hp-Adaptive least squares spectral element method for hyperbolic partial differential equations

Árpád Galvão\textsuperscript{a}, Marc Gerritsma\textsuperscript{a,∗}, Bart De Maerschalck\textsuperscript{b}

\textsuperscript{a}Department of Aerospace Engineering, Delft University of Technology, Kluyverweg 1, 2629 HS Delft, The Netherlands
\textsuperscript{b}Von Karman Institute for Fluid Dynamics, Waterloosesteenweg 72, 1640 Sint Genesius, Belgium

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Abstract

This paper describes a hp-adaptive spectral element formulation which is used to discretize the weak formulation obtained by minimizing the residuals in the $L^2$-norm. The least-squares error indicator will be briefly discussed. Refinement of the numerical approximation is based on an estimate of the regularity of the underlying exact solution; if the underlying exact solution is sufficiently smooth polynomial enrichment is employed, in areas with limited regularity $h$-refinement is used. For this purpose the Sobolev regularity is estimated. Functionally and geometrically non-conforming neighbouring elements are patched together using so-called mortar elements. Results of this approach are compared to uniform $h$- and $p$-refinement for a linear advection equation.

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1. Introduction

The least-squares spectral element method (LSQSEM) is a novel approach to solve systems of partial differential equations. The method combines the least-squares formulation with a spectral approximation. The method was developed simultaneously by Poot and Gerritsma\cite{18,16,17} and Pontaza and Reddy\cite{14,15}.

LSQSEM combines the locality of the finite element method, the symmetric positiveness of the least-squares formulation and the higher order accuracy of spectral methods. In addition, the least-squares formulation circumvents compatibility requirements between approximating function spaces in mixed problems, such as the $\text{inf}–\text{sup}$ condition for the incompressible Navier–Stokes equations.

Despite these advantages LSQSEM becomes a very expensive method when higher order approximations are used uniformly throughout the whole computational domain. Therefore, an adaptive scheme has been developed, which signals regions that require refinement and takes the appropriate steps to reduce the error locally.

∗ Corresponding author.

E-mail addresses: M.I.Gerritsma@LR.TUDelft.nl (M. Gerritsma), demaersc@vki.ac.be (B. De Maerschalck).
This technique requires three new ingredients compared to the LSQSEM algorithms published previously. First of all, a method should be developed which patches together elements of different sizes and with different numerical representations such as different polynomial degrees. One way of doing so is to use the discontinuous least-squares formulation [4], but in the current paper, the mortar element method (MEM) is employed [2,5,10].

Next, an error indicator needs to be used to flag which elements need to be refined. Having established which elements will be refined, we now need to decide how to refine; decrease the element size, \( h \)-refinement, or increase the polynomial degree, \( p \)-enrichment. This decision is based on the estimated regularity of the exact solution. A more thorough discussion of \( hp \)-adaptive refinement applied to the LSQSEM can be found in [2].

The outline of this paper is as follows: Section 2 gives a brief introduction to the LSQSEM. Section 3 presents a way to patch together elements with different sizes and different approximating function spaces. Section 4 introduces a least-squares error estimator which flags the elements eligible for refinement. In order to establish how to refine we need a regularity estimator as described in Section 5. The resulting \( hp \)-adaptive LSQSEM scheme is applied to a space–time linear advection equation in Section 6. Conclusions are drawn in Section 7.

2. The least-squares spectral element method

The LSQSEM combines the least-squares formulation with a spectral element discretization. In this section, both ingredients will be addressed succinctly.

2.1. The least-squares formulation

The least-squares formulation is based on the minimization of the residual in a suitable norm. For convenience, one usually minimizes the residual in the \( L^2 \)-norm. In addition, we rewrite the differential equation in an equivalent first order system of differential equations to mitigate continuity requirements between adjacent elements and reduce the condition number of the resulting system of algebraic equations.

Introduce

\[
\mathcal{L} u = f, \quad x \in \Omega,
\] (2.1)

as a system of first order partial differential equations defined on the domain \( \Omega \) and supplemented with the boundary conditions

\[
\mathcal{R} u = g, \quad x \in \Gamma \subset \partial \Omega.
\] (2.2)

Let \( \mathcal{L} \) be a linear differential operator which maps elements from the function space \( X \) into the function space \( Y \), \( \mathcal{L} : X \rightarrow Y \), such that there exist two constants \( C_1, C_2 > 0 \) for which we have

\[
C_1 \| u \|_X \leq \| \mathcal{L} u \|_Y \leq C_2 \| u \|_X \quad \forall u \in X.
\] (2.3)

Both inequalities, coercivity and continuity, respectively, assert that \( \| \mathcal{L} u \|_Y \) defines a norm equivalent to \( \| u \|_X \). So minimizing \( \| u - u_{\text{ex}} \|_X \) is equivalent to minimizing \( \| \mathcal{L} (u - u_{\text{ex}}) \|_Y = \| \mathcal{L} u - f \|_Y \). Here \( u_{\text{ex}} \) denotes the exact solution.

If we chose for \( Y \) the Hilbert space \( Y = L^2(\Omega) \), minimization of the residual amounts to

Find \( u \in X \) such that

\[
(\mathcal{L} u, \mathcal{L} v)_{L^2(\Omega)} = (f, \mathcal{L} v)_{L^2(\Omega)} \quad \forall v \in X.
\] (2.4)

Instead of using the infinite-dimensional function space \( X \) to look for a minimizer, we generally restrict ourselves to a finite-dimensional space \( X^h \) in which case the least-squares formulation reads

Find \( u^h \in X^h \) such that

\[
(\mathcal{L} u^h, \mathcal{L} v^h)_{L^2(\Omega)} = (f, \mathcal{L} v^h)_{L^2(\Omega)} \quad \forall v^h \in X^h.
\] (2.5)

For a more extensive treatment of the least-squares formulation, see [7,8].
2.2. Spectral element approximation

For the finite-dimensional subspace $X^h$, mentioned in the previous subsection, we use a spectral approximation. The domain $\Omega$ is sub-divided into $K$ non-overlapping quadrilateral sub-domains $\Omega^k$:

$$\Omega = \bigcup_{k=1}^{K} \Omega^k, \quad \Omega^k \cap \Omega^l = \emptyset, \quad k \neq l. \quad (2.6)$$

Each sub-domain is mapped onto the unit cube $[-1, 1]^d$, where $d = \dim \Omega$. Within this unit cube the unknown function are approximated by Lagrangian functions

$$u^h(\xi, \eta) = \sum_{i=0}^{N} \sum_{j=0}^{M} u_{ij} h_i(\xi) h_j(\eta) \quad \text{for } d = 2, \quad (2.7)$$

where

$$h_i(\xi) = \frac{\left(\xi^2 - 1\right) L_N'(\xi)}{N(N+1)L_N(\xi)(\xi - \xi_i)}. \quad (2.8)$$

Here the points $\xi_i$ are the Gauss–Lobatto–Legendre (GLL) points given by the zeroes of $(1-x^2)L_N'(x)$, where $L_N(x)$ is the Legendre polynomial of degree $N$. Instead of Legendre polynomials Chebyshev polynomials may be used [12,19], or more general Jacobi polynomials [3]. In this paper only Legendre polynomials will be considered.

After transformation of the least-squares formulation (2.5) to the unit cube and insertion of the higher order approximation (2.7), an algebraic system for the unknowns $u_{ij}$ can be set up.

The integrals appearing in (2.5) are evaluated using Gauss–Lobatto integration

$$\int_{-1}^{1} f(x) \, dx \approx \sum_{p=0}^{P} f(x_p) \, w_p, \quad (2.9)$$

where $x_p$ are the GLL points and the GLL weights $w_p$ are the solution of the linear system

$$\sum_{j=0}^{P} x^i_j w_j = \int_{-1}^{1} x^i \, dx \quad \text{for } i = 0, \ldots, N. \quad (2.10)$$

Note that Gauss–Lobatto integration is exact for polynomials of degree $2P-1$. If we assemble the numerical integration weights $w_p$ in a diagonal matrix $W = \text{diag}(w_0, \ldots, w_P)$ the discrete least-squares formulation at elemental level can be written as

$$L^T W \vec{u}^k = L^T \vec{f}^k, \quad (2.11)$$

here $L_{ij} = \mathcal{L} \psi_j(x_i)$ denotes the differential operator acting on the $j$th two-dimensional basis function $\psi_j = h_k(\xi)h_l(\eta)$, evaluated at the $i$th Gauss–Lobatto integration point $x_i = (\xi, \eta)$, where $0 \leq j \leq (N+1)(M+1)$ within one spectral element and $0 \leq i \leq (P+1)^2$. The right-hand side vector $\vec{f}_i = f(x_i)$ is the load-vector in the original differential equation evaluated at the integration point $x_i = (\xi, \eta)$. The vector of unknowns $\vec{u}^k$ are the unknown expansion coefficients in the two-dimensional representation (2.7) in element $k$. In general the matrix $L$ will have more rows than columns, thus comprising an over-determined, but consistent system of algebraic equations.

3. The mortar element method

In the MEM, neighbouring elements in $\mathbb{R}^d$ are patched together by mortar-like elements in $\mathbb{R}^{d-1}$. In $\mathbb{R}^2$ the mortar elements consist of line segments as sketched in Fig. 1. The $i$th boundary of element $k$, denoted by $\Gamma^k_i$, is associated with a number of mortars, $\gamma_j$. The solution on the mortars, $\phi$, is connected to the solution at the border of the two neighbouring elements. This establishes a connection between the solution at the edge of an element, denoted by $u_b$,
and the mortar solution $\phi$. If we choose a polynomial approximation for $\phi$ on the mortar, we can express the expansion coefficients at the boundary of the element, $\tilde{u}_b$, in terms of the expansion coefficients of the solution on the mortar, $\tilde{\phi}$, as

$$
\tilde{u}_b = \tilde{Z} \tilde{\phi}.
$$

(3.1)

The precise relation is inconsequential as long as the matrix $\tilde{Z}$ is of full rank for at least one of the elements associated with the mortar. This condition prevents the appearance of spurious mortar solutions.

Having established the relation between the elemental boundary unknowns and the mortar unknowns, we can express the global system in terms of the inner element unknowns, $\tilde{u}_i$ and the mortar unknowns $\tilde{\phi}$ only:

$$
\tilde{u}^k = \begin{bmatrix}
\tilde{u}_b \\
\tilde{u}_i
\end{bmatrix} = \begin{bmatrix}
\tilde{Z} & 0 \\
0 & I
\end{bmatrix} \begin{bmatrix}
\tilde{\phi} \\
\tilde{u}_i
\end{bmatrix} = [Z^k] \tilde{u}^k,
$$

(3.2)

where $\tilde{u}^k$ represents the true unknowns, i.e. the projected mortar values and the internal unknowns.

This transformation converts the least-squares formulation at the element level, as given in (2.11), into

$$
L^T W L \tilde{u}^k = L^T W \tilde{f}^k \iff [Z^k]^T L^T W L [Z^k] \tilde{u}^k = [Z^k]^T L^T W \tilde{f}^k.
$$

(3.3)

Assembling all element contributions by summing over the projected element matrices gives the global system to be solved.

In this paper the solution on the mortar is defined by an $L^2$-projection of the element boundary solution

$$
\int_{I^k_l} (u_{\Omega} - \phi) \psi \, ds = 0 \quad \forall \text{sides } l \text{ and } k = 1, \ldots, K,
$$

(3.4)

where $\psi \in P_M(\tilde{T}^k_l)$ and $M$ is the polynomial degree of the mortar solution. $M$ should be greater or equal than the degree of the solution in the adjoining elements to prevent spurious mortar solutions. When the Lagrangian basis functions defined in Section 2 are employed, the vertex condition [10] is automatically satisfied. For a more extensive treatment of the MEM the reader is referred to [2,5,10].

4. The error estimator

Having discussed how to match spectral elements with different size and polynomial representation, we now have to find a way to detect those elements that need refinement.

In the least-squares formulation we select the solution which minimizes the residual globally over the whole domain $\Omega$. Having obtained such a minimizing solution we can evaluate the least-squares functional locally over every subdomain $A \subset \Omega$. This gives

$$
\eta^2_A = \|L^T u^h - f\|^2_{L^2(A)} = \|L^T (u^h - u_{\text{ex}})\|^2_{L^2(A)},
$$

(4.1)

due to the linearity of $L^T$. Well-posedness of problem (2.3) then implies that

$$
C_1 \|e\|^2_X(A) \leq \eta^2_A \leq C_2 \|e\|^2_X(A),
$$

(4.2)
where \( e = u_h - u_{\text{ex}} \). This means that the effectivity index \( \theta_{A,X} \), defined by

\[
\theta_{A,X} = \frac{\eta_A}{\|e\|_{X(A)}},
\]

which compares the estimated error \( \eta_A \) to the exact error in the \( X \)-norm is bounded by

\[
\sqrt{C_1} \leq \theta_A \leq \sqrt{C_2}.
\]

Alternatively, we may compare the estimated norm \( \eta_A \) with the residual norm \( \|R\|_{L^2(A)} \) using the fact that the residual norm is norm equivalent to \( \|e\|_X \). Denoting this effectivity index by \( \theta_{A,R} \) gives the rather trivial result

\[
\theta_{A,R} := \frac{\eta_A}{\|L^2 u_h - f\|_{Y(A)}} \equiv 1.
\]

Based on this observation \( \eta_A \) will be used to identify those regions (elements in case \( A = \Omega^k \)) which are selected for refinement. This estimator has also been used by Liu [9] and Berndt et al. [1].

5. Estimation of the Sobolev regularity

Having found a way to match functionally and geometrically non-conforming elements and an indicator \( \eta_{\text{ele}} \) which flags elements for refinement, we now have to determine how to refine. This choice is based on the smoothness of the underlying exact solution. If the exact solution is locally sufficiently smooth, polynomial enrichment is employed. However, if on the other hand, the underlying exact solution has limited smoothness \( h \)-refinement is used.

Let \( \kappa \) be a spectral element with size parameter \( h_\kappa \) and polynomial degree \( p_\kappa \). Let \( u_{\text{ex}}^\kappa \) be the exact solution in that element, where \( u_{\text{ex}}^\kappa \in H^{k_\kappa} \), where \( k_\kappa \geq 0 \) denotes the Sobolev regularity of the exact solution. Let \( u_h^{b_\kappa} \) denote the LSQSEM solution with \( u_h^{b_\kappa} \in H^q, 0 \leq q \leq k_\kappa \) then

\[
\|u_{\text{ex}}^\kappa - u_h^{b_\kappa}\|_{H^q} \leq C \left( \frac{(h_\kappa)^{s_k - q}}{(p_\kappa)^{s_k}} \right) \|u_{\text{ex}}^\kappa\|_{H^{k_\kappa}},
\]

where \( s_k = \min(p_\kappa + 1, k_\kappa) \) and \( C \) is a generic constant. This error estimate tells us that if the solution is very smooth \( (k_\kappa \text{ very large}) \) then the error decreases more rapidly by increasing \( p_\kappa \) in the denominator. For practical purposes the function is considered smooth if \( k_\kappa > p_\kappa + 1 \) and non-smooth when \( k_\kappa \leq p_\kappa + 1 \), in which \( h \)-refinement is more effective.

So the choice between \( h \)-refinement and \( p \)-enrichment is dictated by the Sobolev index of the exact solution. Although the exact solution is in general not available, we can still estimate this index from its numerical approximation. Houston et al. [6] have developed a method to estimate the Sobolev index from a truncated Legendre series. They assume that the one-dimensional solution is in \( L^2(-1, 1) \) which allows for a Legendre expansion

\[
u(x) = \sum_{i=0}^{\infty} a_i L_i(x) \quad \text{with} \quad a_i = \frac{2i + 1}{2} \int_{-1}^{1} u(x) L_i(x) \, dx.
\]

By Parseval’s identity the fact that \( u \in L^2(-1, 1) \) is equivalent to convergence of the series

\[
\sum_{i=0}^{\infty} |a_i|^2 \leq \frac{2}{2i + 1}.
\]

In [6] it is shown that if

\[
\sum_{i=k+1}^{\infty} |a_i|^2 \leq \frac{2}{2i + 1} \frac{\Gamma(i + k + 1)}{\Gamma(i - k + 1)}.
\]
converges, then \( u \in H^k_w([-1, 1]) \), where

\[
H^k_w = \left\{ u \in L^2([-1, 1]) \sum_{j=0}^{k} \int_{-1}^{1} |D^{(j)}u(x)|^2 (1 - x^2)^j \, dx < \infty \right\},
\] (5.5)

for integer values of \( k \). By using the \( \Gamma \)-function in (5.4) this identity can be extended to fractional Sobolev spaces, see [6] for details.

Given the Legendre coefficients \( a_i \), convergence of the series in (5.4) can be established by well-known techniques such as the ratio test, or the root test.

In this work the root test is employed. This leads to the calculation of

\[
l_k = \frac{\log((2k+1)/2|a_k|^2)}{2 \log k}.
\] (5.6)

If \( \lim_{k \to \infty} l_k > \frac{1}{2} \) then \( u \in H^{1/2-\varepsilon}([-1, 1]) \) \( \forall \varepsilon > 0 \). Else \( u \in L^2([-1, 1]) \). Since in a numerical solution only a finite number of Legendre coefficients \( a_i \) are available, this test is applied to the highest Legendre coefficient available in the numerical approximation. Based on the estimated Sobolev index \( l - \frac{1}{2} \), the decision is made whether to refine the mesh, or to increase the polynomial degree locally.

This one-dimensional estimate of the Sobolev index can be extended to multi-dimensional problems by treating each co-ordinate direction separately, see [6] for details. Several tests have been conducted to establish the validity of this estimator.

**Proposition 5.1.** If an element \( k \) at refinement level \( r \) with characteristic mesh size \( h^r_k \) and polynomial degree \( p^r_k \) is flagged for refinement by the error indicator, we calculate \( l_{p_k} \) by (5.6). Then for the Sobolev index \( k_{p_k} = l_{p_k} - \frac{1}{2} \) we have

\[
\begin{align*}
\text{If } k_{p_k} > p^r_k + 1 & \quad \text{then } p^{r+1}_k = p^r_k + 1, \\
\text{If } k_{p_k} \leq p^r_k + 1 & \quad \text{then } h^{r+1}_k = h^r_k/2.
\end{align*}
\] (5.7)

6. Application to the space–time linear advection equation

This section uses the one-dimensional, linear advection problem to validate the presented \( hp \)-adaptive theory. The application of LSQSEM to hyperbolic equations has been studied by De Maerschalck [11,13,12].

The model problem is defined as

\[
\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0 \quad \text{with } 0 \leq x \leq L, \quad t \geq 0, \quad a \in \mathbb{R},
\] (6.1)

\[
u(0, t) = 0,
\] (6.2)

\[
u(x, 0) = \begin{cases} 
\frac{1}{2} - \frac{1}{2} \cos \left( \frac{2\pi x - x_0}{L_0} \right) & \text{if } x_0 \leq x \leq x_0 + L_0, \\
0 & \text{if elsewhere},
\end{cases}
\] (6.3)

where \( a \) is the advection speed and \( L \) is the length of the domain in spatial direction. On the left boundary of the domain a Dirichlet boundary condition, \( u(0, t) = 0 \), is imposed. The initial disturbance, \( u(x, 0) \), is a cosine-hill with offset \( x_0 \) and width \( L_0 \). We use a space–time formulation that treats the one-dimensional advection problem with a two-dimensional least-squares formulation and considers the time variable \( t \) as second spatial variable. Instead of calculating the solution over the whole domain at once, we use a semi-implicit approach. The domain is subdivided into several space–time strips for which the solution is approximated using the LSQSEM, see [11] for details. In the following, 32 time strips are used within the domain \( \Omega = [0, 1] \), where each time strip has initially 32 cells. Each time strip uses the solution at the previous strip as initial condition, except for the first strip that uses the prescribed initial condition (6.3). All time strips use the Dirichlet condition (6.2) on the left boundary. The advection speed \( a = 0.85 \), \( x_0 = 0.13 \) and \( L_0 = x_0 + 0.5 \). The exact solution of this problem \( u_{ex} \in H^{5/2-\varepsilon}(\Omega) \), for all \( \varepsilon > 0 \). The regularity of the
The exact solution is limited in space–time along the lines $x - at = x_0$ and $x - at = x_0 + L_0$. For all other points in the space–time domain the solution is infinitely smooth.

### 6.1. Illustration of a hp-adaptive strategy

Note that even though only the second derivative is discontinuous, the regularity estimator accurately identifies the region with limited regularity as depicted in Fig. 2. No $h$-refinement is used in the smooth parts of the domain.

Fig. 3 shows the final polynomial degree distribution. We imposed the so-called one-level adaptivity, where the difference in refinement level between neighbouring elements may not be more than one. In the regions where the exact solution is zero neither $p$-enrichment nor $h$-refinement is used. Along the cosine-hill polynomials of degree $N = 4$ are used, the light grey strip. The only place where the algorithm uses higher order elements is along the lines with limited regularity. Along these lines both $p$-enrichment and $h$-refinement are employed.

The reason high order elements are used along these lines is that in order to predict the Sobolev regularity accurately enough, one needs sufficiently high Legendre coefficients. This is also illustrated by the convergence plots for one time strip, Figs. 4 and 5.

Note that no coarsening is applied in this example.

In both figures it can be seen that adaptive $p$- and adaptive $hp$-refinement is much more efficient than adaptive $h$-refinement, even for a relatively smooth problem as considered in this paper. Initially, in the refinement process only polynomial enrichment is employed which is illustrated by the fact that the curves for $p$- and $hp$-refinement coincide at low $NDOF$. Once the available Legendre coefficients are sufficiently high to identify the regions with limited regularity, $h$-refinement is applied locally. Figs. 4 and 5 show that once $h$-refinement is used $p$-refinement converges faster than $hp$-convergence. This behaviour is deceptive, because the $hp$-adaptive scheme could be improved by simultaneously lower the polynomial degree in those elements that are split.

Another way to improve the performance of the algorithm is to adapt only a certain percentage of the elements flagged for refinement. Elements with high errors generally pollute neighbouring elements and by adapting only the elements with the highest error, the error in the other elements decreases as well although these elements get no special treatment.

Both these techniques, adaptive coarsening and adapting only a certain percentage of elements flagged for refinement, are incorporated in the code.
Fig. 3. Polynomial degree distribution for $hp$-adaptivity with in each element.

Fig. 4. The $L^2$-error as function on the degrees of freedom, adaptive $h$-refinement (diamonds), adaptive $p$-refinement (circles) and adaptive $hp$-refinement (squares).

In this example refinement is applied to all elements flagged for refinement and no coarsening is applied. The results show that no elements are refined where nothing happens and refinement takes place in the interesting areas.

The example demonstrates that the current algorithm couples elements with different size and polynomial representation, identifies the correct regions where refinement is necessary and is also capable of identifying the regions where the local regularity is limited.
7. Conclusions

We have shown that the MEM is an elegant way to match functional and geometrical non-conforming neighbouring elements. Moreover, it appears that the solution propagates continuously across the element boundaries.

The error indicator marks correctly the elements which need refinement.

The Sobolev regularity estimator leads indeed to $h$-refinement where it is to be expected, near the foot of the cosine-hill, despite the fact that for the Sobolev regularity estimator only low order Legendre coefficients are available. Since LSQSEM does not require artificial diffusion to stabilize the numerical scheme, no smearing of the numerical solution takes place, which would increase the estimated Sobolev regularity.

No coarsening of the grid has been applied. Once the critical regions in the problem have been resolved, small elements may be merged if their estimated error is below a certain tolerance. Alternatively, the polynomial degree may be lowered if the estimated error is below a certain tolerance. The choice whether to merge elements or to decrease the polynomial degree can be based on the estimated Sobolev regularity.

References