DEVELOPING SOFTWARE PACKAGES FOR ELECTROMAGNETIC SIMULATIONS*

J. Xu#, M. Min, and B. Mustapha, ANL, Argonne, IL 60439, U.S.A.

Abstract

In addition to previous developments on parallel beam dynamics software packages, our efforts have been extended to electromagnetic simulations. These efforts include developing new software packages solving the Maxwell equations in 2D and 3D for time domain and eigenvalue simulations. This paper focuses on software packages for eigenvalue simulations. These new solvers are based on high order numerical methods. Comparative studies of different expansion bases, continuous and discontinuous GALERKIN methods will be discussed. Benchmarks and simulation results will be presented at the end.

INTRODUCTION

Most current high energy particle accelerators make use of electromagnetic fields to accelerate charged particles. Therefore, accurate electromagnetic simulations have great importance in the success of accelerator modeling. Most accelerating devices have resonating Radio Frequency (RF) fields, which needs to solve eigenvalues of the Maxwell's equation. Many different numerical methods have been successfully used for electromagnetic simulations, such as finite difference method (FDM), finite volume method (FVM), finite element method (FEM), etc. Due to its flexibility, FEM has been broadly applied in EM simulations [4, 7]. Standard nodal based FEM produces spurious modes which troubled researchers for long time. These problems come from the poor representation of the large null space of the curl operator. In 1980's Nédélec proposed revolutionary vector bases which overcome this difficulty. There are some commercial software packages available now, but most of them only run on desktop computer. With peta and exa scale supercomputers arrive, efficient methods need to be sought for fully making use of them. There are also some groups currently making efforts in this direction but definitely need more. For better understanding the performance of nodal and vector bases, we have developed both eigen solvers based on nodal and vector bases. Benchmarks and comparisons will be given. The eigen solver with the Nédélec vector base has been applied in a real resonator simulation.

MAXWELL'S EQUATION

Consider the Maxwell's equations in general three dimensional domain Ω, with vacuum we have:

$$\frac{\partial \vec{D}}{\partial z} = \nabla \times \vec{H} - \vec{J}, \qquad \nabla \cdot \vec{D} = \rho \tag{1}$$

$$\frac{\partial \vec{B}}{\partial z} = -\nabla \times \vec{E}, \qquad \nabla \cdot \vec{B} = 0 \tag{2}$$

$\rho(\vec{x},t)$ is the charge distribution, and the current $\vec{J}(\vec{x},t)$ related to the electric field $\vec{E}(\vec{x},t)$ through Ohms law, $\vec{J} = \sigma\vec{E}$, where σ is the finite conductivity. The electric field $\vec{E}(\vec{x},t)$ and the electric displacement $\vec{D}(\vec{x},t)$, the magnetic field $\vec{B}(\vec{x},t)$ and the magnetising field $\vec{H}(\vec{x},t)$ have the following constitutive relations:

$$\vec{D} = \varepsilon\vec{E} = \varepsilon_0\varepsilon_r\vec{E}, \qquad \vec{B} = \mu\vec{H} = \mu_0\mu_r\vec{H} \tag{3}$$

Here ε_r and μ_r are relative permittivity and permeability of the material respectively. For our simulations of vacuum, they are both equal to one. The permittivity ε_0 and permeability μ_0 satisfy $c^2 = 1/(\varepsilon_0\mu_0)$.

Transforming the fields into the Fourier space,

$$\hat{\vec{E}}(\vec{x},t) = \int_{-\infty}^{\infty}\vec{E}(\vec{x},t)e^{-i\omega t}d\omega, \quad \hat{\vec{H}}(\vec{x},t) = \int_{-\infty}^{\infty}\vec{H}(\vec{x},t)e^{-i\omega t}d\omega \tag{4}$$

Then the Maxwell's equation can be written in curl-curl form as:

$$\nabla\times\nabla\times\hat{\vec{E}} = \mu\varepsilon\omega^2\hat{\vec{E}} = \frac{\omega^2}{c^2}\hat{\vec{E}} = \lambda\hat{\vec{E}}, \qquad \nabla\cdot(\varepsilon\hat{\vec{E}}) = 0 \tag{5}$$

$$\nabla\times\nabla\times\hat{\vec{H}} = \mu\varepsilon\omega^2\hat{\vec{H}} = \frac{\omega^2}{c^2}\hat{\vec{H}} = \lambda\hat{\vec{H}}, \qquad \nabla\cdot(\mu\hat{\vec{H}}) = 0 \tag{6}$$

For perfect electrically conducting (PEC) wall, the boundary conditions for the fields satisfy:

$$\vec{n}\times\hat{\vec{E}} = 0, \qquad \vec{n}\cdot\hat{\vec{H}} = 0 \tag{7}$$

NUMERICAL METHOD

We have studied different numerical methods for the eigenvalue computation. These include using different expansion bases and different numerical methods. These methods are explained first in the following, then benchmarks and comparisons of them will be present in the next section.

The first two eigen solvers are based on the nodal Finite Element Method (FEM) [2, 3, 5]. Nodal FEM uses nodal expansion bases, which is one at particular node and zero at all other nodes. Detailed information can be found at [3]. The difference of the first two eigen solvers is that they adopt different numerical methods. The first one uses continuous GALERKIN (CG) method, and the second one uses discontinuous GALERKIN (DG) method. The third eigen solver is based on the Nédélec vector base which shows some advantages over the previous two.

Nodal Bases with CG and DG Methods

For CG method, the weak form of the eigenvalue problem is as following:

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#jin_xu@anl.gov

For fixed $\alpha > 0$, find $(\lambda, \vec{\tilde{E}}) \in R \times P_n^3(D)$, such that $\vec{\tilde{E}} \neq 0$ and

$$(\nabla \times \vec{\tilde{E}}, \nabla \times \vec{\phi})_\Omega + \alpha(\nabla \cdot \vec{\tilde{E}}, \nabla \cdot \vec{\phi})_\Omega = \lambda(\vec{\tilde{E}}, \vec{\phi})_\Omega \quad (8)$$

The local stiffness matrix has the following form, which are mapped to different locations in the global stiffness matrix.

	ϕ_x	ϕ_y	ϕ_z
ϕ_x	$\frac{\partial}{\partial z}\frac{\partial}{\partial z}+\frac{\partial}{\partial y}\frac{\partial}{\partial y}$	$-\frac{\partial}{\partial x}\frac{\partial}{\partial y}$	$-\frac{\partial}{\partial x}\frac{\partial}{\partial z}$
ϕ_y	$-\frac{\partial}{\partial y}\frac{\partial}{\partial x}$	$\frac{\partial}{\partial z}\frac{\partial}{\partial z}+\frac{\partial}{\partial x}\frac{\partial}{\partial x}$	$-\frac{\partial}{\partial y}\frac{\partial}{\partial z}$
ϕ_z	$-\frac{\partial}{\partial z}\frac{\partial}{\partial z}$	$-\frac{\partial}{\partial z}\frac{\partial}{\partial y}$	$\frac{\partial}{\partial x}\frac{\partial}{\partial x}+\frac{\partial}{\partial y}\frac{\partial}{\partial y}$

DG method was first proposed in [6], and became popular recently. A thorough review of this method can be found in [1, 3]. For DG method, first we define the jump of function $\vec{f}$ across the boundary surface as:

$$[\vec{f}] = \vec{f}(\vec{x}^-) - \vec{f}(\vec{x}^+) \quad (9)$$

, where $\vec{f}(\vec{x}^-)$ represents the local field, while $\vec{f}(\vec{x}^-)$ represents the neighbouring field. Two integration operators are needed for DG method, they are:

$$(\tilde{\nabla}_D \times \vec{\tilde{E}}, \vec{\phi})_\Omega = (\nabla \cdot \vec{\tilde{E}}, \vec{\phi})_\Omega - \sum_k \left(\frac{a^+}{a^+ + a^-} \vec{n} \times \left[\vec{\tilde{E}}\right], \vec{\phi}\right)_{\partial D^k \setminus \partial\Omega} - \left(\vec{n} \times \left[\vec{\tilde{E}}\right], \vec{\phi}\right)_{\partial D^k \cap \partial\Omega} \quad (10)$$

$$(\tilde{\nabla}_N \times \vec{\tilde{E}}, \vec{\phi})_\Omega = (\nabla \cdot \vec{\tilde{E}}, \vec{\phi})_\Omega - \sum_k \left(\frac{a^+}{a^+ + a^-} \vec{n} \times \left[\vec{\tilde{E}}\right], \vec{\phi}\right)_{\partial D^k \setminus \partial\Omega} \quad (11)$$

Then the Maxwell's equation can be written as:

$$\lambda(\vec{\tilde{E}}_N, \vec{\phi})_D = (\tilde{\nabla}_D \times \vec{\phi}, \vec{p}_N)_D - \tau(\vec{n} \times \left[\vec{\phi}\right], \vec{n} \times \left[\vec{\tilde{E}}_N\right])_{\partial\Omega} \quad (12)$$

$$(\vec{p}_N, \vec{\phi})_D = (\tilde{\nabla}_N \times \vec{\tilde{E}}, \vec{\phi})_D \quad (13)$$

This is the weak form of the eigenvalue problem for the DG method which is different than for CG.

Nédélec Vector Bases

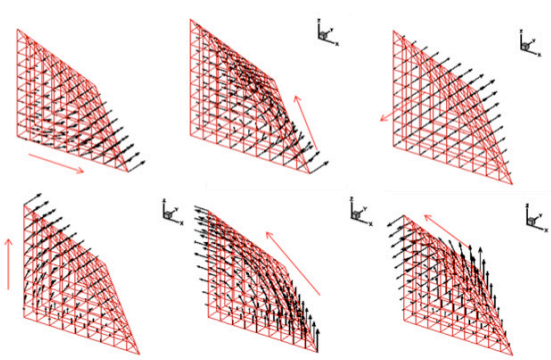

Figure 1: 6 Nédélec Edge Vector Bases with P=0 on 3D tetrahedron element.

During the history of computational electromagnetics, people have found that there are many shortcomings associated with traditional nodal base and CG method. Our investigation with the CG method has verified this, while DG method also shows some inefficiency which will be shown in the comparisons below. Therefore, we tried Nédélec vector base also. There are many different types of bases, and we choose the hierarchical Nédélec vector base introduced in [8]. 2D bases will be introduced first and then 3D bases.

The 2D Nédélec vector bases from the $H^p(curl)$ space can be divided into the following subspaces:

$$H^p(curl) = \underbrace{W^1_{tv,e,ng} \oplus \nabla W^{p+1}_{s,e}}_{W^p_{tv,e}} \oplus \underbrace{W^{p+1}_{tv,f,ng} \oplus \nabla W^{p+1}_{s,f}}_{W^p_{tv,f}}$$

It consists of different order edge, face vector bases. The edge and face vector bases can also be divided into gradient and non-gradient types. In order to make it complete in order p for both the vector and curl bases, we need the bases complete in order p-1 plus (p+1)-th gradient bases and non-gradient bases. The total degree of freedom is (P+1)(P+3).

The 3D Nédélec vector bases from the $H^p(curl)$ space can be divided into the following subspaces:

$$H^p(curl) = H^0(curl) \oplus \underbrace{\nabla(W^{p+1}_{s,e} \oplus W^{p+1}_{s,f} \oplus W^{p+1}_{s,v})}_{p\text{th-order gradient bases}} \oplus \underbrace{(W^{p+1}_{tv,f,ng} \oplus W^{p+1}_{tv,v,ng})}_{(p+1)\text{th-order non-gradient bases}}$$

It consists of different order edge, face, and volume vector bases. The edge, face, and volume vector bases can also be divided into gradient and non-gradient types. In order to make it complete in order p for both the vector and curl bases, it needs bases which are complete in order p-1 plus (p+1)-th gradient bases and non-gradient bases. The total degrees of freedom is (P+1)(P+3)(P+4)/2. Figure 1 shows the 6 edge vector bases on 3D tetrahedron element.

All three methods will be used to solve the general eigenvalue problem $A \cdot \vec{x} = \lambda B \cdot \vec{x}$. ARPACK software has been used as well as new solvers been developed with the standard ARNOLDI and LANCZOS algorithms. In order to improve the convergence rate, shift-and-invert method has been used.

BENCHMARKS AND SIMULATION RESULTS

Benchmarks

First we test our first and second eigenvalue solvers based on nodal bases and using CG and DG methods. The domain is a box $\Omega = (0,0.8421) \times (0,0.5344) \times (0,0.2187)$. The analytical solution is $\lambda = 48.4773$. Table 1 shows the first eigenvalue computed with CG and DG methods. Although the results are close, there are many spurious modes and it is hard to identify the correct one.

Next, we test our third eigen solver using the Nédélec vector base. As can be seen in Table 2, with low order P (<2), accurate eigenavlues can be obtained, and there is no spurious mode. But with P=2, there still exist some spurious modes, which need to be investigated more in the future. Using 55k tetrahedron elements, very accurate results have been obtained.

Table 1: The First Eigenvalue with CG and DG Methods

P=4	CG	DG
λ	48.4765	48.9599

Table 2: The first 5 Digenvalues with Nédélec Vector Base on box $[-1, 1]^3$.

Mode	Theory	P=0, E=203	P=1, E=203	P=2, E=203	P=0, E=55k
1	4.935	4.828	4.856	4.909	4.935
2	4.935	4.909	4.869	4.929	4.934
3	4.935	4.945	4.870	4.930	4.934
4	7.402	7.132	7.140	4.940*	7.395
5	7.402	7.376	7.183	5.391*	7.396

Comparisons

Besides spurious modes free, using the Nédélec vector base has other advantages as shown in Table 3. DG solver has the largest global degree of freedom, which is about 6~10 times larger than using the Nédélec vector base. This brings many difficulties in the matrix inversion which is the most time consuming part. From this study, we can see that the DG method has some shortcoming in dealing with eigenvalue simulation.

Table 3. Degree of Freedom for Different Methods with Different Order P

P	CG	DG	Vector Base
3	537	4902	165
4	2094	10184	1038
5	6618	18310	3231

Application

At last we have applied the third eigen solver for the simulations of a Half Wave Resonator (HWR) shown in Fig.2. The mesh has been partitioned to 256 processors. The result has been compared with CST MWS, and given in Table. 4. Close result has been obtained. It is also found that high order P brings many challenges on the speed and convergence of the simulations which needs to also be improved in the future.

Table 4. Comparison of the First Eigenvalues of HWR

Solver	New	CST MWS
Mesh (k)	5.765	500
P	0	N/A
CPU	256	1
Frequency (MHz)	235.7	234.4

SUMMARY

This paper presents our efforts on developing parallel eigen solvers with different numerical methods. This includes using nodal bases with CG and DG methods, as well as using Nédélec vector bases on 3D tetrahedron element. ARPARCK software as well as self developed solvers has been used to extract eigen values in these three different eigen solvers. Similar to previous researchers, we found that both CG and DG eigen solvers produce spurious modes, and it is hard to separate them from the true physical modes. Using the Nédélec vector base can overcome this, but there are still spurious modes when using high order P. The new eigen solver using Nédélec vector base has been used for a HWR simulation, and correct results have been obtained. This work provides many future research areas and makes a solid ground for future developments and applications of electromagnetic modeling for accelerators.

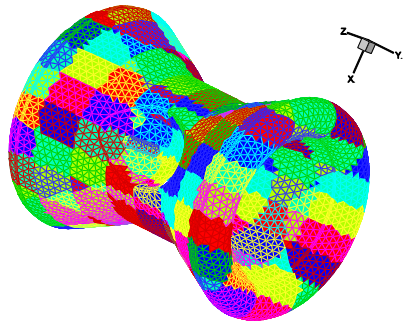

Figure 2: Partition mesh (256) for Half Wave Resonator (E=120k)

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