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An Overview of the Claps Package

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Outline

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

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What is Claps?

A collection of domain decomposition preconditioners and solvers for

$$\boxed{Ax = b}$$

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

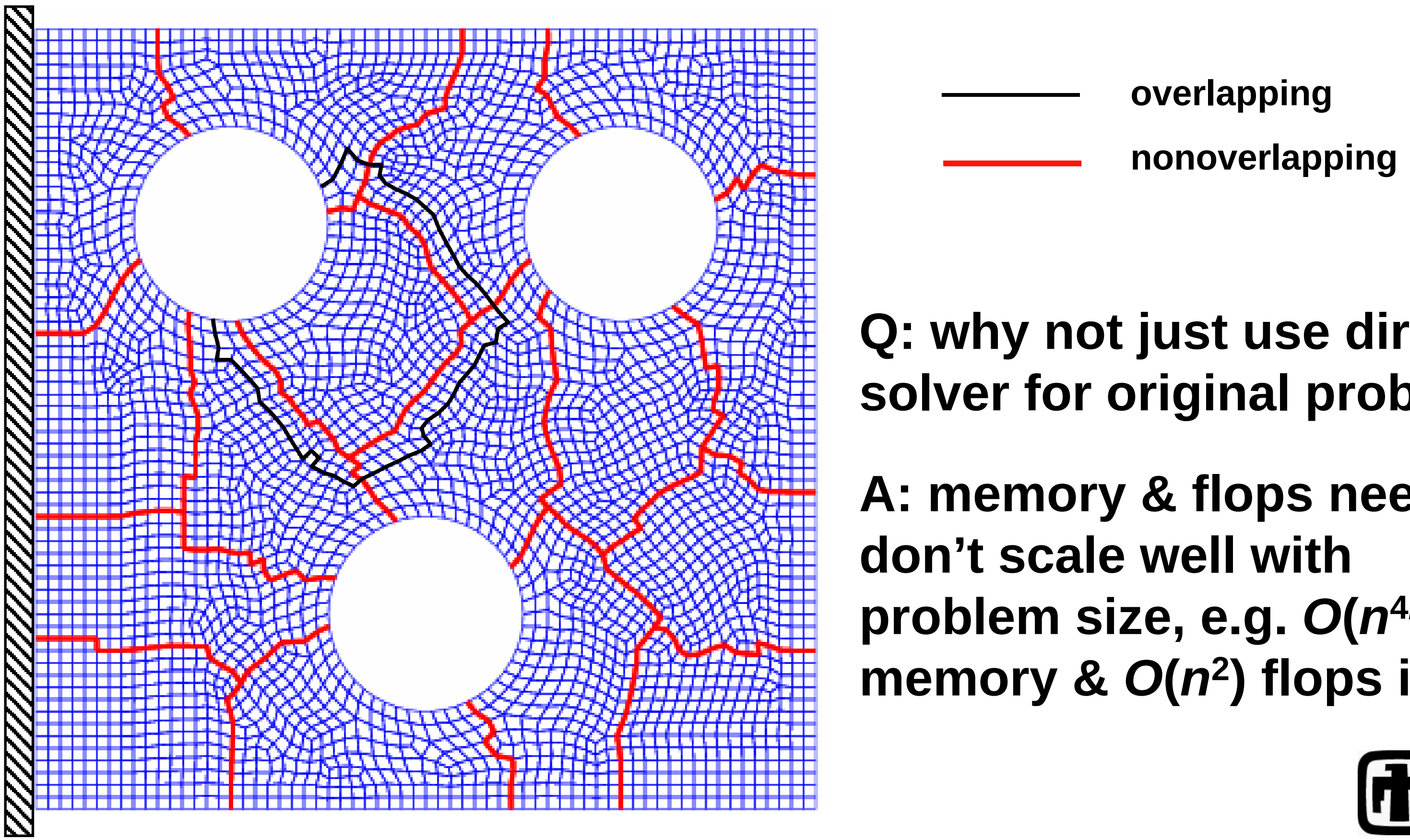
Some introductory books:

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.



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

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Why Domain Decomposition?

1. **Previous success using FETI algorithms for difficult problems in Salinas**

2. **Parallel communications straightforward**

3. **Conceptually simple**

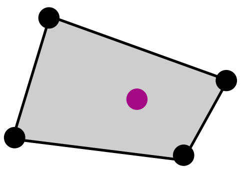
4. **Existing theory**

5. **Can use efficient sparse solvers**

Claps Workhorses

- CLIP
  - an interface (substructuring) preconditioner
  - can be viewed as primal counterpart of FETI-DP
  - multilevel extensions and inexact solves possible
- CLOP
  - an overlapping preconditioner
  - coarse problem more challenging than CLIP, but avoids unexpected subdomain singularities
- CLOP_IFD
  - for incompressible fluid dynamics 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** $x^T A x / 2 - x^T b$ **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

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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*.

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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:

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

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

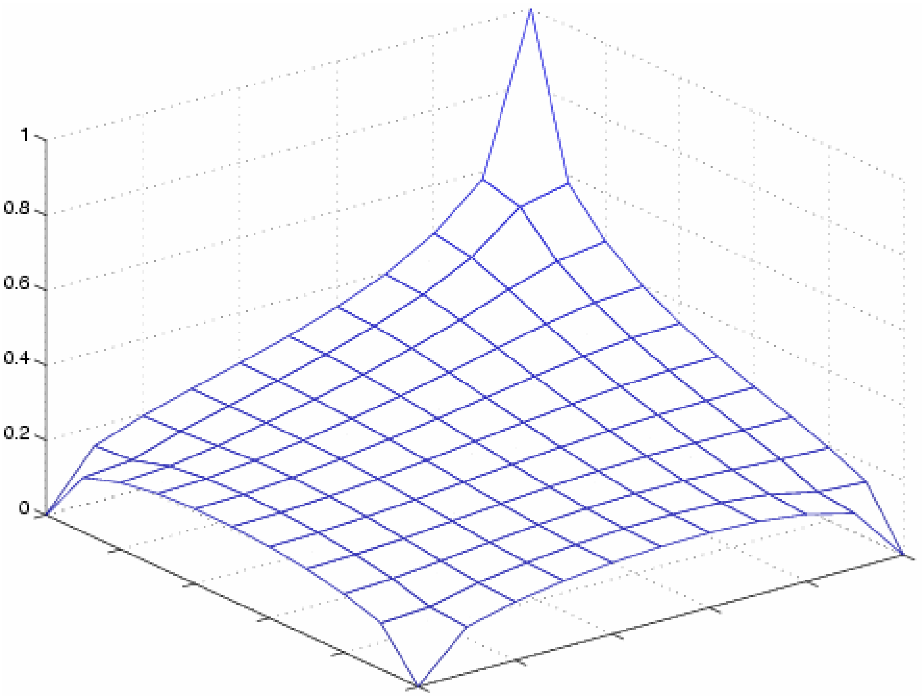
$v_3 \leftrightarrow$ **Dirichlet preconditioner**

Coarse Grid and Substructure Problems

coarse problem:

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

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



- 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

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Coarse Space

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

- multiply rigid body modes by partition
- reduce coarse space energy furthur 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:

$$\begin{pmatrix} A & B^T \\ B & -C \end{pmatrix}\begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}$$

$A > 0$ on kernel of B, $C \geq 0$

$A^T = A$, $C^T = C$, B full rank

penalized (regularized) system: Axelsson (1979)

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

$\tilde{C} > 0, \quad \tilde{C}^T = \tilde{C}$

exact solution of penalized system

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

is

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

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

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

primal rather than dual Schur complement considered

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