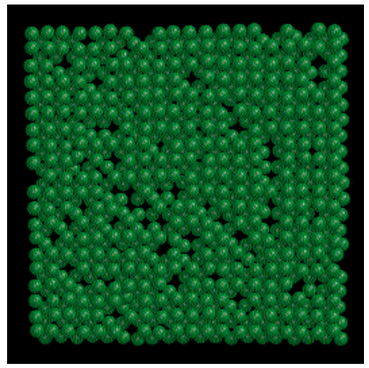
PDC Newsletter

Molecular Dynamics Simulations of Condensed Matter

Sergei Simdyankin, Fredrik Zetterling, and Mikhail Dzugutov, Department of Numerical Analysis and Computing Science, KTH

The results presented here were obtained using an efficient molecular dynamics code developed by the authors. The most time-consuming part of any molecular dynamics program is the computation of the force exerted on an atom by all its neighbors. It is enough to take into account only those neighbors that lie within the limit of an interaction range. The execution time required by this procedure – the selection of interacting neighbors in the general case – scales as $O(N^2)$ where N is the number of atoms. This is because all pairs of atoms must be examined to determine which atoms actually interact.



Distribution of voids in a structural layer of the bcc crystal.

In our algorithm, the information about atoms' positions is organized so that the execution time scales as $O(N)$. The atoms' coordinates are sorted so that the geometric neighbors are stored close to each other in memory. By following this strategy, we achieve a better locality in the data storage; for the RISC architecture, this results in reducing the number of cache misses. Due to the efficient use of the cache memory, the execution time of the program scales linearly with the processor clock frequency.

Because the program does not use any vendor-specific software libraries, it is easy to move it between different computer platforms. For system sizes on the order of ten to twenty thousand particles, we use one SMP node on the IBM SP as a powerful individual computational processor. To monitor the evolution of the system, the nodes are used interactively. The interactive runs are particularly useful while dealing with supercooled liquids and other sysems with extremely slow dynamics. Regular analysis of the output makes it possible to interfere with the course of the simulation. This significantly reduces the overall computation time. The data allocation pattern used in our implementation makes the program easily and efficiently parallelizable for computers with both distributed and shared memory. The parallel versions of the programs are used for large-scale projects.

In This Issue

Computer Simulation of Vacancy Dynamics in Solids

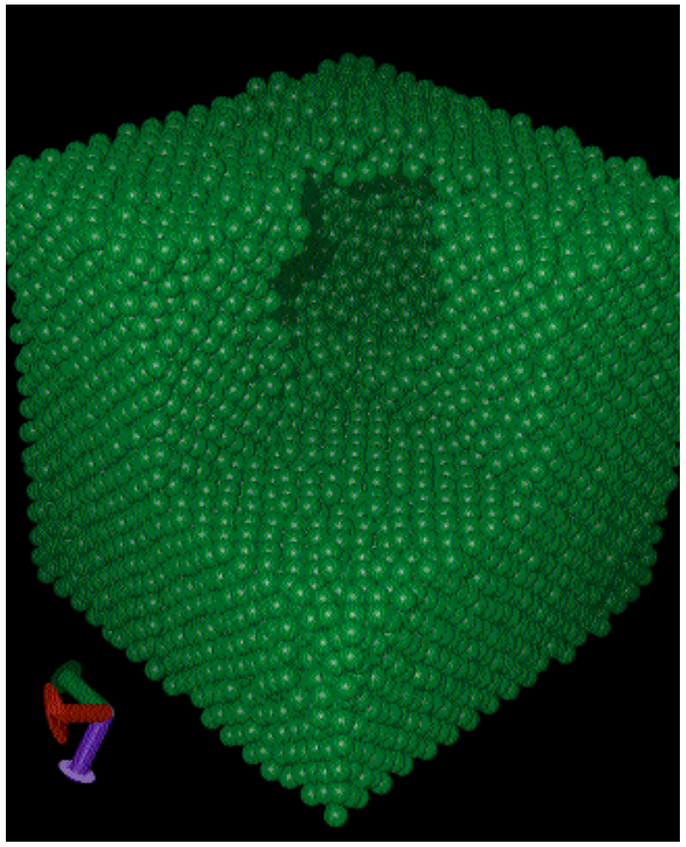


Fig. 1. A large-scale aggregation of vacancies in the fcc crystal.

S. Simdyankin and M.Dzugutov

Formation mechanism and evolution of vacancies in solids is a problem of considerable technological significance that has recently attracted much research interest. It is known that vacancies created by radiation damage in construction materials used in nuclear energy production facilities have a tendency to evolve in macroscopic-size voids. This process may lead to deterioration of mechanical properties of these materials. Atomistic computer simulations may give an important insight into the microscopic mechanism of this phenomenon, providing unique information which cannot be accessed by real experiments.

A particular problem that can be addressed by such a simulation is how the kinetics of the vacancy network in a solid depends on its structure and interatomic interaction forces.In the present study, this problem is investigated by using a molecular dynamics simulation of a crystalline solid containing vacancies.

We simulated a simple monatomic system consisting of 16 128 particles arranged in an fcc lattice with uniformly distributed vacancies interacting via the Lennard-Jones (LJ) pair potential. The presence of vacancies in the system facilitated the process of atomic diffusion whereby the moving particles exchanged positions with vacancies. In the case of the LJ system we observed a tendency for large-scale density fluctuations in the distribution of vacancies. The amplitude of such fluctuations was found to increase with time, which eventually lead to formation of a large void region. This separation of the system in two phases with different densities of vacancies invariably occurred at different thermodynamical conditions and different total numbers of vacancies (see fig.1).

On the other hand, the effect of void formation described above appears to be related to the interparticle interaction potential. We found that with a different form of the potential, which lacked the long-range attraction characteristic of the LJ potential, the vacancy distribution remained uniform even after a considerable run-time (see figure on front page).

The preliminary results described provide a ground for the conclusion that the void-forming vacancy dynamics in solids is related to the energetics of interatomic interactions rather than to the particular structure of the systems in question. Nevertheless, further investigation is needed to analyze the details of the kinetics of void formation. Another interesting extension of this study would be to simulate the dynamics of vacancies in amorphous solid materials.

From the Editor

An important step in the development of HPC in Sweden will be taken in June. The first meeting of the Swedish National Allocations Committee for High Performance Computing (SNAC) will be held at PDC. Applications for computer resources at HPC2N, NSC, and PDC will be evaluated by SNAC. The application process is drastically simplified, because one application covers computing time for all the three centers.

Lennart Johnsson (of the University of Houston, in Texas) serves as chair of SNAC, and members come from the fields of bioscience, chemistry, computing science, engineering, geoscience, mathematics, and physics. All the leading Swedish universities are represented. The committee will evaluate the applications and recommend allocation of computer resources.

The formation of SNAC follows earlier efforts to coordinate the application processes,first between HPC2N and PDC and then among all three centers. We hope that this volunteer cooperation between the HPC centers will increase substantially in the near future. The centers in Lund, Göteborg, and Uppsala could be included, and the coordination should expand to educational activities and a number of technical issues. The goal must be to simplify and streamline not only the application process but also the overall use of the Swedish academic HPC facilities.

We can learn from the HPC partnerships in the United States. The National Science Foundation sponsors two partnerships that support academic users throughout the country. Each partnership comprises 30-50 members with a variety of research interests and equipment. With this structure, the large main resources can be focused at one leading-edge site, while distributed high level HPC activities can take place at all the leading universities.

PDC is an international affiliate of NPACI, which is one of these partnerships. NPACI's motto, “Building the Computational Infrastructure for Tomorrow’s Scientific Discovery,” would also fit a Swedish partnership or metacenter. Similar ideas are now being introduced in other European countries.

Our vision of the future should contain more than the cooperation between HPC centers. An infrastructure of supporting hardware and software should be built such that all research groups can transparently access our different computational and mass storage facilities as well as other systems, which might even include experimental equipment. PDC is part of the Globus project, which is one of the international efforts to build software for such a system.

Finally, I would like to join all others in thanking Britta Svensson for the wonderful job she has done at PDC during all these years.

Björn Engquist

Director

Fond Far ewell

The staff of PDC and NADA, along with many other people, wish Britta Svensson the greatest happiness in her retirement.

She has been the head receptionist and secretary at PDC for ten years.But more importantly, she has been a font of knowledge, a kind smile and laugh, a wealth of resources, and a help when no one else knew what to do.

Britta, you will be sorely missed.

Formation of a Percolating Icosahedral Amorphous Cluster in a Supercooled Simple Monoatomic Liquid

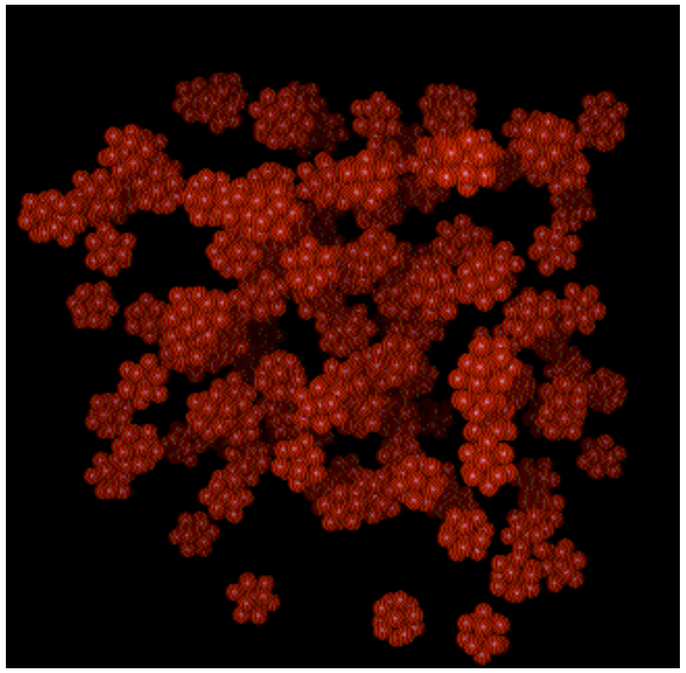


Fig. 1. Spatial distribution of icosahedral atomic configurations at T = 1.40.

A full description of VMD is available via the VMD Web page, **<http://www.ks.uiuc.edu/Research/vmd/>**. The authors of VMD request that any published work that uses VMD include a reference to the VMD Web page and/or the following reference: W. Humphrey, A. Dalke, and K. Schulten, "VMD: Visual Molecular Dynamics," *J. Molec. Graphics*, 1996, vol. 14, pp. 33-38.

F. Zetterling and M.Dzugutov

The current interest in glassy materials is motivated by the potentially vast scope of their technological application. Metallic glasses possess many properties that cannot be obtained in crystalline metallic alloys. Numerical simulation is crucial for a deeper understanding of the formation mechanisms and the microscopic properties of these materials.

A most prominent feature of the glass-forming metallic alloys of simple constitution is the icosahedral local order. It is well known that icosahedral packing of spheres is incompatible with periodic long-range order. Therefore, icosahedrally ordered liquids can easily circumvent the crystalline nucleation and form a solid amorphous phase, provided that the cooling rate is sufficiently high. Nevertheless, at slower cooling rate these systems are known to crystallize into the periodic Frank-Kasper phase. Avoiding such a crystallization is the most important problem of the metallurgy of metallic glasses.

In this simulation, we explore glass formation in a simple one-component system composed of 16 384 particles. We demonstrate that the Frank-Kasper crystallization in a simple monoatomic liquid possessing pronounced icosahedral local order can be inhibited by using a properly designed form of pair potential. The main purpose of the design of the potential used here is to suppress the possibility of the structural elements with six-fold symmetry which are crucial ingredients of the Frank-Kasper crystal. As a result, we produce a liquid which under supercooling increases the degree of local icosahedral ordering without forming long-range periodic order. We observe that the local icosahedral configurations show the tendency for clustering. The process of cluster growth is found to proceed in a low-dimensional way since the bulk growth of icosahedral structure is inhibited by frustration inherent in the icosahedral packing.

These results demonstrate a possibility of a perfect structural glass transition in a simple system of particles with a pair potential imitating that of a glass forming metallic alloy. This simulation provides convincing evidence that the process of glass formation in these systems can be viewed as formation of a global percolating cluster composed of local icosahedrally ordered structural units.

The growth of the percolating cluster of icosahedra is depicted in figures 1 and 2.

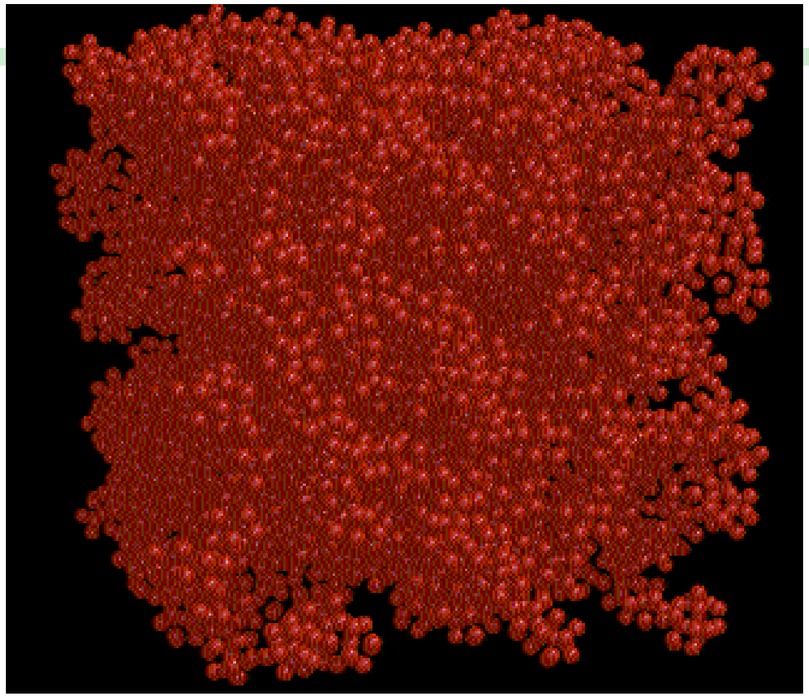


Fig. 2. Spatial distribution of icosahedral atomic configurations at T = 0.45. The icosahedra form a globally percolating cluster.

International Visitors to the VR-CUBE

Six people affiliated with Iowa State University (ISU) came to PDC in late February; they were Carolina Cruz-Neira, Gary Lindahl, Pete Evans, Tom Whetstone, Roger Graden, and Michael Hancock. They visited PDC's VR-CUBE as part of a trip to see five- and six-sided immersive VR environments in Europe.

Cruz-Neira developed the CAVE – the first multi-person, room-sized, high-resolution, 3D video and audio environment – and Lindahl provided technical support for the original CAVE. They are currently coordinating the design and construction of a six-sided system at the Iowa Center for Emerging Manufacturing Technology (ICEMT) at ISU. Cruz-Neira and Lindahl visited PDC to learn about its experiences with the VR-CUBE. Other members of the group were interested in the architectural details, the construction, and the installation of the VR-CUBE.

Carolina Cruz-Neira is ICEMT's associate director, and Gary Lindahl is a research scientist at ICEMT. Pete Evans and Tom Whetstone are architects from Brooks-Borg-Skiles Architectural Engineers (BBSAE), the firm under contract for the new engineering building on campus – which will house the 3D device – as well as the architectural details of the enclosure for the device. Roger Graden is an ISU staff architect who is managing BBSAE's efforts. Michael Hancock is a project manager at MechDyne Corp., the company under contract to design, build, and integrate the six-sided 3D device into the new engineering building.

Calendar of Events

General

June

2–6 2d Workshop on Large-Scale Scientific Computation
Sozopol, Bulgaria
http://orca.st.usm.edu/~marcin/mp/cfp/SciCom99.html

3–4 MMA99: Fourth International Conference on Mathematical Modelling and Analysis
Vilnius, Lithuania
http://www.aldona.mii.lt/mma99/

7–12 Fluid99 Summer School: Industrial Mathematics
Lisboa, Portugal
http://www.math.ist.utl.pt/~calves/CMA/fluid99

10-12 International Conference on Preconditioning Techniques for Large Sparse Matrix Problems in Industrial Applications
Minneapolis, Minnesota
http://www2.msi.umn.edu/Symposia/sparse99/index.html

11 Computational Methods in Engineering Workshop
Uppsala University, Sweden
http://www.tdb.uu.se/CMEworkshop

11–14 SP World '99: Thinking Deeply
Singapore
http://www.rs6000.ibm.com/spworld/

21-22 Data Mining: Principles and Practice
Chicago, Illinois
http://www.gordianknot.com

22 INET'99: Internet Global Summit
San Jose, California
http://www.isoc.org/inet99

23-25 Workshop on Randomized Computing & Communication
Fremantle, Australia
Contact: wei@cs.fordham.edu

27–30 HiPer'99: High Performance Computing on Hewlett-Packard Systems
Tromsø, Norway
http://www.hpc.uit.no/hiper99

28–30 Network Storage '99
Monterey, California
http://www.periconcepts.com

28–July 3 Fluid99 Summer School: Navier-Stokes Equations and Related Topics
Lisboa, Portugal
http://www.math.ist.utl.pt/~calves/CMA/fluid99

July

7–8 The Black Hat Briefings '99
Las Vegas, Nevada
http://www.blackhat.com/

12–17 Fluid99 Summer School: Computational Fluid Dynamics
Lisboa, Portugal
http://www.math.ist.utl.pt/~calves/CMA/fluid99

13–16 International Conference on Applied Partial Differential Equations
Tongji University, Shanghai, China
e-mail contact:
hzpsyhk@online.sh.cn

29–31 QBIC '99: Quantum BioInorganic Chemistry; WATOC '99 Satellite Symposium
University of Warwick, England
http://www.warwick.ac.uk/~mssbq/qbic99.html

August

1–2 HUG'99: 3d Annual HPF User Group Meeting
Redondo Beach, California (note change in location and dates)
http://www.icase.edu/hug99

1–6 5th World Congress of Theoretically Oriented Chemists
Imperial College, London, England
http://www.chemsoc.org/watoc99/satmtg.htm

31–3 Sep Euro-Par '99
Toulouse, France
http://infosun.fmi.uni-passau.de/

September

1–3 5th International Conference on Virtual Systems and Multimedia
Dundee, Scotland
http://www.vsmm.org/vsmm99/

13–14 Data Mining: Principles and Practice
San Francisco, California,
http://www.gordianknot.com

PDC Events

NGSSC Summer School

Introduction to High-Performance Computing; August 16-27

Annual Conference

Simulation and Visualization on the Grid; December 15-17

Call for Papers: PDC Annual Conferenc e

The theme of the 1999 PDC annual conference is "Simulation and Visualization on the Grid." The proceedings for the December conference will be published by Springer-Verlag in its Lecture Notes in Computational Science and Engineering series.

PDC invites contributed papers for presentations of approximately twenty minutes. An extended abstract, not exceeding two pages (800-1100 words), should be sent to PDC by September 3. Authors will be notified two weeks later if their papers have been accepted.

Abstracts will be submitted electronically. Please see **<http://www.pdc.kth.se/conference/1999/>** for instructions and further information.

README

- **Log In**. Because of the upgrade in March of 1999,there is a separate log-in node to get access to an SMP (silver) node environment. Instead of logging in to **strindberg.pdc.kth.se**, you can use **august.pdc.kth.se** for SMP nodes.
- **Kerberos travel kit for Windows NT/98/95** The kerberos travelkit is available in versions for Windows NT. Several users are successfully using this with Windows 9x. The download location can be found at **<http://www.pdc.kth.se/support/>**,under "Kerberos Travelkit."
- **Missing some software?** Software is installed at PDC on request. If there are sufficient requests for a specific piece of software, we will be happy to install it for your convenience. Send e-mail to **<pdc-staff@pdc.kth.se>** to initiate a discussion regarding your needs.
- **Documentation.** See **<http://www.pdc.kth.se/doc/>** for a complete list of on-line documentation available at PDC for both software and hardware.

Low-Cost Tool for Medical Imaging

Modern hospitals produce tens of thousands of volumetric images every year, using magnetic resonance imaging (MRI), computed tomography (CT), nuclear medical imaging (NMI), and ultrasound (US). There is a growing demand for affordable computing techniques to visualize, analyze, and manage these 3D images.

However, much of the hardware required to run currently available software is prohibitively expensive, and much of the software itself is difficult to use.

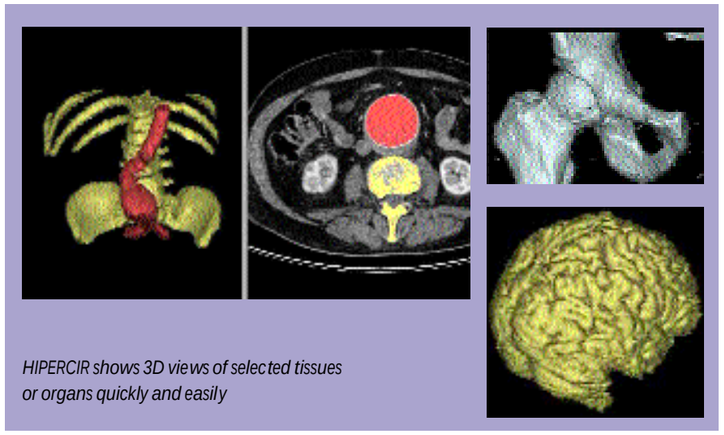
The High-Performance Computing Integrated Radiology (HIPERCIR) suite is a new software package for 3D real-time visualization and semi-automatic segmentation of medical images. This tool, which can be useful for diagnosis,surgical planning, and therapy, uses high-performance computing techniques and yet only requires a network of PCs running on standard operating systems.

Because HIPERCIR uses resources that are already available, it is affordable even for small hospitals, and the amount of training needed for the users is reduced. This minimal training will in turn reduce the possibilities of misleading and incomplete diagnoses; and the users' familiarity and comfort level will allow them to address a wider variety of problems.

The image treatment algorithms that were developed by the members of the HIPERCIR consortium use the latest technology, in terms of expert systems and knowledge bases.

Peset University Hospital in Spain produces hundreds of CT and MR images per week.They currently use a commercial CT solution running on a UNIX workstation. HIPERCIR runs on four PCs, costs five times less, and delivers twice as much performance as this UNIX system. Using parallel computing in this way provides medical professionals with a low-cost 3D image analysis tool that will reduce the execution time and will make diagnosis easier and faster.

Contact Point
Vicente Hernández, Project Manager of HIPERCIR, DSIC-UPV
Camino de Vera s/n,46022 Valencia,SPAIN
Tel: +34 96 387 73 56
Fax +34 96 387 73 59
e-mail:vhernand@dsic.upv.es



HIPERCIR shows 3D views of selected tissues or organs quickly and easily

Correction

The caption for the HPCN TTN article on page 7 of the Winter 1999 PDC Newsletter includes, "Red indicates slower flow, and green and blue indicate faster flow." This should be, "Red indicates faster flow, and green and blue indicate slower flow." We regret this error.

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Sverige
Porto
Betalt

PORT PAYÉ

PDC,KTH
SE-100 44 Stockholm
SWEDEN

VETENSKAP OCH KONST
KTH

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Editor: Björn Engquist

Editorial staff: Faith Short

E-mail: pdc-quarterly@pdc.kth.se

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How to Contact PDC

Visiting address: Lindstedtsvägen 3, Plan 5, KTH, Stockholm

Mail: PDC,KTH
SE-100 44 Stockholm
SWEDEN

E-mail: pdc-staff@pdc.kth.se

WWW: http://www.pdc.kth.se/

Phone: +46 8 790 78 00

Fax: +46 8 24 77 84

PDCTTN

Contact: Marina Backer Skaar

E-mail: pdcttn@pdc.kth.se

WWW: http://www.pdc.kth.se/pdcttn/

Phone: +46 8 790 69 23

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