Accelerated Solvers for CFD

Co-Design of Hardware/Software for Predicting MAV Aerodynamics

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People

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Overview

- Current Efforts
- Long Term Plan
  - Parallel, Accelerated Solvers and Preconditioners for CFD Applications
- Quick Intro to Krylov Methods and Preconditioners
- Recycling Krylov Subspaces for GenIDLEST
  - (but results for an acoustics problem)
- GPU Preconditioners for SENSEI (LDC)
- Conclusions and Future Work

Current Efforts

- Integrating innovative iterative solvers and preconditioners in CFD codes
  - GENIDLEST (Tafti) – Recycling Solvers rGCROT (+ rBiCGStab)
  - SENSEI (Roy) – Fast Preconditioning (plus recycling)
- Faster Krylov-based time integrators (Sandu)
- Solvers that have better convergence, especially for sequences of problems – Krylov recycling
- GPU Acceleration, especially preconditioners
- New solvers with better opportunities to optimize multiple matvecs, precvecs, orthogonalizations in addition to faster convergence
- Updating preconditioners and further efficient variants of preconditioners

Long Term Plan (including CFD appl.s)

- Basic issue is "#iterations vs cost per iteration"
- All methods consist of different arrangements of matvecs, precvecs, dots, daxpy (and computing preconditioners)

<u>Faster Preconditioners on GPUs</u>

- Preconditioners with high level of fine grained parallelism and little data movement
  - Often not as effective (more iterations)
- Precludes ILU and preconditioners related to/based on it
  - Domain decomposition has local (approx) solve
- SAI very fast on GPUs (matvec); can improve convergence by multilevel extension
- FSAI promising too (matvec-like but more effective than SAI)
- Multigrid also promising if smoother fast

Long Term Plan

<u>Solvers and Preconditioners</u>

- Many problems require solving slowly changing systems for many parameters, many rhs, in nonlinear iteration or optimization, etc: Improve convergence across systems
- Recycling Krylov subspaces (select and reuse)
- Recycling preconditioners (update and reuse)
- Faster solver allows weaker preconditioner for cheaper iterations
- Solver variants that allow substantially faster implementations of main kernels by rearranging parts of algorithm (possibly over multiple iterations) – recycling solvers have advantageous over standard solvers
- Use model reduction to solve multiple systems much faster

Important Trends

- Simulations increasingly part of larger analysis, including design, uncertainty/reliability, inverse problems
- Simulations often involve parameters/parameter space
- Simulations involve wide ranges of scales and multi-physics. Drastically reduce effective number of unknowns: model reduction, parameterizing problems, adaptive meshing
- Move from generic models with idealized properties to realistic models individualized by parameterization (with uncertainty) – models first calibrated and then simulated
- Simulation also used to find parameters that cannot be measured directly
- New architectures for HPC require new algorithms, but significant support for solving many related problems

Krylov Methods Crash Course

Solve $Ax = b$, initial solution x_0, residual $r_0 = b - Ax_0$

Solve for error, $Ae_0 = r_0$; find update from search space

Generate space: $K_m\left(A, r_0\right) = \mathrm{span}\left\{r_0, Ar_0, A^2 r_0, \ldots, A^{m-1} r_0\right\}$

Find update $z_m \in K_m\left(A, r_0\right)$ by minimizing

- error in suitable norm (typically special matrices only)
- residual in suitable norm (e.g., GMRES)

Implemented through orthogonal projection (in suitable inner product) – can be expensive.

Alternatively, give up on minimization and compute a cheap projection. Fast but possible robustness problems, e.g, BiCGStab.

Preconditioning

What if convergence slow? Precondition the system.

Replace $Ax = b$ by $P_1AP_2\tilde{x} = P_1b$ and $x = P_2\tilde{x}$

Where

1. Fast convergence for P_1AP_2 and
2. Products with P_1 and P_2 is cheap
3. Computing P_1 and P_2 not too expensive

Often $A \approx LU$ (ILU) and use $L^{-1}AU^{1}$ or $U^{-1}L^{-1}A$

Forward-backward solve often slow on GPUs
Generally problematic for parallelism – do only for diagonal blocks (subdomain or grid line, etc)

Sparse Approx. Inverse Preconditioners

Preconditioners are matvec like (no solves)

Consider $Ax = b \rightarrow AM\tilde{x} = b$

(1) Sparse Approximate Inverse – SAI / SPAI

Pick sparsity pattern of M and min. $\left\| AM - I \right\|_F$

Embarrasingly parallel, many tiny LS problem

Pattern often subset of A^k (dynamic possible)

(2) Factorized Sparse Approximate Inverse – FSAI

Compute $A^{-1} \approx ZDW^T$ (biconjugation process)

with Z, W sparse, uppertriangular, D diagonal

Krylov Methods Crash Course

Consider $Ax = b$ (or prec. system $PAx = Pb$)
Given x_0 and $r_0 = b - Ax_0$, find optimal update z_m in

$$K^m(A, r_0) = \text{span}\{r_0, Ar_0, \ldots, A^{m-1}r_0\}:$$

$$\min_{z \in K^m(A,r_0)} \left\| b - A(x_0 + z) \right\|_2 \quad \Leftrightarrow \quad \min_{z \in K^m(A,r_0)} \left\| r_0 - Az \right\|_2$$

Let $K_m = \left[r_0 \; Ar_0 \; A^2 r_0 \cdots A^{m-1} r_0 \right]$, then $z = K_m \zeta$,

and we must solve the least squares problem

$$AK_m \zeta \approx r_0 \quad \Leftrightarrow \quad \left[Ar_0 \; A^2 r_0 \cdots A^m r_0 \right] \zeta \approx r_0$$

Set up and solve in elegant, efficient, and stable way:
GCR – Eisenstat, Elman, and Schulz '83
GMRES – Saad and Schulz '86

Minimum Residual Solutions: GMRES

Solve $Ax = b$: Choose x_0; set $r_0 = b - Ax_0$;

$v_1 = r_0 / \left\| r_0 \right\|_2$, $k = 0$.

while $\| r_k \|_2 \geq \varepsilon$ do

$k = k + 1$; $\tilde{v}_{k+1} = Av_k$;

for $j = 1 \ldots k$,

$h_{j,k} = v_j^* \tilde{v}_{k+1}$; $\tilde{v}_{k+1} = \tilde{v}_{k+1} - h_{j,k} v_j$;

end

$h_{k+1,k} = \left\| \tilde{v}_{k+1} \right\|_2$; $v_{k+1} = \tilde{v}_{k+1} / h_{k+1,k}$; $\quad (A V_k = V_{k+1} \underline{H}_k)$

Solve/Update LS $\min_\zeta \left\| \eta_1 \left\| r_0 \right\|_2 - \underline{H}_k \zeta \right\|_2$

end

$x_k = x_0 + V_k \zeta$;

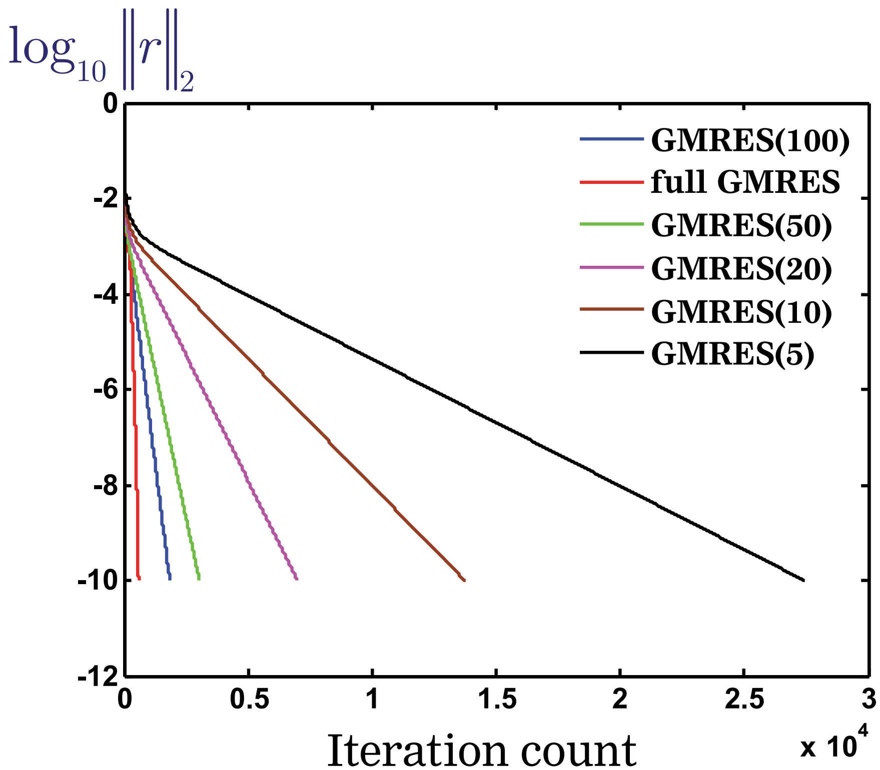
$r_k = r_0 - V_{k+1} \underline{H}_k \zeta$ or $r_k = b - Ax_k$

Convergence restarted GMRES

Test problem on unit square: 202×202 grid points

Interior: $-\nabla \cdot (\nabla u) = 0$ Boundary $u = 1$ for $x = 0$ and $y = 1$

$u = 0$ elsewhere



GMRES(m)	200 x 200 unknowns	
	time (s)	iterations
full	72.888	587
100	40.256	1851
50	41.087	3043
20	63.604	6985
10	111.26	13761
5	199.42	27451

BiCGStab

van der Vorst '92

from: Iterative Solvers for Large Linear Systems, H.A. van der Vorst Cambridge University Press

x_0 is an initial guess; $r_0 = b - Ax_0$
Choose $\widetilde{r}$, for example, $\widehat{r} = r_0$
for $i = 1, 2, \ldots$
  $\rho_{i-1} = \widetilde{r}^T r_{i-1}$
  if $\rho_{i-1} = 0$ method fails
  if $i = 1$
    $p_i = r_{i-1}$
  else
    $\beta_{i-1} = (\rho_{i-1}/\rho_{i-2})(\alpha_{i-1}/\omega_{i-1})$
    $p_i = r_{i-1} + \beta_{i-1}(p_{i-1} - \omega_{i-1}v_{i-1})$
  endif
  $v_i = Ap_i;$
  $\alpha_i = \rho_{i-1}/\widetilde{r}^T v_i$
  $s = r_{i-1} - \alpha_i v_i$
  check $\|s\|_2$, if small enough: $x_i = x_{i-1} + \alpha_i p_i$ and stop
  $t = As$, $\omega_i = t^T s / t^T t$
  $x_i = x_{i-1} + \alpha_i p_i + \omega_i s$
  $r_i = s - \omega_i t$
  check convergence; continue if necessary
  for continuation necessary that $\omega_i \neq 0$
end

Solving Sequences of Linear Systems

- Many applications involve a sequence/group of systems with small or localized changes in space or structure
  - Time-dependent/time-like problems, nonlinear problems and optimization, adaptive discretizations
  - Systems depend (nonlinearly) on multiple parameters
  - Inverse problems, parameter estimation, Monte Carlo and MCMC methods, design, model reduction
  - Uncertainty quantification, reliability (with design)
- Application requires solution of hundreds to thousands of large, sparse, linear systems (millions for MCMC)
- Recycle previously computed results for faster solution
  - Update old solutions
  - Update and reuse search spaces – Krylov recycling
  - Update preconditioners

What to Recycle?

- Krylov methods build search space; solution by projection
- Building search space often dominates cost
- Initial convergence often poor, reasonable size search space needed, then superlinear convergence
- Get fast convergence rate and good initial guess immediately by recycling selected search spaces from previous systems
- How to select the right subspace to recycle?
  - Approximate invariant subspaces
  - Canonical angles between successive spaces
  - Subspace from previous solutions

How to Recycle?

(GCRO, dS'95)

Solve $Ax = b$ with recycled subspace $\tilde{U}$ (for new A):

Compute $A\tilde{U} = \tilde{C}$, $CR = \tilde{C}$ (QR), $U = \tilde{U}R^{-1}$ (implicit)
Now $AU = C$ and $C^*C = I$

Set $r_0 = \left(I - CC^*\right)b$, $x_0 = UC^*b$, and $v_1 = r_0 / \|r_0\|$
Augmented Arnoldi: $AV_m = CB + V_{m+1}\underline{H}_m$
Minimize:

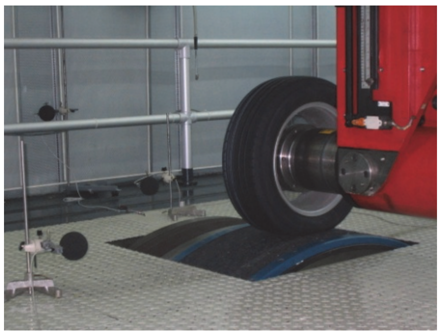
$$\left\|b - A\left(x_0 + Uz + V_m y\right)\right\| = \left\|V_{m+1}\left(e_1\|r_0\| - \underline{H}_m y\right) - C\left(z + By\right)\right\|$$

Solve $\underline{H}_m y \approx e_1\|r_0\|$ and set $z = -By$ (optimal)
$x_m = x_0 + Uz + V_m y$ and $r_m = V_{m+1}\left(e_1\|r_0\| - \underline{H}_m y\right)$

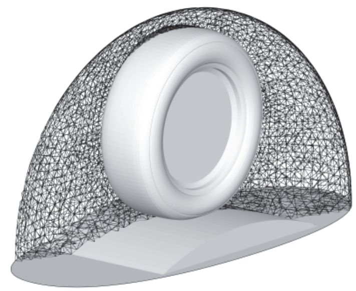
Multiple matvecs/precvecs at once, orthogonalizations not in lock-step (GMRES), m small more U / C vectors

Example: Acoustics Problem

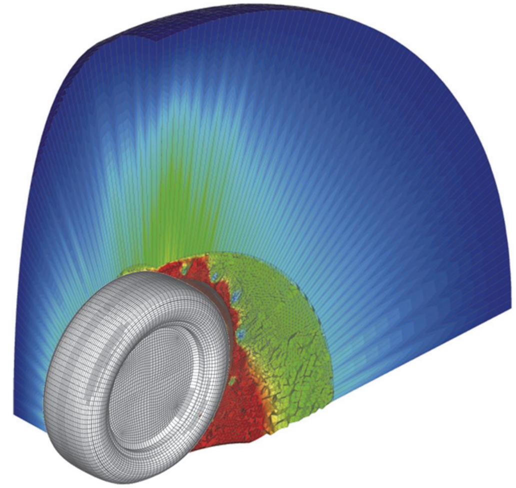
with Bierman (BMW)



Real
experiment



Part of the
acoustic
FE mesh



Acoustic FE/IFE mesh
with solution

Details small model problem:

- 2nd order acoustic Finite Elements
- 6th order acoustic Infinite Elements
- ~10,000 degrees of freedom
- about 150 frequencies to be evaluated

On large realistic problem factor 6 to 10 speedup in time

Discretization

Variational form and resulting matrix components:

$$\int_{\Omega} (\nabla p \cdot \nabla \bar{q} - k^2 p \bar{q}) \,\mathrm{d}V - \int_{\mathsf{S}_N} \mathrm{i}\rho\omega v_n^o p \bar{q} \,\mathrm{d}\mathsf{S} - \int_{\mathsf{S}_R} \mathrm{i}k\alpha p \bar{q} \,\mathrm{d}\mathsf{S} = 0$$

$$K_{ij} = \int_{\Omega^e} \nabla N_i \nabla N_j \,\mathrm{d}V,$$

$$K_{ij} = \int_{\Omega^e} (\nabla D \Phi_i + \nabla \Phi_i D) \nabla \Phi_j \,\mathrm{d}V,$$

$$M_{ij} = 1/c^2 \int_{\Omega^e} N_i N_j \,\mathrm{d}V,$$

$$M_{ij} = 1/c^2 \int_{\Omega^e} (1 - (\nabla \mu \nabla \mu)) \Phi_i \Phi_j D \,\mathrm{d}V,$$

$$C_{ij} = \rho \int_{\mathsf{S}_R^e} \alpha N_i N_j \,\mathrm{d}S.$$

$$C_{ij} = 1/c \int_{\Omega^e} (\nabla \mu \nabla \Phi_j) D \Phi_i - (\nabla D \nabla \mu) \Phi_i \Phi_j - (\nabla \Phi_i \nabla \mu) D \Phi_j \,\mathrm{d}V, + 1/c \int_{\mathsf{S}_R^e} \alpha \Phi_i \Phi_j D \,\mathrm{d}S.$$

$$f_i = -\mathrm{i}\omega \int_{\mathsf{S}_N^e} \rho v_n^o N_i \,\mathrm{d}S.$$

Tire Rolling Noise Modeling

Equations interior and exterior acoustics simulation

$$A(\omega)p = \left(K + i\omega C - \omega^2 M\right)p = f(\omega)$$

RHS depends on excitation frequency (from road texture)

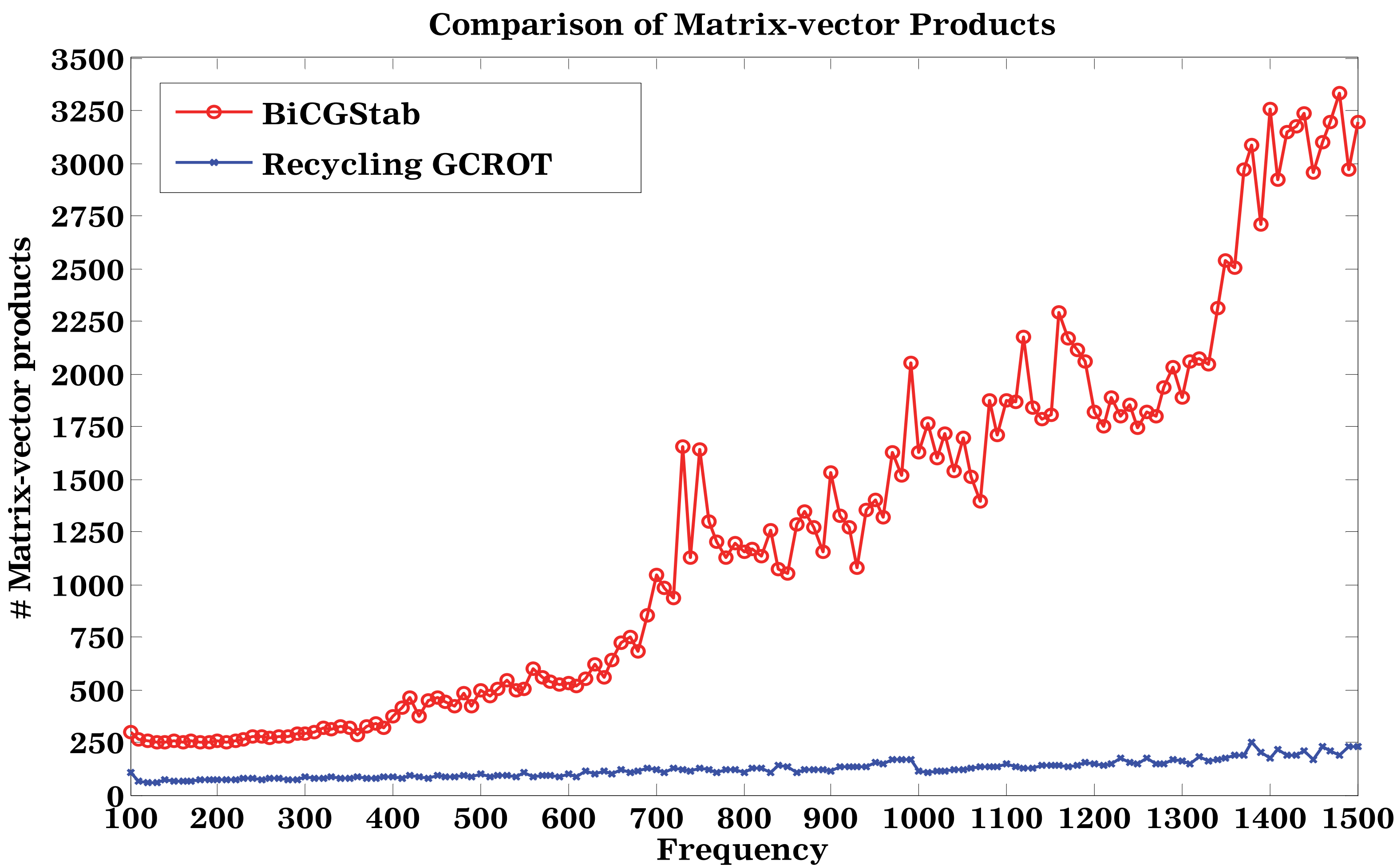
Problem to be solved for $\omega = 100, \ldots, 1500$ and $\Delta\omega = 10$

Must solve 140 linear systems (for small model problem)
For full problem up to 500 frequencies

Matrix components from interior domain are symmetric; the components from exterior domain are nonsymmetric

In general, the exterior domain component is not a low rank update

Acoustics – rGCROT vs BiCGStab in # Matvecs



Preconditioning in SENSEI (LDC)

- Standard ILU type preconditioners require mostly sequential forward/backward solve
  - Mitigated by Block ILU (#blocks - #threads)
- Parallelizes poorly on GPUs (not high level of fine-grained parallelism)
- In contrast sparse MatVec very fast
- Replace by other preconditioners that are more sparse MatVec like
  - Variants of Sparse Approximate Inverses (vary solver)
  - Next, combine with multilevel acceleration for convergence
  - Block Jacobi (small blocks)
- Solver GMRES, BiCGStab, recycling GCROT (almost)

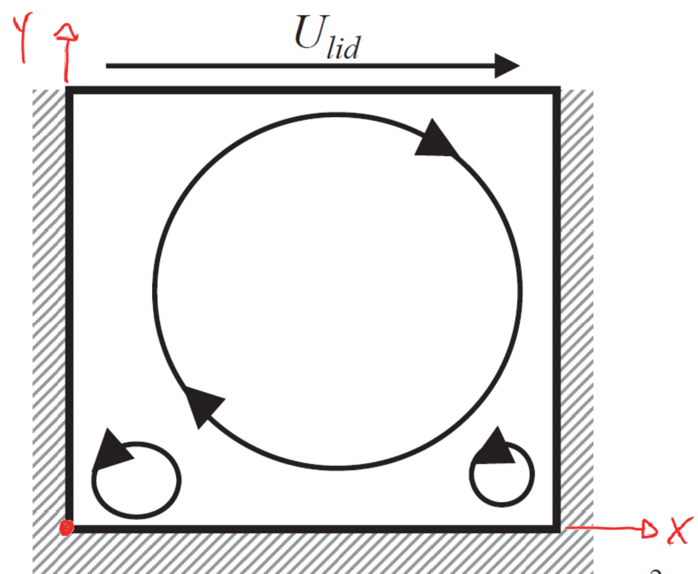
LDC Problem

Incompr. Navier-Stokes with Artificial Viscosity

$$\frac{1}{\beta^2}\frac{\partial p}{\partial t} + \rho\frac{\partial u}{\partial x} + \rho\frac{\partial v}{\partial x} = -C_1\left(u,v\right)\frac{\partial^4 p}{\partial x^4} - C_2\left(u,v\right)\frac{\partial^4 p}{\partial y^4}$$

$$\rho\frac{\partial u}{\partial t} + \rho u\frac{\partial u}{\partial x} + \rho v\frac{\partial u}{\partial y} + \frac{\partial p}{\partial x} = \mu\frac{\partial^2 u}{\partial x^2} + \mu\frac{\partial^2 u}{\partial y^2}$$

$$\rho\frac{\partial v}{\partial t} + \rho u\frac{\partial v}{\partial x} + \rho v\frac{\partial v}{\partial y} + \frac{\partial p}{\partial y} = \mu\frac{\partial^2 v}{\partial x^2} + \mu\frac{\partial^2 v}{\partial y^2}$$



Comparison Iterative Solution in LDC

Average iterative solution times for LDC step

- Solution time in ms
- Iterations in (preconditioned) matrix-vector products (BiCGStab – 2/iteration)

Problem	GMRES(40) ILUT ms	MV	GMRES(40) SAI ms	MV	Bicgstab ILUT ms	MV	Bicgstab SAI ms	MV
101 (30.6K)	207	(21)	189	(99)	213	(23)	47.4	(116)
151 (68.4K)	392	(24)	186	(83)	423	(27)	48.3	(96)
251 (190K)	769	(23)	253	(73)	807	(25)	75.9	(80)
301 (272K)	1.18e3	(23)	293	(72)	1.27e3	(26)	93.3	(80)

Speedups

Problem	GMRES(40) ILUT ms	GMRES(40) SAI Speedup	Bicgstab ILUT Speedup	Bicgstab SAI Speedup
101 (30.6K)	207	1.10 (189)	.972 (213)	4.37 (47.4)
151 (68.4K)	392	2.11 (186)	.927 (423)	8.12 (48.3)
251 (190K)	769	3.04 (253)	.953 (807)	10.1 (75.9)
301 (272K)	1.18e3	4.03 (293)	.929 (1.27e3)	12.6 (93.3)

Observations

- Although SAI less effective preconditioner (iterations), much faster runtimes due to higher flop/s GPU
- For ILUT versions, most time spent in preconditioner
- GMRES expensive in orthogonalizations
  - dot product + vector update (axpy)
- Improvement for GMRES limited by cost of orthogonalizations
- BiCGStab more effective in spite of further increase in iterations
- Results depend on (problem dependent)
  - Convergence vs cost per iteration
  - Relative costs of SMV, PV, orthogonalizations

GMRES Runtime - Breakdown

Problem		GMRES(40)		PrecVec Mult		GS orthog.	
		ms	#PMV	ms	%	ms	%
101	30.6K	207	20.6	183	89	17.9	7
151	68.4K	392	23.8	360	92	25.3	5
251	190K	769	23.2	721	94	36.4	5
301	272K	1.18e3	23.4	1.12e3	95	43.5	4

Problem		GMRES(40)		PrecVec Mult		GS orthog.	
		ms	#PMV	ms	%	ms	%
101	30.6K	189	99.3	11.1	6	157	83
151	68.4K	186	83.5	12.7	7	160	85
251	190K	253	73.4	21.5	8	200	79
301	272K	293	71.9	26.4	9	229	78

Conclusions and Future Work

- Good insight into cost issues of solvers/preconditioners
- Much better GPU performance for solver and preconditioner (BiCGSTAB / SAI) – factor 12
  - and working on other preconditioners (BILUT, …)
  - add multilevel correction to SAI for better convergence
- Recycling solvers implemented for CFD codes, start testing and combine with appropriate preconditioners
  - Explore additional optimization space for these solvers
- Explore solver variants that allow faster (fused) implementations of kernels (across iterations?)

- Extract lessons for Computational Dwarfs

Preconditioned BiCGStab

x_0 is an initial guess; $r_0 = b - Ax_0$
Choose $\widetilde{r}$ (for example, $\widetilde{r} = r_0$;
for $i = 1, 2, \ldots$
    $\rho_{i-1} = \widetilde{r}^T r_{i-1})$
    if $\rho_{i-1} = 0$ **method fails**
    if $i = 1$
        $p_i = r_{i-1}$
    else
        $\beta_{i-1} = (\rho_{i-1}/\rho_{i-2})(\alpha_{i-1}/\omega_{i-1})$
        $p_i = r_{i-1} + \beta_{i-1}(p_{i-1} - \omega_{i-1}v_{i-1});$
    endif
    Solve $\widehat{p}$ from $K\widehat{p} = p_i$
    $v_i = A\widehat{p}$
    $\alpha_i = \rho_{i-1}/\widetilde{r}^T v_i$
    $s = r_{i-1} - \alpha_i v_i$
    if $\|s\|$ small enough **then**
        $x_i = x_{i-1} + \alpha_i \widehat{p}$, quit
    Solve $\widehat{s}$ from $K\widehat{s} = s$
    $t = A\widehat{s}$
    $\omega_i = t^T s / t^T t$
    $x_i = x_{i-1} + \alpha_i \widehat{p} + \omega_i \widehat{s}$
    if x_i is accurate enough **then** quit
    $r_i = s - \omega_i t$
    for continuation it is necessary that $\omega_i \neq 0$
end