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PRESERVING POSITIVITY OF SOLUTIONS TO THE DIFFUSION EQUATION FOR HIGHER-ORDER FINITE ELEMENTS IN UNDER RESOLVED REGIONS

T. A. Brunner

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PRESERVING POSITIVITY OF SOLUTIONS TO THE DIFFUSION EQUATION FOR HIGHER-ORDER FINITE ELEMENTS IN UNDER RESOLVED REGIONS

Thomas A. Brunner
Lawrence Livermore National Laboratory
7000 East Ave, Livermore, CA 94550
brunner6@llnl.gov

ABSTRACT

Higher order finite element methods hold a lot of promise for doing more useful work per memory accessed and stored, which might be advantageous on future computer architectures. But in problems where there are under-resolved features such as boundary layers, the higher order methods often produce non-physical solutions. Traditionally, for linear finite elements, the mass matrix is lumped to preserve positivity. But this technique fails to restore positivity for higher-order elements. We propose a different solution where the higher order zone is refined and a low-order method used to discretize the zone, all while keeping number of unknowns and their locations fixed so that they can be interpreted using both the low-order and high-order basis functions. This restores positivity in a simple test problem while preserving the convergence rate of the high-order method.

Key Words: Finite elements, positivity

1 INTRODUCTION

Higher order finite element methods hold a lot of promise for doing more useful work per memory accessed and stored, which might be advantageous on future computer architectures. But in problems where there are under-resolved features such as boundary layers, the higher order methods often produce non-physical solutions. This is implied by Godunovs theorem that states a method cannot be linear, higher-order, and non-oscillatory all at the same time. Traditionally, for linear finite elements, the mass matrix is lumped to preserve positivity [1, 2]. But this technique fails to restore positivity for higher-order elements [3].

1.1 A Diffusion Example

The application we are targeting is radiation diffusion. Here we are solving a simple steady-state diffusion problem, namely

$$-\nabla\cdot\frac{1}{3\sigma(\vec{x})}\nabla E+\sigma(\vec{x})E=S(\vec{x}) \tag{1}$$

where the source S, and the opacities σ_t and σ_a are functions of space. If we solve a simple one-zone problem using a third order method [4], where $\sigma = 10$ and $S = 0$ over the domain

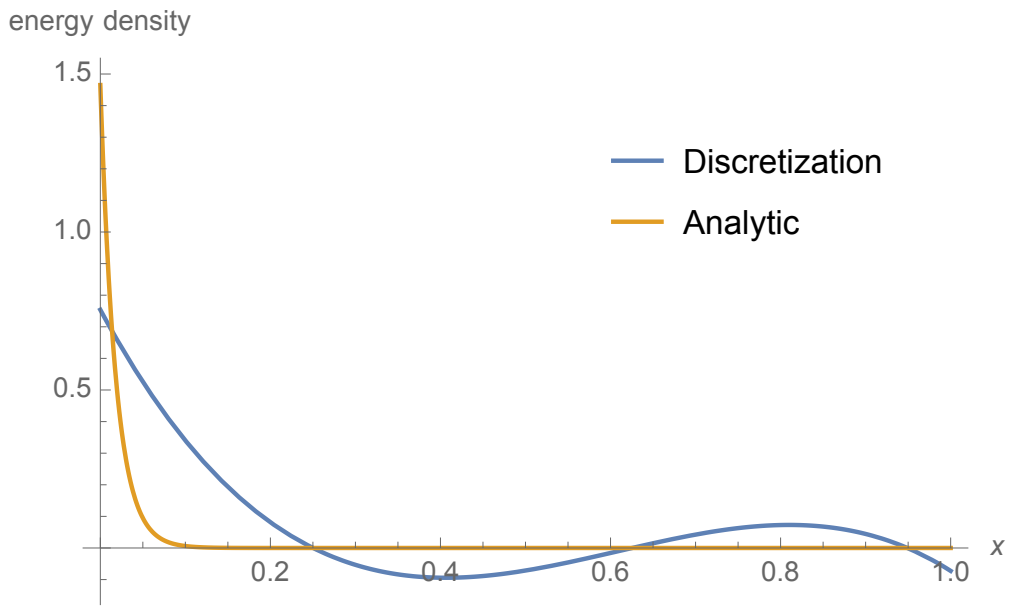


Figure 1. Exact solution and a one-zone, third order finite element solution showing the oscillations in the under-resolved problem

$0 < x < 1$, driven at $x = 0$ with a net incoming flux of 1 and a vacuum boundary at $x = 1$, we get the results in Fig. 1. The equation is dominated by the mass term (absorption), but the stiffness term (diffusion) still moves particles. Approximating the steep exponential analytic solution with a polynomial is oscillatory, since the Galerkin finite element method minimizes the error of the approximate solution. The higher order terms that are not in the solution space contain the all error in the solution.

1.2 What about mass matrix lumping?

Lumping the mass matrix for linear elements is the traditional route to solve these oscillations. But Maginot [3] showed this only works some of the time. Any basis set that spans a polynomial space gets the same, oscillatory solution.

This can be seen in Fig. 2 and Equations 2-4, where the basis function and mass matrices are

shown for a cubic basis set.

$$M_{\text{Lobatto}} \approx \begin{bmatrix} 0.71428 & 0.26620 & -0.26620 & 0.11905 \\ 0.26620 & 3.5714 & 0.59524 & -0.26620 \\ -0.26620 & 0.59524 & 3.5714 & 0.26620 \\ 0.11904762 & -0.26619857 & 0.26620 & 0.71428 \end{bmatrix} \xrightarrow{\text{lump}} \begin{bmatrix} 0.83333 & & & \\ & 4.1667 & & \\ & & 4.1667 & \\ & & & 0.83333 \end{bmatrix} \tag{2}$$

$$M_{\text{Gauss}} \approx \begin{bmatrix} 1.7393 & 0 & 0 & 0 \\ 0 & 3.2607 & 0 & 0 \\ 0 & 0 & 3.2607 & 0 \\ 0 & 0 & 0 & 1.7393 \end{bmatrix} \tag{3}$$

$$M_{\text{Bernstein}} \approx \begin{bmatrix} 1.4286 & 0.71429 & 0.28571 & 0.071429 \\ .71429 & 0.85714 & 0.64286 & 0.28571 \\ .28571 & 0.64286 & 0.85714 & 0.71429 \\ .071429 & 0.28571 & 0.71429 & 1.4286 \end{bmatrix} \xrightarrow{\text{lump}} \begin{bmatrix} 2.5 & & & \\ & 2.5 & & \\ & & 2.5 & \\ & & & 2.5 \end{bmatrix} \tag{4}$$

Lobatto basis functions are commonly used for continuous finite elements. The exact mass matrix is approximately diagonal*, and lumping does not change the discretization much, and the solution is still oscillatory. Gauss basis functions are commonly used for discontinuous finite elements, and form an orthogonal basis set. This means that the mass matrix is automatically lumped, and the "self-lumped" solution is exactly the same as the unmodified solution. Bernstein basis functions are strictly positive, and have a fairly uniform, dense mass matrix, as seen in Eq. 4. Lumping this mass matrix changes the discretization the most, and in this case recovers a positive solution. But there is no proof that this procedure will always be positive. Lumping changes the absorption term discretization in an uncontrolled way that depends on the choice of basis functions, while leaving the discretization of the diffusion term untouched. Now we will explore a procedure to modify the discretization in a controlled manner to recover positivity.

2 CHANGING THE DISCRETIZATION EXPLICITLY

We hope to ensure physical, non-oscillatory solutions by doing two solutions in a (barely) nonlinear process, with the goal of also recovering higher order convergence when we have smooth solutions. The main steps are:

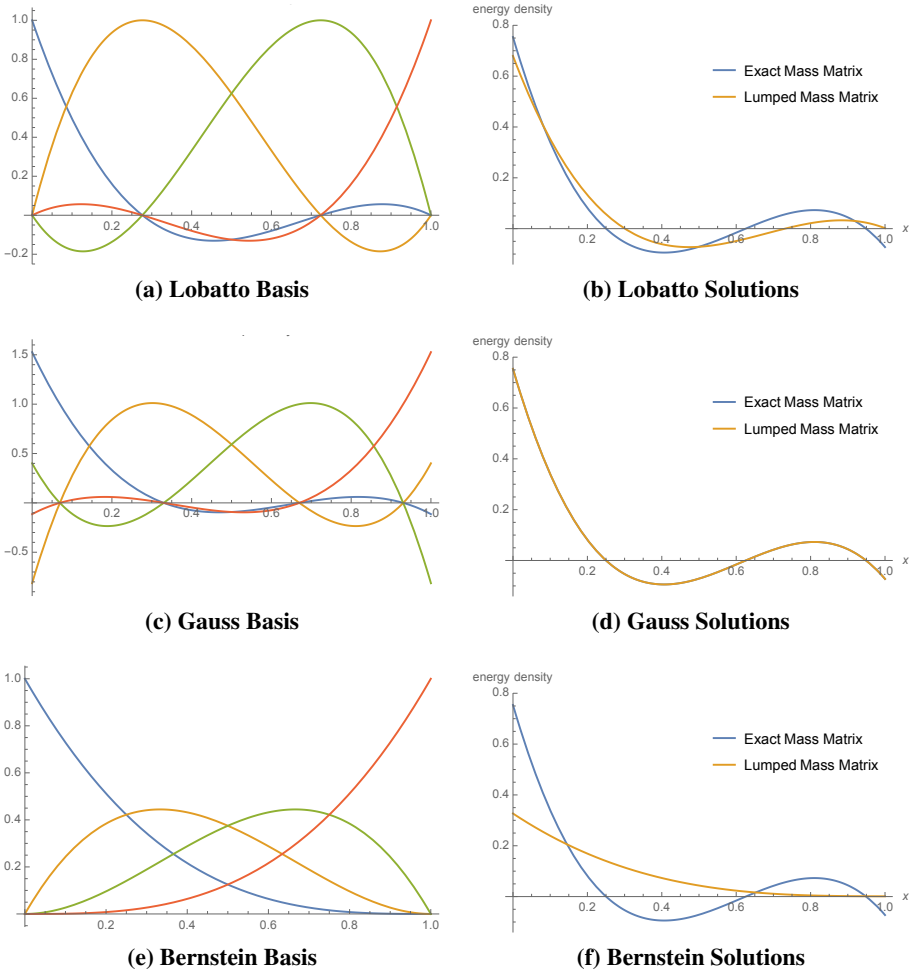
1. *Discretize the system using the standard Galerkin finite element method.* We can use arbitrary-order continuous finite elements to discretize the diffusion equation [4]. The mass matrix is not lumped.

2. *Solve the linear system for the high-order energy density, E^{HO}.*

3. *Detect where oscillations are likely in the solution.* This usually happens in regions where the gradient is extremely high. We compute a gradient length scale at each higher order node of the solution using

$$l_n = h_z \frac{|\nabla E_n^{HO}|_2}{E_n^{HO}}, \tag{5}$$

*In that the ratio of the diagonal to the diagonal of the lumped mass matrix is close to one. See Eq. 2



(a) Lobatto Basis **(b) Lobatto Solutions**

(c) Gauss Basis **(d) Gauss Solutions**

(e) Bernstein Basis **(f) Bernstein Solutions**

Figure 2. Three different sets of basis functions are on the left along with the exact finite element method solution and a lumped mass matrix solution for the sample one-zone problem.

where h_z is the size of the zone and E_n^{HO} is the solution of the full high-order solution at each node. We flag the zones for the low order method if

- the maximum length scale $l_n > \epsilon$, where typically $\epsilon = 2$, *and*
- the opacity length scale is large, namely $h_z\sigma_z > 1.5$, *or*
- the solution E_n^{HO} is negative within the zone.

4. *Re-solve the system with some zones selectively discretized using a low-order method.* We rebuild the matrix. For any unflagged zone, we use the standard high order finite element method. For flagged zones, we refine the mesh within the zone in such a way to maintain the same number of unknowns and their locations as the higher order basis.

   This can be viewed as replacing the p^{th}-order polynomial basis functions with p linear basis functions. In addition to using lower-order basis functions, we also lump the contribution to the mass matrix from the tagged zone.

   This method changes both the mass and the stiffness matrix for the low-order element. This is in contrast to pure mass matrix lumping, where only the mass matrix is modified.

   We call this solution E^{LO}.

5. **Re-interpret the low order solution using the higher order basis functions.** This solution can then be used in other parts of the algorithm without the need to "know" that a different method was used locally.

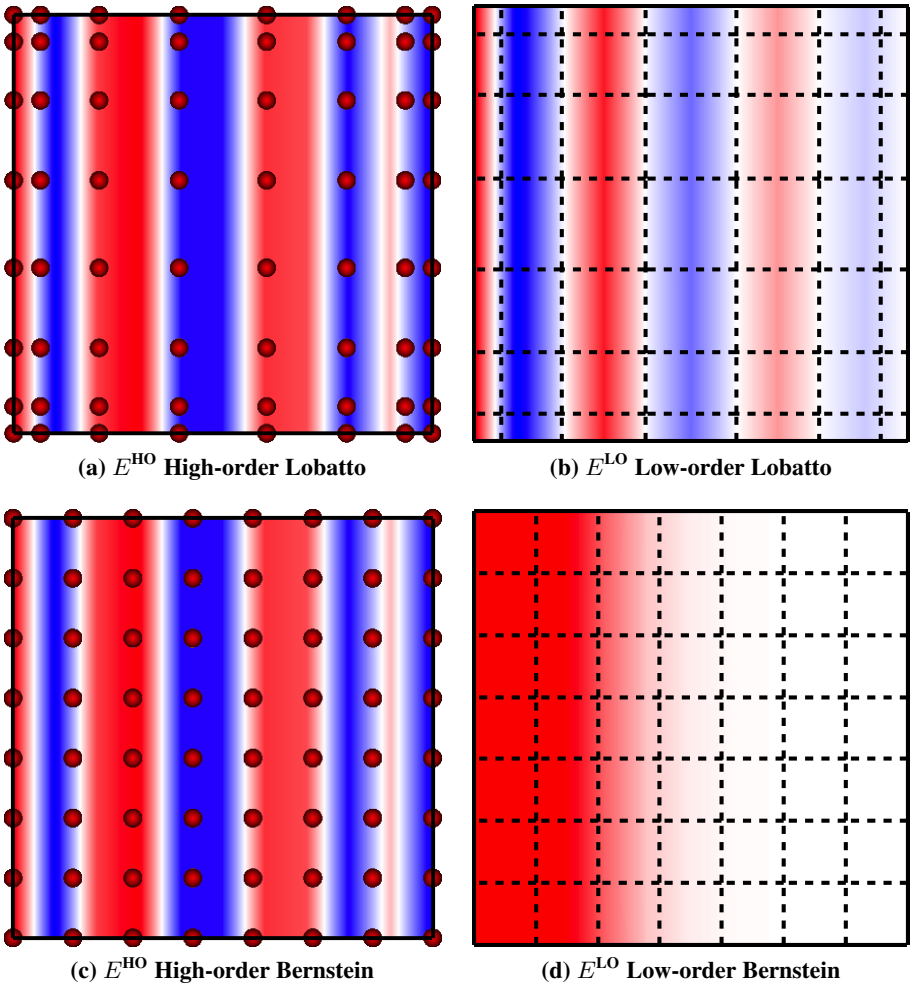
Using the one-zone problem from Section 1.1, the results of this procedure can be seen in Fig. 3. The circles on the left sub-figures represent the support points for the basis functions. These are replaced with "nodes" in virtual low-order refinement of the mesh on the left. Both Lobatto and Bernstein basis functions recover positive solutions at the support points in this case. But reinterpreting the low order solution with the higher order basis functions results in the reconstructed solution between the interpolation points to become negative. For the strictly positive Bernstein basis, the reconstruction is also positive within the zone.

It is important to note that this refinement and going to low-order polynomials changes both the mass and stiffness matrix, while normal mass matrix lumping only changes the mass matrix.

3 RESULTS

A simple two-material test problem was used to test this method. The left side has low absorption, a large diffusion coefficient, and a large source term. The right side has large absorption, small diffusion coefficient, and a small source term. The parameters are loosely based on a NIF laser hohlraum wall, where the thin left side is the vacuum, and the thick right is the hohlraum wall. Table I lists the numerical values used here for the problem[†].

[†]The origin of the source sizes are that the material temperature in the left, thin material is 100 eV=1 160 451.9 K and the right, thick temperature is 36 696.712 K, scaled so that $T_r^4 = 10^{-6} T_l^4$. The source term is found using $S = \sigma a T^4$, where $a = 4\sigma_{\text{SB}}/c$ is the black body constant, which is related to the Stephan-Boltzmann constant $\sigma_{\text{SB}} = 5.670\,373 \cdot 10^{-8}\ \text{W}^2\ \text{m}^{-1}\ \text{K}^{-4}$ and the speed of light $c = 299\,792\,458\ \text{m}\,\text{s}^{-1}$. The wall is $5 \cdot 10^{-5}$ m thick.



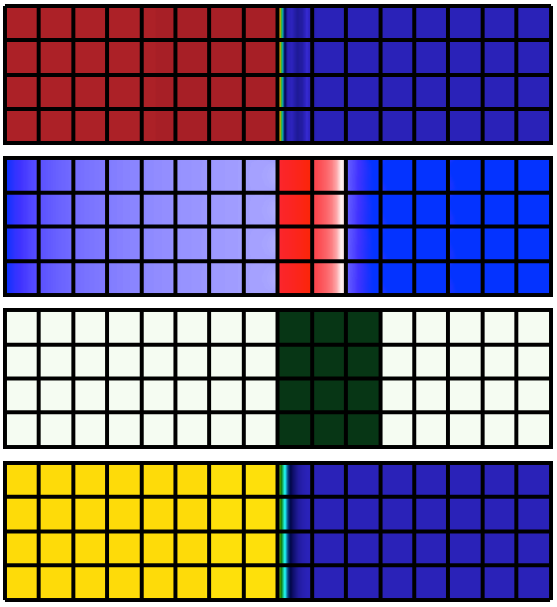
(a) E^{HO} **High-order Lobatto** **(b)** E^{LO} **Low-order Lobatto**

(c) E^{HO} **High-order Bernstein** **(d)** E^{LO} **Low-order Bernstein**

Figure 3. The sub-zonal reconstruction of the seventh order solution for the one zone problem using both the exact high order method and the low-order formulation reconstructed using the basis functions for both Lobatto and Bernstein basis sets. Red is positive, blue is negative, white is zero.

Table I. Material properties for the test problem, loosely based on a laser hohlraum.

Property	Left value	Right value
Absorption: σ	10^2	10^6
Source: S	1.372×10^{11}	1.372×10^9
x_{left}	0	
x_{middle}	5×10^{-5}	
x_{right}	1×10^{-4}	



Exact high-order method computed. We get oscillations at the material boundary.

Solution length scale l_n is computed using exact solution.

Zones identified with large length scale or negative solution.

Low order method used only in the green zones, coupled to exact high-order method in other zones. Final solution projected to higher order basis function is positive!

Figure 4. Sample problem with 16 zones across the thickness. The phases of the solution process are shown.

The different phases of the solution method are shown in Fig. 4. The low-order method is only used in some of the zones near the material boundary.

Figure 5 shows the convergence rates for various order finite elements of both the unmodified finite element method and the hybrid high-low order method. The low-order method maintains positivity at the expense of accuracy, but once the mesh is fine enough to resolve the analytic solution, it switches to the accuracy of the high-order method because no zones are tagged with a high gradient length scale.

4 CONCLUSIONS

High-order methods are known for their oscillatory behavior. This new two-step method maintains physical solutions in under-resolved regions while transitioning to the higher order convergence once the solution is resolved. The combination of two ideas was key to allowing this. First, we used a low-order method to recover positive degrees of freedom. Second, we needed to use a strictly positive set of basis functions (the Bernstein basis) to ensure the interpolated solution is also positive

5 ACKNOWLEDGMENTS

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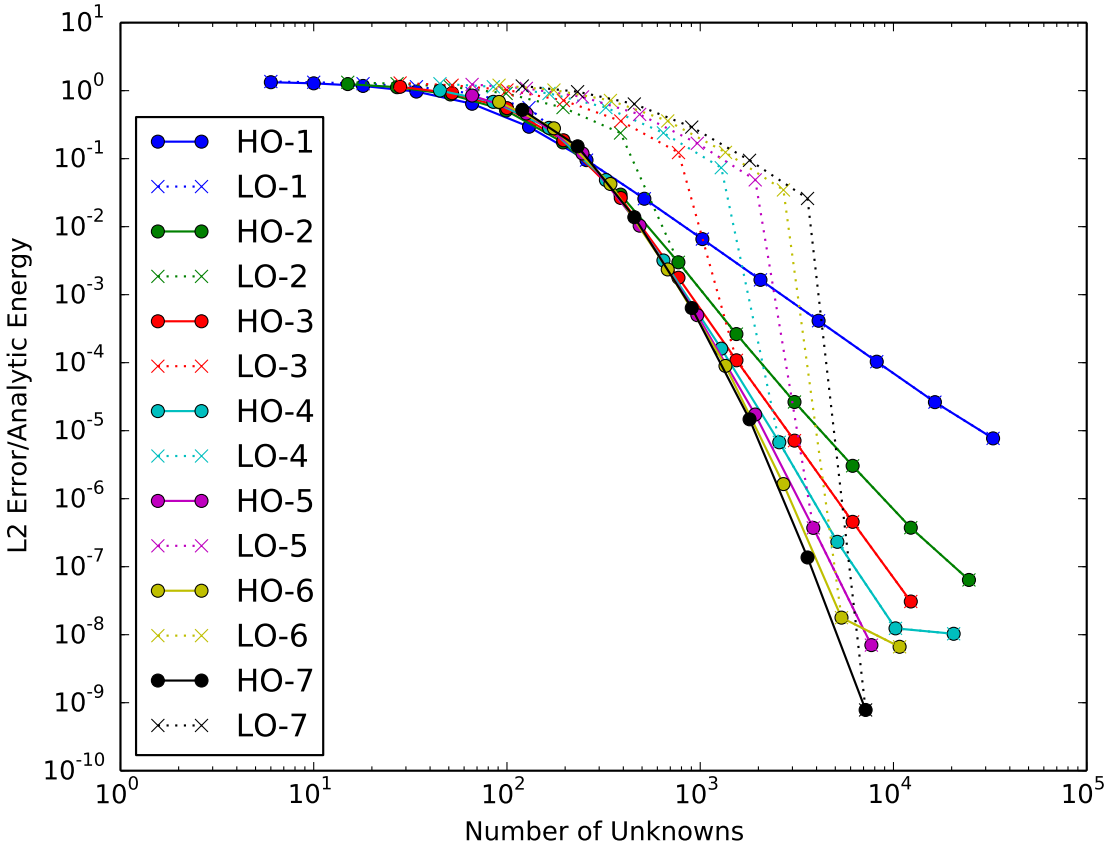

Figure 5. Convergence as a function of the number of unknowns in the system. Solid lines are for the unmodified high-order finite element method. The dotted lines are for the second, partially-low order method. Note that the low-order method eventually snaps to the high-order solution once the jump is resolved.

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