First-Order System Least Squares FOSLS

DOE & NSF & IBM

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HISTORICAL GAP

fast solvers

&

uniform performance

Reynolds number, Lamé constants,...

Outline

no frills

I. Basic FOSLS

II. FOSLS Tools

III. Anatomy of FOSLS for C-D

IV. FOSLL* & Results

V. Concluding Remarks

FOSLoSophy

PHYSICAL PROCESS

CONTINUUM MODEL

ALGEBRAIC MODEL

ALBEGRAIC SOLVER

IMPLEMENTATATION

design effort

I. Basics
II. Tools
III. C-D
IV. LL*
V. End

My Matrix Grail

symmetry

$$Lx = b, \qquad L \text{ general}$$

Normal Equations: $A = L^{\mathrm{T}}L$

$$L^{\mathrm{T}}Lx = L^{\mathrm{T}}b$$

Dual Equations: $A = LL^{\mathrm{T}}$

$$LL^{\mathrm{T}}y = b$$

Dual Matrix Equations

dual (ghost) variables

$x = L^{\mathrm{T}} y$

$Lx = b$ solvable

$\Leftrightarrow$ solution $x \quad \eta \;\; (L) \; = Range(L^{\mathrm{T}})$

$\Leftrightarrow$ $x = L^{\mathrm{T}} y$

$$LL^{\mathrm{T}} y = b$$

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Matrix Minimization Principles

"energy" functionals

$$Lx = b, \qquad L \text{ general}$$

Normal Equations:

$$\|Lx - b\|^2 = \langle L^T L x, x \rangle - 2\langle x, L^T b \rangle + \langle b, b \rangle$$

Dual Equations:

$$\langle L L^T y, y \rangle - 2\langle y, b \rangle$$

My REAL Matrix Grail

symmetry & positive definiteness

$$AX = b, \qquad A \text{ spd}$$

error = $e = x - X$

Energy Functional: solving = minimizing energy error

$$F(x) = \langle Ax, x\rangle - 2\langle x, b\rangle$$

$$= \langle A(x-X), x-X\rangle - \langle AX, X\rangle$$

$$= \langle Ae, e\rangle + \text{constant}$$

↑ ?nice?

My ACTUAL Real Grail

spd & nice (elliptic perhaps)

Let $L = -\Delta^h$ be a discrete Laplacian.

$A = L^2$ O(h^{-4}) condition number!

TROUBLE!

But "no" trouble with $A = L$:

minimize $\langle Ae, e\rangle \sim \|\ e\|^2 = H^1$ semi-norm ^{2}

H^1-ellipticity multigrid

Bottom Line

Objective:

$L \longrightarrow A$ spd & H^1-elliptic.

Trouble:

$L = (\Delta^h)^2$ is spd & H^2-elliptic!?

Cure:

Compute $A = L^{1/2}$?!

Solution:

Get access to the PDE !

FOSLS Illustration

$$p'' + ap' = f$$

ignore boundary

second order

First-Order System: $u = p'$

$$Lu = u' + au = f$$

FOSLS Functional:

$$F(u; f) = \|Lu - f\|^2$$

$$= \int (u' + au - f)^2 dx$$

$$\sim \int (e')^2 dx$$

H^1-ellipticity

Multigrid

$\min F(q^h)$

Relaxation: $\varepsilon_i^h \quad S^h \quad H^1$

$$F(q^h + s\varepsilon_i^h; f) = \min_{t \in \mathbf{R}} F(q^h + t\varepsilon_i^h; f)$$

Coarsening: $S^{2h} \quad S^h$

$$F(q^h + p^{2h}; f) = \min_{q^{2h} \in S^{2h}} F(q^h + q^{2h}; f)$$

Optimality **(Oswald, Zhang, Bramble, ...)**:

homogeneous/bilinear part

$$F(p + e; f) - F(p; f) = E(e) \sim \|e\|_1^2$$

Minimization Principle Advantages

$\min F(q)$

- sense of optimality
- error monitor $F(q)$
- monotone: $T \quad S \qquad \min_T F \leq \min_S F$
- continuum functions & subspaces
- approximation theory analysis
- elliptic
  - standard FE & MG with theory
  - final H^1 accuracy

FOSLS Essence

divide & conquer

Motivation: scalar (esp. elliptic) problems are "well" understood

scalar (elliptic) energy minimization principle

Plan: imbue PDE with "nice" energy principle

Objective: PDE → loosely coupled scalar equations

Purpose: *standard* finite elements and multigrid methods

Approach: PDE → First Order System → Energy

Issues

FOSLS

- New variables
- New equations
- New boundary conditions
- Scaling
- Other norms

Error Measure

Objective: approximation + *reasonable* error measure

Ideal: optimal approximation in the measure

Reasonable:

- always accurate values: L^2
- often accurate derivatives: H^1

Conventional Measure (L = ″)**:**

- residual = $\|Lp\text{-}f\,\|_0 = \|L(p\text{-}p^*)\|_0 = \|Le\|_0 = \|e''\|_0$
- oscillatory error → overly large residuals

FOSLS Error Measure

for *any* approximation **w**
to the exact solution **w***

Absolute :

$$F(\mathbf{w};\mathbf{f}) = \|L\mathbf{w} - \mathbf{f}\|_0^2 = \|L(\mathbf{w} - \mathbf{w}^*)\|_0^2$$

$$\sim \|\mathbf{w} - \mathbf{w}^*\|_1^2$$

Relative :

$$\frac{F(\mathbf{w};\mathbf{f})}{F(\mathbf{0};\mathbf{f})} = \frac{\|L\mathbf{w} - \mathbf{f}\|_0^2}{\|L\mathbf{w}^*\|_0^2} \sim \frac{\|\mathbf{w} - \mathbf{w}^*\|_1^2}{\|\mathbf{w}^*\|_1^2}$$

!!! powerful tool for adaptive refinement !!!

!avoids patch test for nonconforming elements!

#1: New Variables

reducing order

Poisson:

$$\cdot \quad p = f$$

$$\mathbf{u} = \quad p$$

CFD/Elasticity:

$$-\Delta\mathbf{u} + \mathrm{Re}(\quad \mathbf{u}^t)^t\mathbf{u} + \quad p = f$$

$$\cdot\ \mathbf{u} + \alpha p = g$$

$$\mathbf{U} = \quad \mathbf{u}^t$$

#2: New Equations

good norm equivalence

Poisson :

$$\mathbf{u} - \quad p = \mathbf{0}$$

$$\cdot\ \mathbf{u} + f = 0$$

$$\times\ \mathbf{u} = \mathbf{0}$$

CFD/Elasticity :

$$\mathbf{U} - \quad \mathbf{u}^{t} = \mathbf{O}$$

$$- \quad \cdot\ \mathbf{U} + \mathrm{Re}\,\mathbf{U}^{t}\mathbf{u} + \quad p = \mathbf{f}$$

nonlinearity across variables only

$$\cdot\ \mathbf{u} + \alpha p = g$$

$$\times\ \mathbf{U} \qquad = \mathbf{O}$$

$$\& \qquad trace\,\mathbf{U} + \alpha \quad p = \mathbf{0}$$

Curl Option

Poisson system :

$$\mathbf{u} - \quad p = \mathbf{0}$$

$$\cdot\, \mathbf{u} \quad = f$$

$$\times\, \mathbf{u} \quad = \mathbf{0}$$

Div - free error : $\quad \cdot\, \mathbf{e} = 0$

$$\mathbf{u} + \mathbf{e} - \quad p - \mathbf{0} = \mathbf{e}$$

$$\cdot\, (\mathbf{u} + \mathbf{e}) - f = 0$$

$$\times (\mathbf{u} + \mathbf{e}) = \quad \times\, \mathbf{e}$$

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#3: New Boundary Conditions

good norms

Poisson Case: $\mathbf{u} = \quad p$

Neumann:

$$\mathbf{n}\cdot \quad p = 0 \qquad\qquad \mathbf{n}\cdot\mathbf{u} = 0$$

Dirichlet:

$$p = 0 \qquad\qquad \mathbf{n}\times\mathbf{u} = \mathbf{0}$$

Robin/Radiation:

$$\mathbf{n}\cdot \quad p + \alpha p = 0 \qquad\qquad \mathbf{n}\cdot\mathbf{u} + \alpha p = 0$$

Tangential Boundary Condition

y = constant line

$$p = 0$$

$$p_x = 0$$

$$p \parallel \mathbf{n}$$

$$\mathbf{n} \times p = 0$$

#4: *Preconditioners*

nonsmooth data or L^2 measure

ILLUSTRATE WITH POISSON:

$$\mathbf{u} - \quad p = \mathbf{0}$$

$$(-\Delta)^{-\frac{1}{2}}(\quad \cdot \mathbf{u} + f) = 0$$

$$(-\Delta)^{-\frac{1}{2}}(\quad \times \mathbf{u}) = \mathbf{0}$$

$$F_{-1}(\mathbf{u}, p; f) =$$

$$\|\mathbf{u} - \quad p\|_0^2 + \| \quad \cdot \mathbf{u} - f\|_{-1}^2 + \| \quad \times \mathbf{u}\|_{-1}^2$$

$$F_{-1}(\mathbf{u}, p; 0) \sim \| \quad p\|_0^2 + \|\mathbf{u}\|_0^2$$

Inverse Norm

Precondition $L\mathbf{w} = \mathrm{f}$ by $B = (-\Delta)^{-1/2}$:

$$BL\mathbf{w} = B\,\mathbf{f}$$

$$\|q\|_{-1}^{2} \equiv \sup_{r \quad H^{1}} \frac{<q,r>^{2}}{\|r\|_{1}^{2}}$$

$$= <(-\Delta)^{-1}q,q>$$

$$= \|(-\Delta)^{-1/2}q\|_{0}^{2}$$

direct computation by MG

#5: *Scaling*

balanced equivalence

Poisson Case: $\mathbf{u} = \quad p$

$$F_\varepsilon(\mathbf{u}, p; f) =$$

$$\varepsilon\|\mathbf{u} - \quad p\|^2 + (1-\varepsilon)(\| \quad \cdot \mathbf{u} + f\|^2 + \| \quad \times \mathbf{u}\|^2)$$

Stage I:

$$F_0(\mathbf{u}; f) = \| \quad \cdot \mathbf{u} + f\|^2 + \| \quad \times \mathbf{u}\|^2$$

$$F_0(\mathbf{u}; 0) \sim \| \quad \mathbf{u}\|^2$$

StageII:

$$F_1(p; \mathbf{u}) = \| \quad p - \mathbf{u}\|^2$$

$$F_1(p; \mathbf{0}) = \| \quad p\|^2$$

III. FOSLS for Convection Diffusion

convection-diffusion

$$- \quad \cdot \quad p + ap_x = f, \qquad 0 \le x, y \le 1$$

$$p(0,y) = p(1,y) = 0$$

$$p_y(x,0) = p_y(x,1) = 0$$

Guide

$$- \quad \cdot \quad p + ap_x = -e^{ax}(e^{-ax}p_x)_x - p_{yy}$$

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Convection Diffusion 1-3

#1 : New Variables

$$u = e^{-ax} p_x$$
$$v = \quad p_y$$

flux

#2 : New Equations

$$-e^{ax} u_x - v_y + f = 0$$

div

$$e^{ax} u_y - v_x \quad = 0$$

'curl'

#3 : New Boundary Conditions

$$p(0,y) = p(1,y) = 0$$
$$v(0,y) = v(1,y) = 0$$
$$v(x,0) = v(x,1) = 0$$

Convection Diffusion 5

tool #5

$f = 0$ for simplicity

First Stage :

$$e^{-ax/2} \quad \text{X} \quad \begin{cases} -e^{ax}u_x - v_y = 0 \\ e^{ax}u_y - v_x = 0 \end{cases}$$

Troublesome Scaling :

$$\left\| -e^{ax}u_x - v_y \right\|^2 + \left\| e^{ax}u_y - v_x \right\|^2$$

$$= \left\| e^{ax}u_x \right\|^2 + 2 < e^{ax}u_x, v_y > + \left\| v_y \right\|^2$$

decoupled u & v ?

$$+ \left\| e^{ax}u_y \right\|^2 - 2 < e^{ax}u_y, v_x > + \left\| v_x \right\|^2$$

?

Convection Diffusion 5

continued

Better Scaling : $s_{\pm}(x,y) = e^{\pm ax/2}$

$$\left\| -s_+ u_x - s_- v_y \right\|^2 + \left\| s_+ u_y - s_- v_x \right\|^2$$

$$= \left\| s_+ u_x \right\|^2 + 2 < u_x, v_y > + \left\| s_- v_y \right\|^2$$

divided & conquered

$$+ \left\| s_+ u_y \right\|^2 - 2 < u_y, v_x > + \left\| s_- v_x \right\|^2$$

- ***uniform*** scaled H^1 equivalence
- scaling damps boundary layer behavior
- valid for more general convection term
- Poisson equation for recovering p

More General Form

$$s_{-} \sim e^{-ax/2}$$

$$\mathbf{u} = \quad p$$

$$- \quad \cdot \mathbf{u} + au = f$$

$$F_0(\mathbf{u}; f) =$$

$$\| s_{-} [- \quad \cdot \mathbf{u} + au - f] \|^2$$

$$+ \| s_{-} [\quad \times \mathbf{u}] \|^2$$

$$F_0(\mathbf{u}; 0) \sim$$

$$\| s_{-} \quad \mathbf{u} \|^2 + \| s_{-} \quad \mathbf{v} \|^2$$

IV. FOSLL*

L^2 error minimization

Energy Functional: $LL^*V = f, \quad U = L^*V$

$$< LL^*v, v > - 2 < v, f >$$

$$= < L^*v, L^*v > - 2 < v, LL^*V > \pm < V, LL^*V >$$

$$= < L^*v, L^*v > - 2 < L^*v, L^*V > \pm < L^*V, L^*V >$$

$$= \| L^*v - U \|^2 - \text{constant}$$

precise L^2 error minimization

*FOSLL**

theoretical issues

L is a first-order differential operator
with boundary conditions.

L^* is a first-order differential operator
with adjoint boundary conditions.

The solution of $Lu = f$ is in the range of L^*.

L^* is H^1-elliptic: $\| L^* v \| \sim \| \nabla v \|$.

*FOSLL**

sample application
2D

Problem:

$$\bullet a \quad p + \mathbf{b}\bullet \quad p = f$$

First-Order System: $\mathbf{u} \; = \; a^{1/2} \quad p$

$$\bullet a^{1/2}\mathbf{u} + \mathbf{b}\bullet a^{-1/2}\mathbf{u} \; = \; f$$

$$\times\, a^{-1/2}\mathbf{u} \; = 0$$

*FOSLL**

formal dual *LL**

2D

$$\begin{pmatrix} \cdot\ a^{1/2} + \mathbf{b}\cdot \\ \times\ a^{-1/2} \end{pmatrix} \left(-a^{1/2} \quad + \mathbf{b} \quad a^{-1/2} \quad \times\right) \begin{pmatrix} w \\ z \end{pmatrix}$$

$$= \begin{pmatrix} (\ \cdot\ a^{1/2} + \mathbf{b}\cdot\ )(-a^{1/2} \quad + \mathbf{b}) & \left(\mathbf{b}\cdot\ a^{-1/2} \quad \times\right)^* \\ \mathbf{b}\cdot\ a^{-1/2} \quad \times & \times\, a^{-1} \quad \times \end{pmatrix} \cdot \begin{pmatrix} w \\ z \end{pmatrix}$$

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FOSLL* Numerical Example

two stage

problem:

$$\bullet a \quad p + \mathbf{b}\bullet \quad p = f, \qquad a = \begin{cases} 1, & x \le 0.5 \\ \sigma, & x > 0.5 \end{cases}$$

solution:

$$p = \begin{cases} ((2\sigma - 4)x^2 + (4 - \sigma))\sin(\pi y), & x \le 0.5 \\ (-6x^2 + 7x - 1)\sin(\pi y), & x > 0.5 \end{cases}$$

method:

FE uniform linears & AMG W(1,1) cycles

Results

fine grids: h=1/128 $\mathbf{b}^t = (0,0)$ & $\mathbf{b}^t = (6,9)$

jump σ	||MG||	FE accuracy
1	0.08	$O(h^2)$ for p in L^2
10	0.13	$O(h)$ for p in H^1
100	0.25	$O(h)$ for $\mathbf{u}$ in L^2

convection scales: σ = 1 $\mathbf{b}^t = (6,9)$

h =	1/4	1/8	1/16	1/32	1/64	1/128
||MG|| =	0.34	0.64	0.51	0.31	0.15	0.08

FOSLS/FOSLL Advantages*

- minimization principle advantages
- systematic once functional is properly posed
- ‘decoupled’ elliptic or “nice” equations in each variable
- avoids LBB/staggering/artificial diffusion/stabilization...
- final H^1 or L^2 accuracy for all variables
- F is its own practical performance measure
- generally excellent numerical performance

FOSLS/FOSLL* Disadvantages

- possibly more variables
  - but possibly smaller grids
- H^1 equivalence for FOSLS needs smoothness/regularity
  - but FOSLL* does not
- conservation is not automatic
  - but can be done
- very tricky to get the functional & spaces just right

✓ new variables & equations + careful scaling

FOSLS Applications

various stages of development

- diffusion-convection
- neutron transport
- Stokes & Navier-Stokes
- elasticity
- electromagnetics
- eigenproblems
- elliptic grid generation
- boundary functionals
- discontinuities
- highly convective flows
- inverse problems
- time-dependent problems
- coupled systems: flow/structure/em/egg

FURTHER INFO

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