

# Modelling and Efficient FEM for Thermo-Mechanical Problems in High Explosives

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## Abstract

This talk discusses efficient and reliable Finite Element Methods to simulate the thermo-mechanical response of high explosives. A key motivation is the modelling of the initiation of shear bands in materials such as HMX. The localised plastic deformation associated with a shear band leads to the formation of hot spots and can subsequently lead to thermal runaway and potentially serious consequences. To prevent and predict thermal runaway it is often typical practise to use standard finite element methods which struggle to accurately resolve the sharp gradients associated with these thermal and mechanical features which may lead to unphysical predictions of the dynamics within high explosives. The numerical methods presented in this talk aim to provide efficient and reliable tools towards modelling the initiation of shear banding and thermal runaway. We consider two approaches: adaptively generated meshes based on mathematically rigorous estimates of the numerical errors, and enriched finite elements. These methods are demonstrated for thermal and elastic problems respectively, as they arise in reduced models when either the thermal or mechanical dynamics can be eliminated in the modelling. We first present results based on adaptive finite elements for non-linear thermal problems. Steep temperature gradients are resolved by appropriate mesh refinement procedures. Steered by indicators for the accuracy of the solution, the algorithm automatically resolves hot spots on a refined mesh, significantly reducing computational costs, see for example (Gimperlein and Stoczek 2019). Secondly, we consider space-time enriched finite elements (also known as generalised finite elements) which include a priori physical information into the approximation space. This a priori information could represent localised wave-like features. The modelling can effectively capture features occurring at different spatial and temporal scales (Laghrouche et al. 2005; Perrey-Debain et al. 2005). Here we consider a first order formulation of the wave equation (Barucq et al. 2017) and choose plane-wave enrichments (Petersen et al. 2009).

## 1. Introduction and Motivation

Improper handling of energetic materials, such as accidental mechanical or thermal insults, may lead to thermal runaway with its potentially disastrous consequences, as seen with Beirut disaster on 4<sup>th</sup> August 2020 Ghantous; Prothero (2020). Of particular interest is the initiation of shear bands, a strain-localisation phenomenon which is expected to play a role in HMX plasticity. The localised plastic deformation leads to the formation of hot spots, which may subsequently cause ignition on time scales long after an initial

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mechanical insult. While experiments can provide insights into the dynamical evolution, they are limited by experimental, financial and safety constraints. Mathematical models may provide qualitative and quantitative means to determine the behaviour of a material under an insult, taking into account the coupled mechanical, chemical and thermal dynamics inside the energetic material. They may predict the internal deformation and the location and time scales of a potential ignition Hager et al. (2012). To understand and quantitatively predict key mechanisms of the onset of a reaction in an energetic material, based on a mathematical model, requires efficient and reliable numerical methods. Current hydrocodes can fail to represent the extreme localised thermal and mechanical effects in shear bands, due to the severe temperature and strain gradients associated with these problems (Peter Hicks). For example, Peter Hicks discusses the failing of various numerical packages when modelling shear bands. It is further of interest to separate the uncertainties of the mathematical from the challenges of its numerical simulation. We here present preliminary results for two complementary numerical approaches based on advanced finite element methods. *Adaptive finite elements* efficiently resolve localised features by automatic mesh refinements in the regions of large numerical error. The underlying a posteriori error estimates allow us to quantify the accuracy of the numerical result and refine it until a prescribed tolerance is achieved. This is illustrated in recent work (Gimperlein and Stoczek 2019) on contact problems corresponding to a mechanical insult or friction. We here describe its analogue for situations potentially leading to thermal runaway. The second numerical approach, *enriched finite elements* (EFEM), allows us to include available physical information into the numerical approximation spaces. Such information about the solution may circumvent the numerical difficulties and in this way achieve engineering accuracy with a numerical cost reduced by orders of magnitude (Iqbal et al. 2017; Drolia et al. 2017). The approach we present here relates to recent work on Trefftz methods (Barucq et al. 2017; Moiola and Perugia 2018).

To be specific, we consider thermo-mechanical models relevant for energetic materials of the form of a heat equation

$$\rho C_v \frac{\partial u}{\partial t} = \sigma_{ij} \dot{\epsilon}_{ij} + \rho \dot{r} + \kappa \Delta u \quad (1.1)$$

for the temperature  $u$ . Here  $\dot{r}$  is the rate of heat, per unit mass, being produced by a chemical reaction in a material,  $\kappa$  the thermal conductivity,  $\rho$  the density and  $C_v$  the specific heat capacity. The mechanical properties  $\dot{\epsilon}$  and  $\sigma_{ij}$  correspond to the strain rate, respectively the stress. As governing equations for the mechanics, a combination of non-linear elastic and viscous behaviour may be relevant. Bebernes and Lacey (2004) discuss such models for shear banding and Ohmic heating. By integrating the mechanical problem analytically for specific geometries, Bebernes and Lacey (2004) derives effective non-linear heat equations of the form

$$\frac{\partial u}{\partial t} - \Delta u = \lambda r(u) + g(u) \cdot \left( \int_{\Omega} g(u) d\Omega \right)^{-p}, \quad (1.2)$$

where the non-local, non-linear term  $g$  is determined by the temperature dependence of the mechanical properties. In this way, a large class of heat-like equations is obtained, and their efficient numerical approximation becomes relevant. On the other hand, we consider elastic problems under a localised point insult. To illustrate our approach, the model problem of the scalar wave equation is considered. Extensions to elastic problems will be addressed in future work.

## 2. FEM Set Up and Discontinuous Galerkin Formulation

In the following sections we will be discussing the two methods mentioned above: Adaptive FEM and EFEM. To do this effectively we will be considering the basic set up of both methods initially and then discussing how we extend from a standard FEM method into these more complex regimes. We will be considering toy mathematical problems in the form of a heat equation for adaptive FEM and an acoustic system in EFEM.

### 2.1. Thermal Problem

First we discuss the set up of a standard and then adaptive FEM scheme. The theory of the finite element method approximations Thomée (2006) and its implementation as a MATLAB algorithm was largely informed by Larson and Bengzon (2013). For a convenient example let us consider a heat equation,

$$\frac{\partial u}{\partial t} - \Delta u = f(u), \quad (2.3)$$

where the temperature  $u$  maybe be dependent on space and time. Now we give a general template for FEM. To do this we follow a five step approach to obtain an approximate solution to the variational form:

- (a) Reformulate the PDE into variational form
- (b) Discretise the domain,  $Q = \Omega \times [0, T] = \Omega \times \mathcal{T}$ , into elements
- (c) Define a suitable basis for  $S_h$  given the discretisation
- (d) Generate the system of algebraic equations
- (e) Solve the system and obtain the approximate solution.

In step one we are tasked with finding the variational formulation

$$\int_{\Omega} u_t v + \int_{\Omega} \nabla u \cdot \nabla v = \int_{\Omega} f(u) v \quad (2.4)$$

where  $v$  is a *test function* such that  $v \in H_0^1$ .

Step 2 of the process, discretising  $\overline{\Omega}$ , is done by splitting the domain into a finite family of disjoint elements. This discretised domain shall be denoted by  $\mathcal{T}_h$  and the nodes by  $N_h$ . The collection of these nodes are denoted as  $\{P_i\}_{i=1}^{N_h}$ . We know that the variational solution,  $u$ , belongs to  $H_0^1$  and that this is an infinite dimensional space. The aim to approximate  $u$  from an  $N_h$ -dimensional subspace  $S_h$ . To the  $i$ th node,  $P_i$ , we assign a piecewise linear function,  $\phi_i$  which takes the value 1 at  $P_i$  and 0 otherwise. The set  $\{\phi_i\}_{i=1}^{N_h}$  defines a basis (in our case piecewise linear) for the subspace  $S_h$ , from which we shall approximate the solution of (2.4). This approximation shall be defined as  $u_h \in S_h$  and clearly for some  $\{\alpha_i\}_{i=1}^{N_h}$ , such that  $\alpha_i : (0, T] \rightarrow \mathbb{R}$  for all  $i \in \{1, \dots, N_h\}$ , we have

$$u_h(., t) = \sum_{i=1}^{N_h} \alpha_i(t) \phi_i, \quad (2.5)$$

for some fixed  $t$ . Now we substitute this approximation into equation (2.4). Note, every basis function  $\phi_j$  belongs to  $H_0^1$  and as a result constitutes a suitable test function.

For the discrete parabolic problem we introduce the space-time bilinear form  $B_{DG}(\cdot, \cdot)$  given by

$$B_{DG}(u, v) = \sum_{k=1}^{N_h} \int_{\mathcal{T}} \langle \partial_t u, v \rangle + \Delta(u, v) dt, \quad (2.6)$$

whereby we immediately draw the weak formulation,

$$B_{DG}(u_{h\tau}, v_{h\tau}) + \sum_i^{N_h} \langle u_{h\tau}^-, [v_{h\tau}] \rangle_\Omega = \langle f, v_{h\tau} \rangle_Q, \quad (2.7)$$

for  $\tau$  the particular time step in  $\mathcal{T}$  and where  $[\cdot] = [v_h n_t^+ + v_h n_t^-]$  represents a jump in time for  $+$  being from above and  $-$  from below. Now, since (2.7) holds for each  $j \in \{1, \dots, N_h\}$ , for every fixed  $t > 0$  we have a system of equations. This can be written more compactly as the matrix equation

$$\mathbb{I}(\alpha(t+h) - \alpha(t)) + A\alpha(t+h) = \mathbf{F}(t). \quad (2.8)$$

The matrices  $\mathbb{I}$  and  $A$  are each  $N_h \times N_h$  matrices. As mentioned previously the matrices  $\mathbb{I}$  and  $A$  are called the *mass* and *stiffness* matrices respectively and the vector  $\mathbf{F}(t)$  is referred to as the *load vector* (Thomée 2006). We look to improve the standard scheme to fully resolve complex physical problems by employing the following adaptive algorithm for elements within the mesh:

### Adaptive Algorithm

1. Set up the problem
  - Create a coarse mesh
  - Define the accuracy level that is desired
2. Solve the linear system
3. Compute the error indicators for each element
  - Stop iterating if the desired accuracy is attained
4. Mark the elements in need of refinement
5. Refine the marked elements
6. Repeat the process from (2)

### 2.2. Wave Propagation of an Elastic Problem

As discussed in Section 1 we will also be considering enriched finite elements for an acoustic system. The motivation behind focusing on the acoustic wave equation is because of its practical applications - ranging from deformation in energetic materials to railways and tidal power. In this paper we will be considering the first order acoustic system,

$$\begin{cases} \frac{1}{c^2 \rho} \frac{\partial p}{\partial t} + \nabla \cdot \underline{v} = f_1 \\ \rho \frac{\partial \underline{v}}{\partial t} + \nabla p = f_2 \\ p(\cdot, 0) = v(\cdot, 0) = 0 \\ p_t(\cdot, 0) = v_t(\cdot, 0) = 0 \end{cases}, \quad (2.9)$$

where we have unknowns as the pressure ( $p$ ) and velocity ( $\underline{v}$ ) with constants of density ( $\rho$ ) and acoustic wave speed ( $c$ ). For this preliminary work we will consider these constants as 1, to ease the numerical experimentation. Before continuing on we should point out the acoustic equation above can easily be re-written as the wave equation by differentiating with respect to space in one PDE and time in the other. Once we do this we can eliminate the common term to form the wave equation,

$$\frac{\partial^2 p}{\partial t^2} - \Delta p = f. \quad (2.10)$$

Our work first starts to differ in the initial stage of the the set-up when compared to a standard FEM scheme. We pose the above system in the following space-time domain,  $Q = \Omega \times [0, T]$  - where  $\Omega$  is the spatial domain and  $T$  is the final time. We further require that each element,  $\mathbf{K}$ , must be a subset of  $Q$  and thus spans both spatial and temporal nodes. The main advantage of this is to allow us to enrich in both space and time, unlike the previous works discussed in Section 1.

Now that the preliminaries have been set up, we should consider how we formulate the problem. From (2.9) we find that the weak formulation is, noting that  $\eta$  and  $q$  are the test functions,

$$\sum_{\mathbf{K}} - \int_{\mathbf{K}} p \frac{\partial \bar{q}}{\partial t} + \underline{v} \cdot \nabla \bar{q} dV + \int_{\partial \mathbf{K}} p^- [\bar{q} n_t^+ + \bar{q} n_t^-] ds = \sum_{\mathbf{K}} \int_{\mathbf{K}} f_1 \bar{q} dV, \quad (2.11a)$$

$$\sum_{\mathbf{K}} - \int_{\mathbf{K}} v \frac{\partial \bar{\eta}}{\partial t} + p \nabla \cdot \bar{\eta} dV + \int_{\partial \mathbf{K}} v^- [\bar{\eta} n_t^+ + \bar{\eta} n_t^-] ds = \sum_{\mathbf{K}} \int_{\mathbf{K}} f_2 \bar{\eta} dV, \quad (2.11b)$$

where  $\eta$  is now a vector of two variables  $(\eta_1, \eta_2)$ . This subtle change to the weak formulation requires extra care when we compute these relevant gradients and divergences. Now we should note that we will be considering the enriched finite element method in 2.5 dimensions. Now we define the ansatz function for the pressure (noting the approximation for the velocity and the test functions are analogous),

$$p_h(\underline{x}, t) = \sum_m^{\tilde{T}} \sum_b^Q P_m \Pi(t)_m G_{j,m}^{(b)}(\underline{x}, t). \quad (2.12)$$

This is easily derived from the general FEM formulation (Section 2.1), with the multiplication of an enrichment function  $G(\underline{x}, t)$ ,

$$p_h(\underline{x}, t) = \sum_m^{\tilde{T}} \sum_{i,j}^N \sum_b^Q P_{j,m} \Lambda_{i,j}(\underline{x}) \Pi(t)_m G_{j,m}^{(b)}(\underline{x}, t), \quad (2.13)$$

where we include summations for space to account for the piecewise linear hat functions,  $\Lambda_{i,j}(\underline{x})$ . To arrive at (2.12) we simply need to bring the summation through onto the spatial hat functions, noting that  $\sum_{i,j} \Lambda_{i,j} = 1$ . We can easily apply the same idea to the matrices of the system. A reasonable question, at this point, is why would we want to remove the spatial hat functions? This is because we are computing a two-dimensional Fourier series, where  $P_m$  is a Fourier coefficient. As a result we are able to use a Fourier series approximation to populate a solution for all nodes in the problem. By this we mean that we take one node in space, due to the removal of the hat functions, and then solve the system with the appropriate enrichments before generalising the Fourier modes into solutions for any given domain.

### 3. Numerical Experiments

#### 3.1. Adaptive FEM

Here we will consider the applications of adaptive finite elements to a heat equation in a qualitative manner. We will see that the problem being considered has the introduction of a thermal insult in the centre of the circular domain, we should expect that the heat diffuses across the domain, in a somewhat uniform radial manner. If we first consider the static problem in a circular domain and with an initial condition of 0. We clearly see,

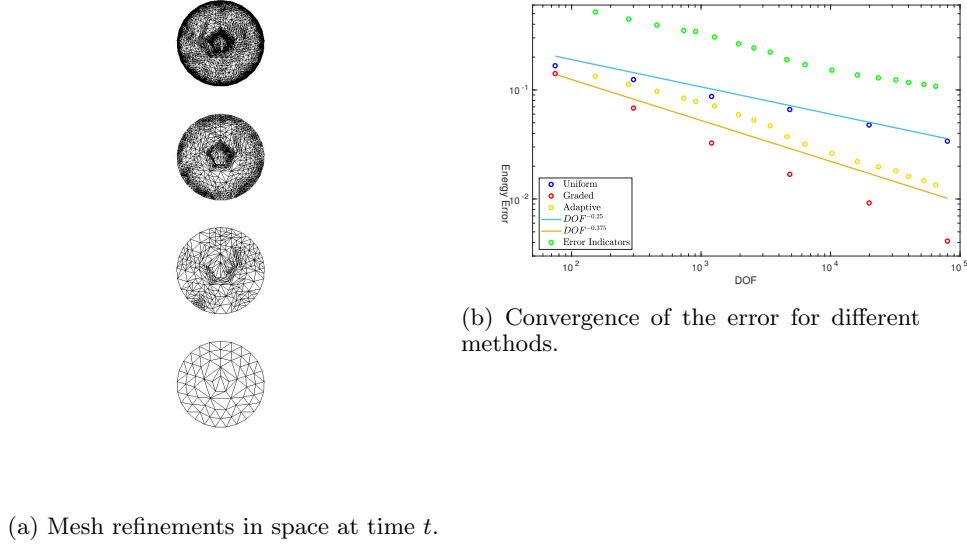
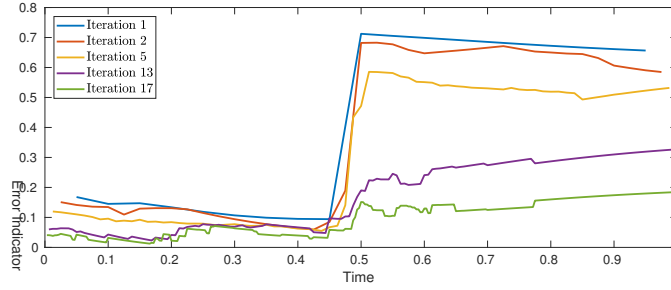


Figure 1: Implementation of an Adaptive Finite Element Scheme.


 Figure 2: Error indicators of adaptively refined meshes in time with the initial condition given by  $\tilde{u}_0$ .

as expected, that the meshes will refine rapidly in time. As the insult occurs; we expect a rapid increase in the number of elements around the *impact* point - Figure 2 This is expected as one would reasonably think that the error will increase at this time. Then when the heat transfer disperses we start to see some coarsening in the meshes as we no longer have the large errors which are found in the steep temperature gradients between elements. We can see that this refinement occurs in the following error plot.

Figure 1 shows how a static problem reacts to the introduction of a thermal insult. In the image we can that there is some clustering around the centre of the mesh, where the insult occurs. This is evidenced over four iterations above as we see the density of the mesh increasing in each step. We then see from Figure 1b that there is clear convergence within this method and that it is significantly quicker than the uniform FEM case. We see that the rates of convergence for the adaptive FEM is  $\frac{3}{8}$  compared to the uniform case of  $\frac{1}{4}$  so there is a significant speed increase on this method as expected. As a result we can clearly see that there are significant advantages of using adaptive FEM when we are considering problems associated with high explosives.

## 3.2. Enriched FEM for Wave Propagation

## 3.2.1. Gaussian Impact

Now we consider an applicable application in the form of a Gaussian Impact. We first define system (2.9) with the right hand side,

$$f(x, y, t) = \begin{cases} f_1(t)f_2(x, y) & \begin{cases} 0 < t < 2t_0 \\ (x - x_0)^2 + (y - y_0)^2 < R^2 \end{cases} \\ 0 & \text{otherwise} \end{cases}, \quad (3.14)$$

where  $f_1$  and  $f_2$  given by (Collino and Tsogka 2001),

$$f_1(t) = 4 \exp\left(-\pi^2 f_0^2 (t - t_0)^2\right), \quad (3.15a)$$

$$f_2(x, y) = \left(1 - \frac{(x - x_0)^2 + (y - y_0)^2}{R^2}\right)^3. \quad (3.15b)$$

Here  $t_0 = \frac{1}{f_0}$ ,  $f_0 = \frac{c_0}{hN_L}$  is the central frequency,  $N_L$  the number of points per wavelength,  $h$  is the mesh size and  $c_0$  is the wave-speed. Qualitatively this function represents a circular source centred at  $(x_0, y_0)$  which emits radial waves until the time reaches  $t = 2t_0$  and these will travel throughout the domain before *reflecting* (noting that the boundary conditions are periodic) back into the emitting wave - this will show the complex structure of interference patterns. This type of problem could therefore be related to many aspects in the real world, for example these could be in a mechanical regime whereby we might have an explosion or impact which expels a pressure wave - similarly to how we would expect an explosive to detonate. To successfully consider this problem we need to choose an appropriate set of enrichments functions. Noting that this problem will expel pressure waves, it is reasonable to choose a plane-wave in the following form:

$$G^{(\underline{b})}(\underline{x}, t) = \exp(i(\underline{k}^{(\underline{b})} \underline{x} + \omega^{(\underline{b})}(t - t_0))) = \exp(i(k_1^{(b_1)}x + k_2^{(b_1)}y + \omega^{(\underline{b})}(t - t_0))), \quad (3.16)$$

where  $\underline{k} = (k_1, k_2)$  are the wavenumbers,  $\omega$  is the frequency and  $\underline{b} = (b_1, b_2) \in \mathbb{Z}$  represents the differing combinations of enrichments. We should further establish that one must make a symmetric choice in the wavenumbers and the frequency. This means that for every  $k, \omega > 0$  we also chose its corresponding negative value such that  $-k, -\omega < 0$ . The reasoning behind this is it allows one to choose a larger number of frequencies as well as removing the complications from the additionally complex terms that are present within the enrichments. If we now consider the results of this experiment, for  $k \in [-10, 10]$  and  $\omega = |k|$ , we initially see that the pressure at the source is far larger compared to the other areas of the domain. As time progresses we see that the wave propagates radially in a uniform manner until the wavefront hits the boundaries of the region.

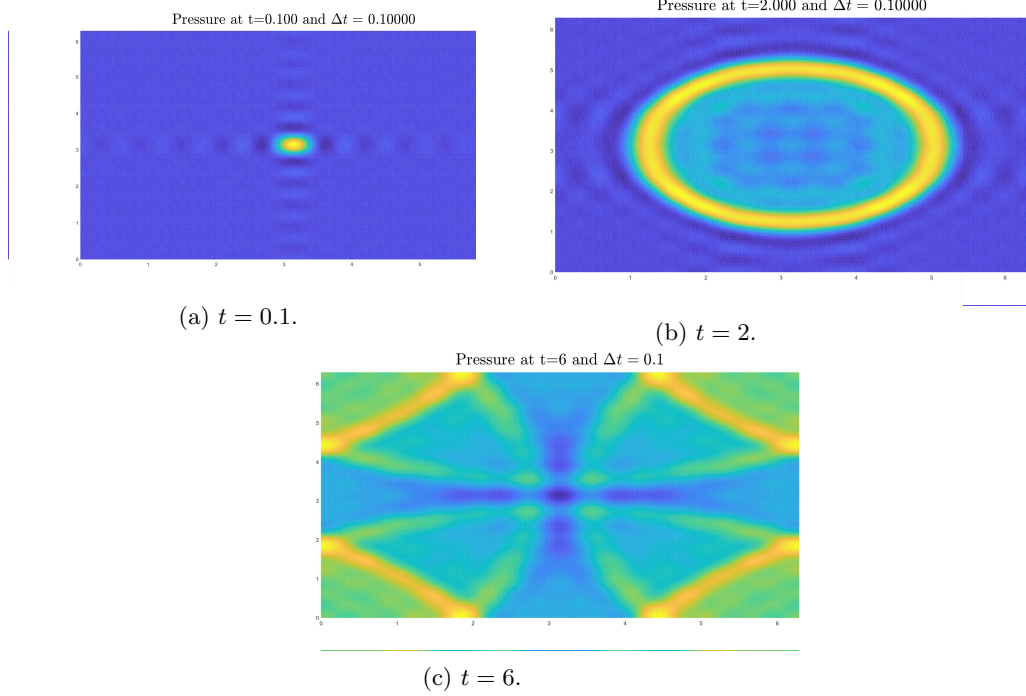


Figure 3: The time progression of the continuous Gaussian explosion over time for a space-time enriched FEM.

Once the wave ‘hits’ the boundary we see that the periodic boundary conditions causes a symmetric reflection on each corner. This then leads to both constructive and destructive interference, as we see in Figure 3c. This phenomena could be associated with a wave impacting a hard surface and reflecting back into a material, in a simplified manner. This approach could be further expanded by placing hard blocks of material in the domain to see how to pressure interacts and reflects.

#### 4. Conclusion

In this paper we have considered two problems: Adaptive FEM (Section 2.1) and Enriched FEM (Section 2.2) for thermal and mechanical problems respectively. The purpose of these approaches have been demonstrated by taking examples of thermal insults, say an external heating of a high explosive. As one can appreciate when an explosive is near its ignition energy we could expect a standard numerical scheme to struggle to capture the intricate nature of runaway whereas using adaptivity we see that we are able to resolve these complex dynamics. In a similar vein we see that Enriched FEM can comfortably capture the wavelike dynamics of a Gaussian explosion - consider an external mechanical insult on an explosive. The pre-requisite for this method is that we needed a priori information to include in the scheme as seen with the inclusion of symmetric plane waves. Then by the nature of the method we can generalise the Fourier modes to an arbitrary mesh - as seen in Figure 3. In future works we will look to consider enriched FEM with the inclusion of the spatial basis functions as well as looking to couple the thermo-mechanical problem.

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