ENHANCING SIMULATIONS OF ADDITIVE MANUFACTURING PROCESSES USING SPATIOTEMPORAL MULTISCALING

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Abstract

The three integral components which are common to all additive manufacturing machines are energy source(s), material(s) and geometrical representation(s). The interaction of these components lead to coupled multiscale thermomechanical phenomena. The overall response due to dynamic localized boundary conditions leads to travelling thermomechanical waves with their origin at the point/line or plane of energy input and finite boundaries located at the extremities of the build chamber of the machine. At these finite boundaries, three phenomena occur, namely reflection, absorption and transmission of the thermomechanical travelling wave. Based on the boundary conditions, any combinations of the mentioned finite boundary phenomena are activated leading to a finite mismatch between the boundary condition and ordinate of the travelling wave at the finite boundary abscissae. This finite mismatch leads to another thermomechanical travelling wave which travels from the finite boundary towards the location of energy input and the process of generation of thermomechanical waves continues till a standing steady state thermomechanical wave converges at each snapshot in time. An important aspect of these forward and backward moving travelling waves is their spatiotemporal thermomechanical curvature as a function of space which leads to spatiotemporal multiscale modeling of these processes. Spatial and temporal examples with multi-order and multi-rank updates of thermal eigensolutions with inhomogeneity in the –z direction and thermal stiffness as a function of time stepping were thus studied to understand their effects on efficient Finite Element simulations of metal additive manufacturing processes.

Introduction and Background

All Selective Laser Melting (SLM) process models are computationally expensive to solve using traditional FEM methods, as they require fine-scale resolution across a part volume that is many orders of magnitude larger than the fine-scale lengths. This has led to efforts to solve the problem using asymptotic behaviors, modal space methodologies or beam theories. The intent behind this new EigenSolver strategy is to solve for dominant modes in the macroscopic domain and local high frequency modes in the microscopic domain. These can be accurately applied at certain locations (e.g. 5 layers) below the melt pool.

Beam and plate theories are meant to take benefit of asymptotic theories involved in dimensionally reducible structures. Beam theories for complicated geometries such as aircraft wings and ship hulls and for material variations across the cross-section and length of a component have been an area of intense research. An analytical method, namely the Variational Asymptotic Method (VAM) [1], has been used extensively to derive these beam theories. One of the limitations of this methodology lies in the difficulty of deriving beam theories for very complicated beams. To overcome this problem we have developed a new EigenSolver beam theory derivation

for use with FEA. This novel method can consider any complicated shape and cross-sectional variation and derives beam or plate theories involved in it. Further it has applications in problems which do not fall in the categories of beams or plates (e.g. prismatic bodies or any general structural configuration). The importance of this methodology lies in calculating eigenvectors of the cross-section or group of nodes in FEM matrices (such as the stiffness matrix). It is well known that eigenvalues and eigenvectors are computationally expensive to calculate. To overcome this difficulty, any set of orthogonal vectors can be employed for this purpose and their coupling is calculated to derive simplified simultaneous equations. Various material and geometrical nonlinearities can be incorporated in this beam theory with the help of our other existing solver tools.

This methodology can be further generalized to work with groups of nodes in banded FEM meshes for large size problems. These can then be solved on desktop computers. In summary this methodology is capable of:

- Representing complicated geometry and material inhomogeneity in beams.
- Inexpensive computations leading to global-local coupled response.
- Generalization to be used for any problem with some hidden unknown asymptotics.
- Solving large size FEM problems (for example 10 million Degrees of Freedom or much larger in some specific cases) on desktop computers.
- Simplified and fast assembly of FEM matrices.

In addition, an analytical method using a multi-dimensional, multi-resolution wavelet based eigentheory is in development. This methodology can solve both linear and non-linear problems provided a space transformation between the cross-sections is available. The theory has been extended to account for inhomogenous material distributions which are very common among powder based additive manufacturing technologies where solid and powder continuously interact in a non-linear mode with the applied thermal and resulting deformation based boundary conditions.

A schematic diagram which represents the concept of an EigenSolver is illustrated in Figure 1. This strategy works with polynomial basis functions such as orthonormal polynomial shape functions formulated for finite element method resulting in the creation of the stiffness matrix first followed by finding the eigenvalue and eigenvector of the thermomechanical propagator matrix extracted from the stiffness matrix. The eigenmodes transform the problem in its frequency domain. Some other methods of interest in this case and which may require further investigation are the Spectral Finite Element Methods (SFEM). Although the method and its variants has not been attempted in this description- the research in this direction has been reviewed.

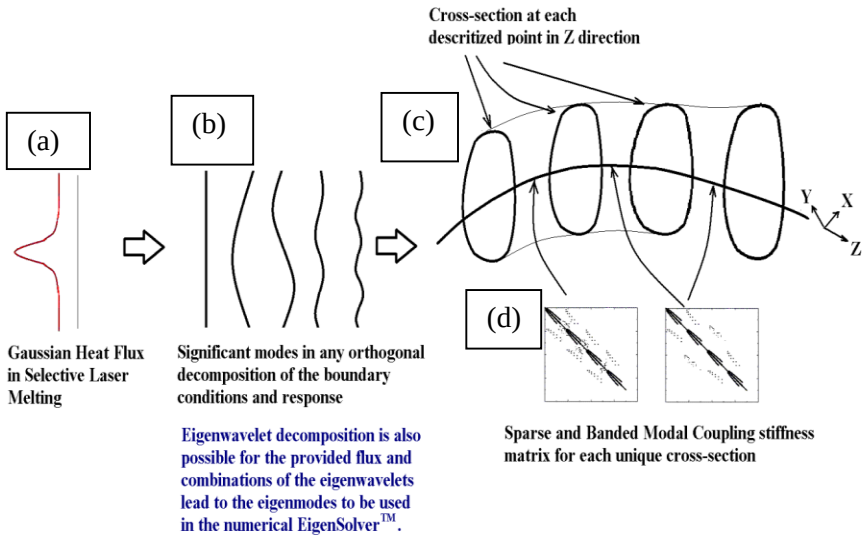

Figure 1: Schematic Diagram illustrating the Concept of an EigenSolver. In (a), first a Gaussian heat flux is applied to the material followed by the split of the flux in orthogonal modes in (b). These orthogonal modes are a function of geometry and the material (in-homogeneity and non-linearity) which traverse forward through the cross-sections shown in (c) followed by their temperature counterparts which traverse backwards towards the source as the flux modes hit the fixed temperature boundary. In (d), the stiffness modal coupling of flux and temperature modes between changing cross-sections is shown, where black regions represent numbers in a matrix and white regions represent insignificantly small numbers. These matrices will assume an identity matrix or integral multiples of the identity matrix along the matrix diagonal since consecutive cross-sectional material properties/geometry are assembled in a fashion such that they are integral multiples w.r.t one another whereas if the material properties/geometry is continuously changing, this will lead to off-diagonal terms comprising an interaction of one cross-section w.r.t the other.

For general wave propagation related problems, the traditional finite element method (FEM) is the most used and trustworthy numerical technique for its capabilities of analyzing complex structures and capturing dynamic response with high accuracy. However, for reliable predictions of dynamic response of wave propagation, the number of elements required is typically large, which induces enormous computational costs. SFEM uses exponential functions instead of polynomial functions as basis functions and the finite element method is implemented based on variational integration in a frequency-dependent domain. SFEM has been studied in stationary vibrations of fluid-filled pipes, [2] railway car structures [3] and wave propagation in composite tubes[4], composite plates [5, 6] and composite beams [7-9], and diagnosis of crack/damage of structures [10-13]. SFEM has good reliability and efficiency compared to traditional FEM for these types of problems.

The Fast Fourier transform (FFT) based spectral finite element (FSFE) method is known for its ability to simulate inverse wave motion problems. However, due to the Fourier series approximation in the spatial domain and discrete assumption in the temporal domain, the lateral boundary responds with an inaccurate wrap around response for short length waves [14]. The wavelet based spectral finite element (WSFE) method, which is similar to the FSFE method, alleviates this problem by using compactly orthonormal and supported Daubechies scaling

functions [15] approximation both in time and space. The WSFE method allows imposition of initial values with no periodicity assumption and thus is free from wrap around problems [16]. The wave equations are reduced to the ordinary differential equations (ODEs) in both temporal and spatial domains and are typically decoupled using eigenvalue analysis and solved for obtaining the element shape functions.

Methodology

A novel solution strategy for prediction of thermo-mechanical variables away from the point of laser exposure has been formulated. The involved strategy has been borrowed from structural vibrations and image analysis algorithms where modal contributions (eigenmodes) are computed in terms of orthogonal functions. The typical approach for determination of modes using sine or cosine functions has been extended to fit a finite element framework where an eigenvalue problem of the thermomechanical propagator matrices (these matrices compute the propagation of the thermomechanical field from one cross-sectional layer to another along the –z direction) is computed in order to determine the orthogonal basis functions (eigenvectors) for thermomechanical fields. It has been observed that very near to the point of laser exposure the number of modes required to reconstruct the solutions is very high (the number of modes is limited by the number of nodal points in each cross-section) and as the distance from the point of laser exposure increases, the number of modes required to accurately predict the solution drops very quickly. For performing these calculations, therefore, the region very close to the point of laser exposure in the –z direction where non-linear thermal conductivity relations and melt pools are active is solved using a unique Feed Forward Dynamic Adaptive Mesh Refinement and De-Refinement (FFDAMRD) finite element method. When more than 4-9 layers from the top surface, the problem is solved using the thermal eigensolver approach (as illustrated in Figure 2). For performing the calculations on the current time step, first the thermal evolutions in the first 4-9 layers are calculated using FFDAMRD and the thermal distribution of the deeper layers as a boundary condition. This is followed by using the new thermal distribution calculated for the 4^{th} to 9^{th} layers as flux boundary conditions to solve for the deeper layers in the current time step.

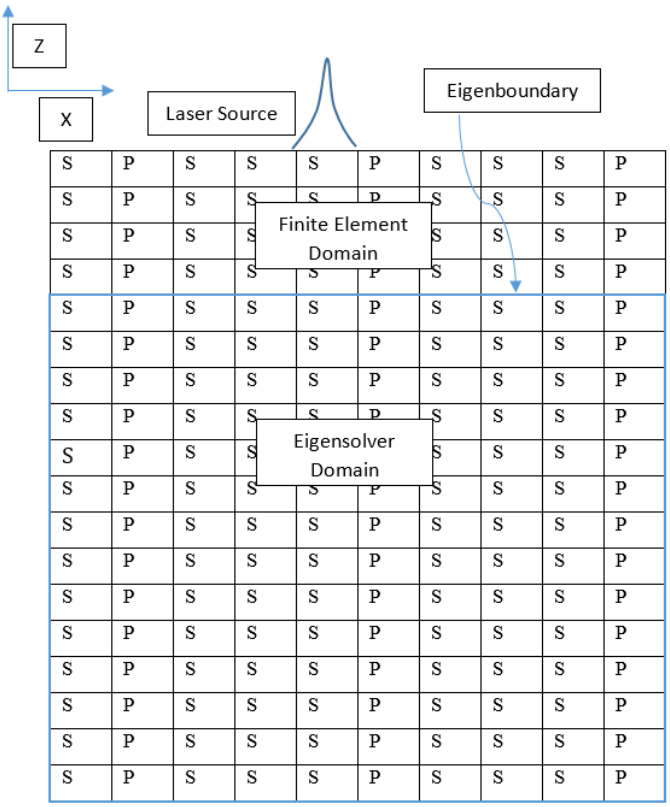

Figure 2: XZ plane cross-section elements viewed from the -Y direction. The Solid-Powder pattern in the +X direction is repeated and extruded in the –Z direction, illustrating a part with the same cross-sectional geometry between layers. S denotes the portion of the powder bed which has converted from powder to solid following laser exposure and P denotes the portion of the powder bed which didn't change its state and remained as powder.

In an another development, a new solution methodology has been formulated such that the thermal solution using our FFDAMRD algorithm can be updated in a manner such that LU factorization need not be calculated more than once to obtain the thermal distribution for every time step (shown by red dots) in Figure 3 for each offset location (Figure 3 compared to Figure 4 show how the fine mesh moves by one coarse mesh division in the direction of laser motion, thus defining one offset). The method used for this development is a multi-rank/order update for changing thermal stiffness as a function of time step/offset.

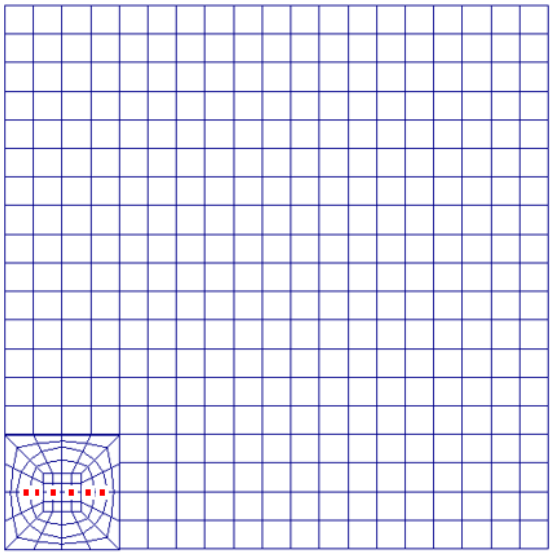

Figure 3: Figure showing the combined fine and coarse mesh at offset 1 with red dots showing the time stepping.

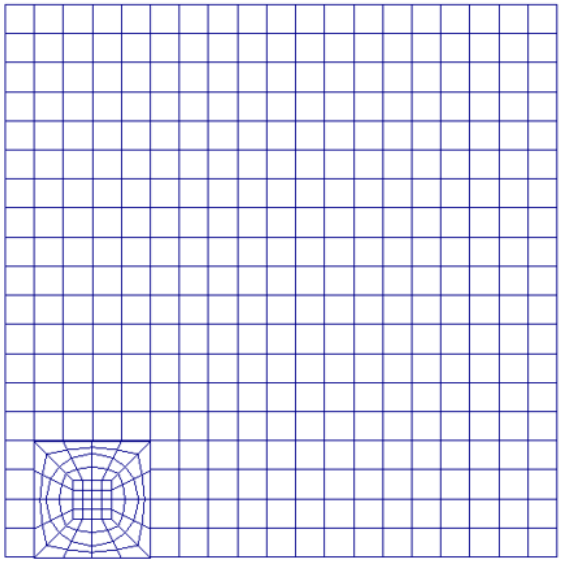

Figure 4: Fine mesh movement from offset1 to offset2.

Results and Discussion

Thermal Eigensolver

In the case of Ti6Al4V, accurate thermomechanical solutions can be calculated almost instantaneously 4 or more layers away from the point of laser exposure using a limited number of modes. A part with 2.5 dimensional properties (where the geometry is extruded in the z direction) in the powder bed, due to the scalar nature of eigenmode decay equations, turns out to be extremely uncomplicated, as shown in Figures 5, 6 and 7. The amount of error introduced using this approach is negligibly small for a point energy source (see Figure 5) while the speed improvement is substantial. For cases of a line energy source (see Figure 6), the match is good but not excellent.

For cases of a large area source, due to unrefined orthogonal modes, the trend of solutions is replicated but the error is much worse when compared to a point energy-source solution (see Figure 7). The use of Arnoldi and other methods for refinement of modes [17] for this scenario would be relevant for manufacturing processes in which point sources of energy are not used. For focused energy sources such as for SLM and EBM, this approach completely eliminates the need to re-compute thermomechanical fields using fine-scale FFDAMRD for the problem domains which are more than a few layers away from the laser; thus eliminating the vast majority of the computational time necessary to simulate real parts (which are made up of thousands or tens of thousands of layers).

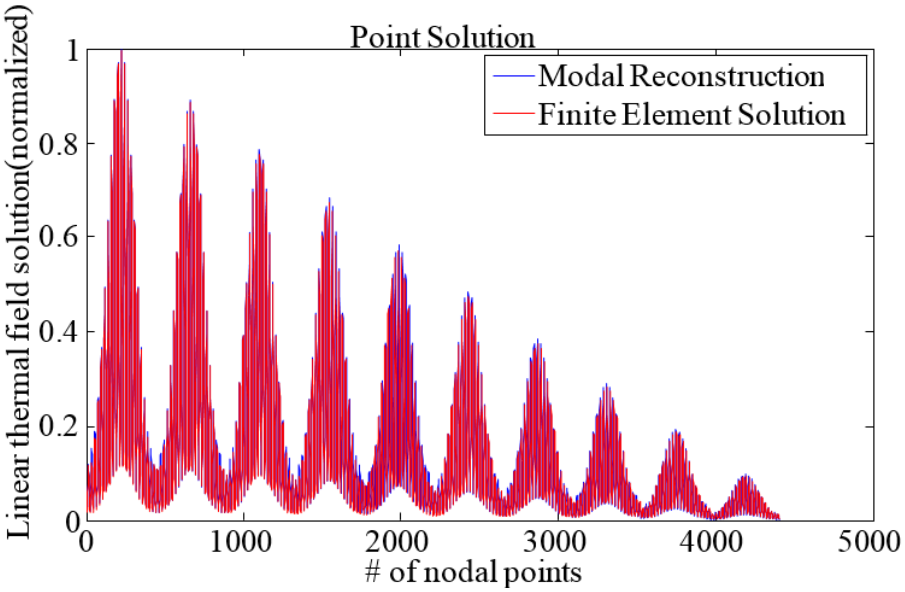

Figure 5: Nodal point by point match of a finite element solution for a thermal field with a Modal reconstructed (eigensolver) solution for a Gaussian point energy source. The error is negligibly small (<0.1%) and the results lie right on top of each other.

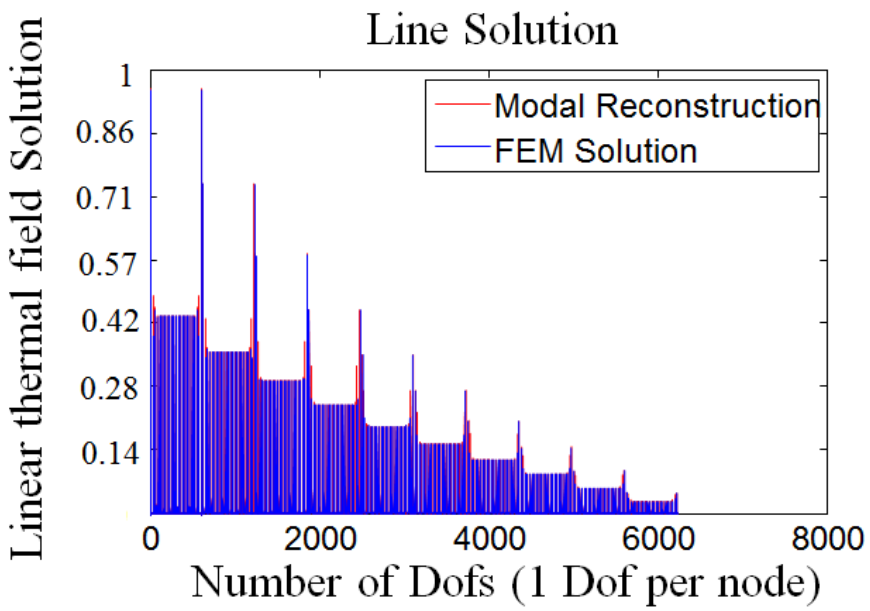

Figure 6: Nodal Point by point comparison of a finite element solution with a Modal reconstructed solution for a constant line energy source. The match is good but not excellent when compared to Figure 5.

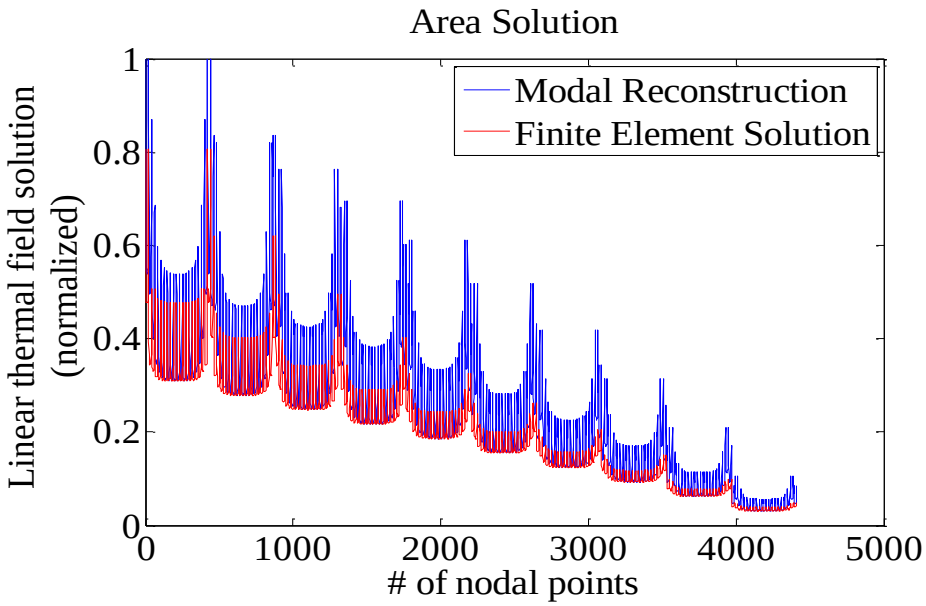

Figure 7: Nodal Point by point comparison of a finite element solution with a Modal reconstructed solution for an area energy source. The modally reconstructed solution matches the trend but not the magnitude of the solution due to unrefined orthogonal modes. This result is irrelevant for moving point energy problems associated with SLM or EBM, but should be taken into account when seeking the correct solution for area energy sources.

For problems which do not have an extruded geometry from the top surface to the bottom surface the solution becomes intractable since the extruded geometry eigensolutions could no

longer be used for these cases and they require further mathematical corrections to account for the inhomogeneity. The finite element solution has been superposed on an extruded homogenous eigensolution in Figure 8 for a case shown in Figure 9. It can be clearly seen that there exists a significant mismatch between the finite element and thermal eigensolver results for this case if no correction is implemented.

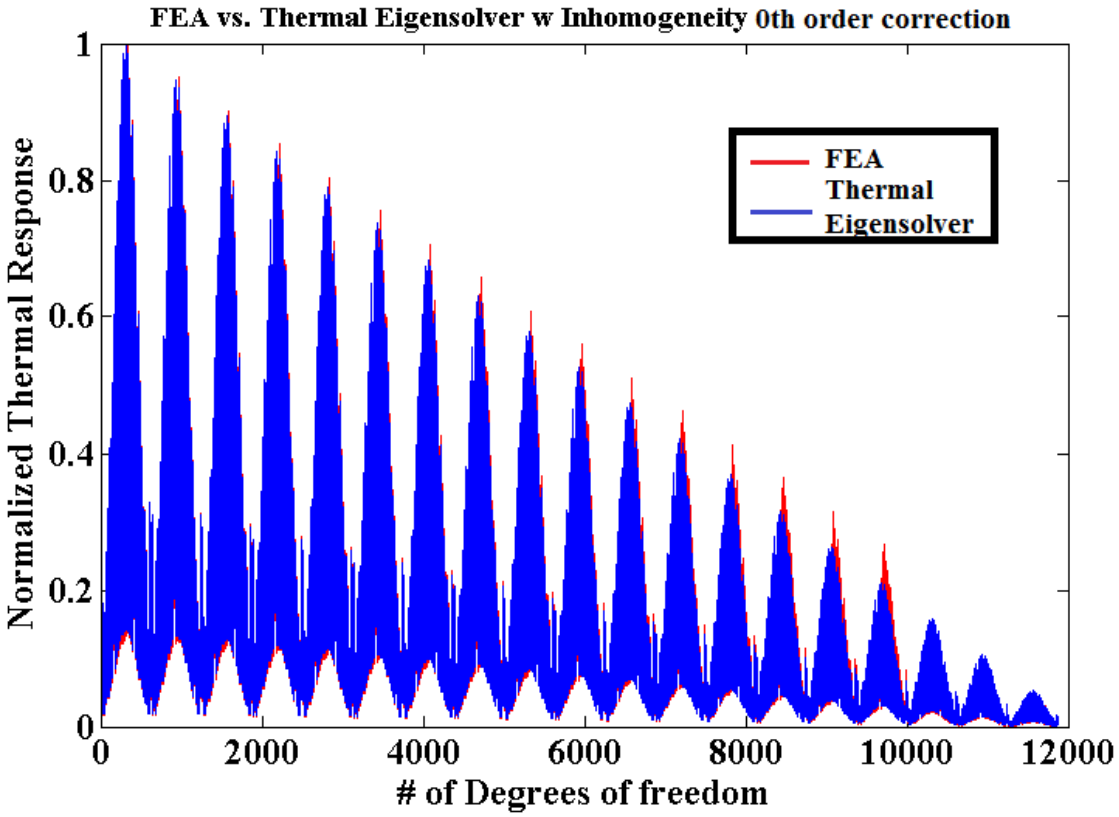

Figure 8: FEA and Thermal eigensolver with 0^{th} order correction for node-by-node comparison using homogenous modes for computation

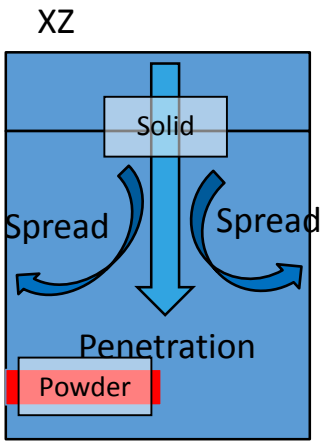

Figure 9: Inhomogeneous case in the -z direction showing a solid part with an internal cavity and entrapped powder

Using a first order correction, the results match with a relative error of 0.14%. FEM results superimposed on the thermal eigensolver results with first order correction are shown in Figure 10. The eignesolver solution is ~8000 times faster for this small problem, but.the computational advantage will be even greater for larger problems as the matrix size grows exponentially with number of layers.

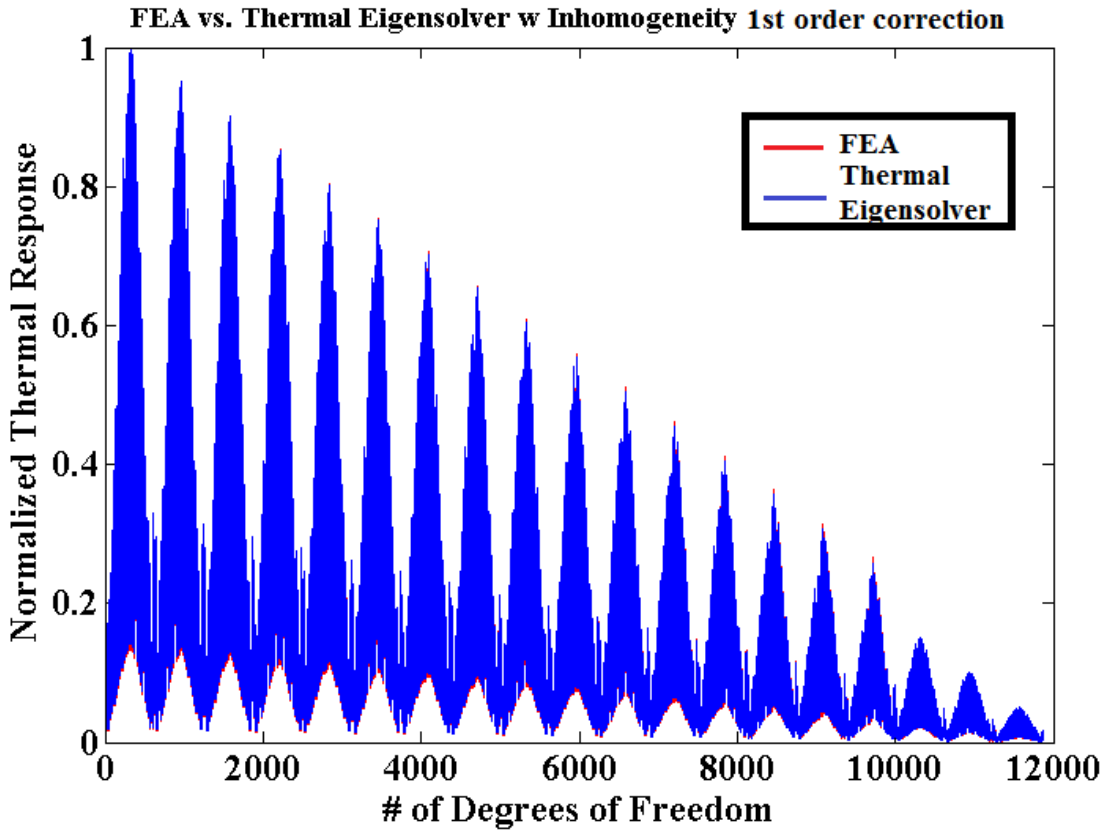

Figure 10: FEA and Thermal eigensolver with 1st order correction one-on-one DOF comparison using homogenous modes for computation.

It should be noted that, so far, eigenvalues have been identified and reconstructed for the thermal case only. A parallel architecture is required for solving the deformation problem using our dislocation density based crystal plasticity (DDCP) finite element solver. For DDCP, the eigenvalue problem has orders of magnitude higher complexity than for the FFDAMRD thermal problem and will thus require a very fine refinement to compute the dispersion matrix and penetration matrices correctly in order to obtain the propagator matrix for its eigenvalue determination.

Multi-rank updates

In order to use the multi-rank updates for computing the approximate inverse of the changing thermal stiffness as a function of offsets, the convergent singular values have been plotted against the total number of singular values in Figure 11. It is clear from this illustration that the singular values converge as a function of increasing number of mesh transfers. Another important aspect from Figure 11 is that the singular values follow a steeply decreasing curve similar to a rectangular hyperbola and hence the number of singular values required for computing the inverse should be less than the full size of the matrix. This results in even more savings in computational effort and time along with convergence of the singular values as a function of number of offsets. A one-to-one match between the thermal distributions obtained using the LU

decomposition and a much lower rank 1000 update of the thermal stiffness (including dynamic *C*) is shown in Figure 12.

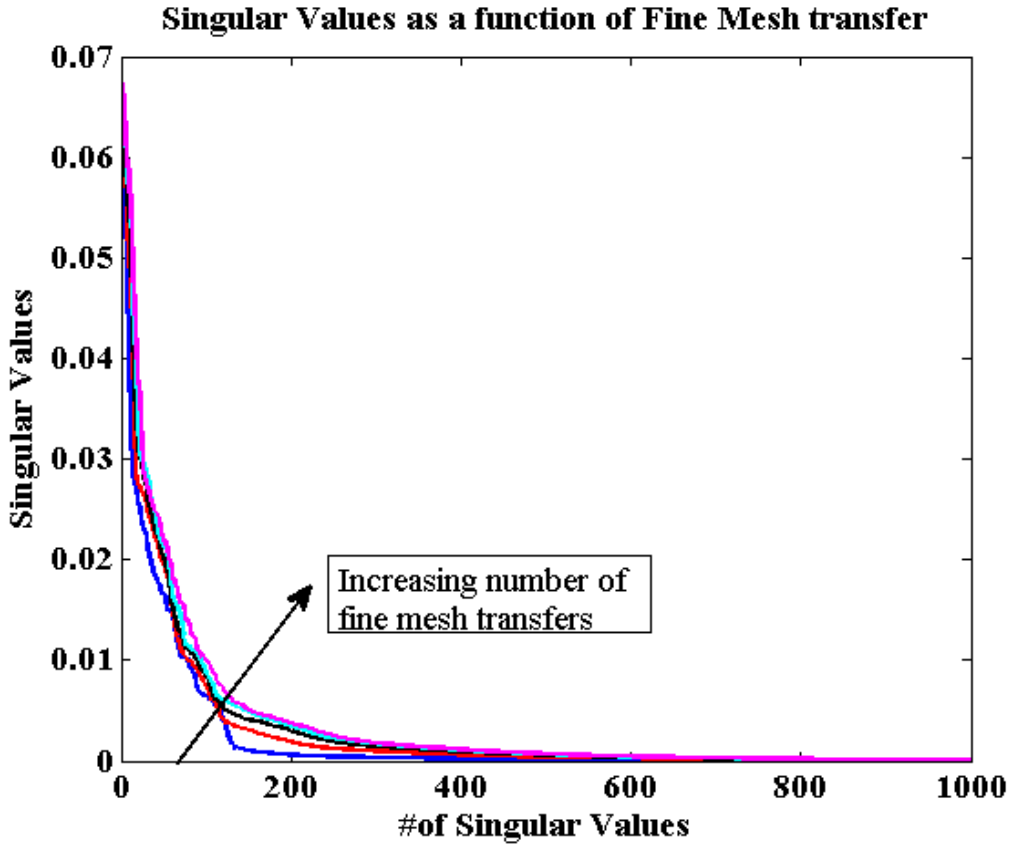

Figure 11: Singular values as a function of fine mesh transfer offsets

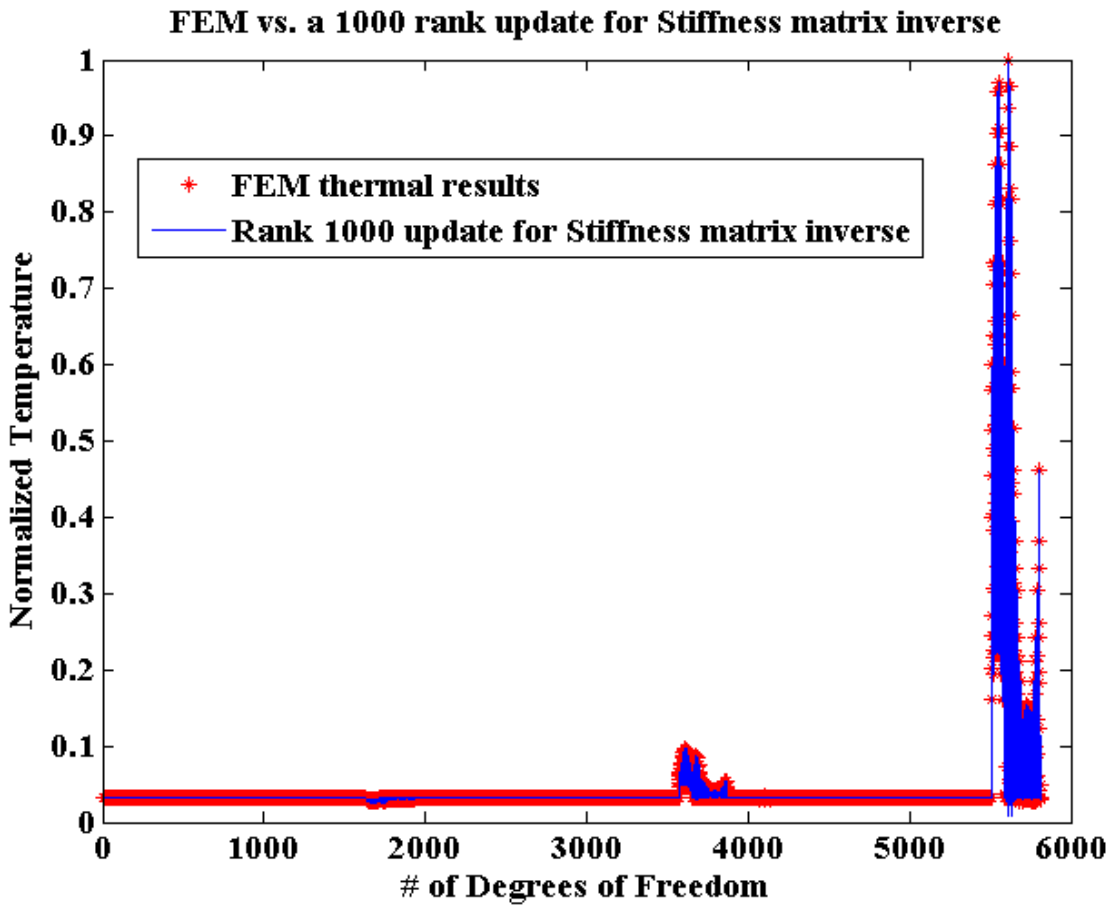

Figure 12: Thermal distributions computed by performing the LU/Cholesky Decomposition of the full thermal stiffness matrix against a much lower rank update of the inverse.

Multi-order updates

For using the multi-order updates, the inverse of the thermal stiffness for the current time step has been updated using the thermal stiffness of the previous time step. While multi-rank updates were found to be more beneficial and faster in the case of fine mesh offset transfers, multi-order updates are more suitable for updating the thermal distribution as a function of time steps. A one-to-one thermal DOF comparison using Cholesky factorization in Finite Element and using the 4^{th} order thermal stiffness update is shown in Figure 13. The results are in excellent agreement with the thermal distribution obtained using the finite element method.

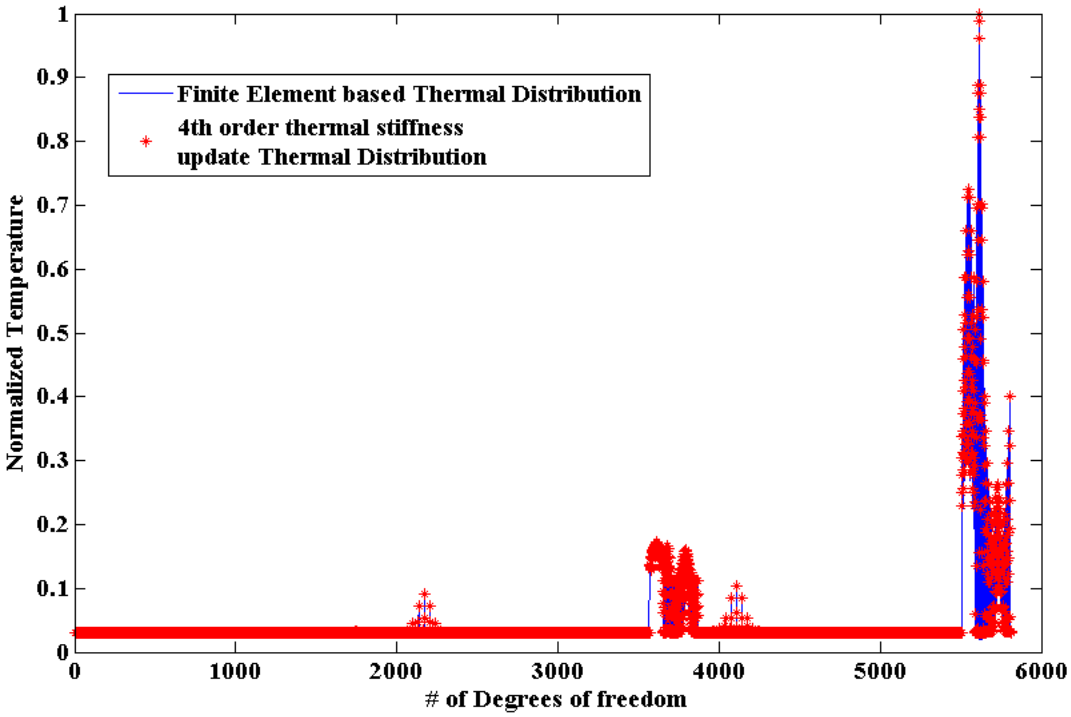

Figure 13: Thermal distributions computed by performing the LU/Cholesky Decomposition of the full thermal stiffness matrix against a much lower order update of the inverse.

Conclusions & Future Work

Three algorithms have been developed to increase the efficiency of computation of thermal fields in metal melting based additive manufacturing. The first algorithm deals with propagation of the macroscopic thermal response in the –z directions (a multi-order update followed by update of the macroscopic 3 dimensional thermal response). The other two algorithms provide two different methods for computing thermal distribution as a function of fine mesh transfer offsets and time steps inside a particular fine mesh offset configuration. The results of these algorithms have been found to be in an excellent agreement with their inefficient finite element counterparts. These algorithms are being implemented in the commercial code being developed by 3DSIM, LLC in close collaboration with University of Louisville personnel.

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