

TECHNICAL REPORT

Large Scale Parallel Solution of Incompressible Flow Problems using Uintah and hypre

John Schmidt, Martin Berzins, Jeremy Thornock, Tony Saad, James Sutherland

UUSCI-2012-002

Scientific Computing and Imaging Institute
University of Utah
Salt Lake City, UT 84112 USA

May 4, 2012

Abstract:

The Uintah Software framework was developed to provide an environment for solving fluid-structure interaction problems on structured adaptive grids on large-scale, long-running, data-intensive problems. Uintah uses a combination of fluid-flow solvers and particle-based methods for solids together with a novel asynchronous task-based approach with fully automated load balancing. As Uintah is often used to solve compressible, low-Mach combustion applications, it is important to have a scalable linear solver. While there are many such solvers available, the scalability of those codes varies greatly. The hypre software offers a range of solvers and pre-conditioners for different types of grids. The weak scalability of Uintah and hypre is addressed for particular examples when applied to an incompressible flow problem relevant to combustion applications. After careful software engineering to reduce start-up costs, much better than expected weak scalability is seen for up to 100K cores on NSF's Kraken architecture and up to 200K+ cores, on DOE's new Titan machine.

Large Scale Parallel Solution of Incompressible Flow Problems using Uintah and hypre

John Schmidt*, Martin Berzins†, Jeremy Thornock‡, Tony Saad § and James Sutherland¶

*Scientific Computing and Imaging Institute
University of Utah, Salt lake City, UT 84112 USA
Email: John.Schmidt@utah.edu

†Scientific Computing and Imaging Institute
University of Utah, Salt Lake City Ut 84112 Email: mb@sci.utah.edu

‡Institute for Clean and Secure Energy
Email: Jeremy.Thornock@utah.edu

§Institute for Clean and Secure Energy
Email: saadtony@gmail.com

¶Institute for Clean and Secure Energy
University of Utah, Salt Lake City Ut 84112 Email: James.Sutherland@utah.edu

Abstract—The Uintah Software framework was developed to provide an environment for solving fluid-structure interaction problems on structured adaptive grids on large-scale, long-running, data-intensive problems. Uintah uses a combination of fluid-flow solvers and particle-based methods for solids together with a novel asynchronous task-based approach with fully automated load balancing. As Uintah is often used to solve incompressible flow problems in combustion applications it is important to have a scalable linear solver. While there are many such solvers available, the scalability of those codes varies greatly. The hypre software offers a range of solvers and preconditioners for different types of grids. The weak scalability of Uintah and hypre is addressed for particular examples of both packages when applied to a number of incompressible flow problems. After careful software engineering to reduce startup costs, much better than expected weak scalability is seen for up to 100K cores on NSF's Kraken architecture and up to 260K cpu cores, on DOE's new Titan machine. The scalability is found to depend in a critical way on the choice of algorithm used by hypre for a realistic application problem.

Keywords-Uintah, hypre, parallelism, scalability, linear equations

I. INTRODUCTION

In this paper we consider solving a pressure projection formulation of the Navier-Stokes equations within Uintah [8], [12], [29], [30], an open-source software framework (www.uintah.utah.edu). In recent previous work we showed that Uintah scales well to about 200K cores for some applications, [8], [24], including a sympathetic explosion modeling problem, funded by the NSF PetaApps Program, that is one of our main applications driving examples. In these cases the solution techniques were all fully explicit and did not require the solution of a system of equations. In many of the Uintah applications the flow is incompressible and chemically reacting [17], [18] with the formulation of the governing equations requiring the use of a linear

solver at each timestep [13]. Such problems arise at Institute for Clean & Secure Energy Program, Utah, whose mission is to perform research to utilize the 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. Typical problems consist of the prediction of the performance and stability of oxygen-fired burners in boilers and industrial furnaces for CO₂ capture or determining flare combustion efficiency and VOC content of flares through combination of online measurements and high-fidelity codes, [17], [33]. In tackling such problems, as we approach problem sizes requiring greater than 100K cores on machines such as Kraken¹ and Jaguar,² it is far from clear that the linear solvers available today will perform efficiently on such large core counts, never mind on architectures such as the Titan machine.³ In this paper we will address the scalability of the Uintah software applied to incompressible flow problems when using one particular class of solvers from the hypre software. [2], [3], [14]. The test problems used will be a model incompressible flow problem and on a challenging example taken from the modeling of Helium plumes. The rest of this paper is organized as follows. The Uintah software, including the ARCHES and Wasatch software used for incompressible flow combustion problems, is described in Section II. Section III describes the hypre software and how it is used in conjunction with Uintah including the

¹Kraken is an NSF supercomputer located at the University of Tennessee/Oak Ridge National Laboratory with 112,896 cores.

²Jaguar is a DOE supercomputer located at the Oak Ridge National Laboratory with 224,256 cores that was in service until December 2011.

³Titan is a DOE supercomputer at the Oak Ridge National Laboratory with approx 299,008 cpu cores and 18,600 GPUs.

improved performance obtained by avoiding start-up costs by preserving data structures. In Section IV the results of numerical experiments are given that show the weak scaling obtained on two test problems. The first problem is a straightforward test problem while the second is a more challenging example that is representative of real applications. Section V presents a model for the weak scalability of the linear solver. Section VI provides conclusions and described future work in extending the ideas here to other applications and Uintah components.

II. OVERVIEW OF UINTAH SOFTWARE

The Uintah Software was originally a product of the University of Utah Center for the Simulation of Accidental Fires and Explosions (C-SAFE) [12]. C-SAFE, a Department of Energy ASC center. The aim of Uintah was to be able to solve complex multi-scale multi-physics problems, with a particular emphasis on combustion and fluid-structure interaction problems. Uintah is available as open source software⁴ and extended to run on about 260K cores [8], [24], Uintah makes use of a component design that enforces separation between large entities of software and can be swapped in and out, allowing them to be independently developed and tested within the entire framework. This has led to a very flexible simulation package that has been able to simulate a wide variety of problems, see [7]. A novel feature of Uintah, and one that directly leads to its scalability is its use of a task-based paradigm, with complete isolation of the user from parallelism. The individual tasks are viewed as part of a directed acyclic graph (DAG) and are executed adaptively, asynchronously and now often out of order [25]. Uintah uses a novel adaptive meshing approach, [23], as well as a particle solution methods, however neither of these components is necessary here.

Uintah currently contains five main simulation algorithms, or components, the ICE compressible multi-material CFD formulation (based upon [19]), the particle-based Material Point Method (MPM) for structural mechanics, the combined fluid-structure interaction algorithm MPMICE [15] and the ARCHES combustion component. The focus in this paper is on the fixed-mesh ARCHES and Wasatch components designed for simulation of compressible turbulent reacting flows with participating media radiation [26], [34].

A. The ARCHES Combustion Component

ARCHES is a three-dimensional, Large Eddy Simulation (LES) code developed by Prof. P.J. Smith and his group in Utah. The ARCHES code is currently used for a broad class of industrial and industrial-strength research simulations, [7]. The ARCHES component uses a low-Mach number ($Ma < 0.3$), variable density formulation to simulate heat, mass, and momentum transport in reacting flows. The Large

Eddy Simulation algorithm used in ARCHES solves the filtered, density-weighted, time-dependent coupled conservation equations for mass, momentum, energy, and particle moment equations in a Cartesian coordinate system [18], [20].

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. Spatial discretization is handled with central differencing where appropriate for energy conservation or flux limiters (e.g., scalar mixture fractions) to avoid unphysical solutions. The low-Mach, pressure formulation requires a solution of an implicit pressure projection at every time sub-step. The solution of these equations has been tackled with a number of different solvers. Most recently both the PETSc [4]–[6] and the hypre packages [13] have been used.

ARCHES uses a dynamic, large eddy turbulence closure model for the momentum and species transport equations is used. The dynamic model accounts for sub-grid velocity and species fluctuations. Various combustion models exist within ARCHES for doing gas phase and particle phase combustion chemistry, including sub-grid turbulence and chemistry interactions. For gas phase combustion, the dimensionality of the problem is reduced by parameterizing the thermo-chemical state space $(\rho, T, x_1, x_2, \dots, x_{n-1})$, where x_i represents a chemical species (from set n), into a small set of variables which are tracked on the resolved mesh. These parameters then map back the state space as a function of space in time through the computational mesh. The combustion chemistry is pre-processed in a tabular form for dynamic table look-up during the course of the LES simulation. The energy balance includes the effect of radiative heat-loss/gains in the IR spectra by solving the radiative intensity equation using a discrete-ordinate solver [20]. The solution procedure solves the intensity equation over a discrete set of ordinances and, like the pressure equation, is formulated as a linear system that is solved using a linear solver package such as hypre. Solid particulate fuel phases are represented using the direct quadrature method of moments (DQMOM) This Eulerian reference frame approach solves a discrete set of moments of the number density equation using numerical quadrature. The number density function is described by the solid fuel properties including particle number, size, and fuel properties (e.g., velocity, volatile mass fraction, fixed fuel mass fraction, energy content, size). Various physical models for coal combustion are implemented to include the effect gas devolatilization, char oxidation, particle drag, and size changes, which in turn effect the coal number density function. The DQMOM description of the coal phase is completely coupled with the gas phase description to produce a completely coupled, gas/solid phase description of the flow with closed mass, momentum, and energy balances.

The ARCHES code is essentially a stencil-based p.d.e.

⁴see www.uintah.utah.edu

code and so achieves good weak and strong scalability for its discretization by making use of the Uintah infrastructure [31], [32]. The potential bottleneck to scalability arises from the use of parallel solvers like hypre [2], [13] and PETSc, [21], as this is where most of the compute time is spent on incompressible flow calculations.

B. Wasatch Component

The extension to ARCHES is an approach, named Wasatch, proposed by one of the authors (Sutherland), see [9] that is a Domain Specific Language (DSL) for the very large and complex p.d.e. systems that arise in certain combustion applications. The complexity of the combustion problems to which simulation is applied naturally increases with available computing power. For example, turbulent combustion simulation of typical fuels involves perhaps hundreds of species and quite possibly thousands of reactions. Solving such large sets of highly coupled, nonlinear PDEs may be problematic. In such highly dynamic, multi-physics systems, one may not be able to determine *a priori* the most appropriate models. One possible solution to this is to make use of programming models which allow significant flexibility in the complex couplings that may occur for different model sets in multi-physics applications.

In the approach proposed by Sutherland, [27], the programmer writes code that calculates various mathematical expressions, explicitly identifying what data the code requires and produces/calculates. In order to create an algorithm, the programmer selects one or more expressions to be evaluated and the dependencies are recursively “discovered” resulting in a dependency graph. The dependency graph may be inverted to obtain the execution graph, which may be traversed in parallel if desired. Wasatch uses an operator approach over strongly typed fields to form a domain specific language to achieve abstraction of field operations, including application of discrete operators such as interpolants, gradients, etc, so as to make sure that each task executes as efficiently as possible on each core or accelerator. In this work Wasatch was used to automatically generate code for the discretization of the first examples used to test the Uintah interface to hypre.

III. USING HYPRE WITH UINTAH

The hypre software [2], [3], [14] is a library of high performance preconditioners and solvers for the solution of large linear systems of equations on massively parallel machines. The hypre library has an emphasis on multi-grid preconditioners, including algebraic multigrid. While hypre has three conceptual interfaces [2] the interface that is most applicable here is the Structured Grid Interface (Struct). This interface is designed for stencil-based p.d.e. codes that use grids, such as those in Uintah, that consist of unions of logically rectangular (sub)grids. The specialized structured grid multigrid solvers in hypre make use of the conceptual

interface to introduce problem-specific algorithmic aspects by taking advantage of the the structure of the problem and are thus the most scalable part of hypre [2]. In particular the structured multigrid solver used here, PFMG, adopts this approach.

PFMG [1] is a semi-coarsening multigrid method for solving scalar diffusion equations on logically rectangular grids discretized with up to 9-point stencils in 2D and up to 27-point stencils in 3D, [2] with anisotropies that are uniform and grid-aligned throughout the domain. The solver is designed to deal with anisotropies and so attempts to automatically determine the *best* direction of semi-coarsening. PFMG interpolation is determined algebraically. The coarse-grid operators are also formed algebraically, either by Galerkin or by the alternative method [1] for 5-point (2D) and 7-point (3D) problems. PFMG has many options to deal with solution anisotropies. Baker et al. [2] report that various version of PFMG are between 2.5 and 7 times faster than the equivalent algebraic multigrid (AMG) options inside hypre because they are able to take account of structure.

In general a multigrid method such as PFMG has a setup phase and a solve phase. The setup phase consists of defining the coarse grids and the interpolation and coarse grid operators. This phase can be computationally very intensive as will be demonstrated below. In contrast the solve phase which performs the multigrid cycles is often less expensive.

Note that in the use of hypre described here multigrid methods are not used as linear solvers but are used as a preconditioners for Krylov or other iterative methods provided by hypre. In the cases considered here, the Conjugate Gradient (CG) method was used with the PFMG preconditioner based upon a Jacobi and red-black Gauss Seidel relaxation methods used as part of the structured multigrid approach.

A. hypre Setup Costs

As mentioned above, hypre setup (preconditioning and communication) time is significant at large core counts upwards to twenty times that of the solve phase. The setup phase is slower than the solve phase, due primarily to the assumed partition and global partition components of the code. The global partition requires $O(P \log P)$ communications in the setup phase, where P is the number of cores, while the current implementation of the assumed partition requires $O((\log P)^2)$ communications, [2] also reported setup phase scales quite poorly, likely due to the $O((\log P)^3)$ number of coarse grids. It is important to configure hypre to not use a global partition especially for very large core count runs.

Table I show the start-up costs for a simple Poisson equation solve in two space dimensions as described in Section IV-A. We see a considerable growth in start-up costs in this weak scaling case in which each core has roughly

the same computational load in terms of equations and unknowns. Experiments were performed on both the old XT5 and new XK6 configurations of Jaguar/Titan. At the time of the experiments this system consists of approximately 262,144 AMD Interlagos cores arranged so that there are 16 cores per node and connected through the new Cray Gemini interconnect. It is interesting to note that the set-up costs are greater for the slower interconnect found on the older XT5 configuration. The set-up overhead is a significant component of the overall solution time for each linear solve.

Titan Cores and Start-Up	2K	4K	8K	16K	32K	64K	128K
	0.02	0.13	0.25	0.25	0.50	0.75	3.89
Jaguar Cores and Start-Up	3K	6K	12K	24K	48K	96K	192K
	1.54	1.10	1.22	2.04	2.4	2.9	22.11

Table I
HYPRE START-UP TIMES FOR TITAN AND JAGUAR CORES

Our first experiments using hypre with Wasatch and ARCHES involved doing matrix allocation and setup at every timestep. The high setup costs on each solve made both weak and strong scalability impossible to achieve. As a result work was undertaken to ensure that the interface for the pressure solve to the external hypre library is handled efficiently. This led to code speed-up through the removal of redundant operations in the setup phase.

B. Avoiding hypre Setup Costs Using Uintah’s Data Warehouse

The key observation is that in the incompressible formulation for the pressure solve found in both ARCHES and Wasatch, the matrix did not change between timesteps and so the setup only needed to be done as often as the mesh changed. In the case of the fixed mesh calculations reported here the setup only needed to occur at the beginning of the simulation.

While allowing hypre to completely control the memory allocation allowed for a certain simplicity in the initial implementation of the integration of hypre with Uintah, ultimately a more cooperative memory management strategy needed to be implemented. Within Uintah, the DataWarehouse is the key component for storing data for all calculations. The DataWarehouse is essentially a large hash table that stores pointers to allocated blocks of memory. From an application point of view, the vast majority of data are represented by one of four types of grid variables, i.e. node, face, cell, and particles. The node, face, and cell grid variables present a high level interface to the underlying I,J,K block of raw memory that represents the patch/patches on a given processor. The DataWarehouse manages the complete lifetime of data including the allocation, deallocation, reference counting, and ghost data exchanges which greatly simplifies data management for the simulation algorithm implementations [22].

While this simplifies native Uintah application developments, it does complicate the interaction between external third party software packages such as hypre. To provide a more cooperative memory management strategy, we developed a new C++ templated variable type named SoleVariable for Uintah that acted as a container object for the raw memory pointers from within the DataWarehouse. Unlike the typical Uintah variable, the SoleVariable variables are not dependent on the underlying grid/patch layout, instead they represented data that encompassed the entire grid.

For maximal memory efficiency and reuse, the following hypre data structure needed to be allocated with its lifetime intelligently managed by the DataWarehouse. At the beginning of the simulation and then reused on all subsequent linear system solves: solver, preconditioner, A matrix, B and X vectors. These five data types can be combined into a straightforward reference counted C++ structure:

```
struct hypre_solver_struct {
    HYPRE_StructSolver solver;
    HYPRE_StructSolver preconditioner;
    HYPRE_StructMatrix* HA;
    HYPRE_StructVector* HB;
    HYPRE_StructVector* HX;
};
```

From within the Uintah, this data structure would be the template argument to the SoleVariable as in:

```
SoleVariable<struct hypre_solver_struct>
```

The pointers to the matrix and vectors are then used in the native hypre APIs to do the initial memory management and the set-up of the communication patterns. Once the various hypre data structures were created, the SoleVariable container object managed the lifetime and reuse. For the computational experiments presented below, the setup phase and data structure creation phase were done prior to the first timestep.

In the case of combustion problems involving radiation, the external hypre solves for the pressure and radiative intensity equations represent the bulk of the overall execution time.

IV. COMPUTATIONAL EXPERIMENTS

In this section we describe two computational experiments that illustrate the weak scalability that is possible when using hypre as the linear solver for incompressible flow calculations. For each experiment, the solution of the Navier-Stokes equations is required where the Navier-Stokes equations describe the spatio-temporal motion of a fluid and are given by

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0 \quad (1)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} = \mathbf{F} - \nabla p; \quad \mathbf{F} \equiv -\nabla \cdot \rho \mathbf{u} \mathbf{u} + \mu \nabla^2 \mathbf{u} + \rho \mathbf{g} \quad (2)$$

Here, $\mathbf{u} = (u_x, u_y, u_z)$ is the velocity vector describing the speed of fluid particles in three orthogonal directions, ν is the kinematic viscosity - a fluid property that reflects its resistance to shearing forces, ρ is the fluid density, and p is the pressure.

The numerical solution of the Navier-Stokes equations requires evaluation of the pressure field while enforcing the continuity constraint given by (1). One standard approach for deriving an explicit equation for the pressure is to take the divergence of (2) and make use of (1) to act as the constraint. At the outset, one obtains a Poisson equation for the pressure

$$\nabla^2 p = \nabla \cdot \mathbf{F} + \frac{\partial^2 \rho}{\partial t^2} \equiv R \quad (3)$$

Equation (3) is known as the pressure-Poisson-equation (PPE). Its solution requires the use of a solver such as hypre for large sparse systems of equations.

A. Taylor Green Vortex Example

The Taylor-Green vortex is a well-known benchmark for the verification of CFD codes [10]. It simplifies the system by assuming constant density so that the continuity equation reduces to

$$\nabla \cdot \mathbf{u} = 0. \quad (4)$$

The initial condition is a divergence-free (solenoidal) velocity field that evolves in time according to the Navier-Stokes equations.

To test this formulation, we call upon the 3D Taylor-Green vortex. The initial condition is given by the following specification

$$u_x(\mathbf{x}, t = 0) = \frac{2}{\sqrt{3}} \sin(\theta + \frac{2}{3}\pi) \sin x \cos y \cos z \quad (5)$$

$$u_y(\mathbf{x}, t = 0) = \frac{2}{\sqrt{3}} \sin(\theta - \frac{2}{3}\pi) \cos x \sin y \cos z \quad (6)$$

$$u_z(\mathbf{x}, t = 0) = \frac{2}{\sqrt{3}} \sin \theta \cos x \cos y \sin z \quad (7)$$

where θ is an arbitrary phase angle. If the PPE equation is correctly implemented, then the evolution of the flow from this solenoidal initial condition should remain solenoidal for all subsequent times.

In the current study, we set $\theta = 0$ and solve the Navier-Stokes equations on the domain $0 \leq (x, y, z) \leq 2\pi$ with periodic conditions. We used a first-order forward-Euler method for time integration. This may be summarized as follows

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \mathbf{F}^n - \frac{1}{\rho} \nabla p^n \quad (8)$$

with the following PPE

$$\nabla^2 p^n = \rho \nabla \cdot \mathbf{F}^n \quad (9)$$

For spatial discretization, we used second order central differencing on a staggered grid. A staggered grid is one on which the velocity components are located on staggered cells while all scalars (including pressure) are located at cell

centroids. Furthermore, all fluxes are stored at the faces of scalar or staggered volumes.

For each simulation, the mesh was composed of multiple patches with 32^3 cells per patch. One patch per core was used and the resolution and domain sizes were increased to achieve a constant workload as the core count increased. For the smallest core count case of 192, the approximately 6.2 million (192×32^3) unknowns were solved using hypre with the PFMG pre-conditioner and the Jacobi smoother. The largest core count case of 192K cores required the solution over 6.4 billion ($196,068 \times 32^3$) unknowns.

In the experiments that follow not only was the new Titan machine used but the calculation was also done but also the older Jaguar machine at Oak ridge before it was upgraded to Titan. For the older XT5 configuration, the core count increased as multiples of 12 reflecting the 12 cores per node. Results for core counts ranging from 192 cores up to 196,068 cores were obtained prior to the transition from the XT5 configuration to the XK6 configuration. The new Titan machine did not have its GPUs yet and so has only 16 cores per node and thus the nodes may be viewed as XE6 nodes with only half the cores or XK6 nodes without the GPUs. For simulations running on the new XK6 configuration, the core count increased by multiples of 16 reflecting the 16 cores per node up to a maximum of 131,072 cores that were available at the time of the experiments. Figure 1 shows the

Weak Scaling for Taylor Green Vortex using HYPRE (PFMG) for Jaguar's XT5 and XK6

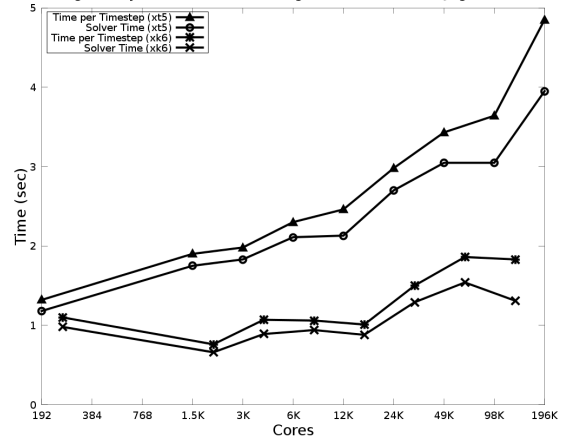


Figure 1. Weak scalability of Wasatch with hypre using the the PFMG pre-conditioner for the Taylor-Green Problem

weak scalability of Wasatch on a test incompressible flow problem - The Taylor-Green Vortex problem as described by equations (1-3).

Not only is the new machine faster per core but the improved communications network results in better weak scaling (constant workload per core) than on the original Jaguar. The top line 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 line down. The bottom two lines correspond to the same times on the new XK6 type nodes (as mentioned above without GPUs) in the Titan machine.

B. Helium Plume problem

Although the Taylor-Green vortex illustrates of simple incompressible flow problem, it neglects the effects of density variation which are paramount in combustion applications. The second example is a Helium plume problem, which requires the full solution of Equations 1 and 2 including the density variations. In addition, various sub-models are used to account for any unresolved turbulence scales that are not directly resolved by the computational mesh.

The helium plume represents the essential characteristics of a real fire without introducing the complexities of combustion and thus serves as an important validation problem for the ARCHES code. Experimental data collected by O'Hern et al. [28] at the Sandia FLAME facility in Albuquerque, NM serve as the validation data for ARCHES simulations.

The computational scenario consists of a $3m^3$ domain with a $1m$ opening that introduces the helium into a quiescent atmosphere of air with a co-flow of air. Velocity and density conditions at these boundaries are known. The sides and top of the computational cube are modeled using pressure and outlet boundary conditions respectively. The outlet boundary condition allows flow to leave the domain while the pressure conditions make it possible for air flow to enter (as driven by the buoyancy forces) through the side of the domain. Both the outlet and pressure conditions are driven by the resulting pressure field solution. The CFD solution procedure exercises major components of the overall ARCHES algorithm, including the modeling of small, sub-grid turbulence scales. Additionally, the coupled problem combines the effects of fluid flow and turbulent scalar mixing for a full spectrum of length and time scales without introducing the complications of combustion reactions. CFD results are compared to time-averaged velocity of both vertical and horizontal components, mixture fraction variables, and turbulence statistics. For this more complex problem the XK6 does not show such an advantage over the XT5 per core unless we factor in the smaller number of floating point units per core on the XK6.

V. LINEAR SOLVER WEAK SCALABILITY MODEL

A model for the weak scalability of the linear solver time as a function of the number of cores (C) can be described by a simple power law:

$$time = a * C^b \quad (10)$$

taking the logarithm of each side

$$\log(time) = \log(a) + b * \log(C). \quad (11)$$

and performing a linear least squares fit yields the coefficients for each problem shown in Table II. Figure 2 shows

Problem	a	b
Taylor-Green (xt5)	0.496	0.165
Taylor-Green (xk6)	0.182	0.179
Helium Plume (xk6)	0.0095	0.447

Table II
LEAST SQUARES COEFFICIENTS FOR A AND B IN (10)

the linear least squares fit of equation 11. The results suggest that the scalability of the linear solver depends significantly on the system of equations that are being solved for. What is interesting to note is that while the network infrastructure is quite different from the XT5 and the XK6 machines, the scalability of the linear solver for the Taylor-Green case is quite similar and scales roughly to the power of $\frac{1}{6}$. The scalability of the Helium Plume problem is quite different scaling approximately to the power of $\frac{1}{2}$. The power law relationship for linear solver scalability demonstrates a remarkably accurate predictive model over a very wide distribution of core counts. It appears to be suggestive of the scalability of the linear solvers for future machines. In

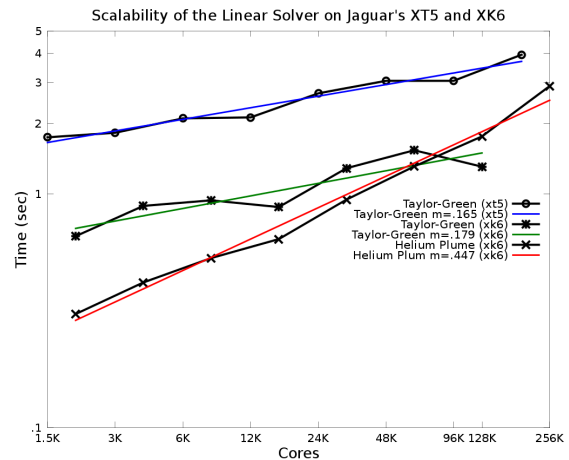


Figure 2. Scalability of the Linear Solvers with a Least Squares Fit for (11)

order to try and improve the scalability of the Helium Plume Problem experiments were undertaken with the different options in hypre. These experiments included using non-symmetric red black Gauss Seidel preconditioner and skipping levels during the multi-grid solves. Instead of solving at every level during the multi-grid, results were interpolated to the "skipped" levels. This reduced the amount of work being done and improved the solve times. These experiments also made it possible to improve the scalability of the Taylor-Green Problem as shown in Figure 3 Applying these algorithmic improvements to the Helium Plume Problem

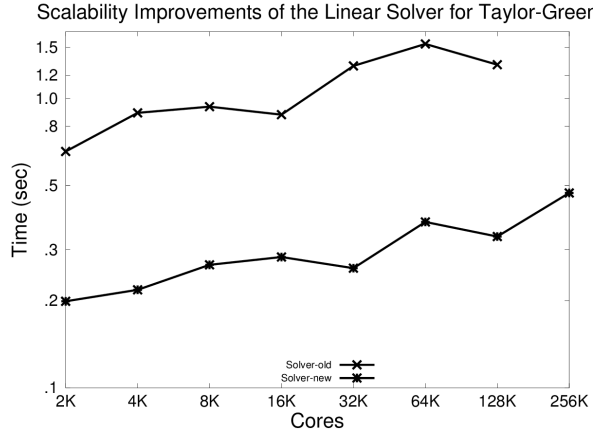


Figure 3. The Effects on Performance of Different hydre Options

gives rise to the results shown in Figure 4. In particular when running the Helium Plume problem with the improved options on the old XT5 Kraken machine we see that its performance scales better than when running on the newer Jaguar XK6 with the original Jacobi method. The same figure also shows a plot of a $\log(p)$ curve that shows that the Helium plume with appropriate algorithms has a scaling that is close to $\log(p)$ where p is the number of cores.

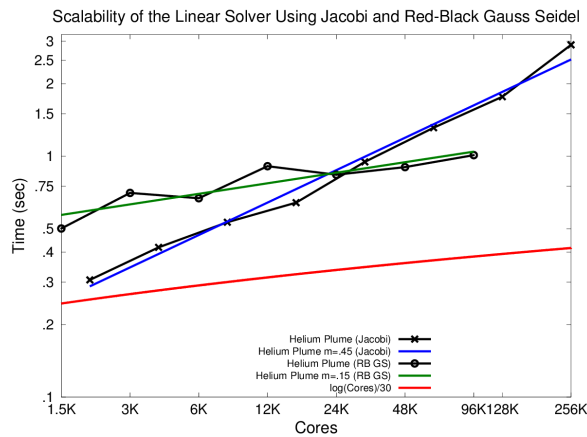


Figure 4. The Effects on Performance of Different hydre Options

VI. CONCLUSIONS AND FUTURE WORK

The overall conclusion of this paper is that it is possible to get quite reasonable weak scaling at large core counts when using hydre with Uintah. The only provisos are that care has to be taken with the start-up costs of hydre and in the choice of algorithms. In the case of Uintah this involved some careful software engineering to ensure continuity of the hydre work spaces and considerable experimentation with the differet hydre options. The results show that effective use of the hydre linear solver package has led to better-than-expected weak scalability on 100K+ cores of Uintah

on incompressible flow problems that range from a simple example problem to an industrial-strength helium plume problem.

In addition, a simple power law relationship for the weak scalability of the linear solver is developed and shows a good range of applicability from the smallest core counts to the full machine capacity. Further work is needed to determine the applicability of the results to the scalability of the linear solvers for future machines and offers insight into the upper limits of current algorithms.

VII. ACKNOWLEDGMENTS

This work was supported by the National Science Foundation under subcontracts No. OCI0721659, the NSF OCI PetaApps program, through award OCI 0905068 and by DOE INCITE award CMB015 for time on Jaguar and DOE NETL for funding under NET DE-EE0004449, Uintah was written by the University of Utah's Center for the Simulation of Accidental Fires and Explosions (C-SAFE) and funded by the Department of Energy, subcontract No. B524196. We would like to thank the hydre team for offering assistance and insight into maximizing the full capabilities of hydre. We would like to thank all those previously involved with Uintah and TACC, NICS and Oak Ridge for access to large numbers of cores.

REFERENCES

- [1] S. F. Ashby and R. D. Falgout. A parallel multigrid preconditioned conjugate gradient algorithm for groundwater flow simulations. *Nuclear Science and Engineering*, 124(1):145–159, 1996.
- [2] A.H. Baker, R.D. Falgout, T. Kolev, and U.M. Yang. Scaling hydre's multigrid solvers to 100,000 cores. In M.W. Berry, K.A. Gallivan, E. Gallopoulos, A. Gram, B. Philippe, Y. Saad, and F. Saied, editors, *High-Performance Scientific Computing*, pages 261–279. Springer London, 2012.
- [3] A.H. Baker, T. Gamblin, M. Schulz, and U.M. Yang. Challenges of scaling algebraic multigrid across modern multicore architectures. In *IPDPS*, pages 275–286, 2011.
- [4] S. Balay, J. Brown, K. Buschelman, V. Eijkhout, W.D. Gropp, D. Kaushik, M.G. Knepley, L.C. McInnes, B.F. Smith, and H. Zhang. PETSc users manual. Technical Report ANL-95/11 - Revision 3.2, Argonne National Laboratory, 2011.
- [5] S. Balay, J. Brown, K. Buschelman, W.D. Gropp, D. Kaushik, M.G. Knepley, L.C. McInnes, B.F. Smith, and H. Zhang. PETSc Web page, 2011. <http://www.mcs.anl.gov/petsc>.
- [6] S. Balay, W.D. Gropp, L.C. McInnes, and B.F. Smith. Efficient management of parallelism in object oriented numerical software libraries. In E. Arge, A. M. Bruaset, and H. P. Langtangen, editors, *Modern Software Tools in Scientific Computing*, pages 163–202. Birkhäuser Press, 1997.
- [7] M. Berzins. Status of release of Uintah computational framework. Technical Report SCI UUSCI-2012-001, SCI Institute University of Utah, 2012.

- [8] M. Berzins, J. Luitjens, Q. Meng, T. Harman, C.A. Wight, and J.R. Peterson. Uintah - a scalable framework for hazard analysis. In *TG '10: Proceedings of the 2010 TeraGrid Conference*, New York, NY, USA, 2010. ACM.
- [9] M. Berzins, Q. Meng, J. Schmidt, and J.C. Sutherland. DAG-based software frameworks for PDEs. In M. Alexander et al., editor, *Proceedings of Euro-Par 2011 Workshops, Part I*, Lecture Notes in Computer Science (LNCS) 7155, pages 324–333. Springer-Verlag Berlin Heidelberg, August 2012.
- [10] M.E. Brachet, D.I. Meiron, S.A. Orszag, BG Nickel, R.H. Morf, and U. Frisch. Small-scale structure of the Taylor-Green vortex. *Journal Fluid Mechanics*, 130(41):1452, 1983.
- [11] A. D. Brydon, S. G. Bardenhagen, E. A. Miller, and G. T. Seidler. Simulation of the densification of real open-celled foam microstructures. *J. Mech. Phys. Solids*, 53:2638–2660, 2005.
- [12] J. D. de St. Germain, J. McCorquodale, S. G. Parker, and C. R. Johnson. Uintah: A massively parallel problem solving environment. In *Ninth IEEE International Symposium on High Performance and Distributed Computing*, pages 33–41. IEEE, Piscataway, NJ, November 2000.
- [13] R.D. Falgout, J.E. Jones, and U.M. Yang. The design and implementation of hypre, a library of parallel high performance preconditioners. In *Numerical Solution of Partial Differential Equations on Parallel Computers*, pages 267–294. Springer-Verlag, 2006.
- [14] R.D. Falgout and U.M. Yang. hypre: A library of high performance preconditioners. In Peter M. A. Sloot, Chih Jeng Kenneth Tan, Jack Dongarra, and Alfons G. Hoekstra, editors, *International Conference on Computational Science (3)*, volume 2331 of *Lecture Notes in Computer Science*, pages 632–641. Springer, 2002.
- [15] J. E. Guilkey, T. B. Harman, and B. Banerjee. An Eulerian-Lagrangian approach for simulating explosions of energetic devices. *Computers and Structures*, 85:660–674, 2007.
- [16] J. E. Guilkey, J. B. Hoying, and J. A. Weiss. Modeling of multicellular constructs with the material point method. *Journal of Biomechanics*, 39:2074–2086, 2007.
- [17] P. J. Smith, M. Hradisky, J. Thornock, J. Spinti, and D. Nguyen. Large eddy simulation of a turbulent buoyant helium plume. In *Proceedings of the 2011 companion on High Performance Computing Networking, Storage and Analysis Companion*, SC '11 Companion, pages 135–136, New York, NY, USA, 2011. ACM.
- [18] J. Spinti, J. Thornock, E. Eddings, P. Smith, and A. Sarofim. Heat transfer to objects in pool fires, in transport phenomena in fires. In *Transport Phenomena in Fires*, Southampton, U.K., 2008. WIT Press.
- [19] B. A. Kashiwa. A multifield model and method for fluid-structure interaction dynamics. Technical Report LA-UR-01-1136, Los Alamos National Laboratory, Los Alamos, 2001.
- [20] G. Krishnamoorthy, S. Borodai, R. Rawat, J. P. Spinti, and P. J. Smith. Numerical modeling of radiative heat transfer in pool fire simulations. In *ASME 2005 International Mechanical Engineering Congress (IMECE2005)*, November 2005.
- [21] G. Krishnamoorthy, R. Rawat, and P. Smith. Parallelization of the p-1 radiation model. *Numerical Heat Transfer Part B: Fundamentals*, 49(1):1–17, 2006.
- [22] J. Luitjens. *The Scalability of Parallel Adaptive Mesh Refinement Within Uintah*. PhD thesis, University of Utah, 2011.
- [23] J. Luitjens and M. Berzins. Improving the performance of Uintah: A large-scale adaptive meshing computational framework. In *Proceedings of the 24th IEEE International Parallel and Distributed Processing Symposium (IPDPS10)*, page (accepted), 2010.
- [24] Q. Meng, M. Berzins, and J. Schmidt. Using hybrid parallelism to improve memory use in Uintah. In *Proceedings of the Teragrid 2011 Conference*. ACM, July 2011.
- [25] Q. Meng, J. Luitjens, and M. Berzins. Dynamic task scheduling for the uintah framework. In *Proceedings of the 3rd IEEE Workshop on Many-Task Computing on Grids and Supercomputers (MTAGS10)*, 2010.
- [26] P. Moin, K. Squires, and S. Lee. A dynamic subgrid-scale model for compressible turbulence and scalar transport. *Phys. Fluids*, 3(11):2746–2757, 1991.
- [27] P.K. Notz, R.P. Pawlowski, and J. C. Sutherland. Graph-based software design for managing complexity and enabling concurrency in multiphysics pde software. *ACM Transactions on Mathematical Software* (accepted).
- [28] J. O'Hern, E.J. Weckman, A.L. Gerharti, S.R. Tieszen, and R.W. Schefer. Experimental study of a turbulence buoyant helium plume. Technical Report SAND2004-0549, Sandia National Laboratories, 2004.
- [29] S. G. Parker. A component-based architecture for parallel multi-physics PDE simulation. *Future Generation Comput. Sys.*, 22:204–216, 2006.
- [30] S. G. Parker, J. Guilkey, and T. Harman. A component-based parallel infrastructure for the simulation of fluid-structure interaction. *Engineering with Computers*, 22:277–292, 2006.
- [31] R. Rawat, J. Spinti, W. Yee, and P. Smith. Parallelization of a large scale hydrocarbon pool fire in the uintah pse. In *ASME 2002 International Mechanical Engineering Congress and Exposition (IMECE2002)*, pages 49–55, November 2002.
- [32] P. Smith, R. Rawat, J. Spinti, S. Kumar, S. Borodai, and A. Violi. Large eddy simulation of accidental fires using massively parallel computers. In *AIAA-2003-3697, 18th AIAA Computational Fluid Dynamics Conference*, June 2003.
- [33] P. J. Smith, J. Thornock, D. Hinckley, and M. Hradisky. Large eddy simulation of industrial flares. In *Proceedings of the 2011 companion on High Performance Computing Networking, Storage and Analysis Companion*, SC '11 Companion, pages 137–138, New York, NY, USA, 2011. ACM.
- [34] J. Spinti, J. Thornock, E. Eddings, P. Smith, , and A. Sarofim. *Transport Phenomena in Fires*, chapter Heat Transfer to Objects in Pool Fires. WIT Press, 2008.