Meros

TUG

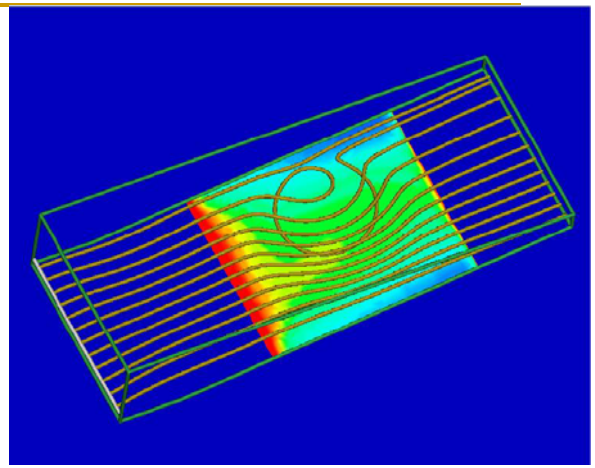
Tuesday, November 7

Robert Shuttleworth
Victoria Howle, Ray Tuminaro

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company,
for the United States Department of Energy under contract DE-AC04-94AL85000.

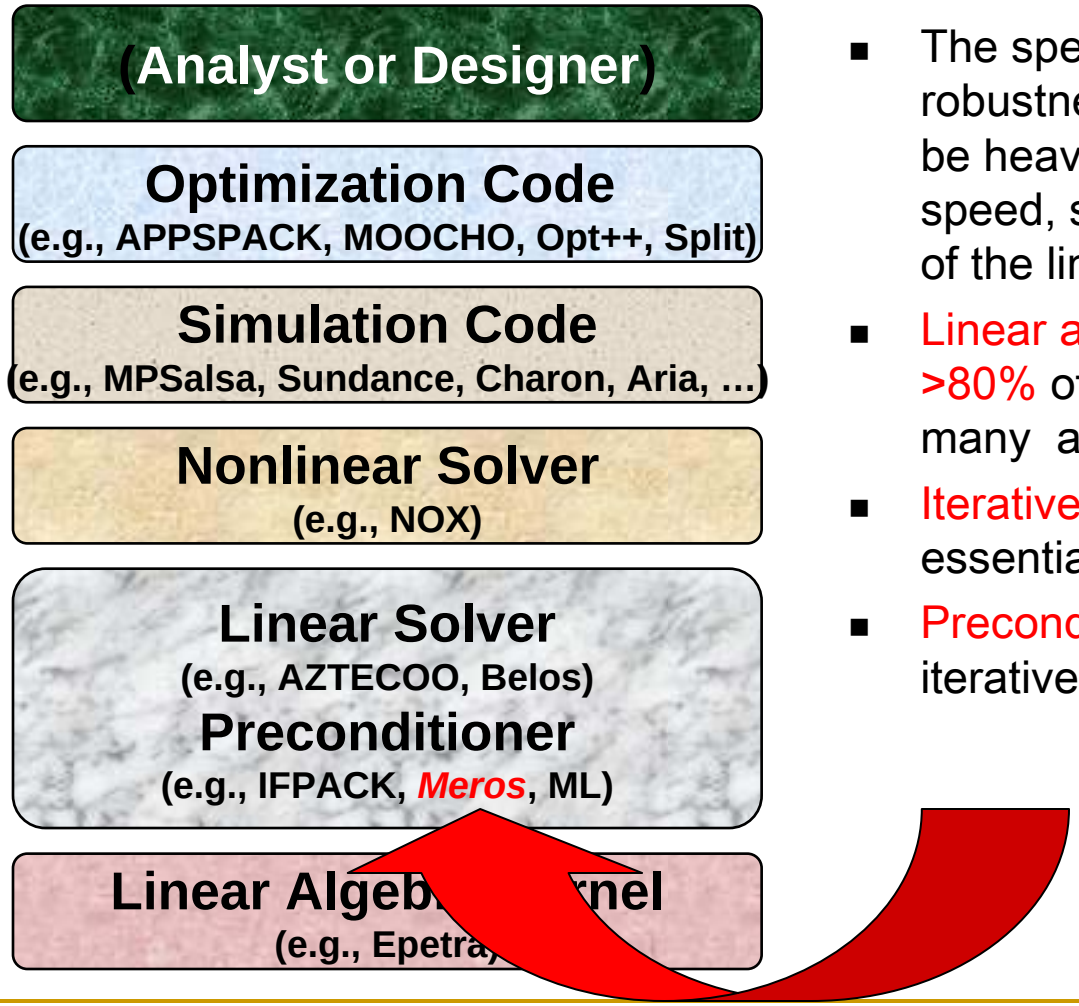
Sandia National Laboratories

Outline



- Background
  - Incompressible Navier-Stokes Eq.
  - Schur Complement Preconditioners (LSC, PCD, SIMPLE)
- Implementation
  - Meros – Block Preconditioner Package
  - MPSalsa – Stabilized FEM Fluid Flow Code
- Steady State Results
  - Lid driven cavity problem (3D)
  - Flow over a diamond obstruction (2D)
- Conclusions

Food Chain (a.k.a. vertical integration)



- The speed, scalability, and robustness of an application can be heavily dependent on the speed, scalability, and robustness of the linear solvers
- Linear algebra often accounts for >80% of the computational time in many applications
- Iterative linear solvers are essential in ASC-scale problems
- Preconditioning is the key to iterative solver performance

Introduction

Given the Incompressible Navier-Stokes Equations:

$$\text{Momentum}: \quad -\nu\Delta \mathrm{u} + (\mathrm{u}\cdot\nabla)\mathrm{u} + \nabla p = f$$

$$\text{Mass}: \quad -\nabla\cdot\mathrm{u} = 0$$

Nonlinear Term:

Picard:

$$(u^{(old)}\cdot\nabla)u$$

Newton:

Jacobian of Momentum Eq.

Discretization and Linearization:

$$\begin{pmatrix} F & B^T \\ B & -C \end{pmatrix}\begin{pmatrix} \mathbf{u} \\ p \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ 0 \end{pmatrix}$$

Block Preconditioners

- Discretization: $\begin{bmatrix} F & B^T \\ \hat{B} & -C \end{bmatrix} \begin{bmatrix} \mathrm{u} \\ p \end{bmatrix} = \begin{bmatrix} \mathrm{f} \\ 0 \end{bmatrix}$
- Consider: $P = \begin{bmatrix} F & B^T \\ & S \end{bmatrix}$
  - Optimal preconditioner is when S is the Schur Complement, $S = C + \hat{B} F^{-1} B^T$.
  - Question: How to approximate the Schur complement?

$$P^{-1} = \begin{bmatrix} F^{-1} & \\ & I \end{bmatrix} \begin{bmatrix} I & B^T \\ & I \end{bmatrix} \begin{bmatrix} I & \\ & S^{-1} \end{bmatrix}$$

Preconditioners in Meros

- PCD (Kay, Loghin, Silvester, Wathen)
- BFB^T (Elman)
- LSC (Elman, Howle, Shadid, Shuttleworth, Tuminaro)

$$P^{-1} = \begin{bmatrix} F^{-1} & \\ & I \end{bmatrix} \begin{bmatrix} I & B^T \\ & I \end{bmatrix} \begin{bmatrix} I & \\ & S^{-1} \end{bmatrix}$$

$$S = F_p^{-1}(A_p)$$

$$A_p \approx \Delta$$

- Pressure Projection – *coming soon*
  - SIMPLE
  - SIMPLEC
  - SIMPLER

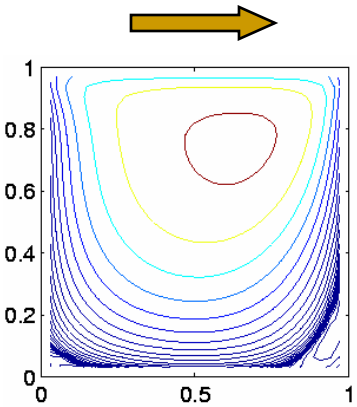
$$P^{-1} = \begin{bmatrix} I & -D^{-1}B^T \\ 0 & I \end{bmatrix} \begin{bmatrix} F & 0 \\ \hat{B} & S \end{bmatrix}^{-1}$$

$$S = \hat{B}D^{-1}B^T$$

Meros & Trilinos

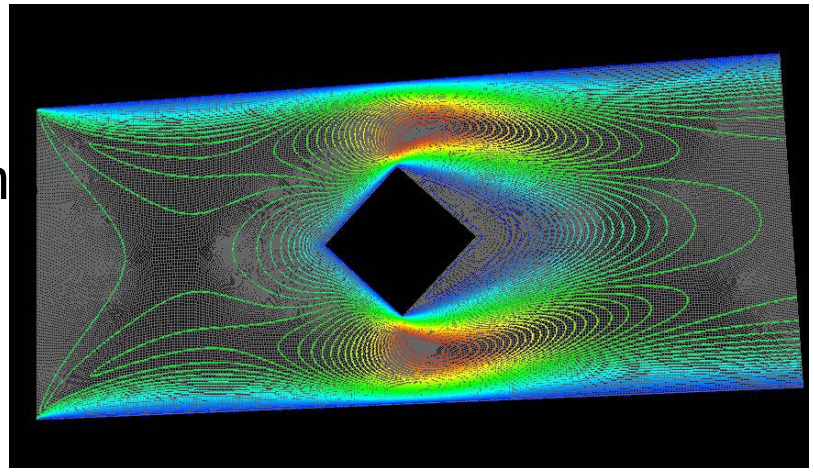
- Meros 1.0 released with Trilinos 7.0 in 9/2006
- Meros is Trilinos package as well as a user of other packages
  - Thyra
  - Teuchos
  - Epetra
  - AztecOO
  - ML

Benchmark Problems



- Lid Driven Cavity
  - Flow in a unit box (2D) or a unit cube (3D)
  - Contains many features of harder flows – recirculation/eddies
  - Structured Mesh

- Flow over a diamond obstruction
  - Inflow/Outflow boundary condition
  - Harder flow
  - Unstructured Mesh



MPSalsa Steady Problem Results

3D Lid driven cavity

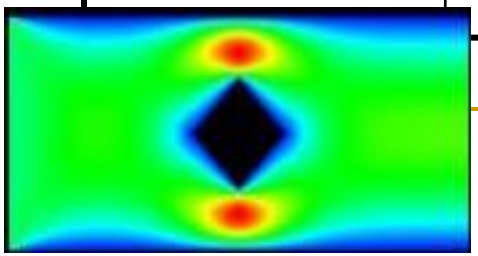
Re Number	Mesh Size	DD	PCD	Nprocs
10	32x32x32	67.0 (634.6)	28.0 (803.2)	1
	64x64x64	159.8 (2316.9)	28.4 (1265.2)	8
50	32x32x32	62.2 (615.5)	40.2 (946.9)	1
	64x64x64	162.6 (2301.6)	47.8 (1861.6)	8
100	32x32x32	61.7 (730.7)	56.0 (1432.7)	1
	64x64x64	168.5 (3069.6)	62.1 (2597.8)	8

The values in each column represent the average number of outer linear iterations per Newton Step, while the number in () represents the total CPU time for the experiment.

MPSalsa Steady Problem Results

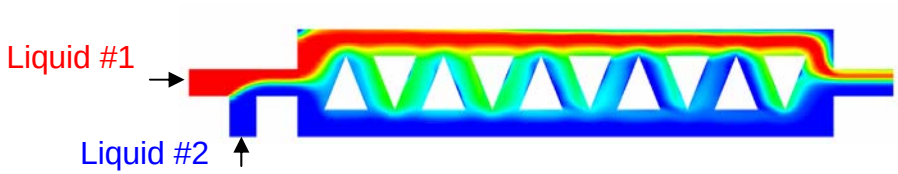
2D Flow over a Diamond Obstruction

Re #	Unknowns	DD	PCD	Nprocs
10	64K	110.8 (186.6)	20.5 (138.8)	1
	256K	284.6 (1657.4)	22.5 (266.2)	4
	1M	1329.0 (7825.5)	22.9 (501.0)	16
	4M	NC (NC)	29.4 (1841.7)	64
25	64K	101.7 (198.8)	32.9 (248.0)	1
	256K	273.8 (1583.1)	35.9 (480.6)	4
	1M	1104.8 (7631.5)	38.3 (956.9)	16
	4M	NC (NC)	48.0 (4189.8)	64
40	64K	70.4 (267.2)	54.6 (565.8)	1
	256K	203.9 (1420.7)	70.1 (1280.9)	4
	1M	997.1 (8188.2)	65.4 (2011.7)	16
	4M	NC (NC)	79.8 (9387.9)	64



Future Work

- **Sundance**
  - Microfluidics/Bio-briefcase
  - 10 microns
  - Flow at low Re
  - Shape and topology optimization



- **Aria**
  - Improve the scalability of Neutron Generator problems
- **Xyce**
  - Interested in preconditioning harmonic balance methods
- **Charon**
  - Interested in preconditioning semiconductor modeling

Wrap-up

- We have developed methods to enable scalable solvers for incompressible flow applications
- Available to any application using Trilinos
  - Tested in MPSalsa
  - Early user: Sundance
- Meros 1.0 released in September
- Work this year to develop methods needed by Aria, Charon, and Xyce
- Several core methods currently implemented; more on the way

- software.sandia.gov/Trilinos/packages/meros