

中間評価に関する質問への回答（文部科学省）

質問 2) スケジュールについて

- 2 - 1) 資料 7 のスケジュールで、開発計画は富士通（スカラ部）しか記載されていない。ベクトル部は 2011 年 3 月および 2012 年 3 月にどのような性能を出すか。

ベクトル部については、2011 年 3 月時点で 1 PF、2012 年 3 月時点で 3 PF の性能を達成する計画となっている。

- 2 - 2) 資料 7 で、DOE の Sequoia の 20PF 達成が、2012 年 7 月付近に記載されているが、報道発表資料等によると、2011 年 4Q に完成するとの意見もある。2012 年 7 月付近と判断した根拠資料は何か。

- 1 .Sequoia の 20PF 達成時期については、平成 2 0 年 8 月の提案依頼書(Request for Proposal)提出時には、「Sequoia with a mandatory 20-petaFLOPS peak with target delivery in 2011 2012」とされていた。(出典 1)
- 2 .その後、平成 2 1 年 2 月 3 日付けのエネルギー省プレスリリースにおいて、「be delivered starting in 2011 and deployed in 2012」(出典 2)との表現になったことを受け、システム設置完了から演算可能となるおおよその期間(約 2 ヶ月)を考慮して、資料 7 については、Sequoia の 20PF の達成時期予測期間を 2012 年 2 月付近からとしたもの。

(出典 1)「ASCeNEWS (平成 2 0 年 9 月号)」(米国サンディア国立研究所(エネルギー省所管)の HP に掲載)(<http://www.sandia.gov/nnsa/asc/enews/0908/0908.html>)

The ASC Sequoia Supercomputer Request for Proposals (RFP) was approved for release by DOE/NNSA in July, and proposals were submitted by industry on August 21, 2008. The contract award should be announced by the end of the year. The RFP specified two machines: Sequoia with a mandatory 20-petaFLOPS peak with target delivery in 2011 2012 and Dawn with a mandatory peak of 0.5 petaFLOPS peak with target delivery in 2009. Bidders were required to run a series of benchmarks and include the results as part of their proposals and make projections of the performance of these benchmarks on the Dawn and Sequoia platforms.

(出典 2)米国エネルギー省プレスリリース(平成 2 1 年 2 月 3 日付)

IBM will deliver two systems: Sequoia, a 20 petaflop (quadrillion floating operations per second) system based on future BlueGene technology, to be delivered starting in 2011 and deployed in 2012;



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The New Fiscal Year Cometh...



Editorial by Bob Meisner

For the past two years our budget has been determined by continuing resolution and it seems that we are facing that situation at least for the immediate future. There will be a continuing resolution up to the election and beyond and we are waiting to find out if the level of funding will be at 2008 levels or at the lower of the House and Senate marks. With a \$66M difference between the marks, that decision will have a substantial impact on how we will be able to proceed.

[Complete story...](#)

Third Annual Modeling and Simulation Expo Held on Capitol Hill

On Tuesday July 15, 2008, the ASC Division exhibited for the second time in the third annual Modeling and Simulation (M&S) Expo sponsored by the National Training and Simulation Association (NTSA) and the Congressional M&S Caucus, co-chaired by Congressman J. Randy Forbes and Congressman Solomon P. Ortiz.

[Complete story...](#)

Earthquake Simulations Broaden Scientific Understanding

Using the ASC BlueGene/L supercomputer, Lawrence Livermore's modern simulation tool, Wave Propagation Program (WPP), helps seismologists and earthquake engineers understand the ground motion hazard posed by earthquakes and other seismic events. The code computes ground motions for any seismic event in the San Francisco Bay Area region using a 3D geology/seismic wave-speed model of the area provided by the U.S. Geological Survey. Moderate earthquakes, such as the magnitude 5.6 quake that rocked the Calaveras Fault near the town of Alum Rock (east of San Jose) on October 30, 2007, can be used to validate earthquake simulations by testing the 3D model and allowing scientists to constrain uncertainties for large, less frequent earthquakes.

[Complete story...](#)

Multi-Agency Workshop Addresses Issues Facing Network

Technologies

The Institute for Advanced Architectures and Algorithms (IAA), which is jointly operated by Sandia National Laboratories (SNL) and Oak Ridge National Laboratory (ORNL), hosted a highly successful workshop on advanced interconnection network technologies in San Jose, California on July 21 and 22. The workshop was organized by Scott Hemmert from Sandia and Jeff Vetter from Oak Ridge National Laboratory and sought to characterize the challenges facing interconnect technologies, looking toward building exascale supercomputers within the next decade.

[Complete story...](#)

Project Provides Thirteen Years of Industry-Shaping Deliverables

Over the past 13 years, the ASC File Systems and I/O project has provided products used by the ASC program directly, leveraged and shaped the HPC industry, and built and shaped the HPC file systems and I/O community.

The (former) ASCI Path Forward Program had two projects that were particularly noteworthy. The first Path Forward Global Parallel File System project was instrumental in guiding the design of the Panasas® File System, one of the most popular global parallel file systems in industry and used in production at Los Alamos. The second project was the guiding force behind the Lustre® file system, also a top parallel file system industry competitor and in use at Sandia and Lawrence Livermore national laboratories.

[Complete story...](#)

ASC's Roadrunner Supercomputer Energy Efficient



In addition to breaking the petaFLOPS record, the Roadrunner supercomputer located in Los Alamos is #3 on the June 2008 Green500 list (<http://www.green500.org/lists/2008/06/green500.php>).

To illustrate the dramatic improvements in power efficiency, the first vector supercomputer installed at Los Alamos in 1976 needed 115 kW to deliver about 100 megaFLOPS on highly optimized matrix operations hand-coded in assembly language. To match Roadrunner's performance, ten million such machines would require 1,150,000 megaWatts of power — more than the entire electricity-generating capacity of the United States.

[Complete story...](#)

Red Storm Supercomputer Upgraded to 284 teraFLOPS

Located at Sandia, Red Storm is undergoing its second large-scale upgrade in four years of active duty. Sixty-five of the 135 compute cabinets are being upgraded from dual-core to quad-core Opteron processors by swapping dual-core modules for newer, quad-core boards. Processing power will increase from a theoretical maximum of 124 teraFLOPS to 284 teraFLOPS across 38,400 cores (12,960 nodes). To hold the computational results, roughly 1.5 petabytes of disk space are being deployed. A corresponding memory upgrade will provide 2 gigabytes of memory per core across the entire machine.

[Complete story...](#)

Maximizing Use of the ASC's Purple Supercomputer

In the fall of 2005, the ASC Program appointed a team to formulate a governance model for allocating resources and scheduling the stockpile stewardship workload on ASC capability systems.

Since October 2006, the ASC Purple capability system at Lawrence Livermore has successfully run as a national user facility using this model. The two primary objectives of the model are to ensure the capability system resources are allocated on a priority-driven basis according to program requirements and to use ASC capability systems for the large capability jobs for which they were designed and procured.

[Complete story...](#)

Collaborative Campaign Funding Aids Researchers to Develop New Modeling Capabilities

Researchers in Sandia's ASC Verification and Validation Program, leveraging funding from NW Campaign 6 experiments, have developed new failure modeling capabilities within Sandia's SIERRA Mechanics software framework. This new capability permits quasistatic and dynamic modeling of complex failure modes in composite materials, which are used in many weapon and non-weapon applications. This study employed Sandia's DAKOTA software toolkit to generate over 800 SIERRA simulations, which were used to optimize parameters in the composite material failure models to match experimental test data, and, to perform sensitivity studies that identified the most critical parameters out of SIERRA's 37-parameter material failure model.

[Complete story...](#)

Sandia System Software Researchers Receive SC08 Best Paper Nomination

A paper authored by Sandians Kurt Ferreira and Ron Brightwell together with Patrick Bridges from the University of New Mexico has been nominated for the Best Paper and Best Student Paper awards at the upcoming SC08 conference in Austin, Texas <http://www.sc08.supercomputing.org/>

The paper was one of four such papers selected from a total of 59 accepted papers. The paper entitled "Characterizing Application Sensitivity to OS Interference using Kernel-Level Noise Injection" is a detailed study performed on the ASC Red Storm machine of how operating system activity can impact the performance of parallel applications on very large-scale machines. The paper describes how the Catamount lightweight compute node operating system was extended to allow for creating various kinds of artificial noise to provide more insight into the important characteristics of applications and operating systems that influence performance and scalability.

Roadrunner Technical Seminar Videos Now Streaming on Web

Now available to the high-performance computing community are Roadrunner technical seminars presented by Computer, Computational, and Statistical Sciences (CCS) Division staff at Los Alamos National Laboratory.

These presentations about the first multi-core petaFLOPS speed computer, Roadrunner, were given March–June 2008 at Los Alamos. Using Flash Media Server, the hour-long sessions can now be seen in their entirety, including question and answer sessions, and can be used as tutorials as the adoption of similar systems increases. Visit the website at <http://www.lanl.gov/roadrunner/rseminars.shtml>.

Sequoia Request for Proposals Approved, Proposals Accepted



The ASC Sequoia Supercomputer Request for Proposals (RFP) was approved for release by DOE/NNSA in July, and proposals were submitted by industry on August 21, 2008. The contract award should be announced by the end of the year. The RFP specified two machines: Sequoia with a mandatory 20-petaFLOPS peak with target delivery in 2011–2012 and Dawn with a mandatory peak of 0.5 petaFLOPS peak with target delivery in 2009. Bidders were required to run a

series of benchmarks and include the results as part of their proposals and make projections of the performance of these benchmarks on the Dawn and Sequoia platforms.

"Designing scalable benchmarks is hard, but estimating the performance of a machine that is 20-50x faster than BlueGene/L and has not yet been designed poses even greater challenges," said Mark Seager, assistant department head of advanced technologies.

Roadrunner Supercomputer Installed at Los Alamos

The first Roadrunner Phase 3 Connected Unit (CU) was delivered to Los Alamos on July 15, 2008. Shortly after delivery, IBM successfully kicked off a Linpack burn-in run on the first CU in the Metropolis Center for Modeling and Simulation.

[Complete story...](#)

Roadrunner Phase 3 System Stabilization Proposals Selected

Proposals have been selected in a competitive process to help with the Roadrunner Phase 3 system stabilization efforts once the machine is accepted at Los Alamos National Laboratory.

To advance science and programming knowledge, LANL has selected open-science and weapons-science projects.

[Complete story...](#)

ASC Salutes Matthew L. Leininger



As a deputy for Advanced Technology Projects within the ASC Program at Lawrence Livermore National Laboratory, Matt Leininger works at the center of advances in supercomputing that are enabling predictive scientific simulations.

"It's exciting to see the direct impact advanced supercomputing architectures and predictive models are having on both scientific discovery and real-world problems such as stockpile stewardship," said Matt.

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NEWS

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NNSA awards IBM Contract to Build Next Generation Supercomputer

WASHINGTON, D.C. - The Department of Energy's National Nuclear Security Administration (NNSA) announced today a contract with IBM to bring world-leading supercomputing systems to its Lawrence Livermore National Laboratory to help continue to ensure the safety and reliability of the nation's aging nuclear deterrent.

"The longstanding partnership of NNSA, Lawrence Livermore National Laboratory, and IBM is ushering in an era of multi-petaflops computing," said NNSA Administrator Thomas D'Agostino. "These powerful machines will provide NNSA with the capabilities needed to resolve time-urgent and complex scientific problems, ensuring the viability of the nation's nuclear deterrent into the future. This endeavor will also help maintain U.S. leadership in high performance computing and promote scientific discovery."

IBM will deliver two systems: Sequoia, a 20 petaflop (quadrillion floating operations per second) system based on future BlueGene technology, to be delivered starting in 2011 and deployed in 2012; and an initial delivery system called Dawn, a 500 teraflop (trillion floating operations per second) BlueGene/P system, scheduled for delivery in the first quarter of 2009. Dawn will lay the applications foundation for multi-petaflops computing on Sequoia.

With a speed of 20 petaflops Sequoia is expected to be the most powerful supercomputer in the world and will be approximately over 10 times faster than today's most powerful system. To put this into perspective, if each of the 6.7 billion people on earth had a hand calculator and worked together on a calculation 24 hours per day, 365 days a year, it would take 320 years to do what Sequoia will do in one hour.

Sequoia and Dawn will serve NNSA's tri-lab Advanced Simulation and Computing (ASC) program, which unites the scientific computing resources and expertise of Los Alamos, Sandia and Lawrence Livermore National Laboratories. The Sequoia systems will be focused on strengthening the foundations of predictive simulation through running very large suites of complex simulations called uncertainty quantification (UQ) studies. In addition, the machines will be used for weapons' science calculations necessary to build more accurate physical models. This work is a cornerstone of NNSA's Stockpile Stewardship program to ensure the safety, security and reliability of the U.S. nuclear weapons stockpile today and into the future without underground testing.

Sequoia will have 1.6 petabytes of memory, 96 racks, 98,304 compute nodes, and 1.6 million cores. Though orders of magnitude more powerful than such predecessor systems as ASC Purple and BlueGene/L, Sequoia will be 160 times more power efficient than Purple and 17 times more than BlueGene/L.

Established by Congress in 2000, NNSA is a semi-autonomous agency within the U.S. Department of Energy responsible for enhancing national security through the military application of nuclear science in the nation's national security enterprise. NNSA maintains and enhances the safety, security, reliability, and performance of the U.S. nuclear weapons stockpile without nuclear testing; reduces the global danger from weapons of mass destruction; provides the U.S. Navy with safe and effective nuclear propulsion; and responds to nuclear and radiological emergencies in the U.S. and abroad.

質問 8) グランドチャレンジ・アプリケーションについて

プロジェクト終了時に大きな成果となるグランドチャレンジ・アプリケーションを明確化し、その目的、計算性能、科学技術的意義を示してください。(これまで、評価が行われる毎に、グランドチャレンジ・アプリケーションが異なっているため、何がコミットする成果かが明確化されてない)

1. 次世代ナノ統合シミュレーション

1 - 1. 目的及び科学的意義

ペタスケールのシミュレーション技術により、ナノスケールの領域で初めて発現する特有の現象・特性を解明し、予測することのできる計算科学理論・方法論を確立することで、ナノテクノロジー・材料分野はもとより、ライフサイエンス分野やエネルギー分野等との融合領域において、飛躍知の発見・発明にとどまらず、産業力の強化に繋げることを目的とする。

各小分野の目的及び科学的意義については以下のとおり。

- (1) 次世代ナノ情報機能・材料
ナノ物質内の電子制御をシミュレートできる方法論を確立する。
- (2) 次世代ナノ生体物質
ナノスケールの生体物質に対して、自由エネルギーレベルでの相互作用、自己組織化、また動的な振るまいを、シミュレートできる方法論を確立する。
- (3) 次世代エネルギー
高効率の触媒・酵素の設計ができる方法論を確立する。

また、次世代ナノ統合シミュレーションの中核となる「中核アプリケーション」を 6 本定めて重点的に開発するとともに、中核アプリケーションに連動する「付加ソフトウェア」を開発している。(計算性能については、資料 3 参照)

なお、研究開発課題の明確化については、チャレンジングでシンボリックなテーマを提示するとともに、研究会等を通して、実験研究者、企業研究者との連携を強化し、ナノサイエンス分野の今日的な課題(緊急課題)にも取り組むこととしている。

【シンボリックなテーマ】

高速、高機能、省エネルギー電子デバイスの開発へ

複合的ナノ電子デバイスシミュレーション

感染症の克服に向けて

ウィルス全原子シミュレーション

セルロースからバイオマスエタノール生成へ

酵素反応のまるごと解析

2. 次世代生命体統合シミュレーション

2 - 1 . 目的及び科学的意義

基礎方程式に基づく解析的アプローチと大量の実験データから未知の経路と法則に迫る実験的アプローチにより、異なるスケールの研究とデータ解析を統合的かつ有機的に進め、ペタスケールという桁違いの性能を持つスーパーコンピュータの性能をフルに発揮し、生体で起こる種々の現象を理解し医療に結びつけるためのソフトウェアを開発する。ライフサイエンス分野に仮説 - 検証型アプローチに基づく新たな研究手法を提供し、生命プログラムの理解・再現・予測を実現するとともに、創薬・ヘルスサイエンスへの貢献、新規医療技術を実用化する。

各スケールの目的及び科学的意義については以下のとおり。また、計算性能については、平成 21 年度に生命体基盤ソフトウェア開発・高度化チームが、優先的に高速化に取り組んでいるソフトウェア(分子動力学計算、量子化学計算、構造流体連成)について実行性能等の評価を実施する計画。

() 分子スケール

数万原子レベルで、ミリ秒オーダーの分子シミュレーションを目指す。これにより、薬剤設計の基盤となる計算科学的手法の構築につなげる。

() 細胞スケール

ペタフロップス級の計算力を活かして細胞を 10 万のボクセルに区画し、そこに包括的な実証データを組み込んだシミュレーションの実現を目指す。これにより、薬剤等の作用や副作用の予測を行うシミュレーションの開発につなげる。

() 臓器全身スケール

ペタフロップス級の計算量を用いて、数時間で実行可能な臓器全身シミュレーションの構築を目指す。これにより、病態予測や治療予測等の医療支援ツールの開発につなげる。

() データ解析融合

ペタフロップス級の計算によって、創薬ターゲット探索や個人差を考慮した医療のための基盤情報技術の構築を目指す。これにより、ヒト全遺伝子(現行、全遺伝子の数%レベル)を対象とした創薬ターゲット遺伝子探索の実現につなげる

() 生命体基盤ソフトウェア開発・高度化

プロジェクトで開発される各種ソフトウェアの高性能化、特に次世代スーパーコンピュータ向けの最適化を行い、次世代スーパーコンピュータの生命科学への応用を促進すると同時にグランドチャレンジを実現する。

() 脳・神経系

神経細胞の発達・可塑(学習) 神経細胞集団の活動、昆虫の嗅覚系やほ乳類の視覚系の活動など、単一神経細胞から脳全体にわたるシミュレーションを行うことで、脳神経系の機能の解明、さらには発達・学習障害など機能障害の機序の理解につなげる。

研究開発課題の明確化については、 長期的目標として、サイエンスとしてのインパクトと、スケールを超えた生命現象の統合的理解を目指すこととし、 短期的目標として、次世代スパコンの性能を最大限に利活用すること及びライフサイエンス分野への貢献度を考慮した、ライフサイエンスの各分野の取組を進めることとしており、長期と短期のそれぞれの目標にむけて研究開発課題の明確化を図った。