Curved mesh correction and adaptation tool to improve COMPASS electromagnetic analyses

Xiaojuan Luo¹, Mark Shephard¹, Lie-Quan Lee², Cho Ng² and Lixin Ge²

¹Rensselaer Polytechnic Institute, Troy, NY 12180, USA ²Stanford Linear Accelerator Center (SLAC), Menlo Park, CA 94025, USA

E-mail: xluo@scorec.rpi.edu, shephard@scorec.rpi.edu, liequan@slac.stanford.edu,cho@slac.stanford.edu and lge@slac.stanford.edu

Abstract. SLAC performs large-scale simulations for the next-generation accelerator design using higher-order finite elements. This method requires using valid curved meshes and adaptive mesh refinement in complex 3D curved domains to achieve its fast rate of convergence. ITAPS has developed a procedure to address those mesh requirements to enable petascale electromagnetic accelerator simulations by SLAC. The results demonstrate that those correct valid curvilinear meshes can not only make the simulation more reliable but also improve computational efficiency up to 30%.

1. Introduction

SLAC has been successfully taking advantage of higher-order finite elements [1] to perform analyses for the design of next-generation accelerators which are regarded as critical to basic energy research [2, 3, 4]. The short-range wakefield calculations in electromagnetic analysis using the higher-order elements requires the meshes must be properly curved to the 3D complex geometric domains and adaptively control refinement around the particles beams that need sufficiently smaller mesh size than the rest of the domain. The common straight-sided mesh generation procedures [5, 6] can not automatically generate valid curvilinear meshes to meet those requirements. The invalid curved meshes or overrefined meshes lead to infeasibly large problem sizes, inaccurate results, or possible failure of the simulations. The DOE SciDAC center ITAPS has been working with SLAC to develop a procedure that applies Bezier mesh curving and size-driven technologies to address these mesh requirements. SLAC has successfully applied this procedure to generate meshes used in accelerator simulations. The results yield stable and reliable time-domain simulations and improve computational efficiency up to 30%.

2. Curved mesh correction and mesh adaptation dontrol tool

This section discusses the two key technical components – curved mesh correction and adaptive mesh refinement control – to generate valid curvilinear meshes that improve COMPASS electromagnetic analyses.



Figure 1. Bezier control points for a quadratic tetrahedral region.



Figure 2. Computation of det(J) indicates that the mesh entities M_0^0, M_0^1, M_1^1 and M_2^1 are key mesh entities.

2.1. Curved mesh correction

The common approach to the construction of curved meshes is to apply a straight-sided mesh generation procedure [5, 6] and then curve the mesh edges and faces on the curved domain boundaries to the proper orders. This approach takes advantage of the conventional unstructured mesh generators to deal with the complexity of model geometry. However, the resulting meshes may become invalid because the curving of the mesh entities to model boundaries can lead to negative determinants of the Jacobian in the closures of curved elements. The curved mesh correction tool we developed applies Bezier polynomial representations [9] to define hierarchic higher-order shapes for topological mesh entities in their parametric coordinates. Figure 1 shows the Bezier control points for a quadratic tetrahedral region; $b_{|i|}^q$ are the control points used to define the shapes of the Bezier mesh edges, faces, and regions, and |i| = i + j + k + l is the control point net index of a higher-order tetrahedral region in its parametric coordinates $\boldsymbol{\xi} = (\xi_i, \xi_j, \xi_k, \xi_l), \xi_i + \xi_j + \xi_k + \xi_l = 1.$

The Bezier higher-order shapes provide an effective means to form a general validity check algorithm for curved elements. The algorithm takes advantage of the convex hull property to ensure that a valid curved element always has positive determinants of the Jacobian in its closures [7]. Given a qth-order Bezier tetrahedron mesh region, the determinant of the Jacobian J can be represented as

$$det(J) = \sum_{|\mathbf{i}|=r} C^r_{|\mathbf{i}|} c^r_{|\mathbf{i}|} \boldsymbol{\xi}^{|\mathbf{i}|}, \qquad (1)$$

where r = 3(q-1). $C_{|\mathbf{i}|}^r$ and $c_{|\mathbf{i}|}^r$ are the coefficients computed by the control points $b_{|\mathbf{i}|}^q$. The convex hull property of Bezier polynomial indicates [9],

$$\min(c_{|\mathbf{i}|}^r) \le \det(J) \le \max(c_{|\mathbf{i}|}^r).$$

$$\tag{2}$$

Therefore, a curved tetrahedral region is valid in its closure as long as $min(c_{|\mathbf{i}|}^r) > 0$.

The Bezier curved mesh correction tool processes invalid curved elements one at a time by applying a set of local mesh modification operations on the key mesh entities. The computation of the determinants of the Jacobian can provide useful information to determine the key mesh entities and appropriate operations to correct the invalidity. As an example, figure 2 shows an invalid quadratic tetrahedral region, which has a negative determine of Jacobian at control point b_{2000} . Since the control points $b_{2000}, b_{1100}, b_{1010}$, and b_{1001} affect the computation of det(J), the mesh entities M_0^0, M_0^1, M_1^1 , and M_2^1 associated with those control points are key mesh entities,



Figure 3. Before (left) and after (right) refinement of a quadratic curved mesh edge M_0^1 on model edge G_0^1 . New mesh edges M_1^1, M_2^1 have been appropriately curved to the model boundaries.

and applying local mesh modifications on any of them can effectively make the curved element valid. Curved meshes for more complex domains used by SLAC for electromagnetic linear accelerator analysis are shown in Section 3.

2.2. Moving mesh adaptation control in curved domains

The size=driven mesh adaptation procedure [8] has been successfully applied in cardiovascular blood flow simulations [10], metal forming process [11], wave propagation simulations [12], and the other studies, and the results have demonstrated that computational efficiency can be substantially improved b using the isotropic or anisotropic adapted meshes to effectively resolve solution fields. The procedure has been extended to deal with curved meshes for higher-order finite elements to track the needed refinement around the particle beams for short-range wakefield time-domain electromagnetic simulations. The extended procedure maintains the existing functionalities developed for straight-sided meshes such as vertex-based size field specifications and selective local mesh modification applications [8]. In addition, the following two steps have been added in when the mesh is curved.

- The validity check algorithm described in equation 2 must be applied when the affecting cavities for a local mesh modification operation have curved mesh entities. This step ensures that resulting curved meshes are valid after applying the selected local mesh operation.
- Any newly created mesh entities on the curved domain boundaries must be properly curved to the model boundaries to ensure that the geometric approximation of the resulting adapted meshes is maintained. As an example, figure 3 shows the results of the procedure to split a quadratic curved mesh edge M_0^1 that is classified on the curved model edge G_0^1 . The two new created mesh edges M_1^1 and M_2^1 are also curved to the model edge G_0^1 .

Moving adaptively refined meshes for SLAC to perform short-range wakefield electromagnetic simulations is shown in Section 3.

3. Analysis results

3.1. Curvilinear meshes for FETD electromagnetic simulation

The wakefield effects of an 8-cavity cryomodule for the proposed International Linear Collider (ILC) are studied by using the FETD method. Figure 4 shows a snapshot of the electric field distribution excited by a beam in the ILC cryomodule. A curved mesh with 2.97 million quadratic isoparametric tetrahedral elements is used in this FETD simulation, resulting in about 20 million degrees of freedom. The simulation used 256 multistream processors on the Cray-X1E, a leadership-class facility at Oak Ridge National Laboratory. It took a total runtime of

300 wall-hours through multiple jobs with checkpointing for a complete run. Half a terabtye of data was generated.

From the initial given curvilinear mesh 1,583 invalid curved elements have been corrected by using the procedure discussed in Section 2.1. Figure 5 shows the curved mesh for one cavity of the model and the closeup mesh before and after curving.

The corrected curvilinear mesh not only leads to a stable time-domain simulation but also reduced computational cost by 30%.



Figure 4. Snapshot of the electric field distribution excited by a beam in an 8-cavity cryomodule for the proposed International Linear Collider.



Figure 5. Curved mesh for one cavity, closeup mesh before and after curving, and local mesh cavity before and after applying edge swap to correct the invalid element.

3.2. Moving adaptive refined meshes for short-range wakefield calculations

A series of moving adapted meshes in a curved domain was generated by using the procedure described in Section 2.2 for short-range wakefield calculations by SLAC. Figure 6(a) shows the geometric model, which has some complex components in the middle of the domain. The initial location of the beam is at the left end of the domain, the desired mesh size inside the particle dense mesh is 1 and the size for the rest of the domains is 10. Figure 6 shows the moving adapted meshes up to step 5 to track the moving particle beams. The adaptively refined meshes have around $1 \sim 1.15$ million elements comparing to the uniform refined mesh with 6.5 million elements if the mesh size inside the particle beam domains is applied in the entire domain. The increase of the number of elements in the middle of domain is due to the complex geometries as shown in Figure 6(a). The computation effort of short-range wakefield calculations using the moving adaptive refined meshes can reduce by one order of magnitude compared to the uniformly refined mesh.

4. Conclusion

This paper has presented a procedure to track moving adaptive mesh refinement in curved domains. The procedure is capable of generating suitable curvilinear meshes to enable large-scale accelerator simulations. The procedure can generate valid curved meshes with substantially fewer elements to improve the computational efficiency and reliability of the COMPASS electromagnetic analyses. Future work will focus on the scalable parallelization of all steps for petascale simulations.



Figure 6. Moving adapted meshes in curved domain for short-range wakefield simulation.

Acknowledgments

This work is supported by U.S. Department of Energy under DOE grant number DE-FC02-06ER25769 and DE-AC02-76SF00515.

References

- [1] Babuska I, Szabo BA and Katz IN 1981 Int. J. Numer. Meth. Engng. 18(3):515-545
- [2] Akcelik V, Ko K, Lee LQ, Li ZH, Ng CK and Xiao LL 2008 J. Comput. Physics 227(3):1722–1738
- [3] Xiao L, Adolphsen C, Akcelik V, Kabel A, Ko K, Lee LQ, Li Z and Ng CK 2007 in Proc. of 2007 Particle Accelerator Conference
- [4] Lee LQ, Akcelik V, Chen S, G LX, Prudencio E, Schussman G, Uplenchwar R, Ng C, Ko K, Luo XJ and Shephard MS 2007 J. of Physcis: Conference Series 78:012040
- [5] CUBIT geometry and mesh generation toolkit. http://cubit.sandia.gov
- [6] Simmetrix Inc. Enabling simulation-based design. http://www.simmetrix.com
- [7] Luo XJ, Shephard MS, Obara RM, Nastasia R, Beall MW 2004 Engineering with Computers 20:265-285
- [8] Li XR, Shephard MS and Beall MW 2005 Comp. Meth. Appl. Mech. Engng. 194:4915-4950
- [9] Farin G 1992 Curves and Surfaces for Computer Aided Geometric Design. Academic Press
- [10] Sahni O, Muller J, Jansen KE, Shephard MS. and Taylor CA (2006) Comput. Methods Appl. Mech. Engrg. 195(41-43):5634–5655
- [11] Wan J 2006 An Automated Adaptive Procedure for 3D Metal Forming Simulations. PhD Thesis, Rensselaer Polytechnic Institute, New York
- [12] Chevaugeon N, Hillewaert K, Gallez X, Ploumhans P and Remacle JF 2007 J. Comput. Physics 223(1):188– 207