ADVANCED COMPUTATIONAL RESEARCH IN MATERIALS PROCESSING FOR DESIGN AND MANUFACTURING

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INTRODUCTION

Advanced mathematical techniques and computer simulation play a major role in providing enhanced understanding of conventional and advanced materials processing operations. Development and application of mathematical models and computer simulation techniques can provide a quantitative understanding of materials processes and will minimize the need for expensive and time consuming trial- and error-based product development. As computer simulations and materials databases grow in complexity, high performance computing and simulation are expected to play a key role in supporting the improvements required in advanced material syntheses and processing by lessening the dependence on expensive prototyping and re-tooling. Many of these numerical models are highly compute-intensive. It is not unusual for an analysis to require several hours of computational time on current supercomputers despite the simplicity of the models being studied. For example, to accurately simulate the heat transfer in a 1-m³ block using a simple computational method requires 10¹² arithmetic operations per second of simulated time. For a computer to do the simulation in real time would require a sustained computation rate 1000 times faster than that achievable by current supercomputers. Massively parallel computer systems, which combine several thousand processors able to operate concurrently on a problem are expected to provide orders of magnitude increase in performance. This paper briefly describes advanced computational research in materials processing at ORNL. Continued development of computational techniques and algorithms utilizing the massively parallel computers will allow the simulation of conventional and advanced materials processes in sufficient generality.

HIGH PERFORMANCE COMPUTING

In recent years, significant advances have been made in high performance computing. Figure 1. shows the evolution of computers over the last fifty years from early mechanical machines to the current generation state-of-the-art massively parallel machines.¹ As shown in the figure, with the emergence of scalable parallel machines, we are fast approaching TerraFlop level of computational power. These machines will provide unprecedented opportunities for the solution of coupled multi-physics problems in materials processing.

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Figure 1. Evolution of computing.

At ORNL, researchers have the choice of several parallel computing platforms ranging from the 16 processor IBM SP2 and 64 processor Kendall Square KSR1 to several Intel Paragons, the largest of which is a 2048 processor, 150 GFlop machine. These computers, which combine several thousand processors, are able to operate concurrently on a problem, dramatically increasing the scope as well as the speed with which one can simulate complex multi-physics phenomena. For example, recently, a massively parallel finite element code² was successfully used in the analysis of the superplastic forming process. Superplastic forming is a technology that offers advantages in material utilization and cost saving by producing near net shaped parts. Mathematical models of the superplastic forming process are used to predict the pressurization rate which will result in optimum superplastic formability and to predict the distribution of thickness in the formed part. Because of the high sensitivity to variations in strain rate, it is important to use a pressurization schedule during forming which will lead to acceptable formability. Modeling also yields an estimate of forming time, which is needed to estimate the cost of operation. The analysis is computationally expensive and usually takes 3 to 4 weeks on a high end workstation. Recently, a complex 20,000 node problem was solved using 128 processors on the Intel Paragon in 6 hours as opposed to 31 days using a single processor.

The finite element code has also been used for large deformation, contact-impact simulation typical of an automobile car crash. Design for crashworthiness is particularly important as automobiles become increasingly lighter, using new and advanced materials, for improved energy efficiency. In studies of crashworthiness, impact and penetration, it is not unusual for an analysis to require several weeks of CPU time on current supercomputers despite the simplicity of the models being studied. As shown in Fig. 2, a 50% offset, car to car, frontal crash analysis was

Figure 2. Large scale finite element computation on massively parallel computers.

performed on the ORNL Paragon. The analysis which took 48 hours on a CRAY-YMP was completed in 8 hours using 128 processors on the Intel Paragon.

LENGTH SCALES IN COMPUTING

Often, in numerical simulation of materials processes, it is extremely challenging to consider multiple, coupled, phenomena that occur at different length and temporal scales. The continuum mechanics analyses assume that sufficiently smooth density functions such as temperature, stress, strain, displacement, and density exist. As the spatial scale is reduced towards the scale of the microstructure, the validity of this assumption must be considered more carefully.

Melting and solidification during welding is a good example of a complex multi-physics problem with multi-phase flow, electromagnetic and surface-tension effects, transient heat transfer, evaporation, solidification and residual stresses. However, these phenomena occur at different length and temporal scales, and are computationally intensive despite the simplicity of the models considered.

A relatively simple problem for a non-stationary gas tungsten arc (GTA) welding with a gaussian heat source on the top of rectangular domain was considered. The complexity of the numerical model requires intensive computation and large amounts of associated data. These requirements make simulations with moderate and large discretization grids intractable for single processor computers. In order to allow for analysis of such problems, massively parallel machines, together with a domain decomposition approach, were employed.

The analyses used a $200 \times 100 \times 20$ grid in the x, y, and z direction, respectively. Each processing node on the multiprocessor machine was assigned a part of the computational domain on which it performed the analysis. Since computation of one discrete element requires information from its adjacent elements, it is necessary to interchange data between processors. The data from border elements of each region is transmitted to its neighboring regions using a message passing programming model. The smallest number of processors that could be used due to

memory requirements was 16. The average CPU time per time step for Intel Paragon and Kendall Square Research exhibit good scaling over larger number of processors as shown in Table 1.

Typically, the computational time (t) for a particular multi-processor (p) application can be expressed as,

$$t = A + B \cdot p + C/p \quad (1)$$

where A is a constant related to initial setup (usually negligible), B is a constant related to interprocessor communication, and C is the computation time for a single processor. From equation 1, it can be seen that the overall performance is determined by the communication cost that increases with the number of processors and computational cost that decreases with the number of processors. Depending on the relative value of B and C , the overall computation time (t) may initially decrease with increasing number of processors up to a point beyond which t would increase as the number of processors increase.

Figure 3 shows the convective flow in the weld pool as a result of the complex interaction between the various driving forces. Depending on the welding conditions, the resulting convective flow can be a relatively simple recirculating flow, or a more complex flow with several convective cells operating in the weld pool. Most current weld pool heat and fluid flow models ignore the geometric structure of the liquid-solid boundary caused by solidification, i.e., the formation of columnar grains or dendrites. Microstructures which develop in the fusion zone of the weld strongly depend upon the shape of the melt pool and can ultimately influence any solid-state transformations that may subsequently occur during cooling. They also play a major role in defect formation such as microporosity or hot cracking. In this sense, they are an important step in any welding process prediction.

Table 1. Performance of WELDER³

	16 processors	24 processors	32 processors
Paragon	10 sec/iter	7.8 sec/iter	6.4 sec/iter
KSR	28 sec/iter	18 sec/iter	15 sec/iter

Over the last few years, probabilistic modeling of grain structures has emerged in the field of castings^{4,8}. Such techniques are very valuable since they allow for direct visualization of grain structure and prediction of the extension of

Figure 3. Fluid flow in a weld pool.

the columnar zone, the impingement of the equiaxed grains, the columnar to equiaxed transition, etc. The models⁴⁻⁶ were based on Monte-Carlo techniques, which were originally developed for grain growth and recrystallization (Potts model)⁹. They lacked a sound physical background since they did not consider specifically the growth kinetics of dendrites or eutectics and the preferential $\langle 100 \rangle$ growth directions of the dendrite trunks. More recently, cellular automata techniques have been able to include such physical mechanisms^{7,8}. A coupling of such models with finite element heat flow calculations can then predict grain structures in realistic situations^{10,11}. Figure 4 shows grain structure

Figure 4. Cellular automata simulation of solidification structure.

Figure 5. MC simulation of a) 2-D and b) 3-D grain growth.

resulting from a simulation of welding polycrystalline sheet metal. The base metal grains were computed by allowing 1500 randomly placed seeds to grow until they impinged each other, following which the epitaxial growth of fusion zone solidification structure was simulated. The curvature of the grains resulting from competitive growth is evident in the calculated result.

The fusion and heat affected zones (HAZ) of welds represent distinct regions from the microstructural point of view. Monte Carlo techniques have been used for grain coarsening in the HAZ^{12,13}. Such methods also have the advantage that they can provide detailed information about the distribution of grain sizes, i.e., field data, which are otherwise less accessible in models based on overall transformation kinetics. Results from 2D and 3D grain growth simulations are shown in Figure 5. As in the case of heat flow calculations, the calculation domain was split into contiguous subregions or blocks, and each block was assigned to a different processor.

The heat affected zone presents additional problems¹⁴. For example, it has long been known in the welding industry that the gradient in grain size in the heat affected zone cannot be accurately simulated experimentally, because of the so-called thermal pinning effect in which the finer grains away from the fusion boundary restrict the free coarsening of those close to the fusion surface. Recently, it has been shown that Monte Carlo techniques can be used to simulate the thermal pinning phenomenon in the weld HAZ¹¹⁴.

Developments in microstructural models have significant impact on the computation of stress distribution in the solid region. Current models usually assume an elasto-plastic stress-strain relationship that can be a function of temperature and strain hardening. They usually ignore the high temperature strain rate dependence and creep. There is a need to develop models of the stress-strain relationship that are functions of the microstructure. This is particularly important

since the material properties can vary rapidly in the HAZ. Without accurate stress-strain relationships, accurate stress analysis will not be possible.

SUMMARY

Modeling, simulation and high performance computing have evolved as powerful technologies for understanding the fundamental phenomena in materials processing. Microscopic models that couple the heat flow equations with solidification phenomena have been developed. With the help of powerful computers, such models have been now integrated in sophisticated macro-micro models which couple the average continuity equations (e.g., heat flow equation) with microscopic phenomena of grain growth. Using such models, it is now possible to do *computational metallurgy* and to directly visualize the grain structures obtained under given solidification conditions, including those pertaining to welding.

There are several potentially applicable mathematical and computational tools that have emerged in recent years. Parallel computing provides important opportunities for modeling of welding processes. Increasing the awareness and use of state-of-the-art parallel computation and expertise in the process modeling area would be an important step. It is encouraging to see that emerging techniques such as neural networks, cellular automata, and monte-carlo calculations have already found their use in the simulation of materials processes. A strength of these methods is the ease with which they can handle complex non-linear boundary conditions.

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