FINITE ELEMENT COMPUTATION OF LINEARIZED THERMOELECTRIC EFFECTS WITH *p*-ADAPTIVITY

by

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LIST OF SYMBOLS

∇	Gradient
α	Seebeck coefficient (V/K)
φ	Voltage or electric potential (V)
T	Temperature (° C)
ν,β,ε	Coefficient of general partial differential equation for field problems
u	Field variable
Ω	Three dimensional domain
w	Weighting function
ξ	Basis function
Θ	Unknown for field variable approximation
$\mathbf{K}$	Element submatrix for multiphysics problems
$\mathbf{f}$	Source term for multiphysics problems
ρ	Material density (kg/m^3)
C	Specific heat density ($J/kg\cdot K$)
$\dot{q}$	Internal heat generation density (W/m^3)
$\mathbf{J}$	Electric current density (A/m^2)
$\mathbf{E}$	Electric field strength ($V\cdot m^{-1}$)
Π	Peltier coefficient tensor (V)
Θ	Thermal conductivity tensor ($W\cdot m^{-1}K^{-1}$)
ρ	Electric conductivity tensor ($S\cdot m^{-1}$)
$\mathbf{D}$	Electric flux density (C/m^2)
T_0	Reference temperature
$\|\cdot\|_{E(\Omega)}$	Energy norm
η	Error indicator

LIST OF ABBREVIATIONS

FEM	Finite element method
DOF	Degree of freedom
MEMS	Microelectromechanical system
3D	Three dimensional
TEG	Thermoelectric generator
TEC	Thermoelectric cooler
SORCG	Symmetric Successive Over-relaxation Conjugate Gradient
CGS	Constructive solid geometry
BC	Boundary condition

PENGIRAAN KAEDAH UNSUR TERHINGGA BAGI KESAN-KESAN THERMOELECTRIC SECARA LINEAR DENGAN KAEDAH MUDAH SUAI p

ABSTRAK

Dengan kemajuan dalam teknologi mikrosistem, penyelakuan multifizik di mana beberapa fizik berinteraksi antara sama satu lain menjadi semakin penting. Kecekapan dalam pengiraan dengan pelaksanaan kaedah unsur terhingga bagi penyelakuan ini juga menjadi semakin mencabar. Penyelidikan ini mengkaji kecekapan dalam pengiraan komputer terhadap masalah-masalah termoelektrik tiga dimensi di mana ia merangkumi dua sifat fizik iaitu suhu dan voltan. Pengiraan unsur terhingga ini telah dilaksanakan dalam pengaturcaraan komputer. Pada permulaan, satu set persaman pembezaan separa menakluk yang menguraikan kesan-kesan termoelektrik dirumuskan. Persamaan ini diterjemah kemudian kepada 'bentuk lemah' dengan menggunakan kaedah Galerkin. Untuk pengiraan komputer yang lebih cekap, persamaan ini juga dilinearkan dengan sesuatu suhu rujukan. Dengan menggunakan kaedah penggandingan terus, matriks sistem yang simetri dan positif pasti dapat dijanakan. Persamaan algebra sistem ini boleh diselesaikan dengan cekap menggunakan penyelesai *Conjugate Gradient with Successive Over-Relaxation* (SORCG). Selain itu, kaedah mudah suai *p* juga dilaksanakan untuk mengurangkan ralat pendiskretan. Penganggar ralat *a posteriori* digunakan untuk menganggar ralat tersebut. Walaupun penganggar ralat ini didapati tidak mengikut penumpuan teori dalam pemerhatian, tetapi ia memberitahui kualiti penyelesaian tempatan. Ini memenuhi keperluan untuk mengawal mudah suai *p* dengan cekap. Keputusan pengiraan komputer menyakini bahawa kaedah yang digunakan dalam penyelidikan ini dapat menyelesaikan masalah-masalah termoelektrik dengan betul tanpa membazirkan sumber tenaga komputer. Bagi dua kes ujian yang telah dijalankan, kaedah mudah suai *p* dibuktikan bahawa ia boleh memberi penyelesaian dengan lebih cepat iaitu faktor laju sebanyak 1.42 and 2.35.

FINITE ELEMENT COMPUTATION OF LINEARIZED THERMOELECTRIC EFFECTS WITH *p*-ADAPTIVITY

ABSTRACT

With advances in microsystem technology, multiphysics simulations in which more than one physical nature are considered become increasingly important and pose challenges on the efficiency of their implementations through the finite element method (FEM). The research work was to implement an efficient yet accurate FEM computation of thermoelectric problems where two natures, heat and electric potential mutually interact. A set of partial differential equations (PDEs) describing thermoelectric effects were first formulated for three dimensional problems and transformed into the weak form using the Galerkin's method. For a more efficient computation, constitutive thermoelectric equations were linearized with a reference temperature. Theoretically, the speedup of the linear approach is at least twofold of the nonlinear one. By using a direct or strong coupling, the method retains positive definiteness and symmetry of the system matrix. The algebraic equations were consequently amenable to the widely available matrix solver technology including preconditioned iterative solvers like the Conjugate Gradient with Successive Over-Relaxation (SORCG) method. Besides, *p*-adaptivity was implemented to reduce the discretization error by increasing the polynomial order of the approximation function in a similar manner as in single physics problem. The adaptivity strategy was achieved with an *a posteriori* error estimator, which was an explicit error estimation based on element-wise residuals and jumps at element boundaries. It was observed that although the error indicator did not fully contribute to theoretical convergence rate in error for three dimensional problems, it provided useful information on the quality of the local solution to effectively drive the *p*-adaptation. The method established in this work strongly suggests that the thermoelectric problems may well be computed with the *p*-adaptivity so that accurate results can be achieved without an excessive use of computational resources. For two test

cases in the work, the *p*-adaptivity is proven to be able to provide faster solutions with speed factors of 1.42 and 2.35.

Chapter 1
INTRODUCTION

1.1 Introduction

Most of the physical phenomena or systems in the world can be modeled by mathematics equations, for examples, structural dynamics, heat transfer, solid mechanics and electromagnetic waves. Most of the time, it is impractical or impossible to solve these equations exactly. In fact, they are usually solved by using numerical methods to obtain their approximate solutions. Finite element method (FEM) is widely considered one of the most powerful numerical methods designed for computer implementations. It is used to solve boundary value problems by dividing the solution domain into elements and by expressing the unknown field variable in terms of an interpolation function.

Over the last three decades, the rapid growth of the computational power has enable large problems which involve huge numbers of degree of freedoms (DOF) to be solved. Meanwhile, FEM computations become increasingly challenging when more complicated problems are considered especially for problems involving multiple natures. One of the most common practical applications in multiphysics simulations is in microelectromechanical systems (MEMS). It involves multiple fields such as the structural, the thermal, the fluidic and the electric. All fields are mutually influencing due to their coupling behavior. Therefore, a coupled approach is mandatory for these problems in order to obtain an accurate solution.

There are basically two types of coupling methods to solve multiphysics problems which are called the strong or full coupling and the weak coupling. The former solves for all fields simultaneously by coupling all constitutive equations to form a large equation (ANSYS Inc, 2007). The later solves each field separately by feeding previous solutions to each other and the problem is then solved again. This can be solved by a single physics solver and it takes a few iteration for all solutions to converge (Bengzon et al., 2007).

Thermoelectric effects are multiphysics phenomena which are commonly found in microelectronic devices like MEMS. These effects are important when thermoelectric materials such as the Bi_2Te_3 semiconductor are involved in the device (Patiño Lopez et al., 2004). A thermoelectric problem is a coupled field problem which involves two natures i.e. the thermal and the electric fields. In (Vokas and Kasper, 2009), FEM exhibits a great flexibility in solving coupled field problems including thermoelectric problems. However, challenges still exist in the efficiency of the multiphysics FEM implementation especially for three dimensional (3D) problems. This is because solving a 3D problem is computationally more expensive than a 2D problem due to the large number of DOF. In order to obtain an accurate solution, strong coupling FEM is often used to solve thermoelectric problems as in (Antonova and Looman, 2005) which again leads to a higher number of DOF. An overly larger number of DOF may result in an impractically long processing time or an inadequacy of computer memory. Thus the number of DOF has to be conserved in order to obtain a higher efficiency in the computation.

Besides, the time taken to solve a algebraic matrix equation given in a FE problem does not depend solely on the size of the matrix equation. For a problem with nonlinearity, nonlinear solver is required for the solution. The problem will be solved iteratively by the solver in a way that the latest solution is updated by the previous one until the solution converges. This certainly increases the computation time. Also, the nonlinear convergence reliability becomes a concern since the convergence might not be assured all the time. Therefore a linearized approach is more computationally economical and reliable for solving multiphysics problems.

As mentioned earlier, the solution time in FEM computation is depending on the number of DOF in the problem. Problems with larger numbers of DOF normally result in longer solution times. However, to obtain good accuracy in the solution, the number of DOF is usually being increased by using smaller elements or applying higher degree of interpolation functions. These methods are called *h*-refinement and *p*-extension. For multiphysics problems, numbers of DOF increase with numbers of fields as well. Giving the same mesh, the total number of DOF for a multiphysics problem is equivalent to that of a single physics problem multiplied by the number of nature. Not to compromise the solution accuracy, a good control on the number of DOF is still possible to improve the solution efficiency.

An interesting advance in FEM is the use of adaptation in the *h*-refinement and the *p*-extension which is called adaptive FEM. It has been proven to have a faster error convergence, ie. the error of the solution is minimized at a lower number of DOF. The idea of adaptive FEM is by estimating the error of the previous solution, decisions can be made whether to refine the mesh in an element-wise manner. This is called *h*-adaptive FEM. The *p*-adaptive FEM, another type of adaptive procedures, increases the polynomial degree of the interpolation functions (the element order) element-wise having the same goal with the *h*-adaptive FEM. However, *p*-adaptivity is found more effective against problems with smooth solution (Szabo and Babuska, 1991). In addition, the combination of both *h*-and *p*-adaptive procedures is called *hp*-adaptive FEM which can be the most effective method in dealing with high singularity problems.

This thesis discusses the implementation of FEM to solve thermoelectric problems using *p*-adaptation. The rest of this chapter introduces works that have been done to solve multiphysics scalar field problems and the scope of works. Some reviews of previous work about solving thermoelectric problems using FEM and error estimations of the FEM solution will be discussed in Chapter 2. Chapter 3 explains the theory of FEM formulation for thermoelectric problems and the theory of error estimations. The computer code implementation will be presented in chapter 4. Chapter 5 shows results obtained from several test cases to verify the computer code and the effectiveness of the *p*-adaptation in improving the solution efficiency. Conclusions and some future works can be found in the last chapter.

1.2 The need of adaptive FEM for multiphysics problems

With the advances in microsystem technology, challenges in computer simulations to solve multiphysics problems have been growing recently. FEM is arguably one of the best numerical methods for simulation to solve multiphysics problems because of its versatility and expandability. Since more than one nature are to be considered in a system, the problem grows larger. Hence, the size of the matrix equation expands vastly for multiphysics problems. This has imposed greater challenges in the computational efficiency. To achieve a good computational efficiency, a skillful meshing technique of the problem's domain is crucial. This is, however, time consuming and difficult to obtain an optimum mesh.

Adaptation in FEM has shown to be a good option in effective control of the quality of FEM solution and yet able to yield best possible solution efficiency. Refinements or extensions in *h*-, *p*- and *hp*-version are theoretically proven by Szabo and Babuska (1991) that they able to ensure a fast convergence of the error with respect to the increase of the number of DOF. With an error estimation, these procedures can be done automatically and effectively. The error can be estimated by calculating the residual of each element. These element residuals are then used to guide the adaptive procedure. This residual-based adaptation is believed able to ensure an optimum mesh.

1.3 Problem statement

Although there are many FEM software packages that provide solutions to multiphysics problems, they are different in their approaches. Efficiency of the solution is always a great challenge for numerical analysts. By using equivalent computational resources, the efficiency of the solution can be measured by the total time taken to complete the computation of the solution which is called the solution time. The solution time increases with the increase of number of DOF which is also the size of the system matrix. Larger problems have larger numbers of DOF. Therefore the solution time increases when the problem grows larger. Thus the control of the number of DOF is crucial to improve the solution efficiency. Given a single physics problem domain, the number of DOF grows when elements of the domain are *h*-refined or *p*-extended. For strongly coupled multiphysics problems, the growth of the number of DOF is amplified by the number of natures. In order to increase the computation efficiency by controlling the number of DOF, *p*-adaptivity is a very good option due to its maturity. In *p*-adaptivity, element orders are raised element-wise depending on the estimation of the element error. However, it still poses a lot of challenges in its implementation especially for three dimensional multiphysics problems. One of the challenges is the reliability and the efficiency of the error estimation in driving the *p*-adaptivity.

For a thermoelectric problem, the solution incorporates two field variables given by two natures which are the temperature and the voltage (electric potential). However, the computational cost for solving thermoelectric problems further rises due to the nonlinearity found in the constitutive PDEs. A nonlinear solver is usually used to solve the nonlinear thermoelectric problem. As a result, the solution time can be much longer than a linear solver due to the iterative computation that involved in the nonlinear solver. The linearization of the thermoelectric constitutive PDEs would be a convincing method to save computational resources. However, the linearized solution must be assured as close as possible to the nonlinear solution.

In previous works, three dimensional thermoelectric problems are normally computed using FEM without using higher order element and also *p*-adaptivity. For example, ANSYS, a commercial FE tool, uses only element orders up to 2 for the computation. This approach may limit the speed of error convergence with respect to the increase of the number of DOF. To further hasten the error convergence, higher element orders (*p*-extended) is strongly recommanded based on the theoretical proof by Szabo and Babuska (1991) and numerical proof by Abdul-Rahman (2008).

Although the *p*-adaptivity is already implemented for 2D thermoelectric elements in previous version of PolyDE (Vokas and Kasper, 2008; Vokas et al., 2011), some great challenges exist in its implementation in the 3D elements like the efficiency and the reliability of the error estimator used in the 2D elements. Another factor affecting the overall performance of the *p*-adaptivity is the number of adaptation steps. Since the computation load for 3D cases is much heavier than for 2D cases, the number of adaptation steps is much limited in order to achieve higher computation efficiency.

Besides, the previous approach in PolyDE by way of linearization of the thermoelectric effects totally neglect of the Joule heating. This work attempts to incorporate the Joule heating while avoiding nonlinear solution.

1.4 Goal and Objectives

The goal of this work is to solve steady state three dimensional thermoelectric problems with high-order adaptive finite element method efficiently. The achievement of the goal relies on the improvement of the speed of the error reduction with respect to the number of equations.

There are four objectives needed to be achieved. The first objective is to solve the governing PDE of the linearized thermoelectric problems using finite element method. This extends previous works in an in-house FE code named PolyDE from 2D thermoelectric elements to 3D thermoelectric elements. Besides, the 3D thermoelectric elements should now be taking Joule heating effect into account. The basis functions (also called shape functions) of order up to 4 of 3D single nature element from the previous works will be used in this work.

The second objective is to achieve a suitable error estimation for the thermoelectric elements. The error estimator should be able to estimate the local solution errors as well as the global solution error.

The third objective is to have the *p*-adaptivity implemented for the FE computation. By implementing the *p*-adaptivity, the *p*-version FE should be able to increase the element order locally which is driving by the error estimator.

The last objective is to achieve a faster error reduction compared to the conventional *p*-version FE implementation. Speedup of the FE computation is expected in this work.

1.5 Scope of work

The code development is based on an open source FE research code called PolyDE (Schober and Kasper, 2006). The work represents an extension of the code to solve 3D thermoelectric problems. The solution method includes high order tetrahedral elements and *p*-adaptivity. For an effective *p*-adaptive method, a specific choice of *a posteriori* error estimator is implemented. While the assessment of the efficiency of the implementation is of interest, the design aspect of a thermoelectric device is not emphasized. Thus parametric study of the thermoelectric device in this work is beyond the scope of the thesis.

The finite element analysis of the thermoelectric problem assumes steady state systems. The two field variables, the temperature and the voltage, are scalar. All the materials are assumed to be isotropic and temperature independent as well.

The finite element discretization is based on tetrahedral elements only. The scope of the code development covers the development of higher order thermoelectric elements. However, the domain discretization or meshing is excluded by utilizing existing open source code called Netgen (Schoberl, 2010, 1997).

Chapter 2
LITERATURE REVIEW

2.1 Introduction

Today's simulation technology tends to solve problems that take multiple natures into account which are called multiphysics or multi-nature problems. Simulation tools based on the finite element methods have become increasingly popular due to their high flexibility in helping engineers and researchers analyse various multiphysics phenomena such as thermoelasticity, thermoelectricity, electro-optics, etc. It has been observed that a lot of recent research efforts at solving field problems involve multiple natures, in which FEM is the most popular method used to solve these problems. For example, the investigation of design parameters of micro-thermoelectric generators by Jang et al. (2010) showed the capability of FEM in solving multiphysics problems, that is more specifically thermoelectric effects. (Turenne et al., 2010; Ziolkowski et al., 2010) are some other recent FEM applications in solving thermoelectric problems specifically to investigate the performance of thermoelectric generators. This simulation technology has contributed to rapid advances of thermoelectric devices like flexible thermoelectric modules (Mativo and Sirinterlikci, 2010; Shimizu et al., 2009).

A multiphysics problem can be solved by coupling equations from every physical nature to form a larger equation. This type of coupling method is called strong coupling or direct coupling (ANSYS Inc, 2007; Antonova and Looman, 2005). Vokas and Kasper (2008) used this approach to solve several coupled problems while demonstrating the viability of an adaptive method with such an approach. A multiphysics problem does not only consider more than one field variable but it involves mutual interactions among all natures. One of these examples is a thermoelectric problem. It involves thermal field and electrical field in a system where direct two-way interactions called thermoelectric effects take place.

Prior to discussing the implementation of FEM to solve thermoelectric problems, this chapter will introduce the theory of thermoelectricity and will elaborate previous attempts related to this simulation technology. Reviews on previous works in the formulation of error estimators and the implementation adaptive FEM will be discussed as well.

2.2 Thermoelectric effects

Thermoelectric effects are phenomena of energy conversion between heat and electrical energy. They include the Seebeck effect, the Peltier effect, the Thomson effect and the Joule effect (Gurevich and Logvinov, 2007). The Seebeck effect can be found in a simple thermocouple as illustrated in Figure 2.1. A and B represent wires made

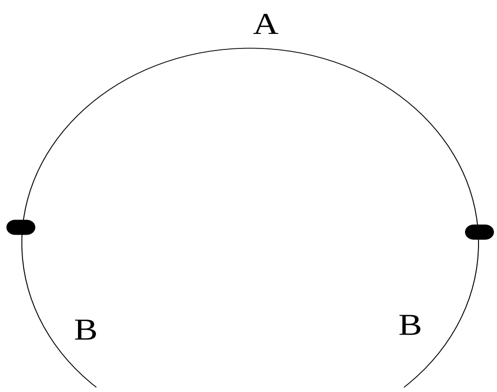

Figure 2.1: Thermocouple.

of different electric conducting materials connected together to form two junctions of different materials. When both junctions are given different temperature value while keeping both free ends of B at the same temperature, electric potential will be generated between both free ends of B. This phenomenon is called the Seebeck effect. The electric potential is linearly depending on the temperature difference (Cochran and Babin, 2007) which is given by

$$\alpha = \frac{d\varphi}{dT} \tag{2.1}$$

where α denotes the Seebeck coefficient, φ denotes the electric potential and T denotes the temperature.

The Peltier effect can be said as the opposite of the Seebeck effect. When a current flows from one free end of B to another, a temperature difference can be found at the two junctions. In other words, one junction will be heated and another will be cooled. The Thomson effect interrelates the Seebeck effect and the Peltier effect. It causes reversible cooling and heating when there exists both a temperature gradient and a flow of current across a material (Goldsmid, 2009).

Thermoelectricity is the electricity generated from heat attributed to the Seebeck effect. This can be observed by subjecting thermal gradient to a thermoelectric material such as doped semiconductors. Researchers are today paying attention at the development of this technology due to its advantages to the environment. One such energy harvesting device is often called thermoelectric generator (TEG) (Turenne et al., 2010; Ziolkowski et al., 2010). In the design of a TEG, FEM simulation packages like ANSYS are usually used to calculate the approximate power gain and its efficiency. For example, Strasser et al. (2004) used ANSYS in the design of micro-machined CMOS TEG to compare the power generated by using two different materials. As opposed to TEGs, TECs produce heating and cooling by consuming electricity (Han et al., 2006; Van Dessel and Foubert, 2010). Basically, a thermoelectric cooler (TEC) can be the same structure as a TEG. These thermal fluxes are caused by a current when it flows through two different materials. These fluxes are not caused by any external or internal heat sources. Thus the Peltier effect is thermodynamically reversible. The change from heating to cooling or vice versa can be done by changing the direction of the current. Gurevich and Logvinov (2007) explained this reversible process in detail.

Despite the low efficiency of thermoelectric devices, their miniature sizes have gained prevalence in many applications such as microchip coolers. In addition, recent research on thermoelectric materials found in (Gonçalves et al., 2009) may potentially improved the performance of those devices. Yet, those reversible thermoelectric effects are always coming with irreversible thermoelectric phenomena namely the Joule effect and the thermal conduction. For this reason, a proper design of a thermoelectric device is very important. Hence reasonably accurate modeling of the thermoelectric behavior is desired.

Thermoelectric coupling can be first modeled using its constitutive partial differential equations (PDE) and then solved by numerical methods like the finite element method. (Gurevich and Logvinov, 2007; Fragoso et al., 2005) are some works that studied the constitutive PDE of the thermoelectric coupling in recent years. Among various types of numerical methods, FEM has shown many applications in research solving two and three dimensional thermoelectric problems. (Van Duyn and Munter, 1992) is an early approach that uses FEM to analyse thermoelectric effect in sensors. (Perez-Aparicio et al., 2007) is another recent work which implemented two dimensional thermoelectric coupling in finite elements. His work was motivated by the device miniaturization toward nanomechanics where multiphysics plays an important role in the thermal interaction and the residual stress. The explanation for the importance of the multiphysics consideration in nanomechanics was found in (Rochus, 2006) based on the scaling laws. In addition, Jaegle (2008) showed the implementation of the thermoelectric field equation in COMSOL which uses a general PDE similar to that of a research code PolyDE (Schober and Kasper, 2006).

PolyDE is a FE software initially developed at the Institute of Micro Systems Technology, Hamburg University of Technology. It is able to solve 2D multiphysics problems which emphasizes on providing solutions to field problems in microsystems. Previous works done by Vokas and Kasper (2008) to solve thermoelastic problems and thermoelectric problems and also by Schober and Kasper (2007) to solve electromagnetic problems have shown the versatility of using FEM to solve multiphysics problems. However, PolyDE is restricted to only two dimensional problems. For industrial-strength FE software package, Antonova and Looman (2005) proved ANSYS to be a good FEM tool to solve thermoelectric problems with its coupled field elements. However, solving the thermoelectric problem using ANSYS requires a nonlinear solver due to the nonlinearity found in the thermoelectric governing equations. Furthermore the resulting system matrix is not symmetric. Thus the overall computation by the nonlinear solver can be very time consuming and it may take multiple iterations for the solution to converge.

Although the wide applications of FEM in solving multiphysics problems, the computational cost of the simulation is seldom discussed. As time is one of the important costs in computer simulation, the necessity of the use of the nonlinear solver in solving thermoelectric problems is still arguable. In fact, linearization is possible and also desirable in order to obtain a faster solution especially for three dimensional problems due to their large matrix equations. Yet, acquiring symmetric and positive definite system matrices from the PDE system can enable a faster linear solver (Van Der Vorst, 1987).

2.3 The coupling of different natures

The art of modeling a multiphysics problem is at describing with reasonable accuracy the way how different physics are interrelated. One can see a multiphysics problem as a phenomenon that consists of many interdependent systems. Consider a thermoelectric problem that involves the heat conduction and the electrical conduction. To solve this problem, each system can be solved separately and iteratively by mutually passing information. The iterations are then ended at the acceptable level of solution convergence. Such procedures are called the weak coupling (ANSYS Inc, 2007). Preis et al. (2006) solved a thermal-electromagnetic problem which was found in a transformer. The electromagnetic equations were first solved to obtain the current density within the transformer. With the current density as the heat source, the thermal conduction equation was then solved. These steps were repeated after recalculating the temperature dependent electrical conductivity in the electromagnetic equations.

On the other hand, one can see a multiphysics problem as a single system where all equations are solved simultaneously. This is known as strong or direct coupling. Unlike the weak coupling, the solution generated by this method is absolute. Besides, convergence problems faced in the iterative computation of the weak coupling can be avoided by using the strong coupling method. This method was found widely used in the simulation of thermoelectric effects (Antonova and Looman, 2005; Vokas and Kasper, 2009; Sandoz-Rosado and Stevens, 2010). However the computation time required by this method is predicted to be longer than the weak coupling due to the larger matrix equation (Angeleri et al., 1989). In fact the size of the matrix equation can be reduced by other means like proper selection of element order and element size. Therefore strong coupling is still highly suggested for multiphysics problems with strong interactions between different natures such as thermoelectric problems. The direct coupling of thermoelectric finite element formulation will be discussed in Chapter 3.

2.4 High order finite elements and *p*-adaptivity

By using higher degree of basis functions (also interpolation functions), higher order finite elements are obtained. The simplest element is the linear element which is also called the first order element. It uses the linear basis function to interpolate the approximate FE solution within an element. A linear one dimensional element has two degree of freedoms (DOF) which are located at both ends while a linear tetrahedral element has four DOF located at each vertex. With the increase of the degree of the basis function, the order of the element increases equally. The higher order elements will give better interpolation of the solution by adding more DOF to the element (Warburton et al., 1999). These additional DOF will be given to the edges, the faces or the body depending on the element order. Detailed explanation about the distribution of DOF for an tetrahedral element is found in Section 4.3.2.

There are a few types of basis functions such as Lagrange basis functions, Hermitian basis functions and hierarchical basis functions (Akin, 2005). Although the Lagrange basis functions are most commonly used, the hierarchical basis functions are more suitable for *p*-adaptivity owing to its simplicity in the implementation. Section 3.5 will discuss the hierarchical basis function in detail.

p-adaptivity is a method designed to automatically control the increase of element order (Babuška et al., 1981). Since higher order elements are computationally expensive, effective control of the element order is important to obtain an optimal number of DOF with respect to the solution error. It is usually steered by an estimate of the solution error to determine the element which needs a higher order element (Babuska and Suri, 1994). Often, the element with high error estimate will be given a higher order element. The adaptation process is iterative and it stops only if any of stopping criteria is reached. Certainly the error estimate will serve as one of the stopping criteria. Other possible stopping criteria are the number of iteration and maximum number of DOF.

2.5 Errors in finite element method

FEM provides only approximate solutions to mathematical models which are always described in partial differential equations. Although the FE solution u_{FE} is always made to be comparable to the exact solution u_{EX}, it is still inevitably subjected to errors. There are two types of errors in computer based solution, the discretization error and the round-off error. Often, the round-off error is insignificant but the discretization error can be large. The discretization error can be described as an error resulting from the polynomial approximation of the solution (Szabo and Babuska, 1991). This error is normally reduced by decreasing the element size which is known as *h*-refinement or by increasing the polynomial order which is known as *p*-extension but at the expense of the computation time. Time is a critical cost in simulation. As a result, a wise decision has to be made to stop the refinement. The error itself is the only criteria for this. Since the exact solution is not known, the true error, $u_{EX} - u_{FE}$, is certainly not known. Therefore the estimate of the error is used. After almost two decades of research, it has shown a concrete advance in the estimation of the discretization error. This error estimation is called *a posteriori* error estimation.

2.6 Advances of error estimates

Following the earliest *a posteriori* error estimation that used for ordinary differential equations, Babuška and Rheinboldt (1978a) started their pioneering attempt in FEM for two point elliptic boundary value problems . This technique measures the error in an energy norm (always represented by η_K) of each element K. Results obtained in (Babuška and Rheinboldt, 1978b) and (Babuška and Rheinboldt, 1981) had contributed to the development of adaptive meshing procedures that are designed for the automatic error reduction. This technique also represents the foundation of explicit error estimates. Further development can be seen in (Verfürth, 1989) where the error estimator was used for the Stokes equation. It was also proven that the explicit error estimator can be used for driving the adaptive FEM by Verfürth (1994). Extensive applications of this estimator in linearized and nonlinear elasticity problems are also summarized in (Verfürth, 1999). A recent review by Segeth (2010) attested that the explicit residual-based error estimator has better suitability for linear second order elliptic equations. Besides, there are some new breed of techniques which are categorized as implicit error estimators. These error estimators are based on the element residual method which can be applied in a variety of problems in physics and mechanics suggested in (Demkowicz et al., 1984) and (Demkowicz et al., 1985). Contemporarily, Bank and Weiser (1985) proposed three similar error estimators of the same category for elliptic PDEs with Neumann boundary conditions.

In 1987, Zienkiewicz and Zhu (1987) introduced another type of error estimators using the recovery based method. This technique assesses the error by comparing the smoothed gradients to the original gradients. The lack of robustness had brought this technique impractical. The improved gradients do not always assure better solutions and it may be worse. Furthermore it is proven effective only for smooth problems when interpolation functions is of $p = 1$ by Carstensen and Funken (2001). Five years later, Zienkiewicz and Zhu successfully improved their error estimators by using the so-called superconvergent points and named this approach as the superconvergent patch recovery technique in (Zienkiewicz and Zhu, 1992a) and (Zienkiewicz and Zhu, 1992b). It was found that there exists points within elements which have more accurate derivatives. These points are able to converge faster to the true value. However, this approach is not effective against problems with material discontinuities.

From the above, there are generally three types of *a posteriori* error estimators: explicit error estimators, implicit error estimators, and recovery-based error estimators. Explicit error estimators are comparatively easier to implement because the error is calculated based on norm of the local residual. Of course, its drawback is the lack of accuracy in comparison to implicit error estimators. In practical applications, an explicit error estimator can still be a wise choice due to its good efficiency in driving the adaptive FEM. On the contrary, implicit error estimators produce higher accuracy of the actual error but it imposes heavier computations. The local error is computed based on the solution of additional auxiliary problems. This means that boundary value problems are locally solved again either on a small patch of elements (subdomain residual method) or on one single element (element residual method) after knowing the local residual and the flux at the boundary (Grätsch and Bathe, 2005).

Studies of the robustness of *a posteriori* error estimators have been done intensively after reaching the maturity in the end of 20th century. Detailed explanation on fundamental theory of explicit, implicit *a posteriori* estimators and estimators that based on gradient recovery can be found in (Ainsworth and Oden, 1997). Of note is their effectiveness on steering the adaptive FEM is case dependent. More importantly, the study of the adaptive FEM on multiphysics problems is still lacking and specifically on thermoelectric problems is rather scarce. A previous attempt by (Larson and Bengzon, 2008) has proven the feasibility of adaptive FEM in solving multiphysics problems.

This approach used multiple solver to solve each nature and passed solutions to others. Similar approaches also found in (Demkowicz et al., 2010). Their approaches are different from the case in this work which uses the direct coupling method. The direct coupling method is expected to be more reliable because it inherently avoids error propagation and accumulation.

In 2005, Schober and Kasper (2007) proved that the residual-based explicit error estimator is sufficient for controlling *h*-, *p*-, and *hp*-adaptation processes for two dimensional electromagnetic propagation problems. Their results show that the problem can be solved by using an optimal number of DOF and hence an optimal computation time can be obtained. The error estimation is based on the local residual error and the jump of the gradient at the element boundary. The L2 norm of the elemental error is then used to steer the *hp*-adaptivity. The numerical result has proven the reliability of the explicit error estimator in steering adaptivity in FEM.

In summary, the explicit error estimator is a more practical approach to guide the adaptive FEM due to its simplicity in implementation and less calculation involved compared to the implicit error estimator. In adaptive FEM, the computational cost imposed by the calculation of the error estimate is a critical factor in determining the success of the adaptive strategy. Heavy computation of the error estimate can lead to a higher computational cost in adaptive FEM than the non-adaptive FEM. However the implementation of the explicit error estimators may be different in their formulations such as the use of different coefficients depending on the type of problems. After the survey, an efficient error estimator is yet to be tailored for the strongly coupled three dimensional thermoelectric problems.

2.7 Finite Element Softwares

Although most of the existing FE softwares like ANSYS and COMSOL are able to solve three dimensional thermoelectric problems, an effient implementation of *p*-adaptivity using high order elements is not found yet. Therefore the in-house FE software, PolyDE, was selected for the implementation and also as a test platform. In order to speed up the computation, PolyDE solves two dimensional thermoelectric problems using the linear approach in which the nonlinear terms describing the Joule effect and the Thomson effect are neglected. As compared to ANSYS, the nonlinear approach is able to yield more accurate result by considering the Joule effect.

PolyDE solver for three dimensional problems covered only single physics problems before this work is being carried out. Thus this work extends the previous works in PolyDE from two dimensional to three dimensional multiphysics elements. Besides, the Joule effect is linearized to a constant for this work to obtain more accurate results.

Chapter 3
FINITE ELEMENT FORMULATION FOR THERMOELECTRIC PROBLEMS

3.1 Introduction

This chapter explains all formulations that used in the computer implementation of finite element method (FEM) to solve thermoelectric problems. It first explains the weak formulation of the thermoelectric constitutive equations. The error estimation of the solution will be discussed next and followed by elaborations on *a posteriori* error estimators and error indicators. The last part of this chapter explains hierarchical basis functions.

3.2 Weak formulation of partial differential equation using Galerkin method

A general field problem can be represented mathematically by a partial differential equation (PDE) (Vokas and Kasper, 2008).

$$-\nabla \cdot (\nu \nabla u) + \beta \nabla u + \varepsilon u = f + \nabla \cdot \vec{g} \tag{3.1}$$

Referring to the left hand side of Eq. (3.1), ν, β and ε are coefficients describing the material properties. For single physics problems, ν is a rank 2 tensor, β is a rank 1 tensor and ε is a scalar constant. The right hand side of Eq. (3.1) describes source terms of the PDE where f is a scalar constant and $\vec{g}$ is a rank 1 tensor. Refer Appendix B for explanation on tensor. In order to include interactions between different natures for multiphysics problems, Eq. (3.1) has been expanded to the following PDE.

$$-\nabla \cdot (\nu_{ij} \nabla u) + \beta_{ij} \nabla u + \varepsilon_{ij} u = f_i + \nabla \cdot \vec{g}_i \tag{3.2}$$

The coefficients ν_{ij}, β_{ij}, ε_{ij}, f_i and $\vec{g}_i$ are now given additional indices i and j that denote the nature. Note that ν_{ij}, β_{ij} and α_{ij} with unequal indices contain the material properties that describe interactions between natures.

For thermoelectric problems, the constitutive PDEs consist of the heat equation and the continuity of electric charge (Antonova and Looman, 2005) which is given by Eqs. (3.3) and (3.4).

$$\rho C \frac{\partial T}{\partial t} + \nabla \cdot \mathbf{q} = \dot{q} \tag{3.3}$$

$$\nabla \cdot \left(\mathbf{J} + \frac{\partial \mathbf{D}}{\partial t} \right) = 0 \tag{3.4}$$

where $\mathbf{q}$ is the vector of heat flux in (w/m^2), ρ is the density in (kg/m^3), C is the specific heat capacity in (J/(kg $\cdot$ K)), $\dot{q}$ is the internal heat generation density in (w/m^3), $\mathbf{J}$ is the electric current density in (A/m^2), $\mathbf{D}$ is the electric flux density in (C/m^2). Note that $\mathbf{q}$, $\mathbf{J}$ and $\mathbf{D}$ are vectors in R^3.

By comparison of the coefficients in Eqs. (3.3) and (3.4) to the general coefficients β_{ij}, ε_{ij} and g_i in Eq. (3.2), we find that $\{\beta_{ij}, \varepsilon_{ij}, g_i\} = 0$. Therefore, the PDE is simplified to

$$-\nabla \cdot (\nu_{ij} \nabla u) = f_i \tag{3.5}$$

To solve Eq. (3.5) using FEM, the Galerkin method is used in which it first transforms the PDE into its weak form by the method of weighted residuals (Akin, 2005). By multiplying a weighting function w_q and integrating both side of Eq. (3.5), its weak form is reached:

$$\int_\Omega (-\nabla \cdot (\nu_{ij} \nabla u)) w_q d\Omega = \int_\Omega (f_i) w_q d\Omega \tag{3.6}$$

According to the Galerkin's method, the variable u can be approximated by u^* such that

$$u^* = \sum_{r=1}^{n} \xi_r \Phi_r \tag{3.7}$$

where ξ_r is the basis function, Φ_r is the unknown and n is the total number of basis functions. The weighting function is also given to be equivalent to the basis function,

$w_q \equiv \xi_q$. Rewriting Eq. (3.6),

$$\int_\Omega -\nabla \cdot (\nu_{ij}(\sum_{r=1}^{n} \nabla\xi_r \Phi_r)\xi_q d\Omega = \int_\Omega \sum_{q=1}^{n} f_i \xi_q d\Omega \tag{3.8}$$

We assume that the material properties is isotropic, i.e. the material property values are identical for all direction. Applying integration by part on the left hand side of Eq. (3.8) leads to

$$\sum_{r=1}^{n} \int_\Omega -\nu_{ij} \nabla\xi_r \nabla\xi_q \Phi_r d\Omega = \sum_{q=1}^{n} \int_\Omega f_i \xi_q d\Omega, \qquad q = \{1,2,\ldots,n\} \tag{3.9}$$

Writing Eq. (3.9) in matrix form for a two nature problems where $i, j = 1,2$,

$$\begin{bmatrix} \mathbf{K}_{11} & \mathbf{K}_{12} \\ \mathbf{K}_{21} & \mathbf{K}_{22} \end{bmatrix} \begin{Bmatrix} \Phi_{1,r} \\ \Phi_{2,r} \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \end{Bmatrix} \tag{3.10}$$

given

$$\mathbf{K}_{ij} = \int_\Omega \sum_{r=1}^{n} \nu_{ij} \nabla\xi_r \nabla\xi_q d\Omega, \qquad q = \{1,2,\ldots,n\}$$

$$\mathbf{f}_i = -\int_\Omega \sum_{q=1}^{n} f_i \xi_q d\Omega$$

Note that $\mathbf{K}_{ij}$ is the square element stiffness matrix while $\Phi_{i,r}$ and $\mathbf{f}_i$ are the unknown vector and the load vector for nature $i = \{1,2\}$.

To apply the thermoelectric constitutive equations in Eq. (3.10), the weak form has to be obtained by using the Galerkin's method mentioned above. The coupling between the heat flux $\mathbf{q}$ and the electric flux $\mathbf{J}$ is given by the thermoelectric constitutive relations as stated in (Antonova and Looman, 2005) and (Jaegle, 2008)

$$\mathbf{q} = \Pi \cdot \mathbf{J} - \Theta \cdot \nabla T \tag{3.11}$$

$$\mathbf{J} = \sigma \cdot (\mathbf{E} - \alpha \cdot \nabla T) \tag{3.12}$$

where $\mathbf{E}$ is the electric field strength in ($\mathrm{V} \cdot \mathrm{m}^{-1}$), Π is the Peltier coefficient tensor in (V), Θ is the thermal conductivity tensor in ($\mathrm{W} \cdot \mathrm{m}^{-1}\ \mathrm{K}^{-1}$), σ is the electric conductivity tensor in ($\mathrm{S} \cdot \mathrm{m}^{-1}$) and α is the Seebeck coefficient tensor in (V/K). For steady state heat flow, Eq. (3.3) becomes