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Fast and Scalable Methods for the Simulation of Incompressible Flow
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A fast algorithm for particle simulations
Switch-Level Timing Simulation of MOS VLSI Circuits
Hardware Accelerators for Electrical CAD, Proceedings of the 4th INT Workshop on Topics in VLSI Held in Oxford, 30th September - 2nd October 1987
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A Fast Adaptive Multiple Algorithm for Particle Simulations. Revision
8th International Conference, ICA3PP 2008, Agia Napa, Cyprus, June 9-11, 2008, Proceedings
An Advanced Monte Carlo Simulation Algorithm for the Fast Equilibration of Atomistic Models of H-shaped Polyethylene Melts
FAST-forward Protein Folding and Design
11th Annual European Symposium, Budapest, Hungary, September 16-19, 2003, Proceedings
Numerical Methods and Computer Models for Simulation of Proteins
Fast Algorithm Development for Large-Eddy Simulation of Circular-Jet Turbulence
Efficient Dynamic Compact Models
Fast Algorithms for N-body Simulations

PATEL BALLARD

Algorithms and Architectures for Parallel Processing John Wiley & Sons
In the field of biology, MD simulations are continuously used to investigate biological studies. A Molecular Dynamics (MD) system is defined by the position and momentum of particles and their interactions. The dynamics of a system can

be evaluated by an N-body problem and the simulation is continued until the energy reaches equilibrium. Thus, solving the dynamics numerically and evaluating the interaction is computationally expensive even for a small number of particles in the system. We are focusing on long-ranged interactions, since the calculation time is O(N^2) for an N particle system. In this dissertation, we are proposing two research directions for the MD simulation. First, we design a new variation of Multigrid (MG) algorithm called Multi-level charge assignment (MCA) that requires O(N) time for accurate and efficient calculation of the electrostatic forces. We apply MCA and back interpolation based on the structure of molecules to enhance the accuracy of the simulation. Our second research utilizes reconfigurable models to achieve fast calculation time. We have been working on exploiting two reconfigurable models. We design FPGA-based MD simulator implementing MCA method for Xilinx Virtex-IV. It performs about 10 to 100 times faster than software implementation depending on the simulation accuracy desired. We also design fast and scalable Reconfigurable mesh (R-Mesh) algorithms for MD simulations. This work demonstrates that the large scale biological studies can be simulated in close to real time. The R-Mesh algorithms we design highlight the feasibility of these models

to evaluate potentials with faster calculation times. Specifically, we develop R-Mesh algorithms for both Direct method and Multigrid method. The Direct method evaluates exact potentials and forces, but requires O(N^2) calculation time for evaluating electrostatic forces on a general purpose processor. The MG method adopts an interpolation technique to reduce calculation time to O(N) for a given accuracy. However, our R-Mesh algorithms require only O(N) or O(logN) time complexity for the Direct method on N linear R-Mesh and NxN R-Mesh, respectively and O(r)+O(logM) time complexity for the Multigrid method on an XxYxZ R-Mesh. r is N/M and M = XxYxZ is the number of finest grid points.

Modern Advances in Software and Solution Algorithms for Reservoir Simulation Elsevier

This book constitutes the refereed proceedings of the 11th Annual European Symposium on Algorithms, ESA 2003, held in Budapest, Hungary, in September 2003. The 66 revised full papers presented were carefully reviewed and selected from 165 submissions. The scope of the papers spans the entire range of algorithmics from design and mathematical analysis issues to real-world applications, engineering, and experimental analysis of algorithms.

Automatic Algorithm Selection for Complex Simulation Problems

Oxford University Press Molecular dynamics simulations are a powerful tool to explore conformational landscapes, though limitations in computational hardware commonly thwart observation of biologically relevant events. Since highly specialized or massively parallelized distributed supercomputers are not available to most scientists, there is a strong need for methods that can access long timescale phenomena using commodity hardware. In this thesis, I present the goal-oriented sampling method, Fluctuation Amplification of Specific Traits (FAST), that takes advantage of Markov state models (MSMs) to adaptively explore conformational space using equilibrium-based simulations. This method follows gradients in conformational space to quickly explore relevant conformational transitions with orders of magnitude less aggregate simulation time than traditional simulations. Since each of the individual simulations are at equilibrium, all of the thermodynamics and kinetics in the final MSM are preserved. Here, I first describe the FAST method then demonstrate that it can be used for a variety of tasks, from folding proteins to finding cryptic pockets. Next, I validate that FAST discovers appropriate transition pathways between states. Lastly, I apply FAST in detailing the mechanism of stabilization for a clinically relevant mutation in TEM-1 [beta]-lactamase. This

mechanistic understanding is then used to design other stabilizing mutations, which are all supported experimentally.

A Fast Sorting Algorithm for a Hypersonic Rarefied Flow Particle Simulation on the Connection Machine Springer Science & Business Media

An adaptive algorithm has been constructed for the rapid evaluation of the potentials and force fields due to large scale ensembles of particles of the type encountered in plasma physics, molecular dynamics, fluid dynamics (the vortex method), and celestial mechanics. The algorithm is applicable whenever the fields to be evaluated are Coulombic or gravitational in nature, and yields the potentials to within round-off error. The asymptotic CPU time estimate for the algorithm is of the order O(N), where N is the number of particles in the simulation, and this estimate is independent of the statistics of the charge distribution. Our numerical experiments indicate a tendency of the scheme to be more efficient for non-uniform distributions than for uniform ones. The storage requirements of the algorithm are of the order O(N), do not depend on the statistics of the distribution, and tend to be quite acceptable even for very large numbers of particles. In this paper, a two-dimensional version of the algorithm is described. Generalizing it to the three-dimensional case is fairly straightforward, and will be reported at a later date.

Guide to Dynamic Simulations of Rigid Bodies and Particle Systems Springer Science & Business Media Molecular Dynamics (MD) simulations provide a molecular-resolution picture of the folding and assembly processes of biomolecules, however, the size and timescales of MD simulations are limited by the computational demands of the underlying numerical algorithms. Recently, Graphics Processing Units(GPUs), specialized devices that were originally designed for rendering images, have been repurposed for high performance computing with signicant increases in performance for parallel algorithms. In this thesis, we briefly review the history of high performance computing and present the motivation for recasting molecular dynamics algorithms to be optimized for the GPU. We discuss cutoff methods used in MD simulations including the Verlet Neighbor List algorithm, Cell List algorithm, and a recently developed GPU-optimized parallel Verlet Neighbor List algorithm implemented in our simulation code, and we present performance analyses of the algorithm on the GPU. There exists an N-dependent speedup over the CPU-optimized version that is ~30x faster for the full 70s ribosome (N=10,219 beads). We then implement our simulations into HOOMD, a leading general particle dynamics simulation code that is also optimized for GPUs. Our simulation code

is slower for systems less than around 400 beads but is faster for systems greater than 400 beads up to about 1,000 beads. After that point, HOOMD is unable to accommodate any more beads, but our simulation code is able to handle systems much larger than 10,000 beads. We then introduce a GPU-optimized parallel Hybrid Neighbor/Cell List algorithm. From our performance benchmark analyses, we observe that it is ~10% faster for the full 70s ribosome than our implementation of the parallel Verlet Neighbor List algorithm.

Microcanonical Monte Carlo Springer Science & Business Media

Only two decades ago most electronic circuits were designed with a slide-rule, and the designs were verified using breadboard techniques. Simulation tools were a research curiosity and in general were mistrusted by most designers and test engineers. In those days the programs were not user friendly, models were inadequate, and the algorithms were not very robust. The demand for simulation tools has been driven by the increasing complexity of integrated circuits and systems, and it has been aided by the rapid decrease in the cost of com puting that has occurred over the past several decades. Today a wide range of tools exist for analYSiS, deSign, and verification, and expert systems and synthesis tools are rapidly emerging. In this book only one aspect of the analysis and design process is examined. but it is a very important

aspect that has received much attention over the years. It is the problem of accurate circuit and timing simulation.
Efficient and Scalable Simulation of Solids and Fluids Springer Science & Business Media
Many physical systems observable in nature are governed by interaction forces between several bodies or particles. Examples of such systems (termed N-body problems) include gravitational, electrostatic, and vortex dynamics problems. For N-body problems, an exhaustive interaction force calculation is O(N2). Fast multipole methods, originally conceived by Greengard, provide a much more efficient O(N) algorithm to achieve the same result within a prescribed error margin. The basic themes of the algorithm rely on multipole expansion of the governing potentials and separation of the near- and far-field effects. A multilevel fast multipole methods (MLFMM) algorithm is developed for applications in free-vortex wake methods, which require computation of mutual interactions between a collection of vortex filaments. When coupled with atmospheric inflow and parallelized, this code can produce fast and accurate simulations of entire wind farms. Simulations of the Lillgrund wind farm have produced power results comparable to actuator line/disk LES simulations, while requiring a much smaller fraction of the computational resources. This MLFMM algorithm is also applied to 2-D dislocation dynamics

simulations, which has applications in nanoscale simulation of materials. In this case, the N-body problem involves the computation of mutual interactions between a set of edge dislocations.
ההנהגה והחיים הקהילתיים של היהודים בשלטון האסלאם עד המאה הי"ג Springer
This book provides a practical guide to molecular dynamics and Monte Carlo simulation techniques used in the modelling of simple and complex liquids.
Computer simulation is an essential tool in studying the chemistry and physics of condensed matter, complementing and reinforcing both experiment and theory. Simulations provide detailed information about structure and dynamics, essential to understand the many fluid systems that play a key role in our daily lives: polymers, gels, colloidal suspensions, liquid crystals, biological membranes, and glasses. The second edition of this pioneering book aims to explain how simulation programs work, how to use them, and how to interpret the results, with examples of the latest research in this rapidly evolving field. Accompanying programs in Fortran and Python provide practical, hands-on, illustrations of the ideas in the text.
Fast and Scalable Methods for the Simulation of Incompressible Flow
Stanford University
Understanding Molecular Simulation: From Algorithms to Applications explains the physics behind the "recipes" of

molecular simulation for materials science. Computer simulators are continuously confronted with questions concerning the choice of a particular technique for a given application. A wide variety of tools exist, so the choice of technique requires a good understanding of the basic principles. More importantly, such understanding may greatly improve the efficiency of a simulation program. The implementation of simulation methods is illustrated in pseudocodes and their practical use in the case studies used in the text. Since the first edition only five years ago, the simulation world has changed significantly -- current techniques have matured and new ones have appeared. This new edition deals with these new developments; in particular, there are sections on: · Transition path sampling and diffusive barrier crossing to simulaterare events · Dissipative particle dynamic as a course-grained simulation technique · Novel schemes to compute the long-ranged forces · Hamiltonian and non-Hamiltonian dynamics in the context constant-temperature and constant-pressure molecular dynamics simulations · Multiple-time step algorithms as an alternative for constraints · Defects in solids · The pruned-enriched Rosenbluth sampling, recoil-growth, and concerted rotations for complex molecules · Parallel tempering for glassy Hamiltonians

Examples are included that highlight current applications and the codes of case studies are available on the World Wide Web. Several new examples have been added since the first edition to illustrate recent applications. Questions are included in this new edition. No prior knowledge of computer simulation is assumed.
Development, Analysis, and Applications of the FAST Sampling Algorithm
CRC Press
ABSTRACT: A major problem associated with freeway operations around major cities is congestion occurrence during peak volume periods. Typically, bottlenecks at merging and diverging junctions as well as incidents create a shockwave that propagates upstream. One of the tools currently examined as a way to dampen the shockwave produced by this bottleneck is variable speed limits (VSL). Current micro-simulators do not provide an interface to easily simulate VSLs and evaluate their impact on traffic, thus simulation must be carried out through additional coding. This study creates a test-bed for simulating and evaluating multiple VSL algorithms using the Corridor Simulation (CORSIM) micro-simulator. Three algorithms for VSL control are selected and simulated to evaluate the effectiveness of each algorithm. The roadway used for the simulation is a 13-mile section of I-95 in Miami, Florida. A run-time extension (RTE) interface is built to

communicate with the CORSIM simulation and replicate the VSL operations. Different threshold values are tested to evaluate the effectiveness of each algorithm under various settings. It was concluded that all but one of the scenarios tested show an improvement in the average travel speed and total travel time after VSL is implemented. The throughput for most scenarios showed an improvement when observed over the time duration of the congestion. Overall, the volume-based algorithm showed the most improvement in the simulations.

GPU-optimized Hybrid Neighbor/cell List Algorithm for Coarse-grained Molecular Dynamics Simulations

Fast Simulation of the Leaky Bucket AlgorithmNumerical Methods and Computer Models for Simulation of ProteinsComputational biology is a multidisciplinary field in which biology, mathematics, physics and computer science are integrated to study biological systems. Main challenges in this field include the speed and scalability of the algorithms to better utilize computer hardware and perform intensive calculations in biological systems, efficiency of the algorithms for better search and predictions, and the accuracy of the models for proteins and macro-molecules. In this work, we studied three different problems, each focusing on one of the challenges mentioned

above. In the first part of the thesis, we introduced a new parallel algorithm to enhance the speed of electrostatic force calculations by better utilizing parallel computer clusters. The fast multipole method (FMM) and smooth particle mesh Ewald (SPME) are well known fast algorithms to evaluate long range electrostatic interactions in molecular dynamics and other fields. FMM is a multi-scale method which reduces the computation cost by approximating the potential due to a group of particles at a large distance using few multipole functions. This algorithm scales like O(N) for N particles. SPME algorithm is an O(N log N) method which is based on an interpolation of the Fourier space part of the Ewald sum and evaluating the resulting convolutions using fast Fourier transform (FFT). Those algorithms suffer from relatively poor efficiency on large parallel machines especially for midsize problems around hundreds of thousands of atoms. A variation of the FMM, called PWA, based on plane wave expansions is presented in this paper. A new parallelization strategy for PWA, which takes advantage of the specific form of this expansion, is described. Its parallel efficiency is compared with SPME through detail time measurements on two different computer clusters. In the second part of this thesis, we studied the accuracy of current force field models to simulate antimicrobial peptides with a dominant helical secondary

structure. Secondary structures of antimicrobial peptides play an important role in their activity. The antimicrobial peptide cecropin P1, like most other anti-microbial peptides, is known to form a helix at the interface of bacterial cell membranes. This structure is fundamental to its activity and its ability to destroy the membrane. In contrast, as reported in experimental measurements, this peptide unfolds in bulk water. We analyzed this behavior using two different force fields, CHARMM22/CMAP and AMBER ff99SB. Although these two force fields are commonly used in molecular dynamics and have been extensively validated, we observed two sharply different results. A sodiumdodecylsulfate (SDS) micelle was used to model the bacterial membrane using Molecular Dynamics simulations. CHARMM22 resulted in a peptide that stays mostly folded in both environments (bulk water and SDS), while AMBER correctly predicted the unfolding in bulk water and produced results that closely match the available experimental data. We further computed the free energy of folding and unfolding, using the adaptive biasing force method, to get a complete picture of the energy barriers and the different metastable states. To get further insights into the interaction of the peptide with its environment, we computed the average number of hydrogen

bonds between different components vs the folding reaction coordinate. In the third part of this thesis, we introduced an algorithm for fast protein structure search and predictions. We particularly applied this algorithm to study a certain type of ion channel, ASIC1a. Gating mechanism is an essential part of ion channel activities. We studied acid sensing ion channel 1a (ASIC1a) to better understand its gating mechanism. Although there are some resolved structures for ASIC1a, the open and conductive conformation of this channel is not yet fully known. We used a two steps method, each step with a different level of fidelity, to efficiently search for the possible open conformations. We searched for conformations which had minimal structural changes from the known closed structure. The two steps search helped reduce the multidimensional search space by splitting the search parameters. In the first step, we searched for conformations at the subunit level dealing with the relative orientation of the two transmembrane helices and their packing agains each other. In the second step, the results from the first step were used to explore the relative orientation of the chains in the transmembrane domain of the channel. We were able to identify several possible stable open conformations for the channel. The obtained candidates for the open structure met

experimentally known characteristics for the open channel. This led to some theories on how the gating mechanism takes place in this channel.Understanding Molecular SimulationFrom Algorithms to Applications As conventional hydrocarbon resources dwindle, and environmentally-driven markets start to form and mature, investments are expected to shift into the development of novel emerging subsurface process technologies. While these processes are characterized by a high commercial potential, they are also typically associated with high technical risk. The time-to-market along comparable development pipelines, such as for Enhanced Oil Recovery (EOR) methods in the Oil and Gas sector, is on the order of tens of years. It is anticipated that in the near future, there will be much value in developing simulation tools that can shorten time-to-market cycles, making investment shifts more attractive. There are two forces however that may debilitate us from delivering simulation as a scientific discovery tool. The first force is the growing nonlinearity of the problem base. The second force is the flip-side of a double edged sword; a rapidly evolving computer architecture scene. The first part of this work concerns the formulation and linearization of nonlinear simultaneous equations; the archetypal inflexible component of all large scale simulators. The proposed solution is an

algorithmic framework and library of data-types called the Automatically Differentiable Expression Templates Library (ADETL). The ADETL provides generic representations of variables and discretized expressions on a simulation grid, and the data-types provide algorithms employed behind the scenes to automatically compute the sparse analytical Jacobian. Using the library, large-scale simulators can be developed rapidly by simply writing the residual equations, and without any hand differentiation, hand crafted performance tuning loops, or any other low-level constructs. A key challenge that is addressed is in enabling this level of abstraction and programming ease while making it easy to develop code that runs fast. Faster than any of several existing automatic differentiation packages, faster than any purely Object Oriented implementation, and at least in the order of the execution speed of code delivered by a development team with hand-optimized residuals, analytical derivatives, and Jacobian assembly routines. A second challenge is in providing a generic multi-layered software framework that incorporates plug-in low-level constructs tuned to emerging architectures. The inception of the ADETL spurred an effort to develop the new generation AD-GPRS simulator, which we use to demonstrate the powers of the ADETL. We conclude with a thought

towards a future where simulators can write themselves. The second part of this work develops nonlinear methods that can exploit the nature of the underlying physics to deal with the current and upcoming challenges in physical nonlinearity. The Fully Implicit Method offers unconditional stability of the discrete approximations. This stability comes at the expense of transferring the inherent physical stiffness onto the coupled nonlinear residual equations that are solved at each timestep. Current reservoir simulators apply safe-guarded variants of Newton's method that can neither guarantee convergence, nor provide estimates of the relation between convergence rate and timestep size. In practice, timestep chops become necessary, and they are guided heuristically. With growing complexity, convergence difficulties can lead to substantial losses in computational effort and prohibitively small timesteps. We establish an alternate class of nonlinear iteration that converges and that associates a timestep to each iteration. Moreover, the linear solution process within each iteration is performed locally. Several challenging examples are presented, and the results demonstrate the robustness and computational efficiency of the proposed class of methods. We conclude with thoughts to unify timestepping and iterative nonlinear methods.

An Q(N) Algorithm for Three-dimensional N-body Simulations Createspace

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A sequential implementation of the algorithm for two-dimensional N-body systems shows the predicted asymptotic scaling. A parallel version on a 16-processor Intel iPSC/860 machine is also in conformance with theoretical expectations.
Scientific and Technical Aerospace Reports
Springer
A recently developed algorithm for simulating statistical systems is discussed. The procedure interpolates between molecular dynamics methods and canonical Monte Carlo. The primary advantages are extremely fast simulations of discrete systems such as the Ising model and a relative insensitivity to random number quality. A variation of the algorithm gives rise to a deterministic dynamics for Ising spins. This model may be useful for high speed simulation of non-equilibrium phenomena. 8 refs., 2 figs.
A fast algorithm for particle simulations
Springer Science & Business Media
This book provides the reader with a complete methodology and software environment for creating efficient dynamic compact models for electro-thermal MEMS devices. It supplies the basic knowledge and understanding for using model order reduction at the engineering level. This tutorial is written for MEMS engineers and is enriched with many case studies which equip readers with the know-how to facilitate the

simulation of a specific problem.
Switch-Level Timing Simulation of MOS VLSI Circuits Springer Science & Business Media
Chapters in Fast Simulation of Computer Architectures cover topics such as how to collect traces, emulate instruction sets, simulate microprocessors using execution-driven techniques, evaluate memory hierarchies, apply statistical sampling to simulation, and how to augment simulation with performance bound models. The chapters have been written by many of the leading researchers in the area, in a collaboration that ensures that the material is both coherent and cohesive. Audience: Of tremendous interest to practising computer architect designers seeking timely solutions to tough evaluation problems, and to advanced upper division undergraduate and graduate students of the field. Useful study aids are provided by the problems at the end of Chapters 2 through 8.
Hardware Accelerators for Electrical CAD, Proceedings of the 4th INT Workshop on Topics in VLSI Held in Oxford, 30th September - 2nd October 1987 Stanford University
This dissertation presents efficient and scalable algorithms for the simulation of incompressible fluids. Physical simulation of fluids is one of the most interesting and challenging problems because of the amount of small scale details that realistic fluids exhibit.

Although a large number of high fidelity simulations can be obtained with existing techniques, the resolution that these techniques can obtain is limited by the amount of computational power available. The simulation of incompressible flow has two main aspects: advection and projection. This thesis addresses performance and scalability issues related to both aspects and demonstrates a number of algorithms that work to massively reduce the computational cost of simulations. In the first chapters we concentrate on improving the performance and scalability of fluid simulations by investigating new conservative advection methods based off the established semi-Lagrangian method. Applying a conservative limiter to the typical semi-Lagrangian interpolation step can guarantee that the amount of the quantity being advected (e.g. mass, momentum, volume, etc.) does not increase. In addition, a new second step can be utilized that forward advects any of the quantity that was not accounted for in the typical semi-Lagrangian advection. Using this new conservative semi-Lagrangian method, mass and momentum can be conservatively advected in order to improve visual fidelity of smoke simulations at large time steps. In addition to conserving momentum during advection, the commonly used vorticity confinement turbulence model can be modified to

exactly conserve momentum as well. It is shown that this new method is amenable to efficient smoke simulation with one time step per frame, whereas the traditional non-conservative semi-Lagrangian method experiences serious artifacts when run with these large time steps, especially when object interaction is considered. This method is then extended for water simulation when taking large time steps where, in contrast to smoke, an extrapolated velocity field is required. Inaccuracies with the extrapolated velocity field are alleviated by not using it when it is incorrect, which is determined via conservative advection of a color function that adds forwardly advected semi-Lagrangian rays to maintain conservation when mass is lost. This method is then coupled to the more visually appealing particle levelset method to obtain both a visually appealing and accurate method for simulating water at large time steps. In the final chapters we discuss improving the performance and scalability of the projection step through the use of faster methods for the pressure solve. This technique coarsens the Eulerian fluid grid during the pressure solve, allowing for a fast implicit update but still maintaining the resolution obtained with a large grid. This allows simulations to run at a fraction of the cost of existing techniques (~60x faster) while still providing the

fine scale structure and details obtained with a full projection. This algorithm scales well to very large grids and large numbers of processors, allowing for high fidelity simulations that would otherwise be intractable.

Algorithms - ESA 2003

Welcome to the proceedings of the 8th International Conference on Algorithms and Architectures for Parallel Processing (ICA3PP 2008). ICA3PP 2008 consist of two keynote addresses, seven technical sessions, and one tutorial. Included in these proceedings are papers whose authors are from Australia, Brazil, Canada, China, Cyprus, France, India, Iran, Israel, Italy, Japan, Korea, Germany, Greece, Mexico, Poland, Portugal, Romania, Spain, Switzerland, Taiwan, Tunisia, UAE, UK, and USA. Each paper was rigorously reviewed by at least three Program Committee members and/or external revi- ers, and the acceptance ratio is 35%. These papers were presented over seven technical sessions. Based on the paper review results, three papers were selected as the best papers. We would like to thank the many people who helped make this conference a successful event. We thank all authors who submitted their work to ICA3PP 2008, and all Program Committee members and additional reviewers for their diligent work in the paper review process ensuring a collection of high-quality papers. We are grateful to Hong Shen University of Adelaide, Australia and

Kleanthis Psarris University of Texas at San Antonio, United States, for their willingness to be the keynote speakers. Our thanks go to Hai Jin and George Papapodoulos, the conference General Co-chairs, and Andrzej Goscinski, W- lei Zhou and Yi Pan, the conference Steering Committee Co-chairs for help in many aspects of organizing this conference. Finally, we thank all the conference participants for traveling to Cyprus.

Fast Simulation of Electro-Thermal MEMS

This thesis considers the numerical simulation of rigid and deformable bodies, as well as compressible fluids. We consider each of these types of simulations independently, and in particular we focus on what it takes to make these simulations both efficient and scalable. First, we develop a robust parallelized method for simulating cloth and we demonstrate simulations consisting of up to 2 million triangles. This added level of detail allows us to achieve high detailed folds and wrinkles. We propose a robust history-based repulsion/collision framework where repulsions are treated accurately and efficiently on a per time step basis. Distributed memory parallelism is used for both time evolution and collisions and we specifically address Gauss-Seidel ordering of repulsion/collision response. Next, we propose a method for alleviating the stringent CFL condition imposed by the sound speed in

simulating inviscid compressible flow with shocks, contacts and rarefactions. Our method is based on the pressure evolution equation, so it works for arbitrary equations of state, chemical species, etc. The relaxed CFL condition allows us to simulate shocks, contacts and rarefactions accurately while taking much larger time steps than before. Then, we turn to the simulation of rigid bodies, where we present an algorithm for conserving energy and momentum when advancing rigid body orientations. Furthermore, we develop a technique for clamping energy gain during contact and collisions. Together, these methods allow us to prevent energy increase during rigid body simulations, regardless of the time step size. This allows us to reduce the computation needed while still producing stable and physically plausible simulations. We also introduce a technique for fast and realistic fracture of rigid bodies using a novel collision-centered prescoring algorithm. Finally, we extend the use of energy preservation techniques to the simulation of deformable bodies, again with the goal of reducing the cost of these simulations. We propose a new spring that, in one spatial dimension, gives the exact solution regardless of the size of the time step chosen. In multiple spatial dimensions, the problem becomes nonlinear because the direction of the spring changes over time, and

thus we propose an iterative approach. Then, we consider the simulation of more complicated elements such as triangles, tetrahedra, and finally full meshes and propose a novel technique that allows us to cut the iterative approach short and instead apply a final correction globally to the mesh.

Fast Algorithm Simulation and Test (FAST) Facility

An algorithm is presented for the rapid evaluation of the potential and force fields in systems involving large numbers of particles whose interactions are Coulombic or gravitational in nature. For a system of N particles, an amount of work of the order O(N2) has traditionally been required to evaluate all pairwise interactions, unless some approximation or truncation method is used. The algorithm of this paper requires an amount of work proportional to N to evaluate all interactions to within roundoff error, making it considerably more practical for large-scale problems encountered in plasma physics, fluid dynamics, molecular dynamics and celestial mechanics. Keywords: N-body problem; Molecular dynamics, Plasma physics, Potential theory. (Author).

Fast Simulation of Computer Architectures

Lists citations with abstracts for aerospace related reports obtained from world wide sources and announces documents that have recently been entered into the NASA Scientific

and Technical Information Database.

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