Optimally Blended Finite/Spectral Element Scheme for Wave Propagation

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Outline

- (Very) Quick Overview of Spectral Element Method
- Typical Practical Application
- Analysis and Properties
- Optimal Blending
Model Problem

Seek $u : (-1, 1) \times (0, T) \mapsto \mathbb{C}$:

$$u_{tt} - u_{xx} = f(x, t) \text{ in } (-1, 1) \times (0, T),$$

subject to $u(x, 0) = u_t(x, 0) = 0$, $x \in (-1, 1)$ and

$$u(-1, t) = g(t), \quad u_x(1, t) + u_t(1, t) = 0 \text{ for } t \in (0, T)$$
Variational Formulation

Seek $u \in H^1(-1, 1) : u(-1, t) = g(t)$

\[
\frac{d^2}{dt^2} (u, v) + \frac{d}{dt} u\bar{v}|_{x=1} + (u_x, v_x) = (f, v),
\]

for all $v \in H^1(-1, 1) : v(-1) = 0$, where $(u, v) = \int_{-1}^{1} u\bar{v} \, dx$. 
Variational Formulation

Seek \( u \in H^1(-1, 1) : u(-1, t) = g(t) \)

\[
\frac{d^2}{dt^2} (u,v) + \frac{d}{dt} u\bar{v}\bigg|_{x=1} + (u_x, v_x) = (f, v),
\]

for all \( v \in H^1(-1, 1) : v(-1) = 0 \), where \( (u,v) = \int_{-1}^{1} u\bar{v} \, dx \).

Discretise by introducing a finite dimensional subspace \( X \subset H^1(-1, 1) \).
Semi-Discretisation in Space

Seek $U \in X : U(-1, t) = g(t)$

$$\frac{d^2}{dt^2}(U, v) + \frac{d}{dt} U v|_{x=1} + (U_x, v_x) = (f, v),$$

for all $v \in X : v(-1) = 0$. 

Modern Techniques for Numerical Solution of PDEs, ACMAC, Crete, September 2011 – p. 5/54
Semi-Discretisation in Space

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$$\frac{d^2}{dt^2} (U, v) + \frac{d}{dt} U v \bigg|_{x=1} + (U_x, v_x) = (f, v),$$

for all $v \in X : v(-1) = 0.$

Introduce basis $\{\phi_i\}_{i=0}^N$ for $X$, and write

$$U(x, t) = \sum_{i=0}^{N} \alpha_i(t) \phi_i(x).$$
Semi-Discrete Scheme

Find \( \{ \alpha_i \}_{i=0}^N \) such that

\[
\sum_{i=0}^N \left( (\phi_i, \phi_j) \frac{d^2 \alpha_i}{dt^2} + \phi_i(1)\phi_j(1) \frac{d \alpha_i}{dt} + (\phi_{i,x}, \phi_{j,x}) \alpha_i \right) = (f, \phi_j)
\]

for \( j = 1, \ldots, N \), with

\[
\alpha_i(0) = \frac{d \alpha_i}{dt}(0) = 0
\]

with \( \alpha_0(t) = g(t), t \in (0, T) \).
Find $\vec{\alpha}$ such that

$$M \frac{d^2 \vec{\alpha}}{dt^2} + C \frac{d\vec{\alpha}}{dt} + K \vec{\alpha} = \vec{r}$$

with

$$\vec{\alpha}(0) = \frac{d\vec{\alpha}}{dt}(0) = \vec{0}$$
Semi-Discrete Scheme

Find $\vec{\alpha}$ such that

$$M \frac{d^2 \vec{\alpha}}{dt^2} + C \frac{d\vec{\alpha}}{dt} + K \vec{\alpha} = \vec{r}$$

with

$$\vec{\alpha}(0) = \frac{d\vec{\alpha}}{dt}(0) = \vec{0}$$

and

$$M_{ij} = \int_{-1}^{1} \phi_i(x) \phi_j(x) \, dx \quad \text{‘Mass Matrix’}$$

$$K_{ij} = \int_{-1}^{1} \phi'_i(x) \phi'_j(x) \, dx \quad \text{‘Stiffness’}$$
Fully Discrete Scheme

Simple leapfrog scheme in time

\[
\frac{1}{(\Delta t)^2} M \left( \ddot{\alpha}^{n+1} - 2\ddot{\alpha}^n + \ddot{\alpha}^{n-1} \right) + \frac{1}{\Delta t} C \left( \dot{\alpha}^n - \dot{\alpha}^{n-1} \right) + K \ddot{\alpha}^n = \ddot{f}^n
\]

where \( \ddot{\alpha}^0 = \ddot{\alpha}^1 = \ddot{0} \), and

\[
M_{ij} = \int_{-1}^{1} \phi_i(x) \phi_j(x) \, dx \quad \text{Mass}
\]

\[
K_{ij} = \int_{-1}^{1} \phi_i'(x) \phi_j'(x) \, dx \quad \text{Stiffness}
\]
**Fully Discrete Scheme**

Simple leapfrog scheme in time

\[
\frac{1}{(\Delta t)^2} M \left( \bar{\alpha}^{n+1} - 2\bar{\alpha}^{n} + \bar{\alpha}^{n-1} \right) + \frac{1}{\Delta t} C \left( \bar{\alpha}^{n} - \bar{\alpha}^{n-1} \right) + K \bar{\alpha}^{n} = \bar{r}^{n}
\]

where \( \bar{\alpha}^{0} = \bar{\alpha}^{1} = \bar{0} \), and

\[
M_{ij} = \int_{-1}^{1} \phi_{i}(x)\phi_{j}(x) \, dx \quad \text{Mass}
\]

\[
K_{ij} = \int_{-1}^{1} \phi'_{i}(x)\phi'_{j}(x) \, dx \quad \text{Stiffness}
\]

... requires inversion of mass matrix \( M \) at each time step.
Spectral Element Method: General Idea

Spectral element spatial discretisation gives

\[
\frac{1}{(\Delta t)^2} \tilde{M} \left( \bar{\alpha}^{n+1} - 2\bar{\alpha}^n + \bar{\alpha}^{n-1} \right) + \frac{1}{\Delta t} \tilde{C} \left( \bar{\alpha}^n - \bar{\alpha}^{n-1} \right) + \tilde{K} \bar{\alpha}^n = \bar{r}^n
\]

where \( \bar{\alpha}^0 = \bar{\alpha}^1 = 0 \), and

\[
\tilde{M}_{ij} \approx \int_{-1}^{1} \phi_i(x)\phi_j(x) \, dx \quad \text{Mass}
\]
\[
\tilde{K}_{ij} \approx \int_{-1}^{1} \phi_i'(x)\phi_j'(x) \, dx \quad \text{Stiffness}
\]
Spectral Element Method: General Idea

Spectral element spatial discretisation gives

\[
\frac{1}{(\Delta t)^2} \widetilde{M} \left( \ddot{\alpha}^{n+1} - 2\dot{\alpha}^n + \alpha^{n-1} \right) + \frac{1}{\Delta t} C \left( \dot{\alpha}^n - \dot{\alpha}^{n-1} \right) + \widetilde{K} \alpha^n = \vec{r}^n
\]

where \( \ddot{\alpha}^0 = \dot{\alpha}^1 = 0 \), and

\[
\widetilde{M}_{ij} \approx \int_{-1}^{1} \phi_i(x)\phi_j(x) \, dx \quad \text{Mass}
\]

\[
\widetilde{K}_{ij} \approx \int_{-1}^{1} \phi'_i(x)\phi'_j(x) \, dx \quad \text{Stiffness}
\]

Spectral element method characterised by particular combinations of

- quadrature rule for integrals
- nature and form of basis functions.
**Spectral Element Method: Quadrature Rule**

Gauss-Lobatto quadrature rule:

\[
\int_{-1}^{1} f(\zeta) \, d\zeta \approx Q_p(f) = \sum_{\ell=2}^{p} w_\ell f(\zeta_\ell) + \frac{2}{p(p+1)} [f(-1) + f(1)],
\]

where

- **Nodes:** \( \{\zeta_\ell\}_{\ell=2}^{p} \) zeros of \( L'_p \)
- **Weights:** \( w_\ell = \frac{2}{p(p-1)}[L_{p-1}(\zeta_\ell)]^2 > 0 \)

with \( L_p \) Legendre polynomial of degree \( p \). Rule exact for \( f \in \mathbb{P}_{2p-1} \).
Lagrange basis functions $\{\phi_\ell\}_{\ell=1}^{p+1}$:

$$\phi_\ell \in \mathbb{P}_p : \phi_\ell(\zeta_m) = \begin{cases} 
1, & \ell = m \\
0, & \ell \neq m 
\end{cases}$$
Lagrange basis functions $\{\phi_\ell\}_{\ell=1}^{p+1}$:

**Quadratic GL–Shape Functions**
Lagrange basis functions $\{\phi_\ell\}_{\ell=1}^{p+1}$:

Cubic GL–Shape Functions
Lagrange basis functions $\{\phi_\ell\}_{\ell=1}^{p+1}$:

Order six GL–Shape Functions
... so what’s the big deal?

Stiffness matrix $\tilde{K}$:

$$\tilde{K}_{\ell m} = Q_p(\phi'_{\ell} \phi'_{m}),$$

recall $\phi'_{\ell} \in \mathbb{P}_{p-1}$ and quadrature rule exact for $\mathbb{P}_{2p-1}$, so

$$\tilde{K}_{\ell m} = (\phi'_{\ell}, \phi'_{m}) = K_{\ell m}$$

Hence, stiffness matrix unchanged.
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Hence, stiffness matrix unchanged.

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... so what’s the big deal?

Mass matrix $\tilde{M}$:

$$\tilde{M}_{\ell m} = Q_p(\phi_\ell \phi_m) = \sum_{k=1}^{p+1} w_k \phi_\ell(\zeta_k) \phi_m(\zeta_k).$$

(recall $\phi_\ell(\zeta_k) = \delta_{\ell k}$)

$$\tilde{M}_{\ell m} = \sum_{k=1}^{p+1} w_k \delta_{\ell k} \delta_{m k} = w_\ell \delta_{\ell m}.$$
... so what’s the big deal?

Mass matrix $\tilde{M}$ is diagonal

$$
\tilde{M} = \begin{bmatrix}
    w_1 & 0 & 0 & \cdots & 0 \\
    0 & w_2 & 0 & \cdots & 0 \\
    0 & 0 & w_3 & \cdots & 0 \\
    \vdots & \vdots & \vdots & \ddots & 0 \\
    0 & 0 & 0 & 0 & w_{p+1}
\end{bmatrix}
$$

... finite elements with ‘Gauss-point mass lumping’

Spectral Element Method

Spectral Element/Gauss-point Mass Lumped Finite Element Scheme

\[
\frac{1}{(\Delta t)^2} \tilde{M} \left( \tilde{\alpha}^{n+1} - 2\tilde{\alpha}^n + \tilde{\alpha}^{n-1} \right) + \frac{1}{\Delta t} C \left( \tilde{\alpha}^n - \tilde{\alpha}^{n-1} \right) + \tilde{K} \tilde{\alpha}^n = \tilde{r}^n
\]

where \( \tilde{\alpha}^0 = \tilde{\alpha}^1 = \tilde{0} \), with

\[
\tilde{M} = \text{Diag}(w_1, \ldots, w_{p+1})
\]
Spectral Element Method

Spectral Element/Gauss-point Mass Lumped Finite Element Scheme

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\frac{1}{(\Delta t)^2} \tilde{M} \left( \tilde{\alpha}^{n+1} - 2\tilde{\alpha}^n + \tilde{\alpha}^{n-1} \right) + \frac{1}{\Delta t} C \left( \tilde{\alpha}^n - \tilde{\alpha}^{n-1} \right) + \tilde{K} \tilde{\alpha}^n = \tilde{r}^n
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Same structure and approach applicable to

- multiple spatial dimensions
- acoustics, electromagnetics, structures, ...
Spectral Element Method

Spectral Element/Gauss-point Mass Lumped Finite Element Scheme

\[
\frac{1}{(\Delta t)^2} \tilde{M} (\tilde{\alpha}^{n+1} - 2\tilde{\alpha}^n + \tilde{\alpha}^{n-1}) + \frac{1}{\Delta t} C (\tilde{\alpha}^n - \tilde{\alpha}^{n-1}) + \tilde{K} \tilde{\alpha}^n = \tilde{r}^n
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Same structure and approach applicable to

- multiple spatial dimensions
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Advantages:

- retains geometric flexibility of finite elements
- obtain extremely efficient time-stepping.
Simulations of Ground Motion in the Los Angeles Basin Based upon the Spectral-Element Method

by Dimitri Komatitsch, Qinya Liu, Jeroen Tromp, Peter Süss,* Christiane Stidham, and John H. Shaw
Application: Seismic Simulation


Surface topography of Southern California viewed from Southeast.
Simulations of Ground Motion in the Los Angeles Basin Based upon the Spectral-Element Method

by Dimitri Komatitsch, Qinya Liu, Jeroen Tromp, Peter Süß,* Christiane Stidham, and John H. Shaw

• Hollywood (Full)
• Hollywood (Zoom)
Seismic Simulation: Computational Details

- average distance between grid points at the surface roughly 335m
- mesh contains 672,768 elements
- time step size of 9 msec and 20,000 timesteps in total.
- polynomial degree $p = 4$
- each element contains $3(p + 1)^3 = 375$ degrees of freedom
- 136 million degrees of freedom in total
- 144 processor Beowulf PC cluster using MPI
- 6.5 hours needed to compute seismograms with a duration of 3 min
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... state of the art back in 2004. Same technology SPECFEM3D being used for global seismic simulation—see cover of *Science*, May 2005.
Seismic Simulation: Cross-Section of Portion of Mesh

Note: Highly structured *translation invariant* mesh in bulk of the domain.
Basic Issues in Computational Wave Propagation

A numerical scheme should, as far as possible:

- propagate waves at correct speed i.e. control numerical dispersion;
- preserve conserved quantities (energy, momentum, ...) i.e. control numerical dissipation;
Basic Issues in Computational Wave Propagation

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- preserve conserved quantities (energy, momentum, ...) i.e. control numerical dissipation;

... but there is no silver bullet.
Basic Issues in Computational Wave Propagation

A numerical scheme should, as far as possible:

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- preserve conserved quantities (energy, momentum, ...) i.e. control numerical dissipation;

Every scheme needs at least two degrees of freedom per wavelength just to resolve the wave, unless we know something about structure of the solution and take it into account.
A numerical scheme should, as far as possible:

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Every scheme needs at least two degrees of freedom per wavelength just to resolve the wave, unless we know something about structure of the solution and take it into account.

Fairly poor understanding of properties and behaviour of high order spectral element schemes for approximation of waves

- how high should the order be?
- how much numerical dispersion? ... numerical dissipation?
- how does behaviour compare with (consistent) finite element scheme?
- how compare to the ‘two degrees of freedom per wavelength’?
Numerical Observations

Consider the model problem with time-harmonic excitation:

\[ u_{tt} - u_{xx} = 0 \]

subject to

\[ u(-1, t) = \exp(i\omega t), \quad u_x(1, t) + u_t(1, t) = 0, \quad t \in (0, T). \]

Solution has form \( u(x, t) = U(x) \exp(-i\omega t) \) where \( U \) satisfies \( U(-1) = 1, \)
\( U'(1) - i\omega U(1) = 0 \) and

\[ -U''(x) - \omega^2 U(x) = 0, \quad x \in (-1, 1). \]

True solution \( U(x) = \exp(i\omega(x + 1)). \)
Finite element method (exact quadrature) on uniform mesh of size $h$:

$$(K - \kappa^2 M + i\kappa C) \vec{U} = \vec{r}$$

where $\kappa = \omega h/2$, $C = \vec{e}_N^t \vec{e}_N$, 

$$K = \frac{1}{h} \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & -1 \end{bmatrix} ; \quad M = \frac{h}{6} \begin{bmatrix} 2 & 1 & 0 & \cdots & 0 \\ 1 & 4 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix}.$$ 

Easy to invert $M$ of course, but becomes more problematic on unstructured grids in higher dimensions.
**Piecewise Linear Approximation**

Spectral element method (GLL quadrature) on uniform mesh of size $h$:

\[
\left( \tilde{K} - \kappa^2 \tilde{M} - i\kappa C \right) \vec{U} = \vec{r}
\]

where $\kappa = kh/2$, $C = \vec{e}_N \vec{e}_N^t$,

\[
\tilde{K} = \frac{1}{h} \begin{bmatrix}
1 & -1 & 0 & \cdots & 0 \\
-1 & 2 & -1 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & -1 \\
0 & 0 & 0 & -1 & 1
\end{bmatrix} ; \quad \tilde{M} = \frac{h}{2} \begin{bmatrix}
1 & 0 & 0 & \cdots & 0 \\
0 & 2 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & 0 \\
0 & 0 & 0 & 0 & 1
\end{bmatrix}.
\]

Mass matrix $\tilde{M}$ diagonal.
Piecewise Linear Approximation

Numerical real wave obtained using the spectral element scheme
Numerical real wave obtained using the finite element scheme
Numerical real wave obtained using the optimal scheme
Exact real wave
Piecewise Linear Approximation

- Finite elements exhibit phase \textit{lead}. Spectral elements phase \textit{lag}.
- Magnitude is \textit{same} for both schemes.
Piecewise Quadratic Approximation
Piecewise Quadratic Approximation

- Finite elements exhibit phase lead. Spectral elements phase lag.
- Magnitude is smaller for spectral elements.
Piecewise Cubic Approximation

Numerical real wave obtained using the spectral element scheme
Numerical real wave obtained using the finite element scheme
Numerical real wave obtained using the optimal scheme
Exact real wave
Piecewise Cubic Approximation

- Finite elements exhibit phase lead. Spectral elements phase lag.
- Magnitude is even smaller for spectral elements.
How to measure this behaviour?

Dispersion relation for wave equation

\[ u_{tt} - u_{xx} = 0 \]

obtained by seeking non-trivial solution of form \( u(x, t) = U(x) e^{-i \omega t} \), where \( U \) has Bloch wave property

\[ U(x + h) = e^{ikh} U(x). \]

Gives \( k = \pm \omega \).
How to measure this behaviour?

Dispersion relation for wave equation

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\[ U(x + h) = e^{ikh} U(x). \]

Gives \( k = \pm \omega \).

Seek non-trivial discrete Bloch wave \( u_h(x, t) = U_h(x) e^{-i\omega t} \) such that

\[ U_h(x + h) = e^{i\tilde{k}h} U_h(x) \]

with \( \tilde{k} \) to be determined.
How to measure this behaviour?

Dispersion relation for wave equation

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Seek non-trivial discrete Bloch wave \( u_h(x, t) = U_h(x)e^{-i\omega t} \) such that

\[ U_h(x + h) = e^{i\tilde{k}h}U_h(x) \]

with \( \tilde{k} \) to be determined.

\[ \tilde{k} - k \] measures phase error
Example: First Order SEM

Spectral elements ($p = 1$):

\[
\frac{1}{h} \left( U_{j-1} + 2U_j - U_{j+1} \right) - \omega^2 h U_j = 0
\]
Example: First Order SEM

Spectral elements ($p = 1$):

\[
\frac{1}{h} \left( U_{j-1} + 2U_j - U_{j+1} \right) - \omega^2 h U_j = 0
\]

Seek non-trivial discrete $U$ of form $U_j = Ce^{i\tilde{k}jh}$, such that

\[
\frac{1}{h} \left( e^{-i\tilde{k}h} - 2 + e^{i\tilde{k}h} \right) - \omega^2 h = 0.
\]

Hence,

\[
\cos \tilde{k}h = 1 - \frac{\Omega^2}{2}, \quad \Omega = \omega h
\]
Example: First Order SEM

Spectral elements \((p = 1)\):

\[
\frac{1}{h} \left( U_{j-1} + 2U_j - U_{j+1} \right) - \omega^2 h U_j = 0
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Seek non-trivial discrete \(U\) of form \(U_j = Ce^{i\tilde{k} j h}\), such that

\[
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\]

Hence,

\[
\cos \tilde{k} h = 1 - \frac{\Omega^2}{2}, \quad \Omega = \omega h
\]

For \(\Omega \ll 1\), obtain

\[
\tilde{k} h - \omega h = \frac{\Omega^3}{24} + \mathcal{O}(\Omega)^5.
\]
**Discrete Dispersion Relation** \((\Omega = \omega h)\)

**Spectral Element Scheme**

<table>
<thead>
<tr>
<th>Order (p)</th>
<th>(R_p(\Omega))</th>
<th>(\cos^{-1} R_p(\Omega) - \Omega)</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>(1 - \frac{\Omega^2}{2})</td>
<td>(\frac{\Omega^3}{24})</td>
</tr>
<tr>
<td>2</td>
<td>(\frac{\Omega^4 - 22\Omega^2 + 48}{2(\Omega^2 + 24)})</td>
<td>(\frac{\Omega^5}{2880})</td>
</tr>
<tr>
<td>3</td>
<td>(\frac{-\Omega^6 + 92\Omega^4 - 1680\Omega^2 + 3600}{2(\Omega^4 + 60\Omega^2 + 1800)})</td>
<td>(\frac{\Omega^7}{604800})</td>
</tr>
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<td>:</td>
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**Discrete Dispersion Relation** \((\Omega = \omega h)\)

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**Finite Element Scheme** *(Ainsworth, SINUM 2004)*

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<td>(-\frac{2\Omega^2+6}{\Omega^2+6})</td>
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<tr>
<td>2</td>
<td>(\frac{3\Omega^4-104\Omega^2+240}{\Omega^4+16\Omega^2+240})</td>
<td>(-\frac{\Omega^5}{1440})</td>
</tr>
<tr>
<td>3</td>
<td>(-\frac{4\Omega^6+540\Omega^4-11520\Omega^2+25200}{\Omega^6+30\Omega^4+1080\Omega^2+25200})</td>
<td>(-\frac{\Omega^7}{201600})</td>
</tr>
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<td>...</td>
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</tr>
</tbody>
</table>
General Form of Dispersion Relation for Finite Elements

Discrete dispersion relation for order $p$ elements:

$$\cos(kh) = R_p(h\omega)$$

where $R_p$ is the rational function

$$R_p(2\kappa) = \frac{\left[2N_o/2N_o - 2\right]_\kappa \cot \kappa - \left[2N_e + 2/2N_e\right]_\kappa \tan \kappa}{\left[2N_o/2N_o - 2\right]_\kappa \cot \kappa + \left[2N_e + 2/2N_e\right]_\kappa \tan \kappa}.$$ 

and $N_e = \lfloor p/2 \rfloor$ and $N_o = \lfloor (p + 1)/2 \rfloor$.

- Simple form in terms of Padé approximants ...

(Ainsworth, SINUM 2004)
General Form of Dispersion Relation Spectral Elements

Define sequences \( \{a_p\}_{p=0}^{\infty} \) and \( \{b_p\}_{p=0}^{\infty} \) recursively by the rule

\[
a_{p+1} = -\frac{2p+1}{\kappa} b_p + a_{p-1},
\]

\[
b_{p+1} = \frac{2p+1}{\kappa} a_p + b_{p-1},
\]

for \( p \in \mathbb{N} \) with \( a_0 = 1, a_1 = 1, b_0 = 0 \) and \( b_1 = 1/\kappa \). Then, the discrete dispersion relation for spectral element method is given by

\[
R_p(2\kappa) = \cos(kh) = (-1)^p \left[ \frac{a_p (\kappa b_{p-1} + p a_p) + b_p (\kappa a_{p-1} - p b_p)}{a_p (\kappa b_{p-1} + p a_p) - b_p (\kappa a_{p-1} - p b_p)} \right].
\]

(Ainsworth and Wajid, SINUM 2008)

Not related to Padé approximants! (c.f. finite element case)
Phase Error for $\omega h \ll 1$

Phase error for finite element method satisfies

$$kh - \omega h = -\frac{1}{2} \left( \frac{p!}{(2p)!} \right)^2 \frac{(\omega h)^{2p+1}}{2p + 1} + O(\omega h^{2p+3})$$

(Ainsworth, SINUM 2004)
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(Ainsworth and Wajid, SINUM 2008)

- Finite elements exhibit phase lead and spectral elements exhibit phase lag.
- Spectral elements a factor $1/p$ times more accurate than finite elements.
Numerical Dispersion for Large Order and Large Wavenumber

Case: $\omega h = 80$, $\omega h \gg 1$

Note: Very sharp transition between garbage and essentially exact
Numerical Dispersion for Large Order and Large Wavenumber

Suppose that $\omega h \gg 1$. Then the error $E^p = \cos kh - \cos \omega h$ in the discrete dispersion relation passes through distinct phases as the order $p \in \mathbb{N}$ is increased:

- **Unstable Phase:** For $p = \mathcal{O}(1)$, $E^p \approx (-1)^p \frac{(\omega h)^2}{2}$.

- **Oscillatory Phase:** For $1 \ll 2p + 1 < \omega h - o(\omega h)^{1/3}$, $E^p$ oscillates and decays to $\mathcal{O}(1)$ as $p$ is increased.

- **Transition Zone:** For $\omega h - o(\omega h)^{1/3} < 2p + 1 < \omega h + o(\omega h)^{1/3}$, the error $E^p$ oscillates without further decrease.

- **Super-Exponential Decay:** For $2p + 1 > \omega h + o(\omega h)^{1/3}$, $E^p$ decreases at a super-exponential rate.

(Ainsworth and Wajid, SINUM 2008)
One Consequence of the Analysis

What is significance of condition $2p + 1 \approx \omega h$ which appears in analysis?
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$$\pi \text{ modes per wavelength are required to resolve wave.}$$

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Ref: Ainsworth and Wajid, SINUM 2008
Blended Finite Element/Spectral Element Schemes
Blended FEM/SEM Schemes

Idea: Can we obtain better scheme by averaging (blending) finite elements and spectral elements?
Blended FEM/SEM Schemes

Finite Element Scheme:

\[ \frac{1}{(\Delta t)^2} M (\bar{\alpha}^{n+1} - 2\bar{\alpha}^n + \bar{\alpha}^{n-1}) + \frac{1}{\Delta t} C (\bar{\alpha}^n - \bar{\alpha}^{n-1}) + K \bar{\alpha}^n = \bar{r}^n \]
Blended FEM/SEM Schemes

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Spectral Element Scheme:

$$\frac{1}{(\Delta t)^2} \tilde{M} \left( \bar{\alpha}^{n+1} - 2\bar{\alpha}^n + \bar{\alpha}^{n-1} \right) + \frac{1}{\Delta t} C \left( \bar{\alpha}^n - \bar{\alpha}^{n-1} \right) + K \bar{\alpha}^n = \bar{r}^n$$
**Blended FEM/SEM Schemes**

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\]

Blended FEM/SEM Scheme:

\[
\frac{1}{(\Delta t)^2} M_{\tau} (\vec{\alpha}^{n+1} - 2\vec{\alpha}^{n} + \vec{\alpha}^{n-1}) + \frac{1}{\Delta t} C (\vec{\alpha}^{n} - \vec{\alpha}^{n-1}) + K \vec{\alpha}^{n} = \vec{r}^{n}
\]

where, for \( \tau \in [0, 1] \) (to be determined)

\[
M_{\tau} = (1 - \tau) M + \tau \tilde{M}.
\]
**Blended FEM/SEM Schemes**

- Finite elements exhibit phase *lead*. Spectral elements phase *lag*.
- *Magnitude is same* for both schemes. Suggests a symmetric weighting $\tau = 1/2$. 
Blended FEM/SEM Schemes

![Numerical graphs showing comparisons of different schemes]

- Dashed line: Numerical real wave obtained using the spectral element scheme
- Dashed-dotted line: Numerical real wave obtained using the finite element scheme
- Dotted line: Numerical real wave obtained using the optimal scheme
- Solid line: Exact real wave
Blended FEM/SEM Schemes

- Numerical real wave obtained using the spectral element scheme
- Numerical real wave obtained using the finite element scheme
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- Exact real wave
Blended FEM/SEM Schemes

Dispersion analysis reveals for blended scheme ($\tau \in [0, 1]$):

$$kh - \omega h = \frac{1}{24} (\omega h)^3 (2\tau - 1) + O(\omega h)^5.$$
**Blended FEM/SEM Schemes**

Dispersion analysis reveals for blended scheme ($\tau \in [0, 1]$):

\[
kh - \omega h = \frac{1}{24} (\omega h)^3(2\tau - 1) + O(\omega h)^5.
\]

... so choice $\tau = 1/2$ is optimal and gives

\[
k h - \omega h = \frac{1}{480} (\omega h)^5 + O(\omega h)^7.
\]

- two additional orders of accuracy;
- improved coefficient of leading order term.
Blended FEM/SEM Schemes

A quote taken from the conclusion of the highly influential article of Marfurt (Geophysics, 49, 1984):

*Frequency domain finite element solutions employing weighted average of consistent and lumped masses yield the most accurate results, and they promise to be the most cost-effective method for [several applications in wave propagation].* Marfurt (1984).
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Despite this bold statement, none of the citing articles or any other over the past 20 years presents an optimal blended scheme for elements of higher than first order.
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Is it possible to obtain a general result?
Blended FEM/SEM Schemes

Let $p \geq 2$ and $\tau \in [0, 1]$. Then, error in discrete wavenumber for blended scheme is given by

$$kh - \omega h = \frac{1}{2} \left[ \frac{p!}{(2p)!} \right]^2 \frac{(\omega h)^{2p+1}}{2p+1} \{ (1 + 1/p)\tau - 1 \} + \mathcal{O}(\omega h)^{2p+3}.$$
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**Optimal blending parameter** given by $\tau = p/(p + 1)$. 
**Blended FEM/SEM Schemes**

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**Optimal blending parameter** given by $\tau = p/(p + 1)$.

With this choice, we find that

$$kh - \omega h = \frac{4}{2p - 1} \left[ \frac{(p + 1)!}{(2p + 2)!} \right]^2 \frac{(\omega h)^{2p+3}}{2p + 3} + \mathcal{O}(\omega h)^{2p+5}.$$  

- two additional orders of accuracy;
- coefficient of leading order term much smaller.

Ref: Ainsworth and Wajid, SINUM 2010.
Blended FEM/SEM Schemes

- Numerical real wave obtained using the spectral element scheme
- Numerical real wave obtained using the finite element scheme
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- Exact real wave

"Modern Techniques for Numerical Solution of PDEs, ACMAC, Crete, September 2011 – p. 42/54"
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What about $d > 1$ dimensions?

Can we find $\tau$ such that blending mass matrices for FEM/SEM scheme in 2D has higher accuracy?
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Bad news: there is no choice giving higher accuracy.
What about $d > 1$ dimensions?

Can we find $\tau$ such that blending mass matrices for FEM/SEM scheme in 2D has higher accuracy?

Bad news: there is no choice giving higher accuracy.

Don’t give up yet. Look in detail at structure of 2D equations on tensor product grid:

$$K \otimes M + M \otimes K - \omega^2 M \otimes M \quad (FEM)$$

and

$$K \otimes \tilde{M} + \tilde{M} \otimes K - \omega^2 \tilde{M} \otimes \tilde{M} \quad (SEM)$$
What about \( d > 1 \) dimensions?

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and

\[
K \otimes \tilde{M} + \tilde{M} \otimes K - \omega^2 \tilde{M} \otimes \tilde{M} \quad (SEM)
\]

Suggests that in multi-dimensions should look for blending in the form

\[
K \otimes M_\tau + M_\tau \otimes K - \omega^2 M_\tau \otimes M_\tau \quad (Blended)
\]
What about $d > 1$ dimensions?

Can we choose $\tau$ so that

$$K \otimes M_\tau + M_\tau \otimes K - \omega^2 M_\tau \otimes M_\tau \quad (Blended)$$

has higher order accuracy?
What about \( d > 1 \) dimensions?

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has higher order accuracy?

- Yes ... and for all dimensions \( d \);
- Optimal \( \tau = p/(p + 1) \) ... same as in 1D case;
- Obtain two additional orders of accuracy and improved constant (as in 1D case).
What about $d > 1$ dimensions?

Can we choose $\tau$ so that

$$K \otimes M_\tau + M_\tau \otimes K - \omega^2 M_\tau \otimes M_\tau \quad (Blended)$$

has higher order accuracy?

- Yes ... and for all dimensions $d$;
- Optimal $\tau = p/(p + 1)$ ... same as in 1D case;
- Obtain two additional orders of accuracy and improved constant (as in 1D case).

but ...

- nobody wants to assemble mass matrices for both SEM and FEM or to form Kronecker products.
- what to do with non-affine elements?
New ‘Non-Standard’ Quadrature Rules

For $\tau \in [0, 1)$, define

$$
\int_{-1}^{1} f(x) \, dx \approx Q^{(p)}_{\tau}(f) = \sum_{j=0}^{p} w_j f(\xi_j)
$$

where $\{\xi_j\}$ zeros of $P_{p+1} - \tau P_{p-1}$ and

$$
w_j = \frac{2[p(1 + \tau) + \tau]}{p(p + 1)P_p(\xi_j)[P'_{p+1}(\xi_j) - \tau P'_{p-1}(\xi_j)]}.
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Then

- nodes are distinct and contained in $(-1, 1)$;
- weights well-defined and positive;
- rule has precision $2^p - 1$ (under-integration).

... non-standard but perfectly reasonable quadrature rule.  
(Ainsworth-Wajid, SINUM 2010)
‘AW-Quad’ Quadrature Rules

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</tbody>
</table>

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If you have FEM code on quads/hexahedra: Replace Gauss-Legendre quadrature rule with ‘AW-Quad’ rule with $\tau = p/(p + 1)$, and solve.
‘AW-Quad’ Quadrature Rules

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OR
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OR

If you have SEM code on quads/hexahedra: Replace Gauss-Lobatto quadrature rule with ‘AW-Quad’ rule with $\tau = p/(p + 1)$ and solve (don’t change basis functions).
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Resulting approximation is precisely the optimally blended FEM/SEM approximation.
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... trivial implement the method at virtually no additional overhead.
Planar case: harmonic excitation on line $z_S$.

Axisymmetric case: harmonic excitation at point $z_S$. 
Pekeris Waveguide - True Solution

Real part of pressure. Frequency 200Hz. Line source.
Pekeris Waveguide - Mesh

PML used to truncate domain.
Polynomial order of elements (yellow = quartic, green = cubic).
Mesh size: \( hk/(2p + 1) \approx 0.4 \) at 200Hz.
Pekeris Waveguide - FEM vs Optimal Blending

Magnitude of error for Standard FEM (top) and Optimal Blending (bottom).
In this example, we take a 2D waveguide of 1km and frequency of 200Hz.
Relative error in $L_2$ norm:
Standard FEM 18.1%; Optimally Blended 4.44%.
Comparison of errors in standard FEM and Optimally Blended Method over a range of frequencies.
Pekeris Waveguide - Axisymmetric Case

Same behaviour observed in axi-symmetric case also!
Blended FEM/SEM Schemes: The story so far ...

- general result for optimal blending and error analysis;
- numerical performance is promising;
- novel non-standard quadrature rules means easily implemented in an existing code.
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