Spectral Element Methods for Transient Acoustics in ANSYS LS-DYNA®

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1 Introduction

Increasingly there is an emphasis in the engineering simulation community on ultrasonic devices. They are seen in medical imaging, structural health monitoring, and of course, in the rapidly emerging world of autonomous/semi-autonomous vehicles. These devices operate at frequencies of 50KHz and above, sometimes well above. Wavelengths at those frequencies are measured in millimeters, sometimes even micrometers. The simulation of the propagation of such short waves over any substantial distance is a very demanding endeavor. This is especially true if tri-linear/quadratic iso-parametric finite elements are used. Newer, higher-order finite element methods exist [1]. Among those methods is the spectral element method (SEM). Many SEM references are available in the literature, a sampling being [1-6.] Spectral elements are appealing because they are highly accurate and can be efficiently incorporated in an explicit solver like LS-DYNA. In a massively parallel setting, they allow for the solution of models with billions of degrees-of-freedom in a reasonable amount of time.

2 Governing Equation of Acoustics

A linear acoustic fluid is compressible, irrotational, inviscid and undergoes small displacements. The governing equation in terms of pressure is [7]

$$\frac{\partial^2 p}{\partial t^2} - c^2 \nabla^2 p = c \frac{\partial q_f}{\partial t}$$

where p is the pressure, t time, c sound speed, and q_f is the mass per unit volume source term. When coupled with a structural model, the corresponding system of finite element equations is

$$\begin{bmatrix} M_{ss} & 0 \\ -\rho c^2 T_{fs}^T & M_{ff} \end{bmatrix} \begin{Bmatrix} \ddot{u} \\ \ddot{p} \end{Bmatrix} + \begin{bmatrix} W_{ss} & 0 \\ 0 & W_{ff} \end{bmatrix} \begin{Bmatrix} \dot{u} \\ \dot{p} \end{Bmatrix} + \begin{bmatrix} K_{ss} & T_{fs} \\ 0 & K_{ff} \end{bmatrix} \begin{Bmatrix} u \\ p \end{Bmatrix} = \begin{Bmatrix} r_s \\ r_f \end{Bmatrix}$$

where M_{ss}, W_{ss}, K_{ss} are the structural mass, damping and stiffness. Similarly, M_{ff}, W_{ff}, K_{ff} for the fluid. T_{fs} is the fluid-structure coupling matrix. Vector *u* is the structural displacements and vector *p* is the pressure. The explicit time step used by LS-DYNA is the smallest stable time step in the fluid and structural domains.

3 Spectral Elements

Spectral elements are a type of finite element (sub-parametric) that combine higher-order interpolation of the field variables with GLL integration and unevenly spaced nodes at the integration points. The interpolants used for the acoustic elements in LS-DYNA are based on Legendre polynomials [2,6].

$$\phi_i = \frac{-(1-\xi^2) P_N'(\xi)}{N(N+1) P_N(\xi_i)(\xi - \xi_i)}$$

P_n is the Legendre polynomial of degree N and ξ_i is i[th] integration point. The interpolants and element mass (capacitance) and stiffness (reactance) integrals in three-dimensions are

$$\Phi = \phi_i(\xi)\,\phi_j(\eta)\,\phi_k(\varsigma)$$
$$M_{ff} = \int \Phi\,\Phi^T\,dV, \quad K_{ff} = c^2 \int \nabla\Phi\,\nabla\Phi^T\,dV$$

3.1 Accuracy of spectral elements

One of the principal advantages of spectral elements for the simulation of linear acoustic wave propagation is their rapid convergence with increasing element integration order. This property is illustrated in figure 1. Consider the simple problem of propagating a 50KHz wave packet up and down a 1m column of air. Assume the packet starts at the bottom, hits the top, and bounces back. A 50KHz wave in air has a wavelength of about 7mm, so 1 meter of travel requires 145 cycles of the wave. Any amplitude decay or phase distortion will accumulate over that time.

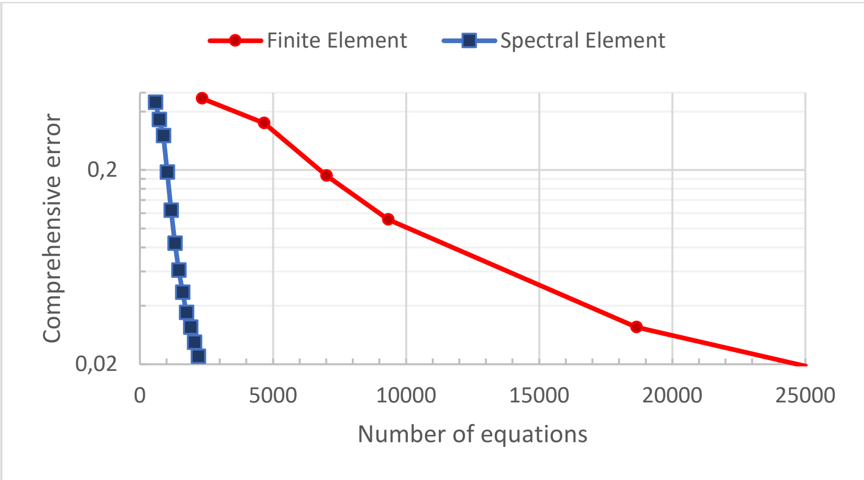

Fig.1: Comprehensive error vs number-of-equations for 1-D wave.

Figure 1 plots the comprehensive error [8] in the pressure history at the middle of the column as a function of the number of equations in the solution. Note that comprehensive error is a measure of both phasing and magnitude error, and that a value of 0.15 is generally considered good agreement between two signals. A value of 0.05 is excellent. The spectral element solutions of figure 1 use 1 element per wavelength and vary the element integration order from 4 to 15. In contrast, the finite element solutions use linear interpolation functions and vary the number of elements per wavelength, starting with 8 elements per wavelength. All solutions use a factor of safety on the time step of 0.1 to minimize the role of the central difference time integrator in the accuracy comparison. It is obvious the spectral element solution is converging much more rapidly than the low-order finite element solution. The spectral elements achieve an error less than 0.15 with 8th order integration and about 1300 equations. The linear finite elements require 48 elements per wavelength and about 7000 equations.

3.2 Variation of time step with spectral element integration order

As you would expect, the stable time step for explicit time integration of spectral elements is sensitive to the element integration order. Figure 2 illustrates how the time step varies for a typical model. The red curve is the time step obtained from the highest frequency of an individual element. The blue curve shows the time step obtained from the more conservative Levy-Harmond-Gerschgorin estimate. All steps are normalized to the step obtained from the maximum frequency of the 2nd order element.

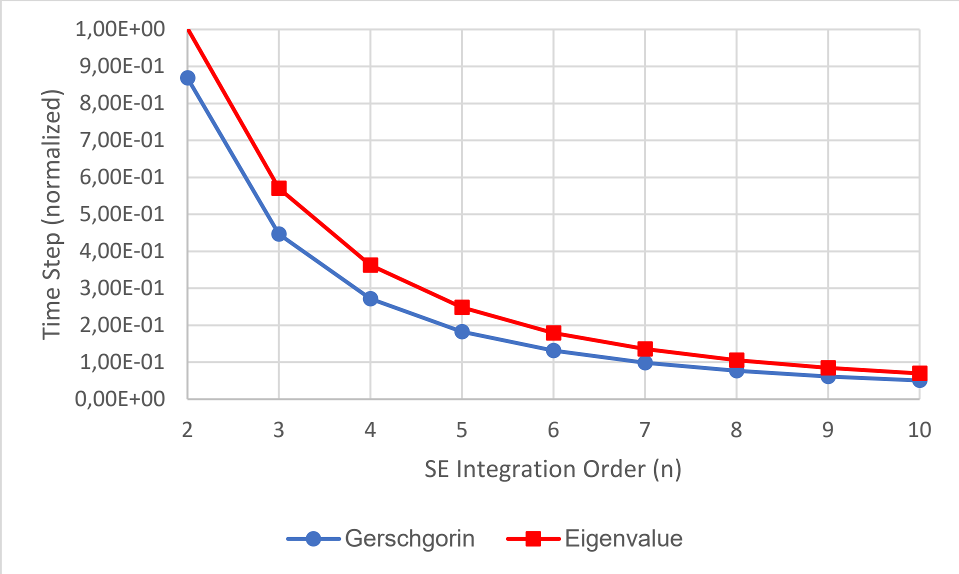

Fig.2: Time step variation with element integration order.

The Gerschgorin estimate is the more conservative estimate of the two and will be the least expensive to calculate. In nonlinear analysis the stable time step is recalculated every time step, so the increased expense of an eigenvalue calculation can be a decisive argument against using it. However, in linear acoustic wave propagation the cost of the maximum eigenvalue method is amortized over thousands of time steps, potentially justifying the higher cost of the approach. Nonetheless, there is a second consideration in ultrasonic applications – distortion introduced by the time integration algorithm. The central difference operator is at best 2nd order accurate. It is often advantageous to use a time step smaller than the stable step when the objective is to accurately model wave propagation over long distances (relative to the wavelength.) For that reason, a time step factor of safety of 0.5 is recommended along with the Gerschgorin time step estimate.

4 Usage within LS-DYNA

When using the spectral elements in LS-DYNA for acoustic wave propagation, a hex8 mesh of the acoustic domain should be provided as if standard, low-order acoustic finite elements are being used (`*section_solid, elform=8`.) From this mesh, the spectral elements and all their internal degrees-of-freedom will automatically be generated by LS-DYNA. The user does not normally see these degrees-of-freedom. The concept is illustrated in figure 3, with the white dots being the internal degrees-of-freedom for N=6 elements.

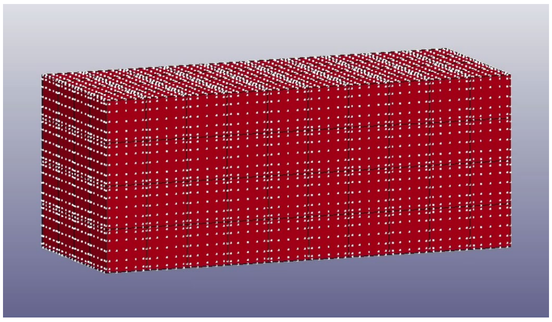

Fig.3: Acoustic model of 160 N=6 spectral elements having 38,125 degrees-of-freedom.

4.1 Applicable keywords

The keywords applicable to acoustic spectral elements and the functions they serve are summarized in table 1 and figure 3.

Required keyword	*control_acoustic_spectral
Material Properties – Ω_F	*mat_acoustic
Structural Coupling - Γ_{FS}	*boundary_acoustic_coupling_spectral
Prescribed Boundary Motion - Γ_U	*boundary_acoustic_prescribed_motion
Prescribed Boundary Pressure - Γ_P	*boundary_acoustic_pressure_spectral
Rigid Boundary - Γ_R	This is a natural condition
Impedance Boundary - Γ_Z	*boundary_acoustic_impedance
Absorbing Boundary - Γ_{NRB}	*boundary_acoustic_non_reflecting
Zero Pressure Boundary – Γ_0	*boundary_acoustic_free_surface
Small Amplitude Wave Boundary - Γ_W	*boundary_acoustic_free_surface
Internal Point Source – Q	*load_acoustic_source
Time history save frequeny	*database_aceout
Locations for nodal time history results	*database_history_acoustic

Table 1: Keywords for transient acoustic spectral elements.

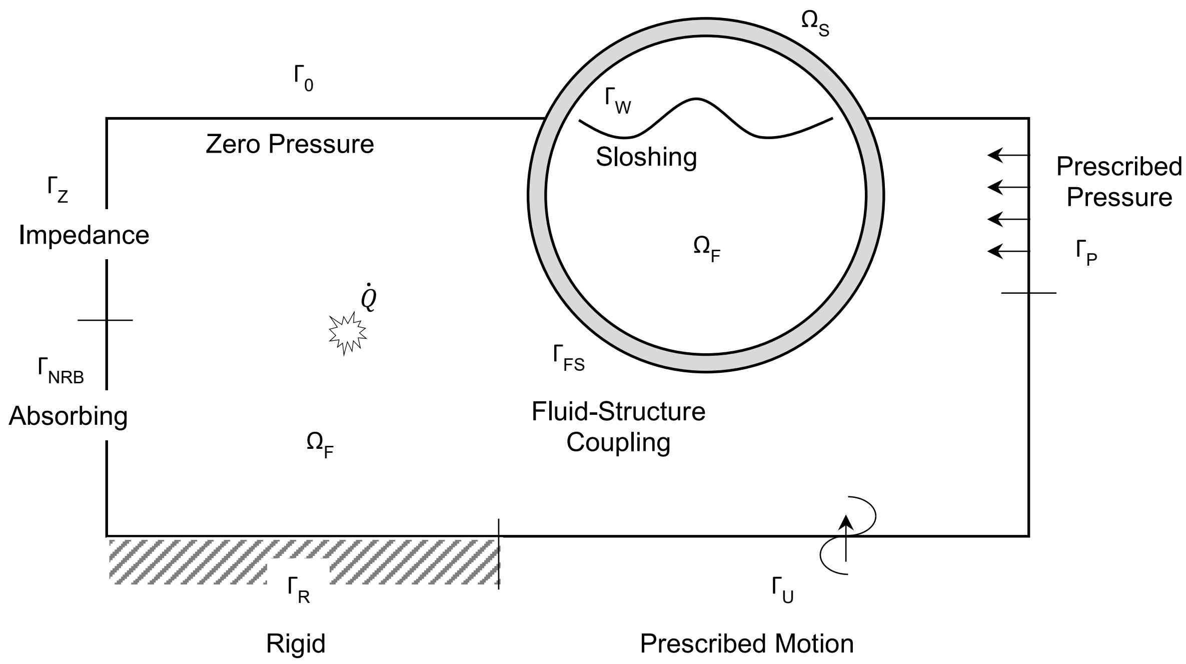

Fig.4: Boundary conditions and loadings for spectral elements.

4.1.1 *control_acoustic_spectral

All acoustic spectral element solutions require the keyword **`*control_acoustic_spectral`**. Without this keyword the solution will default to the iso-parametric solution of **`*mat_acoustic`**.

Variable	MASEORD	MASEHRF	MASEKFL	MASEIGX				
Type	I	I	I	I				
Default	None	0	0	1				

VARIABLE DESCRIPTION

MASEORD	Spectral element integration order	
	2 .LE. MASEORD .LE. 15	
MASEHRF	Optional H-refinement	
	.EQ.0	No splitting unless tetrahedra or wedges are present
	.EQ.1	Split all elements once into hexahedra
	.EQ.2	Split each element a second time into 8 hexahedra
	.EQ.3	Split each element a second time into 27 hexahedra
MASEKFL	Dump flag for H-refined and spectral element meshes	
	.EQ.1	Dump keyword deck of acoustic mesh after H-refinement
	.EQ.10	Dump keyword deck of spectral acoustic element mesh
	.EQ.11	Dump both meshes for review
MASEIGX	Approach to element time-step calculation	
	.EQ.1	Gerschgorin theorem
	.EQ.2	Maximum element eigenvalue

This instruction applies to all `*section_solid, elform=8` elements in the model. Those elements may be hexahedra, tetrahedra, or wedges. Iso-parametric acoustic elements can't be mixed with spectral acoustic elements in the same model. And no acoustic pyramids may be used in spectral element solutions. If wedges or tetrahedra are used anywhere in the acoustic fluid mesh, then all acoustic fluid elements are split once into hexahedra. Boundary and coupling faces are automatically split in the process. Additional splitting is permitted, for instance to accommodate the extreme mesh refinement that is often required in ultrasonic wave propagation problems, without having to generate and manipulate an extremely large mesh. As noted in section 3.2, the Gerschgorin theorem is a faster time step estimation method and will yield a more conservative time step. Typically, the conservative time step is also less dispersive and more accurate. One element per wavelength and 8th order integration gives a very accurate solution over hundreds of cycles of time. Roughly equivalent in accuracy will be two elements per wavelength and a 5th order rule.

*4.1.2 *boundary_acoustic_coupling_spectral*

The other keyword that deserves special mention is `*boundary_acoustic_coupling_spectral`. This is intended for strong coupling between the structural parts of the model and the acoustic spectral element parts. The former will probably be made up of 4-node shell elements and 8 node solid elements. These may be chosen from the list of explicit transient elements available in LS-DYNA. Structural elements are not spectral elements and so should be discretized appropriately for the wavelengths of interest, rather than with the discretization of the acoustic elements. In general, that will require 6-10 elements per wavelength. The surfaces of both the structural elements and the acoustic elements meant to be coupled together should be identified with separate `*set_segment` set identifiers. The faces of the structural elements and the acoustic elements <u>should</u> <u>not</u> be merged. LS-DYNA will form coupling matrices for that acoustic-structural interface.

Descriptions of the remaining keywords in table 1 may be found in the LS-DYNA Keyword Manual.

4.2 Illustrative example

Ultrasound computer tomography is non-invasive medical imaging technology for breast cancer. Envision a well in a table with the patient lying face downward. Each transducer of many in the well emits a high-frequency pulse while the others record the scattered waves. From the character of the scattered waves an image of the tissue and its discontinuities is reconstructed. The higher the frequency of the pulses, the shorter the wavelength, and so the better the resolution of the image. At 500KHz the wavelength of a (sine) pulse in water is about 3mm. For this case, a LS-DYNA model of 6,048,000 n=7 spectral elements has been used, as depicted in figure 5. The model has 2,077,289,341 equations. Pressure iso-surfaces at 24.5µs and 94.5µs are depicted in figures 4 and 5 respectively. Note, in both figures the pressure state is mapped back on the user's hex8 mesh.

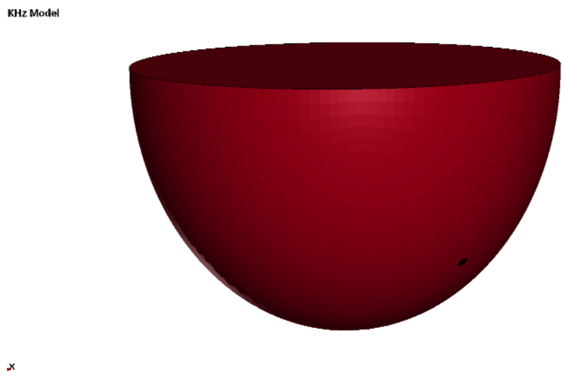

Fig.5: LS-DYNA 500KHz model.

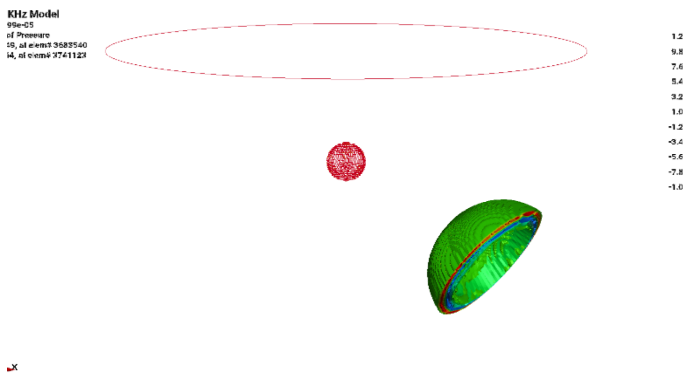

Fig.6: Pressure iso-surfaces at 22.5 μs.

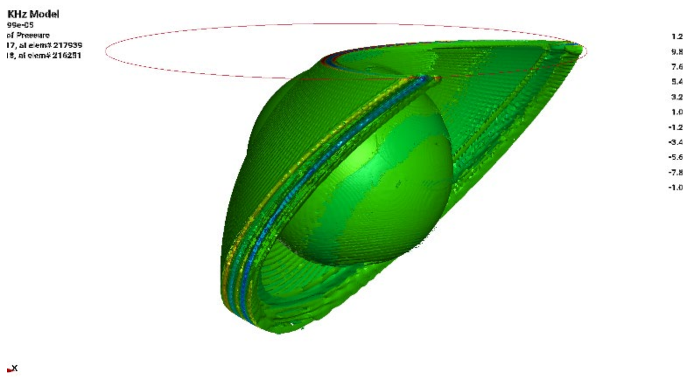

Fig.7: Pressure iso-surfaces at 94.5 μs.

4.3 HPC performance

Acoustic spectral element models for ultrasonic applications can possess hundreds of millions, even billions of equations. For most of these problems the MPP version of LS-DYNA will be required. The 2 billion equation solution depicted in figures 4 and 5 was conducted on an older AVX2 platform. MPP execution with 224 processors required an elapsed time of 14 hours and 9 minutes for 68,745 time steps, double precision.

5 Summary

The R13.0 version of LS-DYNA released in 2021 includes spectral element features for explicit transient acoustics. This paper introduces those features. Enhancements to them are ongoing. Spectral elements are especially effective for high frequency wave propagation because they are both very accurate and very efficient when implemented in an explicit algorithm. We have demonstrated rates of convergence superior to what can be achieved with low-order iso-parametric elements. At the same time, we provide an illustration from medical imaging which used over 2 billion degrees-of-freedom and ran in 14 hours.

6 References

1. Cohen, G.C., Higher-Order Numerical Methods for Transient Wave Equations, Springer-Verlag, Berlin GmbH, 2002.
2. Ronquist, E.M. and Patera, A.T., A Legendre spectral element method for the Stefan problem, Int. J. Numer. Meth. Engng, 1987; 24:2273–2299.
3. Seriani, G., A parallel spectral element method for acoustic wave modeling, Journal Computational Physics, 1997, 05:01:53-69.
4. Komatitsch, D., and J. Tromp, Introduction to the spectral-element method for 3-D seismic wave propagation, Geophys. J. Int., 139, 1999, 806–822.
5. Kaltenbacher, M., Huppe, R., Leerch, R., Mixed spectral finite elements for computational acoustics, DAGA 2008 – Dresden, pp 77-78.
6. Sprague, M.A., and Geers, T.L., A spectral-element method for modelling cavitation in transient fluid–structure interaction, Int. J. Numer. Meth. Engng, 2004; 60:2467–2499.
7. Sandberg, G., Wernberg, P-A., Davidsson, P., Fundamentals of Fluid Structure Interaction, Computational Aspects of Structural Acoustics and Vibration, eds, Sandberg and Ohayon, SpringerWien New York, 2008, 23-102.
8. Russell, D.M., Error measures for comparing transient data: part 1 – development of a comprehensive error measure, Proceedings of the 68th Shock and Vibration Symposium, Nov 3-6, 1997.