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LLNL-TR-821380

High Performance Parallel Processing Project (HPPPP) Advanced Materials Designs for Massively Parall

B. Bosl, T. Keller, J. Northrup

April 12, 2021

Disclaimer

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

High Performance Parallel Processing Project (HPPPP)
Advanced Materials Designs for Massively Parallel Environment

Final Report
CRADA No. TC-0824-94-I

Date: August 21, 1998 Revision: 2

A. Parties

The project is a relationship between the Lawrence Livermore National Laboratory (LLNL), Xerox Palo Alto Research Center and Cray Research Inc.

University of California
Lawrence Livermore National Laboratory
PO Box 808, L-795
Livermore, CA 94550

Xerox Palo Alto Research Center (Xerox PARC)
3333 Coyote Hill Road
Palo Alto, CA 94304

Cray Research Inc.
655 Lone Oak Drive
Eagan, MN 55121

B. Project Scope

This project was a multi-partner CRADA with nine industrial partners. The CRADA with Xerox PARC made available the advanced quantum-level materials modeling (code name: PCGPP) code developed at LLNL to the wider industrial community by porting and optimizing these codes for Cray Research supercomputers.

There were four phases to this project:

Phase 1
LLNL vectorized and parallelized their atomistic simulation codes for the PVP architecture. This work was in progress at the time the CRADA was established, as the vector portions of this code ran at ~200 Mflops on a single Y_MP processor.

Phase 2
LLNL ported and optimized LLNL's materials simulation codes, which included the atomistic ab initio and force field materials simulation programs and the smoothed particle applied mechanics, to the production T3D MPP.

Phase 3
LLNL performed algorithmic and formalism developments on various simulation codes in order to extend their efficiency and functionality to the T3D and other MPPs.

Phase 4
LLNL, in collaboration with Xerox PARC, applied these atomistic *ab initio* materials simulation codes to specific large-scale materials physics problems of significance to DOE and to the Electronic Materials Laboratory at the Xerox PARC, including (but not limited to) [1] investigations of the atomic and electronic structure of a-Si and [2] investigations of defects in III-V materials.

All phases of this project were completed on time and all deliverables were met without significant changes to the original statement of work.

C. Technical
The main goal of this project was to provide U.S. industry with breakthrough capabilities in advanced atomistic materials simulation by using innovative new MPP algorithms, methods, and computers. Moreover, many computational tasks of central importance in materials modeling and simulation had wide applicability, and their optimization would benefit other industrial areas of research outside the confines of ab initio electronic structure calculations of materials. These include parallel input/output and parallel basic linear algebra subroutines for eigenvalue problems.

LLNL completed the initial testing of *ab initio* material simulation (PCGPP) code in March 1996. The next months were spent optimizing the code interfaces for user-friendly use and tuning for better efficiency and performance. Early simulations indicated that a significant speedup with 89% parallel efficiency had been accomplished for processor number up to 64. Further implementations have been made throughout the course of the project.

A parallel implementation of the PCGPP algorithm involves three principal components, namely a complex 3D FFT, input/output and basic linear algebra subroutines (BLAS) such as CAXPY. The parallel algorithm was first implemented using Cray Research Inc.'s Shared Memory Library (SHMEM) and with the MPI library in the latest version for general application in other platforms such as IMB SP system. Our programming strategies contain four major elements:

1. *Automatic domain decomposition.* Based on load balance and data locality, the code automatically assigns the distributions of three indexes for a given number of nodes. In Fig. 1, we illustrate how these assignments have been designed within the PCGPP code.

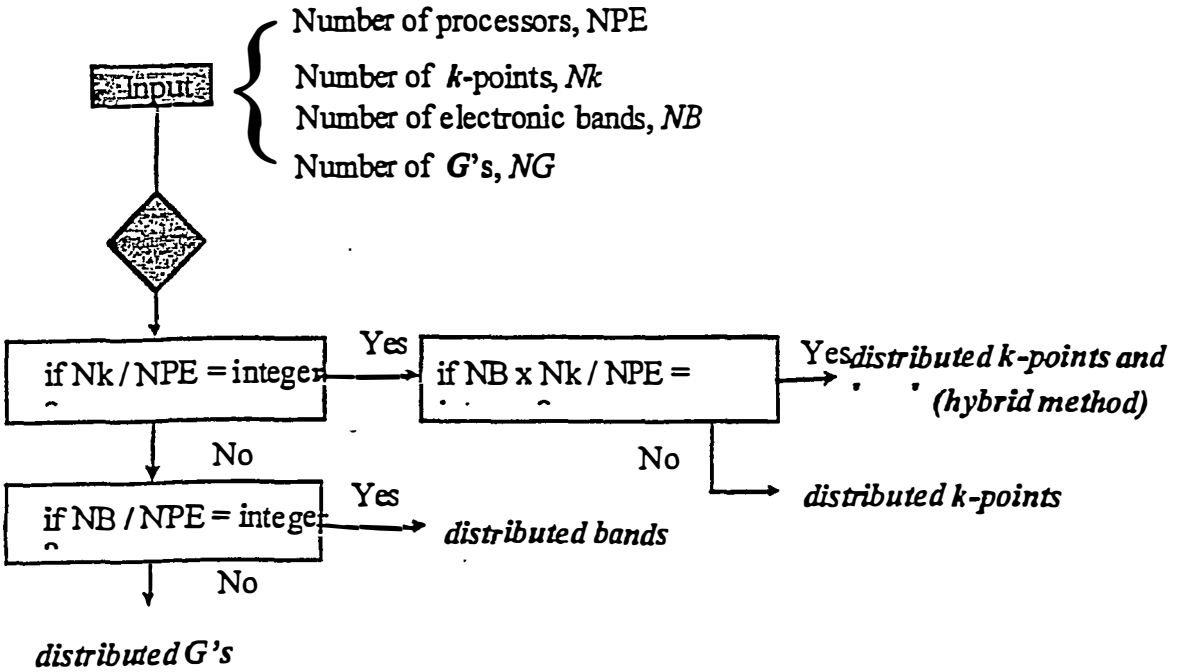

Figure 1. Flow chart shows the automatic domain decomposition according to the data input and number of processors to be used.

2. *Parallel I/O which can speed up the I/O linearly with the number of processors.* An example of a portion of the code is indicated below:

```
file_Rho = fopen("rho.d", "wb+");
ierror = fsetpos(file_Rho, &RhoPosMyPE);
ierror = fwrite (&(Rho[IstartMyPE]), sizeof(double), NrhoMyPE];
ierror = fclose(file_Rho);
```

In such an arrangement, only one single file "rho.d" is necessary for storing all data.

3. *Distributed 3D complex fast Fourier transform (3D CFFT) routines.* In the PCGPP code, applications of CFFTs can be summarized as follows:

- *Perform 3D CFFT on array X from G-space to R-space*
- *Do calculations on array X in R-space using BLAS library*
- *Perform 3D CFFT on array X from R-space to G-space*

Therefore, application of the 3D FFT transforms the array X from G-space to R-space and then transforms it back to the G-space after some calculations have been performed in R-space. There is no need to keep the order of the array index in R-space to be the same as in G-space. In this case, we can express a 3D FFT as three sets of 1D transforms, corresponding to the *x*-, *y*-, and *z*-directions. Each of the 1D transforms in a set is independent of every other transform in that set, and can therefore be performed in parallel. The parallel CFFT routine requires less memory than those found in the parallel Library and allows the user to control the node

assignments. Table I illustrates the data-flow of reduced FFT operations for a transformation from R-space to G-space. We also indicate how step-2 is proceeded in Fig. 2. The data arrangement in R-space is local along z direction but distributed across *x*-*y* planes, while the arrangement in G-space is local along *x* but distributed across *y*-*z* planes. Only two transpose operations and three 1D-FFT calls are needed to transform the data from R-space to G-space. The only drawback with this approach is that tedious book-keeping work is needed at the beginning of the calculations. However, as compared to more than 1,000 3D CFFT calls in a single calculation, the amount of book-keeping work is small.

Step	*x*	*y*	*z*	Operations
1	NPE1	NPE2	1	1D FFT along *z*
2	NPE1	1	NPE2	Transpose *y*-*z*, 1D FFT along *y*
3	1	NPE1	NPE2	Transpose *x*-*y*, 1D FFT along *x*
Output	1	NPE1	NPE2	G-space order: *y*, *z*, *x*

Table I. Three essential steps for transforming a 3D complex array from R-space to G-space. The total number of processors for this transformation is NPE = NPE1 x NPE2.

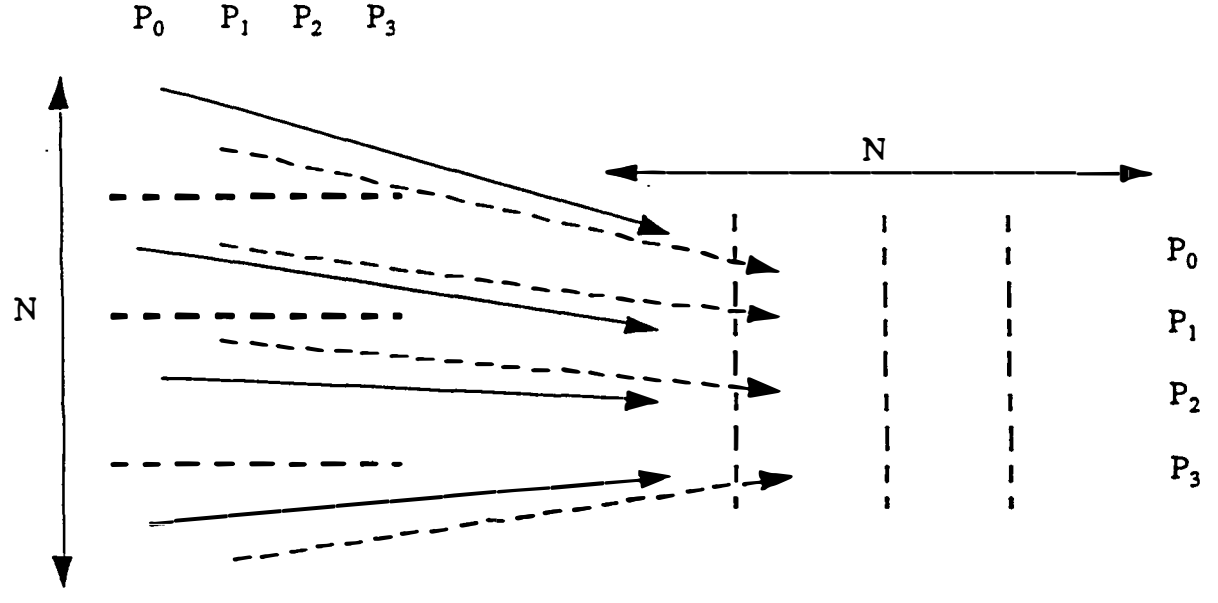

Figure 2. Using 4 processors as an example to illustrate how step-2 in Table I is implemented. First, for each processor the local array is divided into sub-sections according to the number of target processors. Then each sub-section is sent to the target processor simultaneously. After all the data have been sent to the target processors, each individual processor performs 1D FFT operation on its local array.

Figure 3 shows an almost linear speedup of a 3D complex FFT using SHMEM library based on the parallel scheme described above.

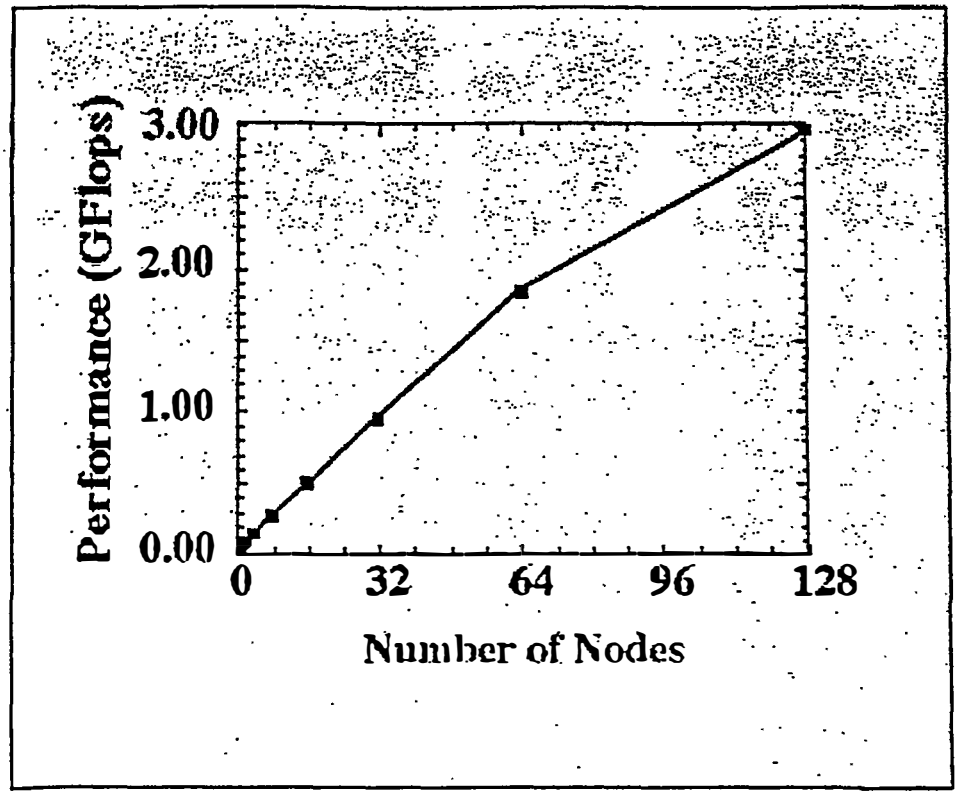

Figure 3. An example shows the performance efficiency in billions of floating-point operations per second (Gflops) vs. the number of nodes of the three dimensional, Fast Fourier Transform routine implemented on the Cray T3D using the SHMEM library. The data size is a 128 x 128 x 128 complex matrix.

Another technical objective was the application of advanced *ab initio* electronic structure methods, at PARC and at LLNL, to specific physics problems of primary importance to research activities in the Electronic Materials Laboratory at Xerox PARC, including (but not limited to) investigations of the atomic and electronic structure of amorphous silicon and defect energetics in III-V semiconductor materials. Investigations of interface band alignment between crystalline and amorphous silicon, and the effect of supercell size on the formation energies of neutral and charged point defects in GaAs semiconductors, were performed and completed during the duration of this project.

D. Expected Economic Impact

The advanced materials modeling codes from LLNL were initially implemented on the Cray Research's T3D system using Shared Memory Library and then were converted to general platform using Message Passing Interfaces (MPI) Library. A user–friendly interfaces have been implemented and thereby became available to industry.

E. Partner Contribution

The main deliverable of this project was the materials simulation codes described above, to run on Cray's heterogeneous PVP-MPP architecture. LLNL, in collaboration with Xerox PARC, applied these codes to specific large-scale materials physics problems. The parties also prepared semi-annual progress reports, held progress meetings, wrote technical reports, and published journal articles describing the research results.

LLNL Milestones

Task Description	Completion Date
- optimization of PCGPP code to CRI's PVP machines	11/95
- ported codes to T3D	3/96
- optimized the PCGPP codes and test production runs	9/97
- conducted detailed numerical simulations	9/97

Xerox PARC Milestones

Task Description	Completion date
- identify and define problems in a-Si and III-V compounds, generate realistic models for numerical simulations	3/96
- identify possible mechanisms and calculate activation energies for self-diffusion in III-V compounds	6/95
- identify possible mechanisms and calculate activation energies for dopant motion in III-V compounds	6/97
- investigate the structural and electronic properties of a-Si	6/96
- use quasiparticle theory to calculate intradefect transition energies	9/97
- study the motion of hydrogen through the amorphous network	3/98

CRI Milestones

Task Description	Completion Date
- determined porting and optimization requirements	9/95
- determined interface requirements	3/96
- developed user interface	9/96
- develop chemical technology	NA
- integrate codes into interface	NA

F. Documents/Reference List

1) Reports

1. "Advanced Quantum-level Materials Simulations in a Massively Parallel Systems," L.H. Yang and C. Mailhiot, *to appear in a book entitled "Industrial Strength Parallel Computing: Programming Massively Parallel Processing Systems."*
2. *"Ab Initio* Data Base of Silica," L.H. Yang and C. Mailhiot, *to appear in J. High Temp. Matts.*
3. "Band Discontinuities at Heterojunctions between Crystalline and Amorphous Silicon," C.G. Van de Walle and L.H. Yang, J. Vac. Sci. & Tech. B13, 1635 (1995).
4. "*DX* center formation in wurtzite and zinc-blende AlGaN," Chris G. Van de Walle, Phys. Rev. B 57, 2033 (1998).
5. "Hydrogen in silicon: fundamental properties and consequences for devices," Chris G. Van de Walle, J. Vac. Sci. Technol. A 16, 1767 (1998).
6. "Hydrogen interaction with polycrystalline and amorphous silicon - theory," Chris G. Van de Walle, in *Hydrogen in Semiconductors II*, edited by N. H. Nickel, *Semiconductors and Semimetals*, Treatise Editors R. K. Willardson and A. C. Beer (Academic Press, Boston), in press.
7. "Exchange of deeply trapped and interstitial hydrogen in silicon," B. Tuttle, C. G. Van de Walle, and J. B. Adams, submitted to Phys. Rev. B.
8. "Possibility of a Mott-Hubbard ground state for the SiC(0001) surface," J. E. Northrup and J. Neugebauer, Physical Review B 57, R4230 (1998).

2) Intellectual Property

i) Subject Inventions

Art. I: "Subject Invention" means any invention of The Regents or Participant conceived or first actually reduced to practice in the performance of work under this CRADA.

Art. XIV: The Parties agree to disclose to each other each and every Subject Invention, which may be patentable or otherwise protectable under the Patent Act.

LLNL Subject Inventions: None

Xerox PARC Subject Inventions: None

CRI Subject Inventions: None

ii) Copyrighted Computer Software:

CRADA Article XIII requires that for all copyrighted computer software produced in the performance of this CRADA, the Party owning the copyright

will provide the source code, an expanded abstract, and the object code and the minimum support documentation needed by a competent user to understand and use the software to DOE's Energy Science and Technology Software Center.

Computer software developed by LLNL: PCGPP was optimized and ported to the Cray T3D MPP. LLNL also ported gang scheduler software to the T3D. LLNL did not assert copyright in any computer software developed under this CRADA.

Computer software developed by Xerox PARC: None

Computer software developed by CRI: None

Licensing Activity:

Appendix C provides that to the extent that LLNL obtains title or authority to license copyrights first arising or produced under this CRADA, LLNL shall negotiate to grant Participant a limited exclusive license to such copyrights for a period from the effective date of the CRADA until six months after the termination of the CRADA, with the period to be extended by mutual consent of the Parties.

Appendix C further provides that, subject to prior commitments, the Parties will negotiate in good faith with each other for licenses, based upon reasonable terms and conditions, in other inventions or copyrighted works, including Background Intellectual Properties, that are necessary either for the practice of the Subject Inventions and Intellectual Property or for the exercise of any license granted by the other Party.

Neither Xerox PARC nor CRI has requested a license to LLNL computer software developed under this CRADA.

G. Acknowledgment

Participant's signature of the final report indicates the following:

1) The Participant has reviewed the final report and concurs with the statements made therein.
2) The Participant agrees that any modifications or changes from the initial proposal were discussed and agreed to during the term of the project.
3) The Participant certifies that:
   a) all reports either completed or in process are listed;
   b) all subject inventions attributable to the project have been disclosed or are included on a list attached to this report; and
   c) appropriate measures have been taken to protect intellectual property attributable to this project.
4) The Participant certifies that if tangible personal property was exchanged during the agreement, all has either been returned to the initial custodian or transferred permanently.
5) The Participant certifies that proprietary information has been returned or destroyed by LLNL.

Tim Keller Date
Cray Research Inc.

Bill Bosl Date
Lawrence Livermore National Laboratory

7/27/00
John Northrup Date
Xerox Palo Alto Research Center

Attachment I - Final Abstract
Attachment II - Project Accomplishments Summary
Attachment III -Final Quarterly Report

High Performance Parallel Processing Project (HPPPP)
Advanced Materials Designs for Massively Parallel Environment

Final Abstract
Attachment I
CRADA No. TC-824-94I

Date: August 4, 1998 Revision: 1

Massively parallel computers, such as the Cray T3D, have historically supported resource sharing solely with space sharing. In that method, multiple problems are solved by executing them on distinct processors. This project developed a dynamic time- and space-sharing scheduler to achieve greater interactivity and throughput than could be achieved with space-sharing alone. CRI and LLNL worked together on the design, testing, and review aspects of this project.

This project was a multi-partner CRADA with nine industrial partners. The CRADA with Xerox PARC made available the advanced materials modeling codes developed at LLNL to the wider industrial community by porting and optimizing these codes for Cray Research supercomputers.

There were separate software deliverables. CRI implemented a general purpose scheduling system as per the design specifications. LLNL ported the local gang scheduler software to the LLNL Cray T3D. In this approach, processors are allocated simultaneously to all components of a parallel program (in a "gang"). Program execution is preempted as needed to provide for interactivity. Programs are also relocated to different processors as needed to efficiently pack the computer's torus of processors. LLNL's advanced quantum-level materials simulation package includes computational tasks of central importance in materials modeling applications. These include parallel input/output and parallel basic linear algebra subroutines for eigenvalue problems. A distributed 3D complex Fast Fourier Transform (3D – CFFT) routine specially designed for *ab initio* materials simulations was implemented. Programs also include a user–friendly interfaces to help industrial users easily adopt and apply the advanced *ab intio* simulation techniques to materials science problems of interest.

LLNL completed the initial testing of *ab initio* material simulation (PCGPP) code in March 1996. The next few months were spent optimizing the code interfaces for user-friendly use and tuning for better efficiency and performance. Early simulations indicated that a significant speedup with 89% parallel efficiency had been accomplished for processor number up to 64. Further implementations have been made throughout the course of the project.

High Performance Parallel Processing Project (HPPPP)
Advanced Materials Designs for Massively Parallel Environment

Project Accomplishments Summary (Attachment II)
CRADA No. TC-0824-94-I

Date: August 21,1998 Revision: 2

A. Parties
The project is a relationship between the Lawrence Livermore National Laboratory (LLNL), Xerox Palo Alto Research Center and Cray Research Inc.

University of California
Lawrence Livermore National Laboratory
PO Box 808, L-795
Livermore, CA 94550

Xerox Palo Alto Research Center
3333 Coyote Hill Road
Palo Alto, CA 94304

Cray Research Inc.
655 Lone Oak Drive
Eagan, MN 55121

B. Background
Massively parallel computers, such as the Cray T3D, have historically supported resource sharing with space sharing only. In that method, multiple problems are solved by executing them on distinct processors, and once a problem begins execution, it cannot be interrupted. When a heavy load exists on such a computer, initialization of jobs may be substantially delayed until other jobs terminate. This paradigm makes interactivity and/or throughput inherently poor. LLNL had experience developing a gang scheduler for the BBN TC2000 massively parallel computer, which successfully addressed these problems.

The prospects for realistic atomic–level materials simulations and prediction of cohesive, structural, mechanical and electronic properties of materials have improved significantly in recent years. *Ab-initio* materials simulation methods based on density functional theory have yielded accurate results for a wide range of materials and have become a *"standard model"* for materials property calculations. Furthermore, advances in numerical algorithms and in computational hardware, particularly the introduction of massively parallel supercomputers, now makes feasible the *ab-initio* treatment of technologically important materials, such as semiconductors used in computer applications. The adaptation of *ab initio*

materials modeling methodology to parallel processing platforms has been implemented within the scope of this work.

C. Description

In the overall CRADA, the project developed a dynamic time- and space-sharing scheduler to achieve greater interactivity and throughput than could be achieved with space-sharing alone. The LLNL Cray T3D was initially configured for a high level of interactivity during working hours, frequently resulting in very poor throughput. When a very heavy interactive load existed, very long delays could be experienced for job initialization. We were also forced to severely limit job size and run times to limit the adverse impact a single job could have. Our objective was to develop a dynamic time- and space-sharing scheduler to resolve all of these problems, providing excellent throughput, excellent interactivity, and permitting the execution of larger and longer running jobs.

CRI and LLNL worked together on the design, testing, and review aspects of this project. There were separate software deliverables for this project. CRI implemented a general purpose mechanism for the preemption of jobs, saving the job's state to disk, and later reloading its state into memory for continued execution. LLNL ported the local gang scheduler software to the LLNL Cray T3D. In this approach, processors are allocated simultaneously to all components of a parallel program (in a "gang"). Program execution is preempted as needed to provide for interactivity. Programs are also relocated to different processors as needed to efficiently pack the computer's torus of processors.

LLNL completed the initial installation of the gang scheduler in March of 1996. Since LLNL's Cray T3D was originally configured for a high level of interactivity with moderate throughput, we were able to reconfigure the computer for dramatically higher throughput. The gang scheduler was able to provide even greater interactivity while utilization was increased from the 30 percent range to the 90 percent range – a phenomenal level of throughput for a massively parallel computer.

In this portion of the CRADA, Cray Research Inc. (CRI), the Xerox Palo Alto Research Center (PARC), and LLNL worked together on the project with each had primary responsibility for certain tasks. LLNL ported and optimized current LLNL atomistic ab-initio materials simulation codes to production on the T3D. Since the T3D was part of a heterogeneous computer architecture consisting of a parallel vector platform (PVP) coupled to a massively parallel component (T3D), porting to the T3D was realized in a staged approach; pieces of LLNL's materials simulation codes were optimized to run on the T3D, while the remaining pieces were executed on the PVP part of the machine. CRI assisted LLNL in porting and optimization to the T3D. LLNL, in collaboration with Xerox PARC, applied the atomistic ab initio materials simulation codes to specific large-scale materials physics problems of significance to DOE and to the Electronic Materials Laboratory (EML) at the Xerox PARC.

D. Expected Economic Impact

The utilization of the LLNL Cray T3D increased by a factor of three. With computers of this size costing tens of millions of dollars, the benefit to taxpayers has been enormous. The LLNL gang scheduler has been provided to other U. S. government agencies with Cray T3D computers. Like LLNL, these sites are expected to enjoy a substantial increase in throughput and interactivity in their Cray T3D supercomputers with minimal expense for the installation of this software.

CRI has also developed its own dynamic time- and space-sharing scheduler, the Dynamic Job Manager (DJM) The development of the DJM has benefited from much of this CRADA's work and has been installed by CRI on a number of their Cray T3D computers leading to significant performance improvements.

The *ab initio* materials modeling codes from LLNL were initially implemented on Cray Research's T3D system using Shared Memory Library and then were converted to general platform using Message Passing Interfaces (MPI) Library. User–friendly interfaces have been implemented and thereby became available to industry.

E. Benefits to DOE

The Cray T3D located at LLNL was able to achieve a dramatic improvement in throughput and interactivity. In the months following the introduction of the gang scheduler, average monthly utilization increased from the 30 % range to the 90 % range while interactivity also increased. LLNL was able to triple the effective use of its Cray T3D without additional hardware cost and with minimal software development costs. Problems using up to 40 hours and 64 processors are executed on a routine basis. Problems have been executed with up to 256 processors (the entire LLNL T3D) and 40 hours of execution time. Problems of this size could not realistically be solved formerly.

High-performance computing and materials simulation are two critical core competencies at LLNL and within the DOE/DP complex in general. The development of quantum-level materials simulation methods, as developed and implemented in this project, directly benefit LLNL and DOE because they are directly applicable to stockpile materials of interest. In particular, such methods form the basis to the prediction of the properties of materials, as a result of aging and/or re-manufacturing, and their effects on stockpile performance, safety, and reliability.

F. Industry Area

This project demonstrated that time- and space-sharing of massively parallel computers is not only possible, but highly advantageous. This work benefits a wide number of industries in which massively parallel computers are used, including: aircraft, automotive, medical, etc. In part due to our success, several other companies are currently pursuing gang schedulers for their parallel computers.

G. Project Status
This project is completed.

H. LLNL Point of Contact for Project Information
Christian Mailhiot
Lawrence Livermore National Laboratory
PO Box 808, L-055
Livermore, CA 94550
925/422-5873
FAX: 925/422-9488

Company Size and Point(s) of Contact
Cray Research has 3700 employees. Primary contact for this project is Shepard Smithline.

The Xerox Palo Alto Research Center has 300 employees. Primary contacts for this project are John Northrup and Chris G. Van de Walle.

J. Project Examples
None

K. Intellectual Property

i) Subject Inventions

Art. I: "Subject Invention" means any invention of The Regents or Participant conceived or first actually reduced to practice in the performance of work under this CRADA.

Art. XIV: The Parties agree to disclose to each other each and every Subject Invention, which may be patentable or otherwise protectable under the Patent Act.

LLNL Subject Inventions: None

Xerox PARC Subject Inventions: None

CRI Subject Inventions: None

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Computer software developed by CRI: None

Licensing Activity:

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Neither Xerox PARC nor CRI has requested a license to LLNL computer software developed under this CRADA

L. Release of Information

I certify that all information contained in this report is accurate and releasable to the best of my knowledge.

Norma E Dunford — 9/12/00

Karena McKinley, Director
Industrial Partnerships and Commercialization

Date

Release of Information

I have reviewed the attached Project Accomplishment Summary prepared by Lawrence Livermore National Laboratory and agree that the information about our CRADA may be released for external distribution.

John E Northrup — 7/27/00

John Northrup
Xerox Palo Alto Research Center

Date

Tim Keller
Cray Research Inc.

Date

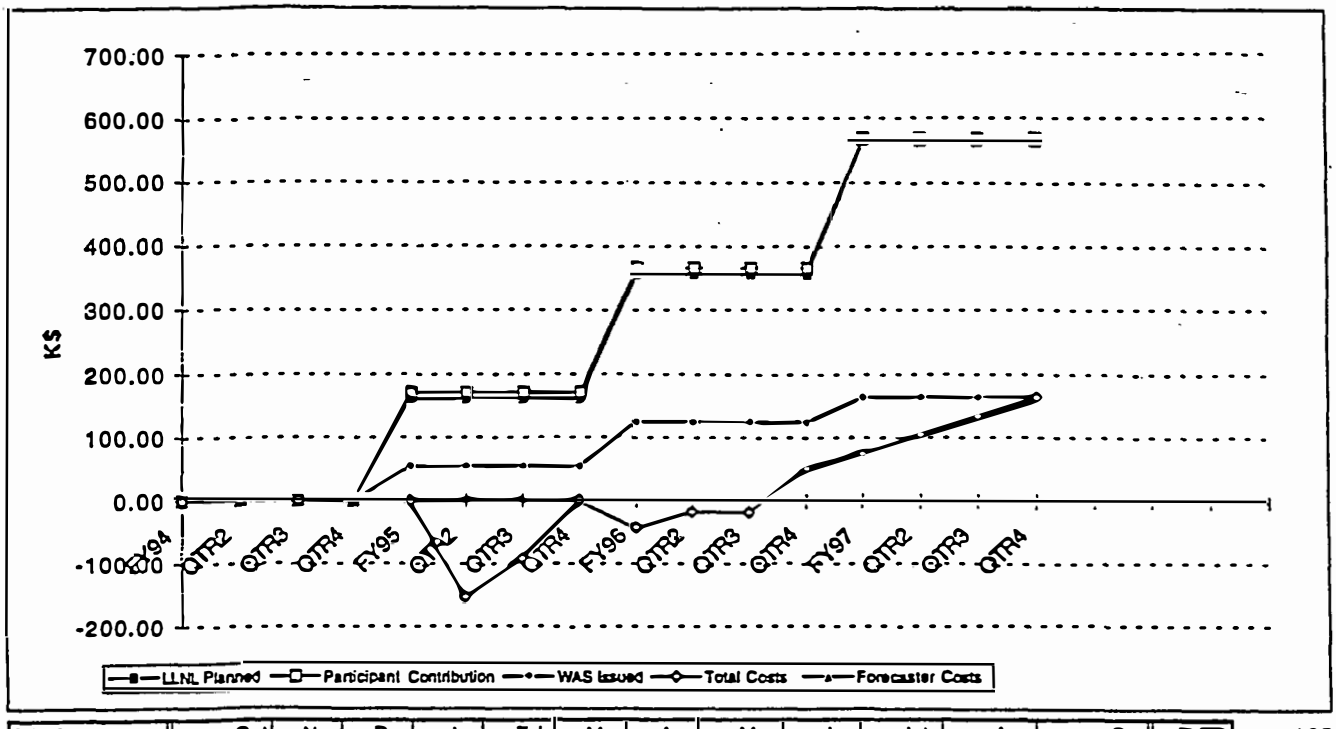
Lawrence Livermore National Laboratory

Title: HPPP Advanced Materials Design
Participant: Xerox
DOE TTI No.: 94-MULT-003-XX-1
CRADA No.: TC-0824-94 (I)
Account Number 4745-77, 87
Accounts Closed N/A

Reporting Period: 07/01/95 - 09/30/97
Date CRADA Executed: 1/30/95
DOE Approval Date: 2/22/95
Scheduled Ending Date: 2/22/98
Project Completion Date: N/A
B & R Code (S): DP0301, YN01000

Approved Funding Profile ($K)

	FY94	FY95	FY96	FY97	FYOUT	Total
LLNL Planned	0	162	195	209	0	566
Participant In-Kind	0	172	195	202	0	569
Participant Funds-I	0	0	0	0	0	0
WAS DP0301	0	55	70	40	0	165
LDRD Funds	0	107	0	0	0	107
Total Costs	0	1	51	113	0	165



DP0301	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun	July	Aug	Sep	FYTD
FY94	0	0	0	0	0	0	0	0	0	0	0	0	0
FY95	0	0	0	0	0	-154	13	21	27	30	54	9	1
FY96	-66	11	11	8	10	8	12	-23	10	11	11	48	51
FY97	9	14	0	9	11	10	10	11	9	14	17	0	113
FYOUT	0	0	0	0	0	0	0	0	0	0	0	0	0

165

YN01000	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun	July	Aug	Sep	FYTD
FY94	0	0	0	0	0	0	0	0	0	0	0	0	0
FY95	0	0	0	0	0	0	0	0	0	0	0	0	0
FY96	0	0	0	0	0	0	0	0	0	0	0	0	0
FY97	0	0	0	0	0	0	0	0	0	0	0	0	0
FYOUT	0	0	0	0	0	0	0	0	0	0	0	0	0

0

STAFF w/phone:

Lab PI: Lin H. Yang (510) 424-4153
Participant: John Northrup (415) 812-4117
Resource Manager: Steve Stinson (510) 423-2888
DOE OAK: Jerry Scheinberg (510) 637-1653
DOE HQ: Alex Larzelere (202) 586-1101

Reporting Period 07/01/95 - 09/30/97
DOE TTI No.: 94-MULT-003-XX-1
CRADA No.: TC-0824-94 (I)

Milestones and Deliverables:

List the complete set of milestones for all phases of the CRADA. Continue on a separate page if necessary.
Report any changes from the original CRADA or previous quarterly report on the CRADA Change Form.

	Completion Date: Scheduled	Actual
1 LLNL: Optimization of current ab-initio code on CRI's T3D machines.	03/95	03/95
2 LLNL: Port codes to T3D.	09/95	07/95
3 LLNL: Fine-tune the codes and test production runs.	12/95	10/95
4 LLNL: Conduct detailed numerical simulations.	12/97	01/98
5 Xerox: Identify and define problems in a-Si and III-V compounds.	09/95	09/95
6 Xerox: Calculate activation energies for self-diffusion in III-V compounds.	06/96	04/97
7 Xerox: Calculate activation energies for dopant diffusion in III-V compounds.	03/97	12/97
8 Xerox: Investigate the structural and electronic properties of a-Si.	12/97	02/96

Verification of participants' In-kind contribution was made in accordance with LLNL policy. Explain basis of verification:

Please initial: YES X NO

List any subject inventions by either party (include IL# for LLNL inventions), additional background intellectual property, patents applied for, software copyrights, publications, awards, licenses granted or reportable economic impacts

See attached

Accomplishments

Describe Technical/Non-Technical lessons learned (address and be specific about milestones, participant contributions)
Summarize causes/justification of deviations from original scope of work. Continue on a separate page if necessary.

See attached

Reviewed by CRADA project Program Manager: Date:

Reviewed by Karena McKinley, Director, LLNL/IP&C: Karena E. McKinley Date: 9/12/97

Direct questions regarding this Report to IP&C Resource Manager, Carol Asher at (925) 422-7618