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Status of Release of the Uintah Computational Framework

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Abstract:

This report provides a summary of the status of the Uintah Computation Framework (UCF) software. Uintah is uniquely equipped to tackle large-scale multi-physics science and engineering problems on disparate length and time scales. The Uintah framework makes it possible to run adaptive computations on modern HPC architectures with tens and now hundreds of thousands of cores with complex communication/memory hierarchies. Uintah was orignally developed in the University of Utah Center for Simulation of Accidental Fires and Explosions (C-SAFE), a DOE-funded academic alliance project and then extended to the broader NSF snd DOE science and engineering communities. As Uintah is applicable to a wide range of engineering problems that involve fluid-structure interactions with highly deformable structures it is used for a number of NSF-funded and DOE engineering projects. In this report the Uintah framework software is outlined and typical applications are illustrated. Uintah is open-source software that is available through the MIT open-source license at http://www.uintah.utah.edu/.

THE UNIVERSITY OF UTAH

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1 Summary

This report provides a summary of the status of the Uintah Computation Framework (UCF) software. Uintah is uniquely equipped to tackle large-scale multi-physics science and engineering problems on disparate length and time scales. The Uintah framework makes it possible to run adaptive computations on modern HPC architectures with tens and now hundreds of thousands of cores with complex communication/memory hierarchies. Uintah was orignally developed in the University of Utah Center for Simulation of Accidental Fires and Explosions (C-SAFE), a DOE-funded academic alliance project and then extended to the broader NSF snd DOE science and engineering communities. As Uintah is applicable to a wide range of engineering problems that involve fluid-structure interactions with highly deformable structures it is used for a number of NSF-funded and DOE engineering projects. In this report the Uintah framework software is outlined and typical applications are illustrated. Uintah is open-source software that is available through the MIT open-source license at `http://www.uintah.utah.edu/`.

2 Introduction to Uintah

The Uintah Computational Framework as distributed to the broader NSF science and engineering community is a general-purpose tool for computational mechanics and fluid dynamics, and has particular strengths in large deformations, fire simulation, and fluid-structure interaction problems. Uintah was originally developed under the University of Utah Center for Simulation of Accidental Fires and Explosions (C-SAFE), a DOE-funded academic alliance project [35], from 1997 until 2007. Since 2007, the development of Uintah has been funded through a number of NSF and DOE grants. For example NSF award OCI-0721659 *SDCI HPC Improvement and Release of the Uintah Computational Framework* from 2007 until 2011 was directly focused on delivering software and resulted in the first formal release of Uintah in 2009 and subsequent releases.

The motivation behind software such as Uintah is that large scale multi-physics computational simulations often provide insight into complex problems that complements existing experiments and defines future physical and computational experiments [59]. Uintah is designed to solve reacting fluid-structure problems involving large deformations and fragmentation on a structured Adaptive Mesh Refinement (AMR) mesh. The underlying methods inside Uintah are a novel combination of fluid-flow methods and material point (particle) methods.

2.1 Fluid-Structure Interaction Methodology

Uintah contains three main simulation algorithms: 1) the ARCHES incompressible fire simulation code, 2) the ICE [42] (in)compressible method with both explicit and implicit versions, and 3) the particle-based Material Point Method (MPM) for structural modeling. In addition these components may be combined, most notably in MPMICE which is Uintah's fluid-structure interaction component. In addition to these primary algorithms, Uintah integrates numerous sub-components including equations of state, constitutive models, reaction models, radiation models and so forth. Here we briefly describe our approach to *full physics* simulations of fluid-structure interactions involving large deformations and phase change. The term *full physics* refers to problems involving strong coupling between the fluid and solid phases with a full Navier-Stokes representation of fluid phase materials and the transient, nonlinear response of solid phase materials which may include chemical or phase transformation between the solid and fluid phases.

The methodology upon which the Uintah approach is built uses a full *multi-material* approach in which each material is given a continuum description and is defined over the complete computational domain. Although at any point in space the material composition is uniquely defined, the multi-material approach adopts a statistical viewpoint whereby the material (either fluid or solid) resides with some finite probability. To determine the probability of finding a particular material at a specified point in space, together with its current state (i.e., mass, momentum, energy), multi-material equations are used. The algorithm that uses a common framework to treat the coupled response of a collection of arbitrary materials is described below. This follows the ideas previously presented by Kashiwa and colleagues [42, 43, 44, 45]. Individual equations of state are needed for each material to determine relationships between pressure, density, temperature and internal energy. Constitutive models are also required to describe the stress for each material based on appropriate input parameters (deformation, strain rate, history variables, etc.). In addition to those parameters, the multi-material nature of the equations also requires closure for the volume fraction of each material.

2.2 The ICE Multi-material CFD Approach

The basis of the multi-material CFD formulation used here is the ICE (Implicit, Continuous-fluid, Eulerian) method [33], further developed by Kashiwa and others at Los Alamos National Laboratory [46]. The use of a cell centered, finite volume approach is convenient for multi-material simulations in that a single control volume is used for all materials. This is particularly important in regions where a material volume goes to zero. By using the same control volume for mass and momentum then as the material volume goes to zero, the mass and momentum also go to zero at the same point. The technique is fully incompressible and compressible, allowing wide generality in the types of problems that can be simulated.

The Uintah implementation of the ICE technique uses operator splitting in which the solution consists of a separate Lagrangian phase where the physics of the conservation laws are computed and an Eulerian fluids phase in which the material state is transported via advection to the surrounding cells. The general solution approach is well-developed and described in [46, 30, 34, 27], with a more recent analysis and positivity preserving improvements in [79].

2.3 The Material Point Method

Uintah uses the particle method known as the Material Point Method (MPM) [73, 74] to evolve the equations of motion for the solid materials. MPM is a powerful technique for computational solid mechanics and has found favor in applications such as those involving complex geometries [31], large deformations [19] and fracture [32], to name but a few. MPM is an extension to solid mechanics of FLIP [16, 15], which is a particle-in-cell (PIC) method for fluid flow simulation [17]. Uintah also uses an implicit formulation of MPM [29]. In this formulation Lagrangian particles or material points are used to discretize the volume of a solid material. Each particle carries state information (e.g. mass, volume, velocity, and stress) about the portion of the volume that it represents. The method typically uses a cartesian grid as a computational scratchpad for computing spatial gradients. This grid may be arbitrary, and in Uintah it is the same grid used by the accompanying multi-material CFD component. The initial physical state of the solid is projected from the computational nodes to the cell centers collocating the solid material state with that of the fluid. This common reference frame is used for all physics that involve mass, momentum, or energy exchange among the materials. This results in a tight coupling between the fluid and solid phases. This coupling occurs through terms in the conservation equations, rather than explicitly through specified boundary conditions at interfaces between materials. Since a common multi-field reference frame is used for interactions among materials, typical problems with convergence and stability of solutions for separate domains communicating only through boundary conditions are alleviated. a A considerable amount of fundamental research in Utah has led to significant improvements in the method and its analysis [78, 70, 71, 72, 83, 84, 63].

2.4 The ARCHES Combustion Simulation Component

The ARCHES component was designed for the simulation of turbulent reacting flows with participating media and radiation. It is a three-dimensional, Large Eddy Simulation (LES) code developed by Prof. Smith and his research group at the University of Utah as part of C-SAFE. ARCHES uses a low-Mach number ($Ma < 0.3$), variable density formulation to simulate heat, mass, and momentum transport in reacting flows.

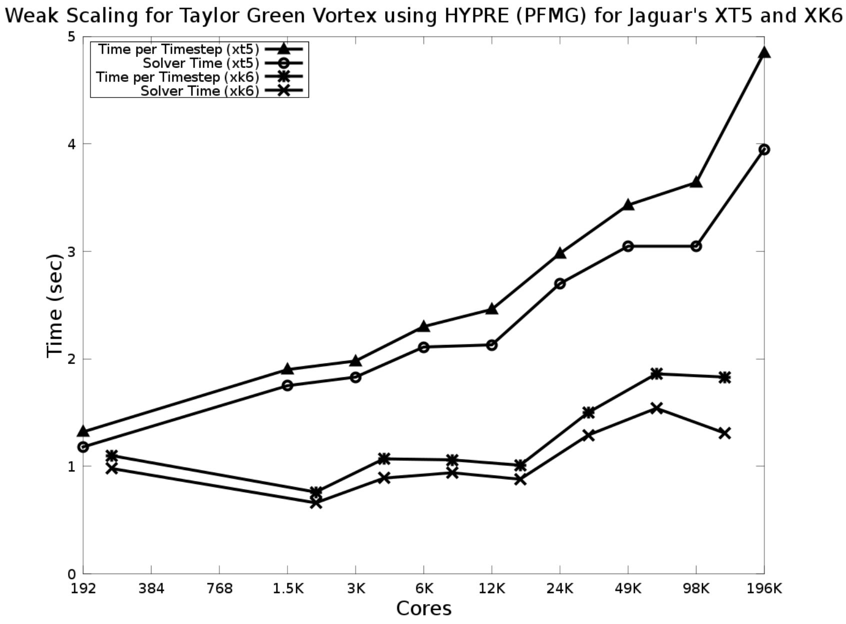

Figure 1: Weak scalability of ARCHES with hypre showing XK6 improved scalability and speedup over XT5 results

The LES algorithm solves the filtered, density-weighted, time-dependent coupled conservation equations for mass, momentum, energy, and particle moment equations in a Cartesian coordinate system [69, 50]. This set of filtered equations is discretized in space and time and solved on a staggered, finite volume mesh. The staggering scheme consists of four offset grids, one for storing scalar quantities and three for each component of the velocity vector. Stability preserving, second and third order explicit time-stepping schemes are used to advance the simulation in time. For the spatial discretization of the LES scalar equations, flux limiting schemes for the convection operator are used to ensure that scalar values remain bounded. For the momentum equation, a central differencing scheme for the convection operator is used for energy conservation. All diffusion terms are computed with a second-order approximation of the spatial gradient. Overall, ARCHES is second-order accurate in space and time. The ARCHES code is massively parallel and highly scalable through Uintah [66, 61] and also through use of third-party parallel solvers like hypre [1, 25] and PETSc, [4, 3, 5, 48]. Figure 1 shows the weak scalability of ARCHES on the standard Taylor Green Vortex test incompressible flow problem using hypre on Oak Ridge's new successor to Jaguar (XK6 nodes without GPUs) and on the original Jaguar (XT5). Not only is the new machine faster per core but the improved communications net-work results in better weak scaling (constant workload per core) than on the original Jaguar. The top graph shows the total average cpu time per timestep on Jaguar with a roughly constant load per core. The amount of time spent in the hypre solver is the next graph down. The bottom two graphs correspond to the same times on the new XK6 type nodes (without GPUs) in the Titan machine. The scalability of ARCHES depends on the scalability of the linear solver used on each timestep. Effective use of the hypre linear solver package has led to better-than-expected weak scalability on 100K+ cores. The ARCHES code apart from the hypre linear solver exhibits good weak and strong scalability through the Uintah framework. As part of the ARCHES development, substantial research has been done on radiative heat transfer using the parallel Discrete Ordinates Method and the P1 approximation to the radiative transport equation [47, 48, 49]. More recent work has been based upon the use of more efficient Reverse Monte Carlo Ray Tracing (RMCRT) methods, e.g. [55, 75, 76, 36]. The ARCHES code is currently used for broad class of industrial and industrial-strength research simulations as described below in Sections 5 and 6.

3 Uintah Parallel Scalability and Software Engineering

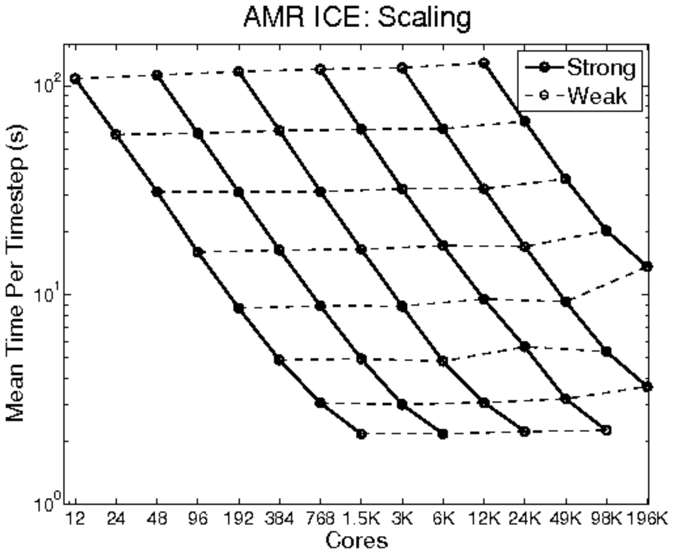

Figure 2: Strong and weak scalability up to 196,608 cores of an ICE simulation with AMR

At the conclusion of the C-SAFE project Uintah was capable of running in a scalable way on approximately 2K cores with adaptive mesh refinement. The NSF project *SDCI HPC Improvement and Release of the Uintah Computational Framework* (2008 until 2011) extended the scalability and use of Uintah, so that it was capable of running on 100K cores with mesh refinement [53, 56, 12]. This project also resulted in a web page `www.Uintah.Utah.edu` that provides access to regular releases of the software, the Uintah documentation and installation user guides [28, 64], as well as publications, images and movies. There is now also a Uintah gateway that allows easier access to NSF XSEDE machines, [65].

NSF-funded research has broadened use of the software and funded developments that made Uintah scale on large parallel architectures. The improved scalability was needed to allow Uintah to began to be used to solve a challenging PetaApps problem, [53, 12]. The first full release of Uintah was in July 2009 and the latest in December 2011, with a release planned for June 2012.

At the heart of Uintah is a sophisticated computational framework that can integrate multiple simulation components, analyze the dependencies and communication patterns between them, and efficiently execute the resulting multi-physics simulation. Uintah's visionary initial design by Parker [58] uses C++ components that follow a very simple interface to establish connections with other components in the system. Uintah uses a Directed Acyclic Graph (DAG) representation of parallel computation and communication to express data dependencies between multiple components. Each task (node) in the DAG task graph reads inputs (in-edges) and produces some output (out-edges), which are in turn the input of some future task. These inputs and outputs are specified for each patch in a structured AMR grid. Each component specifies a list of tasks to be performed and the data dependencies between them. The task graph representation has a number of advantages, including efficient fine-grained coupling of multi-physics components, flexible load balancing mechanisms and a separation of application code development from parallel code development.

The idea of the data-flow task-graph as an organizing structure for execution is well known, see [13]. Uintah's implementation supports data-flow (task-graphs) of C++ based mixed particle/grid algorithms on a structured adaptive mesh, which provides a convenient granularity for parallelism without requiring specific compiler support. The task-graph approach of Uintah also shares many features with the object-based philosophy of Charm++ [41]. Uintah uses a scheduler that sets up MPI communication for data dependencies and then executes the tasks that have been assigned to it. When the task completes, the infrastructure sends data to other tasks that require that task's output. A measurement-based load balancing component is responsible for assigning each detailed task to a core on a processor. This allows parallelism to be integrated between multiple components while maintaining overall scalability. The task-graph allows the Uintah runtime system to analyze the structure of the computation to automatically enable load-balancing, data communication, parallel I/O, and checkpoint/restart. The underlying architecture of Uintah is able to take advantage of the complex hardware topologies of modern HPC platforms so as to enable runtime analysis of communication patterns and other program characteristics. In particular Uintah is able to adapt work assignments to the underlying machine topology based on the observed performance [53]. In the next two sections we describe recent improvements to Uintah. These were funded through NSF award OCI-0721659 *SDCI HPC Improvement and Release of the Uintah Computational Framework* from 2007 until 2011.

3.1 Scalability of Adaptive Mesh Refinement (AMR)

The importance of AMR for allowing refined and coarsened meshes is now well understood in many areas of computational science. In the case of codes like Uintah which solves large systems of partial differential equations on a mesh, refining the mesh increases the accuracy of the simulation. Although Uintah's task-graph structure of the computation makes it possible to improve scalability through adaptive self-tuning, the changing nature of the task-graph from adaptive mesh refinement poses extra challenges for scalability [51, 52].

In the last 4 years, improvements within Uintah to the regridding and load balancing algorithms have led to a 40x increase in the scalability of AMR [53, 54]. Previously, Uintah used the well-known Berger-Rigoutsos algorithm [11] to perform regridding. However, at large core counts this algorithm performed poorly. The new regridder [54] defines a set of fixed-sized tiles throughout the domain. A search of each tile is then made for refinement flags without the need for communication and all tiles that contain refinement flags become patches. This regridder scales well at large core counts because cores only communicate once at the end of regridding when the patches are combined. The load balancing algorithm was also improved to more accurately predict the amount of work a patch requires by using data assimilation and measurement techniques [53]. This approach out-perform traditional cost models. While measurement based load balancing been used by others (e.g. by Charm++ [14]), this feedback mechanism appears to be novel. Through this research Uintah has been able to show strong and weak scalability up to 196,608 cores on DOE's Jaguar for ICE with AMR as seen in Figure 2. The calculation used for this scaling study was a two material compressible Navier Stokes calculation with a prescribed velocity at the inflow boundaries. There were many steps needed to achieve this scalability including using a new dynamic scheduler that now changes the task order during execution to overlap communication and computation. A significant amount of development has also been done on out-of-order execution of tasks, which has produced a significant performance benefit in lowering both the MPI wait time and the overall runtime [56, 12] on 98K cores and beyond.

3.2 Support for Heterogeneous Computing

The message passing paradigm that Uintah initially operated under was that any data that needed communicated to a neighboring core was passed via MPI. For multi-core architectures. The process of passing data that is local to a node by using MPI is both time consuming and duplicates identical data that is shared between cores. Uintah now stores only one copy of global data per multi-core node in its data warehouse. The task scheduler now spins off tasks to be executed on, say, nc cores using a threaded model, [57] which results in the global memory used in a single shared data warehouse being a fraction of nc^{-1} of what is required for multiple MPI tasks, one per each of the nc cores. This memory saving expands the scope and range of problems beyomd those that we have been to explore until now [13]. This architecture is also being extended to spin-off tasks to be executed on other types of processors, such as GPUs. A working prototype that uses as many as 1000 GPUs has recently been tested on the Titan GPU test system at Oak Ridge as well as full capability jobs being run on the Keeneland GPU system at NICS, which has multiple GPUs per node.

4 Uintah Software Engineering and Sustainability

Code development inside Uintah follows a formal structure. Each Uintah component is a C++ class that must implement several virtual methods: *problemSetup, scheduleInitialize, scheduleComputeStableTimestep*, and *scheduletimeAdvance*. Each scheduling task, i.e. *scheduleTimeAdvance*, contains a pointer to a function implementing the actual work of the task. The Uintah documentation describes each of these methods. For example, the purpose of *scheduleTimeAdvance* is to schedule the actual algorithmic implementation. For simple algorithms, there is only one task defined with a minimal set of data dependencies specified. However, for more complicated algorithms, the best way to schedule the algorithm is to break it down into individual tasks. Each task of the algorithm has its own data dependencies and function pointers that reference individual computational methods.

In order to ensure the quality of new codes and the underlying software base, Uintah has had a long history of running daily build and test scripts since the inception of the C-SAFE project in 1997. Following NSF SDCI funding and as required by the SDCI call for proposals, the NMI Build and Test System (`http://nmi.cs.wisc.edu`) was used to build Uintah on several of the common operating systems including Debian, Fedora Core, SLES, CentOS, MacOSX. In addition to the NMI build and test system, the Uintah project uses a continuous integration testing buildbot (http://buildbot.net/trac) to constantly build and regression test every source code modification checked into the Subversion repository. The Uintah testing approach ensures that Uintah builds on a variety of different OS versions and that the current code base will always compile and any regressions are immediately discovered and resolved.

The Buildbot system provides an automated compile and test cycle that is triggered each time the Uintah subversion repository is updated. After the compile checks, a suite of 100 regression tests are performed for the optimized build for the 64-bit architecture. Any failures are reported and potential problems are quickly identified and reported to the individual developer via email and to the internal developer mailing list. In addition, a publicly available web server runs recording the status of the build and tests for the individual check-in and the more comprehensive nightly tests. Finally, each night the buildbot does a comprehensive build and test for both debug and optimized builds for the 64-bit architecture. This process provides a level of confidence to developers that the Uintah code base will always be in a compilable and tested state at any given point in time.

4.1 Uintah Releases

The latest Uintah release (version 1.4.1) is available for download at `www.uintah.utah.edu` under the `Download` link. Uintah release 1.5 is scheduled for June 2012. Previous Uintah releases are as follows.

Figure 3: Geographical Distribution of Uintah Downloads.

12/14/2011 - Uintah version 1.4.1 was released.
9/26/2011 - Uintah version 1.4.0 was released.
12/06/2010 - Uintah version 1.3.1 was released.
9/28/2010 - Uintah version 1.3.0 was released.
3/9/2010 - Uintah version 1.2.0 was released.
8/21/2009 - Uintah version 1.1.0 was released.
7/1/2009 - Uintah version 1.1.0 beta was released.

The Uintah web site also contains images, movies and links to publications. In addition, the Uintah User Guide, and applications guides [28, 64] are also available on the Uintah web site, together with an installation guide which covers installation of Uintah and all supporting libraries including PETSc, hypre, MPI and VisIt.

4.2 Core Uintah Team

Although many applications groups use Uintah the core development is done from two grants.

Petascale Simulation of Sympathetic Explosions, University of Utah. NSF OCI PetaApps award OCI 0905068, $999K. PI Prof M. Berzins. One post-doc and one student are funded from this grant. The post-doc postion has been shared by Dr T. Harman and Dr J.Schmidt. The graduate student is Mr Qingyu Meng who has been instrumental in many of the scalability improvements to Uintah.

Unconventional and Renewable Energy Research Utilizing Advanced Computer Simulations DOE NETL, PI Prof. C.R. Johnson, University of Utah. Award Number: DE-EE0004449. As a co-PI my share of this is one post-doc and ome student, per year. This award presently funds Mr A. Humphries and the remainder of Dr J. Schmidt.

4.3 Uintah Downloads

Uintah has a worldwide user base with a distribution of users as is shown in Figure 3. Current Uintah downloads average about 50-100 per month, after filtering out what appear to be spurious repeated downloads. While the initial philosophy behind the website was not to log users information, we have recently started to monitor user information more carefully.

4.4 Uintah Use of TeraGrid/XSEDE Resources and DOE INCITE

From 2008 much of the large-scale algorithmic and software development and some of the science associated with Uintah has made use of Teragrid Resources. Inially this was mostly on TACCs Ranger and then increasingly and now almost all on NICS Kraken. The details of the Teragrid/XSEDE allocations are

2008-2009 5M SUs awarded
2009-2010 6.6M SUs awarded
2010-2011 7.5M SUs awarded
2011-2012 9.5M SUs awarded
2012-2013 9.5M SUs awarded

In addition in 2011 Uintah was used in a 15M SU award from DOEs INCITE program. This was for the Jaguar system. A Directors allocation of 1M SUs is being used to prepare for the next INCITE call.

5 Previously Funded Uintah Projects Completed before 2012

Uintah has been brought to bear on a number of novel and interesting physical scenarios such as stage separation in rocket motors, behavior of large-scale "agent defeat" devices, blast wave interactions with military vehicles, projectile impact in the human torso, angiogenesis and machining. Several of these new applications have gone on to secure independent funding and in each case, new capability was added to the code. A few of these projects are described in further detail below, but other complex phenomena have also been studied [31, 6, 7, 8, 9].

NSF ITR, (CTS-0218574). A Simulation Approach for Physical Systems Involving Multi-Material Interaction Dynamics. Work during this award had two major components, improvements to the numerical properties of several of the Uintah components, and enabling the use of those components across a wider range of applications. In the former category, improvements to the Material Point Method (MPM) include better time integration, a more accurate method for transferring particle data to the computational domain.

DOE, Center for Simulation of Accidental Fires and Explosions. The University of Utah Center for the Simulation of Accidental Fires and Explosions (C-SAFE) [35] was a Department of Energy ASC center that focused on providing state-of-the-art, science-based tools for the numerical simulation of accidental fires and explosions. The primary objective of C-SAFE was to provide a software system (Uintah) in which fundamental chemistry and engineering physics are fully coupled with nonlinear solvers, visualization, and experimental data verification, thereby integrating expertise from a wide variety of disciplines. Simulations using Uintah helped to better evaluate the risks and safety issues associated with fires and explosions in accidents involving both hydrocarbon and energetic materials.

The C-SAFE target scenario was the simulation of a steel container filled with a plastic-bonded explosive (PBX) subject to heating from a hydrocarbon pool fire. A jet fuel fire impinged on a steel container filled with PBX-9501, heating the container and the PBX. Once the temperature of the PBX reached a threshold, it ignited in an exothermic solid→gas reaction. The products of this reaction pressurized the container, causing it to bulge and eventually rupture, thus allowing the high-pressure product gases to escape the container. Not only was this scenario successfully simulated but the C-SAFE project also led to many advances in each of the numerous disciplines that made up the center.

DOE, Simulation of Foam Compression. Uintah was used by DOE collaborators at Los Alamos National Laboratory to model dynamic foam compaction [19], such as those used to isolate nuclear weapons components from shock loading. Uintah's MPM component was used to carry out these simulations, which allowed for compression of the foam to full densification. This was noteworthy for several reasons as this type of direct numerical simulation allows users to correlate microscopic behavior of the foam constituent material with bulk behavior. At this time a number of other methods failed to solve this problem.

DARPA, Virtual Soldier Project. In the Virtual Soldier project MPM [37, 38] was used to create a model of cardiaci/torso wounding in a collaboration between the University of Auckland, USCD and the University of Utah. The goal of this project was to understand the mechanics of wounding in an effort to improve the chances of recovery for wounds. MPM simulations of cardiac mechanics allowed substantial changes in cardiac anatomy and associated domain topology due to wounding. MPM was used to simulate a penetrating wound with the cardiac/torso computational models. MPM allowed substantial structural changes to be readily computed through the explicit movement of tissue across the mesh. Experience with MPM methods has shown that it provides accurate solutions for problems involving large deformations such as projectile intrusions, without the drawback of mesh distortion that is typically encountered in the finite element method. Results on torso calculations given by [39] showed that Uintah and MPM have an important role to play in the simulation of large deformations in biomedical tissue.

NIH, Mechanics of Angiogenesis. The broad objective of this project was to study biomechanical interactions of angiogenic microvessels with the extracellular matrix (ECM) on the microscale level by developing and applying novel experimental and computational techniques to study a 3D in vitro angiogenesis model. This project developed techniques to simulate the microscale biomechanical behavior of vascularized collagen gels using Uintah. Volumetric confocal images were used as the basis for generating the geometry of the computational domain [31]. These segmented images were automatically converted to a computational distribution of material points for MPM simulations. New constitutive models were used in the MPM code to represent the collagen matrix (based on direct experimental measurements) and the smooth muscle and endothelial cells. Computational algorithms were developed to represent interface conditions between microvessels and the ECM. The MPM code was optimized for implicit time integration using quasi-Newton and full Newton solution methods [29]. Development of these simulation technologies allowed computation of local stresses within 3D vascularized constructs and correlation of mechanical local mechanical stresses with microvessel sprouting.

NIH, Aerodynamic and Acoustic Models of Phonation. The Uintah fluid-structure interaction component, known as MPMICE, was employed by researchers at Bowling Green University [24] in a study of phonation (the production of sound) in human vocal folds. This investigation began by determining the ability of Uintah to capture normal acoustical dynamics, including movement of the vocal fold tissue. Uintah provided the ability to treat large deformation fluid-solid interaction, material models for biological tissue available, as well as tools to convert two and three dimensional image data (microscopic, CT, etc) to a geometric description suitable for use in Uintah's Material Point Method. Lastly, the use of a compressible flow solver for the fluid enabled measurement of "sounds" by recording the computed pressure.

Institute for Clean & Secure Energy Program, Utah. This DOE-funded program's mission is to perform research to utilize the vast energy stored in our domestic resources and do so in a manner that will capture CO2. This Uintah-based research is organized around the theme of validation and uncertainty quantification through tightly coupled simulation and experimental designs and through the integration of legal, environment, economics and policy issues. The results of the research are embodied in the computer simulation tools which predict performance with quantified uncertainty; thus transferring the results of the research to practitioners to predict the effect of energy alternatives using these technologies for their specific future application. The Uintah ARCHES component was the main computational tool for this program, which had three components.

(i) Flare Simulations. Alberta Research Council 04/01/2008 - 03/31/2009 ARC2. This work involved the Institute for Clean and Secure Energy (ICSE) researchers in a study of H2S emissions from flares in high cross winds to provide standard operating procedures. ICSE researchers are used ARCHES to predict combustion efficiency, pollutant emissions, and the sensitivity of operational parameters in industrial flares. They also explored operational conditions in which it is not possible to collect experimental data. In these simulation studies, it was possible to resolve the large length and time scales responsible for controlling flare dynamics.

(ii) Rocket Motor Simulations. ATK Aerospace / NASA 10/30/2007 - 08/07/2008, S71005. ICSE researchers have also used ARCHES in NASA funded work using Teragrid computers to examine the thermal environment in accident scenarios involving rocket motors in large-scale storage facilities by radiation heat transfer predictions at a distance from the large accident scenario.

(iii) Industrial Flares. This was an ICSE study funded by John Zink Company from 12/01/2007 until 11/30/2011 5019856, that involved an evaluation of combustion efficiency of industrial flares.

6 Examples of Current Research Using Uintah

Microscale Fluid Structure Interaction in the Slip Flow Regime, University of Utah. An NSF proposal, 0933574, that is led by Prof. T. Ameel and Prof. T. Harman, in Mechanical Engineering starts from the viewpoint that both rarefaction and fluid-structure-interaction (FSI) effects are significant for many microscale systems such as micro valves, pumps, actuators, particulate flows, porous flows, two-phase flows, micro-air-vehicles, combustion, and heat exchangers. Rarefaction becomes significant for gaseous systems at the microscale. Uintah appears to be unique in its ability to to accurately model FSI and rarefaction effects for a generic microsystem [80, 81, 82].

Petascale Simulation of Sympathetic Explosions, University of Utah. NSF OCI PetaApps award OCI 0905068, September 1, 2009 to August 31, 2013. PI Prof M. Berzins. This project aims to advance the state-of-the-art in the computational modeling of hazards related to explosives through a combination of modeling, algorithmic and computer science developments. This advance will be achieved by performing simulations that have not been previously possible in order to answer fundamental questions about *sympathetic* explosions in which the collective heating by fire and interactions of a large ensemble of explosives results in dramatically increased explosion violence. This work is motivated by a recent transport accident and unexpectedly large detonation that destroyed a highway and railway. The project is predicting the violence (as characterized by fragment velocities, pressures, etc.) and explosive yield (percentage of devices exploded) for common shipping configurations and thus make possible design-for-safety. These computations have required advances in the Unitah models used for explosives, and in the computational infrastructure such as extending adaptivity into the particle-based algorithms [12]. The need to run such simulations at large scale has driven many algorithmic and software developments, particularly in the area of scalability [13] as well as fundamental work on the modeling of detonation.

Clean & Secure Energy Program, University of Utah. PI: Prof. P. Smith, Institute for Clean and Secure Energy. NNSA U.S. Department of Energy / NNSA 10/01/2010 - 09/30/2013 DE-NA0000740 Accelerate deployment of retrofitable CO2 capture technology through V&V/UQ. There are four areas of current research in this program.

The first area is prediction of the performance and stability of oxygen-fired burners in boilers and industrial furnaces for CO_2 capture, and performance of verification, validation and uncertainty quantification of the numerical and modeling error associated with this prediction [23, 77].

The second area is Coal CDP (oxy-coal and gasification) funded by U.S. Department of Energy / NETL 12/01/2008 - 08/31/2013 DE-NT0005015. This area is prediction of the performance of entrained-flow gasifiers and validating these tools with pilot-scale experimental data. The work will quantify numerical uncertainty and identify key model parameters. The approach used in ARCHES is Large eddy Simulation (LES) of oxy-coal and coal gasification systems.

The third area is the extension of ARCHES to fluidized-bed conditions for the simulation of chemical looping combustion, a technique for extracting energy from a fuel and producing a relatively pure CO_2 exhaust that involves two fluidized-bed reactors. The first reactor contains a metal-oxide to provide oxygen for combustion; after combustion this reduced metal oxide is transported to the second bed where it is re-oxidized before being reintroduced back to the first reactor.

The fourth ICSE area is work with Spectral Sciences Inc. 01/21/2011 - 08/01/2012, 10015663 (STTR-DOE 92711S10-I). The project is concerned with determining flare combustion efficiency and VOC content of flares through a combination of online measurements and the ARCHES code, [67, 68].

Schlumberger-Funded Research using Uintah, Schlumberger technology Corporation. PI: J. Guilkey. Schlumberger has been using and supporting Uintah developments in certain areas for the past four years in the following ways. Uintah has been used for the study of fracturing in coalbed methane beds, the modification/design of shaped charges, penetration of shaped charge jets into metals and geomaterials, [18], material selection for shaped charge jet liners and wellbore dynamics modeling. Schlumberger has a full-time Research Engineer on campus in Utah who spends 80% of his time in the use or development of Uintah. There has been and is funded research at the University of Utah to the value of $1 million from 2008 to 2012. This research funding has made it possible to make algorithmic enhancements to MPM as well as to develop and implement material models for geomaterials. Subcontractor Scott Bardenhagen was awarded $40,000 to investigate/incorporate effects of material heterogeneity on failure properties.

Constitutive Modeling Research, University of Utah. PI: R.M.Brannon, Key Investigator and Uintah developer: Biswajit Banerjee (New Zealand). $1.1M ONR-MURI (new grant up to 5 years). This project involves simulations of soil damage and ejecta from underground explosives. The material models and simulation capabilities are being designed specifically for Uintah [20]. There is also an award of $100k from Idaho National Laboratory (previous and continuing grant) to PI: R.M.Brannon for work on Unnotched Charpy impact simulations of metal plasticity and fracture. Finally as a result of a $200k award from Sandia National Laboratories Uintah is being used as one of the frameworks to test constitutive models for ceramics, rock, concrete, and metal.

Soil Deformation Research, Univerity of Newcastle, Australia. PI: Wojciech Solowski, Department of Surveying and Environmental Engineering. This project involves the application of Uintah to soil deformation, with particular focus on the new MPM CPDI integrator developed in the research of Brannon [63].

Energetic Materials Research, Wasatch Molecular. PI: Scott Bardenhagen. Penetration Survivable Advanced Energetics, (2 years). DOD SBIR Phase II, FA8651-10-C-0151. This project is a combined experimental and modeling effort focused on the role of mesoscale structure on the response of plastic bonded explosives in highly confined environments. Uintah is being used to perform mesoscale simulations and rank the importance of various mesoscale characteristics.

Advanced Nuclear Fuels Research, University of Texas at Dallas. PI: Hongbin Lu. (3 years) DOE NEUP, 09-416. Simulation of Failure via Three-Dimensional Cracking in Fuel Cladding for Advanced Nuclear Fuels. A new generation of reactors is under development that operate at higher temperatures and Neuron fluxes than traditional reactors. Fuel cladding failure limits the efficiency of traditional reactors, and must be evaluated for use in more severe environments. Uintah is being used to simulate the failure process in irradiated fuel cladding.

Blast-Induced Injury Modeling using Uintah, University of Utah. PI: Ken Monson. Cerebrovascular Injury in Blast Loading DOD, 2008-2012 Current W81XWH-08-1-0295. This work focuses on understanding the influence of blast waves on cerebral blood vessels. the project uses Uintah to determine internal mechanical quantities (stress, strain, strain-rate) on targets exposed to the 'blast. A follow-on project Blast-Induced Vascular Injury DOD, 2012-2016 is pending and aims to define the loading conditions on intracranial tissues during blast. Uintah will be used to define transfer of the blast wave from air into the intracranial contents and to simulate the response of internal tissues to loading.

Early Science Program for the BG/Q using Uintah, DOE Argonne National Laboratory. PI: Hal Finkel. DOE - 2 years Current DE-AC02-06CH11357. Phase transitions in the very early universe underlie several important classes of models of inflationary cosmology. Studying these highly-nonlinear models requires numerical simulations capable of resolving a wide range of length scales. In the past, the effects of gravity have often been ignored, or treated crudely, and so the current understanding of regimes in which gravity plays an important role is poor. The project currently aims to study phase-transition scenarios, modeled using effective scalar fields coupled to gravity (in the BSSN or generalized harmonic formulations), using adaptive mesh refinement in order to better understand the contribution of gravity to these models.

Aerodynamics and Magnetohydrodynamics with Uintah, Institute of Applied Physics and Computational Mathematics, Beijing, China. PI: Qiang Zhao. At present this appears to be preliminary algorithmic work.

Unconventional and Renewable Energy Research Utilizing Advanced Computer Simulations DOE NETL, PI: Prof. C.R. Johnson, University of Utah, September 2010 until March 2013. Award Number: DE-EE0004449. A small part of this project (one graduate student and one post-doc) is concerned with applying Uintah to novel energy applications and in porting the code to Hybrid GPU architectures.

Green Infrastructure Research, University of Utah. PI: Eric Pardyjak. IDR-Collaborative Research: Understanding the Impact of Green Infrastructure on Urban Microclimate and Energy Use. NSF 2011-2014 CBET-1134580 (current) This project uses large-scale simulation science to investigate the impact of green infrastructure projects on urban energy use and microclimate. A follow project is pending with NASA:Understanding the Impact of Urbaniztion, Orography, and Climate on Urban Energy Budget, Water Cycle and Sustainability. The objectives of this project are to: (i) develop an integrated modeling framework that combines state-of-the-art weather, microclimate, and hydrologic models with remote sensing that can be used to study the urban environment, (ii) use the framework to study the impact of urbanization on urban and regional climate, (iii) develop new models, based on land-use and other characteristics, that can be incorporporated into simulations for future climate.

Landslide modelling, University of Texas at Austin. PI: Eunseo Choi. A pilot project was used to run some landslide models of the proof-of-concept type using Uintah. Title: EAGER: Catastrophic landslide dynamics from seismic wave inversion and satellite remote sensing. Funding source: NSF Grant number: EAR 11-50072 Duration: 09/01/2011-08/31/2012. PIs C. P. Stark and G. Ekstrom (Columbia University). Synopsis: This pilot project seeks to address the following issue: Do the seismic waves generated by catastrophic slope failure retain enough information on the forces driving a landslide to allow inference of its dynamics? The results obtained from this proposal have been included in a full (pending) proposal submitted to NSF. Title: Landslide dynamics from seismic wave inversion, satellite remote sensing and numerical modeling. Funding source: NSF (Pending) Duration: 07/01/2012-06/30/2015 PI G. Ekstrom (Columbia University) Synopsis: The tasks of the proposed research are (i) to develop and improve a method for inverting the long-period seismic waves induced during the motion of massive, rapidly accelerating landslides, and (ii) to evaluate the validity of the forces, accelerations, momenta, trajectories, and energies inferred from the seismological analysis using field and remote-sensing observations, as well as numerical modeling.

Study of material Properties of Wood-Based Composites, FPI Innovations. Dr Edward A. Le, FPInnovations - Composite Products, Vancover Canada. Numerical simulation of creep behavior of wood-based composites. The main focus of the study is to look at the strain and stress deformation under load duration and creep. The study is in its very early stages.

All-Season Vehicle-Terrain Interaction: Modeling and Validation, University of Alaska. PI: Jonah H. Lee Professor and Chair Department of Mechanical Engineering. U.S. Army Tank-automotive and Armaments Command (TACOM), \$1.26 M, Aug. 2008-present. Approximately 30% of the research on this project uses Uintah. Uintah is used primarily to understand the mesoscale mechanical properties of dry snow treated as a porous material with an ice matrix involving viscoplasticity and damage. Extensive test results in compression, indentation, penetration, plowing and sliding, under vehicle traversal conditions, are used to validate the computational model.

Impact problems at asteroid scales, John's Hopkins University. PI: Prof. K.T. Ramesh, Mechanical Engineering. In this project Uintah is being used to study the feasibility solve a problem relating to on impact problems at asteroid scales. The particular problem being investigated is a glass bead impacting a Basalt cube.

Stability Analysis of Aircraft with Wind Gusts, Institute of Applied Physics and Computational Mathematics. PI: M.Xu. The work concerns the stability analysis of aircraft when there are strong wind gusts. the research aims to consider whether or not the plane can be controlled normally under such conditions.

Aerodynamics and Magnetohydrodynamics with Uintah, Institute of Applied Physics and Computational Mathematics, Beijing, China. PI: Qiang Zhao. At present this appears to be preliminary algorithmic work.

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