OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

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July 31, 2012

Dr. Karen Pao
U. S. Department of Energy
SC-21.1/Germantown Building
1000 Independence Avenue, SW
Washington, DC 20585-1290

Dear Dr. Pao:

DOE Program Announcement LAB 12-742: Resilient Extreme-Scale Solvers ("RX-Solvers"), Oak Ridge National Laboratory Field Work Proposal ERKJ247

Enclosed please find the proposal entitled, "MCREX: Using Monte Carlo algorithms to achieve resiliency and performance at scale for linear and non-linear solver applications," for your consideration.

This work addresses the investigation of stochastic, Monte Carlo-based solver algorithms that can be used to address resiliency and efficiency concerns that will arise on the next generation of high-performance computing platforms.

The total request is $1,574,943 with the Oak Ridge National Laboratory receiving $1,340,000 over a period of three years.

Questions regarding this proposal should be directed to the Principal Investigator, Thomas Evans, 865-576-3535 or email: evanstm@ornl.gov.

Sincerely,

J A Nichols

Jeffrey A. Nichols
Program Manager
ORNL ASCR Research

Enclosures

JAN:tme

cc: T. M. Evans, U. F. Henderson, M. W. Hulsey, D. Ingram, W. C. Lin, DOE-ORO, A. B. Maccabe, J. A. Nichols

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U.S. DEPARTMENT OF ENERGY
OAK RIDGE OPERATIONS

FIELD WORK PROPOSAL

PROGRAM: KJ ADVANCED SCIENTIFIC COMPUTING

1. WORK PROPOSAL NO. ERKJ247	2. REVISION NO. 000	3. DATE PREPARED 07/30/2012	94

4. WORK PROPOSAL TITLE: MCREX: Using Monte Carlo Algorithms to Achieve Resiliency and Performance at Scale for Linear and Non-linear Solver Applications	5. BUDGET AND REPORTING CODE KJ0402000

6. WORK PROPOSAL TERM BEGIN: 10/01/2012 END: 09/30/2015	PATENT STATUS This proposal is being transmitted in advance of patent review for evaluation purposes only. No further dissemination or publication shall be made without prior approval of the Assistant General Counsel for Patents, DOE.	7. Is This Work Proposal Included in the Institutional Plan? ☒Yes ☐No

NAME: (Last, First, MI) (Phone Number) 8. HEADQUARTERS/OPERATIONS OFFICE PROGRAM MANAGER: Pao, Karen (301) 903-5384	11. HEADQUARTERS ORGANIZATIONS: **Science**	14. DOE ORGANIZATION CODE: **SC**
9. OPERATIONS OFFICE WORK PROPOSAL REVIEWER: Lin, Wayne C. (865) 576-0639	12. FIELD OFFICE: **Oak Ridge Operations**	15. DOE ORGANIZATION CODE: **ON**
10. CONTRACTOR WORK PROPOSAL PRINCIPAL INVESTIGATOR(S)/MANAGER: Evans, Thomas M. (865) 576-3535	13. CONTRACTOR NAME: **Oak Ridge National Laboratory** **Managed by UT-Battelle, LLC** **For the U.S. Department of Energy** **Post Office Box 2008** **Oak Ridge, TN 37831**	16. DOE CONTRACTOR CODE: **41**

17. WORK PROPOSAL DESCRIPTION (Approach, anticipated benefits in 200 words or less)

The next generation of computational science applications will require numerical solvers that are capable of high performance on proposed HPC platforms. In order to meet this goal, solvers must be resilient to soft and hard system failures, provide high concurrency on heterogeneous hardware configurations, and retain numerical accuracy and efficiency. In light of these requirements, a natural avenue of inquiry would be to adapt the current stable of numerically efficient solvers to this new high-performance computing regime. However, an alternative approach would be to investigate different classes of algorithms that can address issues of resiliency, particularly fault tolerance and hard processor failures, naturally. In this proposal, the team will investigate new stochastic methods for solving linear systems, otherwise termed Monte Carlo Resilient, Exascale (MCREX) solvers. The family of methods that the team has proposed builds on the sequential Monte Carlo work of Halton, 1962. While showing significant promise, this class of solvers has not made inroads into the broader computational science community. The methods that the team has initially developed use Monte Carlo to accelerate a fixed-point iteration; therefore, the team has called them Monte Carlo Synthetic Acceleration (MCSA). Preliminary work using MCSA has demonstrated that they are at least as efficient as Jacobi-preconditioned Conjugate Gradient (PCG) on sparse, SPD systems. These initial results demonstrate that very good efficiency could be attained on non-symmetric systems; thus making MCSA an ideal solver in non-linear Newton schemes. Furthermore, Monte Carlo methods have the benefit of addressing resiliency in a natural way; soft errors can be treated as high variance samples and lost histories from processor failures can be easily discarded without affecting the quality of the solution.

18. CONTRACTOR WORK PROPOSAL MANAGER: (Name and Phone No.) J Nichols 8/6/12 (Signature) Nichols, Jeffrey A. (865)574-6224 (Date)	19. OPERATIONS OFFICE REVIEW OFFICIAL (Signature) (Date)

20. DETAIL ATTACHMENTS: (See instructions for page 3)

☐ a. Facility Requirements	☐ e. Approach	☐ i. NEPA Requirements	☐ m. ES&H Considerations
☐ b. Publications	☐ f. Technical Progress	☐ j. Milestones	☐ n. Human/Animal Subjects
☐ c. Purpose	☐ g. Future Accomplishments	☐ k. Deliverables	☐ o. Other (Specify)
☐ d. Background	☐ h. Relationships To Other Projects	☐ l. Perform Measures/Expectations	

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WORK PROPOSAL REQUIREMENTS FOR OPERATING/EQUIPMENT OBLIGATIONS AND COSTS

PROGRAM: KJ ADVANCED SCIENTIFIC COMPUTING

CONTRACTOR NAME:	WORK PROPOSAL TITLE:		
UT-BATTELLE, LLC	MCREX: Using Monte Carlo Algorithums to Achieve Resiliency and Performance		
	WORK PROPOSAL NO. ERKJ247	REVISION NO. 000	DATE PREPARED 07/30/2012

20. DETAIL ATTACHMENT CONTINUED:

21. STAFFING (in staff years)	FY 2012	FY 2013	FY 2014		FY 2015	FY 2016	TOTAL TO COMPLETE
			REQUEST	AUTHOR.			
a. SCIENTIFIC / OTHER DIRECT - ORNL		1.4	1.4		1.4		
b. OTHER DIRECT - OTHER SITES							
c. TOTAL DIRECT		1.4	1.4		1.4		
22. OPERATING EXPENSE (in Thousands)							
a. TOTAL OBLIGATIONS		433	445		462		
COSTS:							
1) WAGE POOL AND ORG. BURDEN	0	309	320		333		
2) MATERIALS AND SERVICES		13	10		10		
3) SUBCONTRACTS AND CONSULTANTS	0	0	0		0		
4) INDIRECT COSTS		111	115		119		
b. TOTAL COSTS		433	445		462		
23. EQUIPMENT (in Thousands)							
a. EQUIPMENT OBLIGATIONS							
b. EQUIPMENT COSTS							

24. MILESTONE SCHEDULE (TASKS:)	DOLLARS (in Thousands)		SCHEDULE (DATE)	
	PROPOSED	AUTHORIZED	PROPOSED	AUTHORIZED
Demonstrate convergence properties and performance of MCSA algorithm on sparse symmetric and non-symmetric systems			09/13	00/00
Show resiliency of MCSA algorithm for soft and hard errors while solving the linear advection- diffusion and non-linear Navier-Stokes equations			09/14	00/00
Show parallel performance of MCSA algorithm on existing HPC architectures and demonstrate scaling to exascale systems using the MCSA performance model			09/15	00/00

25. REPORTING REQUIREMENTS (DESCRIPTION:)

Results will be reported in periodic highlights to the U. S. Department of Energy and in journals and conference proceedings.

o. Other

(1) OBLIGATIONS FOR OPERATING EXPENSES-Budget Authority (B/A)

	Obligation Estimates FY 2012	FY 2013	FY 2014
Cost (B/O) Estimates	0	433	445
Less: Uncosted Balance (--) at 10/01	0	0	0
Plus: Commitments for Continued Operations	0	0	0
Outstanding Commitment Balance	0	0	0
TOTAL OBLIGATIONS--CHANGE	0	433	445

(2) CAPITAL EQUIPMENT OBLIGATIONS AND COSTS: None

Program Announcement: LAB 12-742
Resilient Extreme-Scale Solvers (“RX-Solvers”)

MCREX: Using Monte Carlo algorithms to achieve resiliency and performance at scale for linear and non-linear solver applications

Oak Ridge National Laboratory
Field Work Proposal # ERKJ247

Contact Information

Principal Investigator at ORNL

Thomas M. Evans
Distinguished R&D Staff
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, Tennessee 37831-6170
Phone: (865) 675-3535; Fax: (865) 576-3513
Email: evanstm@ornl.gov

Official Signing for ORNL

Jeffrey A. Nichols
ORNL ASCR Research Program Manager
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, Tennessee 37831-6163
Phone: (865) 574-6224; Fax: (865) 574-4839
Email: nicholsja@ornl.gov

Funding Requested ($):

	Year 1	Year 2	Year 3	Total
Thomas M. Evans (PI), ORNL	$433,000	$445,000	$462,000	$1,340,000
Michele Benzi (Co-PI), Emory	$76,011	$78,291	$80,640	$234,942
Total	$509,011	$523,291	$542,640	$1,574,942

Funding period: October 1, 2013 – September 30, 2015

Use of human subjects: No

Use of vertebrate animals: No

8/1/12

Principal Investigator Signature / Date

8/6/2012

Laboratory Official Signature / Date

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Budgets

ORNL Budget

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Statement on Reverse

ORGANIZATION OAK RIDGE NATIONAL LABORATORY				**Budget Page No:** YR 1	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Thomas Evans				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested by Applicant	Funds Granted by DOE
	CAL	ACAD	SUMR		
1. Thomas Evans	3.00			$32,832	
2. Steven Hamilton	6.00			$42,048	
3. Wayne Joubert	3.00			$27,072	
4. Christian Engelman	3.00			$21,312	
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (4) TOTAL SENIOR PERSONNEL (1-6)	15.00			$123,264	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER ORNL SERVICES					
TOTAL SALARIES AND WAGES (A+B)				$123,264	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$90,736	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$214,000	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$4,000	
2. FOREIGN					
TOTAL TRAVEL				$4,000	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$9,000	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER ORGANIZATION DIVISION ADMINISTRATION				$95,000	
TOTAL OTHER DIRECT COSTS				$104,000	
H. TOTAL DIRECT COSTS (A THROUGH G)				$322,000	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) PLEASE SEE BUDGET EXPLANATION PAGE FOR DETAILS					
TOTAL INDIRECT COSTS				$111,000	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$433,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$433,000	

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ORGANIZATION OAK RIDGE NATIONAL LABORATORY				Budget Page No: YR 2	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Thomas Evans				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested	Funds Granted by DOE
1. Thomas Evans	3.00			$33,984	
2. Steven Hamilton	6.00			$43,776	
3. Wayne Joubert	3.00			$28,224	
4. Christian Engelman	3.00			$21,888	
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (4) TOTAL SENIOR PERSONNEL (1-6)	15.00			$127,872	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER ORNL SERVICES					
TOTAL SALARIES AND WAGES (A+B)				$127,872	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$94,128	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$222,000	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$4,000	
2. FOREIGN					
TOTAL TRAVEL				$4,000	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$6,000	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER ORGANIZATION DIVISION ADMINISTRATION				$98,000	
TOTAL OTHER DIRECT COSTS				$104,000	
H. TOTAL DIRECT COSTS (A THROUGH G)				$330,000	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) PLEASE SEE BUDGET EXPLANATION PAGE FOR DETAILS					
TOTAL INDIRECT COSTS				$115,000	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$445,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$445,000	

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ORGANIZATION OAK RIDGE NATIONAL LABORATORY				Budget Page No:	YR 3
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Thomas Evans				Requested Duration:	12 (Months)
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested by Applicant	Funds Granted by DOE
	CAL	ACAD	SUMR		
1. Thomas Evans	3.00			$35,712	
2. Steven Hamilton	6.00			$45,504	
3. Wayne Joubert	3.00			$29,376	
4. Christian Engelman	3.00			$23,040	
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (4) TOTAL SENIOR PERSONNEL (1-6)	15.00			$133,632	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER ORNL SERVICES					
TOTAL SALARIES AND WAGES (A+B)				$133,632	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$98,368	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$232,000	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$4,000	
2. FOREIGN					
TOTAL TRAVEL				$4,000	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$6,000	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER ORGANIZATION DIVISION ADMINISTRATION				$101,000	
TOTAL OTHER DIRECT COSTS				$107,000	
H. TOTAL DIRECT COSTS (A THROUGH G)				$343,000	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) PLEASE SEE BUDGET EXPLANATION PAGE FOR DETAILS					
TOTAL INDIRECT COSTS				$119,000	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$462,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$462,000	

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ORGANIZATION OAK RIDGE NATIONAL LABORATORY				**Budget Page No:** YRS 1 - 3	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Thomas Evans				Requested Duration: 36 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applicant	Funds Granted by DOE
1. Thomas Evans	9.00			$102,528	
2. Steven Hamilton	18.00			$131,328	
3. Wayne Joubert	9.00			$84,672	
4. Christian Engelman	9.00			$66,240	
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (4) TOTAL SENIOR PERSONNEL (1-6)	45.00			$384,768	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER ORNL SERVICES					
TOTAL SALARIES AND WAGES (A+B)				$384,768	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$283,232	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$668,000	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$12,000	
2. FOREIGN					
TOTAL TRAVEL				$12,000	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$21,000	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER ORGANIZATION DIVISION ADMINISTRATION				$294,000	
TOTAL OTHER DIRECT COSTS				$315,000	
H. TOTAL DIRECT COSTS (A THROUGH G)				$995,000	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) PLEASE SEE BUDGET EXPLANATION PAGE FOR DETAILS					
TOTAL INDIRECT COSTS				$345,000	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$1,340,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$1,340,000	

ORNL Budget Explanation

Cost estimates presented in this proposal have been reclassified to be comparable with proposals from other research institutions. At the Oak Ridge National Laboratory (ORNL), actual costs will be collected and reported in accordance with the Department of Energy (DOE) approved cost accounting system. Total cost presented in this proposal and actual costs will be equivalent as will the subtotal of direct and indirect costs. Details of the budget breakdown of all budget categories, including salaries, benefits and fringe, and direct costs are described below. In consideration of cost estimates for ORNL staff support, it is important to understand that all ORNL costs are covered by proposals such as this one. There is no "base" funding for DOE Office of Science multiprogram national laboratories, including ORNL.

A. (1-6) Senior Personnel

The ORNL cost accounting system incorporates wage pools which are built around actual salaries for staff with similar salaries. The salary figure listed for Senior Personnel represents the average salary for a staff scientist within a specific wage pool. For budgeting purposes, one calendar month is assumed to be 150.0 hours.

Support is requested for Drs. Christian Engelmann, Thomas Evans, Steven Hamilton and Wayne Joubert as detailed in the budget spreadsheets. Dr. Thomas Evans will serve as Research Coordinator and Project PI.

B. (1-6) Other Personnel

No funds are allocated toward other staff for this proposal.

C. Fringe Benefits

Fringe benefits are included in the ORNL employees wage pool rate and are estimated at 59.0% for FY2012, decreasing to 48.0% for FY2013–2017.

D. Permanent Equipment

No funds for permanent equipment are allocated.

E. Travel

Travel in the amount of $4,000 per year is being included in the proposal in order to interact with M. Benzi and his students and present results at seminars. This sum also allows travel to 1 to 2 meetings per year in order to present results of the project.

G. (1-6) Other Direct Costs

1. Materials & Supplies

Materials and supplies include general and miscellaneous supplies directly related to the project. The additional budget for the first year is provided for software licenses for both toolkits needed to complete work for the proposal and collaboration software that will enable a virtual "one-roof" collaboration between ORNL and Emory.

6. Other — Organization Burden Administration

Organizational Burden Administration costs include utilities (purchased utilities as well as laboratory staff associated with maintaining the utility systems), space charges (building maintenance), division managerial oversight, technical and administrative support, and other support personnel such as plant and equipment, instrumentation and controls, environmental, safety, and health, finance and budget, quality, and health physics provided for the general benefit of all staff and R&D activities. Inclusion of these costs is necessary to provide a full accounting of estimated cost for the project period. All cost will be collected and reported in ORNL's cost accounting system, as approved by DOE.

Emory Budget

RESEARCH & RELATED BUDGET - SECTION A & B, BUDGET PERIOD 1

* ORGANIZATIONAL DUNS: 066469933
*** Budget Type:** ● Project ❍ Subaward/Consortium
Enter name of Organization: Emory University

*** Start Date:** 10-01-2012 *** End Date:** 09-30-2013 **Budget Period: 1**

A. Senior/Key Person

Prefix	* First Name	Middle Name	* Last Name	Suffix	* Project Role	Base Salary ($)	Cal. Months	Acad. Months	Sum. Months	* Requested Salary ($)	* Fringe Benefits ($)	* Funds Requested ($)
1.	Michele		Benzi		PD/PI	196,667.00		0	1	16,389.00	4,917.00	21,306.00
Total Funds Requested for all Senior Key Persons in the attached file												
Additional Senior Key Persons:			File Name:			Mime Type:				**Total Senior/Key Person**		**21,306.00**

B. Other Personnel

* Number of Personnel	* Project Role	Cal. Months	Acad. Months	Sum. Months	* Requested Salary ($)	* Fringe Benefits	* Funds Requested ($)
	Post Doctoral Associates						
1	Graduate Students	9			19,500.00	0.00	19,500.00
	Undergraduate Students						
	Secretarial/Clerical						
1	**Total Number Other Personnel**					**Total Other Personnel**	**19,500.00**
						Total Salary, Wages and Fringe Benefits (A+B)	**40,806.00**

RESEARCH & RELATED Budget {A-B} (Funds Requested)

Tracking Number: **OMB Number: 4040-0001**

RESEARCH & RELATED BUDGET - SECTION C, D, & E, BUDGET PERIOD 1

* ORGANIZATIONAL DUNS: 066469933

*** Budget Type:** ● Project ❍ Subaward/Consortium

Enter name of Organization: Emory University

*** Start Date:** 10-01-2012 *** End Date:** 09-30-2013 **Budget Period: 1**

C. Equipment Description		
List items and dollar amount for each item exceeding $5,000		
	Equipment Item	*** Funds Requested ($)**
Total funds requested for all equipment listed in the attached file		
	Total Equipment	
Additional Equipment:	File Name:	Mime Type:

D. Travel		**Funds Requested ($)**
1. Domestic Travel Costs (Incl. Canada, Mexico, and U.S. Possessions)		6,116.00
2. Foreign Travel Costs		
	Total Travel Cost	**6,116.00**

E. Participant/Trainee Support Costs		**Funds Requested ($)**
1. Tuition/Fees/Health Insurance		
2. Stipends		
3. Travel		
4. Subsistence		
5. Other:		
Number of Participants/Trainees	**Total Participant/Trainee Support Costs**	

RESEARCH & RELATED Budget {C-E} (Funds Requested)

RESEARCH & RELATED BUDGET - SECTIONS F-K, BUDGET PERIOD 1

* ORGANIZATIONAL DUNS: 066469933

*** Budget Type:** ● Project ❍ Subaward/Consortium

Enter name of Organization: Emory University

*** Start Date:** 10-01-2012 *** End Date:** 09-30-2013 **Budget Period: 1**

F. Other Direct Costs	**Funds Requested ($)**
1. Materials and Supplies	
2. Publication Costs	
3. Consultant Services	
4. ADP/Computer Services	
5. Subawards/Consortium/Contractual Costs	
6. Equipment or Facility Rental/User Fees	
7. Alterations and Renovations	
8. Graduate Student Enrollment Fee	2,813.00
Total Other Direct Costs	**2,813.00**

G. Direct Costs	**Funds Requested ($)**
Total Direct Costs (A thru F)	**49,735.00**

H. Indirect Costs

Indirect Cost Type	**Indirect Cost Rate (%)**	**Indirect Cost Base ($)**	*** Funds Requested ($)**
1. Research_On Campus	56	46,922.00	26,276.00
		Total Indirect Costs	**26,276.00**

Cognizant Federal Agency DHHS, Steven Zuraf, (301) 492-4855
(Agency Name, POC Name, and POC Phone Number)

I. Total Direct and Indirect Costs	**Funds Requested ($)**
Total Direct and Indirect Institutional Costs (G + H)	**76,011.00**

J. Fee	**Funds Requested ($)**

K. * Budget Justification File Name: Rev_Budget_Justification1011366606.pdf Mime Type: application/pdf
(Only attach one file.)

RESEARCH & RELATED Budget {F-K} (Funds Requested)

Tracking Number: OMB Number: 4040-0001

RESEARCH & RELATED BUDGET - SECTION A & B, BUDGET PERIOD 2

* ORGANIZATIONAL DUNS: 066469933
*** Budget Type:** ● Project ❍ Subaward/Consortium
Enter name of Organization: Emory University

*** Start Date:** 10-01-2013 *** End Date:** 09-30-2014 **Budget Period: 2**

A. Senior/Key Person

Prefix	* First Name	Middle Name	* Last Name	Suffix	* Project Role	Base Salary ($)	Cal. Months	Acad. Months	Sum. Months	* Requested Salary ($)	* Fringe Benefits ($)	* Funds Requested ($)
1.	Michele		Benzi		PD/PI	202,567.00		0	1	16,881.00	5,064.00	21,945.00
Total Funds Requested for all Senior Key Persons in the attached file												
Additional Senior Key Persons:			File Name:			Mime Type:				**Total Senior/Key Person**		**21,945.00**

B. Other Personnel

* Number of Personnel	* Project Role	Cal. Months	Acad. Months	Sum. Months	* Requested Salary ($)	* Fringe Benefits	* Funds Requested ($)
	Post Doctoral Associates						
1	Graduate Students	11			20,085.00	0.00	20,085.00
	Undergraduate Students						
	Secretarial/Clerical						
1	**Total Number Other Personnel**					**Total Other Personnel**	**20,085.00**
						Total Salary, Wages and Fringe Benefits (A+B)	**42,030.00**

RESEARCH & RELATED Budget {A-B} (Funds Requested)

Tracking Number: **OMB Number: 4040-0001**

RESEARCH & RELATED BUDGET - SECTION C, D, & E, BUDGET PERIOD 2

* ORGANIZATIONAL DUNS: 066469933

*** Budget Type:** ● Project ❍ Subaward/Consortium

Enter name of Organization: Emory University

*** Start Date:** 10-01-2013 *** End Date:** 09-30-2014 **Budget Period: 2**

C. Equipment Description

List items and dollar amount for each item exceeding $5,000

Equipment Item	*** Funds Requested ($)**
Total funds requested for all equipment listed in the attached file	
Total Equipment	

Additional Equipment: File Name: Mime Type:

D. Travel	**Funds Requested ($)**
1. Domestic Travel Costs (Incl. Canada, Mexico, and U.S. Possessions)	6,353.00
2. Foreign Travel Costs	
Total Travel Cost	**6,353.00**

E. Participant/Trainee Support Costs	**Funds Requested ($)**
1. Tuition/Fees/Health Insurance	
2. Stipends	
3. Travel	
4. Subsistence	
5. Other:	
Number of Participants/Trainees **Total Participant/Trainee Support Costs**	

RESEARCH & RELATED Budget {C-E} (Funds Requested)

Tracking Number: **OMB Number: 4040-0001**

RESEARCH & RELATED BUDGET - SECTIONS F-K, BUDGET PERIOD 2

* ORGANIZATIONAL DUNS: 066469933

*** Budget Type:** ● Project ❍ Subaward/Consortium

Enter name of Organization: Emory University

*** Start Date:** 10-01-2013 *** End Date:** 09-30-2014 **Budget Period: 2**

F. Other Direct Costs	**Funds Requested ($)**
1. Materials and Supplies	
2. Publication Costs	
3. Consultant Services	
4. ADP/Computer Services	
5. Subawards/Consortium/Contractual Costs	
6. Equipment or Facility Rental/User Fees	
7. Alterations and Renovations	
8. Graduate Student Enrollment Fee	2,814.00
Total Other Direct Costs	**2,814.00**

G. Direct Costs	**Funds Requested ($)**
Total Direct Costs (A thru F)	**51,197.00**

H. Indirect Costs

Indirect Cost Type	**Indirect Cost Rate (%)**	**Indirect Cost Base ($)**	*** Funds Requested ($)**
1. Research_On Campus	56	48,383.00	27,094.00
		Total Indirect Costs	**27,094.00**

Cognizant Federal Agency DHHS, Steven Zuraf, (301) 492-4855
(Agency Name, POC Name, and POC Phone Number)

I. Total Direct and Indirect Costs	**Funds Requested ($)**
Total Direct and Indirect Institutional Costs (G + H)	**78,291.00**

J. Fee	**Funds Requested ($)**

K. * Budget Justification	File Name: Rev_Budget_Justification1011366606.pdf (Only attach one file.)	Mime Type: application/pdf

RESEARCH & RELATED Budget {F-K} (Funds Requested)

Tracking Number: OMB Number: 4040-0001

RESEARCH & RELATED BUDGET - SECTION A & B, BUDGET PERIOD 3

* ORGANIZATIONAL DUNS: 066469933

*** Budget Type:** ● Project ❍ Subaward/Consortium

Enter name of Organization: Emory University

*** Start Date:** 10-01-2014 *** End Date:** 09-30-2015 **Budget Period: 3**

A. Senior/Key Person

Prefix	* First Name	Middle Name	* Last Name	Suffix	* Project Role	Base Salary ($)	Cal. Months	Acad. Months	Sum. Months	* Requested Salary ($)	* Fringe Benefits ($)	* Funds Requested ($)
1.	Michele		Benzi		PD/PI	208,644.00		0	1	17,387.00	5,216.00	22,603.00

Total Funds Requested for all Senior Key Persons in the attached file

Additional Senior Key Persons: File Name: Mime Type: **Total Senior/Key Person** **22,603.00**

B. Other Personnel

* Number of Personnel	* Project Role	Cal. Months	Acad. Months	Sum. Months	* Requested Salary ($)	* Fringe Benefits	* Funds Requested ($)
	Post Doctoral Associates						
1	Graduate Students	9			20,688.00	0.00	20,688.00
	Undergraduate Students						
	Secretarial/Clerical						
1	**Total Number Other Personnel**					**Total Other Personnel**	**20,688.00**
						Total Salary, Wages and Fringe Benefits (A+B)	**43,291.00**

RESEARCH & RELATED Budget {A-B} (Funds Requested)

Tracking Number: **OMB Number: 4040-0001**

RESEARCH & RELATED BUDGET - SECTION C, D, & E, BUDGET PERIOD 3

* ORGANIZATIONAL DUNS: 066469933

*** Budget Type:** ● Project ❍ Subaward/Consortium

Enter name of Organization: Emory University

*** Start Date:** 10-01-2014 *** End Date:** 09-30-2015 **Budget Period: 3**

C. Equipment Description

List items and dollar amount for each item exceeding $5,000

Equipment Item	*** Funds Requested ($)**
Total funds requested for all equipment listed in the attached file	
Total Equipment	

Additional Equipment: File Name: Mime Type:

D. Travel	**Funds Requested ($)**
1. Domestic Travel Costs (Incl. Canada, Mexico, and U.S. Possessions)	6,598.00
2. Foreign Travel Costs	
Total Travel Cost	**6,598.00**

E. Participant/Trainee Support Costs	**Funds Requested ($)**
1. Tuition/Fees/Health Insurance	
2. Stipends	
3. Travel	
4. Subsistence	
5. Other:	
Number of Participants/Trainees **Total Participant/Trainee Support Costs**	

RESEARCH & RELATED Budget {C-E} (Funds Requested)

RESEARCH & RELATED BUDGET - SECTIONS F-K, BUDGET PERIOD 3

* ORGANIZATIONAL DUNS: 066469933

*** Budget Type:** ● Project ❍ Subaward/Consortium

Enter name of Organization: Emory University

*** Start Date:** 10-01-2014 *** End Date:** 09-30-2015 **Budget Period: 3**

F. Other Direct Costs	**Funds Requested ($)**
1. Materials and Supplies	
2. Publication Costs	
3. Consultant Services	
4. ADP/Computer Services	
5. Subawards/Consortium/Contractual Costs	
6. Equipment or Facility Rental/User Fees	
7. Alterations and Renovations	
8. Graduate Student Enrollment Fee	2,813.00
Total Other Direct Costs	**2,813.00**

G. Direct Costs	**Funds Requested ($)**
Total Direct Costs (A thru F)	**52,702.00**

H. Indirect Costs

Indirect Cost Type	**Indirect Cost Rate (%)**	**Indirect Cost Base ($)**	*** Funds Requested ($)**
1. Research_On Campus	56	49,889.00	27,938.00
		Total Indirect Costs	**27,938.00**

Cognizant Federal Agency DHHS, Steven Zuraf, (301) 492-4855
(Agency Name, POC Name, and POC Phone Number)

I. Total Direct and Indirect Costs	**Funds Requested ($)**
Total Direct and Indirect Institutional Costs (G + H)	**80,640.00**

J. Fee	**Funds Requested ($)**

K. * Budget Justification	File Name: Rev_Budget_Justification1011366606.pdf (Only attach one file.)	Mime Type: application/pdf

RESEARCH & RELATED Budget {F-K} (Funds Requested)

Tracking Number: OMB Number: 4040-0001

RESEARCH & RELATED BUDGET - Cumulative Budget

		Totals ($)
Section A, Senior/Key Person		**65,854.00**
Section B, Other Personnel		**60,273.00**
Total Number Other Personnel	3	
Total Salary, Wages and Fringe Benefits (A+B)		**126,127.00**
Section C, Equipment		
Section D, Travel		**19,067.00**
1. Domestic	19,067.00	
2. Foreign		
Section E, Participant/Trainee Support Costs		
1. Tuition/Fees/Health Insurance		
2. Stipends		
3. Travel		
4. Subsistence		
5. Other		
6. Number of Participants/Trainees		
Section F, Other Direct Costs		**8,440.00**
1. Materials and Supplies		
2. Publication Costs		
3. Consultant Services		
4. ADP/Computer Services		
5. Subawards/Consortium/Contractual Costs		
6. Equipment or Facility Rental/User Fees		
7. Alterations and Renovations		
8. Other 1	8,440.00	
9. Other 2		
10. Other 3		
Section G, Direct Costs (A thru F)		**153,634.00**
Section H, Indirect Costs		**81,308.00**
Section I, Total Direct and Indirect Costs (G + H)		**234,942.00**
Section J, Fee		

Emory Budget Explanation

Salary

One month summer salary in each year of the project is requested to free the PI from teaching in order to conduct a significant portion of the proposed research. Fringe benefits for faculty members at Emory are currently 30% of salary. A 3% raise per year is projected.

The proposed research provides an excellent opportunity for a motivated Ph.D. student working on a dissertation in large-scale scientific computing on emerging architectures. The Ph.D. program in Computational Mathematics at Emory University has a strong history of attracting top graduate students, many of whom went on to successful careers in academia, government, and industry, including several females. Funds to support a full-time (academic year) Ph.D. student are requested for each of the three years of the project. Student salary is $19,500 for the first year, with a 3% raise per year. Additionally, funds to cover the student's enrollment fees totalling $2,813/year are being requested.

Travel

Travel support to attend meetings with the other project investigators plus one relevant conference per year, for a total of $6,116 in year one, $6,353 year two, and $6,598 in year three is requested.

MCREX: Using Monte Carlo algorithms to achieve resiliency and performance at scale for linear and non-linear solver applications

LAB 12-742 Resilient Extreme-Scale Solvers, **Field Work Proposal #: ERKJ247**

Principal investigator (PI): Dr. Thomas M. Evans
Reactor and Nuclear Systems Division
Oak Ridge National Laboratory
tel: (865) 576-3535, fax: (865) 576-3513
e-mail: evanstm@ornl.gov

Funding period: October 1, 2012 to September 30, 2015
Total budget request: ∼$1,575K over 3 years

Abstract.

The next generation of computational science applications will require numerical solvers that are capable of high performance on proposed exascale platforms. In order to meet this goal, solvers must be resilient to soft and hard system failures, provide high concurrency on heterogeneous hardware configurations, and retain numerical accuracy and efficiency. In light of these requirements, a natural avenue of inquiry would be to adapt the current stable of numerically efficient solvers to this new high-performance computing regime. However, an alternative approach would be to investigate different classes of algorithms that can address issues of resiliency, particularly fault tolerance and hard processor failures, naturally. In this proposal we will investigate new stochastic methods for solving linear systems, otherwise termed Monte Carlo Resilient, Exascale (MCREX) solvers. The family of methods that we have proposed builds on the sequential Monte Carlo work of Halton, 1962. While showing significant promise, this class of solvers has not made inroads into the broader computational science community. The methods that we have initially developed use Monte Carlo to accelerate a fixed-point iteration; therefore, we have called them Monte Carlo Synthetic Acceleration (MCSA). Preliminary work using MCSA has demonstrated that they are at least as efficient as Jacobi-preconditioned Conjugate Gradient (PCG) on sparse, SPD systems. These initial results demonstrate that, because MCSA does not require symmetry or positive definiteness, very good efficiency could be attained on non-symmetric systems, thus making MCSA an ideal solver in non-linear Newton schemes. Furthermore, Monte Carlo methods have the benefit of addressing resiliency in a natural way; soft errors can be treated as high variance samples and lost histories from processor failures can be easily discarded without affecting the quality of the solution.

This is a collaborative proposal among team members:

Drs. Christian Engelmann, Thomas Evans, Steven Hamilton, and Wayne Joubert, Oak Ridge National Laboratory, and Dr. Michele Benzi, Emory University

Each institution is independently submitting a proposal. However, each submission has identical technical content.

1 Introduction

In nearly all computational engineering and physics fields, linear and non-linear solvers form the core components of modeling and simulation applications. Recent focus on multiphysics coupling adds additional complexity to common linear and non-linear systems as solution strategies change when physical models are coupled. Furthermore, a desire for predictive simulations to enhance the safety and performance of engineered systems creates a need for extremely high fidelity computations to be performed for these coupled systems as a means to capture effects not modeled by coarser methods. In order to achieve this high fidelity, state-of-the-art computing facilities must be leveraged in a way that is both efficient and considerate of hardware-related issues. As scientific computing moves towards exascale facilities, with machines of $O(1,000,000)$ cores already coming online, new algorithms to solve these complex problems must be developed to leverage this new hardware. Issues such as resiliency to node failures and scaling to large numbers of heterogeneous computing elements (CPUs and GPUs) will be pertinent to robust algorithms aimed at this new hardware.

A natural path of investigation in addressing these issues would be to analyze and adapt the existing class of state-of-the-art solvers (Krylov, multigrid, etc.) in order to make them efficient and resilient on current and future hardware. Instead, we pose the question, "Do algorithms exist that naturally enable resiliency while preserving accuracy, convergence, and robustness?" Our objective is to answer this question by proposing a novel group of stochastic methods to advance solution techniques for linear and non-linear problems with a focus on resiliency against both hard and soft errors.

For many decades, the particle transport community has been utilizing Monte Carlo methods for the solution of transport problems. The partial differential equation (PDE) community has focused on various deterministic methods for solutions to linear problems. In between these two areas are a not widely known small group of stochastic methods for solving sparse linear systems [1–3]. In recent years, we have further developed these methods for transport problems in the form of Monte Carlo Synthetic-Acceleration (MCSA) that have yet to be applied to more general sparse linear systems. Compared to other methods in these regimes, MCSA offers three attractive qualities: (1) the linear operator need not be symmetric or positive-definite, thereby reducing preconditioning complexity, (2) parallelization using modern methods developed by the transport community [4] is possible, and (3) the stochastic nature of the solution method provides a natural solution to the issue of resiliency.

In addition to linear solver advancements, non-linear solvers may also benefit from a general and parallel MCSA scheme. In the engineering community, non-linear problems are often addressed by linearizing the problem and using traditional iterative or direct methods. In the mathematics community, various Newton methods have been popular [5]. Recently, Jacobian-Free Newton-Krylov (JFNK) schemes [6] have been utilized in multiphysics and advanced single physics codes. The benefits of JFNK schemes are that the Jacobian is never formed, simplifying the implementation, and a Krylov solver is leveraged (typically GMRES or Conjugate Gradient), providing excellent convergence properties for well-conditioned and well-scaled systems. However, there are two potential drawbacks to these methods for high fidelity predictive simulations: (1) the Jacobian is approximated by a first-order differencing method on the order of machine precision such that the error can grow beyond that of those in a fine-grained system and (2) for systems that are not symmetric positive-definite (which will be the case for most multiphysics systems and certainly for most preconditioned systems) the Krylov subspace generated by methods utilizing a long recurrence relation such as GMRES may become prohibitively large. To address these issues, this work proposes novel methods for non-linear systems based on the MCSA method. Although the Jacobian must be explicitly formed to use MCSA, for problems that take more than a few GMRES iterations to converge the storage required for the Krylov subspace will likely grow beyond that of the Jacobian. Finally, using MCSA for the linear solve provides its benefits for preconditioning, parallelism, and resiliency.

To present the key and novel components of this work, we first provide background on stochastic methods for solving linear problems and give results from our initial work in this area. We then provide a research plan that aims to drive the development of these methods with an emphasis on addressing the issue of resiliency and performance at the exascale.

2 Background

The idea of using Monte Carlo methods (random walks) to invert linear systems is not new. The earliest referenceable work dates to a 1950 paper by Forsythe and Leibler [7]. Their paper credits the idea to unpublished work by J.v. Neumann and S.M. Ulam dating back to the 1940's. The basic principles of Monte Carlo matrix inversion were further elucidated in Hammersley and Handscomb's 1964 text [1]. These early methods are distinguished by very slow, statistically noisy convergence properties; thus, they have not made any significant impact in the linear solver community.

In order to address the convergence issues plaguing Monte Carlo solvers, Halton [2, 3] proposed a Sequential Monte Carlo method. This algorithm demonstrated dramatically improved convergence over regular Monte Carlo. Nonetheless, this method has not gained widespread use as a production-quality linear solver. In the next sections, we will briefly describe the Monte Carlo methods that can be used to solve linear systems. Furthermore, we will show preliminary results from our extension of Halton's Sequential Monte Carlo method, the Monte Carlo Synthetic Acceleration Method (MCSA) [8].

2.1 Monte Carlo Solver Methods

To establish the mathematical framework for Monte Carlo linear solvers, we consider the following matrix equation:

$$\mathbf{A}\mathbf{x} = \mathbf{b}\,, \tag{2.1}$$

which can be written,

$$\begin{aligned} \mathbf{x} &= (\mathbf{I} - \mathbf{A})\mathbf{x} + \mathbf{b} \\ &= \mathbf{H}\mathbf{x} + \mathbf{b}\,. \end{aligned} \tag{2.2}$$

When the spectral radius of the iteration matrix ($\mathbf{H}$) is less than 1, we can expand $\mathbf{A}^{-1}$ using the *Neumann Series*,

$$\mathbf{A}^{-1} = (\mathbf{I} - \mathbf{H})^{-1} = \sum_{k=0}^{\infty} \mathbf{H}^k\,. \tag{2.3}$$

Thus, when $\rho(\mathbf{H}) < 1$ we can recast the solution vector $\mathbf{x}$ as a series,

$$\begin{aligned} \mathbf{x} &= (\mathbf{I} - \mathbf{H})^{-1}\mathbf{b} \\ &= \mathbf{b} + \mathbf{H}\mathbf{b} + \mathbf{H}^2\mathbf{b} + \mathbf{H}^3\mathbf{b} + \ldots\,. \end{aligned} \tag{2.4}$$

With this knowledge in hand, we can write an iterative method that solves Eq. (2.1) (Richardson's Iteration),

$$\mathbf{x}^{k+1} = \mathbf{H}\mathbf{x}^k + \mathbf{b}\,. \tag{2.5}$$

Equation (2.5) will converge for all $\mathbf{b} \in \mathcal{R}^N$ when $\rho(\mathbf{H}) < 1$ [5]. All of the Monte Carlo methods that are described in §§ 2.1.1 through 2.2 rely on estimating the terms in Eq. (2.4) through random walks.

2.1.1 Direct Method

Now we consider a Monte Carlo method that can be used to estimate the solution to Eq. (2.1) [1]. First, rewrite Eq. (2.4) in order to calculate a component of $\mathbf{x}$,

$$\begin{aligned} x_i &= (\mathbf{b})_i + (\mathbf{H}\mathbf{b})_i + (\mathbf{H}^2\mathbf{b})_i + (\mathbf{H}^3\mathbf{b})_i + \dots \\ &= \sum_{k=0}^{\infty} \sum_{i_1}^{N} \sum_{i_2}^{N} \dots \sum_{i_k}^{N} h_{i,i_1} h_{i_1,i_2} \dots h_{i_{k-1},i_k} b_{i_k} \,. \end{aligned} \tag{2.6}$$

The terms in the Neumann series can be interpreted as a series of transitions from $i_{m-1} \rightarrow i_m$ that can be simulated by a random walk. Let X be a random variable sampled from a random walk with k events that initiates in state i,

$$\begin{aligned} X(i_0 = i) &= \sum_{m=0}^{k} W_m b_{i_m} \\ &= \sum_{m=0}^{k} w_{i,i_1} w_{i_1,i_2} \dots w_{i_{m-1},i_m} b_{i_m} \,. \end{aligned} \tag{2.7}$$

Here, the weight on the m^{th} step is denoted W_m, and each random walk starts with unit weight. At every step, contributions to each component of X are generated only in the starting state of the history, i_0, by the source term in the current state, b_{i_m}. Therefore, for a given random walk permutation, each state must be used as a starting value in order to calculate its component of the expectation value (i.e. a state of size N will have N histories per random walk permutation). When there is a transition between states, for example $i \rightarrow j$, the weight is multiplied by the transition factor.

$$w_{ij} = \frac{h_{ij}}{p_{ij}} \,, \tag{2.8}$$

where p_{ij} denotes the probability of transitioning from state i to j. Then, the expected value of X is

$$\begin{aligned} E[X(i_0 = i)] &= \sum_{\nu} P_\nu X_\nu \\ &= \sum_{k=0}^{\infty} \sum_{i_1}^{N} \sum_{i_2}^{N} \dots \sum_{i_k}^{N} p_{i,i_1} p_{i_1,i_2} \dots p_{i_{k-1},i_k} w_{i,i_1} w_{i_1,i_2} \dots w_{i_{k-1},i_k} b_{i_k} \\ &= x_i \,, \end{aligned} \tag{2.9}$$

where ν denotes a particular random walk permutation. Therefore, the estimator in Eq. (2.7) is an unbiased estimator of the components of $\mathbf{x}$ provided $\rho(\mathbf{H}) < 1$.

We are left to define the transition probabilities. The most straightforward approach is to set

$$p_{ij} = \frac{|h_{ij}|}{\sum_j |h_{ij}|} \,. \tag{2.10}$$

Each row of the transition probability matrix, $\mathbf{P}$, represents a discrete probability density function that can be sampled to select a new state j, given that the current state is i. Random walks can be terminated in two ways: the matrix can be augmented with a terminating event equation that describes the probability that a history ends its walk, or the random walk can be terminated by weight cutoff, W_c. Generally, we choose to terminate random walks using a weight cutoff as opposed to augmenting the matrix such that the random walk terminates when $W_m < W_c$.

2.1.2 Adjoint Method

An alternative approach to the one just described is to calculate contributions to every component of $\mathbf{x}$ during the random walk. In this method, the weight change from state $i \to j$ is

$$w_{ij} = \frac{h_{ji}}{p_{ij}} . \tag{2.11}$$

The transition probabilities may be calculated as

$$p_{ij} = \frac{|h_{ji}|}{\sum_j |h_{ji}|} . \tag{2.12}$$

Note that the indices are reversed so that the probabilities are normalized over a column, as opposed to the forward method in which the probabilities are normalized over a row. This is equivalent to forming the Neumann series in reverse order. Correspondingly, the estimator for this method is

$$\begin{aligned} X &= \sum_{m=0}^{k} W_m \delta_{i_m,i} \\ &= \sum_{m=0}^{k} \hat{b}_{i_0} w_{i_0,i_1} w_{i_1,i_2} \dots w_{i_{m-1},i_m} \delta_{i_m,i} . \end{aligned} \tag{2.13}$$

Here, $\hat{b}_{i_0}$ is the sampled source and initial weight in state i_0. The Kronecker delta implies that tallies are only made in the state where the random walk currently resides. This is the common approach in standard Monte Carlo transport simulations. Unlike the direct method, because tallies are made in the state in which the random walk currently resides, we are no longer required to start a history in each state for each random walk permutation. Instead, sampling the source is sufficient and requires only one random walk per permutation.

Similar to the direct method, the adjoint method random walk process requires a terminating condition. In all of the work that follows we utilize a relative weight cutoff. The weight cutoff is defined as a fraction of the starting weight such that

$$W_f = W_c \hat{b}_{i_0} , \tag{2.14}$$

where W_f is the terminating weight of the random walk and W_c is the input relative weight cutoff. The random walk terminates on the m^{th} step if $W_m < W_f$.

2.2 Monte Carlo Synthetic-Acceleration

The methods presented in § 2 are characterized by slow convergence rates bound by the Central Limit Theorem. Halton [2, 3] proposed a staged residual scheme called Sequential Monte Carlo to speed up the convergence of these methods. A variant of this scheme has been successfully applied to the 1D non-linear thermal radiation diffusion equation in Ref. [9].

Concisely, the Sequential Monte Carlo method solves Eq. (2.1) using the adjoint solution technique described in § 2.1.2. The following iteration scheme is applied:

$$\mathbf{r}^l = \mathbf{b} - \mathbf{A}\mathbf{x}^l , \tag{2.15a}$$

$$\mathbf{A}\delta\mathbf{x}^{l+1} = \mathbf{r}^l , \tag{2.15b}$$

$$\mathbf{x}^{l+1} = \mathbf{x}^l + \delta\mathbf{x}^{l+1} . \tag{2.15c}$$

In this scheme, the Monte Carlo adjoint method is used to estimate the solution to Eq. (2.15b), and the residual is iterated to convergence. This iteration sequence is closely related to iterative refinement; the exception being that there is no update to x^{l+1} between residual iterations.

We propose a modification of this scheme that uses Monte Carlo as a synthetic-acceleration for the fixed-point iteration given by Eq. (2.5). We begin by subtracting Eq. (2.5) from Eq: (2.2):

$$\delta\mathbf{x}^{l+1} = (\mathbf{I} - \mathbf{A})\delta\mathbf{x}^{l} \, , \tag{2.16}$$

where

$$\delta\mathbf{x}^{l} = \mathbf{x} - \mathbf{x}^{l} \tag{2.17}$$

is defined as the error at iteration l. We then subtract $(\mathbf{I} - \mathbf{A})\delta\mathbf{x}^{l+1}$ from Eq. (2.16), giving a linear system to solve for the error:

$$\begin{aligned} \mathbf{A}\delta\mathbf{x}^{l+1} &= (\mathbf{I} - \mathbf{A})(\mathbf{x}^{l+1} - \mathbf{x}^{l}) \\ &= \mathbf{r}^{l+1} \, . \end{aligned} \tag{2.18}$$

The following scheme will then converge in one iteration:

$$\mathbf{x}^{l+1} = (\mathbf{I} - \mathbf{A})\mathbf{x}^{l} + \mathbf{b} \, , \tag{2.19a}$$

$$\mathbf{A}\delta\mathbf{x}^{l+1} = \mathbf{r}^{l+1} \, , \tag{2.19b}$$

$$\mathbf{x} = \mathbf{x}^{l+1} + \delta\mathbf{x}^{l+1} \, . \tag{2.19c}$$

To accelerate the fixed-point method and avoid inverting $\mathbf{A}$ directly in Eq. (2.19b), we can instead use the above ideas to create a new iterative scheme by using the Monte Carlo method to estimate the solution error. With this in hand, the Fixed-Point Monte Carlo Synthetic-Acceleration (MCSA) method can be defined as follows:

$$\mathbf{x}^{l+1/2} = (\mathbf{I} - \mathbf{A})\mathbf{x}^{l} + \mathbf{b} \, , \tag{2.20a}$$

$$\mathbf{r}^{l+1/2} = \mathbf{b} - \mathbf{A}\mathbf{x}^{l+1/2} \, , \tag{2.20b}$$

$$\hat{\mathbf{A}}\delta\mathbf{x}^{l+1/2} = \mathbf{r}^{l+1/2} \, , \tag{2.20c}$$

$$\mathbf{x}^{l+1} = \mathbf{x}^{l+1/2} + \delta\mathbf{x}^{l+1/2} \, . \tag{2.20d}$$

The hat on $\mathbf{A}$ in Eq. (2.20c) indicates that the Monte Carlo solution only approximately inverts this operator. Thus, we have defined a scheme in which the initial estimate of $\mathbf{x}$ in each iteration is updated using a single fixed-point iteration[1]. The residual is calculated and is used as a source to estimate the error, $\delta\mathbf{x}^{l+1/2}$, by solving Eq. (2.20c) via the Monte Carlo adjoint method. The error is then used to calculate an updated iterate of the solution vector, $\mathbf{x}^{l+1}$. The entire sequence is iterated to convergence based on the following stopping criterion [5],

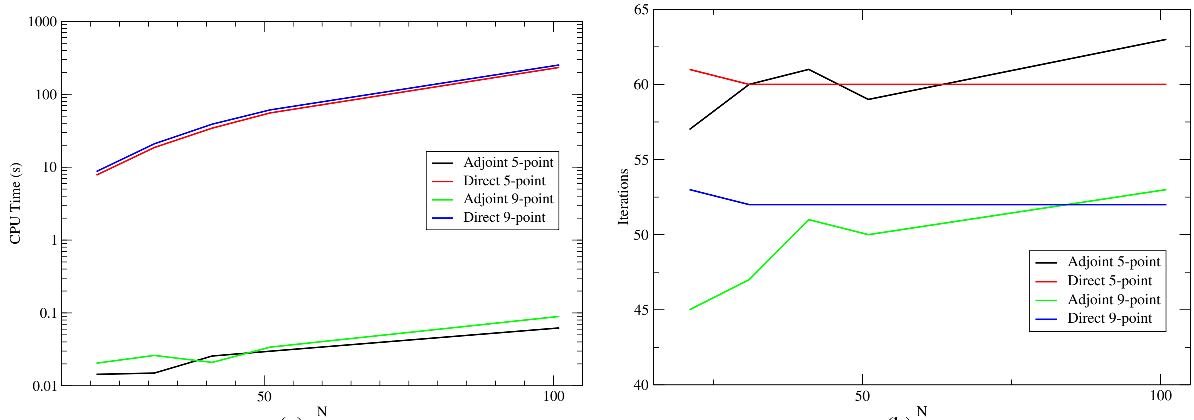
$$\|\mathbf{r}\|_{\infty} < \epsilon \cdot \|\mathbf{b}\|_{\infty} \, . \tag{2.21}$$

2.2.1 Preliminary Results

The MCSA method can use either the direct or adjoint method to solve Eq. (2.20c). We have performed a preliminary study that demonstrates the superiority of the adjoint method within the context of MCSA using the two-dimensional time-dependent Poisson equation as a simple model problem with second and fourth-order finite-difference stencils. A timing and convergence study is used to demonstrate the effectiveness of the adjoint method as compared to the direct method.

We see clearly in Fig. 1a that using the adjoint solver with MCSA results in several orders of magnitude speedup over the direct solver while the number of iterations required to converge is of a similar scale. We expect this for several reasons. First, with an equivalent number of histories specified for both solvers and

[1] Although, a Krylov method could be used instead of a stationary method here.



(a) (b)

Figure 1: Comparison of Direct and Adjoint MCSA methods for varying problem size specified by an $N \times N$ grid, (a) time to solution, (b) iterations required for solution.

a system of size $N \times N$, the direct solver will compute $N \times N$ random walks per permutation while the adjoint solver will only compute one. Initially, this may not seem like a fair comparison, however, we see from Fig. 1b that the number of iterations required to converge is approximately the same and therefore the extra computations performed by the direct method do not improve the error estimation.

In order to gauge the performance of MCSA we have used it to solve the thermal-equilibrium radiation diffusion equation,

$$-\nabla \cdot D^n \nabla \phi^{n+1} + \tilde{\sigma}^n \phi^n = q^n \, , \tag{2.22}$$

where ϕ is the energy-integrated radiation intensity, $\tilde{\sigma}^n$ is the effective absorption plus reemission, D^n is the diffusion coefficient, and q^n is the source at t^n. In operator form, Eq. (2.22) is $\mathbf{D}\boldsymbol{\phi} = \mathbf{q}$ where $\mathbf{D}$ is an SPD operator. Using left-preconditioning, the MCSA algorithm that is applied at each timestep is

$$\begin{aligned}
\boldsymbol{\phi}^{l+1/2} &= (\mathbf{I} - \mathbf{M}^{-1}\mathbf{D})\boldsymbol{\phi}^l + \mathbf{M}^{-1}\mathbf{q} \, , && \text{(fixed-point iteration)} \\
\mathbf{r}^{l+1/2} &= \mathbf{M}^{-1}\mathbf{q} - \mathbf{M}^{-1}\mathbf{D}\boldsymbol{\phi}^{l+1/2} \, , && \text{(compute residual)} \\
\mathbf{M}^{-1}\mathbf{D}\delta\boldsymbol{\phi}^{l+1/2} &= \mathbf{r}^{l+1/2} \, , && \text{(estimate } \delta\phi \text{ using adjoint Monte Carlo method)} \\
\boldsymbol{\phi}^{l+1} &= \boldsymbol{\phi}^{l+1/2} + \delta\boldsymbol{\phi}^{l+1/2} \, . && \text{(update } \boldsymbol{\phi}\text{)}
\end{aligned}$$

As noted above, the residual acts as the source for this simulation. There are two Monte Carlo interpretations that can be applied to this system. The first follows the mathematical presentation given in § 2. Namely, we form probabilities from the iteration matrix and perform random walks to generate unbiased estimates of the solution vector, $\delta\boldsymbol{\phi}^{l+1/2}$, using the estimator in Eq. (2.13).

However, a more natural interpretation is to consider the random walk as a transport process; in the problem above this is equivalent to a particle transport process. In this connotation, the machinery described in § 2.1.2 is used to define Probability Distribution Functions (PDFs) that determine the transport of state transitions through the linear system (matrix). The random walk is a Monte Carlo transport calculation that uses Eq. (2.11) to calculate the weight change at each transition. Equation (2.12) gives the probability of transmission to an adjacent state in the system. We tally the contribution to the solution (ϕ in the above example) in each state using Eq. (2.13). The transport process is terminated using a relative weight cutoff that is defined in Eq. (2.14).

There are two principal degrees of freedom when utilizing the MCSA method: (1) the number of histories per iteration (N_p), and (2) the weight cutoff (W_c). Figure 2a shows the CPU time as a function of the requested number of histories per iteration for a relative weight cutoff of 1×10^{-4} for a Marshak wave problem [10]. For less than 5 histories per iteration the method does not converge. Figure 2b shows the variation in the maximum number of iterations per cycle with number of histories. Analysis of these two figures shows that increasing the number of histories reduces the total number of iterations required to converge the solution. However, the cost of the Monte Carlo transport is high; thus, better performance is attained by running more iterations with fewer histories per iteration [9].

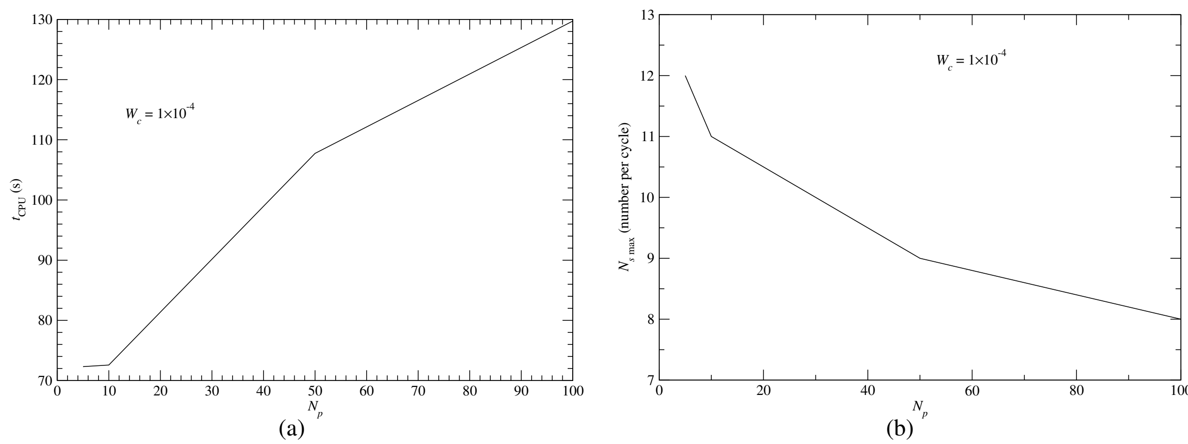


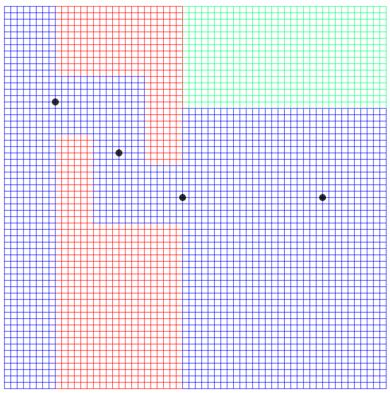
Figure 2: (a) CPU time versus number of histories per iteration, and (b) maximum number of iterations per cycle versus number of histories per iteration for the Marshak problem. The number of histories is the requested number. In each iteration the exact number can vary depending upon the number of cells and source strength per cell.

A similar analysis was done comparing different weight cutoffs. These results indicate that the performance of the MCSA method is relatively insensitive to the weight cutoff. This is especially true when running small numbers of histories per iteration. When larger numbers of histories are used the weight cutoff has a more pronounced effect on the efficiency of the method.

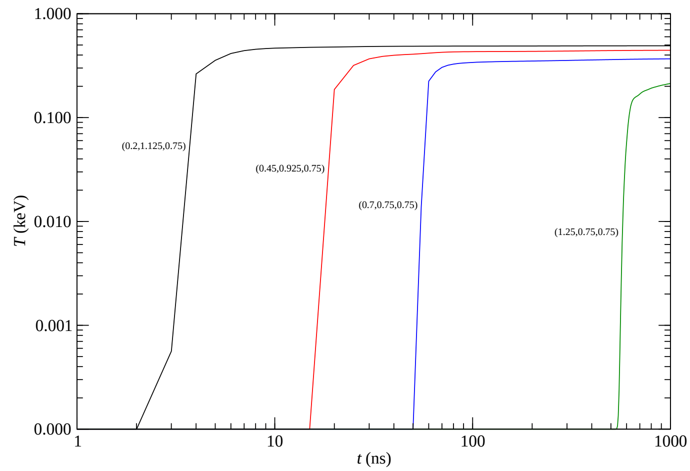
We have compared the MCSA solution algorithm with both Jacobi-preconditioned Conjugate Gradient (PCG) and Jacobi iteration (JACOBI). The model problem is a dog-legged duct through a thick wall where the radiation flows into a thin region bound by a foil on one side. The size of the spatial grid was 60^3 (216,000 spatial cells). All three methods, give numerically identical answers when using a stopping criterion of 1×10^{-8}. The geometry and time-evolution of the temperature is shown at 4 edit points in Fig. 3. Table 1 shows the timing results for the multi-material problem using PCG, PFIX, and MCSA. The results correspond roughly with the results from the Marshak problem. The MCSA is marginally faster than PCG and 43% faster than PFIX.

Table 1: Comparison of solution methods for the multi-material problem. All methods were run with a stopping criterion of 1×10^{-8}. The MCSA method used $N_p = 1000$ and $W_c = 1 \times 10^{-3}$. The problem was run to an elapsed time of 1000 ns.

Method	Max Iterations	Relative CPU Time
PCG	18	1.03
PFIX	38	1.43
MCSA	20	1.00



(a) Edit points



(b) Temperature

Figure 3: (a) Edit points and (b) time-evolution of the temperature at each point. All points are centered in the z-axis.

3 Research Plan

As stated in § 1, we plan to analyze and extend MCSA in order to achieve numerical efficiency, robustness, and accuracy combined with resiliency and performance on current and future HPC architectures. The objective is to obtain resiliency in a manner that naturally fits into the complete MCSA algorithm. Numerical characterization and improvements to MCSA will be performed using the tools of standard numerical analysis. We intend to verify solver resiliency through *fault injection*, described in the following sections. Likewise, we will extrapolate performance estimates to proposed future HPC architectures by developing a *performance model*.

3.1 Numerical and Algorithmic Investigations

Numerical investigations of MCSA will be performed in two phases (a) demonstrating convergence, accuracy, efficiency, and robustness, and (b) determining the applicability of subspace iteration schemes. Algorithmic investigations will be focused on improving parallel performance. Both numerical and algorithmic research will investigate resiliency aspects of the solution process. We define resiliency as the ability to recover from both hard and soft errors. Soft errors consist of logical, floating-point, and other processor evaluation faults short of process failure. Hard errors are full process failures. We will show how we can address each failure type algorithmically through numerical analysis and parallel redundancy.

All numerical and algorithmic investigations will be demonstrated using linear and non-linear forms of the Advection-Diffusion-Reaction (ADR) equations,

$$\partial_t u + \nabla \cdot \mathbf{f}(\mathbf{x}, u - \nabla \cdot \big[d(\mathbf{x}, u)\nabla u\big] + r(\mathbf{x}, u)u = q(\mathbf{x}, t)\,. \tag{3.1}$$

This system is representative of the wide class of problems that the algorithms and methods proposed in this study should solve efficiently. In order to verify the methods on real models, we will also consider the non-linear consistent, incompressible Navier-Stokes equations [11–13]. All investigations will consider two and three-dimensional forms of the models in order to demonstrate broad applicability to relevant science and engineering problems.

3.1.1 Numerical Investigations

The first stage of our numerics research will be demonstrating convergence, accuracy, efficiency, and robustness of the MCSA algorithm. The preliminary results described in § 2.2.1 indicate that the fundamental solver converges and is efficient for sparse SPD systems. However, significant analysis remains to determine

- its convergence properties on non-symmetric systems;
- its effectiveness as the linear solver in non-linear Newton methods;
- an analytical framework that relates weight cutoff and number of histories to problem parameters;
- the effect of high variance events on convergence and robustness.

All of our preliminary studies have focused on sparse SPD systems, in which we have shown MCSA to be competitive with PCG. Because MCSA has no requirements on symmetry or positive-definiteness, it is anticipated that the method will compare favorably to GMRES, BICGSTAB, or TFQMR.

Once the properties of MCSA have been scoped, we can begin investigations using MCSA as the inner solver in non-linear Newton methods. The inner part of each Newton iteration requires the solution to the following linear system,

$$\mathbf{J}(\mathbf{u}^k)\delta\mathbf{u}^{k+1} = -\mathbf{f}(\mathbf{u}^k)\ . \tag{3.2}$$

As opposed to Krylov methods, MCSA requires the formation of the matrix elements to build the probabilities that are used to execute random walks. Thus, the standard inexact Jacobian-Free Newton-Krylov (JFNK) [6] methods that rely on numerical approximations of the matrix-vector product,

$$\mathbf{J}\mathbf{v} \approx \frac{\mathbf{f}(\mathbf{u}+\epsilon\mathbf{v}) - \mathbf{f}(\mathbf{u})}{\epsilon}\ , \tag{3.3}$$

are not feasible with Newton-MCSA. Instead, we can numerically approximate the matrix elements of the Jacobian, $J_{ij} = \partial \mathrm{f}_i(\mathbf{u})/\partial u_j$ directly using automatic differentiation [14, 15]. This technology is available in Trilinos' Phalanx package [16].

For both direct application in linear systems and as an inner solver for non-linear systems, a mathematical framework must be established that can be used to analytically determine the runtime parameters of the solver for a given problem. The problem-dependent runtime parameters for the MCSA solver are number of histories per iteration and weight cutoff. Because the cost of the Monte Carlo is proportional to the total number of random walks, the goal is to minimize the total number of histories. As indicated in Fig. 2 this involves a balance between number of iterations and number of histories per iteration.

The effect of high variance events has significant implications for both robustness and resiliency to soft errors. All of the Monte Carlo methods we are investigating rely on the assumption that

$$E[X] = \sum_{\nu} P_\nu X_\nu\ , \tag{3.4}$$

is an unbiased estimator of X. Soft errors will result in random walk events that appear as high-variance histories. In order to determine algorithmic resiliency we must determine the scale at which high-variance events invalidate Eq. (3.4). We expect that most soft errors will manifest as high-variance events that will be ameliorated during successive random walks. Thus, the MCSA algorithm provides a natural means of dealing with the majority of soft errors. Research must be performed to determine the robustness of the method to high-variance events that result from the numerics of the linear system or from soft errors. We will use the simulator described in § 3.2 to validate solver robustness to these events.

In addition to investigating the numerical features of the proposed MCSA algorithm, we also intend to investigate new iteration sequences that may prove more efficient. In the current MCSA method, Monte Carlo is used to accelerate a stationary fixed-point iteration. Instead, significant performance gains could possibly be achieved by casting MCSA as a preconditioner to a Krylov subspace method. Because the statistical convergence of Monte Carlo methods will inherently lead to variations in the preconditioning operator from one iteration to the next, it will likely be necessary to appeal to flexible Krylov methods [17]. Although the idea of using Krylov subspace methods to accelerate Monte Carlo calculations is not new (see Ref. [18] for an example applied to eigenvalue calculations in neutron transport), significant effort will be necessary to quantify convergence properties of such an approach.

3.1.2 Algorithmic Investigations

In general, deterministic and Monte Carlo solution methods have competing requirements with regard to achieving concurrency; efficient parallelism in deterministic methods is often achieved by decomposing the global phase space as much as possible, whereas in Monte Carlo efficiency is often the result of replicating as much of the phase space as possible. An additional constraint beyond pure performance considerations is the best decomposition strategy that can aid resiliency, particularly to hard system errors. Balancing these requirements, we propose to use a recently developed algorithm for Monte Carlo called Multi-Set, Overlapping Domain (MSOD) [4] (originally named multi-level, overlapping region in Ref. [4]). An illustration of the MSOD algorithm is displayed in Fig. 4 for the ADR equations. The spatial domain (matrix) is decom-

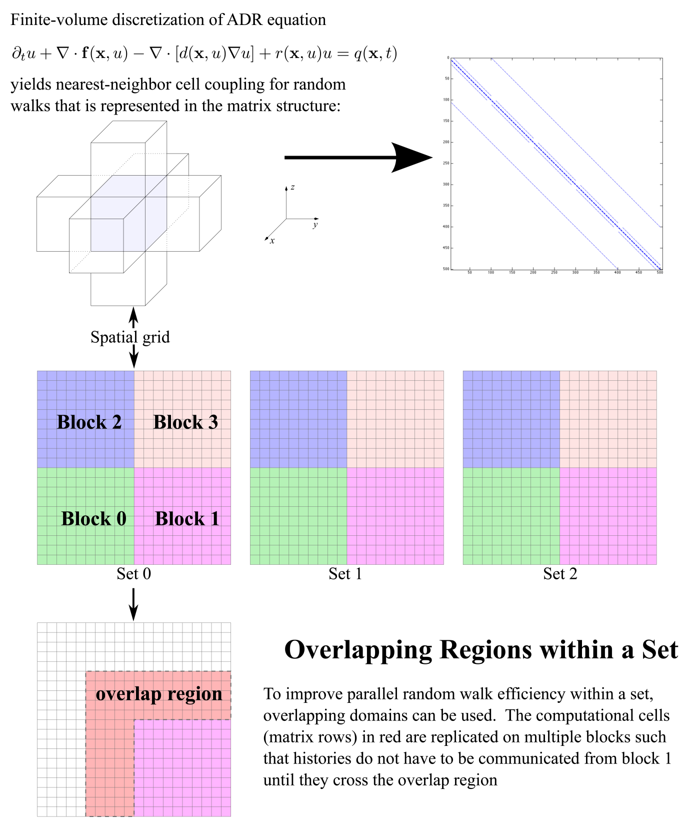


Figure 4: Schematic of the MSOD decomposition algorithm. The spatial grid (matrix) is decomposed into 4 blocks (blue, green, pink, violet); the spatial decomposition is replicated in 3 sets yielding 12 total domains, $N_{\text{domains}} = N_{\text{blocks}} \times N_{\text{sets}}$. The entire matrix/spatial grid is contained in each set. Random walks through the matrix do not cross set boundaries, only block boundaries.

posed into blocks such that the set $\{b_0, b_1, \ldots, b_{N_{\text{blocks}}}\}$ constitutes the complete grid. Each set of N_{blocks} is replicated in N_{sets}. Thus, the total number of domains for any given problem is $N_{\text{blocks}} \times N_{\text{sets}}$.

The potential advantages of this parallel algorithm are

- the intrinsic concurrency patterns of both Monte Carlo and deterministic algorithms are, in part, preserved;
- the algorithm limits to both full *domain decomposition* (single set—multiple blocks) and full *domain replication* (multiple sets—single block);
- problems can be scaled to arbitrarily large size by increasing multiple sets;
- a natural partitioning of work to heterogeneous hardware components is provided, e.g. blocks on GPUs, sets on cores;
- the algorithm enables *redundancy* by replicating the solution domain.

The MSOD algorithm should provide natural resiliency to hard errors through redundancy. In any given MCSA iteration, histories can be rejected as long as this is done in an unbiased manner. Hard errors result in part of the problem domain being unsampled. The MSOD algorithm provides a mechanism for rejecting a complete set in these cases, thus preserving an unbiased random walk. Additionally, a small bias may be tolerable by only rejecting the blocks that encounter hard errors. The amount of bias that negligibly affects the solution will need to be determined.

3.2 Resiliency Modeling

The resilience of the proposed algorithm will be modeled though a series of fault injection campaigns. The impact of a hard or soft error on the algorithm will be investigated by artificially creating such errors during algorithm execution and by observing the resulting runtime behavior, execution time, and output. The two most likely errors in an extreme-scale system are a process failure, e.g., a detected but unrecoverable error leading to process termination, and silent data corruption (SDC), e.g., an undetected bit flip in a memory latch [19–26]. Both error types will be injected based on their probability, i.e., with a certain frequency and probability distribution, targeting specific algorithm vulnerabilities.

The error probability will be modeled using historical log data from ORNL systems and assumptions communicated by HPC vendors, such as Cray and Intel, regarding the reliability of future-generation systems. The algorithm vulnerabilities will be modeled using a whitebox analysis for identifying the most vulnerable execution paths and data structures in combination with runtime profiling for identifying system component (processor, memory, and network) usage. Correlating algorithm vulnerabilities with system component usage provides a number of injection points at which a specific error class is most likely and is expected to result in a significant impact, such as a process fault during a critical collective operation or SDC in the most significant bits of an important value. The fault injection campaigns will utilize different existing technologies to model the resilience of the algorithm on today's and on future-generation HPC systems.

The fault injection campaigns will provide the data points needed to model the resilience of the proposed algorithm, such that the probability of computing a correct result within a certain time to solution can be estimated for both error classes depending on the reliability properties of the HPC system, the scale of the application run, and the problem size.

3.2.1 Hard Errors on Today's HPC Systems

For investigation of hard errors on today's HPC systems, a fault-tolerant MPI solution will be used to implement a fully functional resilient algorithm atop a message passing runtime environment that is capable of detecting and surviving process failures and notifying an application about each failure. Injecting a hard error is as simple as manually killing a process. The fault-tolerant MPI automatically reconfigures to survive the process failure and notifies the application about the failure. The notification can be used to trigger any reconfiguration of the application, including algorithm-level recovery. The PIs have access to two different fault-tolerant MPI solutions, FT-MPI developed by the University of Tennessee in 2001 [27, 28] and the prototype for the MPI 3.x standard with fault tolerance support developed by ORNL in 2011 [29–31]. This fault injection campaign will observe the impact of hard errors on the algorithm's execution time and result.

3.2.2 Soft Errors on Today's HPC Systems

For investigation of soft errors on today's HPC systems, the redundant MPI implementation, redMPI [32–36], will be used to perform comparative studies at runtime. redMPI transparently executes an application in a redundant fashion by utilizing the MPI performance tool interface, PMPI, to transparently intercept MPI calls from an application and to hide all redundancy-related mechanisms. A redundantly executed application runs with $r * m$ native MPI processes, where r is the number of MPI ranks visible to the application and m is the replication degree.

Under normal operation, messages between redundant nodes are replicated and compared for hard and soft error detection and correction. For fault injection campaigns [32], the message replication and comparison protocol performs detection only. This permits the original parallel application to be tainted with data corruption, while the fully redundant parallel application serves as a correct live control for close observation of the error impact, including its propagation, detection, and masking. Differences between the tainted execution and the control are detected and recorded at runtime by the message replication and comparison protocol, providing detailed information about error sensitivity and propagation.

3.2.3 Hard and Soft Errors on Future HPC Systems

For investigation of hard and soft errors on future-generation HPC systems, the Extreme-scale Simulator (xSim) performance investigation toolkit will be utilized. xSim [37–39] is a recently developed performance investigation toolkit that permits running HPC applications in a controlled environment with millions of concurrent execution threads. It allows observing application performance in a simulated extreme-scale system for hardware/software co-design. Using a lightweight parallel discrete event simulation, xSim executes an application on a much smaller HPC system in an oversubscribed fashion with a virtual wall clock time, such that performance data can be extracted based on a processor and a network model with the appropriate simulation scalability/accuracy trade-off. xSim is designed like a traditional performance tool, as an interposition library that sits between the MPI application and the MPI layer, using the MPI performance tool interface. It currently holds the world record in extreme-scale simulation, running up to 134,217,728 (2^{27}) communicating MPI tasks, each with its own process context, using just a 960-core Linux-based cluster.

As part of an LDRD project at ORNL (see Current and Pending Support for Christian Engelmann in § B), xSim is being extended with advanced features to (1) permit the injection of different faults, errors, and failures into the simulation, (2) model various propagation, isolation, and detection properties of the simulated system, (3) support a variety of avoidance, masking, and recovery strategies, (4) model the power consumption of the entire simulated system, and (5) study the performance, resilience, and power consumption impact with different parameter sets for (1), (2), (3), and (4) using standardized methods and metrics. Within this proposal, we will leverage the new xSim capabilities developed under the LDRD project, such as the support for a simulated fault-tolerant MPI, algorithm-based fault tolerance, and SDC injection, for investigating the impact of hard and soft errors on the proposed algorithm in simulated future-generation HPC systems. Both hard and soft errors will be injected into the algorithm execution atop a simulated HPC system, while the simulator allows close observation of the error impact, including its propagation, detection, and masking as well as the algorithm's execution time and result.

3.3 Performance Modeling

The DARPA Exascale Report [40] made clear the multiple challenges facing software and algorithm developers on the path to exascale, including the memory wall, the power wall, resiliency issues and the need for unprecedented levels of parallelism. Exascale application development is made particularly challenging by the uncertainty regarding the final hardware characteristics of these systems due to the multiple innovations that will be required in the coming years.

The Oak Ridge Leadership Computing Facility (OLCF) has successfully navigated application and algorithm migration across multiple generations of new HPC system installations and upgrades, most recently with the Jaguar Istanbul processor upgrade in 2009 and the OLCF-3 Titan installation which is currently underway. Central to this effort has been the performance modeling and analysis of key science applications and their algorithms as input to the system design and procurement process. This effort has required the OLCF to develop and validate predictive models for many of its heavily-used application codes to understand their anticipated performance characteristics on future hardware. The performance models have successfully guided the development teams' code and algorithm changes both for incremental hardware upgrades as well as disruptive hardware changes such as the advent of heterogeneous GPU-based systems.

To insure the success of the MCREX solvers on exascale hardware, a vigorous effort will be undertaken to model the algorithm and code performance characteristics as part of the algorithm design process. This work will take place in the setting of the following interrelated steps.

- **Algorithm Development.** The MCREX solver algorithms will be designed with concern not only for the algorithm numerics and convergence properties but also with anticipated future hardware characteristics in mind, such as the presence of hard and soft errors, increasing time and power costs of communicating off-die and off-node, decreasing relative sizes of high-speed cache memories and register files, and the need to expose increasing amounts of thread-level parallelism.
- **Code Implementation.** The algorithms will be implemented in software, initially as prototypes and then as more full-fledged versions, to be evaluated and tested on current state-of-the-art HPC hardware such as the ORNL Titan system and follow-on hardware.
- **Performance Analysis.** The performance characteristics of these codes will be determined, using tools such as VAMPIR, CrayPat and other profiling tools to understand the performance hot spots of the algorithms and understand how the performance depends on characteristics of the different system hardware components.
- **Performance Modeling.** Quantitative models will be developed to predict the performance of the algorithms for different problem types of interest under the assumption of multiple potential future architecture scenarios, based on possible futures for exascale hardware. These findings will not only provide a feedback loop for further algorithm design but also provide an assessment of the relative effectiveness of alternative system hardware designs for algorithms of this type. The fully developed performance model will be simulated using the performance investigation features of the xSim toolkit, described in § 3.2.3.

4 Research Timetable and Tasks

The research tasks described in § 3 are organized into yearly milestones with concurrent tasks. The yearly milestones for the project are:

Year 1 Demonstrate convergence properties and performance of MCSA algorithm on sparse symmetric and non-symmetric systems.

Year 2 Show resiliency of MCSA algorithm for soft and hard errors while solving the linear advection-diffusion and non-linear Navier-Stokes equations.

Year 3 Show parallel performance of MCSA algorithm on existing HPC architectures and demonstrate scaling to exascale systems using the MCSA performance model.

The full list of major tasks, correlated by yearly milestones, are

Task	Description	Milestone
1	Determine performance on non-symmetric systems	Y1
2	Implement Newton-MCSA method	Y1, Y2
3	Derive and implement linear ADR model equations	Y1, Y2
4	Derive and implement non-linear, incompressible Navier-Stokes equations	Y1, Y2
5	Investigate solver runtime parameters	Y1
6	Analyze robustness of unbiased estimators to high-variance events	Y1, Y2
7	Implement MSOD parallel algorithm	Y2, Y3
8	Develop performance model for MSOD/MCSA algorithm	Y3
9	Model algorithm resiliency using fault injection campaigns	Y2, Y3
10	Estimate algorithm performance on future systems using the performance model and xSim	Y3

The products of this research are twofold:

- Journal and conference articles and lab reports;
- Open-source distribution code base.

All code products produced *directly* as part of this proposal will be hosted on ORNL-managed GIT repositories. All code products will be available through open-source distribution, but access to the development repositories will be controlled through ORNL.

5 Management Plan

This is a highly focused proposal with a limited scope. Accordingly, the management plan specifies an agile development model in order to optimize the work output and allow maximum flexibility in pursuing new avenues of investigation. The project has two PIs, Drs. Thomas Evans, ORNL and Michele Benzi, Emory University. Dr. Evans will serve as the Research Coordinator for the project, which will be led at ORNL. The project member roles and responsibilities are shown in Fig. 5. Also illustrated are the institutional roles. ORNL will host the project management site (http://fogbugz.ornl.gov, see http://www.fogcreek.com/fogbugz for details) and GIT software and document repositories. An electronic notebook server using NoteShare (http://www.aguaminds.com) will be maintained at ORNL that allows instant sharing of progress and results.

Because this project only involves 5 professional staff plus one student, the process should be agile so that subsequent investigations can be easily modified to reflect current work. Accordingly, the project lifecycle model that will be employed is based on an agile Kanban [41] process. All milestones and tasks will be tracked on a Kanban board hosted at ORNL. This project will leverage experience gained in the CASL DOE NE Hub (CASL, http://www.casl.gov) for managing an inter-institutional project under a virtual "one roof." The relatively close proximity between ORNL and Emory makes travel between the institutions feasible. Furthermore, bi-weekly and as-needed conference calls/interactive coding sessions using ReadyTalk (http://www.readytalk.com) can be used to easily facilitate collaboration. As noted above, electronic notebooks will be used to provide instant access to current status and results of ongoing research.

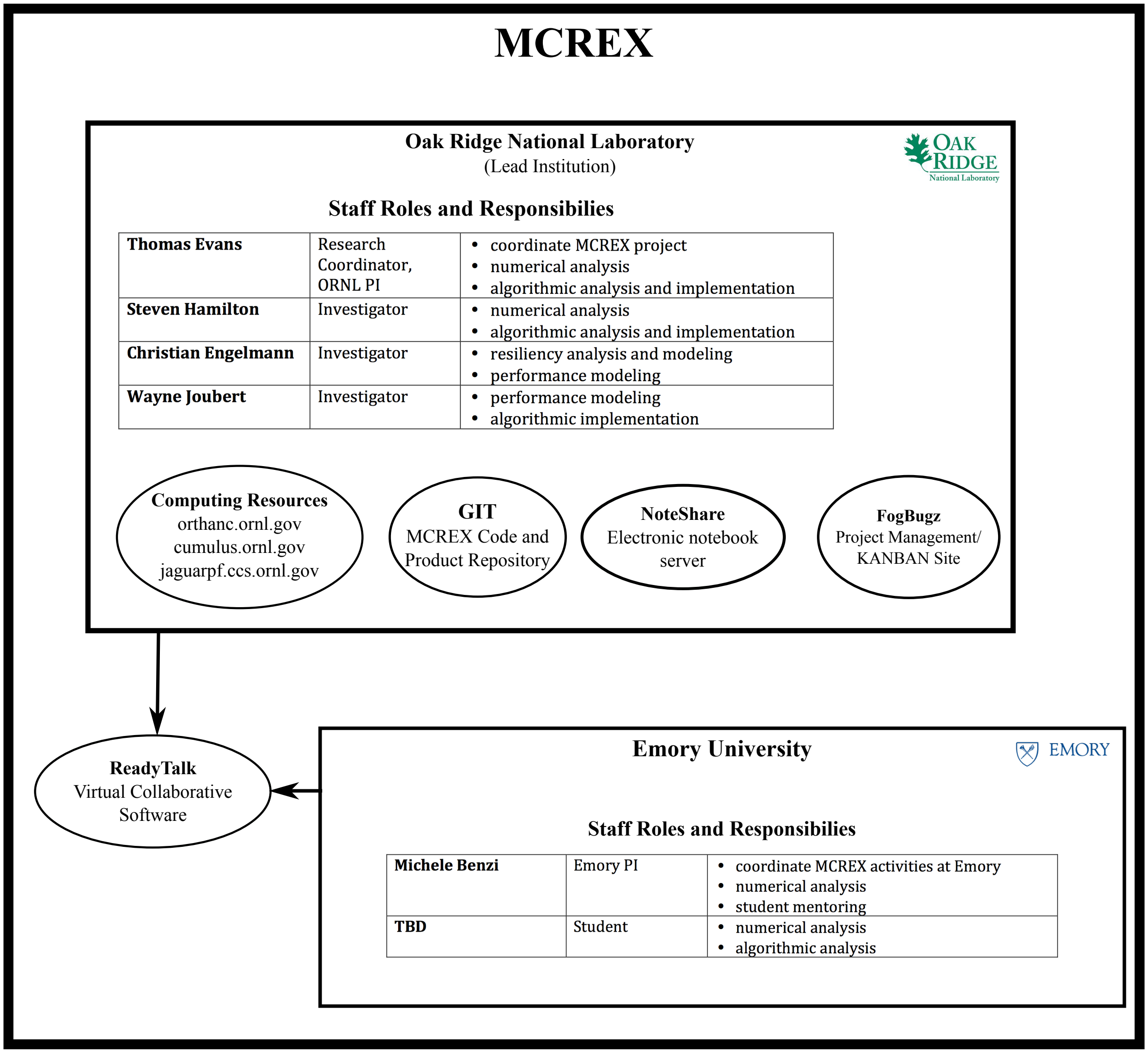


Figure 5: MCREX project member roles and responsibilities.

All code produced in this project will be constructed using a test-driven development model [42]. Test-driven code development is not only essential for production-level code project; it is required for research in order to verify that output is the result of numerics, as opposed to code defects.

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A Biographical sketches

A.1 Biographical Sketch for Michele Benzi

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Education and Training

University of Bologna, Italy	Mathematics	B.S., 1987
North Carolina State University	Mathematics	M.S., 1991
North Carolina State University	Applied Mathematics	Ph.D., 1993

Research and Professional Experience

2012 – present	Samuel Candler Dobbs Professor, Emory University
2006 – 2012	Professor, Emory University
2000 – 2006	Associate Professor, Emory University
1998 – 2000	Staff member, Scientific Computing Group, LANL
1997 – 1998	Director-funded postdoctoral associate, Scientific Computing Group, LANL
1996 – 1997	Postdoctoral Researcher, Parallel Algorithms Group, CERFACS, Toulouse, France
1993 – 1996	Researcher, Department of Mathematics, University of Bologna, Italy

Related Publications

1. M. Benzi and V. Kuhlemann, “Restricted additive Schwarz methods for Markov chains”, Numer. Linear Algebra Appl., **18** (2011), pp. 1011–1029.
2. M. Benzi, M. K. Ng, W. Niu and Z. Wang, “A relaxed dimensional factorization preconditioner for the Navier–Stokes equations”, J. Comp. Phys., **230** (2011), pp. 6185–6202.
3. S. P. Hamilton, M. Benzi and E. Haber, “New multigrid smoothers for the Oseen Problem”, Numer. Linear Algebra Appl., **17** (2010), pp. 557–576.
4. S. P. Hamilton, M. Benzi and J. S. Warsa, “Negative-flux fixups in discontinuous finite element S_N transport”, Proceedings of the International Conference on Mathematics, Computational Methods & Reactor Physics 2009 (M&C 2009), American Nuclear Society, Vol. 4 (2009), pp. 2529-2538, Saratoga Springs, NY, 2009.
5. M. Noskov, M. Benzi, and M. D. Smooke, “An implicit compact scheme solver for two-dimensional multicomponent flows”, Computers & Fluids, **36** (2007), pp. 376–397.
6. M. Benzi, G. H. Golub, and J. Liesen, “Numerical solution of saddle point problems”, Acta Numerica, **14** (2005), pp. 1–137.
7. J. Warsa, M. Benzi, T. Wareing and J. Morel, “Preconditioning a mixed discontinuous finite element method for radiation diffusion”, Numer. Linear Algebra Appl., **11** (2004), pp. 795–811.
8. M. Benzi, “Preconditioning techniques for large linear systems: a survey”, J. Comp. Phys., **182** (2002), pp. 418–477.
9. M. Benzi and M. Tuma, “A parallel solver for large-scale Markov chains”, Appl. Numer. Math., **41** (2002), pp. 135–153.

10. M. Benzi, J. Marin and M. Tuma, “A two-level parallel preconditioner based on sparse approximate inverses”, in Iterative Methods in Scientific Computation IV, D. R. Kincaid and A. C. Elster, eds., IMACS Series in Computational and Applied Mathematics, Vol. 5, IMACS, New Brunswick, NJ (1999), pp. 167–178.

Synergistic Activities

1. Chair, SIAM Activity Group on Linear Algebra (2010-present);
2. Member of the SIAM Council (2009-present);
3. SIAM Fellow (Class of 2012);
4. Program Committeee Co-chair, 2012 SIAM Applied Linear Conference (Valencia, Spain, June 18-22, 2012);
5. Program Committeee Co-chair, SIAM Annual Meeting (Minneapolis, MN, July 9-13, 2012).
6. Editor-in-Charge, SISC Copper Mountain Special Issue (2012-present).

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Graduate and Postdoctoral Advisors and Advisees

Advisors:

1. Wayne Joubert (Postdoc, LANL)
2. Iain Duff (Postdoc, CERFACS)
3. Carl Meyer (PhD, NCSU)

Advisees:

1. Paola Boito (Postdoc)
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A.2 Biographical sketch for Christian Engelmann

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Professional Accomplishments

8 Research grants (2 as Lead)	6 Peer-reviewed journal articles	35 Invited talks and seminars
8 Co-advised M.Sc. theses	33 Peer-reviewed conference papers	70 Committees at 34 conferences
2 Mentored summer faculty	27 Peer-reviewed workshop papers	20 Article & book proposal reviews
10 Direct reports over 7 years	8 Peer-reviewed conference posters	11 Conference booth exhibitions
Erdös number of 5	860+ Total publication citations	H-index of 16 / G-index of 27

Professional Experience

2009–Present : **R&D Staff, Oak Ridge National Laboratory**
- HPC hard-/software co-design: performance/resilience/power modeling & simulation
- Soft-error injection for vulnerability analysis of scientific applications and CMOS logic
- HPC resiliency system software for monitoring, fault prediction, and fault avoidance
- HPC checkpoint storage virtualization and MPI-level redundancy for HPC applications
- HPC hard-/software co-design: performance modeling & simulation
- Light-weight simulation of extreme scale HPC architectures ($\sim$100,000,000 cores)

2004–2009 : **Associate R&D Staff, Oak Ridge National Laboratory**
- Fault tolerance support for MPI: Scalable membership, job pause, and process migration
- 99.9997% high availability for HPC head/service-node services: Torque and PVFS MDS
- Ph.D. thesis research: Symmetric active/active high availability for HPC system services
- Virtual system environments for "plug-and-play" supercomputing with HPC hypervisors
- Enhancing application development productivity via a common view across platforms

2001–2004 : **Post-Master's Research Associate, Oak Ridge National Laboratory**
- Harness Distributed Virtual Machine: Pluggable, lightweight, adaptive, and fault tolerant
- Light-weight simulation of HPC architectures at large scale ($\sim$1,000,000 cores)

2000–2001 : **Software Developer, Oak Ridge National Laboratory**
- M.Sc. thesis research: Distributed peer-to-peer control for Harness (a resilient runtime)

Education

2008 Ph.D. in Computer Science, University of Reading, UK
2001 M.Sc. in Computer Science, University of Reading, UK
2001 Dipl.-Ing. (FH) in Computer Systems Engineering, University of Applied Sciences Berlin, Germany

Important Peer-reviewed Publications

[1] D. Fiala, F. Mueller, C. Engelmann, K. Ferreira, R. Brightwell, and R. Riesen. Detection and correction of silent data corruption for large-scale high-performance computing. In *Intl. Conf. on High Performance Computing, Networking, Storage and Analysis (SC)*, 2012.

[2] J. Elliott, K. Kharbas, D. Fiala, F. Mueller, K. Ferreira, and C. Engelmann. Combining partial redundancy and checkpointing for HPC. In *Intl. Conf. on Distributed Computing Systems (ICDCS)*, pages 615–626, 2012.

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[7] X. He, L. Ou, C. Engelmann, X. Chen, and S. Scott. Symmetric active/active metadata service for high availability parallel file systems. *J. of Parallel and Distributed Computing (JPDC)*, 69(12):961–973, 2009.

[8] A. Nagarajan, F. Mueller, C. Engelmann, and S. Scott. Proactive fault tolerance for HPC with Xen virtualization. In *Intl. Conf. on Supercomputing (ICS)*, pages 23–32, 2007.

[9] C. Wang, F. Mueller, C. Engelmann, and S. Scott. A job pause service under LAM/MPI+BLCR for transparent fault tolerance. In *Intl. Parallel and Distributed Processing Symp. (IPDPS)*, pages 1–10, 2007.

[10] J. Varma, C. Wang, F. Mueller, C. Engelmann, and S. Scott. Scalable, fault-tolerant membership for MPI tasks on HPC systems. In *Intl. Conf. on Supercomputing (ICS)*, pages 219–228, 2006.

Important Professional Activities

2010–2012 : PC chair: Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems (ScalA) at the Intl. Conf. on High Perf. Computing, Networking, Storage and Analysis (SC)

2009–2012 : PC chair: Workshop on Resiliency in High-Perf. Computing (Resilience) at the Intl. Symp. on High Perf, Distributed Computing (HPDC), the Intl. Symp. on Cluster Computing and the Grid (CCGrid), and the European Conf. on Parallel and Distributed Computing (Euro-Par)

2006–2010 : PC chair: HPC Resiliency Summit at the Los Alamos CS Symp. (LACSS), and the High Availability and Perf. Workshop (HAPCW) at the Los Alamos CS Inst. (LACSI) Symp.

2012 : PC vice-chair: IEEE Intl. Symp. on Parallel and Distributed Processing and Apps. (ISPA)

2009 : PC vice-chair: IEEE Intl. Conf. on Networking, Architecture, and Storage (NAS)

Professional Memberships

USENIX, ACM + SIGHPC/SIGOPS, IEEE + ComSoc/CS/RL, IEEE CS TCFT/TCDP/TCPP/TCSC

Collaborators and Co-editors in Past 48 Months (Excl. Advisors, Advisees, Junior Pers., and Non-US)

ANL: P. Beckman, A. Chien, R. Gupta, R. Ross, M. Snir; **Cray:** L. Kaplan; **DOE:** L. Nowell; **Emory U:** M. Benzi; **IBM:** M. Elnozahy; **Intel:** S. Borkar; **ISI:** B. Lucas; **LA Tech:** C. Leangsuksun; **LANL:** N. DeBardeleben; **LBNL:** P. Hargrove, E. Roman, J. Wu; **LLNL:** M. Schulz, B. Still; **NCSU:** X. Ma, F. Mueller; **ORNL:** S. Atchley, D. Bernholdt, D. Dillow, T. Evans, S. Hamilton, Y. Kim, T. Naughton, B. Park, G. Shipman, G. Vallée, S. Vazhkudai; **PNNL:** S. Krishnamoorthy, A. Vishnu; **SNL:** A. Gentile, J. Brandt, R. Brightwell, R. Clay, K. Ferreira, M. Heroux; **TN Tech:** S. Gafoor; **UTK:** G. Bosilca, J. Dongarra; **VA Tech:** A. Butt

Graduate and Postdoctoral Advisors

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Education and Training

Haverford College	Physics and Astronomy	B.S. 1992
Georgia Institute of Technology	Health Physics	M.S. 1994
Georgia Institute of Technology	Nuclear Engineering	Ph.D. 1997

Research and Professional Experience

2012 – present	Distinguished R&D Staff, Oak Ridge National Laboratory
2007 – 2012	Senior R&D Staff, Oak Ridge National Laboratory
2003 – 2007	Project Leader , Radiation Transport Group, Los Alamos National Laboratory
1997 – 2003	Techical Staff Member, Los Alamos National Laboratory
1997 – 1997	Post-doctoral Fellow, Los Alamos National Laboratory

Related Publications

1. J.C. Wagner, S.W. Mosher, T.M. Evans, D.E. Peplow, and J.A. Turner, *Hybrid and Parallel Domain-Decomposition Methods Development to Enable Monte Carlo for Reactor Analyses,* Prog. Nuc. Sci. Tech., 2:815-820, 2011.
2. G.G. Davidson, T.M. Evans, R.N. Slaybaugh, and C.G. Baker, *Massively Parallel Solutions to the k-Eigenvalue Problem*, Trans. Am. Nucl. Soc., 103, 2010.
3. T.M. Evans, K.T. Clarno, and J.E. Morel, *A transport acceleration scheme for multigroup discrete ordinates with upscattering*, Nuc. Sci. Eng., 165:1-13, 2010.
4. T.M. Evans, A.S. Stafford, R.N. Slaybaugh, and K.T. Clarno, *Denovo—A new three-dimensional parallel discrete ordinates code in SCALE*, Nuc. Tech., 171:171-200, 2010.
5. T.M. Evans and S.W. Mosher, *A Monte Carlo Synthetic Acceleration Method for the Non-Linear, Time-Dependent Diffusion Equation*, International Conference on Mathematics, Computational Methods and Reactor Physics, Saratoga Springs, NY, ISBN: 978-0-89448-069-0, American Nuclear Society, La-Grange Park, IL, 2009.
6. Ryan G. McClarren, Thomas M. Evans, Robert B. Lowrie, and Jefferey D. Densmore, *Semi-Implicit Time Integration for P_N Thermal Radiative Transfer*, J. Comp. Phys., 227:7561-7586, 2008.
7. J.D. Densmore, T.M. Evans, and M.W. Buksas, *A Hybrid Transport-Diffusion Algorithm for Monte Carlo Radiation-Transport Simulations on Adaptive-Refinement Meshes in XY Geometry*, Nuc. Sci. Eng., 159:1-22, 2008.
8. T.M. Evans and J.D. Densmore *Methods for Coupling Radiation, Ion, and Electron Energies In Grey Implicit Monte Carlo*, J. Comp. Phys., 225:1695-1720, 2007.
9. T.A. Brunner, T.J. Urbatsch, T.M. Evans, and N.A. Gentile, *Comparison of Four Parallel Algorithms for Domain Decomposed Implicit Monte Carlo*, J. Comp. Phys., 212:527–539, 2006.
10. T.M. Evans, T.J. Urbatsch, H.Lichtenstein, and J.E. Morel. A residual Monte Carlo Method for Discrete Thermal Radiative Diffusion. *J. Comp. Phys.*, **189**(2), 539–556, 2003.

Synergistic Activities

1. Project Leader, Denovo parallel S_N and *Shift* Monte Carlo transport codes at Oak Ridge National Laboratory, which are part of the SCALE package.
2. PI, Deterministic S_N Transport, CASL Modeling and Simulation Hub at Oak Ridge
3. PI, 2012–2013 INCITE Project *The Solution of Three-Dimensional PWR Neutronics Benchmark Problems for CASL.*
4. Member, technical committee for several Math and Computation Division (MCD) meetings of the American Nuclear Society
5. Officer, MCD Vice President, 2012–2013; incoming MCD President, 2013–2014; MCD Secretary, 2000–2001.

Co-Authors and Collaborators (last 48 months)

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Graduate Advisor

C.K. Wang, **Georgia Institute of Technology**

PhD Dissertation Advisees

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A.4 Biographical sketch for Steven P. Hamilton

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Education and Training

Georgia Institute of Technology	Nuclear Engineering	B.S. 2006
Georgia Institute of Technology	Nuclear Engineering	M.S. 2007
Emory University	Computational Mathematics	PhD 2011

Research and Professional Experience

2011 – present	R&D Staff, Oak Ridge National Laboratory
2009 – 2010	Instructor,Mathematics and Computer Science Department, Emory University
2008	Research Practicum, Computational Physics (CCS-2), Los Alamos National Laboratory
2006	Intern, Reactor Physics Group, Oak Ridge National Laboratory

Related Publications

1. S. Hamilton, K. Clarno, B. Philip, M. Berrill, R. Sampath and S. Allu. Integrated Radiation Transport and Nuclear Fuel Performance for Assembly-Level Simulations. *Proc. PHYSOR*, 2012.
2. S. Hamilton, K. Clarno, B. Philip, M. Berrill, R. Sampath and S. Allu. Coupled Radiation Transport and Thermomechanics using the AMP and Denovo Codes. *Proc. 11th Copper Mtn. Conference on Iterative Methods*, 2012.
3. S. Hamilton and K. Clarno. Mathematical Framework for Coupling the AMP and Denovo Codes. *Trans. Am. Nucl. Soc.*, **105**, 515–517, 2011.
4. S. Hamilton and M. Benzi. A Davidson Method for the k-Eigenvalue Problem. *Trans. Am. Nucl. Soc.*, **105**, 432–424, 2011.
5. S. Hamilton and M. Benzi. Eigensolvers for Radiation Transport Applications. *Proc. 11th Copper Mountain Conference on Iterative Methods*, 2010.
6. S. Hamilton, M. Benzi and J. Warsa. Negative Flux Fixups in Discontinuous Finite Element SN Transport. *Proc. International Conference on Mathematics, Computational Methods and Reactor Physics*, 2009.
7. S. Hamilton, M. Benzi and E. Haber. New Multigrid Smoothers for the Oseen Problem. Num. Lin. Alg. with Apps. **17**, 557–576, 2010.
8. S. Hamilton, M. Benzi and E. Haber. New Smoothers for the Oseen Problem. *Proc. 14th Copper Mtn. Conference on Multigrid Methods*, 2009.
9. S. Hamilton, K. Clarno and C. de Oliveira. Error Control in a Time-Dependent Slice-Balance Method. *Trans. Am. Nucl. Soc.*, **97**, 533–535, 2007.
10. W. Stacey et. al. Advances in the Subcritical, Gas-Cooled Transmutation Reactor Concept. Nucl. Tech. **159**, 2007.

Synergistic Activities

1. Developer, Denovo parallel S_N transport code and the Advanced Multi-Physics (AMP) Nuclear Fuel Performance package at Oak Ridge National Laboratory.
2. Alumnus, DOE Computational Science Graduate Fellowship program.
3. Member, American Nuclear Society.

Co-Authors and Collaborators (last 48 months)

LANL: James Warsa **ORNL:** Srikanth Allu, Mark Baird, Kevin Clarno, Greg Davidson, Tom Evans, Josh Jarrell, Wayne Joubert, Bobby Philip, Rahul Sampath, **Univ. Arizona**: Barry Ganapol, **Univ. British Columbia**: Eldad Haber, **Univ. New Mexico**: Cassiano de Oliveira, **Univ. Tennessee**: James Banfield

Graduate Advisor

Michele Benzi, **Emory University**.

A.5 Biographical sketch for Wayne Joubert

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Education and Training

University of Louisiana	Mathematics	B.S. 1981
Univerity of Texas	Mathematics	Ph.D. 1990

Research and Professional Experience

2008 – present	Senior R&D Staff, Oak Ridge National Laboratory
2007 – 2008	Computational Scientist, Engineer Research and Development Center
2002 – 2007	Computer Scientist, Xiylon Software
1999 – 2001	Computer Scientist, LizardTech, Inc.
1998 – 1999	Team Leader, Los Alamos National Laboratory
1992 – 1998	Technical Staff, Los Alamos National Laboratory

Related Publications

1. C. Baker, G. Davidson, T. Evans, S. Hamilton, J. Jarrell and W. Joubert. High Performance Radiation Transport Simulations: Preparing for TITAN. *International Conference for High Performance Computing, Networking, Storage and Analysis (SC12)*, 2012.
2. W. Joubert and S. Su. An Analysis of Computational Workloads on the Jaguar Cray XT System. *International Conference on Supercomputing*, 2012.
3. W. Joubert, D. Kothe and H. Nam. PREPARING FOR EXASCALE: ORNL Leadership Computing Application Requirements and Strategy. *ORNL/TM-2009/308*, 2009.
4. B. Philip, M. Pernice, W. Joubert and B. Lally. A Comparison of Multilevel Preconditioners for Solving Multimaterial Equilibrium Radiation Diffusion Problems on Locally Refined Grids. *Nuclear Weapons Highlights*, 2007.
5. W. Joubert and J. Cullum. Scalable Algebraic Multigrid on 3500 Processors. *Electronic Transactions in Numerical Analysis*, **23**, 2006.
6. W. Joubert and G. Carey. PCG: A Software Package for the Iterative Solution of Linear Systems on Scalar, Vector and Parallel Computers. *Scalable High Performance Computing Conference*, 1994.
7. W. Joubert and T. Oppe. Improved SSOR and Incomplete Cholesky Solution of Linear Equations on Shared Memory and Distributed Memory Parallel Computers. *Numerical Linear Algebra with Applications*, **1**, 1994.
8. W. Joubert. Lanczos Methods for the Solution of Nonsymmetric Systems of Linear Equations. *SIAM Journal on Matrix Analysis and Applications*, **13**, 1992.

Synergistic Activities

1. Performance Task Lead, Oak Ridge Leadership Computing Facility.
2. ORNL Center for Advanced Application Readiness, readiness lead for Denovo code, Titan system.

3. Requirements analysis for 100-250 PF ORNL OLCF-4 system.

4. Member, Society for Industrial and Applied Mathematics.

Co-Authors and Collaborators (last 48 months)

LANL: David Moulton. **Mellanox:** Richard Graham. **Cray:** Jeff Larkin, John Levesque, Norm Troullier. **ORNL:** Chris Baker, W. Michael Brown, Kevin Clarno, Greg Davidson, Tom Evans, Steven Hamilton, Rebecca Hartman-Baker, Oscar Hernandez, Josh Jarrell, Ricky Kendall, Doug Kothe, Don Maxwell, Bronson Messer, Hai Ah Nam, Bobby Philip, Steve Poole, Ramanan Sankaran, Shiquan Su, Arnold Tharrington, John Turner, Bogdan Vacaliuc. **SNL:** Richard Barrett. **University of Colorado:** Samuel Skillman.

Graduate Advisor

David M. Young, **University of Texas**.

B Current & pending support

B.1 ORNL senior personnel

B.1.1 C&P support for Christian Engelmann

Current Support

1. *Extreme-scale Algorithms and Software Institute (EASI)*
   DOE OASCR
   10/11 - 9/12, $1M/yr., 12 months/yr for C. Engelmann
2. *Hardware/Software Resilience Co-Design Tools for Extreme-scale High-Performance Computing (PI)*
   ORNL Director's R&D Fund
   10/12 - 9/14, $380K/yr., 12 months/yr for C. Engelmann

Pending Support

1. *MCREX: Using Monte Carlo algorithms to achieve resiliency and performance at scale for linear and non-linear solver applications*
   - **LAB 12-742 Resilient Extreme-Scale Solvers**
     10/12 - 9/15, $1,575K for 3 years, 4 months/yr for C. Engelmann

B.1.2 C&P support for Thomas M. Evans

Current Support

1. *Deterministic Transport Methods (PI)*
   - **DOE Hub - Consortium for the Simulation of LWRs (CASL)**
     10/2011 - 10/2015, $25,000K/yr., 8-9 months/yr for T. Evans
2. *Advanced Mesh-Enabled Monte Carlo Capability for Multi-Physics Reactor Analysis (PI)*
   - **DOE NEUP**
     10/09 - 10/12, $1,000K/yr., 3 months in 2012 for T. Evans
3. *A novel uncertainty quantification paradigm for enabling massively scalable predictions of complex stochastic simulations*
   ORNL Director's R&D Fund
   10/12 - 10/14, $380K/yr., 4 months/yr for T. Evans

Pending Support

1. *MCREX: Using Monte Carlo algorithms to achieve resiliency and performance at scale for linear and non-linear solver applications (PI and Research Coordinator)(this proposal)*
   - **LAB 12-742 Resilient Extreme-Scale Solvers**
     10/12 - 10/15, $1,575K, 4 months/yr for T. Evans

B.1.3 C&P support for Steven P. Hamilton

Current Support

1. *Development of Advanced Multi-Physics Nuclear Fuel Performance Code (AMP)*
   - **DOE NEAMS**
     10/10 - 10/13, $2,250K/yr., 12 months/yr for S. Hamilton

Pending Support

1. *MCREX: Using Monte Carlo algorithms to achieve resiliency and performance at scale for linear and non-linear solver applications (PI and Research Coordinator)(this proposal)*
   - **LAB 12-742 Resilient Extreme-Scale Solvers**
     10/12 - 10/15, $1,575K, 6 months/yr for S. Hamilton

B.1.4 C&P support for Wayne Joubert

Current Support

1. *Oak Ridge Leadership Computing Facility Project*
   - **DOE Oak Ridge Leadership Computing Facility (OLCF)**
     10/2011 - 10/2015, $370,000K/yr., 12 months/yr for W. Joubert

Pending Support

1. *MCREX: Using Monte Carlo algorithms to achieve resiliency and performance at scale for linear and non-linear solver applications (PI and Research Coordinator)(this proposal)*
   - **LAB 12-742 Resilient Extreme-Scale Solvers**
     10/12 - 10/15, $1,575K, 4 months/yr for W. Joubert

B.2 Emory senior personnel

B.2.1 C&P support for Michele Benzi

Current Support

1. *Numerical Linear Algebra Tools for the Analysis of Complex Network*
   - **NSF**
     08/01/11–07/31/14, $303,045 for M. Benzi

Pending Support

1. *MCREX: Using Monte Carlo algorithms to achieve resiliency and performance at scale for linear and non-linear solver applications (PI)(this proposal)*
   - **LAB 12-742 Resilient Extreme-Scale Solvers**
     10/12 - 10/15, $1,575K total, 76–80K/yr for M. Benzi
2. *A Forest for the Trees: An Ecosystem of Generalized N-Body Solvers*
   - **LAB 12-742 Resilient Extreme-Scale Solvers**
     10/12 - 10/15, 76–80K/yr for M. Benzi

C Facilities & resources

Due to ORNL's world class resources for computing, ORNL will be the prinicpal provider of facilities and resources for this collaborative proposal. However, facility descriptions are provided for each institution in the proposal.

C.1 Oak Ridge National Laboratory

1. Oak Ridge National Laboratory

Computer Facilities. The Oak Ridge National Laboratory (ORNL) hosts three petascale computing facilities: the Oak Ridge Leadership Computing Facility (OLCF), managed for the U.S. Department of Energy (DOE); the National Institute for Computational Sciences (NICS) computing facility operated for the National Science Foundation (NSF); and the National Climate-Computing Research Center (NCRC), formed as collaboration between ORNL and the National Oceanographic and Atmospheric Administration (NOAA) to explore a variety of research topics in climate sciences. Each of these facilities has a professional, experienced operational and engineering staff comprising groups in high-performance computing (HPC) operations, technology integration, user services, scientific computing, and application performance tools. The ORNL computer facility staff provides continuous operation of the centers and immediate problem resolution. On evenings and weekends, operators provide first-line problem resolution for users with additional user support and system administrators on-call for more difficult problems.

Other Facilities. The Oak Ridge Science and Technology Park at ORNL is the nation's first technology park on the campus of a national laboratory. The technology park is available for private sector companies that are collaborating with research scientists. Laboratory officials anticipate that the new park will be used to help create new companies from technologies developed at ORNL.

1.1 Primary Systems

Jaguar is a Cray XK6 system consisting of 18,688 AMD sixteen-core Opteron processors providing a peak performance of more than 3.3 petaflops (PF) and 600 terabytes (TB) of memory. A total of 384 service input/output (I/O) nodes provide access to the 10 PB "Spider" Lustre parallel file system at more than 240 gigabytes (GB/s). External login nodes (decoupled from the XK6 system) provide a powerful compilation and interactive environment using dual-socket, twelve-core AMD Opteron processors and 256 GB of memory. Jaguar also includes 960 NVIDIA Tesla M2090 graphics processing units (GPUs) designed to accelerate calculations. Jaguar is the Department of Energy's most powerful open science computer system and is available to the international science community through the INCITE program, jointly managed by DOE's Leadership Computing Facilities at Argonne and Oak Ridge National Laboratories.

Titan will be an upgrade to Jaguar in late 2012. Titan will add next generation NVIDIA GPUs to the nodes of Jaguar resulting in a system with a peak performance of between 10 and 20 PF. The Spider disk subsystem will be upgraded to provide up to 1 TB/s of disk bandwidth and up to 30 PB of storage.

Gaea is a Cray XE6 system delivered in two stages. The first stage, delivered in the summer of 2010, consists of 2,576 socket G34 AMD 12-core Magny-Cours Opteron processors, providing 30,912 compute cores, 82.4 TB of double data rate 3 (DDR3) memory, and a peak performance of 260 teraflops (TF). The second stage consists of 4,896 socket G34 AMD 16-core Interlagos Opteron processors, providing 78,336 compute cores, 156.7 TB of DDR3 memory, and a peak performance of 721 TF.

After the stage two system enters production, the original stage one system will receive an architectural upgrade to the Interlagos processor. The resulting aggregate system will provide 1.106 PF of computing capability, and 248 TB of memory. The Gaea compute partitions are supported by a series of external login nodes and two separate file systems. The FS file system is based on more than 2,000 SAS drives and provides more than 1 PB (formatted) space for fast scratch to all compute partitions. The LTFS file system provides more than 2000 SATA drives and 4 PB formatted capacity as a staging and archive file system. Gaea is the NOAA climate community's most powerful computer system and is available to the climate research community through the Department of Commerce/NOAA.

The ORNL Institutional Cluster (OIC) consists of two phases. The original OIC consists of a bladed architecture from Ciara Technologies called VXRACK. Each VXRACK contains two login nodes, three storage nodes, and 80 compute nodes. Each compute node has dual Intel 3.4 GHz Xeon EM64T processors, 4 GB of memory, and dual gigabit Ethernet interconnects. Each VXRACK and its associated login and storage nodes are called a block. There are a total of nine blocks of this type. Phase 2 blocks were acquired and brought online in 2008. They are SGI Altix machines. There are two types of blocks in this family.

- Thin Nodes (3 blocks). Each Altix contains 1 login node, 1 storage node, and 28 compute nodes within 14 chassis. Each node has eight cores and 16 GB of memory. The login and storage nodes are XE240 boxes from SGI. The compute nodes are XE310 boxes from SGI.
- Fat Nodes (2 blocks). Each Altix contains 1 login node, 1 storage node, and 20 compute nodes within 20 separate chassis. Each node has eight cores and 16 GB of memory. These XE240 nodes from SGI contain larger node-local scratch space and a much higher I/O to this scratch space because the space is a volume from four disks.

Frost (SGI Altix ICE 8200) consists of three racks totaling 128 compute nodes, 5 service nodes (1 batch node and 4 login nodes), 2 rack leader nodes, and 1 administration node. Each compute node has two Intel quad-core Xeon X5560 at 2.8 GHz (Nehalem) processors, 24 GB of memory, a 1 Gb Ethernet connection, and two 4x DDR Infiniband connections. Each rack of compute nodes contains eight Infiniband switches (Mellanox InfiniScale III MT47396, 24 10-Gb/s Infiniband 4X ports) that are used as the primary interconnect between compute nodes and for connection to the Lustre file system. The center-wide Lustre file system is the main storage available to the compute nodes. The Frost cluster is available to ORNL staff and collaborators.

1.2 The University of Tennessee

Kraken is a Cray XT5 system consisting of 18,816 AMD six-core Opteron processors providing a peak performance of 1.17 PF and 147 TB of memory. It is connected to more than 3 PB of disk space for scratch space. At the current time, it is the eleventh fastest computer in the world, the fastest academic computer in the world, and the largest resource on the NSF XSEDE network.

1.3 Joint Institute for Computational Sciences

The University of Tennessee (UT) and Oak Ridge National Laboratory (ORNL) established the Joint Institute for Computational Sciences (JICS) in 1991 to encourage and facilitate the use of high-performance computing in the state of Tennessee. When UT joined Battelle Memorial Institute in April 2000 to manage ORNL for the Department of Energy (DOE), the vision for JICS expanded to encompass becoming a world-class center for research, education, and training in computational science and engineering. JICS advances scientific discovery and state-of-the-art engineering by

- taking full advantage of the computers at the petascale and beyond housed at ORNL and in the Oak Ridge Leadership Computing Facility (OLCF) and
- enhancing knowledge of computational modeling and simulation through educating a new generation of scientists and engineers well versed in the application of computational modeling and simulation to solving the world's most challenging scientific and engineering problems.

Joint Institute for Computational Sciences.

JICS is staffed by joint faculty who hold dual appointments as faculty members in departments at UT and as staff members in ORNL research groups. The institute also employs professional research staff, postdoctoral fellows and students, and administrative staff.

The JICS facility represents a $10M investment by the state of Tennessee and features a state-of-the-art interactive distance learning center with seating for 66 people, conference rooms, informal and open meeting space, executive offices for distinguished scientists and directors, and incubator suites for students and visiting staff.

The JICS facility is a hub of computational and engineering interactions. Joint faculty, postdocs, students, and research staff share the building, which is designed specifically to provide intellectual and practical stimulation. The auditorium serves as the venue for invited lectures and seminars by representatives from academia, industry, and other laboratories, and the open lobby doubles as casual meeting space and the site for informal presentations and poster sessions, including an annual 200+ student poster session.

In June 2004, JICS moved into a new 52,000 ft^2 building next door to the OLCF. The OLCF, which is located on the ORNL campus, is among the nation's most modern facilities for scientific computing. The OLCF includes 40,000 square feet divided equally into two rooms designed specifically for high-end computing systems.

Within JICS, there are three other centers that are the result of three large National Science Foundation (NSF) awards:

The National Institute for Computational Sciences (NICS) at the University of Tennessee is the product of a $65M NSF Track 2B award. The mission of NICS is to enable the scientific discoveries of researchers nationwide by providing leading-edge computational resources and education, outreach, and training for underrepresented groups. Kraken, the fastest, most powerful supercomputer for academic use, is the flagship NICS computing resource.

The UT Center for Remote Data Analysis and Visualization (RDAV) is sponsored by NSF through a 4-year, $10 million TeraGrid XD award. The centerpiece hardware resource at RDAV is Nautilus, a new SGI UltraViolet shared-memory machine featuring 1,024 cores and 4 terabytes of memory within a single system image. A wide range of software tools is available for TeraGrid users to perform data analysis, visualization, and scientific workflow automation on Nautilus. The machine is located at ORNL and is administered by NICS staff.

The Keeneland Project is a 5-year, $12 million Track 2 grant awarded by NSF for the deployment of an experimental high-performance system. The Georgia Institute of Technology and its project partners, UT-Knoxville and ORNL, have initially acquired and deployed a small, experimental, high-performance computing system consisting of an HP system with NVIDIA Tesla accelerators attached. The machine is located at ORNL and is administered by NICS staff.

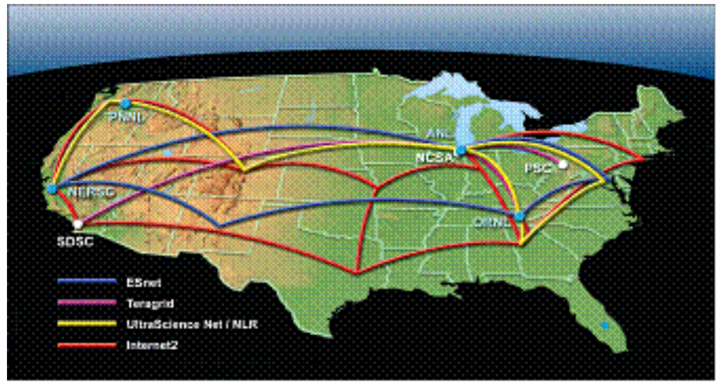
Outside of JICS, ORNL hosts a unique collaborative modeling and simulation center that was awarded in 2010.

The Consortium for Advanced Simulation of Light Water Reactors (CASL) program is a 5-year, $122 million, DOE Office of Nuclear Energy Innovation Hub for Modeling and Simulation. The Virtual Office Community and Computing (VOCC) Project inside of CASL established a state-of-the-art collaborative modeling and simulation laboratory, which houses unique collaborative communication, computing, and 3D immersive visualization instruments. All of its visualization instruments were custom designed and configured to support distributive collaborative coding and reactor engineering simulation activities for the CASL program. CASL's VOCC seeks to play a significant role in improving the way many computational science application programs like CASL collaborate with multiple compute resources and visualization environments. The CASL program is part of the Nuclear Science and Engineering Directorate. The CASL VOCC Laboratory is located in Building 5700 and is managed by CASL's Collaboration and Ideation Officer. CASL works closely with other programs, laboratories and government organizations to create optimal collaborative modeling and simulation environments.

2. Infrastructure

Physical and Cyber Security. ORNL has a comprehensive physical security strategy including fenced perimeters, patrolled facilities, and authorization checks for physical access. An integrated cyber security plan encompasses all aspects of computing. Cyber security plans are risk-based. Separate systems of differing security requirements allow the appropriate level of protection for each system, while not hindering the science needs of the projects.

Network Connectivity. The ORNL campus is connected to every major research network at rates of between 10 GB/s and 100 GB/s. Connectivity to these networks is provided via optical networking equipment owned and operated by UT-Battelle that runs over leased fiber-optic cable. This equipment has the capability of simultaneously carrying either 192 10-GB/s circuits or 96 40-GB/s circuits and connects the OLCF to major networking hubs in Atlanta and Chicago. Currently, 16 of the 10 GB circuits are committed to various purposes, allowing for virtually unlimited expansion of the networking capability. The connections into ORNL provide access to research and education networks such as ESnet, TeraGrid, Internet2, and Cheetah at 10 GB/s; Science Data Net at 20 GB/s; and National LambdaRail at 40 GB/s. ORNL operates the Cheetah research network for NSF. To meet the increasingly demanding needs of data transfers between major facilities, ORNL is participating in the Advanced Networking Initiative that provides a native 100 GB optical network in a loop which includes ORNL, Argonne National Laboratory, Lawrence Berkeley National Laboratory, and other facilities in the northeast.



ORNL network connectivity to university, national laboratory, and industry partners.

Students in the Research Alliance in Math and Science program experience the EVEREST power wall.

The local-area network is a common physical infrastructure that supports separate logical networks, each with varying levels of security and performance. Each of these networks is protected from the outside world and from each other with access control lists and network intrusion detection. Line rate connectivity is provided between the networks and to the outside world via redundant paths and switching fabrics. A tiered security structure is designed into the network to mitigate many attacks and to contain others.

Visualization and Collaboration. ORNL has state-of-the-art visualization facilities that can be used on site or accessed remotely.

ORNL's **E**xploratory **V**isualization **E**nvironment for **RE**search in **S**cience and **T**echnology (EVEREST) is a 30-ft wide by 8-ft high power wall for data exploration and analysis. The facility has a 600 ft^2 projection area and a 1000 ft^2 viewing area known as the EVEREST lab, a venue that serves both as a visualization center and a place for scientists to meet, hold discussions, and present their work. The ORNL visualization team has developed a suite of middleware software tools that offers an intuitive interface with which to operate the power wall and manage multimedia content. Twenty-seven projections are seamlessly edge-matched for an aggregate resolution of 11,520 by 3,072 pixels. This projection environment is driven by an 18-node cluster named Everest. Each node in the Everest cluster contains four dual-core AMD Opteron processors, 4GB of memory, dual NVIDIA GeForce 8800GTX graphics cards, and an Infiniband network. A dedicated Lustre file system provides high bandwidth data delivery to the EVEREST power wall. ORNL also provides Lens, a 77-“fat node” cluster dedicated to data analysis and visualization. 45 nodes of Lens contain 16 AMD cores, 128 GB of memory and an Infiniband network. The remaining 32 nodes of Lens contain 16 AMD cores, 64 GB of memory, Infiniband network, and two graphics cards, an NVIDIA 8800 GTX and a 4GB NVIDIA Tesla C1060. The Lens cluster is a resource of the OLCF and performs a variety of visualization-related functions, including computation, analysis, and rendering, including support for remote visualization for off-site customers. The Lens cluster has been demonstrated with a variety of commercial off-the-shelf software and open-source visualization tools including VisIt, Paraview, CEI Ensight, and AVS-Express. The Everest cluster rendering environment utilizes Chromium and Distributed Multi-Head X (DMX) for tiled, parallel rendering. The Lens cluster cross mounts the Center-wide Lustre file system to allow “zero copy” access to simulation data from other OLCF computational resources.

OLCF tape archive.

High Performance Storage and Archival Systems. To meet the needs of ORNL’s diverse computational platforms, a shared parallel file system capable of meeting the performance and scalability requirements of these platforms has been successfully deployed. This shared file system, based on Lustre, Data Direct Networks (DDN), and InfiniBand technologies, is known as Spider and provides centralized access to petascale datasets from all major on-site computational platforms. Delivering more than 240 GB/s of aggregate performance, scalability to more than 26,000 file system clients, and more than 10-petabyte (PB) storage capacity, Spider is the world’s largest scale Lustre file system. Spider consists of 48 DDN 9900 storage arrays managing 13,440 1-TB SATA drives; 192 Dell dual-socket, quad-core I/O servers providing more than 14 TF in performance; and more than 3 TB of system memory. Metadata are stored on 2 LSI Engino 7900s (XBB2) and are served by three Dell quad-socket, quad-core systems. ORNL systems are interconnected to Spider via an InfiniBand system area network which consists of four 288-port Cisco 7024D IB switches and more than 3 miles of optical cables. Archival data are stored on the center’s High Performance Storage System (HPSS), developed and operated by ORNL. HPSS is capable of archiving hundreds of petabytes of data and can be accessed by all major leadership computing platforms. Incoming data are written to disk and later migrated to tape for long term archiving. This hierarchical infrastructure provides high-performance data transfers while leveraging cost effective tape technologies. Robotic tape libraries provide tape storage. The center has three SL8500 tape libraries holding up to 10,000 cartridges each and is deploying a fourth SL8500 in 2011. The libraries house a total of 24 T10K-A tape drives (500 GB cartridges, uncompressed) and 32 T-10K-B tape drives (1 terabyte cartridges, uncompressed). Each drive has a bandwidth of 120 MB/s. ORNL’s HPSS disk storage is provided by DDN storage arrays with nearly a petabyte of capacity and over 12 GB/s of bandwidth. This infrastructure has allowed the archival system to scale to meet increasingly demanding capacity and bandwidth requirements with more than 21 PB of data stored as of November 2011.

C.2 Emory University

The Department of Mathematics and Computer Science at Emory University maintains appropriate computing facilities for our research needs. These include a shared memory, multi-processor system suited for multi-threaded, CPU-intensive programs. The current hardware is a Sun Microsystems SunFire V40z, with 4 Dual Core AMD Opteron(tm) Processors and 32 GB of memory running Linux.

The department also maintains a second shared memory, multi-processor system suited for multi-threaded, CPU intensive programs. The current hardware is a Sun Microsystems SunFire V880, with 8 CPUs and 16 GB of memory running Solaris.

Additionally, the department maintains *Puma*, a high performance cluster with 32 nodes and 128 processor cores. Each node has two dual core AMD 2214 2.2 GHz Opteron CPUs, 4 GB RAM and an 80 GB drive. The nodes are connected via a High Performance InfiniBand network and also Gigabit Ethernet. The nodes are running Linux CentOS.

The department also maintains a parallel computing cluster with 32 CPUs and 16 GB of memory split across 16 identical systems. All nodes use RedHat Linux/Intel for their operating system. Nodes are interconnected with switched, 100 Mb ethernet. Two build environments are available for MPI programs. One uses the GNU compiler suite [gcc/g++/g77]; the other uses the Portland Group (PGI) compiler suite.

The department also utilizes workstations from the teaching lab to form a compute grid for off-hour and weekend use. The pool of nodes normally includes 32 identical systems each with 2 SPARC CPUs; by arrangement, 16 additional systems could be recruited to bring the total CPU count up to 96.

Emory researchers have also access to a 256 dual-core, dual-socket AMD Opteron-based compute cluster, with a total of 1024 CPUs. Each node uses AMD 2218 processors and has 8 GB DDR2 RAM per node (or 2 GB per core), 250 GB SATA drive local storage per node with Gigabit Ethernet interconnect. The total global storage (parallel file system) is 8 TB.

Further resources for Emory researchers are available at the Emerson Center for Scientific Computation.