

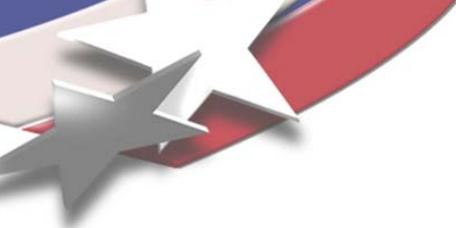


An Overview of the Claps Package

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**Clark R. Dohrmann
Structural Dynamics Research Department
Sandia National Laboratories**



Outline

1. Package Description
2. Some Applications
3. Current & Future Plans
4. Remaining Questions and Comments



What is Claps?

A collection of domain decomposition preconditioners and solvers for

$$Ax = b$$

preconditioner $M^{-1} \Rightarrow M^{-1}Ax = M^{-1}b$

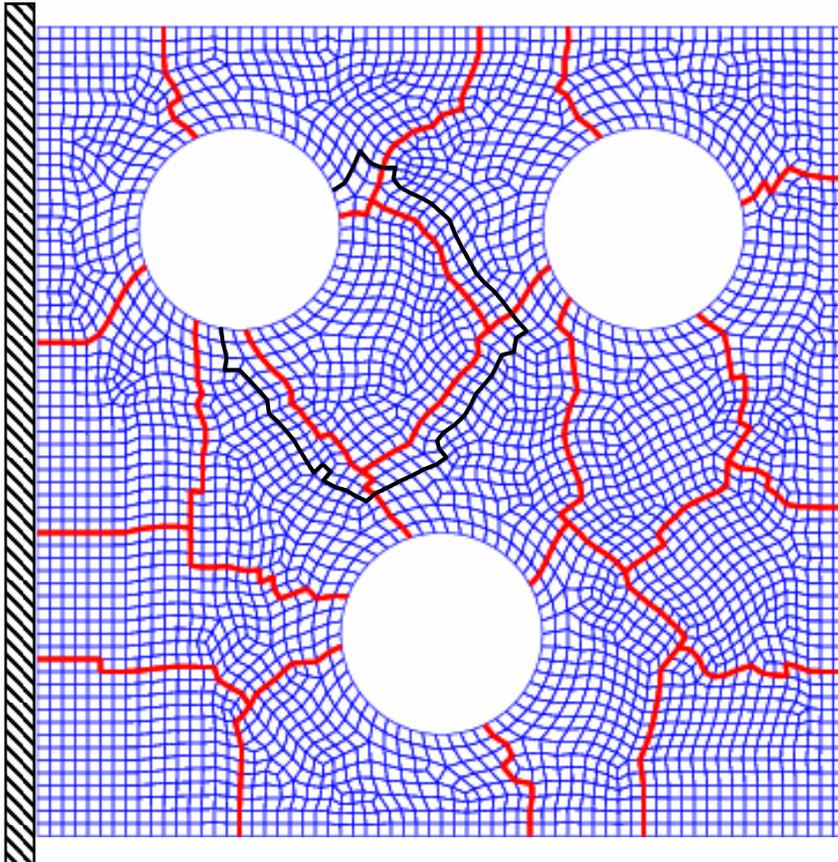
Some introductory books:

Smith, Bjorstad, and Gropp, *Domain Decomposition: Parallel and Multilevel Methods for Elliptic Partial Differential Equations*, Cambridge University Press, 1996.

Toselli and Widlund, *Domain Decomposition Methods: Algorithms and Theory*, Springer Series in Computational Mathematics 34, 2005.

What is Domain Decomposition?

Basic idea: solve smaller problems local to each subdomain (overlapping or nonoverlapping) and add results together. Coarse problem also needed for scalability.



— overlapping
— nonoverlapping

Q: why not just use direct solver for original problem?

A: memory & flops needed don't scale well with problem size, e.g. $O(n^{4/3})$ memory & $O(n^2)$ flops in 3D



Why Domain Decomposition?

- 1. Previous success using FETI algorithms for difficult problems in Salinas**
- 2. Parallel communications straightforward**
- 3. Conceptually simple**
- 4. Existing theory**
- 5. Can use efficient sparse solvers**

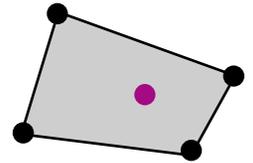


Claps Workhorses

- **CLIP**
 - an **i**nterface (substructuring) **p**reconditioner
 - can be viewed as primal counterpart of FETI-DP
 - multilevel extensions and inexact solves possible
- **CLOP**
 - an **o**verlapping **p**reconditioner
 - coarse problem more challenging than CLIP, but avoids unexpected subdomain singularities
- **CLOP_IFD**
 - for **i**ncompressible **f**luid **d**ynamics problems
 - preconditioner for saddle point systems (not currently part of internal release)

Constraint Equations

- Often appear in Salinas problems
 - tied contact (connecting dissimilar meshes)
 - rigid surfaces (e.g. for joint models)
- Constraint equations have historically presented big challenges to solvers
- Minimize $x^T Ax/2 - x^T b$ subject to $Cx = 0$



$$\begin{bmatrix} A & C^T \\ C & 0 \end{bmatrix} \begin{bmatrix} x \\ \lambda \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix}$$

- Use sparse null space approach $\Rightarrow \tilde{A}\tilde{x} = \tilde{b}$



Some Applications

- **Claps used in current release of Salinas**
 - Milepost 5.4 calculations for hostile blast
 - > 70k constraint equations in models
 - recent structural acoustics work (indefinite)

- **CLOP_IFD currently used in incompressible fluid mechanics code Kachina**
 - primal based penalty preconditioner for saddle point systems
 - applied to Stokes and Navier-Stokes problems



How do I go about using Claps?

- **Store problem components in Epetra form (e.g. Epetra_CrsMatrix, Epetra_IntVector, ...)**
- **Best bet right now is to contact me about your specific application**
 - **documentation limited to comments in the code**
 - **test problems need to be added to package**
 - **all capabilities driven by specific requests**
- **Claps currently available in internal release only**



Current and Future Plans

- **Use inexact solves**
 - **current versions of CLIP and CLOP use sparse direct solvers for subdomain and coarse problems**
 - **maximum number of elements assigned to each processor is constrained primarily by memory requirements of direct solvers**
 - **theory for inexact solves in CLIP recently developed, corresponding theory for overlapping methods (CLOP) already exists**
 - **would allow much larger problems to be run on the same number of processors**



Current and Future Plans (continued)

- Investigate AMG for inexact solves
 - combine simplicity of communications for domain decomposition with optimal complexity of multigrid
 - recent AMG development encouraging

nelem	ndof	nlevel	iter	cond
$(8+2)^3$	2,187	2	8	1.37
$(16+2)^3$	14,739	3	8	1.38
$(32+2)^3$	107,811	4	9	1.39
$(64+2)^3$	823,875	5	9	1.40

3D elasticity
serial AMG
cube geometry
V-cycle, $\nu = 1$
rrtol = 10^{-8}



Current and Future Plans (continued)

- **Investigate new coarse problem for CLOP**
 - current coarse problem based on partition of unity
 - careful attention required for problems with rotational dofs (e.g. shells)
 - new approach based on energy minimization concepts (formulation for scalar PDEs, elasticity, and problems involving shells essentially same)
- **Multilevel Extensions to CLIP and CLOP**
 - currently both are 2-level methods w/ coarse problem solved exactly
 - for larger (>10k) processors, coarse problem will be too large to solve directly



Current and Future Plans (continued)

- **Preconditioners for Different Problem Types**
 - continue work on structural acoustics
 - shifted eigenproblems, direct frequency response
 - non PDE problems (circuits) or different PDEs (e.g. electromagnetics)
- **Move Claps to external release**
 - documentation
 - test problems



Additional References

- **CLIP**

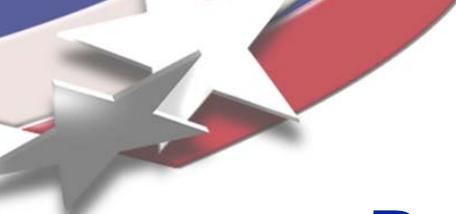
- C.R. Dohrmann, “A Preconditioner for Substructuring based on Constrained Energy Minimization,” *SIAM J. Sci. Comput.*, Vol. 25, No. 1, pp. 246-258, 2003.
- J. Mandel and C.R. Dohrmann, “Convergence of a Balancing Domain Decomposition by Constraints and Energy Minimization,” *Numer. Linear Algebra Appl.*, Vol. 10, pp. 639-659, 2003.
- J. Mandel, C.R. Dohrmann, and R. Tezaur, “An Algebraic Theory for Primal and Dual Substructuring Methods by Constraints,” *Appl. Numer. Math.*, Vol. 54, pp. 167-193, 2005.

- **CLOP**

- C.R. Dohrmann, “A Study of Two Domain Decomposition Preconditioners,” Technical Report SAND2003-4391, Sandia National Laboratories, Albuquerque, New Mexico, 2003.

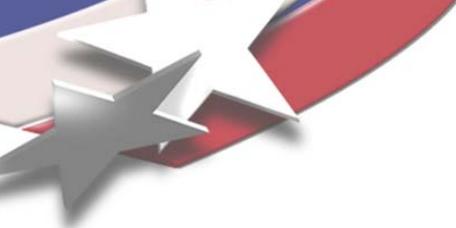
- **CLOP_IFD**

- D. K. Gartling and C.R. Dohrmann, “Quadratic Finite Elements and Incompressible Viscous Flows,” to appear in *Comput. Methods Appl. Mech. Engrg.*
- C.R. Dohrmann and R.B. Lehoucq, “A Primal Based Penalty Preconditioner for Elliptic Saddle Point Systems,” to appear in *SIAM J. Numer. Anal.*



Remaining Questions Comments

- **See additional pages for more details on preconditioners**



CLIP Building Blocks

Additive Schwarz:

- Coarse grid correction v_1
- Substructure correction v_2
- Static condensation correction v_3

$$M^{-1}r = v_1 + v_2 + v_3$$

FETI-DP counterparts:

$$v_2 \leftrightarrow \sum_{s=1}^{N_s} B_r^s K_{rr}^{s^{-1}} B_r^{sT} \lambda^k$$

$$v_1 \leftrightarrow F_{I_{rc}} K_{cc}^{*-1} F_{I_{rc}}^T \lambda^k$$

$$v_3 \leftrightarrow \text{Dirichlet preconditioner}$$

Coarse Grid and Substructure Problems

coarse problem:

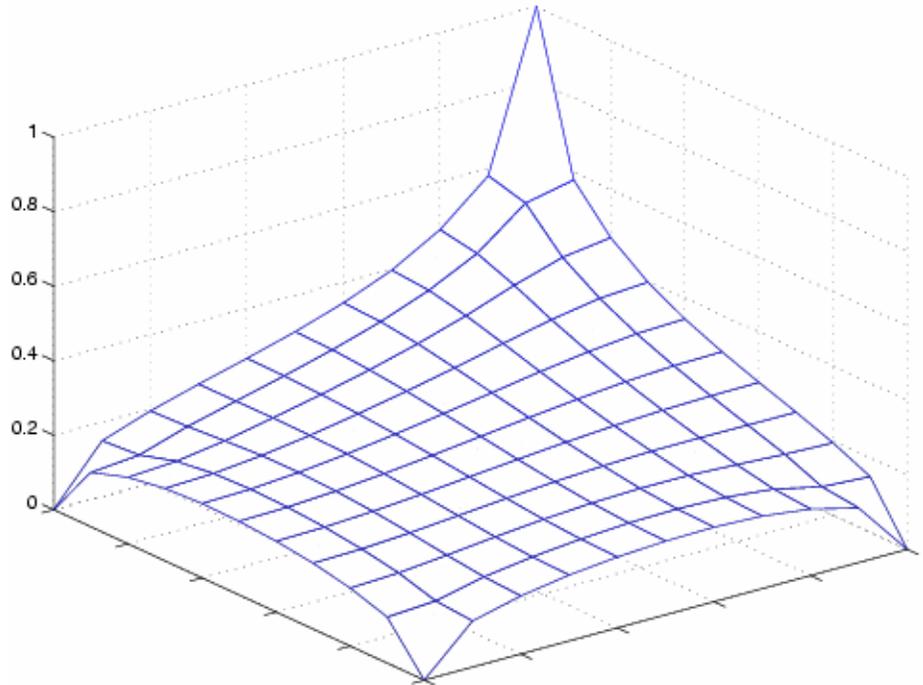
$$\begin{pmatrix} K_i & C_i^T \\ C_i & 0 \end{pmatrix} \begin{pmatrix} \Phi_i \\ \Lambda_i \end{pmatrix} = \begin{pmatrix} 0 \\ I \end{pmatrix}$$

$$\Rightarrow K_{ci} = \Phi_i^T K_i \Phi_i$$

- K_{ci} coarse element matrix
- assemble $K_{ci} \Rightarrow K_c$
- K_c positive definite

substructure problem:

$$\begin{pmatrix} K_i & C_i^T \\ C_i & 0 \end{pmatrix} \begin{pmatrix} v_{2i} \\ \lambda_{2i} \end{pmatrix} = \begin{pmatrix} r_i \\ 0 \end{pmatrix}$$





CLOP Description

Solve $Ax = b$ using pcg

Preconditioned residual $M^{-1}r$ obtained as follows:

1. coarse grid correction $u_1 = \Phi(\Phi^T A \Phi)^{-1} \Phi^T r$
2. residual update $r_1 = r - Au_1$
3. subdomain correction $u_2 = \sum_i R_i^T (R_i A R_i^T)^{-1} R_i r_1$
4. residual update $r_2 = r_1 - Au_2$
5. coarse grid correction $u_3 = \Phi(\Phi^T A \Phi)^{-1} \Phi^T r_2$
6. preconditioned residual $M^{-1}r = u_1 + u_2 + u_3$

Note: Steps 1 and 2 can be omitted after first iteration



Coarse Space

Coarse space (Φ) based on partition of unity (Sarkis)

- multiply rigid body modes by partition
- reduce coarse space energy further by static condensation

Same types of calculations required for subdomain problems are used to construct partition of unity

- takes advantage of existing factorizations/preconditioners for subdomain problems

Specialized treatment needed for problems with rotational dofs

- coarse space for simple treatment still spans rigid body modes, but energy too high



CLOP_IFD Preconditioner

original system:

$$\begin{pmatrix} A & B^T \\ B & -C \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix} \quad \begin{array}{l} A > 0 \text{ on kernel of } B, C \geq 0 \\ A^T = A, C^T = C, B \text{ full rank} \end{array}$$

penalized (regularized) system: Axelsson (1979)

$$\begin{pmatrix} A & B^T \\ B & -\tilde{C} \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix} \quad \tilde{C} > 0, \quad \tilde{C}^T = \tilde{C}$$



exact solution of penalized system

$$\begin{pmatrix} A & B^T \\ B & -\tilde{C} \end{pmatrix} \begin{pmatrix} z_u \\ z_p \end{pmatrix} = \begin{pmatrix} r_u \\ r_p \end{pmatrix}$$

is

$$z_p = \tilde{C}^{-1} (Bz_u - r_p)$$

$$z_u = S_A^{-1} (r_u + B^T \tilde{C}^{-1} r_p)$$

$$S_A = A + B^T \tilde{C}^{-1} B$$

primal rather than dual Schur complement considered

~~$$S_{\tilde{C}} = -(\tilde{C} + BA^{-1}B^T)$$~~