ITR/AP:

Multiscale models for microstructure simulation and process design

J. Dantzig, J. Erickson, M. Garland, R. Haber (PI), R. Jerrard, D. Johnson, L. Kale, J. Sullivan, D. Tortorelli

Center for Process & Simulation Design • Materials Computation Center

University of Illinois at Urbana-Champaign • NSF DMR 01-21695

A collaboration between mechanicians, materials scientists, computer scientists and mathematicians is developing advanced techniques for simulating materials microstructures. Diverse applications, such as dendritic solidification in cryopreservation of biological materials and shock-driven phase transitions in shape memory alloys, pose a number of common challenges. We are addressing these through a coordinated program of information technology research on numerical methods, mesh generation, visualization, and domain-specific abstraction frameworks for parallel applications development.

Cross-discipline research leads to powerful new analysis method

We are developing a new class of space-time discontinuous Galerkin (SDG) finite element methods for solving hyperbolic problems in science and engineering. These methods offer many advantages—but they require new finite element formulations and new techniques for mesh generation, visualization and parallel computing to realize their full potential. Our cross-disciplinary research effort yielded a powerful new analysis tool.

SDG solutions are computed on unstructured spacetime meshes that satisfy a causality constraint that enables an O(N) solution process. Our computational geometry group developed the Tent-Pitcher algorithm to meet this requirement, with support for adaptive mesh refinement (Figs. 1, 2).

Data computed on unstructured spacetime grids requires new visualization technology. Our visualization team developed new data extraction methods and used the latest generation of graphics hardware to implement interactive tools to produce per-pixel-accurate renderings of our solution data (Fig. 3).

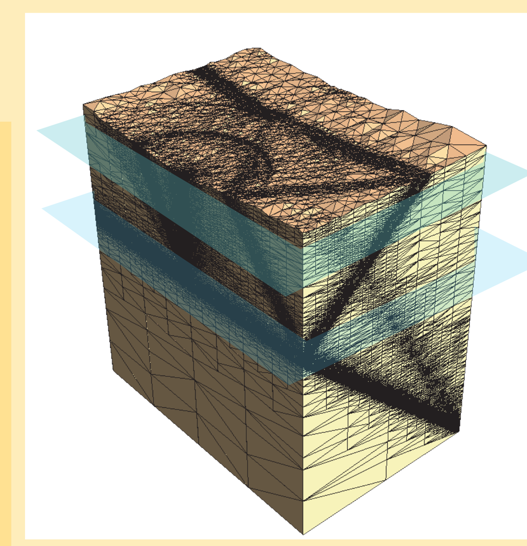


Fig. 1: Adaptive spacetime mesh reveals fine details of shockwave trajectories in crack-tip wave scattering example. Solution data projected onto the transparent constant-time planes generated the animation frames shown below.

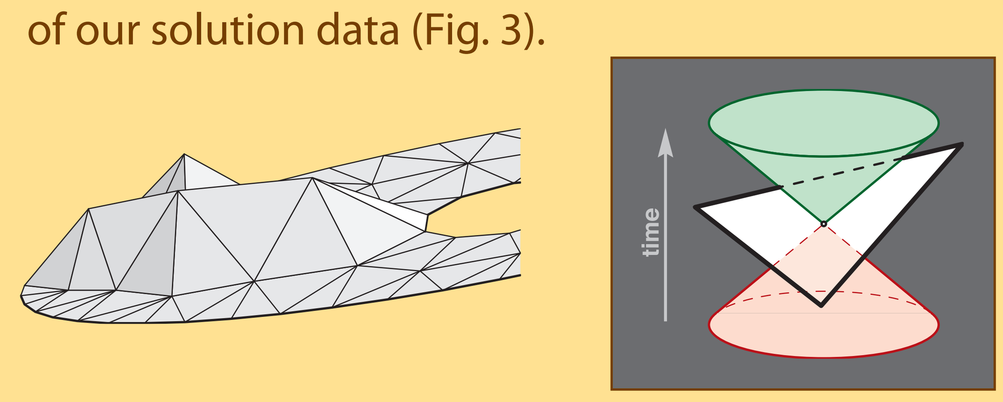


Fig. 2 (above): Tent Pitcher generates causal spacetime meshes that can be solved patch by patch in O(N) time.

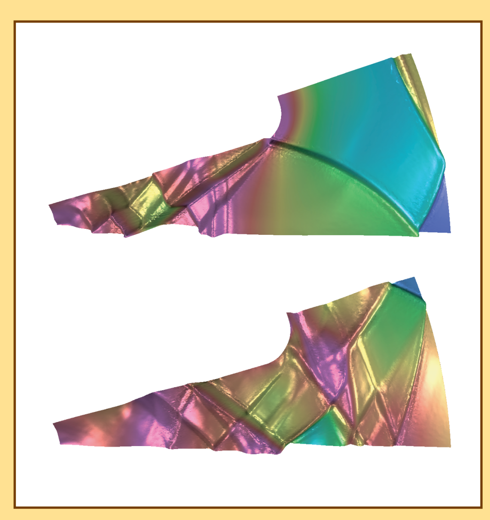
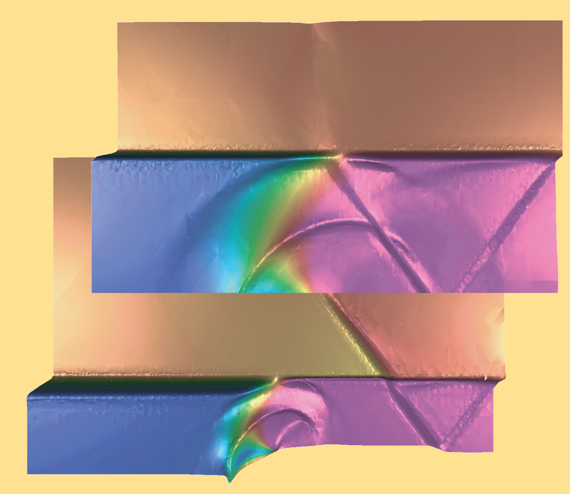


Fig. 3 (left): Per-pixel accurate rendering reveals fine detail of high-resolution SDG solutions. We use the programmable capabilities of contemporary graphics hardware to attain interactive rates.



Research on software environments sparks new science

Simulation of microstructure evolution presents a number of challenges to the analyst, including multiple length and time scales as well as moving interfaces (phase boundaries). Research on dendritic solidification is a case in point. Whether in directional solidification of metallic alloys or in cryopreservation of biological materials, scientific progress in these applications depends on large-scale, adaptive simulations on parallel systems.

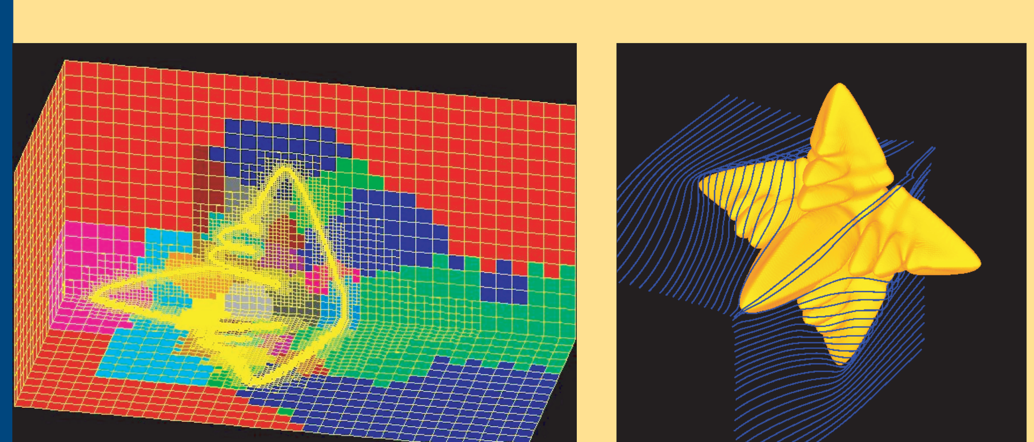


Fig. 4: Simulation of directional solidification in a 3D flow field

CPSD's software environments and parallel computing group works closely with scientists to develop software environments that streamline the development cycle for high-performance applications. The Finite Element Framework uses domain-specific abstractions to relieve applications programmers of the task of managing the complex data structures required for adaptive analysis and parallel computation. Any application developed with the framework has immediate access to Charm^{++}, a parallel computing environment that offers run-time load monitoring and balancing.

Figure 4 (left) shows images from a breakthrough simulation of directional solidification in a 3D flow field that was enabled by the parallel and adaptive capabilities of the FE framework and Charm^{++} (charm.cs.uiuc.edu).

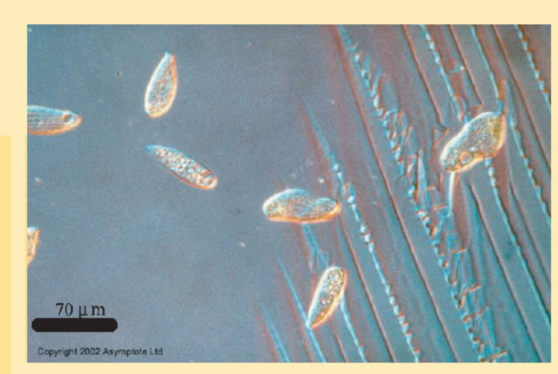


Fig. 5: Dendritic solidification refers to the formation of finger-like structures in solidification processes, such as the microscopic ice crystals seen in the cryogenic preservation process depicted above. Similar structures are responsible for the formation of grain structure in alloy casting processes, as seen in the numerical simulation below (Fig. 7). The ability to predict these structures is essential to the control of material microstructures.

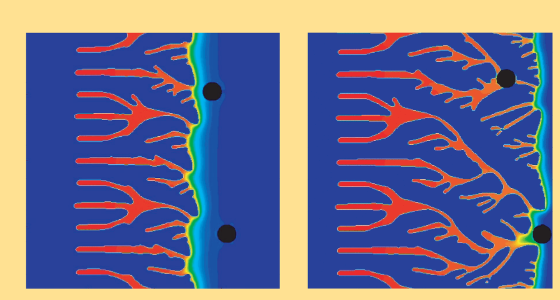


Fig. 6: Particle transport in dendritic solidification

Interdisciplinary training of engineers, scientists & mathematicians

Cross-disciplinary research is essential to the success of this project, as is reflected in the alliance between MCC (atomistic science) and CPSD (continuum science). Training students and postdocs in this style of research is an important part of our mission that is realized through cross-discipline co-advising of students and postdocs and through weekly multidiscipline research meetings:

- SDG systems integration; includes computational geometers (CS, Math), mechanicians (TAM), software and parallel computing environments (CS), and visualization (CS).
- Continuum/atomistic coupling; (MatSE, Physics, TAM)
- PDE theory group; includes pure mathematicians (Math) and finite element experts (TAM)

The project has provided research experience to one undergraduate, and three women are involved at the graduate level.

To date, our graduates have attained two faculty appointments with U.S. universities and two postdoctoral appointments.

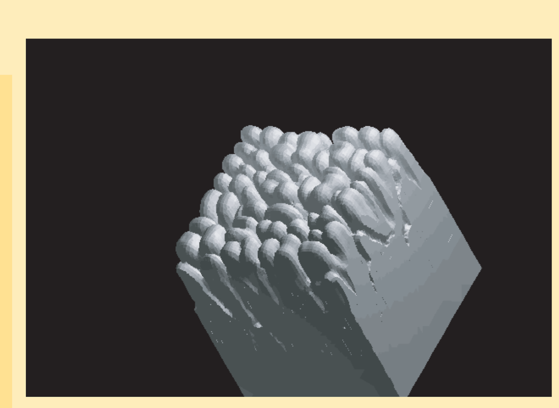


Fig. 7: Three-dimensional simulations of dendritic solidification in a metal alloy are predictive of grain structure in casting processes. In addition to increasing the productivity of applications research, the interdisciplinary research environment in CPSD provides beneficial training to students in computer science, mathematics and the application sciences.

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