DATE: 3/28/97

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Massively Parallel Finite Element Analysis of Three-Dimensional Flows in Materials Processing Systems

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Summer 96

Many of the processes employed to manufacture advanced materials are currently practiced arts which are evolving into engineering sciences, and large-scale numerical simulation represents a modern tool for speeding this evolution onward. As a first step, the use of realistic theoretical models can augment traditional experimental inquiry to develop fundamental understanding of materials processing systems. In the longer term, modeling promises to provide a rational tool for systematic process optimization and design.

New approaches are needed in the study of materials processing systems, since 3D effects often prevail in their operation. The calculation of macroscopic transport effects is routine for virtually any system so long as 2D behavior is assumed. However, fully 3D calculations continue to be extremely challenging to perform, especially since fine spatial discretizations are needed to resolve the length scales relevant to viscous and convective transport in such systems.

Recent advances in massively parallel supercomputers dramatically affect the prospect of studying 3D fluid mechanics and transport phenomena. To take advantage of these advances, the research group of Jeff Derby is developing and applying novel finite element methods to compute 3D, time-dependent, incompressible flows on the CM-5 and the Cray T3D, both distributed memory, multiple processor supercomputers. The large memory and high sustained computation rates provided by these platforms allow for extremely large simulations appropriate for the calculation of 3D phenomena that commonly occur in materials processing systems.

Derby's group is focusing on several research areas, including sintering processes in ceramic and polymeric systems, extension and break-up of drops during processing of polymer blends, microwave heating of food, and growth of large, single crystals of electronic and photonic materials. (These efforts have been supported by the AHPCRC and with grants from the National Science Foundation, Johnson Matthey Electronics, Inc., the Defense Advanced Research Projects Agency, and Lawrence Livermore National Laboratory (LLNL). While much of this work is in a stage of initial development, dramatic progress has already been accomplished in the modeling of time dependent, 3D flows occurring in crystal growth systems.

An example of the calculation of mixing flows in a solution crystal growth system is shown here. Solution crystal growth is

an important means of producing a wide variety of organic and inorganic crystals. In these systems, a single crystal is grown from a supersaturated solution in which the material to be crystallized is dissolved as a solute. Macroscopic transport of solute molecules from the liquid solution phase to the faces of the growing crystal is almost wholly determined by fluid mechanics. Until recently, the extreme challenges posed by modeling flows within the 3D geometry of such systems has limited progress in understanding transport effects; the calculations shown here represent one of the first efforts to rigorously model flows within a solution crystal growth system.

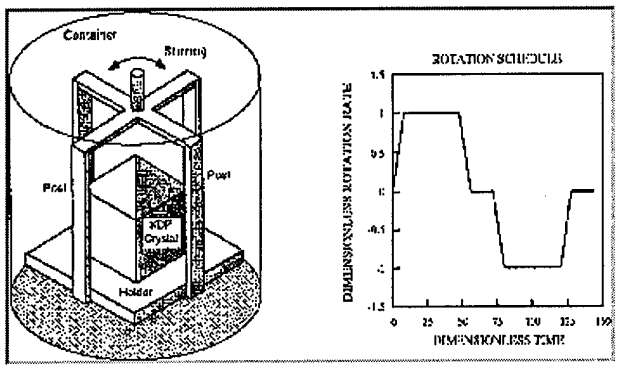

Figure 1. Schematic diagram of the LLNL system for rapid growth of large KDP crystals. The crystal growth habit is prismatic and topped by a pyramidal cap; crystal size is approximately 25 cm. The crystal and platform are rotated to induce mixing in the system.

Figure 1 shows a schematic representation of the rapid growth system for potassium dihydrogen phosphate (KDP) under development by researchers at LLNL. This aggressive program is aimed at growing high-quality KDP, an important nonlinear optical material, at rates greatly surpassing prior approaches. Derby's group has conducted a series of calculations of 3D, time-dependent flows occurring in this system using a massively parallel finite element method implemented on the AHPCRC's Thinking Machines CM-5. These calculations employ 1.4 million mathematical degrees of freedom solved over thousands of time steps.

The crystal and platform are rotated in a time-dependent manner to overcome severe mass transfer limitations in this system, which drives a complicated 3D flow. We consider a stirring schedule representative of the real system, with a short period of spin up, followed by a long period of steady rotation, and ending with a short spin down and rest period. For the calculations shown here, a rotational Reynolds number of 1,267 is employed.

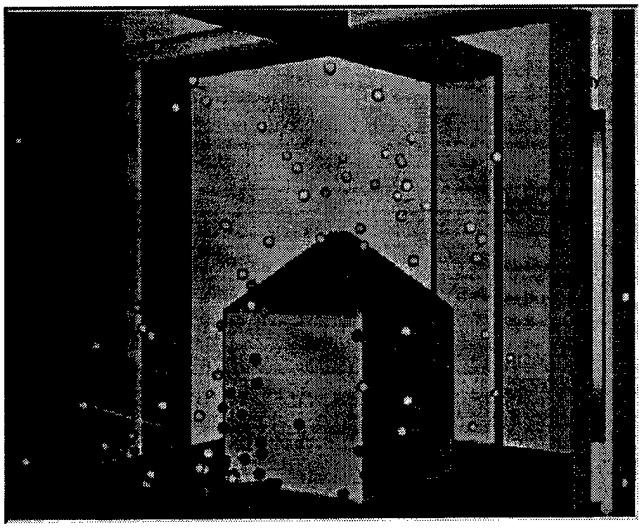

Figure 2. Tracer particles, released in a regular rectangular array aligned with the forward-facing prismatic crystal face, flow away from the face and upward during the spin down portion of the stirring cycle.

Figures 2 and 3 show particle traces during a portion of time after crystal rotation has ceased. This spin down period produces flows which are highly complex in their spatial structure. The large-scale vortical structures of these flows are very important in mixing the solute-rich bulk with fluid regions near the crystalline faces which have been depleted by crystal growth during the steady rotation period. Figure 2 shows upward flow along the prismatic crystal faces during the first portion of the spin down period. Even more important flows for mixing occur via the formation of jets streaming from the bulk toward the prismatic faces, as indicated by the particle paths shown in Figure 3. These flows arise from 3D instabilities triggered by the geometry of the crystal and supports; their discovery was enabled by these calculations.

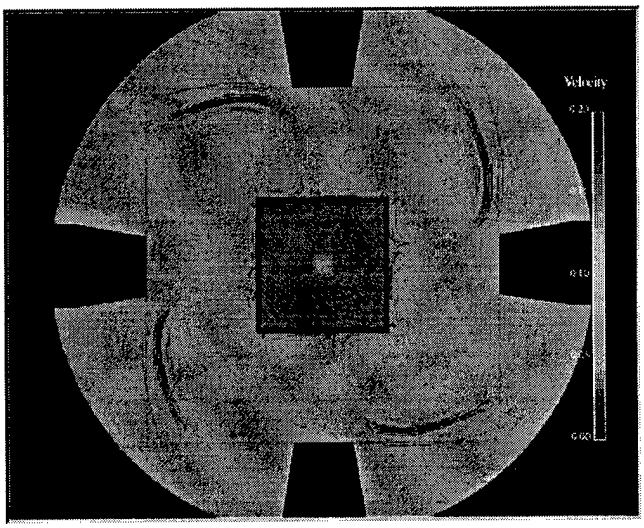

Figure 3. Tracer particles released in selected positions in the bulk clearly show fluid jets impinging on the prismatic faces of the crystal during the spin down portion of the stirring cycle.

These results represent some of the largest simulations ever attempted in crystal growth modeling. Their significance is twofold. First, these simulations specifically represent a meaningful advance in state-of-the-art modeling and analysis of 3D effects in crystal growth systems. Clearly, great advances in understanding and practice are to be expected from the increased use of these techniques in the future. Second, these computations demonstrate the viability of massively parallel algorithms and implementations for the study of real engineering systems. Even now, simulations can be performed which would not be feasible using classical methods on traditional vector architectures. Undoubtedly, continued advances in algorithms and hardware for massively parallel supercomputing will further expand their capability for the study of materials processing systems.