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Parallel Mathematical Libraries Final Reports CRADA No. TC-1117-95

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Final Report
CRADA No. TC-1117-95

Date: 10/13/00   Revision: 1

A.   Parties

The project was a relationship between the Lawrence Livermore National Laboratory (LLNL) and Intel Corporation (Intel). Intel is a member of the United States Industry Coalition (USIC).

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B.   Project Scope

The goal of this CRADA project was to develop parallel mathematical libraries of numerical methods, which are required by a wide range of scientific and engineering simulation codes suitable for use by a wide range of new parallel computer applications for industry, academia, and the national laboratories. The software libraries developed under this CRADA are to be placed in the public domain in order to have the broadest possible benefit.

Under a separate contract between LLNL and Mississippi State University (MSU), LLNL and MSU developed the requirements documents for the base specifications and test plans of all the delivered software components. LLNL/MSU will maintain the mathematical libraries for state-of-the-art supercomputers.

C.   Technical Accomplishments

Subcontracts with both the NIS Institute VNIIEF and the Mississippi State University ("MSU") aided in the completion of the work under this CRADA.

This project developed parallel mathematical libraries for use by parallel computer application code builders. The specific classes of routines to be implemented represent the most commonly needed mathematical functions used when developing large computer simulation codes. For this project, LLNL and Intel identified the following activities: linear algebra (including both dense and sparse solvers, Jacobean calculations, Newton solvers, ODE and DAE solvers, Fast Fourier Transforms (multi-radix), geometric multi-

grid solvers, sorting and graph algorithmic routines, and optimization routines (both constrained and unconstrained). Message Passing Interface (MPI) allows consolidation of parallel algorithm development for specific Massively Parallel Processor (MPP) hardware into a form that can be exploited on a much wider range of parallel computer hardware.

There are two OS targets: the Windows/NT operating system and a generic Unix OS.

Intel defined hardware needs of the commercial market and provided necessary equipment to VNIIEF to develop the libraries and will provide marketing expertise.

VNIIEF conducted testing of the products and libraries developed before submission to LLNL/MSU. VNIIEF developed a test suite which it submitted with the code to LLNL/MSU. The testing assured correctness and robustness over a range of user inputs, and performance over a range of important end user inputs (problem size, concurrence, machine configuration variations). Additional test problems were defined for implementation by VNIIEF to expand the range of inputs that were tested.

VNIIEF studied the design of sparse data formats, Sequential C and F77 data structure converters and Toolbox data structures as a prelude to designing sparse parallel data structures in MPI. VNIIEF developed the prototype interfaces and basic linear algebra routines, provided progress and status reports, created draft Implementation Reference Document and translated an MPI book into Russian. Converted Toolbox Iterative Solver Library to MPI, developed flexible F77interface to Iterative Solver Library, built sparse matrix vector multiplication suite, developed prototype sparse parallel remapping algorithms and Jacobean functions in MPI. VNIIEF developed parallel preconditioner library for Iterative solver and developed prototype ILU and sparse LU libraries as preconditioners for sparse iterative solver.

LLNL/MSU edited the MPI translation, provided MPI for Intel environment for VNIIEF development team and upgrades, provided Multicomputer Toolbox software, evaluated deliverables and provided comments and suggestions. LLNL/MSU evaluated developed software and test plans, completed editing of "Using MPI" and interaction with MIT Press. Evaluated sparse parallel and sequential basic linear algebra software. Reviewed test plans and product quality. Developed and implemented electronic promulgation plans for software to implement wide distribution for public domain release.

LLNL/MSU posted a formal public release of the PMLP library, including web-based documentation.

LLNL/MSU also provided a final report to the DOE Sponsor including recommendations for further software and related follow-on projects.

D.   Expected Economic Impact

The cooperative R&D efforts associated with this partnering program will result in the improvements to the technical base of both DOE and the manufacturing sector in the United States. As the resulting work of this CRADA will be placed in the public domain, it is not possible to predict how substantial any economic impact will be. Other benefits to the DOE program included: (i) facilitation and support defense conversion and nonproliferation activities; (ii) promotion of free markets and economic growth in the NIS; (iii) encouraged emergence of political and economic institutions in the NIS based on free enterprise; (iv) expansion of international markets for U.S. goods and services; and (v) enhanced the international competitiveness of the U.S. private sector.

E.   Partner Contribution

Partner participated by defining the hardware needs of the commercial market and providing marketing expertise and the necessary equipment to VNIIEF to develop the libraries.

F.   Documents/Reference List

F.1 Project Abstract:

LLNL and Intel entered into a CRADA for the development of a parallel mathematical library suitable for use on a wide range of the most commonly available man-market computer hardware. The solvers and preconditioners have been developed in an object-oriented framework that allows the use of each solver and preconditioner for a wide variety of data storage formats, floating-point precisions, etc. Web-based documentation is available for both the entire set of user-accessible routines and internal implementation structure.

F.2   Quarterly Reports:

Quarterly reports were prepared by VNIIEF and LLNL/MSU on a staggered schedule and sent to Participant.

F.3 Final report:

The fully documented, web-based public release serves the role of the final report.

F.4 Intellectual Property:

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.

Under CRADA Article 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.

Since the full source code has been placed in the public domain, no attribute of innovation is required.

Intel Sole Subject Inventions:

Joint LLNL/Intel Subject Inventions: N/A

Sole LLNL Subject Inventions: N/A

Copyrightable Computer Software:

CRADA Article XIII provides that no copyright will be asserted or established over any copyrightable works generated in the performance of this CRADA. Further, the software libraries generated in the performance of this CRADA will be placed into the public domain accompanied by a DOE-approved disclaimer.

Computer software developed solely by Intel: N/A

Computer software developed jointly by Intel and LLNL: N/A

Computer software developed by LLNL or the NIS Institute: N/A

G. Acknowledgement

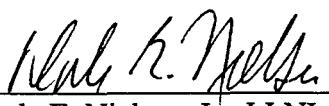Participant's signature of the final report indicates the following:
1) The Participant has reviewed the final report and concurs with the statements made therein.
2) The Participant agrees that any modifications or changes from the initial proposal were discussed and agreed to during the term of the project.
3) The Participant certifies that all reports either completed or in process are listed and all subject inventions and the associated intellectual property protection measures generated by his/her respective company and attributable to the project have been disclosed or are included on a list attached to this report.
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.

FOR RICHARD WIRT
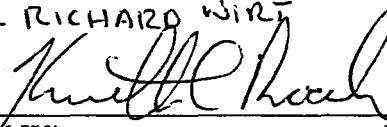
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6 March 2001