Massively Parallel Domain Decomposition Preconditioner for the High-Order Galerkin Least Squares Finite Element Method

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1 Introduction

2 High-Order Galerkin Least Squares

3 Balancing Domain Decomposition by Constraint

4 Results

5 Conclusion and Future Work
Outline

1. Introduction
2. High-Order Galerkin Least Squares
3. Balancing Domain Decomposition by Constraint
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5. Conclusion and Future Work
Motivation

Discretization Requirements

Discretization should support

- **High-Order**: Simulation of unsteady flows with multiple scales benefits from higher-order methods
  - Turbulence (DNS/LES)
  - Acoustics / wave propagation
  - Even in steady aerodynamics, high-order methods are more efficient in terms of error/DOF [Barth, 1997][Venkatakrishnan, 2003]

- **Unstructured Mesh**: Handling complex geometries

Selected Previous Work on High-Order Methods

- High-order schemes have been designed for various frameworks
  - Finite difference [Lele, 1992]
  - Finite volume [Barth, 1993][Wang, 2004]
**Motivation**

**Example: High-Order Discretization**

- Drag convergence for NACA 0012 [Fidkowski, 2005]
- Decay of turbulent kinetic energy in LES modeling [Kosovic, 2000]

- High-order schemes can significantly improve time to achieve engineering required accuracy.
Motivation

Massively Parallel Algorithms

- Modern supercomputers are massively parallel (1000+ procs).
- Parallelization is essential for problems of practical interests.
  - Flow over large, complex geometries
  - Unsteady simulations (e.g. DNS/LES)

Trend of High Performance Computing in Past 15 Years

Statistics from Top500.org

Cart3D, FUN3D, JNWT

#1, #500, Average

Largest, Smallest, Average

FLOPS vs. Processors

Statistics from Top500.org
Typical large jobs remain in $O(100)$ procs.

Range of scales present in viscous flows requires implicit solvers.

“The scalability of most of [CFD] codes tops out around 512 cpus…” [Mavriplis, 2007]

Exceptions:

- FUN3D inviscid matrix-free Newton-Krylov-Schwarz solver using 2048 procs [1999]
- Cart3D inviscid multigrid-accelerated Runge-Kutta solver using 2048 procs [2005]
- NSU3D RANS multigrid solver with line implicit solver in boundary layers using 2048 procs [2005]

Need highly scalable implicit solver to take advantage of the future computers with 10,000+ procs.
Objectives and Approaches

Objectives

1. High-order discretization on unstructured mesh
2. Highly scalable solution algorithm for massively parallel systems

Approaches

1. Galerkin Least Squares (GLS)
   - Study behavior of high-order GLS discretization.
   - Use $h/p$ scaling artificial viscosity for subcell shock capturing.
2. Domain Decomposition (DD) Preconditioner
   - Solve Schur complement system using preconditioned GMRES based on DD.
   - Test the preconditioner for high-order discretization of advection-dominated flows.
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Galerkin Least Squares Discretization

### Background
- Stabilized FEM for advection-dominated flows
- SUPG developed by Hughes [1982]; analyzed by Johnson [1984]
- SUPG extended to GLS by Hughes [1989]

### GLS Discretization for Advection-Diffusion
- Differential operator and bilinear form
  \[ \mathcal{L}u \equiv \beta \cdot \nabla u - \nabla \cdot (\nu \nabla u) = f \]
  \[ a(u, \phi) = (\beta \cdot \nabla u, \phi)_\Omega + (\nu \nabla u, \nabla \phi)_\Omega, \quad \forall u, \phi \in V \subset H^1(\Omega) \]
- Find \( u \in V \) s.t.
  \[ a(u, \phi) + (\mathcal{L}u, \tau \mathcal{L}\phi)_{\Omega,T_h} = (f, \phi)_\Omega + (f, \tau \mathcal{L}\phi)_{\Omega,T_h}, \quad \forall \phi \in V \]
  where \( (\cdot, \cdot)_{\Omega,T_h} = \sum_K \int_K \cdot \, dK \) and \( \tau \sim \begin{cases} h, & P_e \gg 1 \\ h^2, & P_e \ll 1 \end{cases} \).
Stabilization Matrix

**Stability and A Priori Error Estimate for Hyperbolic Case ($\nu = 0$)**

\[
a(u, u) \geq h\|\beta \cdot \nabla u\|_{L^2(\Omega)}^2
\]

\[
\sqrt{h}\|\beta \cdot \nabla (u - u_h)\|_{L^2(\Omega)} + \|u - u_h\|_{L^2(\Omega)} \leq Ch^{p+\frac{1}{2}}\|u\|_{H^{p+1}(\Omega)}
\]

**High-Order Stabilization Matrix**

- In order to keep \(\frac{\text{cond}(L_{\text{stabilized}})}{\text{cond}(L_{\text{unstabilized}})} = O(1)\) as \(p \to \infty\) or \(h \to 0\),

  \[\tau \sim h^2/p^2, \quad P_e \ll 1\]

- One choice of \(\tau\) in \(\mathbb{R}^d\)

  \[
  \tau^{-1} = \sum_{i=1}^{d+1} \left|\beta \cdot \nabla \xi^i\right| + \frac{p^2}{d} \sum_{i=1}^d \sum_{j=1}^d \frac{\partial \xi_i}{\partial x_k} \frac{\partial \xi_j}{\partial x_l} \nu_{kl}
  \]
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Motivation

- Performance of ILU degrades with number of processors even with line partitioning [Diosady, 2007].
- Data parallelism alone is not sufficient to obtain good performance in massively parallel environment (1000+ procs.).

Selected Previous Work (Elliptic)

- Bourgat proposes Neumann-Neumann method for Schur complement system [1988].
- Mandel improves scalability with Balancing DD [1993].
- Dorhmann extends BDD to BDDC [2003].
Schur Complement System

Discrete Harmonic Extension (Elliptic Equation)

- Decompose $\Omega$ into non-overlapping domains $\Omega_i$ and define $\Gamma_i = \partial \Omega_i \setminus \partial \Omega$ and $\Gamma = \bigcup_{i=1}^{N} \Gamma_i$. Decompose $V_h \subset H^1(\Omega)$ into
  
  $$V_h(\Omega \setminus \Gamma) = \{ v \in V_h : v|_{\Gamma} = 0 \}$$
  $$V_h(\Gamma) = \{ v \in V_h : a(v, \phi) = 0, \forall \phi \in V_h(\Omega \setminus \Gamma) \}$$

- $V_h(\Gamma)$ is called the space of discrete harmonic extensions.

Variational Problem

Find $u = \hat{u} + \bar{u} \in V_h(\Omega \setminus \Gamma) \oplus V_h(\Gamma)$ s.t.

$$a(\hat{u}, \psi) = (f, \psi)_{\Omega}, \quad \forall \psi \in V_h(\Omega \setminus \Gamma)$$
$$a(\bar{u}, \phi) = (f, \phi)_{\Omega}, \quad \forall \phi \in V_h(\Gamma)$$

- $\hat{u}$ requires local Dirichlet solves
- $\bar{u}$ requires global interface solve
Schur Complement System

Schur Complement Operator

Schur complement operator $S : V_h(\Gamma) \rightarrow V_h(\Gamma)'$ defined by

$$\langle Sv, \phi \rangle = a(v, \phi), \quad \forall v, \phi \in V_h(\Gamma)$$

where, $\langle \cdot, \cdot \rangle : W' \times W \rightarrow \mathbb{R}$ s.t. $\langle F, v \rangle \equiv F(v), \forall F \in W', \forall v \in W$.

Schur Complement Problem

Find $u \in V_h(\Gamma)$ s.t.

$$\langle Su, \phi \rangle = (f, \phi)_\Omega, \quad \forall \phi \in V_h(\Gamma)$$

- Forming $S$ is expensive; action of $S$ on $v \in V_h(\Gamma)$ is computed via local Dirichlet solves and minimal communication.
- Problem solved using a Krylov space method (e.g. GMRES)
- Scalable preconditioner needed to accelerate convergence
### Features of BDDC
- Equipped with a coarse space that makes subdomain problems wellposed.
- Provides global communication.
- Example of primal constraints:
  - Values at corners of $\Omega_i$.
  - Averages on the edges of $\Omega_i$.

### Spaces
\[
V_h(\Gamma) = \text{global discrete harmonic extension}
\]
\[
\bigoplus_{i=1}^{N} V_h(\Gamma_i) = \text{collection of local discrete harmonic extensions (i.e. discontinuous across } \Gamma)\]
\[
\tilde{V}_h(\Gamma) = \{ v \in \bigoplus_{i=1}^{N} V_h(\Gamma_i) : \text{ } v \text{ continuous on primal constraints} \} \]
BDDC Spaces

Dual and Primal Spaces

Decompose $\tilde{V}_h(\Gamma)$ into $\bigoplus_i V_{h,\Delta}(\Gamma_i)$ and $V_{h,\Pi}(\Gamma)$.

- Dual problems are decoupled
- Primal problem has DOF of $O(N)$

Dual Space ($\Delta$):

$$V_{h,\Delta}(\Gamma_i) = \{ v \in V_h(\Gamma_i) : v = 0 \text{ on primal constraint} \}$$

Primal Space ($\Pi$):

$$V_{h,\Pi}(\Gamma) = \{ v \in \tilde{V}_h(\Gamma) : \sum_{i=1}^{N} \tilde{a}_i(v|_{\Omega_i}, \phi_{\Delta}|_{\Omega_i}) = 0, \forall \phi_{\Delta} \in \bigoplus_{i=1}^{N} V_{h,\Delta}(\Gamma_i) \}$$
Primal and Dual Schur Complement

- **Primal Schur complement:** $S_{\Pi} : V_{h,\Pi}(\Gamma) \to V_{h,\Pi}'(\Gamma)$
  \[
  \langle S_{\Pi} v_{\Pi}, \phi_{\Pi} \rangle = \sum_{i=1}^{N} \tilde{a}_i(v_{\Omega_i}, \phi_{\Omega_i}), \quad \forall v_{\Pi}, \phi_{\Pi} \in V_{h,\Pi}(\Gamma)
  \]

- **Local dual Schur complement:** $S_{\Delta,i} : V_{h,\Delta}(\Gamma_i) \to V_{h,\Delta}'(\Gamma_i)$
  \[
  \langle S_{\Delta,i} v_{\Delta,i}, \phi_{\Delta,i} \rangle = \tilde{a}_i(v_{\Delta,i}, \phi_{\Delta,i}), \quad \forall v_{\Delta,i}, \phi_{\Delta,i} \in V_{h,\Delta}(\Gamma_i)
  \]

**BDDC Preconditioner**

\[
M_{BDDC}^{-1} = \sum_{i=1}^{N} R_{D,i}^T (T_{\text{sub},i} + T_{\text{coarse}}) R_{D,i}
\]

where $T_{\text{sub},i} = R_{\Gamma\Delta,i}^T S_{\Delta,i}^{-1} R_{\Gamma\Delta,i}$ and $T_{\text{coarse}} = R_{\Gamma\Pi}^T S_{\Pi}^{-1} R_{\Gamma\Pi}$

**Condition Number Estimate for Coercive, Symmetric $a(\cdot, \cdot)$**

\[
\kappa(M_{BDDC}^{-1} S) \leq C(1 + \log^2 (H/h))
\]
Background

- Adaptation of N-N condition to nonsymmetric bilinear form
- Proposed by Achdou for BDD [1997]
- Applied to FETI [Toselli, 2001] and BDDC [Tu, 2008]

Robin-Robin IC

- Subtract $\int_{\Gamma_i} \frac{1}{2} \beta \cdot \hat{n}_i u \phi$ from interfaces.
- Modified local bilinear form is

\[
\tilde{a}_i(u, \phi) = (\nu \nabla u, \nabla \phi)_{\Omega_i} + \frac{1}{2} (\beta \cdot \nabla u, \phi)_{\Omega_i} - \frac{1}{2} (\beta \cdot \nabla \phi, u)_{\Omega_i} \\
+ \frac{1}{2} (u, \nu \beta \cdot \hat{n})_{\partial \Omega_i \cap \partial \Omega_N} \\
\]

- $\tilde{a}_i(\cdot, \cdot)$ is positive in local space $V_h(\Omega_i)$: $\tilde{a}_i(u, u) \geq \nu |u|_{H^1(\Omega_i)}$.
- Resulting IC on $\Gamma_i$ is Robin type

\[
(\nu \nabla u - \frac{1}{2} \beta) \cdot \hat{n} = 0 \quad \text{on } \Gamma_i
\]
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Poisson Equation

Poisson Equation Objectives

Test scaling with:
- Number of subdomains
- Size of subdomain
- $p$ for different primal constraints

Solution

Partitioning Examples
Poisson Equation

Scaling with Number of Subdomains and Subdomain Size

- GMRES iteration is independent of number of subdomains and size of subdomain ($p = 1$).
- Corner + state average (C+SA) primal constraint requires approx. half the iterations of just corner constraint (C).

![Graph showing GMRES iterations vs. number of subdomains and DOF per subdomain](image)
Poisson Equation

Scaling with $p$

- Poisson equation solved on unstructured mesh $\sim 8000$ elem.
- Number of iterations nearly independent of $p$ when C+SA primal constraints are used.

Size of Primal Problem

- Corners only: $\approx N_{\text{subdomain}}$
- Corners + Edge State Average: $\approx 3 \times N_{\text{subdomain}}$
Boundary Layer Equation Objectives

Study effect of:
- interface conditions (Neumann-Neumann vs. Robin-Robin)
- $\tau$ scaling ($h^2$ vs. $h^2/p^2$)

Solution ($\nu = 10^{-3}$)

Anisotropic Mesh and Partitioning
Advection Diffusion: Boundary Layer

**Interface Conditions (IC)**

- Robin-Robin IC performs significantly better than Neumann-Neumann IC in advection dominated cases.
- Interface conditions are identical as $\nu \rightarrow \infty$.

**Graphs**

- **Left Graph**: GMRES iterations vs. $\nu$ for $N_{\text{subdomain}} = 16$
  - Advection and diffusion regions are clearly distinguishable.

- **Right Graph**: GMRES iterations vs. $\nu$ for $N_{\text{subdomain}} = 64$
  - Similar to the left graph, but with a higher resolution, showing more detailed behavior near $\nu = 0$. 

**Legend**

- N−N (p=1)
- R−R (p=1)
Advection Diffusion: Boundary Layer

\( \tau \) Matrix Scaling

- Performance of preconditioner degrades for \( p > 1 \) if \( \tau \sim h^2 \) in diffusion dominated cases.
- With \( \tau \sim h^2/p^2 \), the preconditioner performs similar to \( p = 1 \) case.

\[ N_{\text{subdomain}} = 64 \]
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Conclusion

- BDDC preconditioner shows good scalability for:
  - Both diffusion-dominated and advection-dominated flows with Robin-Robin interface condition
  - All ranges of interpolation order $p$ with proper choices of $\tau$ and primal constraints

Future Work

- Extension to 3D
- Inexact solvers for subdomain problems
- Complex geometries and highly anisotropic mesh
Questions
Supplemental Slides
Instability of the Standard Galerkin Method

Discretization

Advection-diffusion equation

\[ \mathcal{L} u \equiv \beta \cdot \nabla u - \nabla \cdot (\nu \nabla u) = f \]

Galerkin: Find \( u \in V \subset H^1(\Omega) \) s.t.

\[ a(u, \phi) = (f, \phi)_\Omega, \quad \forall \phi \in V \]

where \( a(u, \phi) = \int_\Omega \phi \beta \cdot \nabla u + \nu \nabla \phi \cdot \nabla u \).

Stability and A Priori Error Estimate

\[ a(u, u) \geq \nu \| \nabla u \|_{L^2(\Omega)}^2 = \nu \| u \|_{H^1(\Omega)}^2 \]

\[ \nu \| u - u_h \|_{H^1(\Omega)} \leq C h^p \| u \|_{H^{p+1}(\Omega)} \]

Not coercive in \( H^1(\Omega) \) as \( \nu \to 0 \).
Stabilized Methods for Advection-Dominated Flows

- Streamline-Upwind Petrov-Galerkin (SUPG) [Hughes 1982]
- Galerkin Least-Squares (GLS) [Hughes 1989]
- Residual Free Bubbles (RFB) [Brezzi 1994]
- Variational Multiscale based on local Green’s function [Hughes 1995]
Finite Element vs. Finite Volume

Advantages of Finite Element Method

- Maintains element-wise compact stencil for high-order discretization.
  - Ease of boundary condition treatment.
  - Reduces communication volume for DD.
- Straightforward treatment of elliptic operator.
- Rigorous mathematical framework for \textit{a priori} error estimation and DD convergence estimation.

Disadvantages of Finite Element Method

- Requires stabilization term for $H^1(\Omega)$ stability.
- DOF increases with the solution order.
Three types of basis functions (in 2D): Node, Edge, Element.
Basis type defined by its support.
The continuity constraint must be enforced on nodal and edge basis during assembly.
Object-based Block Storage

- Jacobian stored blockwise, with the varying size of blocks
- Matrix converted to CRS format before solved with UMFPACK

Jacobian of $3 \times 3$ Mesh (18 elem, $p = 5$, arbitrary basis)

Galerkin

DG (with compact lifting)
### Comparison with Discontinuous Galerkin

#### Features (common to DG)
- High-order discretization on unstructured mesh
- $H^1(\Omega)$ stability for advection-dominated flows

#### Advantages (compared to DG)
- Straightforward treatment of elliptic operators (no lifting required)
- Fewer DOF required to represent a solution in $H^1(\Omega)$

#### Disadvantages
- Potentially expensive calculation of stabilization terms
- Absence of block-wise compact stencil (more complex preconditioning strategy required)
High-Order SUPG vs. GLS

**p-Refinement with Traditional \( \tau \)**

- If \( h \gg \nu/\|\beta\| \), SUPG \( p \)-refinement fails to converge.
- Asymptotic convergence rates as \( h \to 0 \) are identical \((\|e\|_{H^1(\Omega)} \sim h^p)\)

**Supersonic Solution to advection-diffusion equation \((h = 0.1, \nu/\|\beta\| = 0.01)\)**

![Graphs comparing SUPG and GLS methods](image-url)
$p$-Refinement with High-Order Modified $\tau$

- With the high-order modified $\tau$, both SUPG and GLS $p$-refinement converge to the exact solution.
- GLS converges much rapidly than SUPG with $p$.

Solution to advection-diffusion equation ($h = 0.1, \nu/\|\beta\| = 0.01$)
Shock Capturing

Background
- Artificial viscosity can regularize underresolved features.

Resolution Indicator and $h/p$-Scaling Artificial Viscosity
- high-order resolution indicator based on orthogonal polynomial expansion [Persson, 2006]

$$S_e = \frac{(u - \Pi^{p-1}u, u - \Pi^{p-1}u)_K}{(u, u)_K}, \quad u \in \mathcal{P}_p(K)$$

where $\Pi^{p-1}$ is the $L_2(K)$ projection onto $\mathcal{P}_{p-1}(K)$.
- If $\log_{10}(S_e) \geq s_0$, add piecewise constant viscosity $\nu \sim h/p$ to the element.
Burger’s Equation

Burger’s equation solved on \( \approx 450 \) element mesh.

\[
\frac{\partial}{\partial x} \left( \frac{1}{2} u^2 \right) + \frac{\partial u}{\partial y} + \nabla \cdot (\nu_{\text{artificial}}(u) \nabla u) = 0
\]
Euler Equation: Gaussian Bump

**Formulation**

- Symmetric form using Hughes’ entropy variables [1986]

\[
V = \left( -\frac{s + \gamma + 1}{\gamma - 1}, -\frac{\rho E}{p}, \frac{\rho u_i}{p}, -\frac{\rho}{p} \right)
\]

- The governing equation becomes

\[
\tilde{A}_0 V, t + \tilde{A}_i V, x_i = 0
\]

where \(A_0\) is SPD and \(A_i\) is symmetric (\(K_{ij}\) is SPSD for N-S).

**Gaussian Bump: Pressure and Partitioning**

![Gaussian Bump: Pressure and Partitioning](image)

[Image of Gaussian Bump: Pressure and Partitioning]
Euler Equation:

- BDDC with R-R IC performs well for Euler equation.
- With N-N IC, 400+ GMRES iteration required for 32 subdomains.

Average of GMRES iterations required for last three Newton steps.
Parallel Scalability of ILU

Scalability of ILU for DG Discretization [Diosady 2007]

- Navier-Stokes equation
- Partitioning based on line connectivity
- Line-ordered ILU with $p$-Multigrid within each subdomain

![Graphs showing linear iterations and speed-up vs number of processors](image_url)
Schur Complement for Non-Self-Adjoint Operator

Discrete Harmonic Extension (Non-Self-Adjoint)

Decompose $V_h \subset H^1(\Omega)$ into

$$V_h(\Omega \setminus \Gamma) = \{ v \in V_h : v|_{\Gamma} = 0 \}$$

$$V_h(\Gamma) = \{ v \in V_h : a(v, \phi) = 0, \forall \phi \in V_h(\Omega \setminus \Gamma) \}$$

$$V_h^*(\Gamma) = \{ \psi \in V_h : a(w, \psi) = 0, \forall w \in V_h(\Omega \setminus \Gamma) \}$$

Find $u = \hat{u} + \bar{u} \in V_h(\Omega \setminus \Gamma) \oplus V_h(\Gamma)$ s.t.

$$a(\hat{u}, \phi) = (f, \phi)_\Omega, \quad \forall \phi \in V_h(\Omega \setminus \Gamma)$$

$$a(\bar{u}, \psi) = (f, \psi)_\Omega, \quad \forall \psi \in V_h^*(\Gamma)$$

Schur Complement Operator

Schur complement $S : V_h(\Gamma) \to V_h^*(\Gamma)'$ s.t.

$$\langle Sv, \psi \rangle = a(v, \psi), \quad \forall v \in V_h(\Gamma), \quad \forall \psi \in V_h^*(\Gamma)$$
**Neumann-Neumann Preconditioner**

**Local Spaces and Local Schur Complement**
- Decompose $V_h(\Omega_i) \subset H^1(\Omega_i)$ of $\Omega_i$ into
  \[ V_h(\Omega_i \setminus \Gamma_i) = \{ v_i \in V_h(\Omega_i) : v|_{\partial\Omega_i} = 0 \} \]
  \[ V_h(\Gamma_i) = \{ v_i \in V_h(\Omega_i) : \bar{a}_i(v_i, \phi) = 0, \forall \phi \in V_h(\Omega_i \setminus \Gamma_i) \} \]
- Local Schur complement: $S_i : V_h(\Gamma_i) \rightarrow V_h(\Gamma_i)'$
  \[ \langle S_i v_i, \phi_i \rangle = \bar{a}_i(v_i, \phi_i), \quad \forall v_i, \phi_i \in V_h(\Gamma_i) \]

**Interpolation and Weighting Function**
- Interpolation: $R_i^T : V_h(\Gamma_i) \rightarrow V_h(\Gamma)$ s.t.
  \[ \bigoplus_{i=1}^N R_i^T V_h(\Gamma_i) = V_h(\Gamma) \]
- Weighting Function: $D_i \in V_h(\Gamma_i)$ s.t.
  \[ D_i = 1 / (\text{# of } \Omega_i \text{ sharing DOF on } \Gamma) \]
  Note, $v = \sum_{i=1}^N R_i^T D_i v|_{\Omega_i}, \forall v \in V_h(\Gamma)$
Neumann-Neumann (N-N) Preconditioner

- Precondition $S$ by applying $S_i^{-1} : V'(\Gamma_i) \to V(\Gamma_i)$ on each $\Omega_i$ and interpolate the result back to $V(\Gamma)$

$$M_{NN}^{-1} = \sum_{i=1}^{N} R_i^T D_i S_i^{-1} D_i R_i$$

- For $\tilde{a}_i(u, \phi) = (\nabla u, \nabla \phi)_{\Omega_i}$, application of $S_i^{-1}$ corresponds to solving a local problem with Neumann interface condition on $\Gamma_i$

$$(\nabla u) \cdot \hat{n} = 0 \quad \text{on} \quad \Gamma_i$$

Condition Number Estimate for Coercive, Symmetric $a(\cdot, \cdot)$

$$\kappa(M_{NN}^{-1} S) \leq \frac{C}{H^2} (1 + \log(H/h))^2$$
Balancing Domain Decompositions

Problems of Neumann-Neumann Preconditioner
- Local Schur complement $S_i$ may be singular
- Limited scalability due to lack of coarse space

Coarse Space
- Introduce coarse space $V_{h,0}$ that
  - makes subdomain problems well-posed
  - provides global communication
  - $\text{DOF}_{\text{coarse}} = O(N)$

Examples of DD with a Coarse Space
- BDD: Balancing Domain Decomposition [Mandel, 1993]
- BDDC: BDD by Constraints [Dohrmann, 2003]
Balancing Domain Decomposition

- Define a coarse space: \( V_{h,0}(\Omega) = \text{span}\{R_i^T \delta_i^\dagger\} \), \( \text{Kernel}(S_i) \subset V_{h,0} \)
- Define projection \( P_0 : V_h(\Omega) \rightarrow V_{h,0}(\Omega) \), \( P_0 = R_0^T S_0^{-1} R_0 S \)
- Apply Neumann-Neumann preconditioner to balanced problem

\[
M_{BDD}^{-1} = R_0^T S_0^{-1} R_0 + (I - P_0) \left( \sum_{i=1}^{N} R_i^T D_i S_i^{-1} D_i R_i S \right) (I - P_0)
\]

Examples of DD with a Coarse Space

- BDD: Balancing Domain Decomposition [Mandel, 1993]
  - \( V_{h,0} = \bigoplus_{i=1}^{N} \text{Kernel}(S_i) \).
  - Apply *multiplicative* coarse correction such that residual of subdomain problem is in \( \text{range}(S_i) \). (i.e. 'balanced' problem)
- BDDC: BDD by Constraints [Dohrmann 2003]
  - \( V_{h,0} = \{\psi_i\} \), harmonic extensions satisfying primal constraints.
  - Solve *additive* coarse and constrained subdomain problems.
### Primal Type

Preconditions the Schur complement system by solving Neumann problems using the flux jumps.

- Neumann-Neumann method [Bourgat 1988]
- Balancing Domain Decomposition (BDD) [Mandel, 1993]
- BDD by Constraints (BDDC) [Dohrmann 2003]

### Dual Type

Preconditions the flux equations by solving Dirichlet problems using function jumps.

- Finite Element Tearing and Interconnecting (FETI) [Farhat 1991]
- Dual-Primal FETI (FETI-DP) [Farhat 2001]
  - Spectrum of BDDC and FETI-DP preconditioned operators are identical [Mandel 2005][Li 2005]
BDDC Spaces

**Partially Assembled Spaces**

- Collection of $V_h(\Gamma_i)$: $W_h \equiv \oplus_{i=1}^N V_h(\Gamma_i) \supset V_h(\Gamma)$
- Fully assembled FE space: $\hat{W}_h \equiv V_h(\Gamma) = \oplus_{i=1}^N R_i^T V_h(\Gamma_i)$
- Partially assembled space: $\tilde{W}_h \equiv V_{h,0}(\Gamma) + \oplus_{i=1}^N R_i^T R^T_{\Gamma \Delta, i} V_h(\Gamma_i)$

**Idea**: BDDC preconditioner applies inverse of $\tilde{S}: \tilde{W}_h \rightarrow \tilde{W}'_h$ to Shucr complement system.
Schur Complement System: Matrix Form

**Schur Complement**

Decompose local stiffness matrix and load vector into

\[
A^{(i)} = \begin{pmatrix} A^{(i)}_{II} & A^{(i)}_{I\Gamma} \\ A^{(i)}_{I\Gamma} & A^{(i)}_{\Gamma\Gamma} \end{pmatrix} \quad \text{and} \quad f^{(i)} = \begin{pmatrix} f^{(i)}_I \\ f^{(i)}_\Gamma \end{pmatrix}
\]

Schur complement system is given by

\[
\hat{S}u_\Gamma = \hat{g}
\]

where

\[
\hat{S} = \sum_{j=1}^{N} R^{(j),T} S^{(j)} R^{(j)}, \quad S^{(j)} = A^{(j)}_{I\Gamma} - A^{(j)}_{I\Gamma} \left( A^{(j)}_{II} \right)^{-1} A^{(j)}_{\Gamma\Gamma}
\]

\[
\hat{g} = \sum_{j=1}^{N} R^{(j),T} g^{(j)}, \quad g^{(j)} = f^{(j)}_\Gamma - A^{(j)}_{I\Gamma} \left( A^{(j)}_{II} \right)^{-1} f^{(j)}_I
\]
Application of Schur Complement

Application of $S^{(j)}$

Calculation of $u^{(j)}_\Gamma = S^{(j)} v^{(j)}$ corresponds to solving a local Dirichlet problem:

$$S^{(j)} v^{(j)} = A^{(j)}_{\Gamma\Gamma} v^{(j)} - A^{(j)}_{\Gamma I} \left( A^{(j)}_{II} \right)^{-1} A^{(j)}_{I \Gamma} v^{(j)}$$

Application of $(S^{(j)})^{-1}$

Calculation of $u^{(j)}_\Gamma = (S^{(j)})^{-1} v^{(j)}_\Gamma$ corresponds to solving a local Neumann problem:

$$\begin{pmatrix} A^{(j)}_{II} & A^{(j)}_{I \Gamma} \\ A^{(j)}_{\Gamma I} & A^{(j)}_{\Gamma \Gamma} \end{pmatrix} \begin{pmatrix} u^{(j)}_I \\ u^{(j)}_\Gamma \end{pmatrix} = \begin{pmatrix} 0 \\ v^{(j)}_\Gamma \end{pmatrix}$$
Coarse Correction

Coarse-level correction operator is given by

\[ T_{\text{coarse}} = \psi (\psi^T S \psi)^{-1} \psi^T \]

where

\[ \psi \equiv \left( \psi^{(1)} , \ldots , \psi^{(N)} , T \right)^T \in \mathbb{R}^{\text{DOF}(\bigoplus V_h(\Gamma_i)) \times N_{\text{primal}}} \]

Coarse Basis

The local coarse basis, \( \psi^{(i)} \) is the harmonic extension to \( \Omega_i \) that satisfies the primal constraints, i.e.

\[
\begin{pmatrix}
S^{(i)} & C^{(i),T} \\
C^{(i)} & 0
\end{pmatrix}
\begin{pmatrix}
\psi^{(i)} \\
\Lambda^{(i)}
\end{pmatrix} =
\begin{pmatrix}
0 \\
R^{(i)}_{\Pi}
\end{pmatrix}
\]

where \( C^{(i)} \) enforces primal constraints and \( \Lambda^{(i)} \) is Lagrange multiplier.
Subdomain correction is given by

\[ T_{\text{sub}} = \sum_{i=1}^{N} \begin{pmatrix} R_{\Gamma}^{(i), T} & 0 \end{pmatrix} \begin{pmatrix} S^{(i)} & C^{(i), T} \\ C^{(i)} & 0 \end{pmatrix}^{-1} \begin{pmatrix} R_{\Gamma}^{(i)} \\ 0 \end{pmatrix} \]

- Provides subdomain corrections for which all coarse level, primal variables vanish.
- Primal constraints ensure the local problem is invertible.
Idea [Klawonn, 2004]

Change basis functions on interface to make primal constraints explicit.
- Removes the need for the Lagrange multipliers as primal continuity constraints are satisfied by construction.

Example: State Average

Change of basis $\psi_k \rightarrow \psi_l$ such that

- Dual Variables: $\int_{\text{edge}} \psi_l(\xi) d\xi = 0, \quad l = 1, \ldots, n - 1$
- Primal Variable: $\psi_n(\xi) = 1, \quad \forall \xi \in \text{edge}$

Let $T_{\text{COB}}$ be the weighting matrix that maps from $\psi$ to $\phi$, then new stiffness matrix is

$$A_{\psi,ij} = a(\psi_i, \psi_j) = (T_{\text{COB}}^T A_\phi T_{\text{COB}})_{i,j}$$
Assumption

Consider symmetric, coercive $a(\cdot, \cdot) : V \to V$ and $a_i(\cdot, \cdot) : V_i \to V_i$. Assume $\exists C_0, \omega, E = (\epsilon_{ij})_{i,j=1}^N$ such that

- **Stable Decomposition**
  \[
  \forall v \in V, \exists v_i \in V_i : \sum_{i=0}^N a_i(v_i, v_i) \leq C_0 a(v, v)
  \]

- **Local Stability**
  \[
  \forall i = 1, \ldots, N, \forall v_i \in V_i : a(v_i, v_i) \leq \omega a_i(v_i, v_i)
  \]

- **Strengthened Cauchy-Shwarz Inequality**
  \[
  \forall i, j = 1, \ldots, N, \forall u_i \in V_i, \forall v_j \in V_j : |a(u_i, v_j)| \leq \epsilon_{ij} \sqrt{a(u_i, u_i) a(v_j, v_j)}
  \]

Conditioner Number Estimate [Dryja, 1995]

\[
\kappa \leq C_0 \omega (1 + \rho(E))
\]
Rayleigh Quotient

Applying Rayleigh quotient formula to the inner product $\langle M_{\text{BDDC}} \cdot, \cdot \rangle$,

$$\lambda_{\text{min}} \left( M_{\text{BDDC}}^{-1} S \right) = \min_{v \neq 0} \frac{\langle Sv, v \rangle}{\langle S\eta, \eta \rangle + \sum_{i=1}^{N} \langle S_{\Delta, i} v_{\Delta, i}, v_{\Delta, i} \rangle}$$

$$\lambda_{\text{max}} \left( M_{\text{BDDC}}^{-1} S \right) = \max_{v \neq 0} \frac{\langle Sv, v \rangle}{\langle S\eta, \eta \rangle + \sum_{i=1}^{N} \langle S_{\Delta, i} v_{\Delta, i}, v_{\Delta, i} \rangle}$$
Eigenvalues: Lower Bound

Schur Complement on $\tilde{V}_h(\Gamma)$

$$\langle \tilde{S}v, \phi \rangle = \sum_{i=1}^{N} \tilde{a}_i (v|\Omega_i, \phi|\Omega_i), \quad \forall v, \phi \in \tilde{V}_h(\Omega)$$

Derivation

$$\langle S_{\Pi} v_{\Pi}, v_{\Pi} \rangle + \sum_{i=1}^{N} \langle S_{\Delta,i} v_{\Delta,i}, v_{\Delta,i} \rangle = \langle \tilde{S}v_{\Pi}, v_{\Pi} \rangle + \sum_{i=1}^{N} \tilde{a}_i (v_{\Delta,i}, v_{\Delta,i})$$

$$= \langle \tilde{S}v_{\Pi}, v_{\Pi} \rangle + \langle \tilde{S}v_{\Delta}, v_{\Delta} \rangle$$

$$= \langle \tilde{S}(v_{\Pi} + v_{\Delta}), (v_{\Pi} + v_{\Delta}) \rangle = \langle Sv, v \rangle$$

$$\langle Sv, v \rangle \geq \min_{v=R_D^T R_{\Pi} v_{\Pi} + \sum_{i=1}^{N} R_D^T R_{\Delta,i} v_{\Delta,i}} \left( \langle S_{\Pi} v_{\Pi}, v_{\Pi} \rangle + \sum_{i=1}^{N} \langle S_{\Delta,i} v_{\Delta,i}, v_{\Delta,i} \rangle \right)$$

$$\lambda_{\min} \left( M^{-1}_{BDDC} S \right) \geq 1$$
Eigenvalues: Upper Bound

Derivation

\[
\langle Sv, v \rangle \leq 2[\langle SR_D^T R_{\Gamma n}^T v_n, R_D^T R_{\Gamma n}^T v_n \rangle \\
+ \langle S(\sum_{i=1}^{N} R_{D,i}^T R_{\Gamma \Delta,i}^T v_{\Delta,i}), (\sum_{i=k}^{N} R_{D,k}^T R_{\Gamma \Delta,k}^T v_{\Delta,k}) \rangle] \\
\lesssim \langle SR_D^T R_{\Gamma n}^T v_n, R_D^T R_{\Gamma n}^T v_n \rangle + \sum_{i=1}^{N} \langle S(R_{D,i}^T R_{\Gamma \Delta,i}^T v_{\Delta,i}), (R_{D,i}^T R_{\Gamma \Delta,i}^T v_{\Delta,i}) \rangle
\]

For symmetric, coercive bilinear form with \( p = 1 \),

\[
\langle SR_D^T R_{\Gamma n}^T v_n, R_D^T R_{\Gamma n}^T v_n \rangle \lesssim (1 + \log^2 (H/h)) \langle S_n v_n, v_n \rangle \\
\langle S(R_{D,i}^T R_{\Gamma \Delta,i}^T v_{\Delta,i}), (R_{D,i}^T R_{\Gamma \Delta,i}^T v_{\Delta,i}) \rangle \lesssim (1 + \log^2 (H/h)) \langle S_{\Delta,i} v_{\Delta,i}, v_{\Delta,i} \rangle
\]

Thus,

\[
\langle Sv, v \rangle \lesssim \left( 1 + \log^2 \left( \frac{H}{h} \right) \right) \min_{v=R_D^T R_{\Gamma n}^T v_n+\sum_{i=1}^{N} R_{D,i}^T R_{\Gamma \Delta,i}^T v_{\Delta,i}} \left( \langle S_n v_n, v_n \rangle + \sum_{i=1}^{N} \langle S_{\Delta,i} v_{\Delta,i}, v_{\Delta,i} \rangle \right)
\]

\[\lambda_{\max} \left( M_{\text{BDDC}}^{-1} S \right) \leq C \left( 1 + \log^2 (H/h) \right)\]
GMRES Residual Bound [Eisenstat, 1983]

Let $c$ and $C^2$ be such that

\[
\begin{align*}
    c_0 \langle u, u \rangle & \leq \langle u, Tu \rangle \\
    \langle Tu, Tu \rangle & \leq C_0^2 \langle u, u \rangle
\end{align*}
\]

Then,

\[
\frac{\|r_m\|}{\|r_o\|} \leq \left(1 - \frac{c_0^2}{C_0^2}\right)^{m/2}
\]

Advection-Diffusion Convergence Estimate [Tu, 2008]

With state and flux average as primal constraints, BDDC (R-R) satisfies

\[
\begin{align*}
    c_0 &= 1 - CH(H/h)(1 + \log(H/h)) \\
    C_0 &= C(1 + \log(H/h))^4
\end{align*}
\]
Nonlinear Equation Solution Scheme

Discrete form using Galerkin Method

\[ M_h \frac{dU_h}{dt} + R_h(U_h(t)) = 0 \]

Time Stepping Scheme

\[ U_h^{m+1} = U_h^m - \left( \frac{1}{\Delta t} M_h + \frac{\partial R_h}{\partial U_h} \right)^{-1} R_h(U_h^m) \]

For steady problems \( \Delta t \rightarrow \infty \).

Linear System

\[ A_h x_h = b_h \] must be solved at each time step

\[ A = \frac{1}{\Delta t} M_h + \frac{\partial R_h}{\partial U_h} \quad x = \Delta U_h^m \quad b = -R_h(U_h^m) \]
Parallel GLS Solver

GLS Solver Features

- Many ideas borrowed from ProjectX (Discontinuous Galerkin solver developed at ACDL since 2002)
- High-order GLS discretization on unstructured mesh
- $h/p$-scaling artificial viscosity for shock capturing.
- Parallel communication via MPI
- Local direct solve using UMFPACK
- Equation set: Poisson, advection-diffusion, Burger, Euler
- $\sim 70,000$ lines of C code
**BDDC Spaces**

### Primal and Dual Spaces

Decompose $\tilde{V}_h(\Gamma) = (V_{h,\Pi}(\Gamma)) \oplus (\oplus_{i=1}^{N} V_{h,\Delta}(\Gamma_i))$

Local Dual: $V_{h,\Delta}(\Gamma_i) = \{v \in V_h(\Gamma_i) : v = 0 \text{ on primal constraint}\}$

Primal: $V_{h,\Pi}(\Gamma) = \{v \in \tilde{V}_h(\Gamma) : \sum_{i=1}^{N} \tilde{a}_i(v|_{\Omega_i}, \phi|_{\Omega_i}) = 0, \forall \phi|_{\Omega_i} \in \oplus_{i=1}^{N} V_{h,\Delta}(\Gamma_i)\}$

- Dual space $V_{h,\Delta}(\Gamma) = \oplus_{i=1}^{N} V_{h,\Delta}(\Gamma_i)$ is completely localized
- Primal space has DOF of $O(N)$

### Primal and Dual Schur Complement

- **Primal Schur complement:** $S_{\Pi} : V_{h,\Pi}(\Gamma) \to V'_{h,\Pi}(\Gamma)$
  \[
  \langle S_{\Pi} v_{\Pi}, \phi_{\Pi} \rangle = \sum_{i=1}^{N} \tilde{a}_i(v|_{\Omega_i}, \phi|_{\Omega_i}), \forall v_{\Pi}, \phi_{\Pi} \in V_{h,\Pi}(\Gamma)
  \]

- **Local dual Schur complement:** $S_{\Delta,i} : V_{h,\Delta}(\Gamma_i) \to V'_{h,\Delta}(\Gamma_i)$
  \[
  \langle S_{\Delta,i} v_{\Delta,i}, \phi_{\Delta,i} \rangle = \tilde{a}_i(v_{\Delta,i}, \phi_{\Delta,i}), \forall v_{\Delta,i}, \phi_{\Delta,i} \in V_{h,\Delta}(\Gamma_i)
  \]
BDDC Preconditioner

Injections and Averaging Operator

- $R_{\Gamma\Pi}^T : V_{h,\Pi}(\Gamma) \rightarrow \tilde{V}_h(\Gamma)$
- $R_{\Gamma\Delta}^T : V_{h,\Delta}(\Gamma_i) \rightarrow \tilde{V}_h(\Gamma)$
- $R_{D,i}^T : \tilde{V}_h(\Gamma) \rightarrow V_h(\Gamma)$ s.t. $v = \sum_{i=1}^N R_{D,i}^T v|_{\Omega_i}, \forall v \in V_h(\Gamma)$

BDDC Preconditioner

BDDC preconditioner is given by

$$M^{-1}_{\text{BDDC}} = \sum_{i=1}^N R_{D,i}^T(T_{\text{sub},i} + T_{\text{coarse}})D_i R_{D,i}$$

where $T_{\text{sub},i} = R_{\Gamma\Delta,i}^T S_{\Delta,i}^{-1} R_{\Gamma\Delta,i}$ and $T_{\text{coarse}} = R_{\Gamma\Pi} S_{\Pi}^{-1} R_{\Gamma\Pi}^T$

Condition Number Estimate for Coercive, Symmetric $a(\cdot, \cdot)$

$$\kappa(M^{-1}_{\text{BDDC}} S) \leq C(1 + \log^2(H/h))$$
Galerkin Least Squares Discretization

**Background**

- SUPG developed by Hughes [1982]; analyzed by Johnson [1984]
- SUPG extended to GLS by Hughes [1989]

**GLS Discretization**

Find \( u \in V \subset H^1(\Omega) \) s.t.

\[
a(u, \phi) + (Lu, \tau L\phi)_{\Omega,T_h} = (f, \phi)_\Omega + (f, \tau L\phi)_{\Omega,T_h}, \quad \forall \phi \in V
\]

where \((\cdot, \cdot)_{\Omega,T_h} = \sum_K \int_K \cdot \cdot \ dK\) and \(\tau \sim \begin{cases} h, & P_e \gg 1 \\ h^2, & P_e \ll 1 \end{cases}\).

**Stability and A Priori Error Estimate for Hyperbolic Case \((\nu = 0)\)**

\[
a(u, u) \geq h\|\beta \cdot \nabla u\|_{L^2(\Omega)}^2
\]

\[
\sqrt{h}\|\beta \cdot \nabla (u - u_h)\|_{L^2(\Omega)} + \|u - u_h\|_{L^2(\Omega)} \leq Ch^{p+\frac{1}{2}}\|u\|_{H^{p+1}(\Omega)}
\]
Stabilization Matrix

High-Order Stabilization Matrix

- In order to keep \( \frac{\text{cond}(L_{\text{stabilized}})}{\text{cond}(L_{\text{unstabilized}})} = \mathcal{O}(1) \) as \( p \to \infty \) and \( h \to 0 \),
  \[ \tau \sim \frac{h^2}{p^2}, \quad Pe \ll 1 \]

- One choice of \( \tau \) in \( \mathbb{R}^d \)
  \[ \tau^{-1} = \sum_{i=1}^{d+1} \left| \beta \cdot \nabla \xi^i \right| + \frac{p^2}{d} \sum_{i=1}^{d} \sum_{j=1}^{d} \frac{\partial \xi_i}{\partial x_k} \frac{\partial \xi_j}{\partial x_l} \nu_{kl} \]

Topics Studied in High-Order GLS

- Comparison of SUPG and GLS
- Subcell-shock capturing using \( h/p \) scaling artificial viscosity and resolution based shock indicator
- GLS for highly anisotropic mesh
BDDC Preconditioner

Features of BDDC

- Equipped with a coarse space (primal space) that provides global communication and makes subdomain problems well-posed.

- Operates on partially assembled space: \( V_h(\Gamma) \)

\[
V_h(\Gamma) = \{ v \in L^2(\Omega) : v \in \bigoplus_{i=1}^N V_h(\Gamma_i) \text{ and } v \text{ is continuous on primal constraints} \}
\]

- Examples of primal constraints
  - Values at the corners of \( \Omega_i \)
  - State averages on the edges of \( \Omega_i \)
Decompose $\tilde{V}_h(\Gamma) = (V_{h,\Pi}(\Gamma)) \oplus (\bigoplus_{i=1}^{N} V_{h,\Delta}(\Gamma_i))$

Local Dual: $V_{h,\Delta}(\Gamma_i) = \{ v \in V_h(\Gamma_i) : v = 0 \text{ on primal constraint} \}$

Primal: $V_{h,\Pi}(\Gamma) = \{ v \in \tilde{V}_h(\Gamma) : \sum_{i=1}^{N} \tilde{a}_i(v|_{\Omega_i}, \phi_{\Delta}|_{\Omega_i}) = 0, \forall \phi_{\Delta} \in \bigoplus_{i=1}^{N} V_{h,\Delta}(\Gamma_i) \}$

- Dual space $V_{h,\Delta}(\Gamma) = \bigoplus_{i=1}^{N} V_{h,\Delta}(\Gamma_i)$ is completely localized
- Primal space has DOF of $O(N)$