

SciDAC Scientific Computation Application Partnerships Update

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Strategic ASCR – SC Program Partnerships

Goals and Objectives

Partner with SC Programs to combine domain science expertise with the best applied mathematics and computer science in order to enable advances in program missions of strategic importance

Criteria for successful Partnerships

- 1. Exploit leadership class computing resources to advance scientific frontiers in an area of strategic importance to the Office of Science
- 2. Effectively link to the intellectual resources in applied mathematics and computer science, expertise in algorithms and methods, and scientific software tools at one, or more, SciDAC Institutes
- "Reviewers...will be asked to comment upon the feasibility, benefits, and management of the proposed collaborations between the [domain scientists] supported by [the SC Program] on the one hand, and the computational scientists (i.e., applied mathematicians and computer scientists/engineers) supported by ASCR on the other."



Partnership in Fusion Energy Science

FOA/ LAB	Partner Program	Partner PM	ASCR PM		Max. (\$1,000)	Projects	Duration (Years)
11-571	FES	John Mandrekas	RL	Fusion Plasma Science	\$33,000	1-4	5

- Plasma Edge Physics: highly-scalable simulation codes able to exploit LCF (+NERSC) to address the multi-physics and multi-scale challenges associated with the plasma edge region
- Multiscale Integrated Modeling: integrated simulation codes focused on the prediction, control, and mitigation of instabilities
- Materials Science: predict the properties, behavior, response, and lifetimes of near-surface and bulk materials in the challenging fusion environment (14MeV neutrons, etc.)

Partnership in High Energy Physics

FOA/ LAB	Partner Program	Partner PM	ASCR PM	Topics	Max. (\$1,000)	Projects	Duration (Years)
11-580	НЕР	Lali Chatterjee	RL	High Energy Physics	\$12,000		3

- Cosmic Frontier Simulations: The search for dark matter with N-body simulations of the cosmos
- Lattice Gauge Theory Research: high-energy QCD and "Beyond the Standard Model"
- Accelerator Science Modeling and Simulation

Partnership in Nuclear Physics

FOA/ LAB	Partner Program	Partner PM	ASCR PM		Max. (\$1,000)	Projects	Duration (Years)
11-581	NP	Ted Barnes	RL	Nuclear Physics	\$20,000	1-4	5

Low-Energy

Predict properties of nuclei

Spectroscopy

Extract nuclear forces from QCD

Decay rates and products

Support FRIB & ATLAS experiments

• Medium-Energy

Predict properties of hadrons

Supply parameters for low-energy nuclear properties

Support experiments at JLAB

Heavy-Ion Collisions

Predict quark-gluon plasma properties & QCD EOS

Support experiments at RHIC & LHC



Partnership in Earth System Science

FOA/ LAB	Partner Program	Partner PM	ASCR PM		Max. (\$1,000)	Projects	Duration (Years)
11-588	BER	Dorothy Koch	RL	Earth System	\$32,500	2-5	5

- Develop physics and dynamics for atmosphere, ocean or ice sheets to run efficiently and accurately using high resolution or unstructured grids
- Develop efficient and accurate schemes for simulating atmospheric or oceanic chemical or biogeochemical tracers
- Develop and apply methods to validate and to characterize uncertainty in climate simulations



Partnership in Materials and Chemical Sciences

FOA/ LAB		Partner PM	ASCR PM	_	Max. (\$1,000)	Projects	Duration (Years)
11-593	BES	Jim Davenport, Mark Pederson	CS	Chemistry, Materials	\$30,000	5-12	5

- Development of first-principles treatments of excited states and excited states processes
- Electron correlation in finite and extended systems
- Other priority research directions:
 - solar energy
 - chemical reactions
 - magnetism & superconductivity
 - materials in extreme environments
 - separations
 - energy storage



Five SciDAC Joint FOAs published

August 3 – September 22, 2011

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11-571	FES	John Mandrekas	RL	Fusion Plasma Science	\$33,000	1-4	5
11-580	HEP	Lali Chatterjee	RL	High Energy Physics	\$12,000		3
11-581	NP	Ted Barnes	RL	Nuclear Physics	\$20,000	1-4	5
11-588	BER	Dorothy Koch	RL	Earth System	\$32,500	2-5	5
11-593	BES	Jim Davenport, Mark Pedersor	(3	Chemistry, Materials	\$30,000	5-12	5

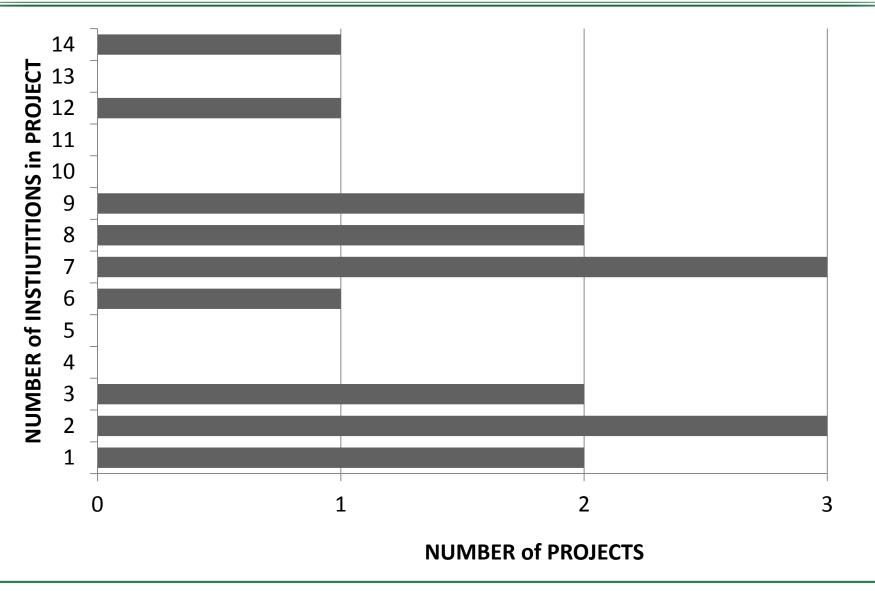
Topics	pre-proposals	proposals	reviewers	recommended w/ASCR support
Fusion Plasma Science	16			
High Energy Physics				
Nuclear Physics	10			
Earth System	11			
Chemistry, Materials	89			
Total	126			

Topics	pre-proposals	proposals	reviewers	recommended w/ASCR support
Fusion Plasma Science	16	15		
High Energy Physics		7		
Nuclear Physics	10	9		
Earth System	11	6		
Chemistry, Materials	89	28		
Total	126	65		

Topics	pre-proposals	proposals	reviewers	recommended w/ASCR support
Fusion Plasma Science	16	15	26	
High Energy Physics		7	27	
Nuclear Physics	10	9	28	
Earth System	11	6	11	
Chemistry, Materials	89	28	42	
Total	126	65	134	

Topics	pre-proposals	proposals	reviewers	recommended w/ASCR support
Fusion Plasma Science	16	15	26	2
High Energy Physics		7	27	3
Nuclear Physics	10	9	28	3
Earth System	11	6	11	3
Chemistry, Materials	89	28	42	6
Total	126	65	134	17

Most Partnership projects involve many institutions





SciDAC Partnerships engage with SciDAC Institutes

Topics	Projects	FASTMath	SUPER	QUEST	SDAV*
Fusion Plasma Science	2	2	2	2	1
High Energy Physics	3	3	1	2	1
Nuclear Physics	3	2	3	1	
Earth Systems	3	3	3	2	
Chemistry, Materials	6	6	3		
Total	17	16	12	7	2

*SDAV started about nine months after other Institutes



SciDAC Partnerships connect ASCR resources to science

- Projects target strategic needs of SC Program partners Began new topics with Partners or restructured topics supported in past SciDAC projects
- 3/5 of ASCR-funded effort for Institute personnel QUEST engaged with Earth Systems and Physics projects SDAV engaged with two projects even though it had been announced after most proposals were due

FASTMath & SUPER engaged all topics and most projects

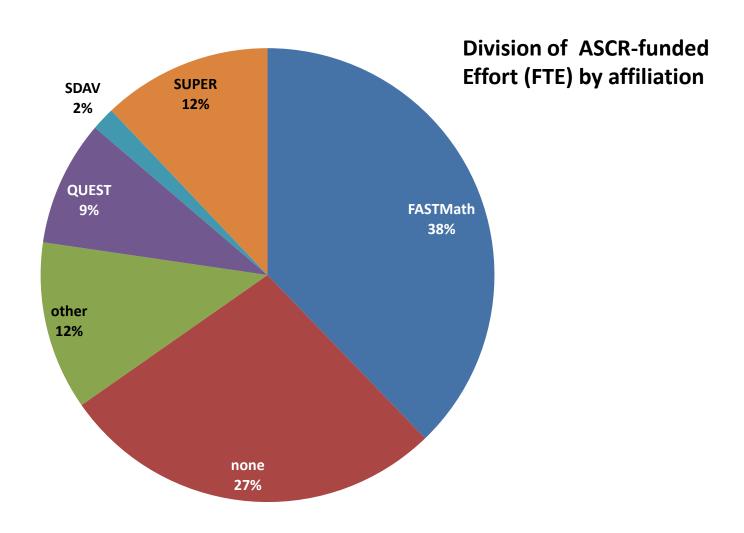
Remainder split between capabilities outside of Institutes or coordination between Partnerships and Institutes

ASCR supports more than 80 named faculty or staff in 25 institutions in multi-disciplinary collaborations with domain scientists

backups



SciDAC Partnerships engage with SciDAC Institutes





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