1 \).

**Integral Formulation Using LG Collocation**  
We will now show that the LG pseudospectral discretization of the state equation has an equivalent integrated formulation. First, using (19), we have

\[
D_0 = -D_{1:N}1,
\]

where \( 1 \) is a column vector of all ones. Multiplying (33) by \( D_{1:N}^{-1} \) gives

\[
D_{1:N}^{-1}D_0 = -1.
\]

Let \( \hat{p} \) be any polynomial of degree at most \( N \). By the construction of the \( N \times (N+1) \) matrix \( D \), we have \( Dp = \hat{p} \) where

\[
p_i = p(\tau_i), \quad 0 \leq i \leq N, \quad \hat{p}_i = \hat{p}(\tau_i), \quad 1 \leq i \leq N.
\]

Multiplying the identity \( \hat{p} = Dp = D_0p_0 + D_{1:N}p_{1:N} \) by \( D_{1:N}^{-1} \) and utilizing (34) gives

\[
p_i = p_0 + \left(D_{1:N}^{-1}\hat{p}\right)_i, \quad 1 \leq i \leq N
\]

Next, we obtain a different expression for \( p_i - p_0 \) based on the integration of the interpolant of the derivative. Let \( L_j^\dagger \) be the Lagrange interpolation polynomials associated with the collocation points:

\[
L_j^\dagger = \prod_{i=0 \atop i \neq j}^{N} \frac{\tau - \tau_i}{\tau_j - \tau_i}, \quad j = 1, \ldots, N.
\]

Notice that the Lagrange polynomials \( L_j \) defined in (3) have degree \( N \) since the product starts at \( i = 0 \), while the polynomials \( L_j^\dagger \) have degree \( N - 1 \) since the product starts with \( i = 1 \).
Since \( \dot{p} \) is a polynomial of degree at most \( N - 1 \), it can be interpolated exactly by the Lagrange polynomials \( L^j_\tau \):

\[
\dot{p} = \sum_{j=1}^{N} \dot{p}_j L^j_\tau(\tau) \tag{38}
\]

Integrating \( \dot{p} \) from \(-1\) to \( \tau_i \), we obtain

\[
p(\tau_i) = p(-1) + \sum_{j=1}^{N} \dot{p}_j A_{ij} = \int_{-1}^{\tau_i} L^j_\tau(\tau)d\tau, \quad 1 \leq i \leq N. \tag{39}
\]

Utilizing the notation (35), we have

\[
p_i = p_0 + (\dot{A} \dot{p})_i, \quad 1 \leq i \leq N. \tag{40}
\]

The relations (36) and (40) are satisfied for any polynomial of degree at most \( N \). We equate (36) and (40) to obtain

\[
\dot{A} \dot{p} = D_{1:N}^{-1} \dot{p}. \tag{41}
\]

Choose \( \dot{p} \) from the columns of the identity matrix to deduce that \( A = D_{1:N}^{-1} \). The dynamics of system (12) can be rewritten as

\[
D_{1:N} X^{LG} = F(X^{LG}, U^{LG}) - D_0 x_0. \tag{41}
\]

Multiply (41) by \( A = D_{1:N}^{-1} \) and utilize (34) to obtain

\[
X_i = X_0 + A_i F(X^{LG}, U^{LG}), \quad 1 \leq i \leq N, \tag{42}
\]

where \( A_i \) is the \( i^{th} \) row of \( A = D_{1:N}^{-1} \). Hence, the differential form of the state equation \( DX = F(X^{LG}, U^{LG}) \) is equivalent to the integrated form (42), where the elements of \( A \) are the integrals of the Lagrange basis \( L^j_\tau \) defined in (37), while the elements of \( D \) in the differential form are the derivatives of the Lagrange basis \( L^j_\tau \) defined in (5). Combining (42) and (11), the integral form of LG collocation can be written as

\[
Y = 1X_0 + \tilde{A} F(X^{LG}, U^{LG}), \tag{43}
\]

where

\[
Y = \begin{bmatrix} X^{LG} \\ X_{N+1} \end{bmatrix} \quad \text{and} \quad \tilde{A} = \begin{bmatrix} A \\ w^T \end{bmatrix}. \tag{44}
\]

In other words, the integral form of LG collocation provides an approximation to the state at each of the LG points plus the terminal point.

To summarize, the approximation to the dynamics given in (42) is in the form of a global implicit integration method while the differential form \( DX = F(X^{LG}, U^{LG}) \) is in the form of a pseudospectral method. The fact that either the integral or the differential form of LG collocation can be used shows that the LG collocation method derived in this paper can be thought of as either a global implicit integration method or a pseudospectral method. In particular, using the pseudospectral form of LG collocation results in a system of equations that has no loss of information from the integral form (because the matrix \( D_{1:N} \) is nonsingular). We call the differential form of LG collocation derived in this paper the Gauss pseudospectral method.*

**Collocation at Legendre-Gauss-Radau (LGR) Points**

The theory in this section follows from the theory for Radau collocation developed in Ref. 11; the only difference is that in Ref. 11, we focused on the Radau points that include \( \tau_1 = -1 \), while here we consider the flipped set of Radau points which includes \( \tau_N = 1 \). These Radau schemes are fundamentally different from those presented in either Ref. 10 or Ref. 18. The scheme in Ref. 10 utilizes a polynomial of degree 1 lower than the degree that we use. By increasing the degree of the polynomial, we are able to approximate the state at both endpoints. The Radau scheme in Ref. 18 imposes the state endpoint constraints at the collocation points; in Ref. 18 it is shown that this strategy for imposing the endpoint constraints leads to a divergence scheme.

*The equivalence between the integral and derivative forms of LG collocation derived in this paper can also be found in Ref. 6.
Consider now collocation using the $N$ backward LGR collocation points $\tau_1, \tau_2, \ldots, \tau_N$ on the interval $[-1, 1]$, with $\tau_1 > -1$ and $\tau_N = +1$. As with the LG scheme, we introduce an additional noncollocated point $\tau_0 = -1$ which is used to describe the approximation to the state variable at $\tau = -1$. Exactly as we did for LG points, each component of the state is approximated by a Lagrange polynomial expansion of the form (4). Again, the discrete system dynamics has the form $DX = F(X^{LGR}, U^{LGR})$. The fundamental difference between LG and LGR collocation is that $\tau_N = +1$ is included in the LGR collocation points. Hence, we do not need to develop a quadrature approximation to the state at the endpoint. Hence, the NLP associated with the backward LGR points has the simplified form

$$\begin{align*}
\text{minimize} & \quad \Phi(X_N) \quad \text{subject to} \quad DX = F(X^{LGR}, U^{LGR}), \quad X_0 = x_0.
\end{align*}$$

Next, the Lagrangian of the NLP of (45) is

$$L(A^{LGR}, \mu, X, U^{LGR}) = \Phi(X_N) + \langle \lambda, F(X^{LGR}, U^{LGR}) - DX \rangle + \langle \mu, x_0 - X_0 \rangle,$$

where $\lambda^{LGR}$ is an $N$ by $n$ matrix of Lagrange multipliers associated with the system dynamics and $\mu$ is a 1 by $n$ row vector of Lagrange multipliers associated with the initial condition. The KKT conditions of the backward LGR collocation are obtained by differentiating the Lagrangian with respect to the state and control variables and are given as follows (see Ref. 19 for details):

$$\begin{align*}
\nabla \Phi(X_N) + \nabla_X \langle \lambda, f(X, U) \rangle &= D_T^N \lambda^{LGR} \\
\sum_{i=1}^N D_{ij} \Lambda_i &= \nabla_X \langle \lambda, f(X_j, U_j) \rangle, \quad 1 \leq j \leq N - 1 \\
\mu &= -D_T^0 \lambda^{LGR} \\
\nabla_U \langle \lambda, f(X_j, U_j) \rangle &= 0
\end{align*}$$

**Transformed Adjoint System Using LGR Collocation**

Analogous to the results given in Ref. 11, the transformed adjoint variables corresponding to Radau collocation can be expressed in terms of the $N$ by $n$ matrix $\lambda$ with $i$-th row

$$\lambda_i = \lambda_i/w_i,$$

and the row vector

$$\lambda_0 = -D_T^0 \lambda^{LGR}.$$  

Here $w$ is the vector of LGR collocation weights. Let $D^\dagger$ be an $N$ by $N$ matrix defined as follows:

$$D^\dagger_{NN} = -D_{NN} + \frac{1}{w_N} \quad \text{and} \quad D^\dagger_{ij} = -\frac{w_j}{w_i} D_{ji} \quad \text{otherwise}.$$  

Using the transformations of (47) and (48), together with $D^\dagger$, we obtain the following transformed KKT conditions for the backward LGR discretization (see Ref. 11 for details):

$$\begin{align*}
\lambda_0 &= \mu, \quad \text{(50)} \\
\lambda_0 - \sum_{i=1}^N w_i \nabla_X \langle \lambda_i, f(X_i, U_i) \rangle &= \nabla \Phi(X_N), \quad \text{(51)} \\
D^\dagger \lambda &= -\nabla_X \langle \lambda, F(X^{LGR}, U^{LGR}) \rangle + \frac{1}{w_N} e_N (\lambda_N - \nabla \Phi(X_N)), \quad \text{(52)} \\
o &= \nabla_U \langle \lambda, F(X^{LGR}, U^{LGR}) \rangle. \quad \text{(53)}
\end{align*}$$

Observe that the discrete and continuous necessary condition for the control (compare (32) and (53)) have exactly the same structure. Moreover, the transformed variable $\lambda_0$ satisfies exactly the same condition (50) as the continuous costate $\lambda(-1)$ in (29). The summation in (51) approximates the integral of $\dot{\lambda}$ over the interval $[-1, 1]$. Hence, the left side of (51) approximates $\lambda(1)$, which corresponds to $\lambda_N$, and the condition (51) is a subtle way of enforcing the equality $\nabla \Phi(X_N) = \lambda_N$, in an approximate sense. Moreover, if $\nabla \Phi(X_N) = \lambda_N$, then last term in the discrete dynamics (52) vanishes. Finally, as has been shown in Ref. 11, the system (52), with the last term dropped, is a pseudospectral scheme for the costate equation. More precisely, if $p$ is a polynomial of degree at most $N - 1$ and $p_j = p(\tau_j), 1 \leq j \leq N$, then

$$D^\dagger p_i = \dot{p}(\tau_i), \quad 1 \leq i \leq N \quad \text{for degree (53).}$$

Thus, we have shown that the transformed KKT conditions are related to a pseudospectral discretization of the continuous costate equation. However, the differentiation matrix $D^\dagger$ in the costate discretization is connected with the derivatives of polynomials of degree at most $N - 1$, while the differentiation matrix in the state discretization is based on the derivatives of polynomials of degree $N$. 

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Integral Formulation Using LGR Collocation
The equivalent integral formulation for LGR collocation has exactly the same form as that of LG collocation; namely,

$$X_i = X_0 + A_i F(X^{LGR}, U^{LGR}), \quad 1 \leq i \leq N,$$

where $A_i$ is the $i^{th}$ row of $A = D^{-1}_{N 	imes N}$. Hence, the differential form of the state equation $DX = F(X^{LGR}, U^{LGR})$ is equivalent to the integrated form (54), where the elements of $A$ are integrals of the Lagrange basis functions $L_i^\tau$, defined in (37) while the elements of $D$ in the differential form are the derivatives of the Lagrange basis function $L_i$, defined in (5).

Summarizing, the approximation to the dynamics given in (54) is in the form of a global implicit integration method while the differential approximation $DX = F(X^{LGR}, U^{LGR})$ is in the form of a pseudospectral method. The fact that either the integral or the differential form can be used shows that the LGR collocation method can be thought of as either a global implicit integration method or a pseudospectral method. In particular, using the pseudospectral form of LGR collocation results in a system of equations that is equivalent to the integral form (because the matrix $D_{1:N}$ is nonsingular). We call the differential form of LGR collocation the Radau pseudospectral method. For more details concerning the analysis of LGR collocation, see Ref. 11.

Collocation at Legendre-Gauss-Lobatto (LGL) Points

Consider now collocation using the $N$ LGL collocation points. Unlike either Gauss or Radau collocation, where additional nodes were introduced at the endpoints, there is no need for additional nodes with LGL since the endpoint $-1$ and $+1$ are collocation points; hence, the state at the endpoints naturally appear in the discrete problem. Each component of the state $x$ is approximated by a polynomial of degree at most $N$. Let $L_i^\tau$, $i = 1, \ldots, N$, be the Lagrange basis associated with the collocation points, which were introduced in (37). The $j^{th}$ component of the state is approximated by a series of the form$^{1,3}$

$$x_j^N(\tau) = \sum_{i=1}^{N} x_{ij} \hat{L}_i^\tau(\tau).$$

Differentiating the series and evaluating at the collocation point $\tau_k$ gives$^{1,3}$

$$\dot{x}_j^N(\tau_k) = \sum_{i=1}^{N} x_{ij} \hat{L}_i^\tau(\tau_k) = \sum_{i=1}^{N} D_{ki} x_{ij}, \quad D_{ki} = \hat{L}_i^\tau(\tau_k).$$

The $N$ by $N$ square matrix $D$ is called the Lobatto Pseudospectral differentiation matrix. It has one row for each collocation point; the $j^{th}$ column contains the derivative of the Lagrange polynomial $L_i^\tau$ evaluated at each of the collocation points. Let $X^{LGL}$ denote the matrix formed from the coefficients $x_{ij}$ in (55). The discrete optimization problem has the form

$$\text{minimize } \Phi(X_N) \text{ subject to } DX^{LGL} = F(X^{LGL}, U^{LGL}), \quad X_1 = x_0.$$  \hspace{1cm} (57)

Notice that the structure of the discrete problem (57) for LGL collocation is the same as that for LGR collocation in (45).

We now develop the first-order optimality conditions for (57). These can be found in a more general context in Ref. 3. The system dynamics in (57) is composed of $NN$ equations. Let $\Lambda^{LGL}$ denote the $N$ by $n$ matrix of Lagrange multipliers associated with the system dynamics, and let $\mu$ be a 1 by $n$ row vector of Lagrange multipliers associated with the initial condition. The Lagrangian associated with (57) is

$$L(\Lambda^{LGL}, \mu, X^{LGL}, U^{LGL}) = \Phi(X_N) + \langle \Lambda^{LGL}, F(X^{LGL}, U^{LGL}) - DX^{LGL} \rangle + \langle \mu, x_0 - X_1 \rangle.$$  \hspace{1cm} (58)

The KKT conditions of the NLP are obtained by differentiating $L$ with respect to each component of $X^{LGL}$ and $U^{LGL}$ and are given as follows:

$$\nabla_X \Phi(X_N) = -\sum_{i=1}^{N} D_{i:N} A_i - \nabla_X \langle A_N, f(X_N, U_N) \rangle$$
$$\sum_{i=1}^{N} D_{ij} A_i = \nabla_X \langle A_j, f(X_j, U_j) \rangle, \quad 2 \leq j \leq N - 1$$
$$\sum_{i=1}^{N} D_{i1} A_i = \nabla_X \langle A_1, f(X_1, U_1) \rangle - \mu$$
$$\nabla_U \langle A_j, f(X_j, U_j) \rangle = 0$$
Note that $F(X^\text{LGL}, U^\text{LGL})$, the right side vector evaluated at the collocation points, depends upon both $X_1$ and $X_N$.

The costate equations can then be rewritten
\begin{align}
\nabla \langle A_1, f(X_1, U_1) \rangle - D_1^T A^\text{LGL} &= \mu, \tag{59} \\
D_N^T A^\text{LGL} - \nabla_X \langle A_N, f(X_N, U_N) \rangle &= \nabla_X \Phi(X_N), \tag{60} \\
D_{2:N-1}^T A_{2:N-1} &= \nabla_X \langle A_{2:N-1}, F(X_{2:N-1}, U_{2:N-1}) \rangle \tag{61}
\end{align}
\begin{footnotesize}
Note that the $N$ by $N$ Lobatto differentiation matrix is singular since $D1 = 0$.
\end{footnotesize}

Transformed Adjoint System for LGL Collocation Using an approach nearly identical to that used for LGR collocation, the KKT conditions of the NLP are now reformulated so that they become a discretization of the first-order optimality conditions for the continuous control problem (1)–(2). Let $w_i, 1 \leq i \leq N$, be the quadrature weights associated with the LGL points; the transformed adjoint is the $N$ by $n$ matrix $\lambda$ defined by
\begin{equation}
\lambda_i = \Lambda_i / w_i. \tag{62}
\end{equation}
Let $D^\dagger$ be the $N$ by $N$ matrix defined as follows:
\begin{align}
D_{ii}^\dagger &= D_{ii}, \quad 2 \leq i \leq N - 1 \\
D_{11}^\dagger &= -D_{11} - \frac{1}{w_1} \\
D_{NN}^\dagger &= -D_{NN} + \frac{1}{w_N} \\
D_{ij}^\dagger &= -\frac{w_j}{w_i} D_{ji}, \quad 1 \leq i, j \leq N, \quad (i \neq j) \tag{63}
\end{align}
The substitutions (62) and (63) in (60)–(61) lead to the following transformed costate equation:
\begin{equation}
D^\dagger \lambda = -\nabla_X \langle \lambda, F(X^\text{LGL}, U^\text{LGL}) \rangle + \frac{1}{w_1} e_1 (\mu - \lambda_1) + \frac{1}{w_N} e_N (\lambda_N - \nabla_X \Phi(X_N)), \tag{64}
\end{equation}
where $e_1$ and $e_N$ are the first and last columns of the $N \times N$ identity matrix. Finally, dividing the last equation in (58) by $w_j$ yields
\begin{equation}
\nabla_U \langle \lambda, F(X^\text{LGL}, U^\text{LGL}) \rangle = 0. \tag{65}
\end{equation}

Observe that the continuous and discrete control necessary conditions (32) and (65) again have the same structure. The discrete and continuous adjoint, however, seem to satisfy quite different conditions. The continuous endpoint conditions (29) and (30) are not present in the discrete system (64). As it turns out, the matrix $D^\dagger$ is a differentiation matrix connected with the quadrature points (see Ref. 19 for details). Note that LGL collocation is the only one of the three schemes for which $D = D^\dagger$. This observation has also been made in Refs. 21 and 22.

Integral Formulation Using LGL Collocation An integral analogue of LGL collocation can be developed as follows: Given a polynomial $p$ of degree at most $N - 1$, its derivative $\dot{p}$ is a polynomial of degree at most $N - 2$. Hence, $p$ can be interpolated exactly by the Lagrange polynomials $L_j$ defined in (37):
\begin{equation}
\dot{p}(\tau) = \sum_{j=1}^{N} \dot{p}_j L_j^\dagger(\tau), \quad \dot{p}_j = \dot{p}(\tau_j) \tag{66}
\end{equation}
Again, we integrate from $-1$ to $\tau_i$ to obtain the relation
\begin{equation}
p(\tau_i) = p(-1) + \sum_{j=1}^{N} \dot{p}_j A_{ij}, \quad A_{ij} = \int_{-1}^{\tau_i} L_j^\dagger(\tau) \, d\tau, \quad 2 \leq i \leq N \tag{66}
\end{equation}
If this is applied to each component of the state variable, then we have
\begin{equation}
X_i = X_0 + A_i F(X^\text{LGL}, U^\text{LGL}), \quad 2 \leq i \leq N, \tag{67}
\end{equation}
where $A_i$ is the $i$-th row of $A$. Note, though, that this integrated scheme is not equivalent to the original LGL collocation system, it is simply a different discrete scheme. In fact, the original LGL discrete system contains $N$ equations, one equation for each collocation point while (67) represents $N - 1$ equations.
COMPARISON OF LG, LGR, AND LGL COLLOCATION

With each of the collocation schemes, the state at the final time is approximated by a quadrature rule associated with the collocation points. For LG collocation, this quadrature rule is embedded in the constraint

\[ X_{N+1} = X_0 + w_{LGL}^T F(X_{LGL}, U_{LGL}). \quad (68) \]

Here \( X_{N+1} \) and \( X_0 \) are the approximations to the state at \( \tau = +1 \) and \( \tau = -1 \) respectively, and \( w_{LGL}^T F(X_{LGL}, U_{LGL}) \) is a quadrature approximation to the integral

\[ \int_{-1}^{+1} \dot{x}(t) \, dt. \]

Now consider the Lobatto differentiation matrix \( D_{LGL} \) and the corresponding quadrature weight \( w_{LGL} \). By the exactness of the LGL quadrature rule, we have

\[ (w_{LGL}^T D_{LGL})_j = \int_{-1}^{+1} \hat{L}_j(t) \, dt = \begin{cases} -1 & \text{for } i = 1, \\ 0 & \text{for } 2 \leq i \leq N - 1, \\ +1 & \text{for } i = N. \end{cases} \]

Hence, multiplying each side of the LGL state equation \( DX_{LGL} = F(X_{LGL}, U_{LGL}) \) by \( w_{LGL}^T \) yields the identity

\[ X_N = X_1 + w_{LGL}^T F(X_{LGL}, U_{LGL}). \quad (69) \]

For Lobatto collocation, \( X_N \) and \( X_1 \) correspond to the state at \( \tau = +1 \) and \( \tau = -1 \) respectively. Hence, the Lobatto identity (69) is analogous to the Gauss identity (68).

Finally, let us consider the LGR collocation scheme. Since the Lagrange polynomials in (3) start from \( i = 0 \), it follows that for the Radau differentiation matrix \( D_{LGR} \) and the corresponding quadrature weights \( w_{LGR} \), we have

\[ (w_{LGR}^T D_{LGR})_j = \int_{-1}^{+1} \hat{L}_j(t) \, dt = \begin{cases} -1 & \text{for } i = 0, \\ 0 & \text{for } 1 \leq i \leq N - 1, \\ +1 & \text{for } i = N. \end{cases} \]

As a result, multiplying each side of the LGR state equation \( DX_{LGR} = F(X_{LGR}, U_{LGR}) \) by \( w_{LGR}^T \) yields the identity

\[ X_N = X_0 + w_{LGR}^T F(X_{LGR}, U_{LGR}). \quad (70) \]

For Radau collocation, \( X_N \) and \( X_0 \) correspond to the state at \( \tau = +1 \) and \( \tau = -1 \) respectively. Hence, each collocation scheme ultimately leads to a state approximation at the terminal time based on the scheme’s quadrature rule [see (68)–(70)].

With each of the schemes, the initial state is introduced in the discretization through interpolation. In particular, for either LG or LGR collocation, the initial value of the state variable appears as the coefficient of \( L_0 \) in the expansion (4). Here \( L_0 \) is the Lagrange basis function associated with the noncollocated point \( \tau_0 = -1 \). For GGL collocation, the initial value of the state appears as the coefficient of \( L_1^1 \) in (55). In this case, \( L_1^1 \) is the Lagrange basis function associated with the collocated Lobatto point \( \tau_1 = -1 \). Figure 2 provides a schematic showing how the three pseudospectral schemes use collocation and interpolation points.

Another interesting feature of the three pseudospectral schemes concerns the discrete mapping from the control to the state. To illustrate this feature, consider the simple scalar dynamics

\[ \dot{x} = u. \quad (71) \]

With either the LG or LGR scheme, the dynamics is approximated by

\[ D_0 x_0 + D_{1:N} X_{1:N} = U, \quad (72) \]

where \( D \) is the GPM/RPM differentiation matrix and \( D_0 \) is the first column of \( D \). We showed that \( D_{1:N} \) was invertible, and \( D_{1:N}^{-1} D_0 = -1 \). Hence, we have

\[ X_{1:N} = I x_0 + D_{1:N}^{-1} U. \]
This shows that there is a unique state associated with each choice for the control, provided the initial condition \(x_0\) is given.

For the Lobatto scheme, the dynamics is approximated by

\[
D^{LPM}_{1:N} \mathbf{X} = \mathbf{U},
\]

where we recall that the matrix \(D^{LPM}_{1:N}\) is square and singular. Thus, the state is not uniquely determined by the control. In fact, the equation (73) only has a solution when \(\mathbf{U}\) lies in the column space of \(D^{LPM}_{1:N}\). Hence, for GPM or RPM, the map from control to state is one-to-one and onto. For LPM, the map from control to state is only defined when the control is orthogonal to the null space of \((D^{LPM})^T\). In general, for nonlinear dynamics, with GPM or RPM, it may be possible to solve for the state in terms of the control and eliminate the state from the problem. With LPM, the representation of the state in terms of the control becomes more complex due to the singularity of the differentiation matrix.

In addition to the properties of the discretized dynamic constraints, the three pseudospectral schemes treat the costate endpoint conditions quite differently. For LG collocation, the endpoint conditions appear explicitly in the transformed adjoint conditions (23) and (24). For LGR collocation, the initial condition appears explicitly in (50) while the terminal condition appears in the approximate form (51). For LGL collocation, the boundary conditions are embedded inside the costate dynamics (64).

EXEMPLARYS

In this section we consider two examples using the aforementioned GPM, RPM, and LPM. The first example has an analytic solution, thus providing the ability to perform an error and convergence analysis for the GPM, RPM, and LPM. The second example is a space flight application that has been studied extensively in the literature (see Ref. 23).

**Example 1**

Consider the following optimal control problem.

\[
\min J = -y(t_f) \quad \text{s.t.} \quad \begin{cases} \dot{y} = -y + yu - u^2 \\ y(0) = 1 \end{cases}
\]

where \(t_f = 5\). The optimal solution to this problem is

\[
\begin{align*}
    y^*(t) &= 4/(1 + 3 \exp(t)) \\
    \lambda_1^*(t) &= -\exp(2 \ln(1 + 3 \exp(t)) - t)/(\exp(-5) + 6 + 9 \exp(5)) \\
    u^*(t) &= y^*(t)/2
\end{align*}
\]
The optimal control problem given in (74) was solved using the GPM, RPM, and LPM for the \( N \) ranging from five to 30 by steps of five using the NLP solver SNOPT with optimality and feasibility tolerances of \( 10^{-15} \) and \( 2 \times 10^{-15} \), respectively. For each method, the initial guess was the exact solution. We compute the \( L_{\infty} \) errors in state, costate, and control at the approximation points (i.e., collocation points for the control and collocation points plus noncollocated endpoints for the state and costate). Figs. 3a–3c show the base 10 logarithm of the \( L_{\infty} \)-norm errors for the state, control, and costate, respectively. First, it is seen in Fig. 3a that the state error using either the GPM or RPM is approximately two to four orders of magnitude smaller than the state error for LPM for \( N \leq 15 \). In Figure 3b, it is seen that the GPM and RPM control is between two and seven orders of magnitude more accurate than the corresponding LPM controls for \( N \leq 15 \). For \( N > 15 \), the GPM and RPM state and control errors drop to machine precision (approximately \( 10^{-16} \)), while the LPM errors achieve machine precision at \( N = 30 \).

In Fig. 3c it is seen that the GPM and RPM costate errors decrease to near the optimizer tolerances (approximately \( 10^{-15} \)) while the LPM costate error remains above \( 10^{-2} \). As a result, it appears as if the LPM costate does not converge for this example. To examine the costate behavior for all three methods in more depth, Fig. 3d shows an enlarged plot of the exact costate and the approximations generated by all three methods for \( N = 30 \). It is seen that the LPM costate oscillates about the exact solution while the GPM and RPM costates are indistinguishable from the optimal solution.

Example 2

Consider the following orbit-raising optimal control problem found in Ref. 23. Minimize the cost functional

\[
J = -r(t_f)
\]

(76)
subject to the dynamic constraints
\[ \begin{align*}
\dot{r} &= v_r, \\
\dot{\theta} &= v_\theta/r, \\
\dot{v}_r &= \frac{v_r^2}{r} - \mu/r^2 + a \sin \beta, \\
\dot{v}_\theta &= -v_r v_\theta/r + a \cos \beta,
\end{align*} \]  
(77)

and the boundary conditions
\[ \begin{align*}
(r(0), \theta(0), v_r(0), v_\theta(0)) &= (1, 0, 0, 1), \\
(v_r(t_f), v_\theta(t_f)) &= (0, \sqrt{\mu/r(t_f)}),
\end{align*} \]  
(78)

where
\[ a \equiv a(t) = \frac{T}{m_0 - |\dot{m}| t}. \]  
(79)

It is noted for this example that \( \mu = 1, T = 0.1405, m_0 = 1, \dot{m} = 0.0749, \) and \( t_f = 3.32. \)

The orbit-raising problem was solved using the GPM, RPM, and LPM for \( N = 64. \) The state, control (after an upwrapping of the angle), and costate solutions are shown in Figs. 4, 5, and 6, respectively (where \( \beta \) is plotted at only the collocation points for each method because each method only determines the control at the collocation points). First, it is observed from Figs. 4 and 5 that the three methods produce qualitatively similar values for the state and control. Next, Fig. 6 shows that the costate obtained using the LPM looks significantly different from the costate obtained using either the GPM or the RPM. In particular, noting that \( \lambda_0(t) \equiv 0 \) for this problem, it is seen that the GPM and the RPM produce a very accurate result for \( \lambda_\theta(t) \) while the LPM produces a value for \( \lambda_\theta(t) \) that oscillates about zero. In addition, it is seen in Fig. 6 that \( \lambda_r(t) \) for LPM also oscillates (unlike the smooth behavior shows for the GPM and RPM). Thus, the GPM and RPM differ significantly from the LPM in costate accuracy, demonstrating a fundamental difference in the nature of the costate estimates obtained using either the GPM or RPM as compared with the LPM.

![Figure 4: GPM, RPM, and LPM State Solutions for Example 3 Using N = 64.](image-url)
Figure 5: GPM, RPM, and LPM Control Solutions for Example 3 Using $N = 64$.

(a) Example 3 Control Using GPM and $N = 64$.

(b) Example 3 Control Using RPM and $N = 64$.

(c) Example 3 Control Using LPM and $N = 64$.

Figure 6: GPM, RPM, and LPM Costate Solutions for Example 3 Using $N = 64$.

(a) Example 3 Costate Using GPM and $N = 64$.

(b) Example 3 Costate Using RPM and $N = 64$.

(c) Example 3 Costate Using LPM and $N = 64$. 

Figure 6: GPM, RPM, and LPM Costate Solutions for Example 3 Using $N = 64$. 

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CONCLUSIONS

A comparison has been given of three different pseudospectral methods based on collocation at Legendre-Gauss (LG), Legendre-Gauss-Radau (LGR), and Legendre-Gauss-Lobatto (LGL) points. The state was expanded in Lagrange polynomials and the dynamics was enforced at the collocation points. For each of the schemes in this paper, (1) the state at the final time can be expressed in terms of a quadrature rule associated with the collocation points, (2) the state at the initial time is approximated by interpolation, and (3) the control and the state are approximated at the collocation point. LG and LGR based schemes presented in this paper employ polynomials to approximate the state that are the same degree as the number of collocation points. In the corresponding LGL scheme, the state approximation is a polynomial that is one degree lower than the number of collocation points. Each of these scheme can be expressed in either a differential or an integral formulation. The LG and LGR differentiation and integration matrices are invertible, and the differential and integral versions are equivalent. The LGL differentiation matrix is singular, and the equivalence between differential and integral forms is lost. A transformed first-order optimality system was developed and compared to the continuous first-order optimality conditions. LGL collocation was the only scheme for which the differentiation matrices for the state and the costate dynamics were the same. Two numerical examples were given. In the first example, the state and control were several orders of magnitude more accurate with either Gauss or Radau collocation when compared to Lobatto. In addition, the Lobatto costate did not seem to converge near the starting time. For the second example, where the exact solution was not known, the state and control for all three methods were qualitatively similar, however, the Lobatto costate oscillated around the correct costate.

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