A highly scalable asynchronous implementation of Balancing Domain Decomposition by Constraints

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BDDC preconditioner

- Overlapped BDDC implementation
- Scalability analysis (overlapped)
- Inexact BDDC
- **5** Scalability analysis (overlapped/inexact)
- 6 Conclusions and future work

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Problem statement

Given a bounded domain Ω and a FE partition \mathcal{T} , we build a conforming (nodal) finite element (FE) space, i.e. $V_h \subset H_0^1(\Omega)$.

• Variational problem: find $u \in V_h$ such that

a(u, v) = (f, v), for any $v \in V_h$,

assuming $a(\cdot, \cdot)$ symmetric, coercive (e.g. Laplacian or linear elasticity)

• Algebraic problem: Equivalent to find $x \in \mathbb{R}^n$ such that

Ax = b

where A is a large and sparse symmetric positive definite matrix

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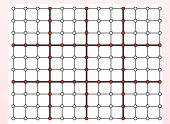
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where A is a large and sparse symmetric positive definite matrix

Motivation:

Efficient exploitation of distributed-memory machines for large scale FE problems \Rightarrow Domain decomposition framework

o: interior DoFs (1); •: interface dofs (Γ)



Interface (Schur complement) problem

• The domain partition induces a block structure

$$Ax = \begin{bmatrix} A_{II} & A_{I\Gamma} \\ A_{\Gamma I} & A_{\Gamma\Gamma} \end{bmatrix} \begin{bmatrix} x_I \\ x_{\Gamma} \end{bmatrix} = \begin{bmatrix} b_I \\ b_{\Gamma} \end{bmatrix} = b,$$

where

$$A_{II} = diag\left(A_{II}^{(1)}, A_{II}^{(2)}, \dots, A_{II}^{(P)}\right)$$

• After the interior correction $[A_{II}^{-1}b_I, 0]$, a reduced system for x_{Γ} is obtained

 $Sx_{\Gamma} = g_{\gamma}$

where $S = A_{\Gamma\Gamma} - A_{\Gamma I} A_{II}^{-1} A_{I\Gamma}$ is the interface Schur complement

- Approach: Consider a Krylov subspace solver for S_x = g → Preconditioning plays a major role for optimality and scalability
- Alternatively, the preconditioner can be extended to Ax = f (equivalent as soon as A_u^{-1} exactly)

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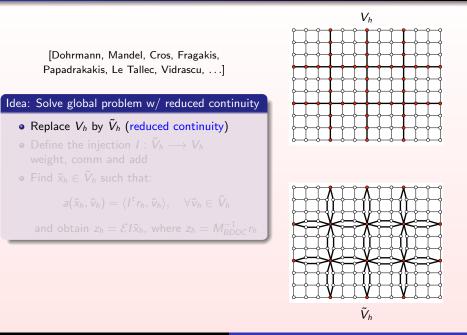
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 V_h [Dohrmann, Mandel, Cros, Fragakis, Papadrakakis, Le Tallec, Vidrascu, ...] Idea: Solve global problem w/ reduced continuity • Replace V_h by \tilde{V}_h (reduced continuity) • Define the injection $I : \tilde{V}_h \longrightarrow V_h$ weight, comm and add 1^t • Find $\tilde{x}_h \in \tilde{V}_h$ such that:

 \tilde{V}_h

[Dohrmann, Mandel, Cros, Fragakis, Papadrakakis, Le Tallec, Vidrascu, ...]

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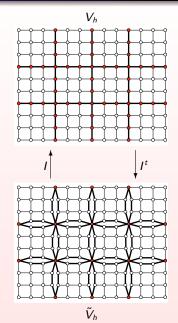
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- Find $\tilde{x}_h \in \tilde{V}_h$ such that:

$$a(\tilde{x}_h, \tilde{v}_h) = \langle I^t r_h, \tilde{v}_h \rangle, \quad \forall \tilde{v}_h \in \tilde{V}_h$$

and obtain $z_h = \mathcal{E}I\tilde{x}_h$, where $z_h = M_{BDDC}^{-1}r_h$

• Last correction: \mathcal{E} is the harmonic extension of the boundary values, which implies local Dirichlet solvers



[Dohrmann, Mandel, Cros, Fragakis, Papadrakakis, Le Tallec, Vidrascu, ...]

Idea: Solve global problem w/ reduced continuity

Alternatively,

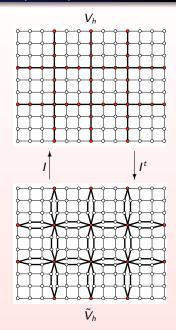
Find $\tilde{x} \in \mathbb{R}^{\tilde{n}}$ such that:

 $\tilde{A}\tilde{x} = I^t r$

and obtain $z = \mathcal{E}I\tilde{x}$, where $z = M_{BDDC}^{-1}r$

 Ã is a sub-assembled global matrix (only assembled the red corners in the figure)

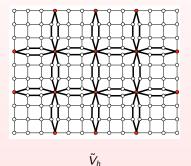
•
$$\mathcal{E} = \begin{bmatrix} 0 & -A_{II}^{-1}A_{I\Gamma} \\ 0 & I_{\Gamma} \end{bmatrix}$$



• Let
$$\tilde{V}_h = [\tilde{v}_{\odot} \ \tilde{v}_{ullet}]$$
 and decompose \tilde{V}_h as

$$ilde{V}_h = ilde{V}_F \oplus ilde{V}_C, \,\, {
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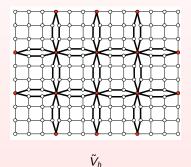
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Fine-grid correction (\tilde{x}_F)

• Find $\tilde{x}_F \in \mathbb{R}^{\tilde{n}}$ such that

$$\tilde{A}\tilde{x}_F = I^t r$$

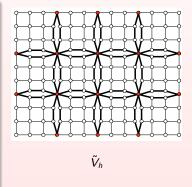
constrained to $(\tilde{x}_F)_{\bullet} = 0$

• Equivalent to P independent problems

Find
$$\tilde{x}_{F}^{(i)} \in \mathbb{R}^{\tilde{n}^{(i)}}$$
 such that

$$A^{(i)}\tilde{x}_F^{(i)}=I_i^t I$$

constrained to $(\tilde{x}_F^{(i)})_{\bullet} = 0$



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Coarse-grid correction (\tilde{x}_C)

Computation of $\tilde{V}_C = \operatorname{span}\{\Phi_1, \Phi_2, \dots, \Phi_{n_C}\}$

• Find $\Phi \in \mathbb{R}^{\tilde{n} \times \mathit{n_{C}}}$ such that

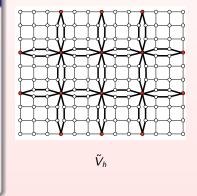
$$\tilde{A}\tilde{\Phi} = 0$$

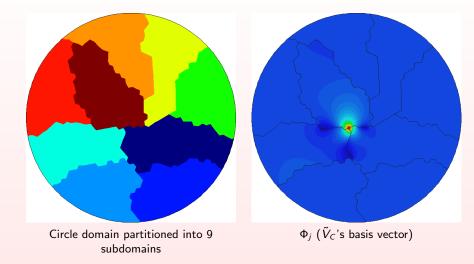
constrained to $\Phi_{\bullet} = I$

• Equivalent to P independent problems Find $\Phi^{(i)} \in \mathbb{R}^{\tilde{n} \times n_C^{(i)}}$ such that

$$A^{(i)}\Phi^{(i)}=0$$

constrained to $\Phi_{\bullet}^{(i)} = I$





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Coarse-grid correction (\tilde{x}_C)

Assembly and solution of coarse-grid problem

$$A_{C} = \text{assembly}(A_{C}^{(i)}) = \text{assembly}(\Phi^{t}A^{(i)}\Phi), \qquad \text{Solve } A_{C}\alpha_{c} = \Phi^{t}I^{t}r, \qquad \tilde{x}_{C} = \Phi\alpha_{C}$$

coarse-grid problem is

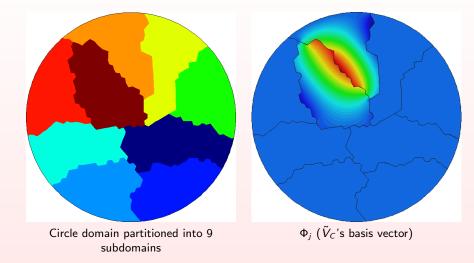
- Global, i.e. couples all subdomains
- But much smaller than S (size n_C)
- Potential loss of parallel efficiency with P

Key aspect: Selection of coarse dofs, i.e. continuity among subdomains

Properties of BDDC preconditioner

- Optimality ($\kappa(M^{-1}S)$ bounded by a constant for fixed N/P and $\uparrow P$)
- $N/P = (H/h)^d$ large in practice (e.g. $\mathcal{O}(10^4)$ for sparse direct solvers)
- In general, BDDC(ce) and BDDC(cef) require much less iterations in 3D
- But at the expense of a more costly coarse-grid problem

Coarse dofs vs. $\kappa(M^{-1}S)$:	<i>d</i> = 2	<i>d</i> = 3
Continuity on corners	$\left[1+d^{-1}\mathrm{log}^{2}\left(rac{N}{P} ight) ight]$	$rac{N}{P}\left[1+d^{-1}\mathrm{log}^{2}\left(rac{N}{P} ight) ight]$
Continuity of mean value on edges too	$\left[1+d^{-1}\mathrm{log}^{2}\left(rac{N}{P} ight) ight]$	$\left[1+d^{-1}\mathrm{log}^{2}\left(rac{N}{P} ight) ight]$
Continuity of mean value on faces too	-	$\left[1+d^{-1}\mathrm{log}^{2}\left(rac{N}{P} ight) ight]$



- The method allows for a (mathematically supported) extremely aggressive coarsening $(10^5 10^6$ size reduction between fine/coarse level)
- Interpretation of the second state of the s
- Ocarse and local components can be computed in a parallel (additive) way
- Local (constrained) Neumann and coarse solvers can be solved in an inexact way (AMG-cycle instead of sparse direct solvers)
- A multilevel extension of the method is possible (for extreme core counts)

- The method allows for a (mathematically supported) extremely aggressive coarsening $(10^5 10^6$ size reduction between fine/coarse level)
- 2 The coarse matrix has a similar sparsity as the original matrix
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- (1)-(2) always exploited in BDDC implementations
- Let us see how to exploit (3), in order to reduce synchromization and boost scalability (overlapped implementation)

BDDC preconditioner

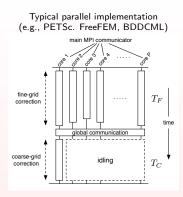
Overlapped BDDC implementation

3 Scalability analysis (overlapped)

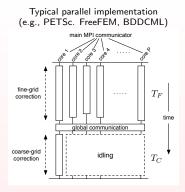
Inexact BDDC

5 Scalability analysis (overlapped/inexact)

Conclusions and future work

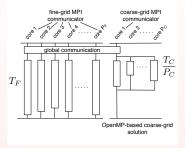


- All MPI tasks have f-g duties and one/several have also c-g duties
- Computation of f-g and c-g correction is serialized (but they are independent!)
- T_C grows as $O(P^2)$ and mem as $O(P^{\frac{4}{3}})$
 - \rightarrow becomes a bottleneck with P
 - \rightarrow mem per core rapidly exceeded
- Parallel coarse solvers / multilevel extensions reduce this effect

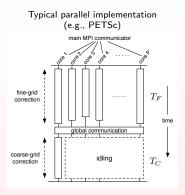


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Highly-scalable parallel implementation Overlapping of fine-grid/coarse-grid duties

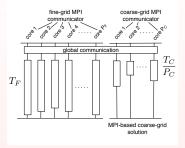


- MPI tasks have either f-g duties or c-g duties (but not both)
- Computation of f-g and c-g correction can be overlapped in time (asynchronous)
- Full node(s) resources (memory and cores) can be devoted to coarse-grid duties
- MPI-based or OpenMP-based (this work) solutions are possible for c-g correction



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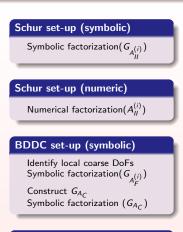
Solve Ax = b via BDDC-PCG

 $\begin{array}{l} \text{Schur complement set-up } (S) \\ \text{Precond set-up } (M_{\mathrm{BDDC}}) \\ g := b_{\Gamma} - A_{\Gamma I} A_{II}^{-1} b_{I} \\ \text{call PCG}(S, M_{\mathrm{BDDC}}, g, x_{\Gamma}) \\ x_{I} := A_{II}^{-1} (b_{I} - A_{I\Gamma} x_{\Gamma}) \end{array}$

PCG

$$\begin{array}{l} r_{0} := g - Sx_{\Gamma} \\ z_{0} := M_{\rm BDDC}^{-1} r_{0} \\ p_{0} := z_{0} \\ \text{for } j = 0, \ldots, \text{ till CONV do} \\ s_{j+1} = Sp_{j} \\ \ldots \\ z_{j+1} := M_{\rm BDDC}^{-1} r_{j+1} \\ \ldots \\ \text{end for} \end{array}$$

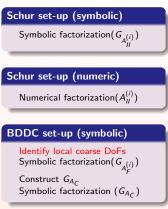
Fine-grid tasks	Coarse-grid task



BDDC set-up (numeric)

Numerical factorization($A_F^{(i)}$) Compute Φ_i $A_C^{(i)} := \Phi_i^* A^{(i)} \Phi_i$ Gather $A_C^{(i)}$ $A_C := assemble(A_C^{(i)})$ Numerical factorization(A_C)

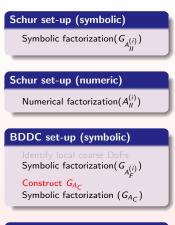
Fine-grid tasks	Coarse-grid task	
Identify local coarse DoFs		Schur
		Symb
		Schur
		Num
		- Turin
		BDDC
		Ident
		Symb
		Cons
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		BDDC
		Num
	1	Com
		$A_C^{(i)}$:
		Gath



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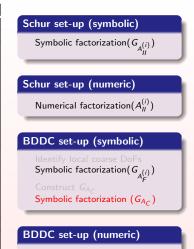
Fine-grid tasks	Coarse-grid task			
Identify local coarse DoFs				
Construct G_{A_C} GC				



BDDC set-up (numeric)

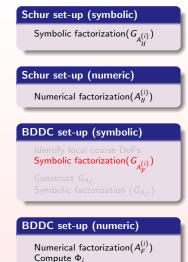
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	Symb fact(G_{A_C}) $\mathcal{O}(P^{\frac{4}{3}})$	
	-	



Numerical factorization $(A_F^{(i)})$ Compute Φ_i $A_C^{(i)} := \Phi_i^t A^{(i)} \Phi_i$ Gather $A_C^{(i)}$ $A_C := assemble(A_C^{(i)})$ Numerical factorization (A_C)

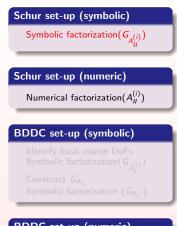
Fine-grid tasks	Coarse-grid task
Identify local coarse DoFs	
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Symb fact $(G_{A_F^{(i)}}) \mathcal{O}(n_i^{\frac{4}{3}})$	Symb fact (G_{A_C}) $\mathcal{O}(P^{\frac{4}{3}})$
	·



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Numerical factorization(A_{C})

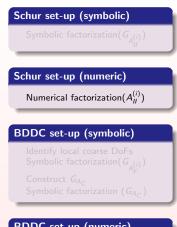
Fine-grid tas	<s< th=""><th>Coarse-grid task</th><th></th></s<>	Coarse-grid task	
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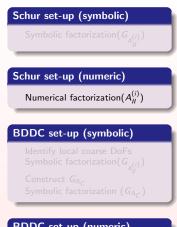
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Num fact $(A_F^{(i)})$	$\mathcal{O}(n_i^2)$	



BDDC set-up (numeric)

Numerical factorization($A_F^{(i)}$) Compute Φ_i $A_C^{(i)} := \Phi_i^t A^{(i)} \Phi_i$ Gather $A_C^{(i)}$ $A_C := assemble(A_C^{(i)})$ Numerical factorization(A_C)

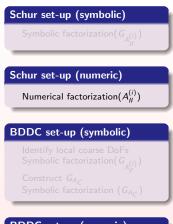
Fine-grid tas	<s< th=""><th>Coarse-grid task</th></s<>	Coarse-grid task
Identify local coars	e DoFs	
Construct G _{AC} GC		
Symb fact($G_{A_F^{(i)}}$)	$\mathcal{O}(n_i^{\frac{4}{3}})$	Symb fact(G_{A_C}) $\mathcal{O}(P^{\frac{4}{3}})$
Symb fact $(G_{A_{F}^{(i)}})$ Num fact $(A_{F}^{(i)})$	$\mathcal{O}(n_i^{\frac{4}{3}})$	
Num fact $(A_F^{(i)})$	$\mathcal{O}(n_i^2)$	
Compute Φ_i	$\mathcal{O}(n_i^{\frac{4}{3}})$	



BDDC set-up (numeric)

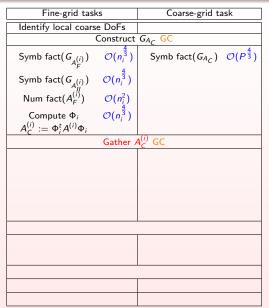
Compute Φ_i $A_C^{(i)} := \Phi_i^t A^{(i)} \Phi_i$ Gather $A_C^{(i)}$ $A_C := assemble(A_C^{(i)})$ Numerical factorization(A_C)

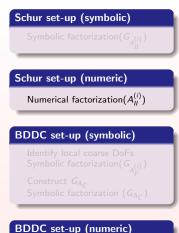
Fine-grid tas	ks	Coarse-grid task
Identify local coars		
Construct G _{A_C} GC		
Symb fact($G_{A_F^{(i)}}$)	$\mathcal{O}(n_i^{\frac{4}{3}})$	Symb fact(G_{A_C}) $\mathcal{O}(P^{\frac{4}{3}})$
Symb fact($G_{A_{II}^{(i)}}$)	$\mathcal{O}(n_i^{\frac{4}{3}})$	
Num fact $(A_F^{(i)})$	$\mathcal{O}(n_i^2)$	
Compute Φ_i $A_C^{(i)} := \Phi_i^t A^{(i)} \Phi_i$	$\mathcal{O}(n_i^{\frac{4}{3}})$	



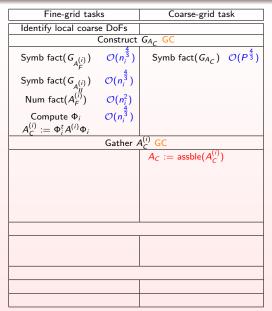
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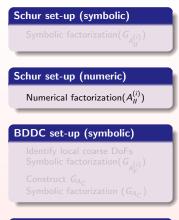
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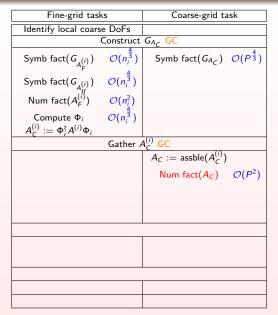
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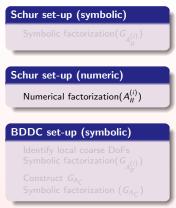




BDDC set-up (numeric)

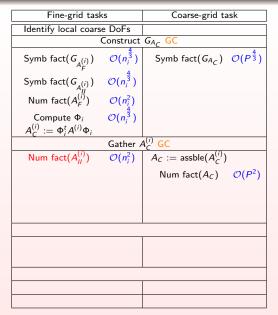
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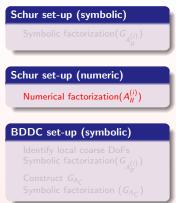




BDDC set-up (numeric)

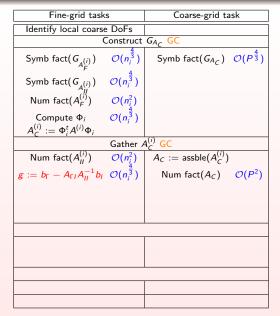
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PCG

$$g := b_{\Gamma} - A_{\Gamma I} A_{II}^{-1} b_{I}$$

$$r_{0} := g - S_{X_{\Gamma}}$$

$$z_{0} := M_{BDDC}^{-1} r_{0}$$

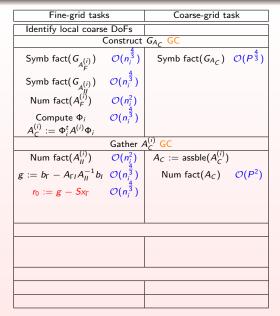
$$p_{0} := z_{0}$$
for $j = 0, ..., \text{ till CONV do}$

$$s_{j+1} = Sp_{j}$$

$$\ldots$$

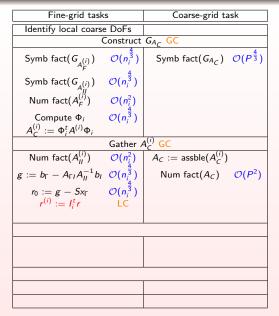
$$z_{j+1} := M_{BDDC}^{-1} r_{j+1}$$
...
end for

BDDC application $r^{(i)} := l_i^t r$ Compute $s_F^{(i)}$ $r_C^{(i)} := \Phi_i^t r^{(i)}$ Gather $r_C^{(i)}$ Gather $r_C^{(i)}$ $r_C := assemble(r_C^{(i)})$ Solve $A_C z_C = r_C$ Scatter z_C into $z_C^{(i)}$ $s_C^{(i)} := \Phi_i z_C^{(i)}$ $z^{(i)} := l_i (s_F^{(i)} + s_C^{(i)})$



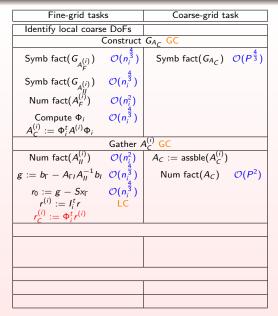
PCG $g := b_{\Gamma} - A_{\Gamma f} A_{II}^{-1} b_{I}$ $r_{0} := g - Sx_{\Gamma}$ $z_{0} := M_{B}^{-1}D_{DC}r_{0}$ $p_{0} := z_{0}$ for j = 0, ..., till CONV do $<math>s_{j+1} = Sp_{j}$ $z_{j+1} := M_{B}^{-1}D_{DC}r_{j+1}$ end for

BDDC application $r^{(i)} := I_i^t r$ Compute $s_F^{(i)}$ $r_C^{(i)} := \Phi_i^t r^{(i)}$ Gather $r_C^{(i)}$ Gather $r_C^{(i)}$ r_C := assemble($r_C^{(i)}$)
Solve $A_C z_C = r_C$ Scatter z_C into $z_C^{(i)}$ $s_C^{(i)} := \Phi_i z_C^{(i)}$ $z^{(i)} := I_i (s_F^{(i)} + s_C^{(i)})$



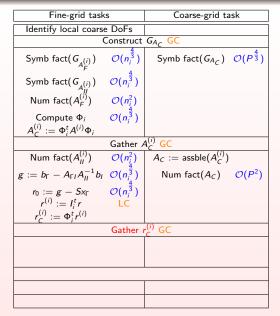
PCG $g := b_{\Gamma} - A_{\Gamma I} A_{II}^{-1} b_{I}$ $r_{0} := g - S_{X\Gamma}$ $z_{0} := M_{BDDC}^{-1} r_{0}$ $p_{0} := z_{0}$ for j = 0, ..., till CONV do $s_{j+1} = Sp_{j}$... $z_{j+1} := M_{BDDC}^{-1} r_{j+1}$... end for

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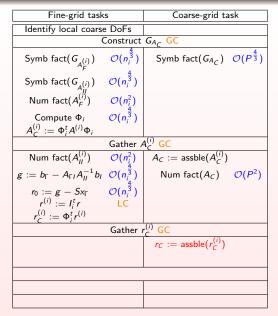
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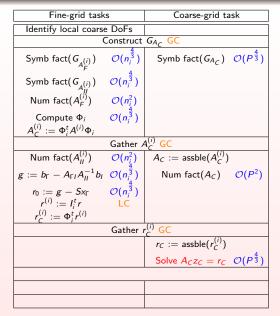
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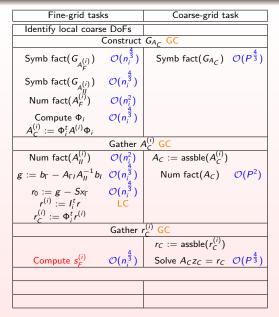
PCG $g := b_{\Gamma} - A_{\Gamma I} A_{II}^{-1} b_{I}$ $r_{0} := g - S_{NT}$ $20 := M_{BDDC}^{-1} r_{0}$ $p_{0} := z_{0}$ for j = 0, ..., till CONV do $s_{j+1} = Sp_{j}$ $z_{j+1} := M_{BDDC}^{-1} r_{j+1}$ end for

BDDC application
$r^{(i)} := l_i^{t} r$
Compute $s_F^{(i)}$
$r_c^{(i)} := \Phi_i^t r^{(i)}$
Gather $r_C^{(i)}$
$r_C := assemble(r_C^{(i)})$
Solve $A_C z_C = r_C$
Scatter z_C into $z_C^{(i)}$
$s_C^{(i)} := \Phi_i z_C^{(i)}$
$z^{(i)} := I_i(s_F^{(i)} + s_C^{(i)})$



PCG $g := b_{\Gamma} - A_{\Gamma I} A_{II}^{-1} b_{I}$ $r_{0} := g - S_{X\Gamma}$ $z_{0} := M_{BDDC}^{-1} r_{0}$ $p_{0} := z_{0}$ for j = 0, ..., till CONV do $s_{j+1} = Sp_{j}$ $z_{j+1} := M_{BDDC}^{-1} r_{j+1}$ end for

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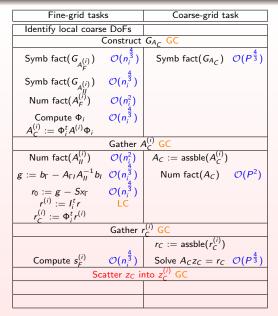
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$$s_{j+1} = Sp_{j}$$

$$...$$

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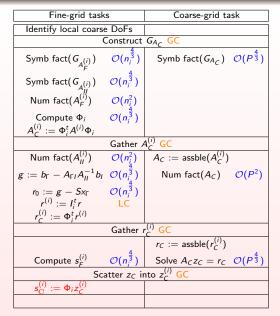


 $:= b_{\Gamma} - A_{\Gamma I}$ $:= \sigma - S_{X \Gamma}$

PCG

$$\begin{aligned} \mathbf{r}_{0} &:= g' - S_{\mathrm{NT}} \\ \mathbf{z}_{0} &:= M_{\mathrm{BDDC}}^{-1} \mathbf{r}_{0} \\ \mathbf{r}_{0} &:= z_{0} \\ \text{for } j = 0, \dots, \text{ till CONV do} \\ s_{j+1} &= Sp_{j} \\ \dots \\ z_{j+1} &:= M_{\mathrm{BDDC}}^{-1} \mathbf{r}_{j+1} \\ \dots \end{aligned}$$

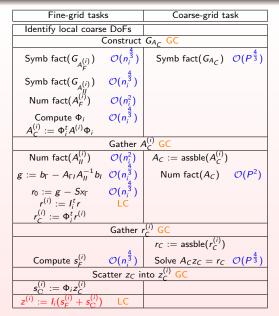
end for **BDDC application** $r^{(i)} := l_i^t r$ Compute $s_F^{(i)}$ $r_C^{(i)} := \Phi_i^t r^{(i)}$ Gather $r_C^{(i)}$ Gather $r_C^{(i)}$ Solve $A_{CZC} = r_C$ **Scatter z_C into z_C^{(i)}** $s_C^{(i)} := \Phi_i z_C^{(i)}$ $z^{(i)} := l_i (s_F^{(i)} + s_C^{(i)})$



PCG $g := b_{\Gamma} - A_{\Gamma I} A_{II}^{-1} b_{I}$ $r_{0} := g - S_{X_{\Gamma}}$ $z_{0} := M_{BDDC}^{-1} r_{0}$ $p_{0} := z_{0}$ for j = 0, ..., till CONV do $s_{j+1} = Sp_{j}$... $z_{j+1} := M_{BDDC}^{-1} r_{j+1}$...

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BDDC application
$s_c^{(i)} := \Phi_i z_c^{(i)}$
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PCG

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...
end for

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BDDC preconditioner

- 2 Overlapped BDDC implementation
- Scalability analysis (overlapped)
- Inexact BDDC
- 5 Scalability analysis (overlapped/inexact)
- 6 Conclusions and future work

FEMPAR (in-house developed HPC software, free software GNU-GPL):

Finite Element Multiphysics PARallel software

- Massively parallel sw for the FE simulation of Multiphysics problems governed by PDEs
- Scalable preconditioning of fully coupled and implicit system via block preconditioning techniques (physics-based preconditioning)
- Scalable preconditioning for one-physics (elliptic) PDEs relies on BDDC, BNN \rightarrow hybrid MPI/OpenMP implementation
- Relies on highly-efficient vendor implementations of the dense/sparse BLAS (Intel MKL, IBM ESSL, etc.)
- Provides interfaces to external multi-threaded sparse direct solvers (PARDISO, HSL_MA87, etc.) and serial AMG preconditioners (HSL_MI20)

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Target machine: HELIOS@IFERC-CSC

4,410 bullx B510 compute blades (2 Intel Xeon E5-2680 8-core CPUs; 64GB)

- Target problem: $-\Delta u = f$ on $\overline{\Omega} = [0, 2] \times [0, 1] \times [0, 1]$
- Uniform global mesh of hexahedral Q1 finite elements
- Uniform partition into rectangular grids of $4m \times 2m \times 2m$ cubic local meshes
- $m = 2^3, 3^3 \dots, 12^3$ blades (8, 432, $\dots, 27648$ cores) devoted to fine-grid duties
- Entire 16-core blade devoted to coarse-grid duties (multi-threaded PARDISO)
- Direct solution (PARDISO) of Dirichlet, Neumann, and coarse-grid corrections
- Gradually larger fixed local problem sizes $\frac{H}{h} = 30^3, 40^3$ FEs/core

BDDC(corners+edges) :: Poisson problem

Weak scaling for BDDC(corners+edges) :: Poisson problem

14 12 Total Wall clock time (secs.) 10 no overlapping Coarse-grid on 2 core(s) Coarse-grid on 4 core(s) Coarse-grid on 8 core(s) Coarse-grid on 16 core(s) 8 6 4 2 H/h³=30³ (27K) FEs/core H/h³=40³ (64K) FEs/core 0 2K 3.5K 5.5K 11.7K 21.3K 128 8K 16K 27.6K #cores

Weak scaling for BDDC(ce)

BDDC preconditioner

- 2 Overlapped BDDC implementation
- 3 Scalability analysis (overlapped)

- 5 Scalability analysis (overlapped/inexact)
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Good features of BDDC towards extreme scales

BDDC has some salient properties that make it an excellent candidate for extreme scale solver design:

- The method allows for a (mathematically supported) extremely aggressive coarsening
- **2** The coarse matrix has a similar sparsity as the original matrix
- Ocoarse and local components can be computed in a parallel (additive) way
- Local (constrained) Neumann and coarse solvers can be solved in an inexact way
- A multilevel extension of the method is possible (for extreme core counts)
- (1)-(2)-(3) always exploited in our overlapped BDDC implementations
- Let us see how to exploit (4), in order to boost scalability further and reduce memory requirements (overlapped/inexact implementation)

- The exact (using direct solvers) BDDC preconditioner leads to the most effective preconditioner
- However, also to the most computationally and memory demanding one
- In order to reduce these demands, one may solve only approximately some (or even all) of the internal problems using, e.g., AMG-based solvers
- Numerical analysis says that inexact BDDC preconditioners are also algoritmically scalable [Dohrmann, 2007]
- Benefit has to be viewed in light of future parallel architectures: the most scalable architectures (e.g., IBM BG) will have more limited memory per core
- Further, the coarse solver time increases as *P* instead of *P*², much less degradation for high core counts

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• Dirichlet problem: approximate $(A_{II}^{(i)})^{-1}$ in $\mathcal{E} = \begin{bmatrix} 0 & -A_{II}^{-1}A_{I\Gamma} \\ 0 & I_{\Gamma} \end{bmatrix}$

Local Neumann problem: approximate (A_c⁽ⁱ⁾)⁻¹, where A_c⁽ⁱ⁾ is the (sub-assembled) local matrix A⁽ⁱ⁾ after eliminating the coarse corner rows/columns

(3) Coarse problem: approximate $(A_C)^-$

• Computation of Φ : approximate $(A_c^{(i)})^{-1}$

From numerical analysis [Dohrmann, 2007]:

• (2)-(3) can be replaced by optimal preconditioners, e.g., AMG-cycle

• (1)-(4) more delicate, additional *null space* preservation required (not true in general)

Key question to be experimentally assessed

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Key question to be experimentally assessed

4 different solvers in BDDC:

- **9** Dirichlet problem: approximate $(A_{II}^{(i)})^{-1}$ in $\mathcal{E} = \begin{bmatrix} 0 & -A_{II}^{-1}A_{I\Gamma} \\ 0 & I_{\Gamma} \end{bmatrix}$
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Sensivity of the algorithm to every inexact solver?

BDDC preconditioner

- Overlapped BDDC implementation
- Scalability analysis (overlapped)

4 Inexact BDDC

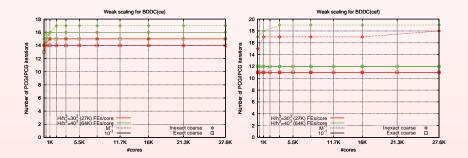
Scalability analysis (overlapped/inexact)

Conclusions and future work

The effect of approximately solving the internal problems

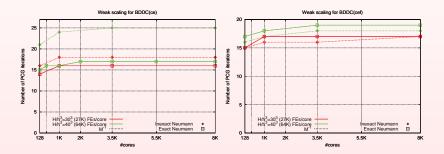
Coarse-grid problem

- The problem that can harm scalability (couples ALL subdomain)
- Fortunately, it can be highly perturbed without impact in the scalability (AMG-cycle suffices)



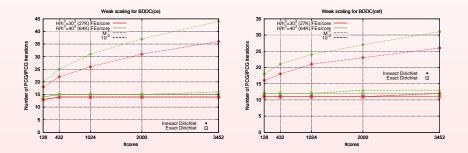
Neumann Problem

Neumann problem can be highly perturbed without impact in the scalability (AMG-cycle suffices)



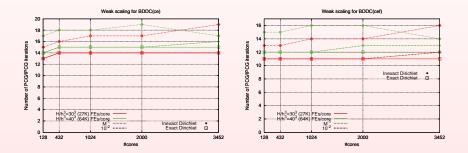
Dirichlet problem

- AMG-cycle wo/ null space preservation (deflation) not algorithmically scalable
- But with loose tolerance enough to make it scalable



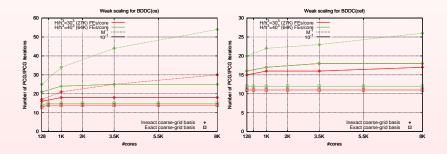
Dirichlet problem

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- But with loose tolerance enough to make it scalable



Coarse-grid basis vectors

- AMG-cycle wo/ null space preservation not algorithmically scalable
- But with loose tolerance enough to make it scalable



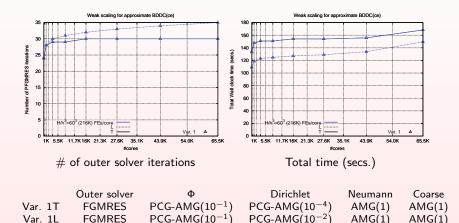
Target machine: JUQUEEN@JSC 28,672 compute nodes (16-core, 64-way threaded IBM PPC A2; 16 GB)

- Target problem: $-\Delta u = f$ on $\overline{\Omega} = [0, 2] \times [0, 1] \times [0, 1]$
- Uniform global mesh of hexahedral Q1 finite elements
- Uniform partition into rectangular grids of $4m \times 2m \times 2m$ cubic local meshes
- $m = 2^3, 3^3 \dots, 16^3$ nodes (8,432, $\dots, 65535$ cores) devoted to fine-grid duties
- Entire node devoted to coarse-grid duties (restricted to only 1 core/GB)
- Gradually larger fixed local problem sizes $\frac{H}{h} = 60^3$ FEs/core

Inexact BDDC(corners+edges) :: Poisson problem

Weak scaling for inexact BDDC(corners+edges) :: Poisson problem

 $\frac{H}{h} = 60$ (216K FEs/core)



Memory usage:

- Fine proc's: 538.6MB (< 1GB)
- Coarse proc's (65.5K cores): 392.7MB (< 1GB)

BDDC preconditioner

- Overlapped BDDC implementation
- 3 Scalability analysis (overlapped)
- Inexact BDDC
- 5 Scalability analysis (overlapped/inexact)



Conclusions:

- Highly scalable asynchronous implementation of BDDC
- Overlapping of fine-grid and coarse-grid computations
- OpenMP parallelization for coarse-grid problem in the exact case
- Exploitation of AMG-based solvers in the inexact case
- Weakly scalable for many ranges of interest
- Memory limitations clearly improved
- High scalability in a memory constrained environment (JUQUEEN)

Conclusions:

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Good features of BDDC towards extreme scales

BDDC has some salient properties that make it an excellent candidate for extreme scale solver design:

- The method allows for a (mathematically supported) extremely aggressive coarsening
- **2** The coarse matrix has a similar sparsity as the original matrix
- Ocoarse and local components can be computed in a parallel (additive) way
- Local (constrained) Neumann and coarse solvers can be solved in an inexact way
- A multilevel extension of the method is possible (for extreme core counts)
- (1)-(2)-(3)-(4) exploited in our inexact/overlapped BDDC implementations
- Next step: Exploit (5), for to boost scalability even further (overlapped/inexact/multilevel implementation)

References

- S. Badia, A. F. Martín and J. Principe. Enhanced balancing Neumann-Neumann preconditioning in computational fluid and solid mechanics. International Journal for Numerical Methods in Engineering. Vol. 96(4), pp. 203-230, 2013.
- S. Badia, A. F. Martín and J. Principe. Implementation and scalability analysis of balancing domain decomposition methods. Archives of Computational Methods in Engineering. Vol. 20(3), pp. 239-262, 2013.
- S. Badia, A. F. Martín and J. Principe. A highly scalable parallel implementation of balancing domain decomposition by constraints. SIAM Journal on Scientific Computing. Vol. 36(2), pp. C190-C218, 2014.
- S. Badia, A. F. Martín and J. Principe. On the scalability of inexact balancing domain decomposition by constraints with overlapped coarse/fine corrections. In preparation, 2014.



Preprints available at http://badia.rmee.upc.edu/sbadia_ar.html

COMFUS team: https://web.cimne.upc.edu/groups/comfus/

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