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LLNL-TR-746744

High Performance Parallel Processing (HPPP) "Detail Simulation of Subsurface Flow and Chemical Migration" Final Report CRADA No. TC-0824-94-H

S. Ashby, K. Loy, K. Lind

February 23, 2018

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High Performance Parallel Processing (HPPP)
"Detail Simulation of Subsurface Flow and Chemical Migration"

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

Date: November 9, 1998 Revision: 2

A. Parties

The project is a relationship between the Lawrence Livermore National Laboratory (LLNL), IT Corporation (IT) and Cray Research Inc (CRI).

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

IT Corporation
4005 Port Chicago Hwy
Concord, CA 94520-1120

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

B. Project Scope

There were three phases to this project model specification, implementation of the simulator on the T3D, and testing and debugging of the simulator.

Phase 1

LLNL and IT developed a preliminary three-dimensional model for fluid flow and chemical contaminant transport in a heterogeneous porous medium. This model was based on a backward Euler time discretization with a finite difference spatial discretization. Preconditioned conjugate gradients were used to solve the inherent linear systems. The main task was to determine the preconditioner that would be most appropriate for the T3D architecture. In addition, LLNL and IT generated hydraulic conductivity "realizations" for the project site. Some initial macros and codes were ported to the T3D by CRI.

Phase 2

The majority of the effort was devoted to porting this simulator to the T3D, and then customizing it to attain superior performance. To do this, LLNL and CRI ported the AMPS message-passing macros to the T3D. IT provided the data for a project site in a format suitable for the T3D.

Phase 3

LLNL and CRI tested, debugged, and refined the simulator by running numerical experiments. The simulator was tested on a sites of interest to IT. In addition, LLNL and CRI conducted a performance analysis on the T3D and compared it to other MPPs.

C. Technical

The main objective in this portion of the CRADA was to use the novel Cray T3D MPP to study the impact of several factors on chemical migration in heterogeneous porous media, under both natural and remedial conditions. To do this, the parties (1) developed a three-dimensional model of fluid flow and chemical migration in heterogeneous porous media; (2) efficiently implemented this model on the T3D; and (3) used this code to perform a preliminary evaluation of flow and transport behavior in nonuniform aquifer materials.

The main deliverable of this project was the simulator described above, customized to run on the T3D manufactured by Cray Research, Inc. The parties also prepared semi-annual progress reports and a final report at the conclusion of the project. In addition, the parties prepared informal working notes, wrote technical reports, and published journal articles describing the research and simulation results.

LLNL Milestones

- Task Description	Month
- develop flow model and choose numerical methods	0- 6
- port AMPS message-passing macros to T3D	3- 9
- implement preconditioned conjugate gradient solver	9-12
- test simulator on representative flow problems	12-18
- develop and implement chemical transport model	15-24
- fine tune the simulator for superior performance	24-30
- conduct detailed numerical simulations	30-36

IT Milestones

- Task Description	Month
- devise hydraulic conductivity realizations	3-15
- provide data for IT test site in suitable format	9-18
- supervise coupling of a preliminary flow and transport models	15-24

CRI Milestones

- Task Description	Month
- aid in port of AMPS message-passing macros	0- 3
- optimize AMPS message-passing macros	3- 9
- optimize basic linear algebra subroutines	6-12
- implement other communication paradigms	9-21
- optimize iterative solver	12-18
- optimize remainder of simulator	18-30
- benchmark code against existing codes	24-36

D. Expected Economic Impact

The new 3-D simulation capability will enable industry to characterize contamination migration and transformation in soils at waste sites to help improve the design and management of engineered remediation strategies.

E. Partner Contribution

LLNL and CRI deliverables were met. However, due to changing business needs at IT and a shift in funding at LLNL toward fundamental math research rather than applications, ParFlow was not validated by IT and is not expected to be used for industrial remediation planning. Its primary use will be in the area of mathematical and theoretical groundwater modeling research. This research may be of use to the environmental remediation community.

F. Documents/Reference List

1) Reports

[1] A. Tompson, S. Ashby, R. Falgout, and S. Smith. On the role of high performance computing for simulating subsurface flow and chemical migration. In *Proc. VIII International Conference on Finite Elements in Fluids—New Trends and Applications*, 1994. Held in Barcelona, Spain, September 20-24, 1993. Also available as LLNL technical report UCRL-JC-114175.

[2] S. F. Ashby, R. D. Falgout, S. G. Smith and A. F. B. Tompson. Modeling groundwater flow on MPPs. In A. Skjellum and D. Resse, editors, *Proc. 1993 Scalable Parallel Libraries Conference*, pages 17-25. IEEE Computer Society Press, 1994. Held at Mississippi State University, October 6-8, 1993. Also available as LLNL technical report UCRL-JC-115602.

[3] A. F. B. Tompson, S. F. Ashby, R. D. Falgout, S. G. Smith, T. W. Fogwell, and G. A. Loosmore. Use of high performance computing to examine the effectiveness of aquifer remediation. In *Proc. X International Conference on Computational Methods in Water Resoorces*, 1994. Held in Heidelberg, Germany, July 19-22, 1994. Also available as LLNL technical report UCRL-JC-115374.

[4] S. F. Ashby, R. D. Falgout, T. W. Fogwell, and A. F. B. Tompson. Numerical simulation of groundwater flow on MPPs. In *Proc. Fifth SIAM Conference on Applied Linear Algebra*, pages 228-232, 1994. Held in Snowbird, UT, June 15-18, 1994. Also available as LLNL technical report UCRL-JC-115895.

[5] S. F. Ashby, R. D. Falgout, S. G. Smith, and T. W. Fogwell. Multigrid preconditioned conjugate gradients for the numerical simulation of groundwater flow on the CRAY T3D. In *Proc. ANS International Conference on Mathematics and Computations, Reactor Physics and Environmental Analyses, 1995*. Held in Portland, OR, April 30-May 4 1995.

[6] S. F. Ashby, R. D. Falgout, S. G. Smith, and A. F. B. Tompson. The parallel performance of a groundwater flow code on the Cray T3D. In *Proc. Seventh SIAM Conference on Parallel Processing for Scientific Computing*, pages 131-136. Society for Industrial and Applied Mathematics, 1995. Held in San Francisco, February 15-17, 1995. Also available as LLNL technical report UCRL-JC-118604.

[7] S. F. Ashby, W. J. Bosl, R. D. Falgout, S. G. Smith, A. F. B. Tompson, and T. J. Williams. A numerical simulation of groundwater flow and contaminant transport on the Cray T3D and C90 supercomputers. In *Proc. 34th Cray User Group Conference*, pages 275-282. Cray User Group, Inc., 1994. Held in Tours, France, October 10-14, 1994. Also available as LLNL technical report UCRL-JC-118635.

Substantial documentation available on the internet at "http://www-lc.llnl.gov/casc/parflow."

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

IT 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: Some development of PARFLOW was done under this CRADA, as well as customization to run on the T3D.

Computer software developed by IT: 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 TI 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.

Kenneth L. Loy 7/24/00
Kenneth Loy Date
IT Corp.

Steven F. Ashby 10/17/00
Steven Ashby Date
Lawrence Livermore National Laboratory

Kevin Lind Date
Cray Research Inc.

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

High Performance Parallel Processing (HPPP)
"Detail Simulation of Subsurface Flow and Chemical Migration"

Final Abstract (Attachment I)
CRADA No. TC-0824-94-H

Date: November 9, 1998 Revision:

This project was a multi-partner CRADA with nine industrial partners. IT Corporation applied high performance computing to a preliminary 3-D model-of fluid flow and chemical transport in heterogeneous porous media. LLNL developed the mathematical methods and computer code. CRI supplied super computer expertise needed to optimize performance of the ParFlow code on the T3D computers.

High Performance Parallel Processing (HPPP)
"Detail Simulation of Subsurface Flow and Chemical Migration"

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

Date: November 9, 1998 Revision:

A. Parties

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

B. Background

On July 13, 1993, Cray Research, Inc. (CRI) submitted a team response to a DOE Solicitation (Number DE-SA03-93DP40010) requesting proposals designed to enhance U.S. competitiveness through a Cooperative Development Project in High Performance Parallel Processing (HPPP). A project was proposed to establish a three year multi-party collaboration to accelerate the availability of commercial MPP software to U.S. government, academic and industrial end-users. The primary collaborators are CRI, Thinking Machines Corporation (TMC), Los Alamos National Laboratory (LANL), and Lawrence Livermore National Laboratory (LLNL). Included in the arrangement were fifteen (15) major U.S. industrial partners.

IT applied high performance computing to a preliminary 3-D model of fluid flow and chemical transport in a heterogeneous porous medium. LLNL developed the mathematical methods and computer code. CRI supplied super computer expertise needed to optimize performance of the Parflow code on the T3D computers.

C. Description

This project developed a 3D groundwater flow and contaminant transport code which would run efficiently on massively parallel super computers. The successful completion of this project required the integration of mathematical and numerical expertise from LLNL, hardware skills and computer science skills from CRI personnel, and scientific experience from IT Corporation. The code has been completed and is being used for scientific research at this time.

IT, LLNL and CRI worked together on all aspects of the project, but each had primary

responsibility for certain tasks. LLNL developed the simulator and ported it to the T3D. IT provided its site data in a format suitable for the T3D. CRI provided expertise in the efficient implementation of numerical algorithms on the T3D.

D. Expected Economic Impact
The new 3-D simulation capability will enable industry to characterize contamination migration and transformation in soils at waste sites to help improve the design and management of engineered remediation strategies.

E. Benefits to DOE
This effort showed that scalable algorithms can be implemented efficiently on large industrial-quality codes. These lessons are being applied to many computational projects at LLNL through the software developed work of the Center for Applied Scientific Computing (CASC).

F. Industry Area
Software and environmental industries

G. Project Status

This project is completed.

H. LLNL Point of Contact for Project Information
Steven Ashby
Lawrence Livermore National Laboratory
PO Box 808, L-561
Livermore, CA 94550
925/423-2462
FAX: 925/422-6675

Company Size and Point(s) of Contact
Cray Research has 3700 employees. Primary contact for this project is Kevin Lind.
612/683-5681 (phone)
612/683-5310 (fax)

IT Corporation has 2200 employees. Primary contact is Kenneth Loy.
925/288-9898 (phone)
925/827-2392 (fax)

J. Project Examples
There are no project examples.

K. Intellectual Property

i) Subject Inventions

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L. Release of Information

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

Karena McKinley, Director
Industrial Partnerships and Commercialization

11/15/00
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.

Kevin Lind
Cray Research Inc.

Date

Ken Loy
IT Corporation

7/24/00
Date

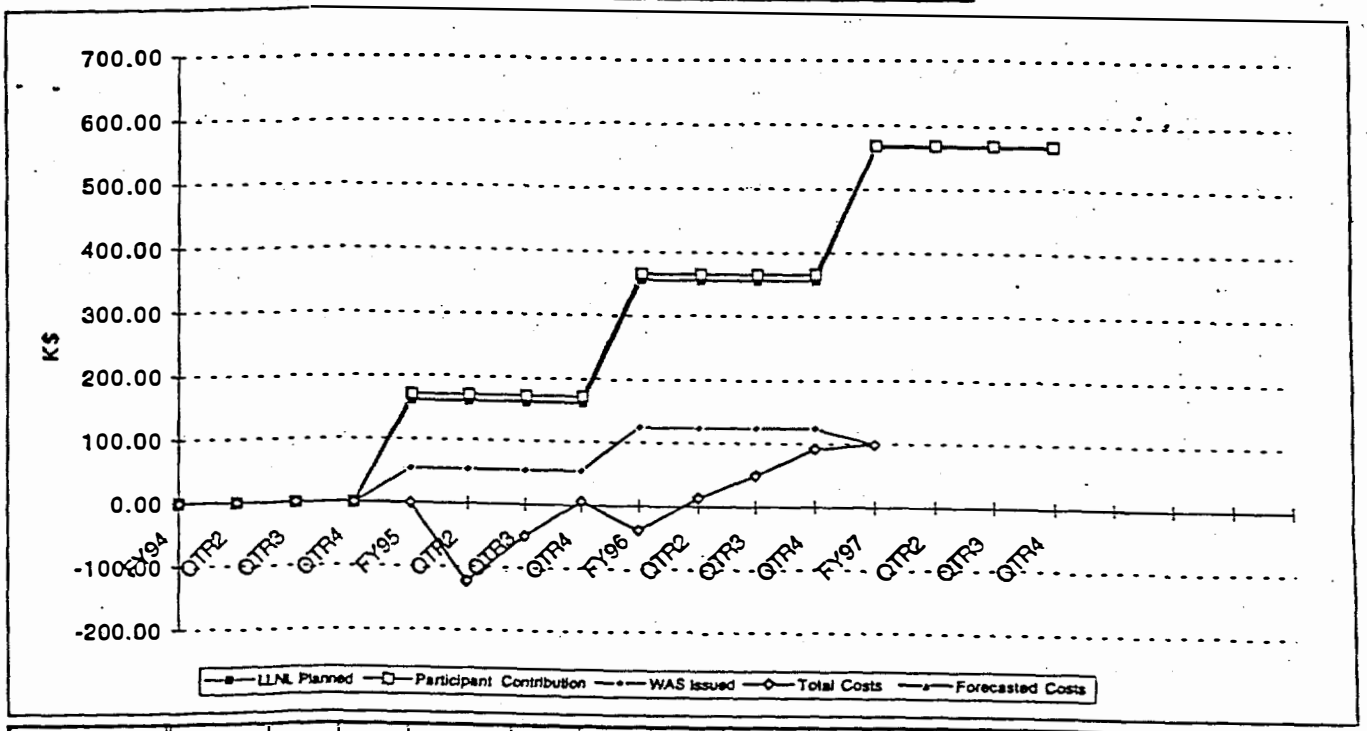
Lawrence Livermore National Laboratory

Title: HPPP Subsurface Flow/Chemical Migration
Participant: International Technology (IT)
DOE TTI No.: 94-MULT-003-XX-1
CRADA No.: TC-0824-94 (H)
Account Number 4745-74, 84
Accounts Closed N/A

Reporting Period: 07/01/95 - 09/30/96
Date CRADA Executed: 2/23/95
DOE Approval Date: 3/3/95
Scheduled Ending Date: 3/1/98
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
Paticipant Funds-In	0	0	0	0	0	0
WAS DP0301	0	55	70	-26	0	99
LDRD Funds	0	0	0	0	0	0
Total Costs	0	6	85	8	0	99



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	-123	17	41	15	27	51	-21	6
FY96	-56	2	9	14	13	27	5	-7	37	8	10	24	85
FY97	1	7	0	0	0	0	0	0	0	0	0	0	8
FYOUT	0	0	0	0	0	0	0	0	0	0	0	0	0

99

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: Steve Ashby (510) 423-2462
Resource Manager: Steve Stinson (510) 423-2888
DOE OAK: Jerry Scheinberg (510) 637-1653

Participant: William Moore (510) 372-9100
DOE HQ: Alex Larzelere (202) 586-1101

Milestones and Deliverables:

List the complete set of milestones for all phases of the CRADA. Continue on a separate page if necessary.

Completion Date: Scheduled / Actual

See attached report

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 report

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 report

Reviewed by CRADA project Program Manager: Date:

Reviewed by Karena McKinley, Director, LLNL/IP&C: Karena McKinley Date: 11/15/00

Direct questions regarding this Report to IP&C Resource Manager, Carol Asher, at (510) 422-7618