Analysis and Application of an Orthogonal Nodal Basis on Triangles for Discontinuous Spectral Element Methods

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In this paper, we propose and analyze an orthogonal non-polynomial nodal basis on triangles for discontinuous spectral element methods (DSEMs) for solving Maxwell’s equations. It is based on the standard tensor product of the Lagrange interpolation polynomials and a “collapsing” mapping between the standard square and the standard triangle. The basis produces diagonal mass matrices for the DSEMs and is easy to implement. Numerical results for electromagnetic scattering in heterogeneous media are provided to demonstrate the exponential convergence of the proposed basis, and its application to the simulation of optical coupling by whispering gallery modes between two microcylinders is presented as well.

1 Introduction

There has been active recent research on the development of discontinuous Galerkin methods (DGMs) for handling material interfaces arising from electromagnetic scattering and porous media flows. The main advantages of the DGMs are their high order accuracy and high suitability for parallel implementation when explicit schemes are utilized. In the DGMs piecewise continuous approximations are used to represent solutions of partial differential equations, while the material interfaces are conformingly approximated in the underlying triangulation of the solution domains. There are three approaches in implementing the DGMs, namely, the \textit{h}-version, the \textit{p}-version, and the \textit{h}-\textit{p} version. Similar to finite element methods [1], the \textit{h}-version allows the mesh size to be decreased to achieve the convergence at a rate of the order of the employed polynomial basis in each element, resulting in a finite order method. The alternative \textit{p}-version, popular in the area of computational electromagnetics due to high wave numbers possibly involved, allows the order of the polynomial basis to be increased while the elements are kept the same as in the initial triangulation. A hybrid \textit{h}-\textit{p} version can also be considered [2]. Since orthogonal polynomials are often used in the \textit{p}-version DGM, it is called a discontinuous spectral element method (DSEM) [3], a term which will be used in this paper.

An important issue in the implementation of a DSEM is the choice of the approximation basis functions. For numerical stability and accuracy concerns, the elementwise mass matrices arising from the DSEM should be made as simple as possible. Because the order of the basis functions may have to be taken large to obtain desired accuracy, in the framework of spectral element methods, it is critical to have elementwise mass matrices that are easy to invert and well-conditioned. The ideal case will be that the elementwise mass matrices are diagonal. This has actually been achieved for both quadrilateral and triangular elements. In the former case, the standard tensor product of the Lagrange interpolation polynomials over the classical Gauss points in the interval \([-1,1]\) will yield diagonal mass matrices [3] in the DSEM. While in the later case, the ingenious construction of the Dubiner orthogonal polynomial basis on triangles [4] provides an answer.

In this paper, we propose a non-polynomial basis on triangles which will be orthogonal, like the Dubiner polynomial basis, and at the same time will be a nodal basis over the appropriately chosen collocation points. This

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orthogonal nodal basis is again based on the standard tensor product of the Lagrange interpolation polynomials over the classical Gauss points in the interval [-1,1]. The resulting basis functions on triangles produce diagonal mass matrices for the DSEM, and are easy to implement. Previous nodal basis functions on triangles have been proposed in [5] by using specially chosen points inside the triangles based on static charge distribution; however, the resulting basis functions are not orthogonal on the triangles.

In the next section, we summarize the DSEM for solving Maxwell’s equations. In Section 3, after reviewing the orthogonal polynomial nodal basis on rectangles and the Dubiner orthogonal polynomial basis on triangles, we present and analyze the orthogonal non-polynomial nodal basis on triangles. In Section 4, numerical results are first provided to demonstrate the exponential convergence of the orthogonal nodal basis for approximating both oscillatory functions and the solutions of electromagnetic scattering by single dielectric cylinder, and numerical simulation of optical coupling by whispering gallery modes between two microcylinders is then presented as well.

2 Discontinuous spectral element method for Maxwell’s equations

Without losing any generality, we consider the non-dimensionalized two-dimensional TM Maxwell’s equations on a domain \( \Omega \). To approximate the Maxwell’s equations in the time domain, we write them in conservation form as

\[
\frac{\partial Q}{\partial t} + \nabla \cdot F = S,
\]

where \( Q = (E_z, H_x, H_y)^T \) with \( E_z \) and \( (H_x, H_y) \) representing the electric field and the magnetic field, respectively, and the flux \( F = (F_x, F_y) = (A_x Q, A_y Q) \) with

\[
A_x = \begin{pmatrix}
0 & 0 & -1/\epsilon \\
0 & 0 & 0 \\
-1/\mu & 0 & 0
\end{pmatrix}, \quad A_y = \begin{pmatrix}
0 & 1/\epsilon & 0 \\
1/\mu & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}.
\]

Here \( \epsilon \) is the material permittivity, and \( \mu \) is the material permeability.

To solve Eq. (2.1) in a general two-dimensional geometry, the physical domain \( \Omega \) under consideration is divided into non-overlapping quadrilateral and/or triangular physical elements. Each physical element is then mapped onto a reference element, either the standard square divided into non-overlapping quadrilateral and/or triangular physical elements. Each physical element is then boundary. Let us generally denote the basis functions by \( \beta_j \), yielding the following equations

\[
\dot{Q}(\xi, \eta, t) \approx \dot{Q}_N(\xi, \eta, t) = \sum_{j=1}^{N} \hat{Q}_j(t) \beta_j(\xi, \eta),
\]

where \( \hat{Q}_j(t) \) are time-dependent expansion coefficients. The residual of the approximation is then required to be orthogonal to the approximation space locally within each element \( K \), yielding the following equations

\[
\left( \frac{\partial Q_N}{\partial t}, \beta_i \right) + \int_{\partial K} \beta_i \cdot F \cdot n \text{d}s - \left( F \cdot \nabla \beta_i \right) = \left( S, \beta_i \right), \quad i = 1, 2, \cdots, N,
\]
where \((u, v) = \int_K uv \, d\xi\) represents the usual \(L^2\) inner product, \(\partial K\) the element boundary, and \(n = (n_x, n_y)\) the outward unit normal to the element boundary.

The integrals in Eq. (2.4) are calculated numerically by quadratures, depending on the element type and the basis functions, and the discretization requires the evaluation of the fluxes along the element boundary. However, the approximation is not continuous across the element boundary. The difference is resolved by solving a local Riemann problem for the numerical normal flux, which is discussed in detail in [6].

Substituting \(\hat{Q}_N\) in Eq. (2.3) into Eq. (2.4), we obtain
\[
\sum_{j=1}^N \left( m_{ij} \frac{d\hat{Q}_j(t)}{dt} + m^\xi_{ij} \hat{\mathbf{F}}_{\xi,j}(t) + m^\eta_{ij} \hat{\mathbf{F}}_{\eta,j}(t) \right) + \int_{\partial K} \beta_i \hat{\mathbf{F}} \cdot \mathbf{n} \, ds = \left( \hat{\mathbf{S}}, \beta_i \right), \quad i = 1, \cdots, N, \tag{2.5}
\]
where \(\hat{\mathbf{F}}_j = \hat{\mathbf{F}}(\hat{Q}_j) = (\hat{\mathbf{F}}_{\xi,j}, \hat{\mathbf{F}}_{\eta,j})\), and the local mass matrix and the local derivative matrices are
\[
\mathbf{M} = (m_{ij}), \quad m_{ij} = \int_R \beta_i \beta_j \, d\xi,
\]
\[
\mathbf{M}^\xi = (m^\xi_{ij}), \quad m^\xi_{ij} = \int_R \frac{\partial \beta_i}{\partial \xi} \beta_j \, d\xi,
\]
\[
\mathbf{M}^\eta = (m^\eta_{ij}), \quad m^\eta_{ij} = \int_R \frac{\partial \beta_i}{\partial \eta} \beta_j \, d\xi.
\]

Equation (2.5) is a system of ordinary differential equations for the time-dependent expansion coefficients \(\hat{Q}_j(t), \ j = 1, 2, \cdots, N\), which can then be solved by explicit methods.

3 Orthogonal bases on rectangles and triangles

As mentioned earlier, for numerical stability and accuracy concerns when we solve Eq. (2.5), the local mass matrix \(\mathbf{M}\) should be made as simple as possible. The ideal case will be that the local mass matrix becomes a diagonal matrix, and this can actually be achieved for both quadrilateral and triangular elements by using appropriate orthogonal bases.

3.1 Orthogonal nodal basis on rectangles

For quadrilateral elements, the approximation space on the standard reference square \(R_0\) is normally chosen as \(P_{M,M} = P_M \times P_M\), where \(P_M\) represents the space of polynomials of degree \(M\) or less. Let \(\tau_i, \omega_i, i = 0, 1, \cdots, M\) be the classical Gauss points and weights in the interval \([-1, 1]\). Then an orthogonal basis for \(P_{M,M}\) is the set of standard tensor products of the Lagrange interpolation polynomials on the interval \([-1, 1]\), i.e.,
\[
q_{mn}(\xi, \eta) = \phi_m(\xi) \phi_n(\eta), \quad 0 \leq m, n \leq M, \tag{3.1}
\]
where
\[
\phi_i(x) = \prod_{j=0, j\neq i}^M \frac{x - \tau_j}{\tau_i - \tau_j}, \quad i = 0, 1, \cdots, M.
\]

Note that \(q_{mn}(\tau_i, \tau_j) = \delta_{mi}\delta_{nj}, \ 0 \leq i, j, m, n \leq M\). Therefore, the basis is also a nodal basis over the collocation points \((\tau_i, \tau_j) \in R_0, \ 0 \leq i, j \leq M\), i.e., for any function \(f(\xi, \eta)\), it can be approximated by
\[
f(\xi, \eta) \approx \sum_{m,n=0}^M f_{mn} q_{mn}(\xi, \eta),
\]
where \(f_{mn} = f(\tau_m, \tau_n)\) are the point values of \(f(\xi, \eta)\) at the collocation points. And for the same reason, we have
\[
(q_{mn}, q_{ij}) = \int_{R_0} q_{mn}(\xi, \eta) q_{ij}(\xi, \eta) \, d\xi \, d\eta = \omega_m \omega_n \delta_{mi} \delta_{nj}. \tag{3.2}
\]

Also note that the above choice of the classical Gauss collocation points requires interpolation of the expansion to the boundary to evaluate the boundary flux terms in the DSEM.
3.2 Orthogonal polynomial basis on triangles

For triangular elements, the approximation space on the standard reference triangle $T_0$ is frequently chosen as

$$\mathcal{P}_M(T_0) = \text{span}\{\xi^m \eta^n, \ 0 \leq m, n, m + n \leq M\}. \quad (3.3)$$

A natural basis for this space is $\{\xi^m \eta^n, \ 0 \leq m, n, m + n \leq M\}$. However, this basis is not orthogonal and works fine only for small expansion order $M$, about 2 or 3. When $M$ is taken large, say $M \geq 7$, the basis is nearly dependent and leads to ill-conditioned approximations.

Investigations of orthogonal polynomials on triangles have been done for long time. In particular, spectral methods on triangles have been studied in [4][7]-[13], where two different approaches have been developed. One approach is to use transformations between triangles and squares and warped tensor product grids within triangles, designed for the accurate approximation of integrals [4][7]-[9], while the other approach is to use critically sampled points in triangles designed for accurate approximation rather than for accurate integration, such as the Fekete points [10]-[13]. However, for triangular spectral element methods, probably the most popular basis is the Dubiner orthogonal polynomial basis discussed in [4]. This basis is briefly summarized in this section, and for more details the readers may consult [4] and [7].

The Dubiner basis on triangles is obtained by transforming the Jacobi polynomials defined on intervals to form polynomials on triangles. The $n$-th order Jacobi polynomials $P_n^\alpha,\beta(x)$ on the interval $[-1, 1]$ are orthogonal polynomials under the Jacobi weight $w(x) = (1 - x)^\alpha (1 + x)^\beta$, i.e.,

$$\int_{-1}^{1} (1 - x)^\alpha (1 + x)^\beta P_n^\alpha,\beta(x) P_m^\alpha,\beta(x) \,dx = \delta_{nm}. \quad (3.3)$$

To construct an orthogonal polynomial basis on the triangle $T_0$, we follow the same idea as in [7] and consider the transformations in Fig. 1 between the reference square $R_0$ and the reference triangle $T_0$. The transformations in Eq. (3.4) basically collapse the top edge of the square $R_0$ into the top vertex (0,1) of the triangle $T_0$.

The transformations in Fig. 1 are defined by

$$\begin{cases}
\xi = \frac{(1 + a)(1 - b)}{4}, \\
\eta = \frac{1 + b}{2},
\end{cases} \quad \text{or} \quad \begin{cases}
a = \frac{2\xi}{1 - \eta} - 1, \\
b = 2\eta - 1.
\end{cases} \quad (3.4)$$

![Fig. 1 Illustration of the mapping between the square $R_0$ and the triangle $T_0$.](image)

The transformations in Eq. (3.4) basically collapse the top edge of the square $R_0$ into the top vertex (0,1) of the triangle $T_0$. The Jacobians of the transformations are

$$J(\xi, \eta) = \frac{\partial(a, b)}{\partial(\xi, \eta)} = \frac{4}{1 - \eta}, \quad (3.5)$$

$$J^{-1}(a, b) = \frac{\partial(\xi, \eta)}{\partial(a, b)} = \frac{1 - b}{8} = \frac{1 - \eta}{4}. \quad (3.6)$$

The Dubiner basis is then constructed by a generalized tensor product (warped product [7]) of the Jacobi polynomials on the interval [-1, 1] to form a basis on the square $R_0$, which is then transformed by the above
“collapsing” mapping to a basis on the triangle $T_0$, i.e., the Dubiner basis on the triangle $T_0$ is defined as

$$g_{mn}(\xi, \eta) = P_m^0(\alpha)(1 - \beta)^m P_n^{2m+1,0}(\beta)$$

$$= 2^m P_m^0\left(\frac{2\xi}{1 - \eta} - 1\right)(1 - \eta)^m P_n^{2m+1,0}(2\eta - 1),$$

$$0 \leq m, n, m + n \leq M.$$  

Note that the Dubiner basis functions are polynomials in $(\alpha, \beta)$ space as well as in $(\xi, \eta)$ space. For example, the first six un-normalized Dubiner basis functions on the triangle $T_0$ are

$$g_{00}(\xi, \eta) = 1,$$
$$g_{10}(\xi, \eta) = 4\xi + 2\eta - 2,$$
$$g_{01}(\xi, \eta) = 3\eta - 1,$$
$$g_{20}(\xi, \eta) = 24\xi^2 + 24\xi\eta + 4\eta^2 - 24\xi - 8\eta + 4,$$
$$g_{11}(\xi, \eta) = 20\xi\eta + 10\eta^2 - 4\xi - 12\eta + 2,$$
$$g_{02}(\xi, \eta) = 10\eta^2 - 8\eta + 1.$$  

Moreover, the Dubiner basis is orthogonal in the Legendre inner product defined by

$$(g_{mn}, g_{ij}) = \int_{T_0} g_{mn}(\xi, \eta)g_{ij}(\xi, \eta)\,d\xi d\eta = \frac{1}{8}\delta_{mi}\delta_{nj},$$

and is complete in the polynomial space $P_M(T_0)$ defined in Eq. (3.3) [7].

However, the Dubiner orthogonal polynomial basis on the triangle $T_0$ is not a nodal basis, which makes its implementation much more inconvenient than that of a nodal basis. Previous nodal basis functions on triangles have been proposed by using specially chosen points inside the triangles based on static charge distribution [5], but the resulting polynomial basis functions are not orthogonal on the triangles. Additionally, for the Dubiner basis a warped tensor product grid has to be employed for the accurate approximation of integrals, but that grid is over-sampled since it requires twice as many grid points as there are degrees of freedom in the polynomial expansion (i.e., the number of polynomial basis functions).

### 3.3 Orthogonal nodal basis on triangles

Similar to the Dubiner orthogonal polynomial basis on the triangle $T_0$, the orthogonal non-polynomial nodal basis is constructed by the standard tensor product of the Lagrange interpolation polynomials on the interval [-1, 1] to form a basis on the square $R_0$, which is then transformed by the same “collapsing” mapping (3.4) to a basis on the triangle $T_0$, i.e.,

$$\psi_{mn}(\xi, \eta) = q_{mn}(\alpha, \beta) = \phi_m(\alpha)\phi_n(\beta)$$

$$= \phi_m\left(\frac{2\xi}{1 - \eta} - 1\right)\phi_n(2\eta - 1), \quad 0 \leq m, n \leq M.$$  

Clearly, this basis is a nodal basis over the collocation points on the triangle $T_0$

$$\left(\xi_i, \eta_j\right) = \left(\frac{(1 + \tau_i)(1 - \tau_j)}{4}, \frac{1 + \tau_j}{2}\right), \quad 0 \leq i, j \leq M,$$

namely, $\psi_{mn}(\xi_i, \eta_j) = \phi_m(\tau_i)\phi_n(\tau_j) = \delta_{mi}\delta_{nj}, 0 \leq i, j \leq M$, and thereby for any function $f(\xi, \eta)$ defined on the triangle $T_0$, it can be approximated by

$$f(\xi, \eta) \approx \sum_{m, n=0}^{M} f_{mn}\psi_{mn}(\xi, \eta),$$

where $f_{mn}=f(\xi_m, \eta_n)$ are the point values of $f(\xi, \eta)$ at the collocation points given by Eq. (3.11). And again, the interpolation of the expansion is required to evaluate the boundary flux terms since all collocation points are interior.
Remark 3.1 Unlike the Dubiner basis defined by Eqs. (3.7) and (3.8), the nodal basis defined by Eqs. (3.9) and (3.10) is no longer a polynomial basis in \((\xi, \eta)\) space even though the basis functions are still polynomials in \((a, b)\) space. Moreover, it has roughly twice as many basis functions as the Dubiner basis does for the same expansion order \(M\). Although it is clear that the computational cost to evaluate a double integral in Eqs. (2.5)-(2.8) by Gaussian quadrature under the non-polynomial nodal basis is only \(O(1)\), one or two orders less than the \(O(M)\) or \(O(M^2)\) computational cost of the polynomial basis, most integrals if not all can be computed in the preprocessing phase. And for these reasons, we are tempted to conclude that in terms of computational cost (CPU time) per time step, the Dubiner polynomial basis should be more efficient than the non-polynomial nodal basis because the latter requires almost twice the number of degrees of freedom as compared to the polynomial basis. Our numerical experiments in Section 4, however, indicate that for some applications the non-polynomial nodal basis is more efficient than the polynomial basis in terms of computational cost.

Remark 3.2 The advantage of a polynomial basis is that the basis functions are easy to differentiate and thereby the derivative matrices (2.7) and (2.8) are easy to compute. The nodal basis is not polynomial in \((\xi, \eta)\) space, but by simply applying the chain rule, we can differentiate the nodal basis functions by

\[
\frac{\partial}{\partial \xi} \psi_{mn}(\xi, \eta) = \frac{2}{1 - \eta} \phi'_m \left( \frac{2\xi}{1 - \eta} - 1 \right) \phi_n (2\eta - 1),
\]

\[
\frac{\partial}{\partial \eta} \psi_{mn}(\xi, \eta) = \frac{2}{1 - \eta} \phi'_m \left( \frac{2\xi}{1 - \eta} - 1 \right) \phi_n (2\eta - 1) + 2\phi_m \left( \frac{2\xi}{1 - \eta} - 1 \right) \phi'_n (2\eta - 1),
\]

where \(\phi'_m\) and \(\phi'_n\) represent the derivatives of the Lagrange interpolation polynomials \(\phi_i(x), i = 0, 1, \cdots, M\) with respect to \(x\), which can be evaluated in many different ways.

Remark 3.3 The nodal basis functions defined by Eq. (3.10), though unconventional compared with traditional polynomial basis functions, appear to but actually do not have singularity at the corner \((\xi, \eta) = (0, 1) \in T_0\) since on the triangle \(T_0\) we always have \(\xi \leq 1 - \eta\). Furthermore, when applied in a DSEM where all grid points are interior [3], the basis (3.10) need not be defined at the corner point at all. On the other hand, the nodal basis is not smooth at the corner \((\xi, \eta) = (0, 1)\), but that does not prevent it from accurately approximating smooth functions. And as pointed out in [4], any spectral element approximation is globally unsmooth. Figure 2 shows the contour shapes of all triangular nodal basis functions and the corresponding collocation points used in the right triangle \(T_0\) for the expansion order \(M = 2\). And the plot clearly suggests that the non-polynomial basis concentrates a lot of resolution in a single corner of the triangle.

As observed earlier, the nodal basis on the triangle \(T_0\) is not a polynomial basis in \((\xi, \eta)\) space, but it still maintains orthogonality. In addition, for the same expansion order \(M\) the approximation space characterized by the nodal basis can be proved without great difficulty to contain the polynomial space \(P_M(T_0)\). In fact, we have the following theorems.

Theorem 3.4 The nodal basis on the triangle \(T_0\) is orthogonal in the Legendre inner product defined by

\[
\langle \psi_{mn}, \psi_{ij} \rangle = \iint_{T_0} \psi_{mn}(\xi, \eta) \psi_{ij}(\xi, \eta) d\xi d\eta = \frac{\omega_m \omega_n (1 - \tau_n)}{8} \delta_{m1} \delta_{nj}.
\]

Proof. Note that for any function \(f(\xi, \eta) \in C(T_0)\), by performing the coordinate transformation (3.4) from \((\xi, \eta)\) to \((a, b)\), we have

\[
\iint_{T_0} f(\xi, \eta) d\xi d\eta = \frac{1}{8} \iint_{R_0} f(a, b)(1 - b) dadb.
\]

Therefore, the inner product in Eq. (3.13) becomes

\[
\langle \psi_{mn}, \psi_{ij} \rangle = \iint_{T_0} \psi_{mn}(\xi, \eta) \psi_{ij}(\xi, \eta) d\xi d\eta
\]

\[
= \frac{1}{8} \int_{R_0} \int_{a} \phi_m(a) \phi_n(b) \phi_i(a) \phi_j(b)(1 - b) dadb
\]

\[
= \frac{1}{8} \left( \int_{-1}^{1} \phi_m(a) \phi_i(a) da \right) \left( \int_{-1}^{1} \phi_n(b) \phi_j(b) (1 - b) db \right).
\]
Now from the property of the Gaussian quadrature that the \((M + 1)\)-point Gaussian quadrature is exact for polynomials of degree up to \(2M + 1\), we see that the first integral in Eq. (3.14) becomes

\[
\int_{-1}^{1} \phi_m(a)\phi_i(a)\,da = \sum_{s=0}^{M} \omega_s \phi_m(\tau_s)\phi_i(\tau_s) = \omega_m \delta_{mi},
\]

and similarly the second integral in Eq. (3.14) becomes

\[
\int_{-1}^{1} \phi_n(b)\phi_j(b)(1 - b)\,db = \sum_{s=0}^{M} \omega_s \phi_n(\tau_s)\phi_j(\tau_s)(1 - \tau_s) = \omega_n (1 - \tau_n) \delta_{nj}.
\]

Therefore, we finally have

\[
(\psi_{mn}, \psi_{ij}) = \frac{\omega_m \omega_n (1 - \tau_n)}{8} \delta_{mi} \delta_{nj}.
\]

An additional point that can be appreciated from the above proof is that integrals involving the inner product of \(\psi_{mn}(\xi, \eta)\) with a function \(f(\xi, \eta)\) can be evaluated in \(O(1)\) operations by using the Gaussian quadrature, i.e.,

\[
(\psi_{mn}, f) \approx \frac{\omega_m \omega_n (1 - \tau_n)}{8} f_{mn},
\]

where \(f_{mn}\) are again the point values of \(f(\xi, \eta)\) at the collocation points defined by Eq. (3.11).
We define \( G_M(T_0) \) as the finite element space on the triangle \( T_0 \) spanned by the nodal basis, i.e.,
\[
G_M(T_0) = \text{span}\{\psi_{mn}(\xi, \eta), 0 \leq m, n \leq M\}.
\]
(3.16)

Then clearly \( \dim(G_M(T_0)) = (M + 1)^2 \) as the basis is truly independent. Moreover, this space contains the polynomial space \( P_M(T_0) \).

**Theorem 3.5** The finite element space \( G_M(T_0) \) contains the polynomial space of degree \( M \) on the triangle \( T_0 \), namely, \( P_M(T_0) \subset G_M(T_0) \).

**Proof.** To demonstrate this result we consider the following functions in \( (a, b) \) space
\[
f(a, b) = \left( \frac{1 + a}{4} \right)^i \left( \frac{1 + b}{2} \right)^j, 0 \leq i, j, i + j \leq M.
\]
Note that every function \( f(a, b) \) is a polynomial in \( (a, b) \) with degrees \( i \) in \( a \) and \( i + j \) in \( b \). Since both \( i \leq M \) and \( i + j \leq M \), the Lagrange interpolation polynomial for \( f(a, b) \) is thus exact, i.e., we have the following polynomial identity in \( (a, b) \) space
\[
f(a, b) = \sum_{m,n=0}^{M} f(\tau_m, \tau_n)\phi_m(a)\phi_n(b), \quad (a, b) \in R_0.
\]
(3.17)

Using the definitions (3.4) and (3.9), we then have the corresponding identity in \( (\xi, \eta) \) space
\[
\xi^i\eta^j = \sum_{m,n=0}^{M} \xi_m^i\eta_n^j\psi_{mn}(\xi, \eta), \quad (\xi, \eta) \in T_0,
\]
which implies that \( P_M(T_0) \subset G_M(T_0) \).

As a matter of fact, it can be shown that the first three finite element spaces \( G_M(T_0) \) are
\[
G_1(T_0) = \text{span}\{1\},
\]
\[
G_2(T_0) = \text{span}\left\{1, \xi, \eta, \frac{\xi}{1-\eta}\right\},
\]
\[
G_3(T_0) = \text{span}\left\{1, \xi, \eta, \xi^2, \xi\eta, \eta^2, \frac{\xi}{1-\eta}, \frac{\xi^2}{1-\eta}, \frac{\xi^2}{(1-\eta)^2}\right\}.
\]

And in general, we have the following theorem.

**Theorem 3.6** The finite element space \( G_M(T_0) \) equals \( \text{span}\{S_M\} \), where the set \( S_M \) is defined as
\[
S_M = \left\{\xi^i\eta^j, 0 \leq i, j, i + j \leq M; \frac{\xi^t}{(1-\eta)^s}, 1 \leq s \leq M, s \leq t \leq M\right\}.
\]

**Proof.** We have already shown above that \( \xi^i\eta^j \in G_M(T_0) \) for \( 0 \leq i, j, i + j \leq M \). For \( \frac{\xi^t}{(1-\eta)^s} \), where \( 1 \leq s \leq M, s \leq t \leq M \), we see
\[
\frac{\xi^t}{(1-\eta)^s} = \frac{1}{2^s} (1 + a)^s \left( \frac{(1 + a)(1 - b)}{4} \right)^{t-s} = \frac{1}{2^{2t-s}} (1 + a)^t (1 - b)^{t-s}.
\]
Note that \( (1 + a)^t(1 - b)^{t-s}/2^{2t-s} \) is a polynomial in \( (a, b) \) with degrees \( t \) in \( a \) and \( t - s \) in \( b \). Again since both \( t \leq M \) and \( t - s \leq M \), in \( (a, b) \) space the polynomial can be exactly represented by its Lagrange interpolating approximation as Eq. (3.17). After transforming coordinate variables from \( (a, b) \) to \( (\xi, \eta) \), we obtain
\[
\frac{\xi^t}{(1-\eta)^s} = \sum_{m,n=0}^{M} \frac{\xi_m^t}{(1-\eta_n)^s} \psi_{mn}(\xi, \eta),
\]
Substituting the above approximation for \( \hat{F} \) where
\[
Q(t) = \sum_{j=1}^{N} Q_j(t)\beta_j(\xi, \eta),
\]
which implies that \( \xi^i/(1-\eta)^s \in \mathcal{G}_M(T_0) \). Therefore, we have \( \text{span}\{S_M\} \subset \mathcal{G}_M(T_0) \).

On the other hand, it is easy to check the set \( S_M \) is linear independent. Recalling that \( \text{dim}(\mathcal{G}_M(T_0)) = (M+1)^2 \), we must have \( \mathcal{G}_M(T_0) = \text{span}\{S_M\} \), i.e.,
\[
\mathcal{G}_M(T_0) = \text{span}\left\{ \xi^i\eta^j, 0 \leq i, j, i + j \leq M; \frac{\xi^i}{(1-\eta)^s}, 1 \leq s \leq M, s \leq t \leq M \right\}.
\]

However, we should point out that the finite element space \( \mathcal{G}_M(T_0) \) is not invariant under rotations and reflections of the triangle because the space contains more resolution in one corner of the triangle than in the other two corners, but the polynomial spaces generated by other choices of basis functions including the Dubiner polynomials are invariant under the same operations of the triangle.

**Remark 3.7** Depending on the Jacobians of the transformations (3.4), one may choose to directly approximate \( Q \) rather than \( \hat{Q} \). Specifically, we have observed that approximating \( Q \) could result in better accuracy when the Jacobian \( J \) of the transformation is degenerate. In this case, similar to Eq. (2.3), \( Q \) can be approximated by
\[
Q(\xi, \eta, t) \approx Q_N(\xi, \eta, t) = \sum_{j=1}^{N} Q_j(t)\beta_j(\xi, \eta),
\]
where \( Q_j(t) \) are again time-dependent expansion coefficients. Then we can approximate \( \hat{Q} \) by
\[
\hat{Q}(\xi, \eta, t) = JQ(\xi, \eta, t) \approx JQ_N(\xi, \eta, t) = J\sum_{j=1}^{N} Q_j(t)\beta_j(\xi, \eta).
\]

Substituting the above approximation for \( \hat{Q} \) into Eq. (2.4), we can write
\[
\sum_{j=1}^{N} \left( \bar{m}_{ij} \frac{dQ_j(t)}{dt} + \bar{m}_{ij}^{\xi} F_{\xi,j}(t) + \bar{m}_{ij}^{\eta} F_{\eta,j}(t) \right) + \int_{\partial\Omega} \beta_i F \cdot \mathbf{n} ds = (J\mathbf{S}, \beta_i), i = 1, \ldots, N,
\]
where \( F_j = F(Q_j) = (F_{\xi,j}, F_{\eta,j}) \), and the local mass matrix and the local derivative matrices become
\[
\bar{M} = (\bar{m}_{ij}), \quad \bar{m}_{ij} = \int_K J \beta_i \beta_j d\xi,
\]
\[
\bar{M}^{\xi} = (\bar{m}_{ij}^{\xi}), \quad \bar{m}_{ij}^{\xi} = \int_K J \frac{\partial \beta_i}{\partial \xi} \beta_j d\xi,
\]
\[
\bar{M}^{\eta} = (\bar{m}_{ij}^{\eta}), \quad \bar{m}_{ij}^{\eta} = \int_K J \frac{\partial \beta_i}{\partial \eta} \beta_j d\xi.
\]

The disadvantage of this approximation scheme is that different elements will have different mass matrices. But more importantly, the mass matrices might not be diagonal even though the basis \( \{\beta_i\} \) is orthogonal. In this case, inverses of the mass matrices have to be calculated, which might be ill-conditioned for high order polynomial basis functions. However, for the non-polynomial nodal basis, if the integrals are approximated by quadrature, every local mass matrix is still numerically diagonal as
\[
\int_{T_0} J(\xi, \eta)\psi_{mn}(\xi, \eta)\psi_{ij}(\xi, \eta) d\xi d\eta = \frac{1}{8} \int_{R_0} J(a,b)\phi_m(a)\phi_n(b)\phi_i(a)\phi_j(b)(1-b) da db \\
\approx \frac{1}{8} \sum_{s,t=0}^{M} \omega_s \omega_t J(t_s, t_t)\phi_m(t_s)\phi_n(t_t)\phi_i(t_s)\phi_j(t_t)(1-t_t) \\
= \frac{1}{8} \delta_{mi}\delta_{nj}\omega_m\omega_n(1-t_n)J(t_m, t_n).
\]
3.4 Spectral derivative matrices

When we solve Eq. (2.5) or Eq. (3.20) by explicit methods, the maximum time step size allowed for numerical stability is always a major concern which, generally speaking, shall depend on the eigenvalues of the derivative matrices as the results of the Galerkin approximation to the derivative operators \( \partial / \partial \xi \) and \( \partial / \partial \eta \). For rectangles, the orthogonal nodal basis (3.1) will produce the standard derivative matrices as in the Galerkin Legendre spectral method [15]. Therefore, the eigenvalues of the derivative matrices \( M^\xi \) and \( M^\eta \) are well-known which grow at a rate of \( O(M^2) \) [15]. For triangles, the derivative matrix \( M^\xi \) produced by the orthogonal nodal basis (3.10) can be easily shown to share in principle the same property as that produced by the orthogonal nodal basis on rectangles. To do so, let us denote \( \beta_i = \psi_{mn}(\xi, \eta) \) and \( \beta_j = \psi_{st}(\xi, \eta) \) be two nodal basis functions on the triangle \( T_0 \). Then the derivative matrix \( M^\xi \) in Eq. (2.7) becomes

\[
m_{ij}^\xi = \int_{T_0} \frac{\partial \psi_{mn}(\xi, \eta)}{\partial \xi} \psi_{st}(\xi, \eta) \, d\xi \, d\eta
\]

which turns out to be exactly the same as the corresponding derivative matrix for the orthogonal nodal basis on the square \( R_0 \) except for a factor of 1/2. On the other hand, the derivative matrix \( M^\eta \) in Eq. (2.8) can be written as

\[
m_{ij}^\eta = \int_{T_0} \frac{\partial \psi_{mn}(\xi, \eta)}{\partial \eta} \psi_{st}(\xi, \eta) \, d\xi \, d\eta
\]

whose spectral property is therefore not clear and will be a subject of further research.

If we choose to directly approximate \( Q \) rather than \( \hat{Q} \), then the property of the consequent derivative matrices \( \hat{M}^\xi \) and \( \hat{M}^\eta \) will depend not only on the choice of the basis but also the underlying geometry of the problem being solved.

Nevertheless, it has been heuristically claimed in [4] and partially analyzed in [8] that, for an orthogonal basis on a triangle constructed by a direct product like (3.9), the explicit time step size has a \( O(1/M^4) \) limitation due to the concentration of a lot of resolution in a single corner of the triangle, while for the Dubiner orthogonal polynomial basis the explicit time step size has only a \( O(1/M^2) \) limitation. To demonstrate such scaling, we consider the spectrum of the inverse of the mass matrix \( M \) times the derivative matrix \( M^\xi \) or \( M^\eta \). And our numerical analysis seems to show that the largest eigenvalue of the inverse of the mass matrix times each derivative matrix does scale as \( O(M^4) \) if using the non-polynomial nodal basis but as only \( O(M^2) \) if using the Dubiner polynomial basis, which is in support of the above heuristic argument. However, at this point it appears to be impossible to have a conclusive mathematical analysis of the spectrum of the inverse of the mass matrix times the derivative matrix and thus the time step restriction of the non-polynomial nodal basis, which therefore shall constitute a separate topic of future research.

4 Numerical results

In this section, we shall give some illustrative examples which demonstrate the exponential convergence property of the orthogonal nodal basis on triangles. The application of the basis to the numerical simulation of optical coupling by whispering gallery modes between microcylinders shall be presented as well.
4.1 Approximation properties of the orthogonal nodal basis on triangles

Because the approximation space spanned by the orthogonal non-polynomial nodal basis $G_M(T_0)$ contains the complete polynomial space $P_M(T_0)$, we expect the standard spectral accuracy of spectral methods [14, 15] over triangles. To show such an approximation property, the first example we consider is the following oscillatory wave function on the square $R_1 = [0, 1] \times [0, 1]$

$$u(x, y) = \frac{1}{2} \left( \sin \left( 2\pi k \left( x + \frac{7}{15} \right) \right) + \cos \left( 2\pi k \left( y + \frac{2}{15} \right) \right) \right),$$

(4.1)

and in Fig. 3 we display the contour plot of this function with the wave number $k = 5$.

![Contour plot of the wave function (4.1) with the wave number $k = 5$.](image)

Fig. 3 The contour plot of the wave function (4.1) with the wave number $k = 5$.

To demonstrate the exponential convergence of the orthogonal nodal basis on triangles and to compare the behaviors of the nodal basis and the Dubiner basis, we first decompose the square $R_1$ into two triangular elements as shown in Fig. 3, and then approximate the oscillatory function $u(x, y)$ with the wave number $k = 2$ by interpolation in terms of the nodal basis and the Dubiner basis with different expansion orders, respectively. When expanding the function in terms of the Dubiner polynomials, we evaluate it at the same collocation points as defined in (3.11), and then solve a linear least square problem to find expansion coefficients. As shown in Fig. 4 are the $L_\infty$ approximation errors plotted with respect to the expansion order. The exponential convergence of both bases are clearly observed as indicated by the asymptotic linear behavior of the curves on this lin-log plot. In addition, the results also suggest that the nodal basis appears to be more accurate than the Dubiner basis, which actually coincides with the fact that the finite element space spanned by the Dubiner basis $P_M(T_0)$ is contained in that spanned by the nodal basis $G_M(T_0)$. On the other hand, however, since most of the extra resolution compared with the Dubiner basis is isolated to a single corner of each triangle, the orthogonal non-polynomial nodal basis only gives a small decrease in the error of the Dubiner polynomial basis.

Next, we shall study the number of points per wavelength required to approximate the oscillatory function $u(x, y)$ to certain degree of accuracy by the orthogonal non-polynomial nodal basis. For this purpose, we define the number of points per wavelength used $N_{ppw}$ as

$$N_{ppw} = \sqrt{2} \frac{M + 1}{k},$$

(4.2)

where the factor $\sqrt{2}$ reflects that the number of total collocation points (and thus the number of total nodal basis functions) is $2(M + 1)^2 = (\sqrt{2}(M + 1))^2$. We investigate two cases, requiring the $L_\infty$ approximation errors being less than 2% and 0.02%, respectively, and the results are shown in Fig. 5. One can note in particular that about 5 to 6 points per wavelength are sufficient to approximate the oscillatory wave with high wave numbers to degree of accuracy of 1%.
4.2 Scattering by single dielectric cylinder

In this test, we shall consider a typical electromagnetic scattering problem as illustrated in Fig. 6 (a), i.e., scattering by a dielectric cylinder in free space with a TM wave excitation. Maxwell’s equations (2.1), together with the boundary condition that at the cylindrical boundary the tangential components of the fields should be continuous, can be used to solve the problem.

We assume that the cylinder is illuminated by a time-harmonic incident plane wave of the form

\[ E_{z}^{\text{inc}} = e^{-i(k_1 x - \omega t)}, \quad H_{y}^{\text{inc}} = -e^{-i(k_1 x - \omega t)}, \]

where \( k_1 = \omega \sqrt{\varepsilon_1 \mu_1} \) is the propagation constant for homogeneous, isotropic free space medium. In this case, the exact solution of the problem is given in [16] and is also available in [17].

We would like to verify the exponential convergence of the nodal basis for solving the above scattering problem. To this end, the cylinder radius is set as \( a = 0.6 \), and the computational domain is chosen as \( \Omega = [-1, 1] \times [-1, 1] \), which is subdivided into quadrilateral and triangular elements as shown in Fig. 6 (b). We should point out that although for this sample scattering problem one doesn’t have to use triangular elements, we employ them so that we can develop more general codes for simulating scattering of not only one cylinder, multiple cylinders of the same size, but also multiple cylinders of different sizes. Regarding the boundary condition at the artificial boundary of the computational domain, we simply use the boundary values obtained by the exact solution so that we can measure the approximation errors and thus investigate the convergence property of the nodal basis. In practical simulations when boundary values are not available, absorbing boundary conditions such as PML boundary conditions should be used [18]-[20].
As described in Section 2, each physical element in the subdivided domain shall be mapped individually onto the reference square $R_0$ or the reference triangle $T_0$ by an isoparametric transformation, which in general can be arrived by the blending function method [1]. Next we only give the transformation required to map those curvilinear triangles shown in Fig. 6 (b) onto the reference triangle $T_0$. For more detailed description of the blending function method as well as more examples the readers may consult [1].

Fig. 7 Transformation between the reference triangle $T_0$ and a curvilinear triangle $\Delta ABC$.

Each triangular element in Fig. 6 (b) has one curved boundary so we need a transformation that can map the reference triangle $T_0$ onto a triangle with one curved boundary. Suppose that the curved boundary $AB$ is parametrizable as shown in Fig. 7 by $(\chi(\xi), \pi(\xi))$ such that $\chi(0) = x_1, \chi(1) = x_2, \pi(0) = y_1$ and $\pi(1) = y_2$. Then the transformation can be written as

$$
x = (1 - \xi - \eta) x_1 + \xi x_2 + \eta x_3 + (\chi(\xi) - (1 - \xi) x_1 - \xi x_2) \frac{1 - \xi - \eta}{1 - \xi},
$$

$$
y = (1 - \xi - \eta) y_1 + \xi y_2 + \eta y_3 + (\pi(\xi) - (1 - \xi) y_1 - \xi y_2) \frac{1 - \xi - \eta}{1 - \xi}.
$$

We consider a situation in which $\epsilon_1 = \mu_1 = 1$, i.e., the material exterior to the cylinder is assumed to be vacuum. The permittivity and the permeability of the cylinder are set as $\epsilon_2 = 9$ and $\mu_2 = 1$, respectively, and the angular frequency $\omega = 2\pi$. Figure 8 shows the contours of the three computed field components at the time $t = 1$ by using the orthogonal nodal basis with $M = 12$, as well as the global $L_\infty$ errors for the three components for several expansion orders. Once again we include corresponding convergence analysis results for the Dubiner basis. All results clearly illustrate the spectral convergence of the two bases, and not surprisingly again that the nodal basis is a little more accurate than the Dubiner basis when high order expansions are employed.

4.3 Optical coupling by whispering gallery modes between microcylinders

Finally, we shall apply the DSEM with the orthogonal nodal bases to study optical coupling by whispering gallery modes between two microcylinders, the building blocks of novel photonic waveguides: Coupled Resonator Optical Waveguide (CROW) [21]. Such waveguides have applications in optical buffering and delay lines in controlling the speed of light propagations, and therefore constitute topics of great interest to the international photonic community. While it is theoretically well-known that in CROW devices waveguiding is provided by the weak coupling of evanescent whispering gallery modes in the individual microresonators, in this example we shall numerically demonstrate that the successful optical coupling between microcylinders can be achieved.

Whispering gallery modes (WGMs) are electromagnetic resonances traveling in dielectric media of circular symmetric structures such as microcylinders, microdisks and microspheres. In the case of a dielectric cylinder, the WGMs were first studied by Lord Rayleigh trying to understand the acoustic waves clinging to the dome of St. Paul’s Cathedral [22]. In this paper, we shall consider electromagnetic WGMs of a circular dielectric cylinder of radius $a$ and infinite length with dielectric constant $\epsilon_1$ and magnetic permeability $\mu_1$, which is embedded in an infinite homogeneous medium of material parameters $\epsilon_2$ and $\mu_2$. With respect to a cylindrical coordinate system $(r, \theta, z)$, for a time factor $\exp(-i\omega t)$, the components of the magnetic field $\mathbf{H} = (H_r, H_\theta, H_z)$ and the electric
The field \( E = (E_r, E_\theta, E_z) \) of the WGMs are given by the following equations \([23, 24]\)

\[
H_r = \left( a_n \frac{nk^2}{\mu \omega \lambda^2} G_n(\lambda r) + b_n \frac{i h}{\lambda} G'_n(\lambda r) \right) F_n,
\]

\[
H_\theta = \left( a_n \frac{ik^2}{\mu \omega \lambda} G'_n(\lambda r) - b_n \frac{nh}{\lambda^2} G_n(\lambda r) \right) F_n,
\]

\[
H_z = b_n G_n(\lambda r) F_n,
\]

\[
E_r = \left( a_n \frac{ih}{\lambda} G'_n(\lambda r) - b_n \frac{\mu \omega n}{\lambda^2} G_n(\lambda r) \right) F_n,
\]

\[
E_\theta = -\left( a_n \frac{nh}{\lambda^2} G_n(\lambda r) + b_n \frac{\mu \omega}{\lambda} G'_n(\lambda r) \right) F_n,
\]

\[
E_z = a_n G_n(\lambda r) F_n,
\]

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where \( F_n = \exp(in\theta + ihz - i\omega t) \) with \( h \) being the axial propagation constant. The function \( G_n \equiv J_n(\omega r) \) for \( r < a \) and \( H_n^{(1)}(\omega r) \) for \( r > a \), where \( J_n \) is the Bessel function of the first kind and \( H_n^{(1)} \) is the Hankel function of the first kind. Prime denotes differentiation with respect to the argument \( \lambda r \). Also, for \( r < a, k = k_1 = \frac{\omega}{c}\sqrt{\epsilon_1\mu_1}, \lambda = \lambda_1 \) where \( \lambda_1^2 = k_1^2 - h^2 \), and for \( r > a, k = k_2 = \frac{\omega}{c}\sqrt{\epsilon_2\mu_2}, \lambda = \lambda_2 \) where \( \lambda_2^2 = k_2^2 - h^2 \).

The coefficients \( a_n \) and \( b_n \) are determined by the boundary condition that, at the cylindrical boundary \( r = a \), the tangential components of the fields are continuous. For a nontrivial solution, the axial propagation constant \( h \) shall satisfy the following eigenvalue equation \([23, 24]\)

\[
\left( \frac{\mu_1}{u} \frac{J_n'(u)}{J_n(u)} - \frac{\mu_2}{v} \frac{H_n^{(1)'}(v)}{H_n^{(1)}(v)} \right) \left( \frac{k_n^2}{\mu_1 u} \frac{J_n'(u)}{J_n(u)} - \frac{k_n^2}{\mu_2 v} \frac{H_n^{(1)'}(v)}{H_n^{(1)}(v)} \right) = n^2h^2 \left( \frac{1}{u^2} - \frac{1}{v^2} \right)^2, \tag{4.5}
\]

where \( u = \lambda_1 a \) and \( v = \lambda_2 a \). For a given mode number \( n \), Eq. (4.5) does not have a unique solution and the electromagnetic WGMs are represented by solutions of Eq. (4.5) when \( n \) is of the order of \( \lambda_1 a \). Note that the mode number \( n \) is also the number of maxima in the field intensity in the azimuthal direction and is thus called the azimuthal number of the WGMs.

In order to investigate optical coupling by WGMs between microcylinders, we shall turn to Maxwell’s equations. For a WGM with the axial propagation constant \( h \), the magnetic field \( H = (H_x, H_y, H_z) \) and the electric field \( E = (E_x, E_y, E_z) \) in a rectangular coordinate system \((x, y, z)\) may be expressed as

\[
H(x, y, z, t) = H(x, y, t)e^{ihz}, \quad E(x, y, z, t) = E(x, y, t)e^{ihz}.
\]

Substituting them into the three-dimensional Maxwell’s equations

\[
\begin{align*}
\mu \frac{\partial H}{\partial t} &= -\nabla \times E, \\
\epsilon \frac{\partial E}{\partial t} &= \nabla \times H,
\end{align*}
\]

we obtain the following hyperbolic system of equations in matrix form

\[
\frac{\partial Q}{\partial t} + A(\epsilon, \mu) \frac{\partial Q}{\partial x} + B(\epsilon, \mu) \frac{\partial Q}{\partial y} = S, \tag{4.6}
\]

where

\[
Q = \left( \begin{array}{c} \mu H \\ \epsilon E \end{array} \right), \quad S = \left( \begin{array}{c} ihE_y \\ -ihE_x \\ 0 \\ -ihH_y \\ ihH_x \\ 0 \end{array} \right),
\]

and

\[
A(\epsilon, \mu) = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -\frac{1}{\mu} \\
0 & 0 & 0 & 0 & \frac{1}{\mu} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & -\frac{1}{\mu} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{\mu}
\end{pmatrix}, \quad B(\epsilon, \mu) = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{\mu} \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}.
\]

The model considered here is a system of two identical circular dielectric cylinders of infinite length in contact. The radiuses of the cylinders are \( r_1 = r_2 = 0.5775 \), and the material parameters are \( \epsilon_1 = 10.24 \) and \( \mu_1 = 1 \) while the external medium is vacuum. Then it can be shown that WGMs exist in such cylinders. In fact, by setting the angular frequency \( \omega = 2\pi \), and the azimuthal number \( n = 8 \), we find that the eigenvalue equation (4.5) has a solution \( h = 6.80842739 \) between \( k_1 = 6.4\pi \) and \( k_2 = 2\pi \), and the corresponding lossless WGM is denoted by \( \text{WGM}_{8,1,0} \).
We will investigate the optical energy transport by WGMs from one cylinder to the other. To this end, in our simulation we assume that initially there exists a WGM in the left cylinder and no fields exist inside the right cylinder. More specifically, the exact values of WGMs in the left cylinder are taken as the initial conditions in the entire computational domain except for the inside of the right cylinder, where a zero field is initialized. In addition, to assure that the initial field satisfies the interface condition on the surface of the right cylinder, in our numerical test we also assume that there exist surface currents over the surface of the right cylinder of the form

\[ J_m(x, t) = J^0_m(x)e^{-\alpha t}, \quad J_e(x, t) = J^0_e(x)e^{-\alpha t}, \]  

(4.7)

where the constant \( \alpha > 0 \) is chosen so that the surface currents become negligible after a short period of time, and \( J^0_m \) and \( J^0_e \) are calculated from the initial fields \( E(x, 0) \) and \( H(x, 0) \) as

\[ J^0_m(x) = n \times \left( E^+(x, 0) - E^-(x, 0) \right), \quad J^0_e(x) = n \times \left( H^+(x, 0) - H^-(x, 0) \right). \]

For such boundary currents, the numerical normal flux in the DSEM can be written as [25]

\[ (F \cdot n)^- = \begin{pmatrix}
  n \times \left( \frac{YE-nH}{Y+} \right)^- + (YE-nH)^+ - J_e - \frac{Y^+}{Y+Y^+} J_m \\
  -n \times \left( \frac{ZH-nE}{Z+} \right)^- + (ZH-nE)^+ + J_m \\
\end{pmatrix}, \]

for the − side of the surface and

\[ (F \cdot n)^+ = \begin{pmatrix}
  n \times \left( \frac{YE-nH}{Y+} \right)^+ + (YE-nH)^- - J_e - \frac{Y^+}{Y+Y^+} J_m \\
  -n \times \left( \frac{ZH-nE}{Z+} \right)^+ + (ZH-nE)^- + J_m \\
\end{pmatrix}, \]

for the + side of the surface. Here \( Z^\pm \) and \( Y^\pm \) are the local impedance and admittance, respectively, and are defined as \( Z^\pm = 1/Y^\pm = (\mu^\pm/\epsilon^\pm)^{1/2} \).

Regarding the boundary condition on the boundary of the computational domain, since most of the electromagnetic energy of a WGM is confined inside the cylinder and fields decay fast away from the cylindrical boundary, a simple matched layer (ML) technique introduced in [26] will be sufficient and is thus used in our simulation.

The computational mesh for this simulation is similar to that shown in Fig. 6 (b), except here we have two touching cylinders. The surrounding ML layer has a width of \( d = r = 0.5775 \). The expansion order \( M = 10 \), while the constant \( \alpha = 10 \) in Eq. (4.7). To demonstrate the dynamics of the optical energy transport by WGMs from the left cylinder to the right cylinder, in Fig. 9 we show the snapshots of the \( E_z \) component at four different times. The initial state of the system is represented by a counterclockwise circulating wave, i.e., the fundamental mode WGMs in the left cylinder. The four sequential snapshots Fig. 9 (a)-(d) then illustrate the generation of a clockwise WGM in the right cylinder due to the optical coupling and the phase matching, and thus confirm the optical energy transport from the left cylinder to the right cylinder. More discussions can be found in [25].

### 4.4 Explicit time step size

As discussed earlier, when we solve Eq. (2.5) or Eq. (3.20) by an explicit method, the explicit time step restriction for numerical stability is always a major concern which generally speaking shall depend on the eigenvalues of the derivative matrices. And as heuristically claimed in [4], partially analyzed in [8] and supported by our numerical experiments, for an orthogonal basis on a triangle constructed by a direct product like (3.9), the explicit time step size has a \( O(1/M^4) \) limitation due to the concentration of a lot of resolution in a single corner of the triangle and is therefore considered unacceptable, while for the Dubiner orthogonal polynomial basis the explicit time step size has only a \( O(1/M^2) \) limitation. However, in practical situations the explicit time step size may also depend on some other factors. For instance, if we choose to approximate \( Q \) instead of \( \tilde{Q} \) in a DSEM as described in Remark 3.7, the eigenvalues of the derivative matrices \( M^x \) and \( M^y \) depend on not only the choice of the basis functions but also the underlying geometry of the problem being solved. Moreover, in practice the expansion order \( M \) normally will not be taken very large so a \( O(1/M^4) \) limitation on the time step size could be still acceptable.

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To numerically compare the explicit time step sizes for the non-polynomial nodal basis and the Dubiner polynomial basis in our applications, we find the “almost optimal” time step sizes for these two bases in those applications described in Sections 4.2 and 4.3, and the results are displayed in Fig. 10. Here we call a step size $X.X \times 10^{-s}$ “almost optimal” when the simulation is stable for $\Delta t = X.X \times 10^{-s}$ but unstable for $\Delta t = (X.X + 0.1) \times 10^{-s}$. As can be seen, for large expansion orders both bases will have to use very small time step sizes, but there is no significant difference between the “almost optimal” step sizes for the two bases except for a factor of around 1.5. And also as indicated in Fig. 10, for the above two applications it appears that the maximum explicit step sizes decrease at a rate faster than $O(1/M^2)$ for both bases. It should be pointed out that the faster-than-$O(M^2)$ growth rate of the explicit time step size for the polynomial basis contradicts most previous work [8]. This difference could be caused by the approximation of $Q$ instead of $\hat{Q}$ in the DSEM, but a full-blown analysis of the difference is not available at this time and it could be another subject of further research.

Fig. 10 Non-quadratic decay of the explicit time step size for both the nodal basis and the Dubiner polynomial basis on triangles in applications as described in Sections 4.2 and 4.3. a) Scattering by a dielectric cylinder; b) Optical coupling between two microcylinders.
4.5 Computational efficiency

In order to make a fair comparison of the effectiveness of the non-polynomial nodal basis and the Dubiner polynomial basis, we measure the computational cost of each basis in terms of the CPU time used to simulate the scattering by a single cylinder. We first investigate the computational cost per time step for each basis. When programming, we have made every effort to identify and optimize those components that are using most of the CPU time, including evaluating most if not all integrals and computing mass matrix inverses in the preprocessing phase. Conducting our numerical experiments on a Pentium Xeon 2.4GHz processor and 2GB of RAM, we have found that most of the CPU time is used to (1) compute the resolved normal fluxes and (2) compute those slope vectors in the Runge-Kutta method. For part (1), both bases use almost the same amount of CPU time because it is primarily determined by the number of element edges. For part (2), however, the situation is a bit complicated and it really depends on the problem being solved. For instance, when simulating the scattering of a single dielectric cylinder, if we employ the total-field formulation in which the source term $S$ in Eq. (2.1) is zero, the polynomial basis will use less CPU time to compute those slope vectors because all integrals can be computed in preprocessing. On the other hand, if we employ the scattered-field formulation, then the nodal basis will use less CPU time since in this case we have to evaluate the right-hand side integral in Eq. (2.5) or Eq. (3.20) at each time step.

For example, the CPU time per time step for the simulation of the scattering by a single cylinder is shown in Table 1. As mentioned earlier we use both quadrilateral and triangular elements, and in this test the same expansion order $M = 14$ is used for the approximation on both elements. It can be seen from the table that it will take about 0.11-0.12s to calculate the resolved normal fluxes and 0.02-0.023s to calculate slopes for quadrilaterals for either basis. If we use the total-field formulation, it will take about 0.01s and 0.026s to compute slopes for triangles by the polynomial basis and the non-polynomial nodal basis, respectively. If we use the scattered-field formulation, however, it will take about 0.082s for the polynomial basis but only 0.028s for the non-polynomial nodal basis to compute the slopes for triangular elements.

<table>
<thead>
<tr>
<th></th>
<th>Total-field Dubiner</th>
<th>Nodal Dubiner</th>
<th>Scattered-field Dubiner</th>
<th>Nodal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal fluxes</td>
<td>0.110</td>
<td>0.121</td>
<td>0.117</td>
<td>0.120</td>
</tr>
<tr>
<td>Slopes for quadrilaterals</td>
<td>0.020</td>
<td>0.020</td>
<td>0.023</td>
<td>0.023</td>
</tr>
<tr>
<td>Slopes for triangles</td>
<td>0.010</td>
<td>0.026</td>
<td>0.082</td>
<td>0.028</td>
</tr>
</tbody>
</table>

Next we consider the total CPU time used to simulate the scattering by a single cylinder to the final time $t = 1$, and the scattered-field formulation is employed since for scattering problem it is often more convenient. Conducted on the same computer, the used CPU time of both bases for different expansion orders is reported in Table 2, where the number in parenthesis represents the ratio of the CPU time of the polynomial basis to that of the non-polynomial nodal basis. As can be seen for the same time step size $\Delta t$, the CPU time of the Dubiner basis is slightly larger than that of the nodal basis. Moreover, this difference broadens with increased expansion orders, which can be partially understood within the fact that the computational cost to evaluate the right-hand side integral in Eq. (2.5) or Eq. (3.20) under the nodal basis is two orders less than that under the Dubiner basis. However, if the stability constraint is taken into account, that is, if we use the corresponding “almost optimal” time step size for each basis, we have found that the computational cost of the Dubiner basis is around 80% of that of the nodal basis.

As our concluding remark, we believe the orthogonal nodal basis on triangles has its applications even the potential $O(1/M^4)$ limitation on the explicit time step size, especially in situations that the computational time is not a major concern. As discussed in Section 3, the orthogonal nodal basis will produce diagonal local mass matrices no matter what approximation scheme is chosen. And compared with the Dubiner polynomial basis, the non-polynomial nodal basis is very much easier to implement. For example, when both quadrilateral and triangular elements are involved, the codes for handling the quadrilateral and triangular elements are almost identical if the orthogonal nodal bases are used in approximating the solution on both types of elements and the values of the solution at the collocation points defined in (3.11) are used in calculating integrals over triangular elements.
Table 2  Total CPU time in seconds for the simulation of the scattering by a single cylinder.

<table>
<thead>
<tr>
<th>Expansion order</th>
<th>$\Delta t_1$</th>
<th>$\Delta t_2$</th>
<th>Nodal Dubiner</th>
<th>Dubiner $\Delta t = \Delta t_1$</th>
<th>Dubiner $\Delta t = \Delta t_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>2.0E−3</td>
<td>2.5E−3</td>
<td>46</td>
<td>46 (1.00)</td>
<td>38 (0.83)</td>
</tr>
<tr>
<td>6</td>
<td>6.1E−4</td>
<td>8.0E−4</td>
<td>213</td>
<td>220 (1.03)</td>
<td>169 (0.79)</td>
</tr>
<tr>
<td>8</td>
<td>2.4E−4</td>
<td>3.2E−4</td>
<td>738</td>
<td>788 (1.07)</td>
<td>593 (0.80)</td>
</tr>
<tr>
<td>10</td>
<td>1.1E−4</td>
<td>1.5E−4</td>
<td>2179</td>
<td>2396 (1.10)</td>
<td>1767 (0.81)</td>
</tr>
<tr>
<td>12</td>
<td>6.0E−5</td>
<td>8.5E−5</td>
<td>5393</td>
<td>6049 (1.12)</td>
<td>4264 (0.79)</td>
</tr>
<tr>
<td>14</td>
<td>3.4E−5</td>
<td>5.0E−5</td>
<td>12884</td>
<td>14604 (1.13)</td>
<td>10218 (0.79)</td>
</tr>
</tbody>
</table>

5 Conclusion

In this paper, we have proposed and analyzed an orthogonal non-polynomial nodal basis on triangles which results in diagonal mass matrices for DSEMs over unstructured grids. By applying this basis to approximate both oscillatory functions and the solution of electromagnetic scattering by single dielectric cylinder, we have demonstrated the exponential convergence of the orthogonal non-polynomial nodal basis. Meanwhile, the same idea can be easily extended to three-dimensional problems for tetrahedral elements or any other elements which can be obtained by a similar “collapsing” mapping from the standard cube.

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