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Nonlinear Fluid Computations in a Distributed Environment

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Abstract

The performance of a loosely and tightly-coupled workstation cluster is compared against a conventional vector supercomputer for the solution of the Reynolds-averaged Navier-Stokes equations. The application geometries include a transonic airfoil, a tiltrotor wing/fuselage, and a wing/body/empennage/nacelle transport.

Decomposition is of the manager-worker type, with solution of one grid zone per worker process coupled using the PVM message passing library. Task allocation is determined by grid size and processor speed, subject to available memory penalties. Each fluid zone is computed using an implicit diagonal scheme in an overset mesh framework, while relative body motion is accomplished using an additional worker process to re-establish grid communication.

Introduction

It is anticipated that the high-order simulation of coupled aerodynamics, body dynamics, and controls on shared memory vector architectures will consume considerable resources. One approach which promises to reduce the cost of such computational prototyping is the use of distributed processor machines.

This effort investigates the use of workstation-class nodes linked by a peak 10 Megabit/s (Mbps) or 250 Mbps network. The work shown here uses a manager-worker Chimera^3 RANS solver^4 first implemented on a network of workstations^5 using the Parallel Virtual Machine (PVM) library. The primary issues of concern here relate to the parallel solution of large moving body problems such as would be encountered in a controlled aircraft simulation.

In order to evaluate the performance of manager-worker computation for realistic problems, three configurations are included in the following sections. Timings for a transonic airfoil, a transonic transport, and a tiltrotor fuselage/wing are given. The two-dimensional airfoil case is used to characterize the effects of boundary information lagging upon convergence and throughput. Scaling effects are shown by further decomposition of the grid system while retaining the highly implicit wall-normal direction. Finally, the addition of moving-body capability is examined using an oscillating airfoil case, with differing lag levels of the intergrid boundary points (IGBP).

Approach

Flow Solver

Solutions to the Reynolds-averaged Navier-Stokes (RANS) equations were computed with the implicit diagonal scheme of Pulliam and Chaussee^8 was used, implemented in the Chimera grid framework of Steger, Dougherty, and Benek. Euler implicit time marching and central second-order spatial differencing was used, with viscous wall conditions specified as no-slip, zero normal pressure gradient, and adiabatic. The Baldwin-Lomax algebraic turbulence model is used for all viscous walls. Information transfer across overset mesh boundaries was implemented using trilinear interpolation of the dependent variable vector, Q = [ρ, ρu, ρv, ρw, c]^T. The flow solver cost is about 6.5μs/cell/step on a Cray C90 head.

The flow solver Overflow-PVM has been developed from the Overflow overset grid flow solver^4 and the PVM (Parallel Virtual Machine) communication libraries. Parallelism is extracted on a coarse grid-by-grid level, and allows multiple grids to be solved on a single processor. During the run, the manager process primarily transfers flow boundary information (QBC)
amongst the worker nodes.

Relative grid motion is accomplished by the addition of a process to run the grid communication code, the Domain Connectivity Function (DCF). The process is directly linked to the manager and worker nodes, and can be executed at a specified frequency. The grid position and speeds may be lagged a given number of steps to allow for the overlap of the flow solver with the computation of the grid communication.

Grid Decomposition

Scaling studies were performed using zone decomposition of the initial overlapping grid system. Given a user-supplied number of subdomains, the decomposition scheme generates a minimal surface area set of grids and an input file for the DCF grid communication code. A search for a nearby decompositions which result in fewer surface points is also performed. The decomposition is constrained not to divide in the C-direction (θ in two-dimensions), which is typically the most implicit direction for wall-bounded viscous flows. This constraint also simplifies the search required by the algebraic turbulence model. The resultant set of grids contain one cell overlap with neighboring grids.

Load Balancing

A static load balancing algorithm has been developed to best match grids with processors such that idle time due to load imbalance is minimized. This first implementation of Overflow-PVM initiated solution on all grids simultaneously, including the case of multiple grids on a single node. Two problems with this approach became apparent for the solution of large problems on a limited cluster. Firstly, the context switching of the UNIX operating system caused system time overhead which is wasted on an otherwise idle processor. Secondly, and more importantly, solution of multiple grids in core can consume available RAM, causing swapping of processes to disk. In order to remove or reduce these losses, a modification to the control structure was made such that only a single grid can be active on each processor of the cluster. This drastically reduces context switching between worker processes, and swapping will only take place at the beginning and end of solution on each grid. Finally, the use of multithreaded code compilation and execution on shared-memory multiprocessor, and generally multiuser, machines was implemented.

In addition to the above improvements, a static load balancing method accounting for available RAM was implemented using the integer branch and bound method of the Microsoft Excel Solver. The method allows a cluster user to input available memory on each node and estimated network bandwidth, latency, and contention for each node. The use of virtual memory is implemented as a penalty rather than a constraint.

The inclusion of a memory variable in the load balancing scheme is required when cluster nodes of differing clock rates, but similar RAM, are considered. For large problems, not accounting for memory will cause the fastest CPU's to be allocated the most work units, eventually exceeding RAM capacity and inducing slow disk-paging virtual memory use.

The load-balancing algorithm for Overflow-PVM requires only node speeds (grid points/s) and available memory (grid points). For problems where grids are in relative motion, the transfer of boundary interpolant information must be periodically re-computed. If the flow solver is to be run sequentially with the grid communication, the above load balance remains unchanged. However, for cases in which DCF can be overlapped with the flow solution, current algorithm can be used by lowering the speed of the node on which DCF and the grid solvers execute to: DCF node speed=1/ [ 1/(p/s)+(IGBP/p) / (IGBP/s) ] where p=grid points, and IGBP=intergrid boundary points.

Non-Prescribed Relative Grid Motion

Loosely coupled body and fluid dynamics problems require the integrated fluid loads to be used as the forcing function of the body dynamics, and the updated body state to be used for boundary conditions of the fluid solver. Elimination of this serial bottleneck caused by the coupling will offer increased throughput, albeit at the sacrifice of some level of accuracy. However, a large class of problems exists for which the low ratio of body natural or forced frequency over fluid motion frequency scales indicate that lagging of boundary interpolants may not cause significant reductions in accuracy.

Figure 1 depicts a comparison of the the sequential and parallel methods. The sequential technique is shown for the case of lockstep update of the IGBP after each flow solver time step and no lead time for DCF. The parallel method overlaps DCF and Overflow by starting the DCF process lead steps before the updated grid communication solution will be required by Overflow. The frequency at which grid communication is re-established is given by idcfreq. Note that the metrics are updated every step, n, based on the load integration from the previous step.

The lagging example shown in Fig. 1a computes the integrated loads acting on the body in Overflow at step n - 1, uses these loads to compute the new body state, sends this state to the grid communication process DCF, and also uses the new body state for the flow solver step n. At time n + 1 the Overflow manager process waits for updated grid communication to be sent to the worker processes before signalling the start of the solution.

It is anticipated that this lagging would adversely effect accuracy when the ratio of applied+aero loads
to mass properties is large, i.e., accelerations are large or when fast relative grid motion exists. One disadvantage of the approach is that more total run-time nodes will be required, most dedicated to the flow solver and a few for the grid communication. However, this separation of flow solver and grid communication codes may make the coupled code more portable and maintainable because each code may be distributed the manner most appropriate.

The scheme implemented here also duplicated grid information for the DCF process, storing temporary grid and search map files in /tmp. This is done due to the requirement that the grid communication scheme generally will access all of the grids during the search for donor/receiver pairs. Accessing grid data from several nodes will incur heavy network load, competing with the flow solver nodes for the shared resource.

Results

In an effort to determine the highest throughput solution process, the Ethernet linked workstation cluster was used to evaluate the impact of lagged boundary updates and computation using 32 versus 64 bit word-sizes.

The cases were executed during low node and network use periods in single cluster-user mode on a set of cross-mounted workstations using PVM 3.2.3. No modification of the network topology was attempted, and the all of the nodes were on either of two subnets. Three gateways separated two of the pool of nodes from the master (measured using traceroute), with a point-to-point transmission time, shown by ping -f for an 8 KB datagram, of 300 ms on an otherwise idle network. This gives an effective bandwidth of 0.21 Mbps to these two distant nodes versus 0.35 Mbps measured between nodes with no intermediary gateways. For smaller datagrams, the lower collision rate increases the effective bandwidth to 8 and 2 Mbps for the near and distant nodes respectively.

The peak transfer rate of Ethernet is 10 million bits per second (Mbps), although during low-use periods the observed bandwidth of the cluster is about 2-9 Mbps, which can drop to 0.2 Mbps during normal use periods. For the large packets typically used in these computations, the discrepancy between observed and peak data transfer rates can be primarily attributed to contention, PVM-required memory to buffer copies, and latency.11

For a typical Chimera application, approximately 10% of the total grid points are IGBP's, each of which require the dependent variable vector, \( Q \), from another zone. In a distributed application, generally this information must be passed to another node. Overflow-PVM is implemented in a manager-worker arrangement, with the manager first parsing the grids to the worker processes, then receiving, updating, and resending large packets of boundary information at a user-specified rate. The solution from the run is collected following the final flow iteration.

Throughput timings for all of the cases were obtained either by monitoring CPU usage or by runs of 5-10 iterations, from which the zero iteration runtime was subtracted. Subtraction of start-up and wind-up costs also allowed good estimates for long-duration runs on an otherwise idle network. Data conversion (XDR) was not required for this set of nodes, and disk swapping not observed for any of the cases.

The static grid version of the code was also run on the High Performance Computing and Communication Program (HPCCP) IBM SP2 located at the Numerical Aerodynamic Simulator (NAS), using the PVMe message passing library. These cases were run in single grid per node mode, with timing numbers obtained in the same manner as on the loosely coupled cluster. Switching of interruptions did not affect timings appreciably for any of the configurations.

Steady Airfoil Case

The solution of the steady transonic flow about a 64a010 airfoil, depicted in Fig. 2, was computed to 1) quantify the effect boundary information lagging upon convergence and 2) to measure the scalability and accuracy of this domain decomposition method.

Figure 3 shows the effect on convergence of decomposing the grid from 3 zones into 30, with single cell overlap. Local time step scaling based on geomet-
ric considerations only was used for all of the cases: 
\[ \Delta t_{(i,j,k)} = \Delta t[1 + 0.005(1/\sqrt{V})]/[1 + 1/\sqrt{V}] \]. The
histories of the L2 norm for both the Ethernet linked workstation (32 bit words) and the IBM SP2 (64 bit words) are of similar trends. The differences in the high-frequency components of the history may be attributable to the elimination of fourth-order dissipation at the zone boundaries and to the inclusion of the overlapping boundary points in the computation of the residuals. The residual on the on the IBM SP2 converges an additional order of magnitude over the 32-bit wordsize cases.

Figure 4 compares \( C_p \) plots for the present cases compared to experiment and a high resolution single zone computation computed on a Cray C-90 (64 bit wordsize).\(^{12}\) The solutions are generally in agreement, although differences exist, and are most significant near the shock.

Figure 5 shows the speedup achieved for the foil problem over a differing number of nodes. The identity line represents ideal speedup, with speeds for single
node flow solver runs included for reference. The difference between ideal and actual speed is broken into two components. The first component contributing to lost capacity is that due to load imbalance, and is the speed the code would run given a perfect network, i.e. infinite bandwidth and zero latency. The second component contributing to the lost computational capacity is that attributable to message passing from one node to another, including time to pack (buffer copy), transmit (network latency and bandwidth), and unpack (buffer copy). The magnitude of this cost will depend both upon the number of IGBP and the ratio of surface area to volume, or IGBP/points. For this case the number of IGBP is 4827, and the total number of points is 49927. In general, the ratio of IGBP/points ranges from about 10 to 15%.

![Graph of capacity vs. number of nodes](image)

**Fig. 5: 64a010 Airfoil case: Scaling study**

Figure 5 also shows that it is advantageous to reserve the manager processor for communication alone for jobs where network contention is high. When the processor which contains the manager also has worker processes, the CPU is busy with the worker process when messages from completing remote processes return. The interrupted CPU then processes the incoming message before returning control to the worker process, with the concomitant adverse effect on throughput.

The difference in throughput seen between the 1 and 5 iterations per boundary Q update cases shown in Fig. 5 is indicative of the contention that is occurring for the network. Since exchange of boundary information comprises the bulk of the message traffic, decreasing this communication / computational time ratio decreases time to solution even though the number of CPU cycles is the same in either case.

An estimate of the loss in throughput due to the network can be computed from the time required to serially communicate the boundary Q information. The communication time for this geometry and precision is about 0.25 seconds: 5 words/point x 32 bits/word x 4.8 x 10^3 boundary points x 2 transmissions (one receive + one send) ÷ 6 x 10^6 bits/second. This communication cost causes a loss in throughput of about 30 kpts/s for the 10 node case. For the 5 iteration per boundary update cases, some of this loss is covered by computation as the different processes finish with larger intervening times.

By comparison of the 5 and 1 iteration per boundary update cases, it can be seen that the cost of updating the boundary information, Q, at each step is high. For the 10 node case, the throughput would be 35% higher, provided that convergence is unaffected.

However, inspection of Fig. 6 shows the marked effect lagging of boundaries has upon convergence for the 30 zone problem. When the boundary update is lagged for a single step (iter=2) the convergence rate drops dramatically, and is monotonically worse for increased lagging. The integrated C_{tp} includes the single cell overlap, and are presented for a comparison of the lagging levels only. Upon convergence the maximum Courant number was approximately 800 and the Courant number across the intergrid boundaries near the foil was about 10.

Figure 7 shows the computation of the airfoil case on the IBM SP2, a tightly coupled cluster of workstations connected by a 240 Mbps peak network. The native implementation, PVMe (similar to PVM 3.2.5), of the message passing library permitted runs with only a single process per node. Although throughput for the 30 zone case exceeds that of a Cray C-90 head, the code remains communication bound, as can be seen from inspection of the 5 and 1 iteration per boundary update cases. The resultant throughput for the single update per iteration case is 40% of that achievable on an ideal network. By taking the difference in times between the perfectly load balanced case and the single iteration per boundary update, the effective bandwidth for this problem was estimated at 35 Mbps. The peak network performance for PVMe on the machine is approximately 240 Mbps for large message sizes (100 KB), dropping off to about 120 Mbps for the estimated primary message size of 8 KB for the airfoil problem.

**Three-Dimensional Static Geometries**

Two geometries were used to evaluate the performance of Overflow-PVM for viscous problems in three-dimensions: a tiltrotor fuselage-wing, and a transonic transport. Scaling of the tiltrotor geometry, shown in Figs. 8 and 9, was computed by subdivision of the 9
zone grid system into 27 zones using the same preprocessing technique as used with the airfoil. The transport case, shown in Fig. 10, did not use additional subdivision for this study, resulting in significant load imbalance for large node number cases.

Figure 7 shows the throughput seen on the tightly coupled cluster for these cases. Comparison of the 9 and 27 zone tiltrotor cases shows that the throughput as a fraction of capacity increases, and is higher than that of a C-90 head for the more distributed case. However, for the 9 zone configuration the loss is primarily due to load imbalance, while network associated losses dominate for the 27 zone case. Again, the 5 iteration per boundary update case is shown to exemplify the communication losses, which consume roughly half of the total time per step. The 26 node
transport case shows much of the reduction from capacity is due to load imbalance. Comparison of the 26 node transport case and the 28 node tiltrotor case shows that the load imbalance for the former partially masks the communication with computation. The 28 node tiltrotor case, with a single step per boundary Q update (QBC), shows a throughput of 51% of the load balanced capacity, while the transport case shows 80% of the throughput that would be seen on an ideal net.

A summary of the results obtained on the Ethernet linked cluster is shown in Fig. 11 for both 32 and 64 bit words. The performance of the code on single nodes is shown for 64 bit floats, with the 32 bit values from Fig. 5 applicable for these cases. The 64 bit performance of the PA-RISC and MIPS nodes used for these cases was approximately half that seen with 32 bit words. The IBM RS6000 node, which performs similarly using single or double precision, is shown for reference only.

![Fig. 11: Three-dimensional cases](image)

The 64 bit transport case, which load balances to 90% efficiency, loses about 14 s per iteration to communication, implying an effective bandwidth of 5.5 Mbps. Using 5 iterations per boundary update decreases the communication overhead to 6 s. The nine zone tiltrotor case executed at 70% capacity using 5 iterations per update.

The 32 bit float tiltrotor cases given in Fig. 11 for 6 and 10 node machines again show the advantageous effect of using the manager node for communication alone. While the efficiency drops when the manager processor is allocated work according to processor speed, a positive trend is evident when the processor is allocated no grids. However, although throughput increases with increasing processors, the communication cost remains constant, with partial overlap of communication and computation due to higher load imbalance for the large machine cases. The communication cost is approximately 6 s for these tiltrotor cases, implying an effective bandwidth of 6 Mbps.

The 32 bit transport cases shown in Fig. 11 show increasing throughput from the 6 node to the 10 node case, but a negative trend from 10 to 18 nodes, despite the potentially communication covering high load imbalance. Using a 6 Mbps bandwidth, the communication cost for the 6, 10, and 18 node cases can be estimated at 6.4 s. Inspection of Fig. 11 shows that the difference between the ideal network cases and the 1 step per QBC update could be explained by 15 s /step communication cost. However, since the communication pattern is similar between the airfoil and tiltrotor cases, that is a large messages, a loss in effective bandwidth is not expected. The poor performance of the transport cases could be caused by cache misses owing to the large grids of this case, effectively lowering the load balanced throughput. The largest grids for the transport case had $1.2 \times 10^5$ points, as opposed to the $3 \times 10^4$ grids used in the tiltrotor case. However, the load balance plotted for the Fig. 11 cases uses the higher single node throughput values to uniformly represent the geometries.

Relative Grid Motion Cases

An oscillating 64a010 foil was used to measure the performance of the loosely coupled cluster for the coupled fluid/grid communication code. The grid system shown in Fig. 2 was used for this case, with the 14 foil-attached zones oscillating about the mid-chord with the remaining 16 grids fixed in inertial space. The interface between the moving and static grids is circular with uniform circumferential spacing. This topology removes effect of differing grid resolution between the zones, and provides a single relative grid speed to be evaluated for the boundary lagging cases.

The mean angle of attack was $-0.21^\circ$ with an oscillation magnitude of $1.01^\circ$ at a frequency of 25.6 Hz. The Reynolds number was $12 \times 10^6$ at a freestream Mach of 0.796, with a wall normal spacing of $10^{-5}$ of chord. A time step of $\Delta t = 10.2\mu s$ was chosen to maintain a Courant number near 0.7 across the zonal boundaries, although at the viscous wall the Courant number is approximately 700. Using this time step, the number of steps required per oscillation was approximately 3830.

The single node throughput speeds along the identity line in Fig. 12 were computed using the estimate of 10% of the grid points being IGBP, and that the grid communication is re-established at each time step. The single node computational cost of the coupled
code for large idcfrq would asymptotically approach about 1.1 times the static grid cases shown in Fig. 5 due to the computation of metrics at each time step. The body dynamics calculation is performed by the manager process, and adds a small computational cost at each step, and requires an additional manager to workers message of 57 floats and 9 integers. Although specified grid motion cases allow this 6-DOF computation to be distributed, the manager was allocated this work for the more general case of aerodynamically determined grid motion.

The load balance used for the 11 node lead=0, idcfrq=1 point was based on the flow solver speeds alone, since no overlap of the flow and grid communication calculation is possible. The breakdown of the times for this point are the sum of 0.5 s for the flow computation, 2.8 s for DCF, and 0.5 s for the IGBP communication. The communication of the boundary Q array is covered by the DCF process. The throughput for the corresponding 19 node case is improved only by the reduction in flow solver compute cost from 0.5 s to 0.34 s, since synchronization losses dominate.

In an attempt to reduce the impact of the grid communication process on the throughput, the use of multiple flow solution steps per IGBP update was investigated. However, for these moving body cases the QBC and the grid metrics were updated at each step. The 11 node lead=0, idcfrq=10 case shows that a speedup of 2.4 was achieved over the lead=0, idcfrq=1 case. However, based on the sum of the DCF communication, IGBP communication, flow computation, and QBC communication, speedup of 3.6 should be seen. This discrepancy of 0.26 s per flow step may be caused by decreased effective bandwidth or increased computation by the DCF process due to the larger search distance. For this case the flow processes were again idled during the DCF computation and communication. Again, only a marginal increase in throughput is seen for the corresponding 19 node case.

Reduction in the idle time of the flow processors was achieved by overlapping the grid communication process with the flow processes, shown as the lead=5, idcfrq=10 cases in Fig. 12. The 0.2 s per step difference between the lead=0, idcfrq=10 case and the lead=5, idcfrq=10 can be explained by the partial overlap of the DCF communication and the QBC communication with the Overflow processes. This overlap was confirmed by inspection of runtime node usage. However, as with the lead=0, idcfrq=10 case, the throughput seen by the coupled code was 60% of that expected based on the summation of the Overflow time and the QBC communication. Finally, the improvement seen by using 19 nodes is limited due to the loss of full overlap of the DCF and Overflow processes.

Figure 13 compares the lift and drag histories for the overlapping scheme and the reference case. The integrated loads include the single cell overlap, and are presented for a comparison of the lagging proce-
dure with the tightly coupled computation. The differences between the overlapping process, where lead=5, idcfrq=10, and the more tightly coupled lead=0, idcfrq=1 case is less than 1% at peak loading for this short time history.

The relative grid motion case of the oscillating airfoil showed performance of up to 80% of the Cray benchmark on the Ethernet linked cluster, albeit by lagging of grid communication information. The lagging and infrequent updates of the grid communication caused lift and drag coefficient errors of 1% for this case. Throughput losses over the steady cases included additional message volume due to the changing grid communication, and synchronization of the grid communication and flow solver processes.

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**Conclusions**

The results of this research would provide the designer with a means of computationally prototyping control systems in problematic nonlinear flight regimes, potentially avoiding costly loss of life and aircraft. However, large simulations of this type will be computationally expensive, providing the impetus for the development of parallel codes.

Currently, workstation clusters using using serial- ized networks provide capability for solution of moderately-sized steady CFD problems for the low-communication flow solvers of the type investigated here. For the airfoil problem considered here, the highest throughput would be achieved by exchanging boundary information at each iteration, using the manager processor for communication only. The well decomposed 2- and 3-D geometries on up to 19 nodes executed at approximately 50% of cluster capacity. The Ethernet linked cluster of HP (PA-RISC) and SGI (MIPS) nodes reached half of the throughput of a Cray C-90 head. Communication became the dominant source of scaling loss for increasing number of nodes.

Porting the code to the IBM SP2 (PVMe) resulted in performance exceeding that Cray C-90 head for the 2- and 3-D cases. However, the poor effective bandwidth observed with this manager-worker code again resulted in communication dominated losses. The well load balanced cases showed efficiencies of 40% of the corresponding zero-communication case.

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