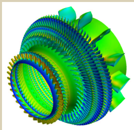

TFLO ALGORITHM DEVELOPMENT

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Motivation

- TFLO has access to a variety of ASCI computational facilities. Different processor/machine combinations effect the overall execution duration, but estimates for job length are now provided in months/years.

Component	Blade Rows	Grid Points (million)	% Wheel	Total CPU Hours (million)	Execution Duration
Turbine	9	94	16	3.0	510 days [1]
Compressor	23	N/A	16	7.7	1300 days [1]

[1] Estimates based on 500-1000 processors at 8 hours per day.

- For TFLO to be utilized as an effective tool for the design engineer, the execution time should be quantified in hours.
- TFLO is currently based on a fully implicit dual time stepping algorithm utilizing a nested system of loops. The outer iteration advances the solution forward in physical time, while the inner iterations minimize the residual at each time step.
- Three separate approaches are currently under development to improve the efficiency of TFLO.
  - Improve the discretization of the time accurate equations. This potentially provides efficiency improvements in the time accurate resolution of the solution (the outer loop).
  - Improve the convergence rates of the multigrid solver, offering a potential reduction in the computational effort per time step (the inner loop).
  - Take advantage of the forced periodicity in the solution, and use a non-linear frequency domain method to provide an efficient initial solution for a fully time accurate calculation.

Non-Linear Frequency Domain Methods

- Time accurate solvers capture any arbitrary time history in the solution field. In turbomachinery applications end users are only concerned with the data once the solution has reached a periodic steady state.
- Conventional solution algorithms waste computational effort resolving the decay of the initial transients; hence the efficiency of any time accurate solver is a function of the decay rate of these transients. In compressor/turbine calculations the blades and stators reflect the unsteady pertubations. The transmission of these waves back and forth through the machine effectively decreases the decay rate of the initial transients.
- In engineering applications it seems possible to obtain sufficient accuracy in practice with a small number of temporal modes, some-times only a single dominant mode.
- The Non-Linear Frequency Domain (NLFD) method could be used to obtain a reduced order solution. The cost of this solution is an order of magnitude less than the current state of the art in time-accurate calculations. If additional accuracy is required, this solution could be used to seed a fully time accurate simulation.
- Advantage: The cost of the NLFD solver is a function of the number of temporal modes multiplied by the cost of a single steady state computation. The computational cost is decoupled from the physical decay rates of the problem.
- Disadvantage: NLFD methods fall under the larger class of reduced order modeling. Because we are intentionally neglecting temporal modes to improve computational efficiency it is impossible to determine the temporal accuracy a priori.

Linearized Scheme

- Approximating the flux vectors as a Taylor series expansion.

$$f(w^{n+1}) = f(w^n) + A\Delta w + \mathcal{O}(||\Delta w^{(n)}||^2)$$
$$g(w^{n+1}) = g(w^n) + B\Delta w + \mathcal{O}(||\Delta w^{(n)}||^2)$$

- We can obtain the linearized scheme expressed below.

$$\left\{I + \frac{2\Delta t}{3}(D_x A + D_y B)\right\}\Delta w^n = \frac{1}{3}\Delta w^{n-1} - \frac{2\Delta t}{3}R(w^n)$$

- Advantage: The scheme has the advantage of being second order accurate in time, and A-stable if the physical equations are stable
- Disadvantage: The scheme requires a nested system of loops. The inner loop requiring a number of multigrid cycles to solve the above equation. The outer loop advances the solution forward in physical time.

Fully Implicit Dual Time Stepping Scheme

- TFLO currently implements a fully implicit dual time stepping algorithm. The time derivative is discretized as a backward difference formula and solved at each time step.

$$\frac{\partial w}{\partial \tau} + \left[\frac{3w^{n+1} - 4w^n + w^{n-1}}{2\Delta t} + D_x f(w^{n+1}) + D_y g(w^{n+1})\right] = 0$$

- Advantage: If the inner iterations converge fast enough, we solve a fully nonlinear BDF, giving an efficient A-stable scheme allowing very large time steps.
- Disadvantage: No way of accessing accuracy unless the inner iterations are fully converged. If a large number of inner iterations are required, the scheme becomes expensive.

Lower Upper Symmetric Gauss-Seidel

- The conservation equations can be expressed with an linearized implicit scheme. If $\mu = 1$ and $\Delta t \to \infty$ this becomes a Newton iteration.

$$\{I + \mu\Delta t\,(D_x A + D_y B)\}\,\delta w + \Delta t R = 0$$

- The symmetric Gauss-Seidel scheme can be conveniently illustrated for a one-dimensional problem. Consider the following flux-split scheme.

$$\left\{I + \lambda\left(\delta_x^+ A^- + \delta_x^- A^+\right)\right\}\delta w + \Delta t R = 0$$

where $\lambda = \frac{\Delta t}{\Delta x}$

- A symmetric Gauss-Seidel scheme can be applied to the above equation. After some mathematical manipulation the scheme can be expressed in the following equation.

$$\left\{I + \lambda\left(A_i^+ - A_i^-\right)\right\}\delta w_i^{(2)} + \lambda A_{i+1}^- \delta w_{i+1}^{(2)} = \left\{I + \lambda\left(A_i^+ - A_i^-\right)\right\}\delta w_i^{(1)}$$

- This expression can be expressed as the matrix multiplication of a lower, diagonal, and upper matrix.

$$LD^{-1}U\delta w = -\Delta t R$$

- Following this line of reasoning, the LU-SGS scheme can be recast in a fully non-linear form. In the limit as the time step goes to infinity, these equations represent the SGS Newton iteration.

$$\{I + \frac{\Delta t}{\Delta x}|A|\}\delta w_i^{(1)} = -\Delta t R_i^{(01)}$$
$$\{I + \frac{\Delta t}{\Delta x}|A|\}\delta w_i^{(2)} = -\Delta t R_i^{(12)}$$

Non-Linear Equations Recast in the Frequency Domain

- The Navier-Stokes equations can be expressed in simplified form

$$\frac{\partial w}{\partial t} + \frac{\partial}{\partial x}f(w) + \frac{\partial}{\partial y}g(w) = 0$$

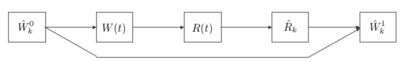
- Using finite volume techniques the above equation can be rewritten as the sum of volumetric and surface integrals. Approximating the volumetric integral as the product of the cell volume and the time derivative, we can rewrite the above equation in simplified form.

$$V\frac{\partial W}{\partial t} + R(W) = 0$$

- Assuming that the solution and residual are periodic over the same time period. We can recast the above equation into the frequency domain. Adding in a pseudo time derivative term allows us to march this transformed system forward to a stationary state.

$$V\frac{d\hat{W}_k}{d\tau} + ikV\hat{W}_k + \hat{R}_k = 0$$

- The non-linear residual term is calculated in physical space and time. The term is transformed to the frequency domain using a Fast Fourier Transform. A typical solution iteration implements the following data flow diagram.



ADI Scheme with BDF

- Replacing the left hand side of the linearized BDF scheme by an approximate factorization will produce the modified ADI scheme.

$$\left(I + \frac{2\Delta t}{3}D_x A\right)\left(I + \frac{2\Delta t}{3}D_y B\right)\Delta w^n = \frac{1}{3}\Delta w^{n-1} - \frac{2\Delta t}{3}R(w^n)$$

- Advantage: Nominally second order accurate in time. The scheme can be solved at a low computational cost in two steps.
- Disadvantage:The factorization error dominates at large CFL numbers. The scheme is not amenable to parallel processing if applied separately in each of a large number of blocks.

Hybrid Scheme

- The proposed hybrid scheme with take an ADI step in real time yielding nominal second order accuracy without iterations.

$$\left[I + \frac{2\Delta t}{3}D_x A\right]\left[I + \frac{2\Delta t}{3}D_y B\right]\Delta w^{(1)} + \frac{2\Delta t}{3}R(w^n) - \frac{1}{3}\Delta w^{n-1} = 0$$

- Then follow it with the iterative multistage time stepping scheme augmented by multigrid to drive the solution in the steady state limit towards the fully non-linear BDF.

$$\Delta w^{(k)} - \Delta w^{(k-1)} + \beta_k\left\{\frac{3w^{n+1} - 4w^n + w^{n-1}}{2\Delta t} + D_x f(w^{n+1}) + D_y g(w^{n+1})\right\} = 0$$

- Advantage: Formal second order accuracy is guaranteed with any number of iterations. It should not be necessary to iterate to convergence within each time step.
- Disadvantage:The additional iterations with multigrid should provide information exchange between processors which is needed to stabilize the ADI scheme separately in each processor.

LU-SGS Convergence

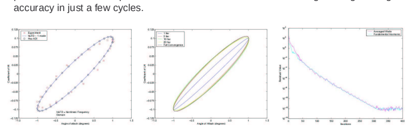
- The convergence rates of the global characteristics in the solution field are provided below. The data in the table verify that the lift and drag coefficients are within 1% of their iteratively converged values after only 3 multigrid cycles, and to within a fraction of 1% after only 5 cycles.

Case	MG Cycles	E-CUSP CL	ECUSP CD	HCUSP CL	HCSUP CD
RAE 2822	50	1.1452	0.0488	1.1417	0.0485
M=0.75	5	1.1469	0.0488	1.1434	0.0485
Alpha=3.00	3	1.1543	0.0496	1.1515	0.0497
NACA 0012	50	0.3812	0.0578	0.3753	0.0575
M=0.85	5	0.3787	0.0576	0.3721	0.0573
Alpha=1.00	3	0.3742	0.0575	0.3634	0.0566
NACA 0012	50	0.3742	0.0239	0.3725	0.0238
M=0.80	5	0.3760	0.0239	0.3744	0.0239
Alpha=1.25	3	0.3840	0.0240	0.3829	0.0240

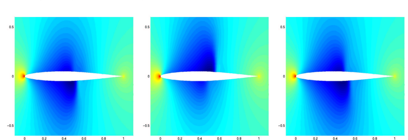
- The asymptotic convergence rates of the scheme are significantly faster than previous results using the well tuned Runge-Kutta multigrid method of Jameson and the diagonalized method of Caughey.
- The CPU time per multigrid cycle is about 50% less than that of the above mentioned methods, indicating that converged solutions can be obtained with almost an order of magnitude less computer time.
- Tests have been carried out for one-dimensional channel flow with area change. With increasing number of blocks, the monotonicity of the convergence is hard to maintain, although the overall convergence rate remains very similar.

NLFD - Pitching Airfoil

- Temporal Resolution: Provided below is a comparison of the coefficient of lift produced by NLFD, hybrid ADI and experimental results. The NFLD results show excellent agreement with the other simulations while using only one harmonic.
- Convergence Results: Plots of the residual and coefficient of lift convergence are provided below. Global parameters such as coefficient of lift converge to engineering accuracy in just a few cycles.



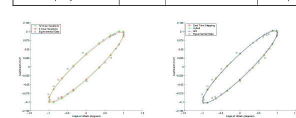
- Solution Contours: Contours of pressure are provided below at different instances in time corresponding to different angles of attack.



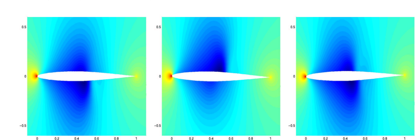
Hybrid-ADI Pitching Airfoil

- The unsteady Euler equations were solved for an oscillating airfoil. The parameters of this numerical experiment were chosen to allow comparison to experimental results from AGARD Report 702.

Parameter	Value	Parameter	Value
Angle of attack variation	1.01 degrees	Mach number	0.796
Reduced frequency of oscillation	0.212	Grid size	161 x 33 points



- Solution Contours: Contours of pressure are provided below at different instances in time corresponding to different angles of attack.



LU-SGS Dual Time Stepping Scheme

- The non-linear LU-SGS scheme can also be applied to unsteady flow calculations. The factorization and linearization errors can be eliminated from this algorithm. Furthermore, the computational cost of this scheme is similar to that of a 4-stage Runge-Kutta explicit scheme.
- Applying LU decomposition to the fully implicit backward difference formula results in the following expression.

$$LD^{-1}U\Delta w^n + \frac{2\Delta t}{3}R(w^n) - \frac{1}{3}\Delta w^{n-1} + \mathcal{O}(||\Delta w^2||) + \mathcal{O}(\Delta t^2) = 0$$

- To permit large time steps, the factorization and linearization errors are eliminated by the introduction of additional terms. After some mathematical manipulation, the expressions are simplified into the following form.

$$LD^{-1}U\quad(\Delta w^k - \Delta w^{k-1}) + \underbrace{\left\{I + \frac{2\Delta t}{3}(D_x A + D_y B + D_z C)\right\}\Delta w^{k-1} + \frac{2\Delta t}{3}R(w^n) - \frac{1}{3}\Delta w^{n-1}}_{\text{linearized total residual}} + \mathcal{O}(||\Delta w^2||) = 0$$

- Following the approach of the non-linear LU-SGS scheme the linearization error can be eliminated. The final form of the proposed algorithm can be recast as follows.

$$LD^{-1}U(\Delta w^k - \Delta w^{k-1}) + \underbrace{\frac{3}{2\Delta t}w^{k-1} - \frac{2}{\Delta t}w^n + \frac{1}{2\Delta t}w^{n-1} + R(w^{k-1})}_{\text{nonlinear total residual}} = 0$$

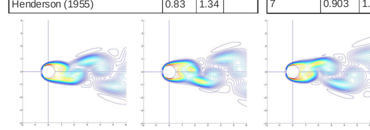
- The evaluation of the modified residual requires no more effort than regular dual time stepping algorithms. The first iteration is basically a non-linear LU-SGS scheme with factorization. The following iterations are used to eliminate the factorization error. Since each time step is formally second order accurate, only a small number of iterations should be required.

NLFD - Unsteady Cylinder

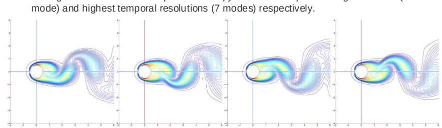
- The unsteady Navier-Stokes equations were solved for cylinder flow at a Reynolds number of 180. Numerical results for global coefficients are compared below to experimental data as a function of temporal resolution used to compute the solution.

Experiment	$-C_{pb}$	C_d	S_t
Williamson and Roshko (1990)	0.83		
Roshko (1954)			0.185
Wieselsberger (1922)		1.3	
Henderson (1955)	0.83	1.34	

Modes	$-C_{pb}$	C_d
1	0.832	1.257
3	0.895	1.306
5	0.903	1.311
7	0.903	1.311



- The figures above and below provide entropy contours computed using the lowest (1 mode) and highest temporal resolutions (7 modes) respectively.



Conclusions

- The Stanford ASCI team has successfully developed three new numerical schemes in a methodical approach to improve the efficiency of unsteady solver technologies. An LU SGS scheme was developed to improve the convergence rates of inner iterations within the TFLO solver. A Hybrid ADI scheme was developed as a method to improve the efficiency of the outer iterations in the TFLO solver. Finally, NLFD methods were developed to offer a reduced order model capable of quickly finding an initial solution to seed a time accurate calculation.
- Lower Upper Symmetric Gauss-Seidel: This scheme was developed and tested on the steady Euler equations. This scheme exhibited an order of magnitude improvement in computational cost as compared to current TFLO schemes. Modifications to the scheme have been developed for the unsteady Navier-Stokes equations.
- Hybrid Alternating Direction Implicit: This scheme was developed and tested on the unsteady Euler equations. This scheme provides a guaranteed second order accuracy with a nominal number of inner iterations.
- Non-Linear Frequency Domain: This scheme was developed and tested on both the unsteady Euler and Navier-Stokes equations. The results show that a limited number of temporal modes can accurately resolve complex viscous fluid mechanics. The cost of the scheme is proportional to the cost of the steady calculation multiplied by the number of temporal modes specified by the user.