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A PARALLEL TIME DOMAIN THERMAL SOLVER FOR TRANSIENT ANALYSIS OF ACCELERATOR CAVITIES*

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Abstract

Simulation of thermal effects in accelerator cavity is normally performed assuming steady state solution where a static thermal solver suffices to evaluate temperature gradients and impacts on mechanical design. However, during the rf pulse ramp up or the machine system cooldown process, when the field in the cavity changes rapidly, transient effects need to be taken into account. Although commercial software packages are available to handle these kinds of transient effects, they become less effective for solving large-scale problems arising from the fine details of a geometry or at the system scale. A time domain thermal solver has been developed in the parallel finite element multi-physics code suite ACE3P with integrated electromagnetic, thermal and mechanical modeling capabilities. The implementation takes advantage of the parallel computation infrastructure of ACE3P and shares most of the ingredients in mesh generation, matrix assembly, time advancement scheme and postprocessing. In this paper, we will outline the finite element formulation of the transient thermal problem and verify the implementation against analytical solutions and existing numerical results. The thermal solver has also been coupled to ACE3P mechanical solver, allowing stress and strain analysis during the transient stage. Application of the transient thermal solver to realistic accelerator cavities will be presented.

INTRODUCTION

SLAC has been developing the parallel finite element electromagnetics simulation suite ACE3P (Advanced Computational Electromagnetics 3D Parallel) [1, 2] for accelerator modeling using high performance computing (HPC) platform. A key advantage of the method is the conformal (tetrahedral) mesh for high-fidelity representation of geometry, and further accuracy can be obtained through the use of quadratic surface and high-order elements (orders 1–6) resulting in reduced computational cost. An equally important advantage is the power of parallel processing, which both increases memory and speed, allowing large problems to be solved in far less time through scalability. The application modules in ACE3P include electromagnetics in frequency and time domains, particle tracking, and multi-physics analysis with integrated electromagnetic, thermal, and mechanical effects. ACE3P primarily runs on the National Energy Research Scientific Computing Center (NERSC) supercomputers [3] and its modules have demonstrated favorable scalability using thousands of compute cores. ACE3P multi-physics modeling capabilities have been disseminated to the user community [1], and its further development has been driven often by computational needs of users. In this paper, we present a new modeling capability in ACE3P by expanding the present static thermal solver to include transient effects for studying temperature time evolution in accelerator cavities.

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THERMAL STATIC SOLVER

The multi-physics capabilities of ACE3P have been applied to the analysis of complex accelerator structures and systems. Often the analysis includes the electromagnetic modules Omega3P or S3P for field calculations in a cavity, thermal solvers in TEM3P for heat loads determination and mechanical solvers in TEM3P for deformation or displacement calculations of the cavity closure. Figure 1 shows the temperature calculation for a simplified rf gun cavity [4]. The accelerating mode is first determined by the eigenmode solver Omega3P and then the electromagnetic fields at the vacuum-metal interface are used as boundary conditions for the thermal solver in TEM3P to calculate the temperature distribution in the metal cavity walls.

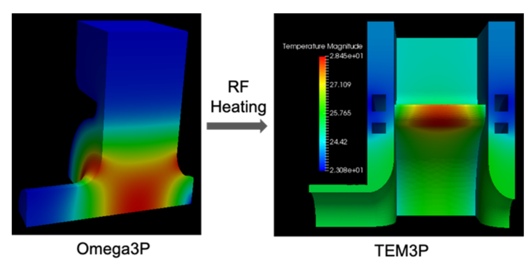

Figure 1: Temperature distribution in cavity enclosure due to rf fields of the cavity accelerating mode.

Parallel computation using ACE3P has enabled calculations of large complex geometries including all relevant fine details of accelerator component design, providing critical analysis for prototyping and installation of the component in accelerator. A recent application of TEM3P static thermal solver to the LCLS-II spare rf gun is presented in another paper in these proceedings [5]. In this application, the cavity enclosure is modeled using a mesh with 2.2 M elements, corresponding to about 7 M degrees of freedom in solving a linear system of equations. The runtime was 40 minutes using 640 compute cores on NERSC Cori supercomputer, demonstrating the efficient performance of ACE3P's parallel computation.

THERMAL TRANSIENT SOLVER

While static analysis can address most thermal analysis for accelerator cavities, the development of a thermal solver in the time domain will provide additional useful evaluation during the transient of a thermal evolution process. Below we will present the details of the implementation of a thermal transient solver in ACE3P. The validity of

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the code development is benchmarked against an analytical solution and an application example.

Heat Diffusion Equation

The heat diffusion equation for governing the temperature evolution is described in Eq. (1) [6]

$$c\rho \frac{\partial T}{\partial t} = \nabla \cdot (k\nabla T) + Q_V \quad \text{in } \Omega, \tag{1}$$

$$T = T_0 \qquad \text{on } \Gamma_D \ \text{(Dirichlet)}, \tag{2a}$$

$$\kappa \frac{\partial T}{\partial n} = q_0 \qquad \text{on } \Gamma_N \ \text{(Neumann)}, \tag{2b}$$

$$-\kappa \frac{\partial T}{\partial n} = h(T - T_f\,) \quad \text{on } \Gamma_h \ \text{(Robin)}. \tag{2c}$$

Here c, ρ and κ are the specific heat capacity, mass density and thermal conductivity of a material, respectively. Q_V sets volumetric heat sources. Eq. (1) is subject to different types of boundary conditions, which may be time dependent. Eq. (2a) is the Dirichlet boundary condition for a fixed temperature, Eq. (2b) the Neumann boundary condition for a fixed heat flux, and Eq. (2c) the Robin boundary condition for heat convection due to temperature difference, respectively. At steady state, the left-hand side of Eq. (1) vanishes, and hence the static temperature solution is controlled by the material thermal conductivity κ. The time evolution during transient is descrribed by additional material parameters c and ρ.

Finite Element Formulation

In the finite element discretization scheme, the spatial domain is divided into a number of elements. The temperature T in an element is expanded as the summation of nodal basis functions N_i with coefficient T_i as $T = \sum_i T_i \, N_i$. In the weak form of the finite element method, Eq. (1) is cast into a matrix representation given by

$$\sum_{i=1}^{n} [M_{ji} \frac{\partial T_i}{\partial t} + K_{ji} T_i] = f_j, \tag{3}$$

where M is the mass matrix (volume integral involving scalar product of 2 basis functions), and K includes the stiffness matrix (volume integral involving scalar product of 2 gradient basis functions) and the temperature dependence matrix (surface integral) in the Robin boundary condition, and f concatenates all possible heat sources, respectively. The time evolution is advanced with a time step Δt using the unconditionally stable backward Euler scheme [7], which leads to

$$\left(\frac{1}{\Delta t}[M^{n+1}] + [K^{n+1}]\right)\{T^{n+1}\} = \frac{1}{\Delta t}[M^{n+1}]\{T^{n}\} + \{f^{n+1}\}. \tag{4}$$

For static solution, the first terms on both sides of Eq. (4) vanish and the solution is equivalent to that of a Poisson equation. The time domain implementation takes advantage of the finite element framework such as parallel matrix assembly and data structures for time advancement that has been in place in ACE3P time domain electromagnetic module. The task of assembling the additional mass matrix M can also be readily performed using existing code components. The object-oriented code structure in C++ renders a fast implementation of the transient solver. The solution of Eq. (4) at every time step is obtained by solving a large sparse linear system $Ax = b$ using an iterative solver in ACE3P software library.

Verification of Time Evolution Constant

The validity of the time domain algorithm is verified using a simple example of a sphere with an initial temperature (25 ºC) subject to a background temperature (200 ºC) as shown in Fig. 2. A Robin boundary condition is imposed on the sphere surface allowing it to reach the background temperature through heat convection. The plot in Fig. 2 shows the time evolution of the sphere temperature whose approach to steady state is governed by the material properties of the sphere. The temperature at a time can be evaluated by analytical formula [8]. Perfect agreement is observed between ACE3P and the analytical value, verifying the correct calculation of the time evolution constant.

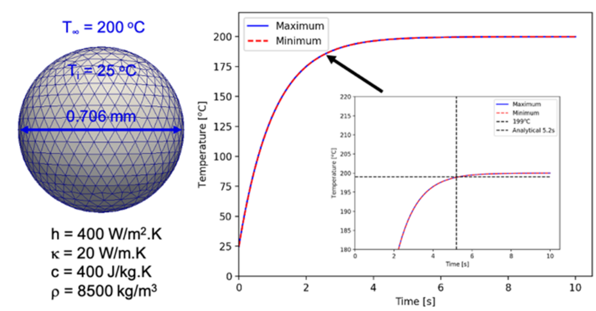

Figure 2: (Left) Simulation model and material properties; (Right) Maximum and minimum temperatures in sphere as a function of time, with insert showing agreement with analytical solution at a time step.

Time Domain Simulation

The transient thermal solver is applied to the simplified rf gun example used for static temperature calculation in a previous section. The initial temperature of the cavity is set to a room temperature of 25 ºC. The heat source is due to rf heating from the accelerating mode on the copper wall surface. Two cooling channels on each side above the cavity iris are used to suppress the temperature increase from surface rf heating and the cooling surfaces are imposed as Robin boundary condition with the water ambient temperature at 22 ºC. For simplicity, the rf heating source and the Robin boundaries are assumed to be time independent. Figure 3 shows the minimum and maximum temperature inside the cavity enclosure as a function of time. It can be seen that they start with the initial temperature and evolve to steady state values, which are in good agreement with

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those obtained by the static solver. Figure 4 shows the steady state temperature distribution, which exhibits the same pattern as that obtained from the static solver.

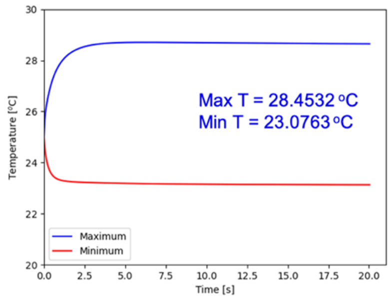

Figure 3: Evolution of minimum and maximum temperatures inside rf gun cavity.

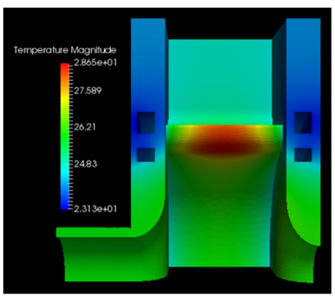

Figure 4: Temperature distribution at steady state.

COUPLING TO MECHANICAL SOLVER

The multi-physics module TEM3P can perform integrated electromagnetic, thermal and mechanical simulations. Once the temperature distribution is calculated by the thermal solver, it can be fed into the mechanical solver to calculate mechanical stress and structural displacement. This has been implemented in the static multi-physics solvers. In a similar manner, the transient thermal solver has been enabled to couple to the static mechanical solver. The instantaneous temperature distribution at a time step of the thermal time evolution is input into the mechanical solver to determine the mechanical quantities. Since the mechanical solution takes more computer time to obtain than the thermal solution, the mechanical calculation can be sampled at a larger time interval than the time step. Using the simplified rf gun cavity, we performed mechanical calculation at specified time intervals by including as loading the temperature distribution obtained from the thermal transit solver as well as Lorentz force due to the electromagnetic force of the accelerating mode. Figure 5 shows the maximum of the cavity displacement as a function of time sampled at every 50 time steps. Figure 6 shows that the displacement distribution of the cavity. Again, the displacement calculations at steady state agree with those using the static mechanical solver [4].

CONCLUSION

A parallel time-domain thermal solver has been added to the multi-physics simulation suite ACE3P. Further development will include the proper treatment for the rise of external sources and boundary conditions. The tool will provide fast and high-fidelity simulation to address transient effects in cavity design and its operation reliability.

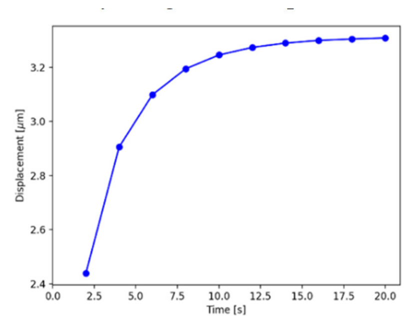

Figure 5: Evolution of maximum displacement of cavity.

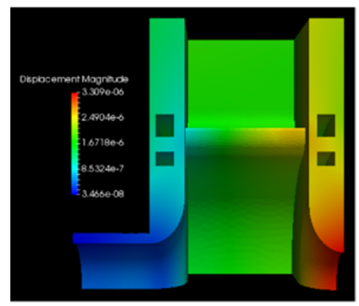

Figure 6: Displacement distribution at steady state.

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