3 – Efficient Solvers and Time Integration

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Summer School on Discontinuous Galerkin Methods
International Center for Numerical Methods in Engineering
Barcelona, Spain

University of California Berkeley

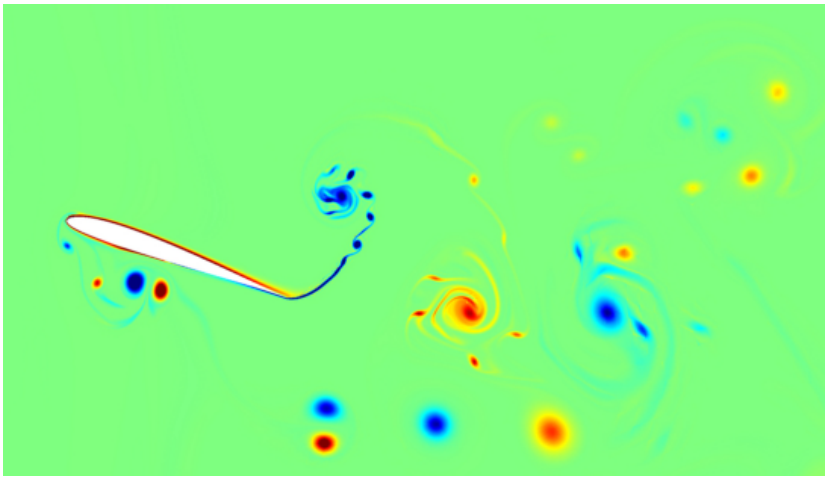
June 11-15, 2012

Berkeley Lab

Outline

Implicit Time Integration

- Implicit solvers typically required because of CFL restrictions from viscous effects, low Mach numbers, and adaptive/anisotropic grids
- Jacobian matrices are large even at $p = 2$ or $p = 3$, however:
  - They are required for non-trivial preconditioners
  - They are very expensive to recompute
- Therefore, we consider matrix-based Newton-Krylov solvers
- In [Persson/Peraire, SISC'08], we proposed efficient preconditioners with block-ILU(0) and automatic element ordering
- Distributed parallel versions developed in [Persson '09]



Problem Formulation

- Consider time-dependent systems of conservation laws:

$$\frac{\partial u}{\partial t} + \nabla \cdot F(u, \nabla u) = S(u, \nabla u)$$

- Standard DG discretization using degree p simplex elements
- Approximate Riemann solver for inviscid fluxes, the Compact Discontinuous Galerkin (CDG) method for viscous fluxes [Peraire/Persson, SISC'08]
- Leads to system of ODEs of the form $\boldsymbol{M}\dot{\boldsymbol{u}} = \boldsymbol{r}(\boldsymbol{u})$
- Implicit BDF or DIRK methods with Newton's method lead to linear systems with matrices of the form

$$\boldsymbol{A} \equiv \alpha_0 \boldsymbol{M} - \Delta t \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{u}} \equiv \alpha_0 \boldsymbol{M} - \Delta t \boldsymbol{K}$$

- Strong dependence on the timestep Δt

Diagonally Implicit Runge-Kutta (DIRK) Methods

- General form of Runge-Kutta methods

$$k_i = f\left(t_n + c_i h, u_n + h\sum_{j=1}^{s} a_{ij}k_j\right), \quad i = 1, \ldots, s$$

$$u_{n+1} = u_n + h\sum_{j=1}^{s} b_j k_j$$

- DIRK schemes:

  Lower triangular

  RK tablaux

c_1	a_{11}		
$\vdots$	$\vdots$	$\ddots$	
c_s	a_{s1}	$\cdots$	a_{ss}
	b_1	$\cdots$	b_s

- Solve with Newton's method

$$F_1(k_1) = k_1 - f(t_n + c_1 h, u_n + h a_{11} k_1)$$

$$F_2(k_2) = k_2 - f(t_n + c_2 h, u_n + h a_{21} k_1 + h a_{22} k_2)$$

$$\vdots$$

for s systems of N equations.

Examples of DIRK Schemes

2-stage, 2nd order DIRK, L-stable

$$\begin{array}{c|cc} \alpha & \alpha & 0 \\ 1 & 1-\alpha & \alpha \\ \hline & 1-\alpha & \alpha \end{array}$$

where $\alpha = 1 - \frac{\sqrt{2}}{2}$

2-stage, 3rd order DIRK, A-stable, not L-stable

$$\begin{array}{c|cc} \alpha & \alpha & 0 \\ 1-\alpha & 1-2\alpha & \alpha \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

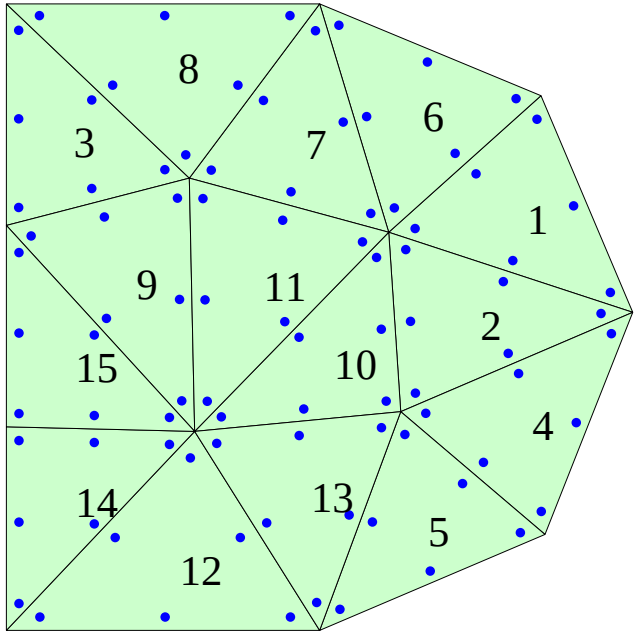
where $\alpha = (3 + \sqrt{3})/6$.

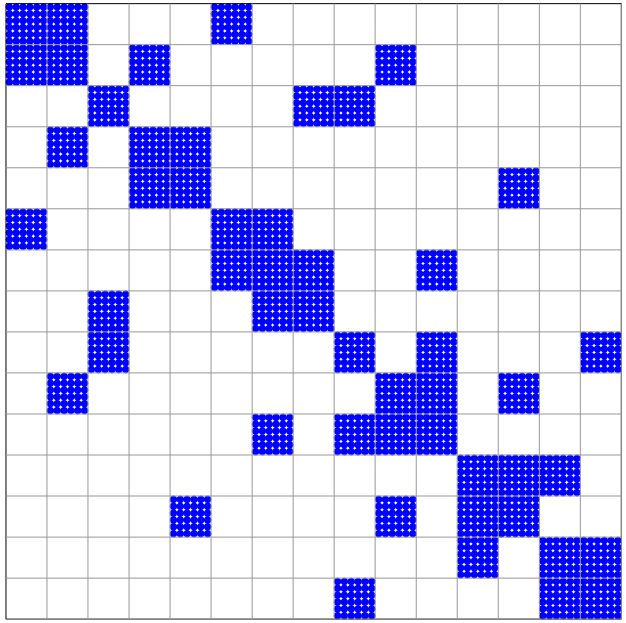
3-stage, 3rd order DIRK, L-stable

$$\begin{array}{c|ccc} 0.43586652 & 0.43586652 & 0 & 0 \\ 0.71793326 & 0.28206673 & 0.43586652 & 0 \\ 1 & 1.2084966 & -0.64436317 & 0.43586652 \\ \hline & 1.2084966 & -0.64436317 & 0.43586652 \end{array}$$

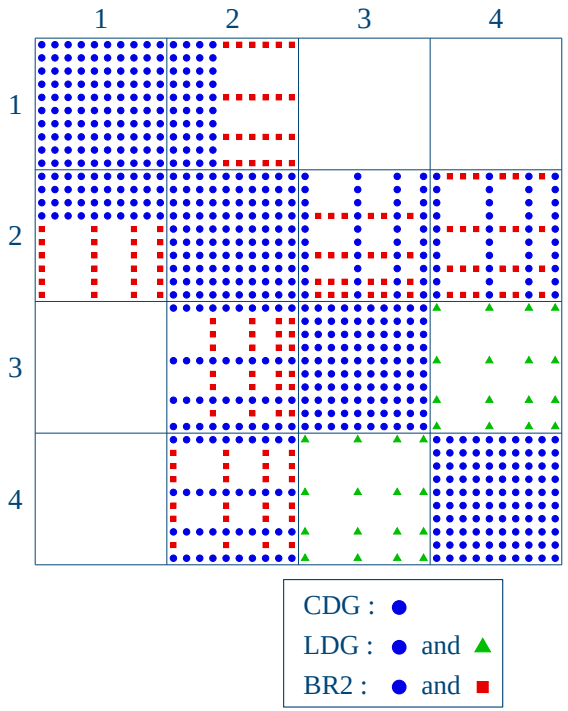
Jacobian Matrix Sparsity Structure

- Dual mesh connectivity, with each entry a large complete graph $\boldsymbol{A}_{ij}$
- Off-diagonal blocks actually sparser with CDG, but assume dense for simplicity
- Size N of submatrices $\boldsymbol{A}_{ij}$ is often > 100
- Block-based storage format essential for high performance using BLAS routines
- For other structures (e.g. elimination matrices), use block-wise compressed column





Computational Cost – DG Jacobian Matrices



- Number of non-zeros in Jacobian matrix for nodal DG (C solution components, T simplex elements, degree p, dimension D)
- Nodes per element $S = \binom{p+D}{p} = \mathcal{O}(p^D)$, nodes per face $s = \binom{p+D-1}{D-1} = \mathcal{O}(p^{D-1})$
- Example: 3-D Navier-Stokes, $p = 3$, $T = 100,000$:

Quantity	Size	Example storage
Solution vector	SCT	80 MB
Inviscid Jacobian	$(S^2 + (D+1)s^2)C^2T$	16 GB
CDG Jacobian	$(S^2 + (D+1)Ss)C^2T$	24 GB
BR2/IP Jacobian	$(S^2 + (D+1)(S+s)s)C^2T$	32 GB
Full block Jacobian	$(D+2)S^2C^2T$	40 GB

Outline

Data Structures for Sparse Matrices

Full:

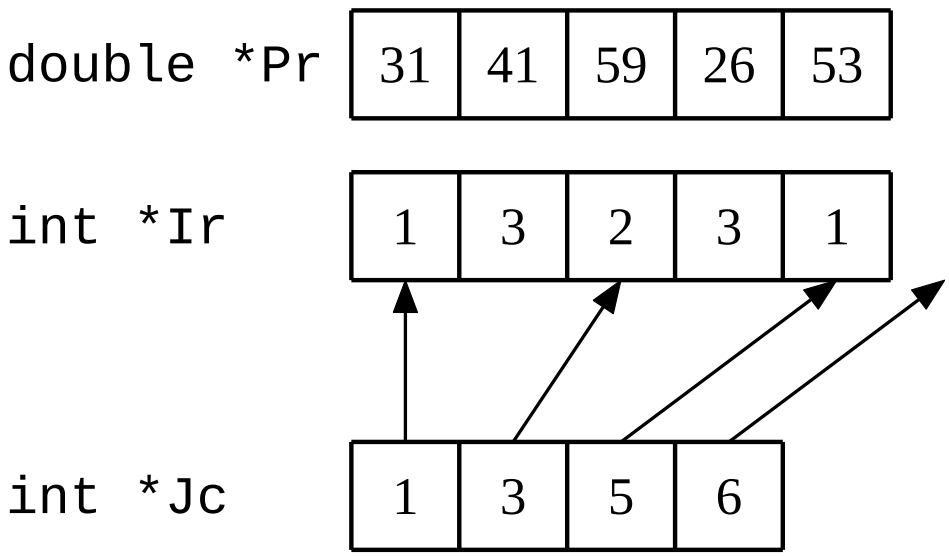
- Storage: Array of real (or complex) numbers
- Memory: `nrows*ncols`

31	0	53
0	59	0
41	26	0

`double *A`

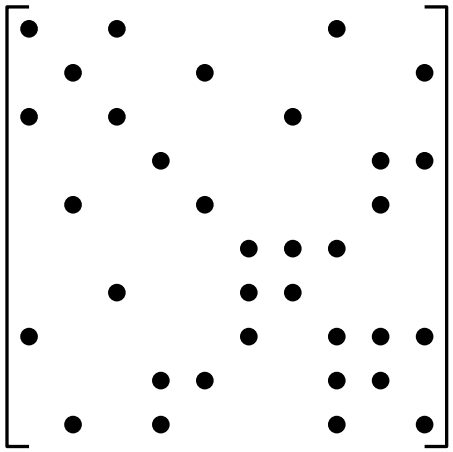
Sparse:

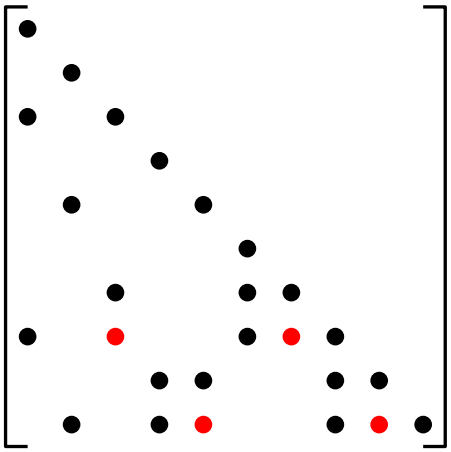
- Compressed column storage
- Memory: About `1.5*nnz+.5*ncols`



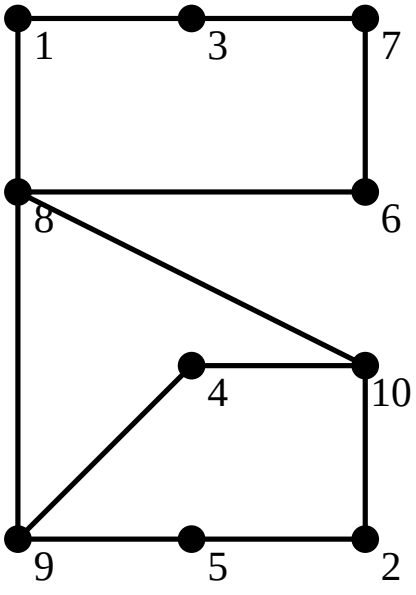
- Element look-up: $\mathcal{O}(\log$ #elements in column$)$ time
- Insertion of new nonzero very expensive
- Sparse vector = Column vector (not Row vector)

Graphs and Sparsity: Cholesky Factorization

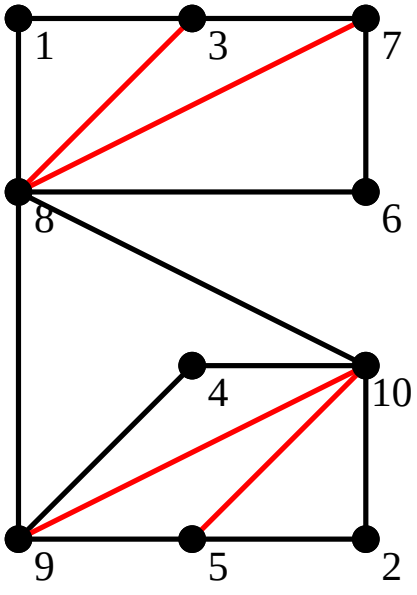




Fill: New nonzeros in factor



$G(A)$



$G^+(A)$

Symmetric Gaussian Elimination:

for $j = 1$ **to** N

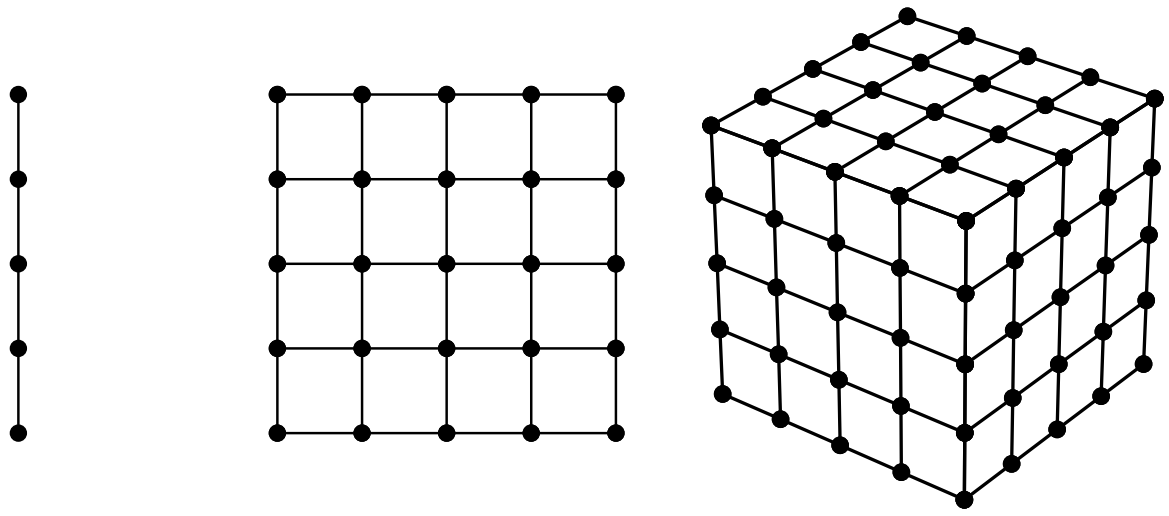
Add edges between j's higher-numbered neighbors

Heuristic Fill-Reducing Matrix Permutations

- Banded orderings (Reverse Cuthill-McKee, Sloan, etc):
  - Try to keep all nonzeros close to the diagonal
  - Theory, practice: Often wins for "long, thin" problems
- Minimum degree:
  - Eliminate row/col with fewest nonzeros, add fill, repeat
  - Hard to implement efficiently – current champion is "Approximate Minimum Degree" [Amestoy, Davis, Duff]
  - Theory: Can be suboptimal even on 2-D model problem
  - Practice: Often wins for medium-sized problems
- Nested dissection:
  - Find a separator, number it *last*, proceed recursively
  - Theory: Approximately optimal separators $\Longrightarrow$ approximately optimal fill and flop count
  - Practice: Often wins for very large problems
- The best modern general-purpose orderings are ND/MD hybrids

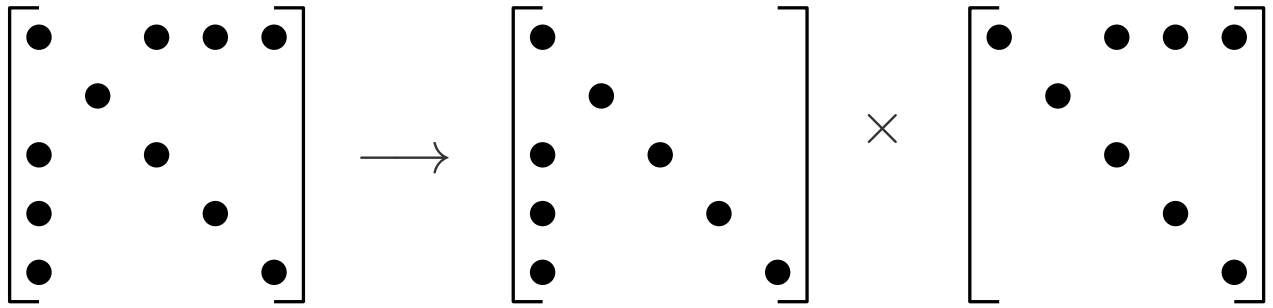
Complexity of Direct Methods

- Time and space to solve any problem on any well-shaped finite element mesh with N nodes:



	1-D	2-D	3-D
Space (fill):	$\mathcal{O}(N)$	$\mathcal{O}(N \log N)$	$\mathcal{O}(N^{4/3})$
Time (flops):	$\mathcal{O}(N)$	$\mathcal{O}(N^{3/2})$	$\mathcal{O}(N^{2})$

Incomplete Cholesky Factorization (IC, ILU)

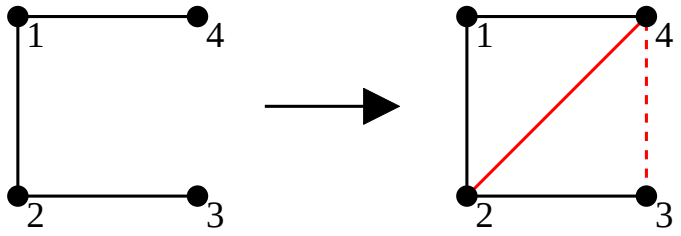


A $\qquad$ R^T $\qquad$ R

- Compute factors of A by Gaussian elimination, but ignore fill
- Preconditioner $B = R^T R \approx A$, not formed explicitly
- Compute $B^{-1}z$ by triangular solves in time $O(\texttt{nnz(A)})$
- Total storage is $O(\texttt{nnz(A)})$, static data structure
- Either symmetric (IC) or nonsymmetric (ILU)

Incomplete Cholesky and ILU: Variants

- Allow one or more "levels of fill"
  - Unpredictable storage requirements



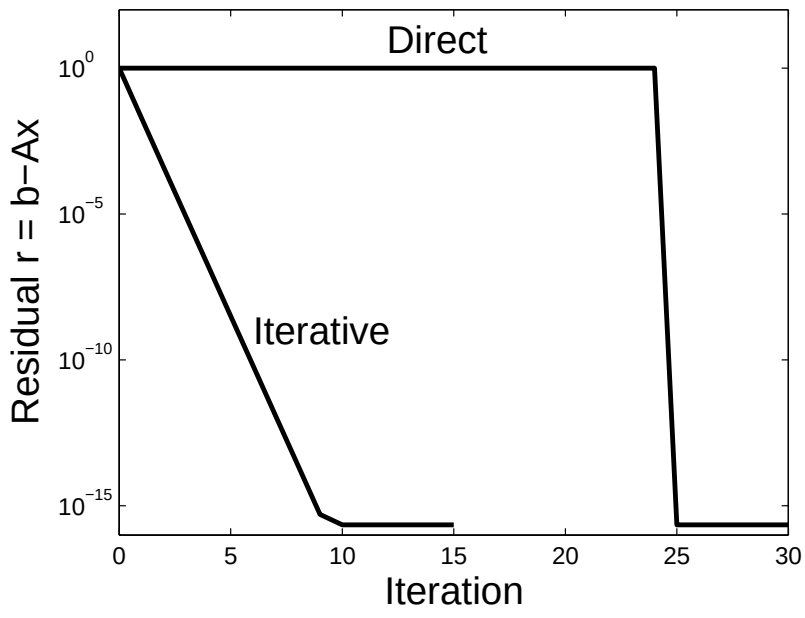
- Allow fill whose magnitude exceeds a "drop tolerance"
  - May get better approximate factors than levels of fill
  - Unpredictable storage requirements
  - Choice of tolerance is ad hoc
- Partial pivoting (for nonsymmetric A)
- "Modified ILU" (MIC): Add dropped fill to diagonal of U (R)
  - A and $R^T R$ have same row sums
  - Good in some PDE contexts

Incomplete Cholesky and ILU: Issues

- Choice of parameters
  - Good: Smooth transition from iterative to direct methods
  - Bad: Very ad hoc, problem-dependent
  - Trade-off: Time per iteration vs # of iterations (more fill $\rightarrow$ more time but fewer iterations)
- Effectiveness
  - Condition number usually improves (only) by constant factor (except MIC for some problems from PDEs)
  - Still, often good when tuned for a particular class of problems
- Parallelism
  - Triangular solves are not very parallel
  - Reordering for parallel triangular solve by graph coloring

Iterative Methods for Linear Systems

- *Direct methods* for solving $Ax = b$, e.g. Gaussian elimination, compute an exact solution after a finite number of steps (in exact arithmetic)
- *Iterative algorithms* produce a sequence of approximations $x^{(1)}, x^{(2)}, \ldots$ which hopefully converges to the solution, and
  - may require less memory than direct methods
  - may be faster than direct methods
  - may handle special structures (such as sparsity) in a simpler way



Two Classes of Iterative Methods

- *Stationary methods* (or classical iterative methods) finds a splitting $A = M - K$ and iterates $x^{(k+1)} = M^{-1}(Kx^{(k)} + b) = Rx^{(k)} + c$
  - Jacobi, Gauss-Seidel, Successive Overrelaxation (SOR), and Symmetric Successive Overrelaxation (SSOR)
- *Krylov subspace methods* use only multiplication by A (and possibly by A^T) and find solutions in the Krylov subspace $\{b, Ab, A^2b, \ldots, A^{k-1}b\}$
  - Conjugate Gradient (CG), Generalized Minimal Residual (GMRES), BiConjugate Gradient (BiCG), etc

Krylov Subspace Algorithms

- Create a sequence of *Krylov subspaces* for $Ax = b$:

$$\mathcal{K}_n = \left\langle b, Ab, \ldots, A^{n-1}b \right\rangle$$

  and find approximate solutions x_n in $\mathcal{K}_n$
- Only matrix-vector products involved
- For SPD matrices, the most popular algorithm is the *Conjugate Gradients* method [Hestenes/Stiefel, 1952]
  - Finds the best solution $x_n \in \mathcal{K}_n$ in the norm $\|x\|_A = \sqrt{x^T A x}$
  - Only requires storage of 4 vectors (not all the n vectors in $\mathcal{K}_n$)
  - Remarkably simple and excellent convergence properties
  - Originally invented as a direct algorithm! (converges after m steps in exact arithmetic)

The Conjugate Gradients Method

Algorithm: Conjugate Gradients Method

$x_0 = 0, r_0 = b, p_0 = r_0$

for $k = 1, 2, 3, \ldots$

$\alpha_n = (r_{n-1}^T r_{n-1})/(p_{n-1}^T A p_{n-1})$	step length
$x_n = x_{n-1} + \alpha_n p_{n-1}$	approximate solution
$r_n = r_{n-1} - \alpha_n A p_{n-1}$	residual
$\beta_n = (r_n^T r_n)/(r_{n-1}^T r_{n-1})$	improvement this step
$p_n = r_n + \beta_n p_{n-1}$	search direction

- Only one matrix-vector product Ap_{n-1} per iteration
- Operation count $O(m)$ (excluding the matrix-vector product)

Properties of the Conjugate Gradients Method

- The errors $e_n = x_* - x_n$ are minimized in the A-norm
- Monotonic: $\|e_n\|_A \leq \|e_{n-1}\|_A$, and $e_n = 0$ in $n \leq m$ steps
- CG also minimizes the quadratic function $\varphi(x) = \frac{1}{2}x^T Ax - x^T b$
- Conjugate Gradients finds an optimal polynomial $p_n \in P_n$ of degree n with $p(0) = 1$, minimizing $\|p_n(A)e_0\|$ with initial error $e_0 = x_*$
- Important convergence results can be obtained from the polynomial approximation:
  1. If A has n distinct eigenvalues, CG converges in at most n steps
     Proof. The polynomial $p(x) = \Pi_{j=1}^{n}(1 - x/\lambda_j)$ is zero at $\Lambda(A)$
  2. If A has 2-norm condition number κ, the errors are

$$\frac{\|e_n\|_A}{\|e_0\|_A} \leq 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^n \approx 2\left(1 - \frac{2}{\sqrt{\kappa}}\right)^n$$

- In general: CG performs well with clustered eigenvalues

Preconditioners for Linear Systems

- Main idea: Instead of solving

$$Ax = b$$

  solve, using a nonsingular $m \times m$ *preconditioner* M,

$$M^{-1}Ax = M^{-1}b$$

  which has the same solution x

- Convergence properties based on $M^{-1}A$ instead of A
- Trade-off between the cost of applying M^{-1} and the improvement of the convergence properties. Extreme cases:
  - $M = A$, perfect conditioning of $M^{-1}A = I$, but expensive M^{-1}
  - $M = I$, "do nothing" $M^{-1} = I$, but no improvement of $M^{-1}A = A$

Preconditioned Conjugate Gradients

- To keep symmetry, solve $(C^{-1}AC^{-*})C^*x = C^{-1}b$ with $CC^* = M$
- Can be written in terms of M^{-1} only, without reference to C:

Algorithm: Preconditioned Conjugate Gradients Method

$x_0 = 0, r_0 = b$

$p_0 = M^{-1}r_0, z_0 = p_0$

for $n = 1, 2, 3, \ldots$

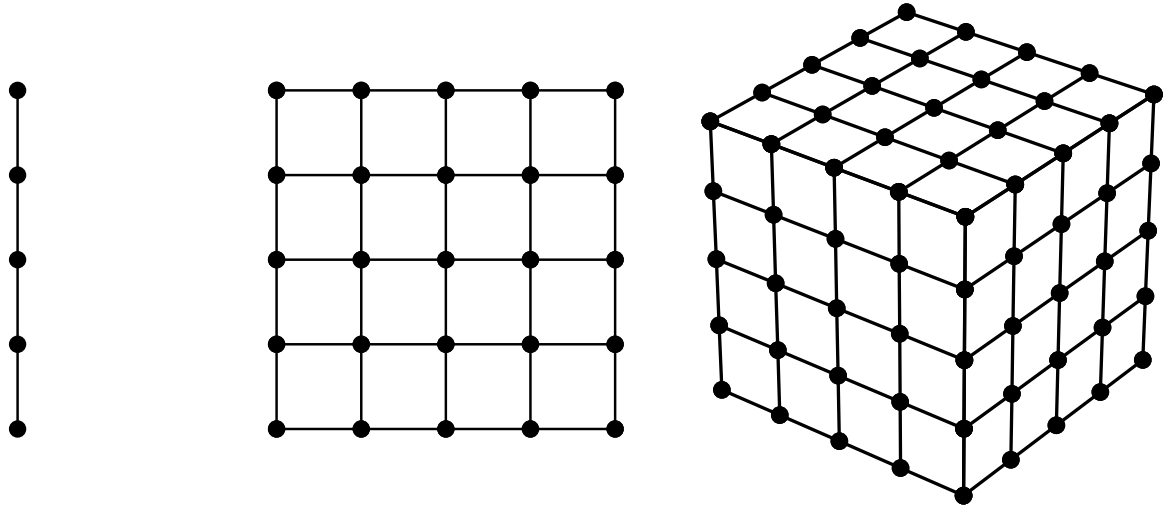
$\alpha_n = (r_{n-1}^T z_{n-1})/(p_{n-1}^T A p_{n-1})$	step length
$x_n = x_{n-1} + \alpha_n p_{n-1}$	approximate solution
$r_n = r_{n-1} - \alpha_n A p_{n-1}$	residual
$z_n = M^{-1} r_n$	preconditioning
$\beta_n = (r_n^T z_n)/(r_{n-1}^T z_{n-1})$	improvement this step
$p_n = z_n + \beta_n p_{n-1}$	search direction

Commonly Used Preconditioners

- A preconditioner should "approximately solve" the problem $Ax = b$
- **Jacobi preconditioning** - $M = \mathrm{diag}(A)$, very simple and cheap, might improve certain problems but usually insufficient
- **Block-Jacobi preconditioning** - Use block-diagonal instead of diagonal. Another variant is using several diagonals (e.g. tridiagonal)
- **Classical iterative methods** - Precondition by applying one step of Jacobi, Gauss-Seidel, SOR, or SSOR
- **Incomplete factorizations** - Perform Gaussian elimination but ignore fill, results in approximate factors $A \approx LU$ or $A \approx R^T R$
- **Coarse-grid approximations** - For a PDE discretized on a grid, transfer the residual to a coarser grid, solve a smaller problem, then transfer back an error correction (*multigrid*)

Complexity of Linear Solvers

- Work to solve a Poisson problem on regular mesh with N nodes:



Solver	1-D	2-D	3-D
Sparse Cholesky	$O(N)$	$O(N^{1.5})$	$O(N^2)$
CG, exact arith.	$O(N^2)$	$O(N^2)$	$O(N^2)$
CG, no precond.	$O(N^2)$	$O(N^{1.5})$	$O(N^{1.33})$
CG, modified IC	$O(N^{1.5})$	$O(N^{1.25})$	$O(N^{1.17})$
Multigrid	$O(N)$	$O(N)$	$O(N)$

Outline

Preconditioners for DG

- Preconditioner critical for good performance with Krylov methods
- Various standard methods for block matrices:
  - Block diagonal: $\boldsymbol{A} \approx \mathrm{blockdiag}(\boldsymbol{A})$
    - Poor in general
  - Block Incomplete LU: $\boldsymbol{A} \approx \tilde{\boldsymbol{L}}\tilde{\boldsymbol{U}}$
    - Good for convection (with the right ordering, more later)
  - p-multigrid (low-degree) preconditioner
    - Good for diffusion
- Highly efficient combination [Persson/Peraire 06,08]
  - Use block ILU(0) as post-smoother for coarse scale correction
  - Combines advantages of ILU and low-degree preconditioners
  - Cheap general purpose preconditioner

Incomplete LU Factorization

- For our low-degree dual meshes, it is uncommon that an element k is a neighbor of both element j and i when j is a neighbor of i
- This simplifies the Block-ILU(0) algorithm:

$\tilde{\boldsymbol{U}} \leftarrow \boldsymbol{A}, \tilde{\boldsymbol{L}} \leftarrow \boldsymbol{I}$

for $j = 1$ **to** $n - 1$

  for neighbors $i > j$ of j

$\tilde{\boldsymbol{L}}_{ij} = \tilde{\boldsymbol{U}}_{ij} \tilde{\boldsymbol{U}}_{jj}^{-1}$

$\tilde{\boldsymbol{U}}_{ii} \leftarrow \tilde{\boldsymbol{U}}_{ii} - \tilde{\boldsymbol{L}}_{ik} \tilde{\boldsymbol{U}}_{ki}$

  end for

end for

- This means $\tilde{\boldsymbol{U}}_{ij} = \boldsymbol{A}_{ij}$ when $j > i$, or $\tilde{\boldsymbol{U}}$ only differs from $\boldsymbol{A}$ in the diagonal blocks
- Store only diagonal blocks of $\tilde{\boldsymbol{U}}$!

Computational Cost

- Pre-calculation cost (block-size N, dimension D, ne elements):

Operation	Flop count
Jacobi Factorization $\tilde{\boldsymbol{A}}^{J}$	$(2/3)N^3ne$
Gauss Seidel Factorization $\tilde{\boldsymbol{A}}^{GS}$	$(2/3)N^3ne$
ILU(0) Factorization $\tilde{\boldsymbol{A}}^{ILU}$	$(2D+8/3)N^3ne$

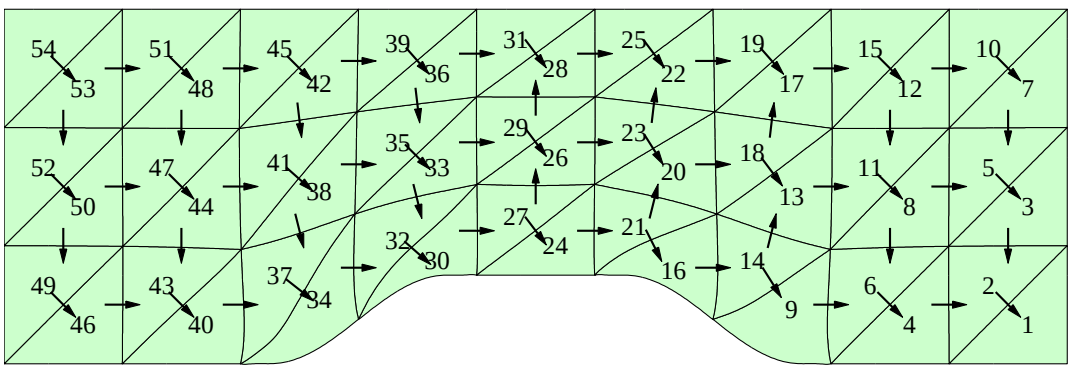
- This assumes full blocks (CDG is significantly cheaper)
- Cost of assembling a nonlinear $\boldsymbol{A}$ is $\mathcal{O}(N^3ne)$ with large constant
- Cost per iteration:

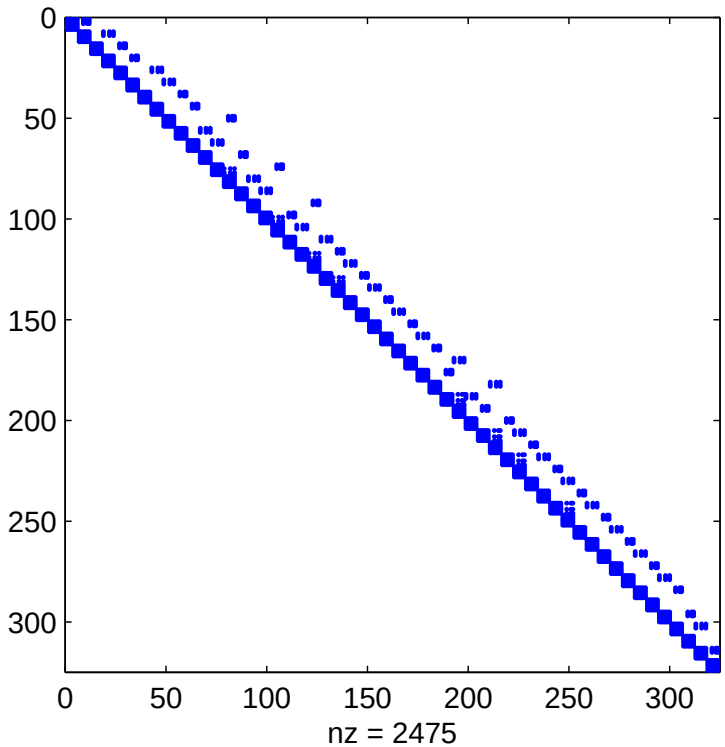
Operation	Flop count
Jacobi solve $(\tilde{\boldsymbol{A}}^{J})^{-1}p$	$(2)N^2ne$
Gauss Seidel solve $(\tilde{\boldsymbol{A}}^{GS})^{-1}p$	$(D+3)N^2ne$
ILU(0) solve $(\tilde{\boldsymbol{A}}^{ILU})^{-1}p$	$(2D+4)N^2ne$
Matrix-vector product $\boldsymbol{Ax}$	$(2D+4)N^2ne$

- Only factor of 2 between ILU + MATVEC and Jacobi + MATVEC

Element Order Dependency

- Properties of Gauss Seidel and ILU preconditioners highly dependent on the ordering of the elements
- For *upwinded scalar convection*, “ordering by lines” gives an optimal upper triangular matrix
- But for viscous or multivariate problems, best ordering not clear
- Matrix-approach: Minimize error in the approximations, rather than using physical observations





Minimum Discarded Fill Element Ordering

- Greedy algorithm for element ordering [Persson/Peraire '08]:
  At step j, if j' is chosen next, we would discard the fill

$$\Delta\tilde{\boldsymbol{U}}_{ik}^{(j,j')} = -\tilde{\boldsymbol{U}}_{ij'}\tilde{\boldsymbol{U}}_{j'j'}^{-1}\tilde{\boldsymbol{U}}_{j'k}, \quad \text{for neighbors } i \geq j, k \geq j \text{ of element } j'$$

- Choose the j' that minimizes the norm of the discarded fill

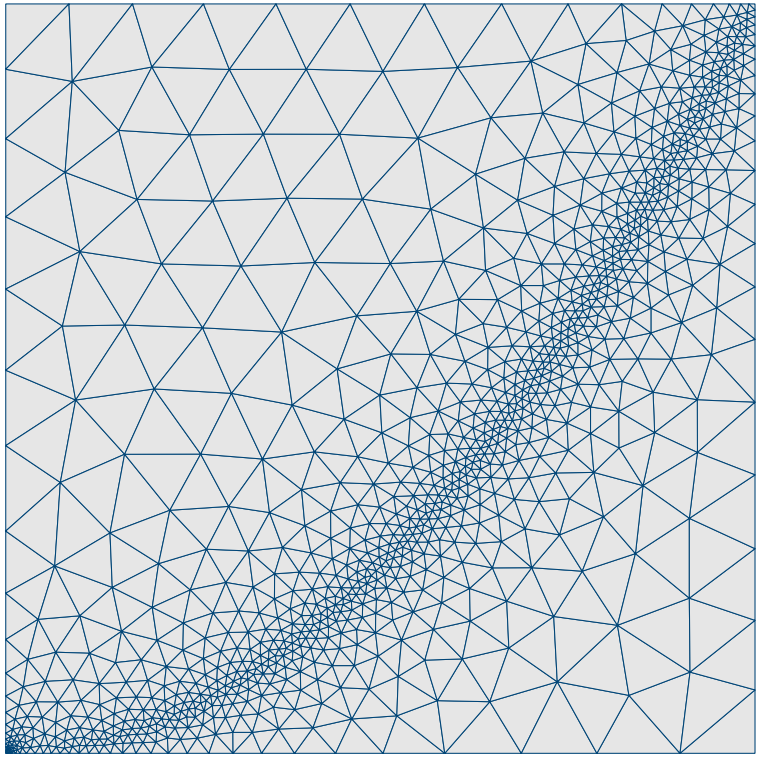
$$w^{(j,j')} = \|\Delta\tilde{\boldsymbol{U}}^{(j,j')}\|_{\mathrm{F}}$$

- Some simplifications, min-heap data structure $\Longrightarrow \mathcal{O}(n \log n)$ cost
- Increased locality: Consider only neighbors for j'

Effect of Ordering on Convection-Diffusion

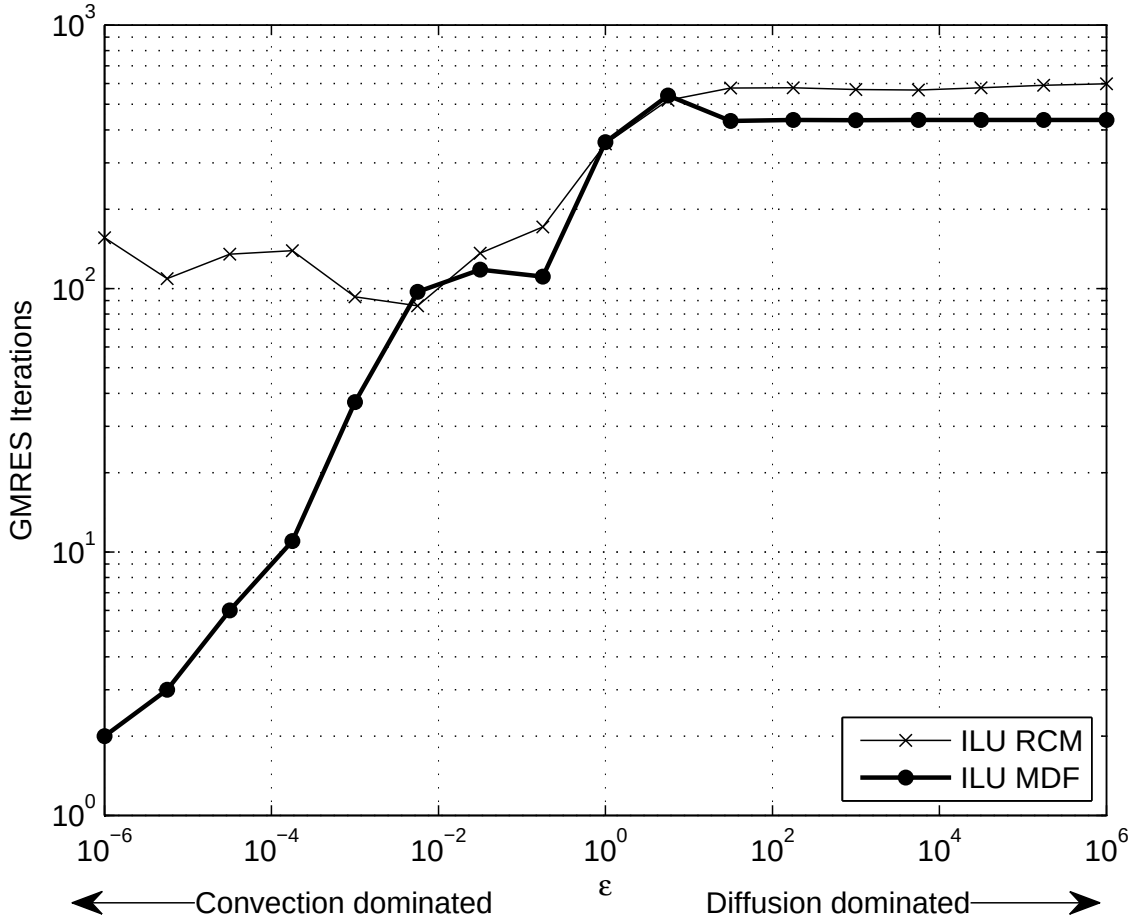
- Convection-Diffusion model problem, with $(\alpha, \beta) = (1, 2x)$, $\varepsilon \geq 0$:

$$\frac{\partial u}{\partial t} + \nabla \cdot \begin{bmatrix} \alpha u \\ \beta u \end{bmatrix} - \nabla \cdot \begin{bmatrix} \varepsilon u_x \\ \varepsilon u_y \end{bmatrix} = 0$$



Effect of Ordering on Convection-Diffusion

- Reverse Cuthill-McKee vs. Minimum Discarded Fill ordering
- MDF makes ILU perfect for convection
- Ordering less important for diffusion, ILU remains poor



The ILU(0)-p1 Preconditioner

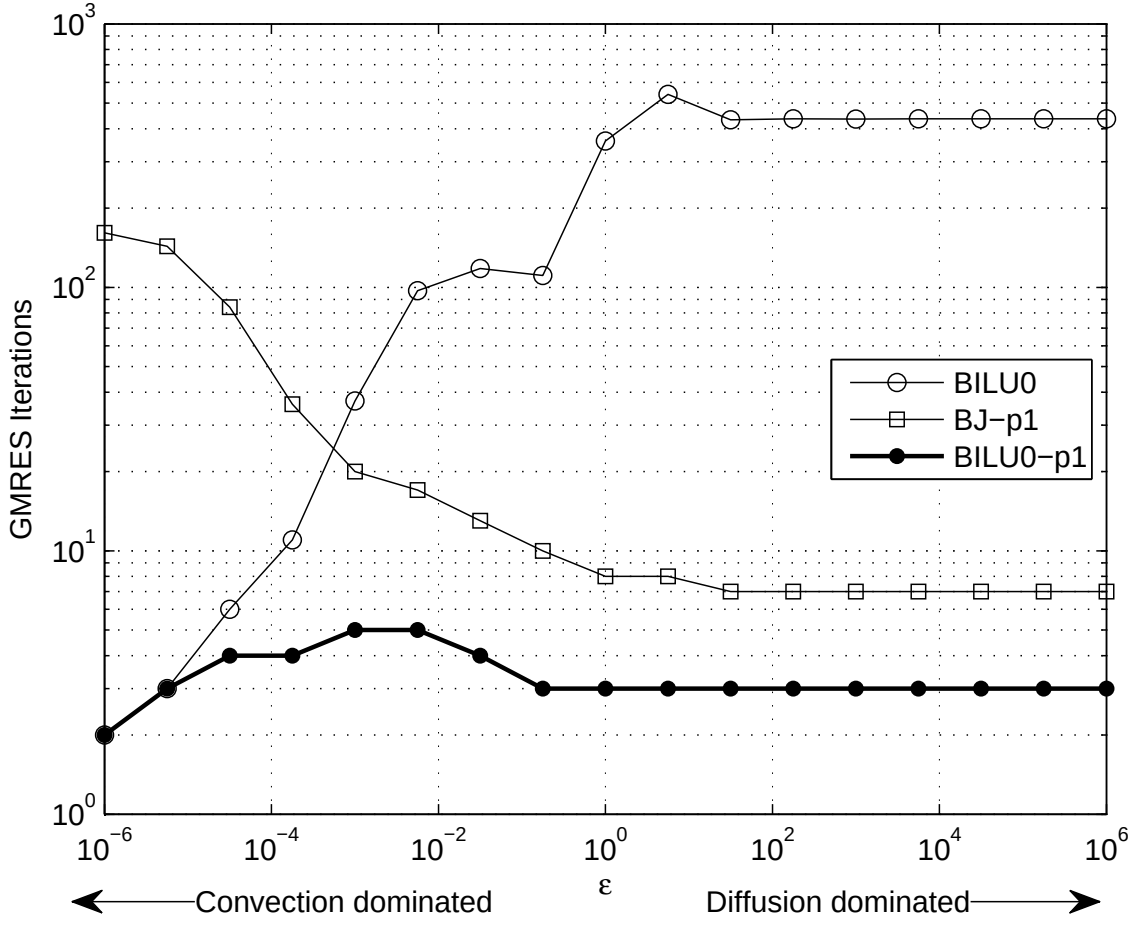
- Combination of block ILU and multigrid [Persson/Peraire 06,08]
- Coarse scale correction + post-smoothing by $\tilde{\boldsymbol{A}} = \tilde{\boldsymbol{L}}\tilde{\boldsymbol{U}}$:

0. $\boldsymbol{A}^{(0)} = \boldsymbol{P}^T\boldsymbol{A}\boldsymbol{P}$	*Precompute coarse operator, block wise*
1. $\boldsymbol{b}^{(0)} = \boldsymbol{P}^T\boldsymbol{b}$	*Restrict residual element/component wise*
2. $\boldsymbol{A}^{(0)}\boldsymbol{u}^{(0)} = \boldsymbol{b}^{(0)}$	*Solve coarse scale problem*
3. $\boldsymbol{u} = \boldsymbol{P}\boldsymbol{u}^{(0)}$	*Prolongate solution element/component wise*
4. $\boldsymbol{u} = \boldsymbol{u} + \alpha\tilde{\boldsymbol{A}}^{-1}(\boldsymbol{b} - \boldsymbol{A}\boldsymbol{u})$	*Apply smoother $\tilde{\boldsymbol{A}}$ with damping α*

- Restriction/prolongation operator $\boldsymbol{P}$ block diagonal, based on orthogonal Koornwinder polynomials
- Coarse scale problem solved directly (2-D problems, serial) or iteratively by GMRES or h-multigrid

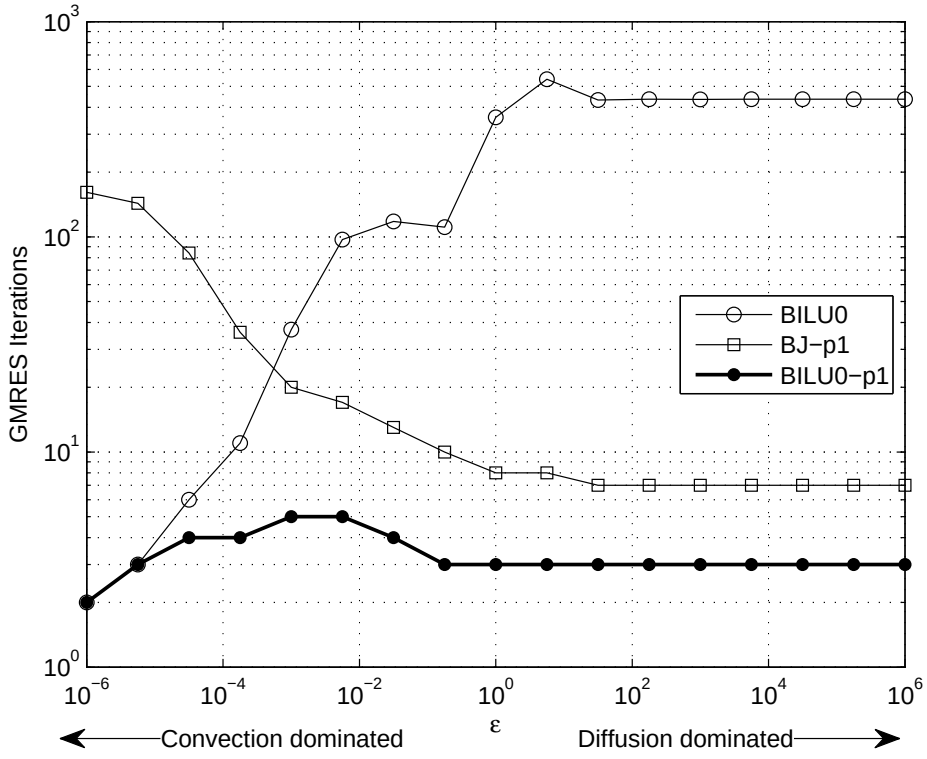
The ILU-p1 Preconditioner - Convection-Diffusion

- Block ILU perfect for convection, multigrid perfect for diffusion
- Block ILU-smoothed multigrid (BILU0-p1) almost perfect for any ε



Effect of Ordering on ILU

- MDF ordering makes block-ILU0 with coarse grid correction almost perfect for convection-diffusion
- Good element ordering critical for Navier-Stokes as well:



Problem	Element Ordering		
	Random	RCM	MDF
Inviscid	51	27	12
Laminar, Re=1,000	200	135	12
Laminar, Re=20,000	197	139	27
RANS, Re=10^6	98	99	18

Convergence – Model Navier-Stokes Problem

$\times$ = No convergence after 1,000 iterations, from [Persson/Peraire '08]

Problem	Parameters		Preconditioner/Iterations					
			Block Jacobi		Block G-S		Block ILU0	
	Δt	M	BJ	BJ-p1	BGS	BGS-p1	BILU0	BILU0-p1
Inviscid	10^{-3}	0.2	24	19	14	11	5	4
	10^{-1}	0.2	187	85	73	49	12	6
	∞	0.2	840	142	456	72	40	9
	10^{-3}	0.01	200	112	111	67	15	6
	10^{-1}	0.01	$\times$	$\times$	$\times$	532	94	10
	∞	0.01	$\times$	$\times$	$\times$	$\times$	374	16
Laminar	10^{-3}	0.2	50	34	25	19	4	4
Re=1,000	10^{-1}	0.2	$\times$	597	477	225	11	5
	∞	0.2	$\times$	$\times$	$\times$	$\times$	37	7
	10^{-3}	0.01	98	66	51	33	8	5
	10^{-1}	0.01	$\times$	619	$\times$	207	27	9
	∞	0.01	$\times$	$\times$	$\times$	748	135	12

Convergence – Model Navier-Stokes Problem

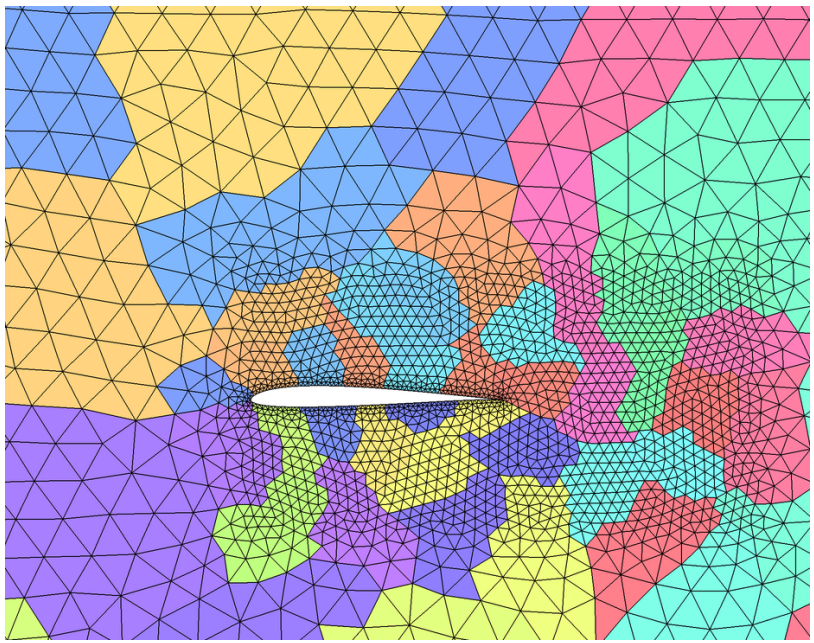
$\times$ = No convergence after 1,000 iterations, from [Persson/Peraire '08]

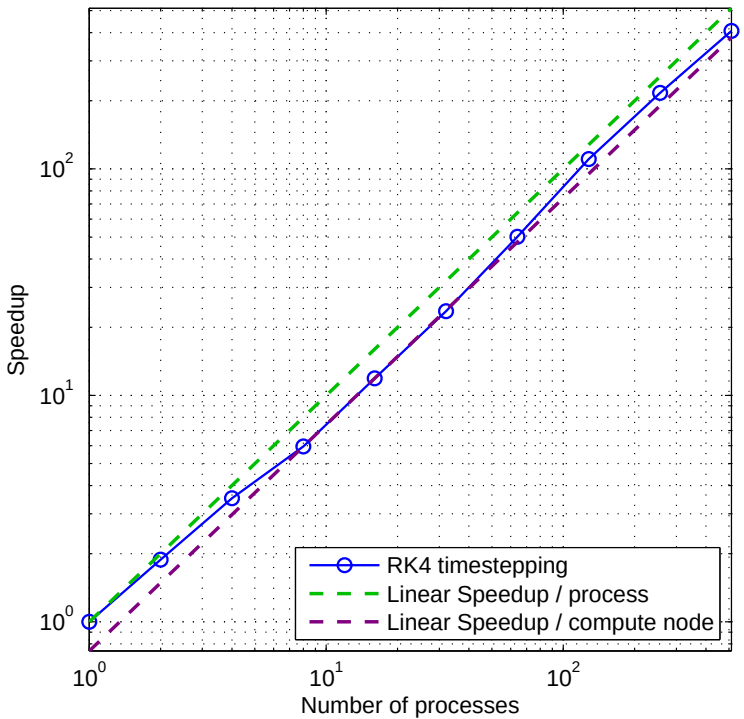
Problem	Parameters		Preconditioner/Iterations					
			Block Jacobi		Block G-S		Block ILU0	
	Δt	M	BJ	BJ-p1	BGS	BGS-p1	BILU0	BILU0-p1
Laminar	10^{-3}	0.2	26	19	14	11	4	4
Re=20,000	10^{-1}	0.2	456	220	219	113	16	8
	∞	0.2	$\times$	$\times$	$\times$	$\times$	236	20
	10^{-3}	0.01	160	90	61	38	12	6
	10^{-1}	0.01	$\times$	$\times$	$\times$	735	80	16
	∞	0.01	$\times$	$\times$	$\times$	$\times$	$\times$	35
RANS	10^{-3}	0.2	76	56	33	28	8	7
Re=10^6	10^{-1}	0.2	$\times$	$\times$	$\times$	$\times$	35	25
	∞	0.2	$\times$	$\times$	$\times$	$\times$	70	18
	10^{-3}	0.01	411	231	174	110	14	9
	10^{-1}	0.01	$\times$	$\times$	$\times$	$\times$	46	16
	∞	0.01	$\times$	$\times$	$\times$	$\times$	132	28

Outline

Parallelization of Residual Evaluation

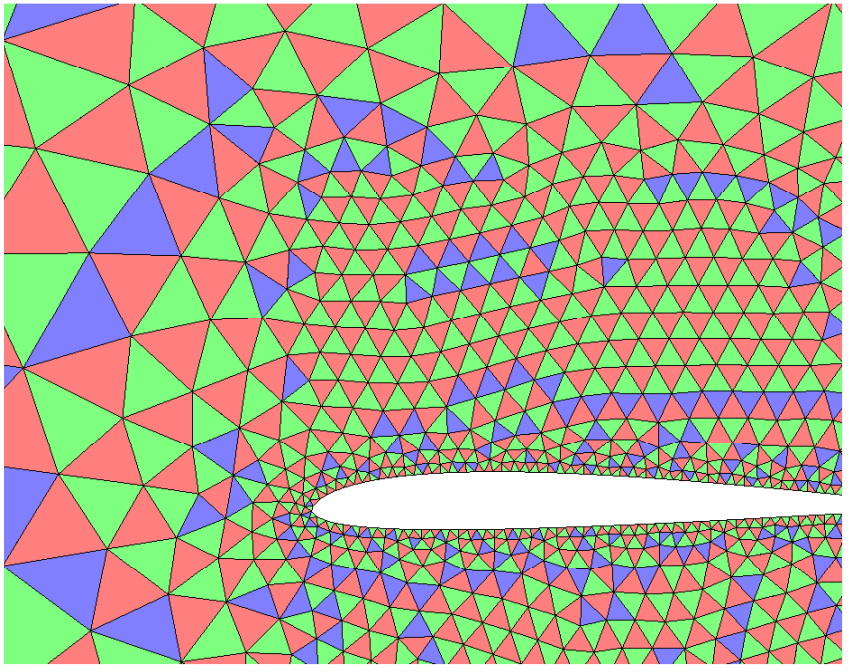
- Two critical properties for parallelization:
  - High computational cost per degree-of-freedom
  - Memory accessed in localized chunks
- Essentially perfect speed-up of residual calculation in MPI
- Communication not an issue with overlapping computations
- However, memory bandwidth limitations for 8 cores on single node





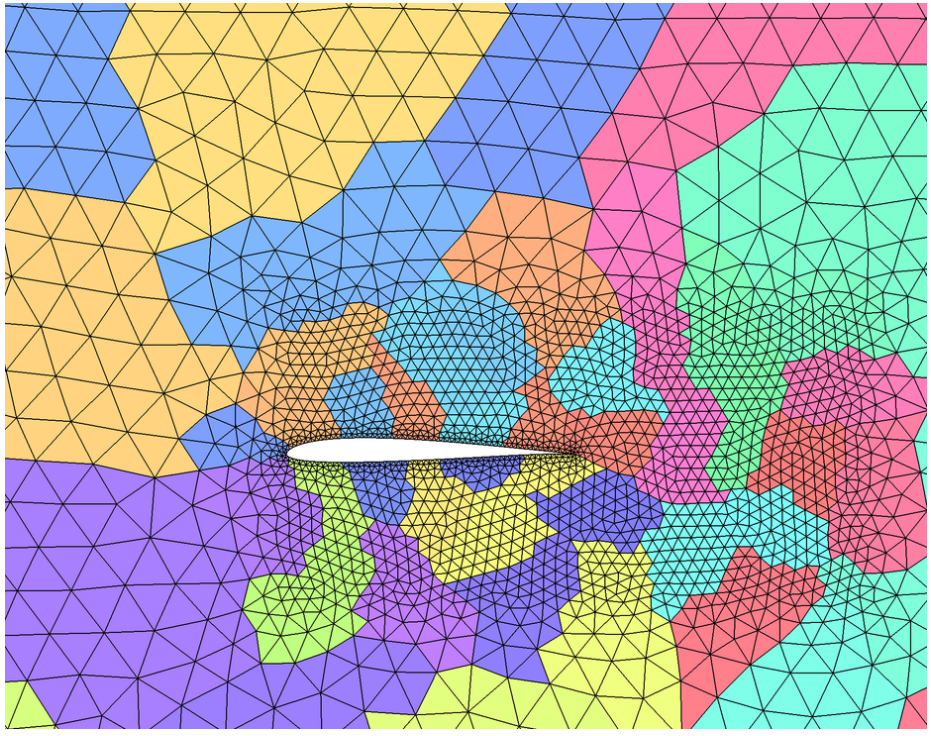
ILU Parallelization – Coloring

- Serial nature of Gaussian elimination – Hard to parallelize ILU(0)
- Standard approach: *Color* the graph to find independent sets
- Elements of the same color can be updated independently
- But this is typically a poor ILU-ordering for convective problems!
- The coloring eliminates the sequential dependencies found by the MDF ordering



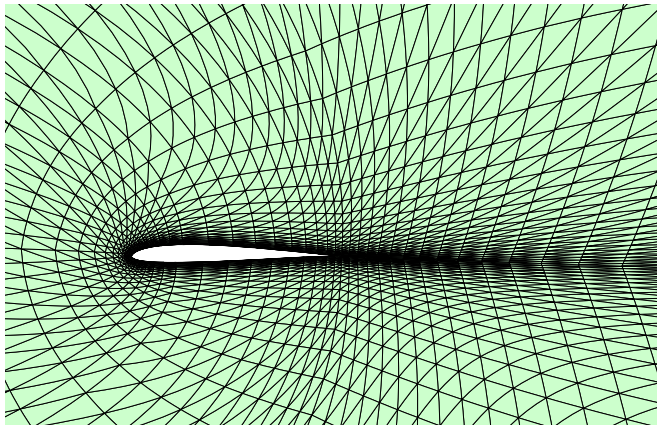
ILU Parallelization – Domain Decomposition

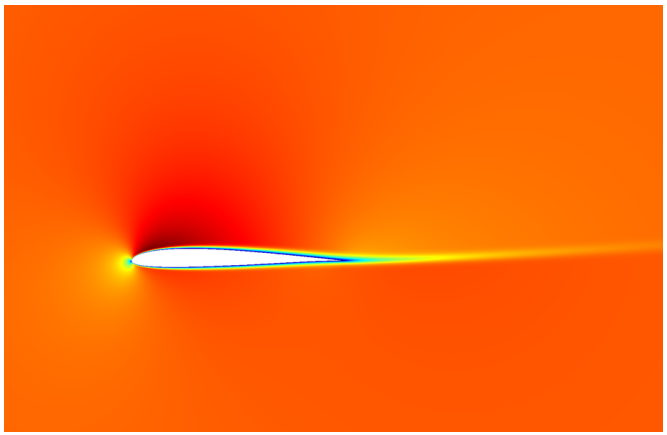
- Better approach: Partition-wise ILUs with MDF ordering
- Partition using the weights $C_{ij} = \|\boldsymbol{A}_{ii}^{-1}\boldsymbol{A}_{ij}\|_F$
- Essentially a “non-overlapping Schwartz preconditioner with incomplete solutions”
- Approaches Jacobi as # partitions $\rightarrow$ # elements
- Good option for many problems – GMRES iterations cheap compared to matrix creation

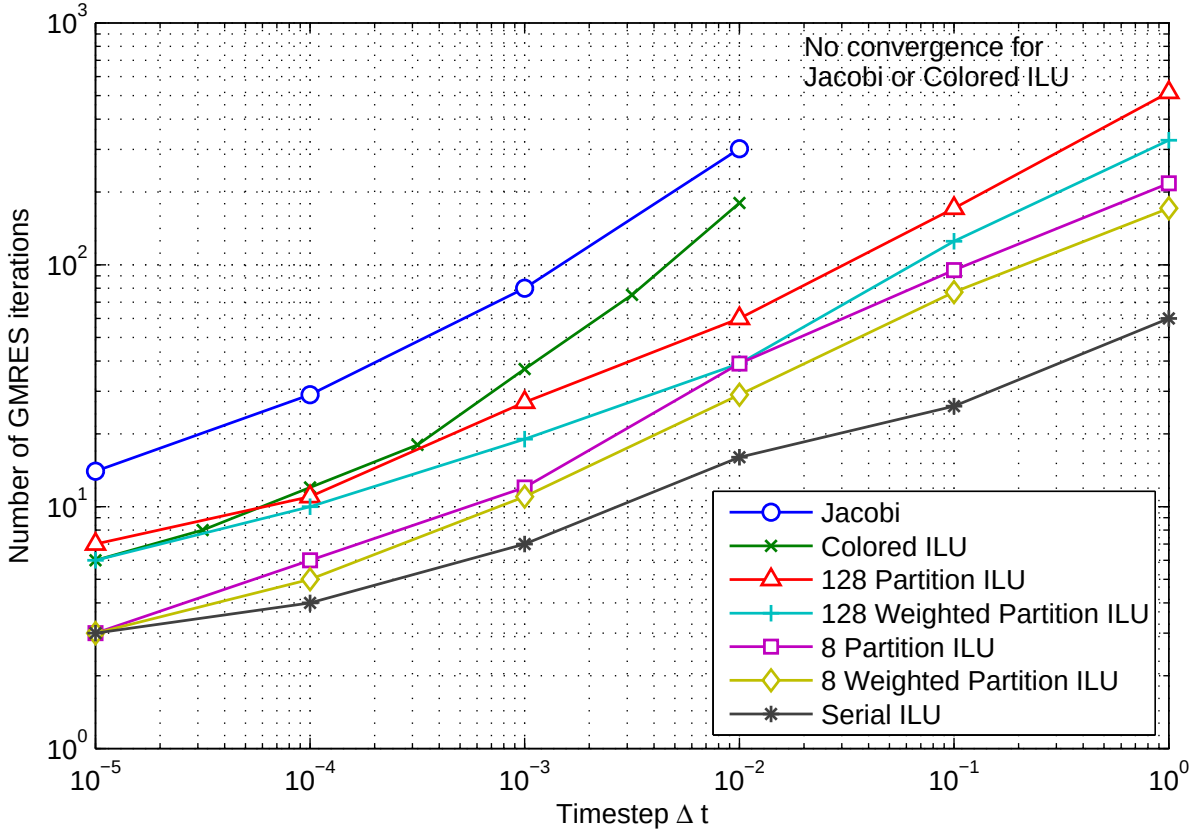


Iterative Solver Convergence Properties

- SD7003 test problem: $\mathrm{Re} = 8000$, $M = 0.1$, CFL $\Delta t < 10^{-6}$
- Coloring essentially destroys the excellent convergence of MDF
- Partition-wise ILUs scale better, only 2-3 times slower for large Δt

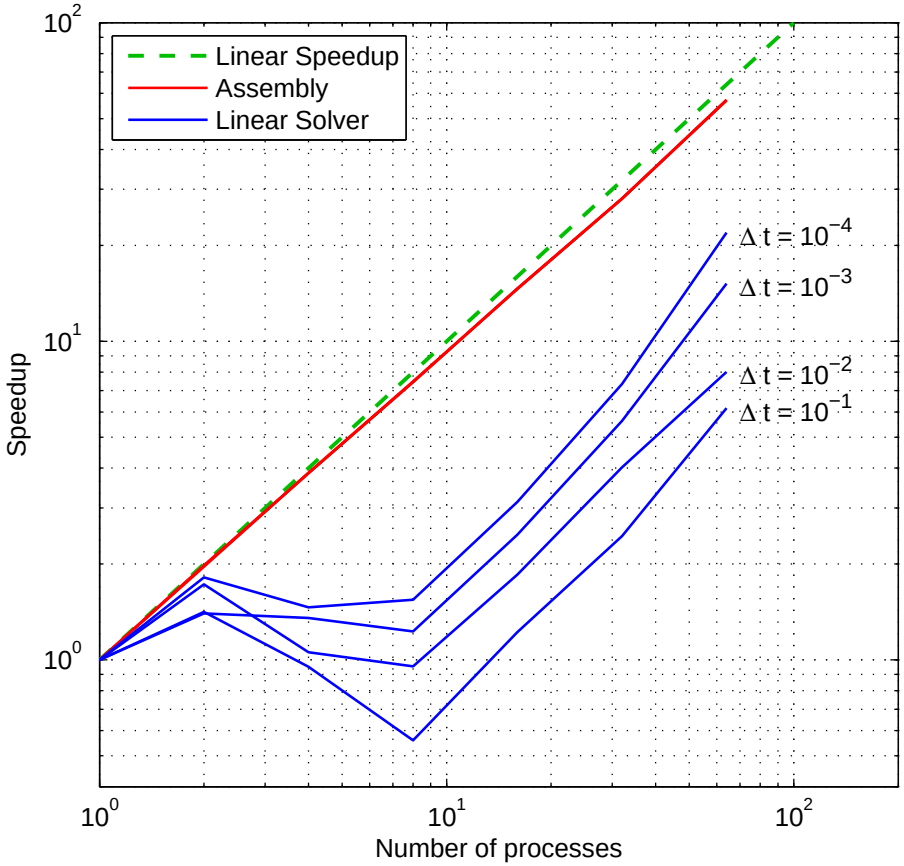


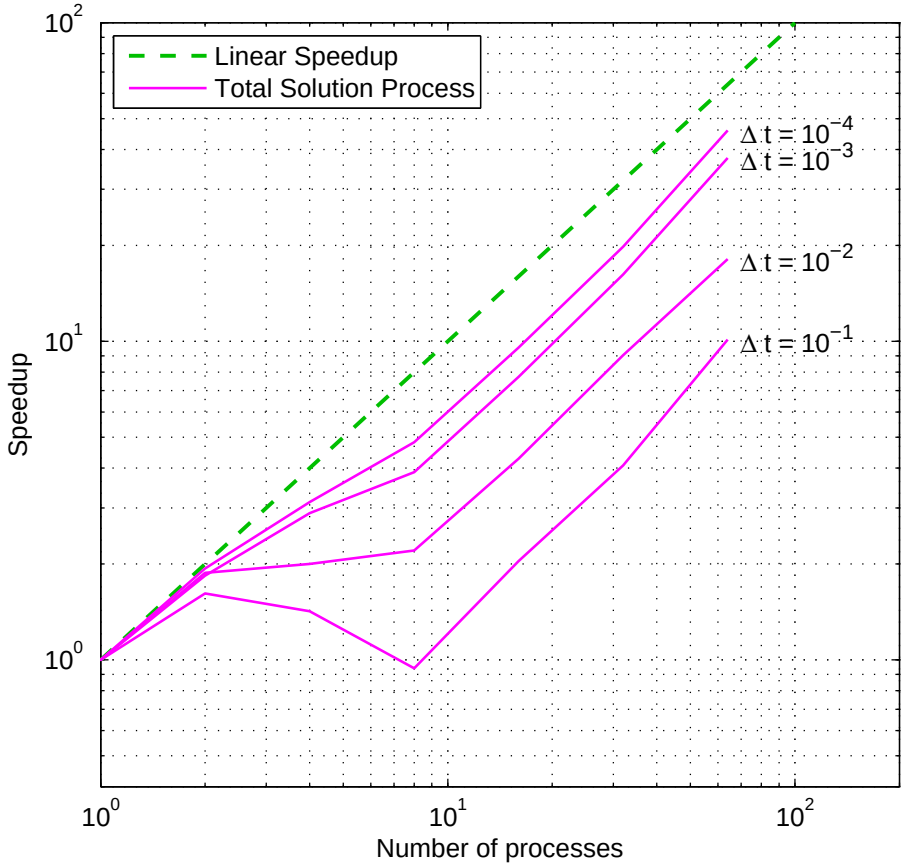




SD7003 Test Problem – Timings and Speedup

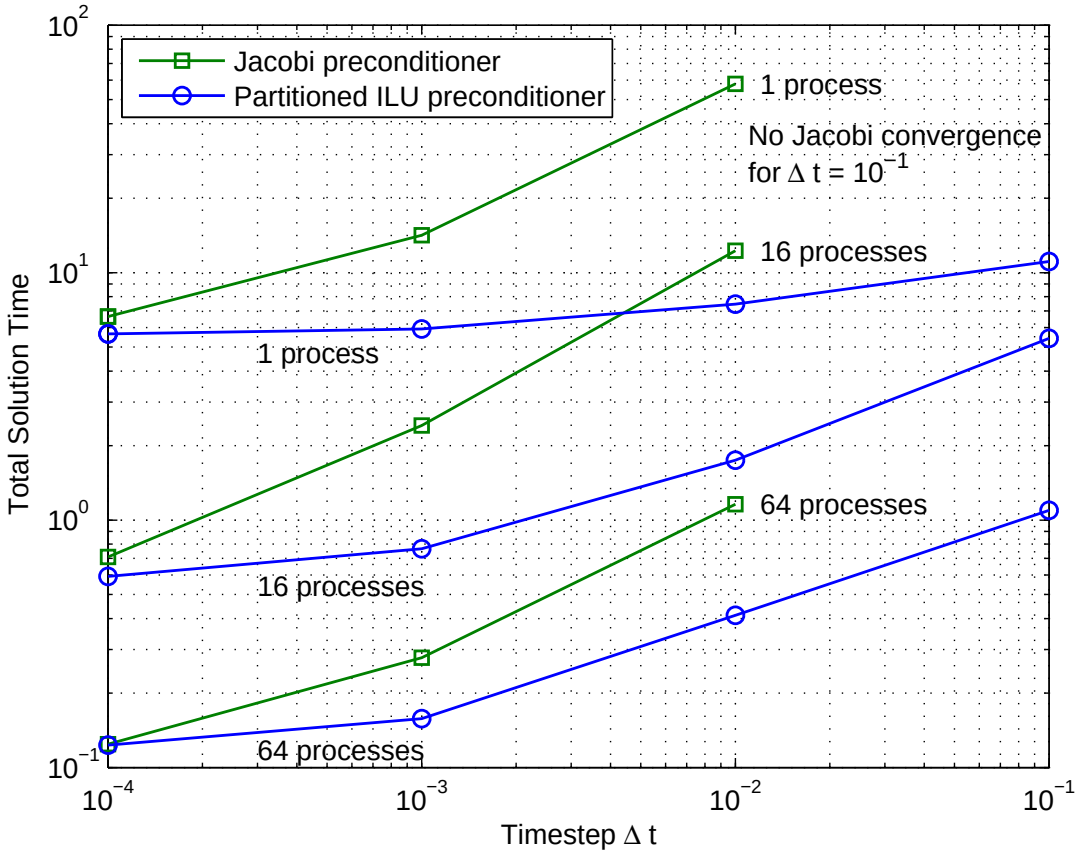
- Assembly scales almost perfectly, as expected
- Linear solver scales poorly up to the 8 cores in each compute node, due to increased iterations and limited memory bandwidth
- Beyond the 8 cores, the scaling per compute node is excellent





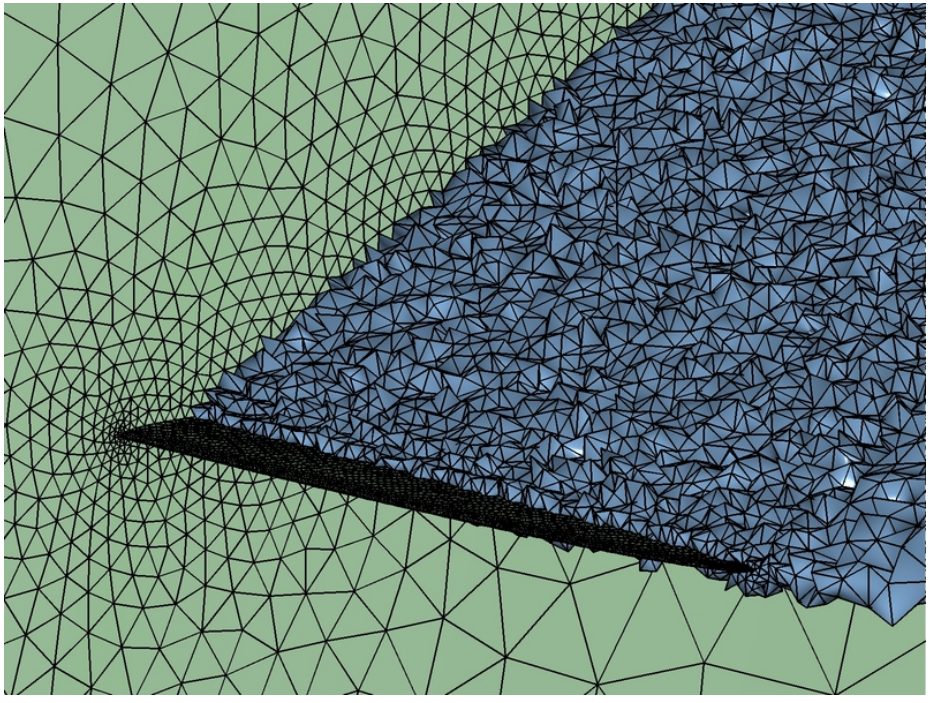
SD7003 Test Problem – Jacobi Comparison

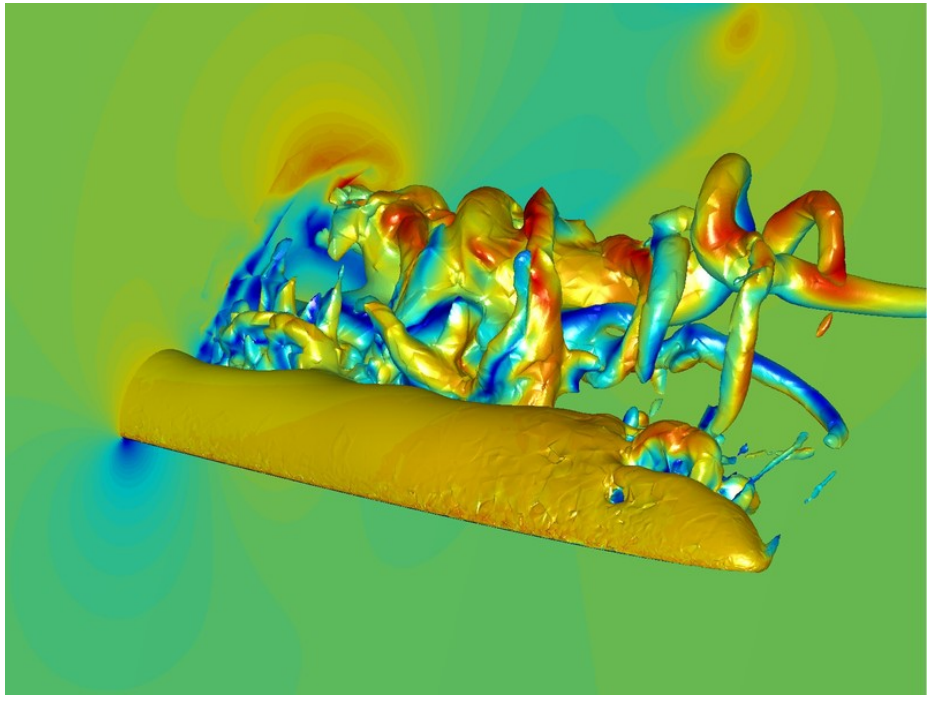
- Partition-wise block-ILU outperforms block-Jacobi even at moderate timesteps Δt
- Jacobi's good scalability does not compensate for its poor preconditioning properties



Elliptic Wing Problem

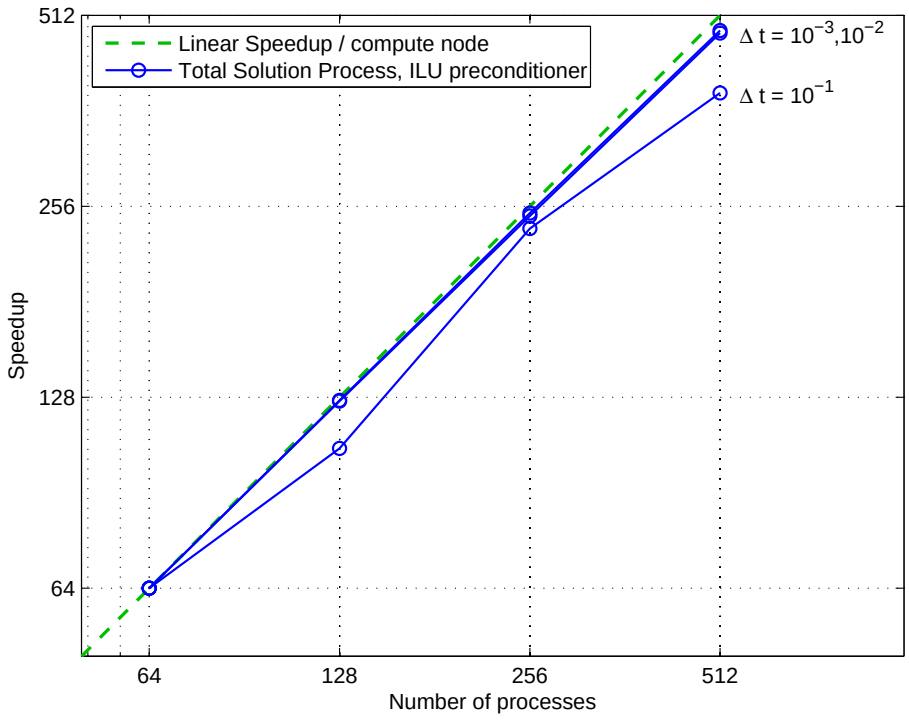
- Elliptic wing, $\mathrm{Re} = 2000$, $M = 0.3$, $\mathrm{AoA} = 30°$
- 190,000 tetrahedral elements, $p = 3$, about 19 million DOFs
- Time integration by 2-stage, 3rd order accurate DIRK scheme
- Jacobian storage 36GB, no comparison with serial possible

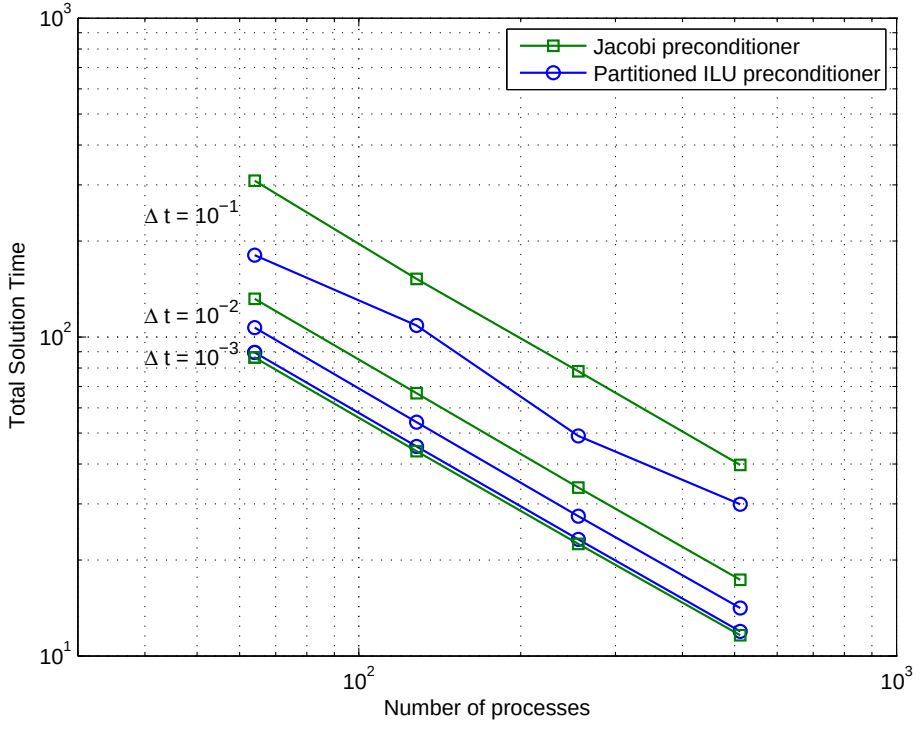




The Elliptic Wing Problem – Timings and Speedup

- Almost perfect speedup per compute node with 512 processes
- Solution time dominated by assembly for small Δt





Outline

Implicit-Explicit Runge-Kutta Methods

- [Persson 2011]: Combine implicit and explicit time stepping
- Based on a splitting $\frac{du}{dt} = f(u) + g(u)$ where $f(u)$ is considered nonstiff terms and $g(u)$ stiff terms
- Two Runge-Kutta schemes
  1. Diagonally Implicit Runge-Kutta (DIRK) scheme c, A, b for $g(u)$
  2. Explicit Runge-Kutta (ERK) scheme $\hat{c}, \hat{A}, \hat{b}$ for $f(u)$
- Combined scheme alternates explicit/implicit:

$\hat{k}_1 = f(u_n)$

for $i = 1$ **to** s

Solve for k_i in $k_i = g(u_{n,i})$, where $u_{n,i} = u_n + \Delta t \sum_{j=1}^{i} a_{i,j} k_j + \Delta t \sum_{j=1}^{i} \hat{a}_{i+1,j} \hat{k}_j$

Evaluate $\hat{k}_{i+1} = f(u_{n,i})$

end for

$u_{n+1} = u_n + \Delta t \sum_{i=1}^{s} b_j k_j + \Delta t \sum_{i=1}^{s+1} \hat{b}_j \hat{k}_j$

IMEX Schemes

IMEX1: 2-stage, 2nd order DIRK + 3-stage, 2nd order ERK

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} = \begin{array}{c|cc} \alpha & \alpha & 0 \\ 1 & 1-\alpha & \alpha \\ \hline & 1-\alpha & \alpha \end{array} \qquad \begin{array}{c|c} \hat{c} & \hat{A} \\ \hline & \hat{b}^T \end{array} = \begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \alpha & \alpha & 0 & 0 \\ 1 & \delta & 1-\delta & 0 \\ \hline & 0 & 1-\alpha & \alpha \end{array}$$

where $\alpha = 1 - \frac{\sqrt{2}}{2}$, $\delta = -2\sqrt{2}/3$. 2nd order, L-stable.

IMEX2: 2-stage, 3rd order DIRK + 3-stage, 3rd order ERK

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} = \begin{array}{c|cc} \alpha & \alpha & 0 \\ 1-\alpha & 1-2\alpha & \alpha \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \qquad \begin{array}{c|c} \hat{c} & \hat{A} \\ \hline & \hat{b}^T \end{array} = \begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \alpha & \alpha & 0 & 0 \\ 1-\alpha & \alpha-1 & 2(1-\alpha) & 0 \\ \hline & 0 & \frac{1}{2} & \frac{1}{2} \end{array}$$

where $\alpha = (3 + \sqrt{3})/6$. 3rd order accurate, no L-stability.

IMEX Schemes

IMEX3: 3-stage, 3rd order DIRK + 4-stage, 3rd order ERK

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} = \begin{array}{c|ccc} 0.43586652 & 0.43586652 & 0 & 0 \\ 0.71793326 & 0.28206673 & 0.43586652 & 0 \\ 1 & 1.2084966 & -0.64436317 & 0.43586652 \\ \hline & 1.2084966 & -0.64436317 & 0.43586652 \end{array}$$

$$\begin{array}{c|c} \hat{c} & \hat{A} \\ \hline & \hat{b}^T \end{array} = \begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ 0.43586652 & 0.43586652 & 0 & 0 & 0 \\ 0.71793326 & 0.32127888 & 0.39665437 & 0 & 0 \\ 1 & -0.10585829 & 0.55292914 & 0.55292914 & 0 \\ \hline & 0 & 1.20849664 & -0.64436317 & 0.43586652 \end{array}$$

3rd order accurate, L-stable.

Mesh-Size Based Splitting of Residual

- Associate each component of the solution vector U with an equation in the residual $R(U)$
- Split based on stiff components U_{im} in mesh elements smaller than a given size, and the remaining nonstiff components U_{ex}:

$$R(u) = \begin{bmatrix} R_{\text{im}}(U) \\ R_{\text{ex}}(U) \end{bmatrix} = \begin{bmatrix} 0 \\ R_{\text{ex}}(U) \end{bmatrix} + \begin{bmatrix} R_{\text{im}}(U) \\ 0 \end{bmatrix} = f(U) + g(U)$$

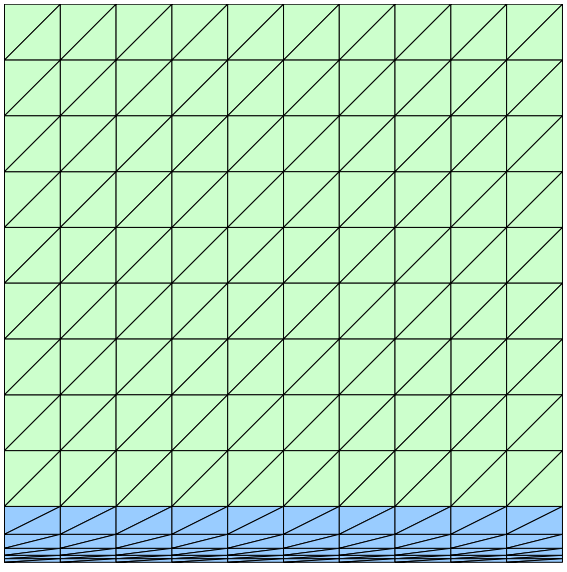
- Assumption: The CFL condition of the explicit scheme will not be affected by the small elements

Preconditioned Quasi-Newton-Krylov Methods

- Need to solve nonlinear systems of equations $k_i = g(u_{n,i})$
- Use quasi-Newton method with Jacobian $J = M - \alpha \Delta t dR/dU$
- Re-use J and its factorizations between iterations and between timesteps, as long as convergence acceptable
- Linear systems solved by preconditioned Newton-Krylov, with ILU-preconditioned CGS solvers and MDF element ordering

Absolute Stability – Flow Over a Flat Plate

- Simple flat plate model problem to evaluate IMEX approach
- Unit square, free-stream left/top, wall bottom, outflow right
- Mach number 0.2, Reynolds number 10,000
- Meshes created by n_{ref} anisotropic refinement of 10-by-10 Cartesian grid, with smallest element height $h_{\text{min}} = 0.1/2^{n_{\text{ref}}}$



Implicit/Explicit Mesh

Density

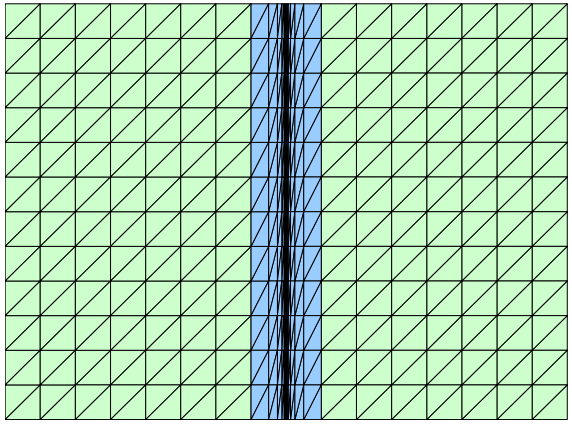
Absolute Stability – Flow Over a Flat Plate

- Determine largest stable timesteps $\Delta t_{\max}$ of ERK method for entire problem, with $\Delta t^0_{\max}$ on the initial mesh
- Confirm that the IMEX schemes are stable with timestep $\Delta t^0_{\max}$ regardless of the number of refinements
- Ratio close to 4 between successive $\Delta t_{\max}$ indicate CFL condition determined by viscous terms

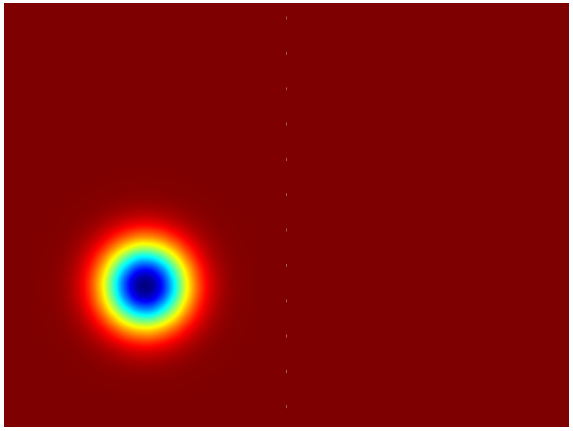
Scheme	ERK1		IMEX1	ERK2		IMEX2	ERK3		IMEX3
$\Delta t^0_{\max}$	$3.26 \cdot 10^{-4}$			$3.35 \cdot 10^{-4}$			$2.61 \cdot 10^{-4}$		
n_{ref}	$\frac{\Delta t_{\max}}{\Delta t^0_{\max}}$	Ratio		$\frac{\Delta t_{\max}}{\Delta t^0_{\max}}$	Ratio		$\frac{\Delta t_{\max}}{\Delta t^0_{\max}}$	Ratio	
0	1.0000		Stable	1.0000		Stable	1.0000		Stable
1	0.6612	1.51	Stable	0.6671	1.50	Stable	0.4958	2.02	Stable
2	0.1747	3.79	Stable	0.1762	3.79	Stable	0.1298	3.82	Stable
3	0.0457	3.82	Stable	0.0461	3.82	Stable	0.0337	3.85	Stable
4	0.0118	3.89	Stable	0.0119	3.89	Stable	0.0086	3.92	Stable
5	0.0032	3.62	Stable	0.0033	3.62	Stable	0.0023	3.72	Stable

Order of Accuracy – Euler vortex problem

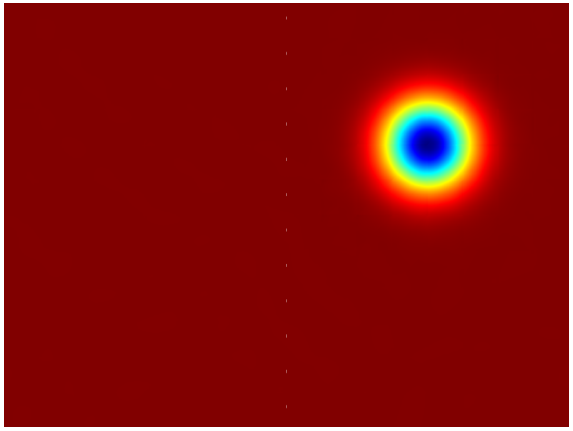
- Validate accuracy of IMEX scheme on unsteady model vortex problem
- Rectangular domain, periodic boundary conditions
- Mesh obtained by anisotropic refinement through center of the domain, a total of $n_{\text{ref}} = 5$ times



Implicit/Explicit Mesh



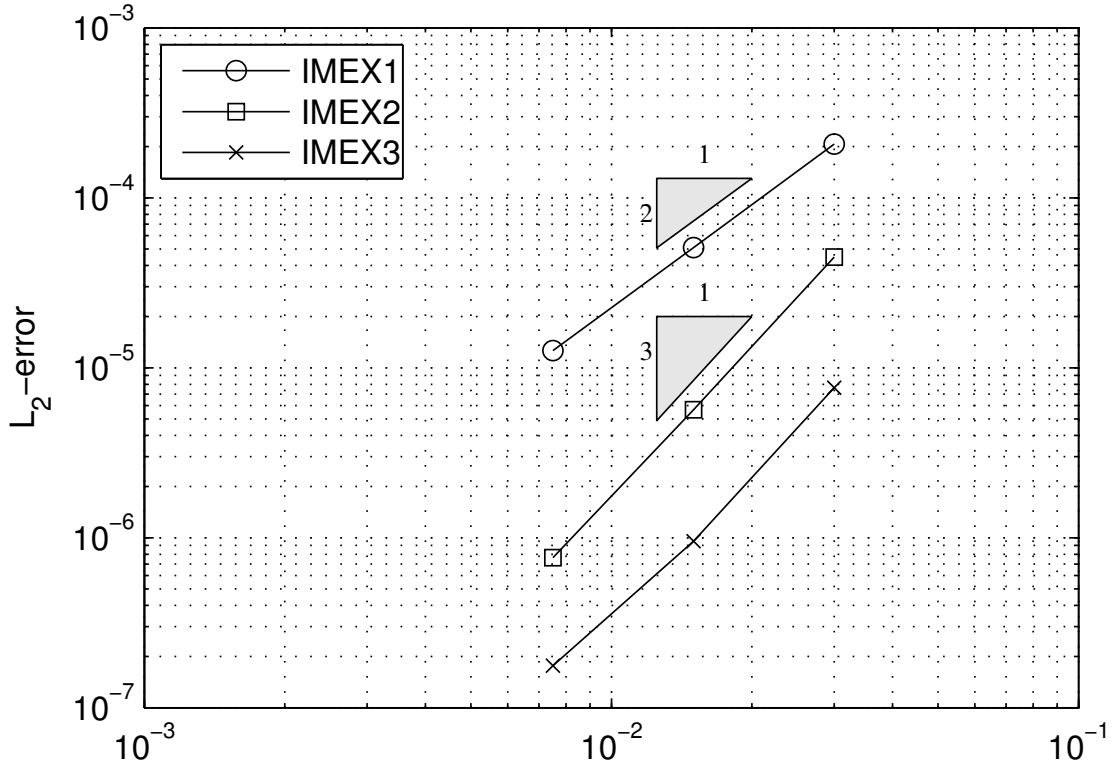
Initial density



Final density

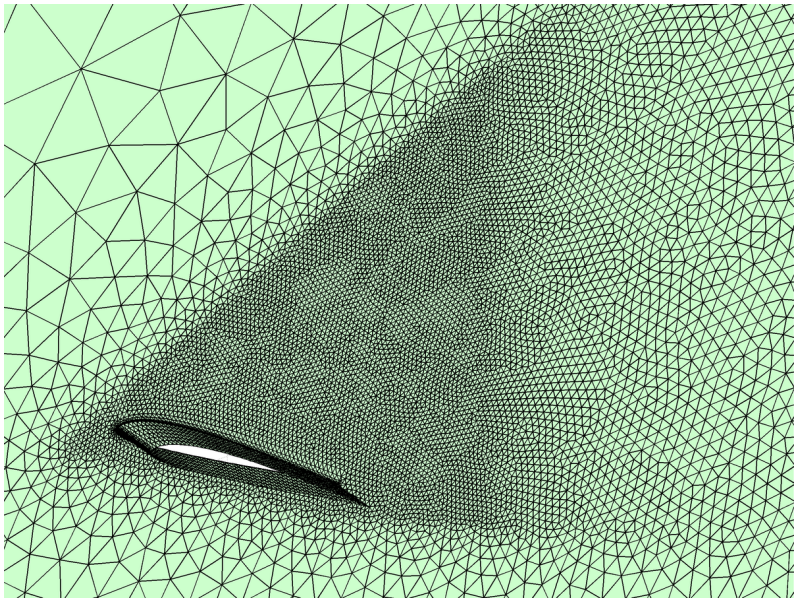
Order of Accuracy – Euler vortex problem

- $\Delta t^0_{\max}$ is again the explicit timestep limit for the unrefined mesh
- Compute L_2-errors for IMEX solutions for three timesteps $\Delta t^0_{\max}$, $\Delta t^0_{\max}/2$, and $\Delta t^0_{\max}/4$
- Expected orders of 2, 3, and 3 obtained, which is not entirely trivial since implicit part is far from the convergent regime



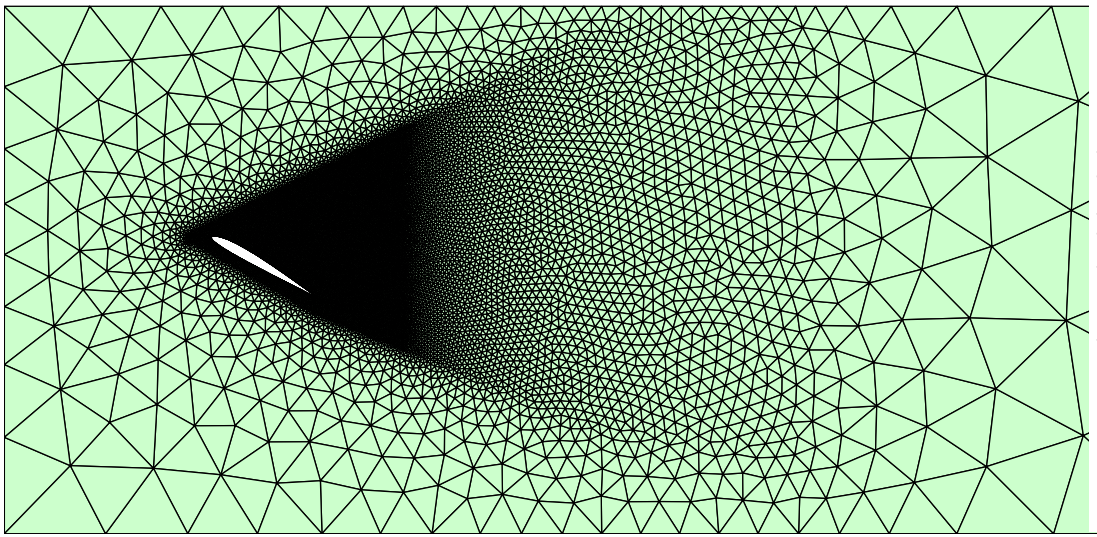
Large Eddy Simulation of Flow over Airfoil

- Consider the flow over an SD7003 airfoil at Reynolds number 100,000 and 30° angle of attack
- LES-type hybrid mesh, with DistMesh for unstructured triangles [Persson '04], each extruded as 6×3 prisms elements spanwise
- 312,000 elements, 31M DOFs, elements curved to align with boundaries using nonlinear elasticity approach [Persson '09].

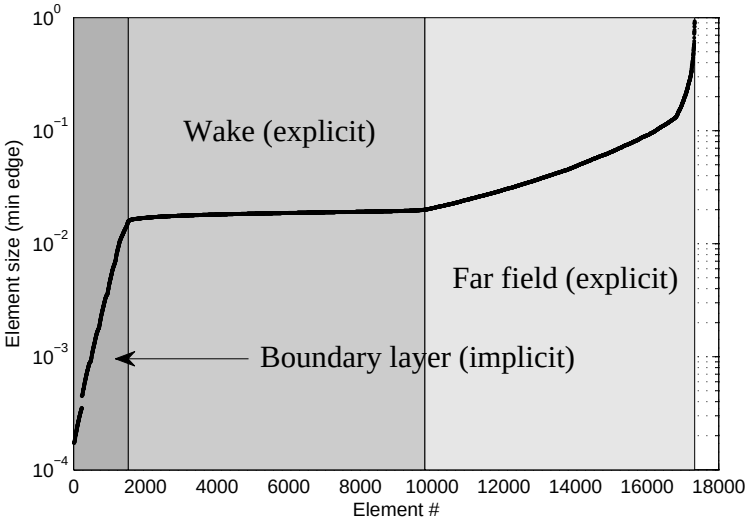


Large Eddy Simulation of Flow over Airfoil

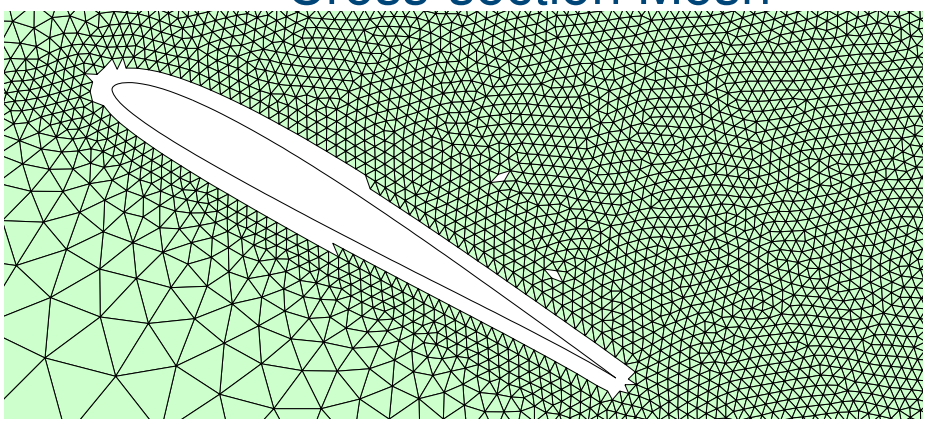
- Split based on smallest element edge sizes



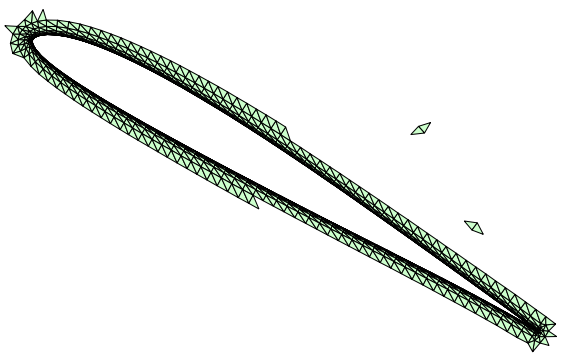
Cross-section Mesh



Element size distribution



Explicit elements



Implicit elements

Large Eddy Simulation of Flow over Airfoil

- Solve the flow problem using the **IMEX1** scheme
- ERK1 on explicit portion only: maximum $\Delta t = 2.0 \cdot 10^{-4}$
- ERK1 on entire mesh: maximum $\Delta t = 2.2 \cdot 10^{-8}$
- IMEX1 on entire mesh with splitting: Stable with $\Delta t = 2.0 \cdot 10^{-4}$
- Improvement of a factor 10,000, at the cost of solving non-linear equations involving 9% of the unknowns

Large Eddy Simulation of Flow over Airfoil

Visualization by Mach number on an isosurface of the entropy