LAWRENCE
LIVERMORE
NATIONAL
LABORATORY

LLNL-TR-745043

High Performance Parallel Processing (HPPP) Finite Element Simulation of Fluid Structure Interactions Final Report CRADA No. TC-0824-94-A

R. Couch, D. P. Ziegler

January 24, 2018

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 (HPPP) Finite Element Simulation Of Fluid Structure Interactions

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

Date: August 21, 1998 Revision: 2

A. Parties

The project is a relationship between the Lawrence Livermore National Laboratory (LLNL) and Aluminum Company of America (ALCOA).

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

Aluminum Company of America (ALCOA)
100 Technical Drive
Alcoa Center, PA 15069-0001

B. Project Scope

This project was a multi-partner CRADA. This was a partnership between Alcoa and LLNL. Alcoa developed a system of numerical simulation modules that provided accurate and efficient three-dimensional modeling of combined fluid dynamics and structural response.

Alcoa and LLNL worked together on all aspects of the problem, but each had primary responsibility for certain tasks. Alcoa provided input and data related to material models and aluminum forming processes. LLNL was responsible for developing the simulation software and porting it to the T3D platform. Alcoa was responsible for providing the benchmark forming data and validating code performance against these benchmarks.

Alcoa and LLNL defined the type of material descriptions and the relevant physical data required. They also defined a set of benchmark forming simulations that provided validation for the simulation techniques developed.

LLNL established a computations strategy based on the physical simulation requirements and the need for efficient parallel processing implementation. Alcoa provided data on material properties and participated with LLNL in the development of related material models. Alcoa also generated the appropriate data on the set of benchmark forming processes for use in the software validation

activities at the various stages of development. A software prototype was developed which Alcoa utilized at their facility while LLNL began the T3D implementation.

Software validation of took place via simulation of the chosen benchmarks. Both Alcoa and LLNL participated in this activity. Funding was not available for the final year of the project. The software product was provided to Alcoa in its then current state, but not all the tasks were completed.

C. Technical Accomplishments

The following milestone chart highlights Alcoa's participation in the CRADA:

Milestones

Task Description	Completed?	Agency
- assembly of relevant physical data	Y	Alcoa
- assembly of initial benchmark problems	Y	Alcoa
- initial solidification model	Y	Alcoa/LLNL
- surface tension model	N	LLNL
- viscosity model	Y	LLNL
- implement explicit Lagrangian coding	Y	LLNL
- assembly of final benchmark problems	Y	Alcoa
- completion of initial heat transfer modules	Y	LLNL
- implement advection routines	Y	LLNL
- completion of heat transfer modules	Y	LLNL
- implement heat conduction modules	Y	LLNL
- development of material models	Y	Alcoa/LLNL
- simulation of initial benchmarks	Y	LLNL/Alcoa
- implement implicit Lagrangian coding	N	LLNL
- simulation of final benchmarks	N	Alcoa/LLNL
- documentation	N	LLNL

D. Expected Economic Impact

This project assists the entire U.S. metals industry in developing improved forging, extrusion and casting processes.

E. Partner Contribution

Alcoa contributed validated material models and data from aluminum forming activities that could be used in the code benchmarking process. They also participated directly in this benchmarking process.

F. Documents/Reference List

Reports

"Improved Utilization and Responsiveness with Gang Scheduling," Dror G. Feitelson and Morris A. Jette, *Job Scheduling Strategies for Parallel Processing Workshop*, (publication pending) April 1 997.

"The Gang Scheduler Timesharing on a Cray T3D," Morris Jette, David Storch, and Emily Yim, Cray User Group Meeting, March 1996.

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

Documentation consisted of an unpublished user's manual that was provided to Alcoa.

Background Intellectual Property

The Regents of the University of California

Software code titled, "Finite Element Simulation of Fluid Structure Interaction".

CRADA Intellectual Property

No inventions were created as part of this CRADA.

Licensing Status:

CRADA Article XIV Reporting Inventions

A. The Parties agree to disclose to each other each and every Subject Invention that may be patentable or otherwise protectable under the Patent Act. The Parties acknowledge that The Regents will disclose Subject Inventions to the DOE within two (2) months after the inventor first discloses the invention in writing to the person(s) responsible for patent matters of the disclosing Party.

B. These disclosures should be in such detail as to be capable of enabling one skilled in the art to make and use the invention under 35 USC 112. The disclosure shall also identify any known, actual, or potential statutory bars (i.e., printed publications describing the invention or a public use or on sale of the invention in this country). The Parties further agree to disclose to each other any subsequent known actual or potential statutory bar that occurs for an invention disclosed but for which a patent application has not been filed. All invention disclosures shall be marked as confidential under 35 USC 205.

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:
   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.

Donald P. Ziegler March 9 1999
Donald P. Ziegler Date
Aluminum Company of America

Richard Couch 4/20/99
Richard Couch Date
Lawrence Livermore National Laboratory

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

High Performance Parallel Processing (HPPP)
Finite Element Simulation Of Fluid Structure Interactions

Final Abstract
Attachment I
CRADA No. TC-0824-94-A

Date: August 21, 1998 Revision: 2

This project was a multi-partner CRADA with nine industrial partners. This was a partnership between Alcoa and LLNL. Alcoa provided data and expertise that assisted in the development of a system of numerical simulation modules that provided accurate and efficient three-dimensional modeling of combined fluid dynamics and structural response with a focus on ingot casting problems.

High Performance Parallel Processing (HPPP) Finite Element Simulation Of Fluid Structure Interactions

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

Date: September 10, 1998 Revision: 4

A. Parties

The project is a relationship between the Lawrence Livermore National Laboratory (LLNL) and Aluminum Company of America (ALCOA).

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

Aluminum Company of America (ALCOA)
100 Technical Drive
Alcoa Center, PA 15069-0001

B. Background

This project was a multi-partner CRADA with nine industrial partners. This was a partnership between Alcoa and LLNL. Alcoa provided data and expertise that assisted in the development of a system of numerical simulation modules that provided accurate and efficient three-dimensional modeling of combined fluid dynamics and structural response with a focus on ingot casting problems.

This project had two components. One involved the development of models and simulation software capable of modeling a broad range of phenomena related to aluminum casting technology. The other consisted of the implementation of the software system on the CRAY T3D platform.

C. Description

The objective of this project was to provide Alcoa with a tool that can be utilized for the design and understanding of casting processes. This software will be incorporated in the software system being developed under an existing CRADA with Alcoa.

Alcoa and LLNL worked together on all aspects of the problem, but each had primary responsibility for certain tasks. Alcoa provided input and data related to material models and aluminum forming processes. LLNL was responsible for developing the simulation software and porting it to the T3D platform. Alcoa was responsible for providing the benchmark forming data and validating code performance against these benchmarks.

D. Expected Economic Impact

This project assists the entire U.S. metals industry in developing improved forging, extrusion and casting processes.

E. Benefits to DOE

The product of this project was a numerical modeling tool, ALE3D, with enhanced capabilities in thermo-mechanically coupled dynamic systems. This project also produced a prototype parallel version of the code. This tool was capable of dynamic 3D simulations at timescales appropriate for both industrial processes and shock hydrodynamics. Such a coupled tool is now playing a significant role in the ASCI project as a code being developed for assessing response of systems to a variety of abnormal environments and understanding issues associated with manufacturing. This CRADA activity saved the DOE ASCI program approximately two years in development time. ALE3D, while still under development, is already being applied to weapons-related problems.

F. Industry Area

This work benefits a wide number of industries including: aircraft, automotive, medical, etc.

G. Project Status

Funding for the project was terminated after two years. Not all the tasks had been completed at that time.

H. LLNL Point of Contact for Project Information

Richard Couch
Lawrence Livermore National Laboratory
PO Box 808, L-170
Livermore, CA 94550
925/422-1655

Company Size and Point(s) of Contact

Alcoa has 81,600 employees.

Primary contact: Donald P. Ziegler
Aluminum Company of America
100 Technical Drive
Alcoa Center, PA 15069-0001
(724) 337-5466
(724) 337-2005 (fax)

J. Project Examples

None

K. 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 — Date 4/9/99
Industrial Partnerships and Commercialization

Release of Information

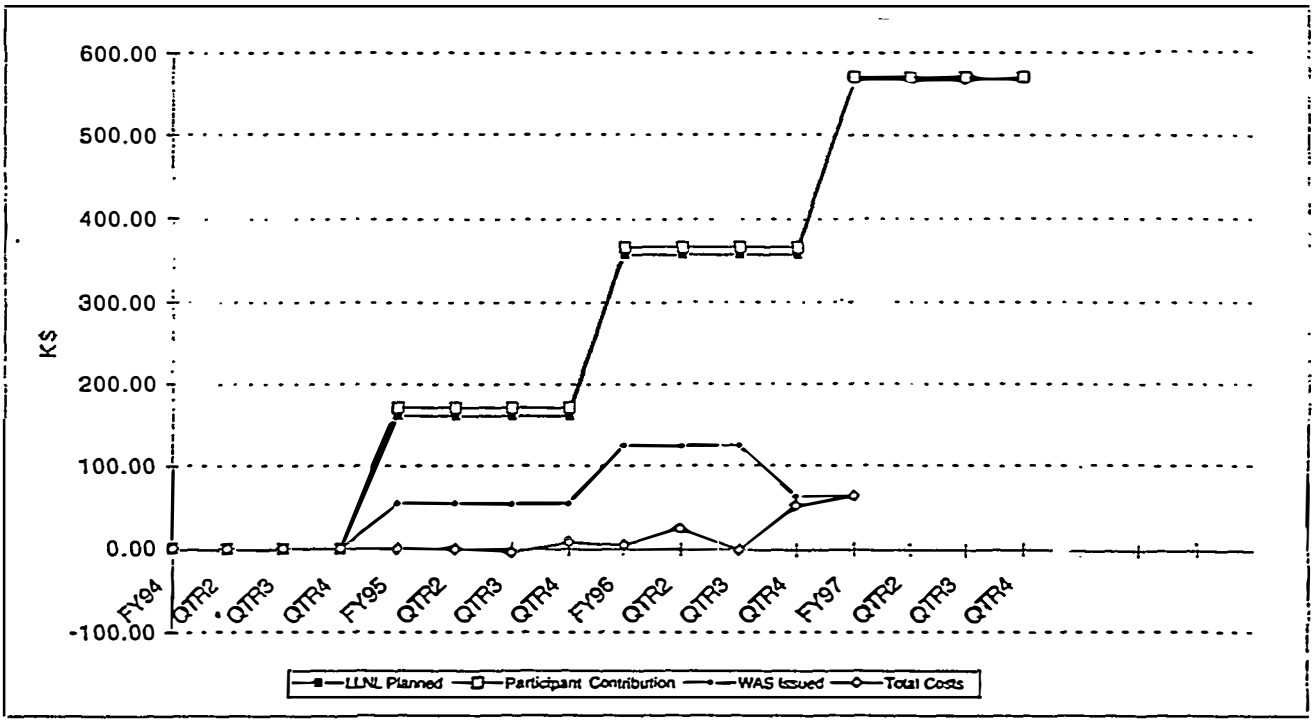
I have reviewed the attached Project Accomplishment Summary prepared by Lawrence Livermore National Laboratory and agree that the information about our CRADA may be released for external distribution.

Donald Ziegler, Program Manager — Date March 9, 1999
Aluminum Company of America

Title:	HPPP Finite Element Sim. of Fluid Structure Interactions	Reporting Period:	07/01/95 - 09/30/96
Participant:	Aluminum Company of America (ALCOA)	Date CRADA Executed:	1/30/95
DOE TTI No.:	94-MULT-003-XX-1	DOE Approval Date:	11/18/94
CRADA No.:	TC-0824-94 (A)	Scheduled Ending Date:	1/30/98
Account Numbers	4745-80	Project Completion Date:	10/31/96
Accounts Closed:	12/21/96	B & R Code (S):	DP0301, YN01000

Approved Funding Profile (SK)

	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	9	0	0	64
LDRD Funds	0	0	0	0	0	0
Total Costs	0	8	44	11	0	64



DP0301	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun	July	Aug	Sep	FYTD	64
FY94	0	0	0	0	0	0	0	0	0	0	0	0	0	
FY95	0	0	0	0	0	0	9	26	-40	27	-56	42	8	
FY96	-44	22	18	18	1	1	2	-30	2	2	18	34	44	
FY97	11	0	0	0	0	0	0	0	0	0	0	0	11	
FYOUT	0	0	0	0	0	0	0	0	0	0	0	0	0	

YN01000	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun	July	Aug	Sep	FYTD	0
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	

STAFF w/phone:

Lab PI: Richard Couch (510) 422-1655 Participant: Don Ziegler (412) 337-5466

Resource Manager: Steve Stinson (510) 423-2888

DOE OAK: Jerry Scheinberg (510) 637-1653 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.
Report any changes from the original CRADA or previous quarterly report on the CRADA Change Form.

Completion Date: Scheduled / Actual

See attached

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.

Verification that all equipment and proprietary information has been returned to the initial owner or permanently transferred.

Please initial: YES X NO

Accomplishments

Describe Technical/Non-Technical lessons learned and other observations.
Summarize causes/justification of deviations from original scope of work.
See Final Report.

Reviewed by CRADA project Program Manager: Date:

Reviewed by Karena McKinley, Director, LLNL/IP&C: Karena McKinley Date: 7/9/97

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