On scalable space-time balancing domain decomposition solvers

Santiago Badia, Marc Olm

LSSC Team at Centre CIMNE
Universitat Politècnica de Catalunya
Barcelona, Spain

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Outline

1. The BDDC Preconditioner
2. Space-Time BDDC
3. Numerical results
4. Conclusions and future work
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2. Space-Time BDDC
3. Numerical results
4. Conclusions and future work
Preliminaries

- Element-based (non-overlapping DD) distribution (+ limited ghost info)

- Gluing info based on objects
  - **Object:** Maximum set of interface nodes that belong to the same set of subdomains
Preliminaries

- Element-based (non-overlapping DD) distribution (+ limited ghost info)

- Gluing info based on objects
  - **Object**: Maximum set of interface nodes that belong to the same set of subdomains
Automatic hierarchical mesh generator

Classification of objects (vef’s at the next level) in 3D

- **Faces**: Objects that belong to 2 subdomains
- **Edges**: Objects that belong to more than 2 subdomains
- **Corners**: Edges and faces with cardinality 1
Coarser triangulation

- Similar to FE triangulation object but \textit{wo/} reference element
- Instead, \textit{aggregation info}

object level 1 = aggregation (vef’s level 0)
Coarser FE space

- On top of coarser triangulation, we create a FE-like functional space
- DOFs on geometrical objects at the coarser level (as in FEs)
- Aggregation info for DOFs: functionals over objects i.e. mean value
Coarser FE space

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- **DOFs on geometrical objects at the coarser level** (as in FEs)
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• Aggregation info for DOFs: functionals over objects i.e. mean value

\[ u^\alpha = \mathcal{F}_\alpha(u) \]

\[ u^\alpha = \frac{1}{|\mathcal{E}_\alpha|} \int_{\mathcal{E}_\alpha} u \, ds \]
Hierarchical FE spaces

- The under-assembled space \( \tilde{V}_0 = \{ v \in \tilde{V}_0 | \text{continuous } F_1(v) \} \)

- \( \tilde{V}_0 \) is a multiscale space (multiscale solvers)

Application 1: Compute sol’n in \( \tilde{V}_0 \) (multiscale solver)

Application 2: Compute sol’n in \( V_0 \) using \( \tilde{V}_0 \) correction as preconditioner (multilevel precond)

BDDC DD preconditioner (Dohrmann, 2003) is a particular realization of \( \tilde{V}_0 \)
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- BDDC DD preconditioner (Dohrmann, 2003) is a particular realization of $\bar{V}_0$
Hierarchical FE spaces

The under-assembled space $\bar{V}_0$ can be decomposed as:

- Its bubble space $\bar{V}_0^b = \{v \in \bar{V}_0 | F_\alpha(v) = 0\}$
- The coarser FE space $V_c = \{v \in \bar{V}_0 | v \perp \tilde{A} \bar{V}_0^b\}$

$$\bar{V}_0 = \bar{V}_0^b \oplus V_c$$
Hierarchical FE spaces

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Coarse corner function

- Compute via local problems a basis for $V_c = \{\Phi_1, \ldots, \Phi_{n_c}\}$
- Every $\Phi$ is a coarse shape function related to a coarse DoF
Coarse edge function

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BDDC problem

The problem in \( \tilde{V}_0 = V_c \oplus \tilde{V}_0^b \):

\[
\tilde{u}_0 \in \tilde{V}_0 : a(\tilde{u}_0, \tilde{v}_0) = (f, \tilde{v}_0) \quad \forall \tilde{v}_0 \in \tilde{V}_0
\]

can be decomposed as \( \tilde{u}_0 = \tilde{u}_0^b + u_c \) (orthogonality \( V_c \perp \tilde{V}_0^b \))

\[
u_0^b \in \tilde{V}_0^b : a(u_0^b, v_0^b) = (f_0, v_0^b) \quad \forall v_0 \in \tilde{V}_0^b
\]

\[
u_c \in V_c : a(u_c, v_c) = (f_c, v_c) \quad \forall v_c \in V_c
\]

- Bubble component is local to every subdomain (parallel)
- Coarse global problem
BDDC problem

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LSSC BDDC implementation: FEMPAR

Software

FEMPAR (Finite Element Multiphysics PARallel) is an in-house developed HPC software:

- Free software GNU-GPL licensing (to be distributed soon)
- Massively parallel software for the FE simulation of multiphysics PDEs
- Scalable preconditioning of fully coupled and implicit systems via block preconditioning
- Interfaces to external multi-threaded sparse direct solvers (PARDISO, HSL_MA87 etc.) and serial AMG preconditioners (HSL_MI20)
Why BDDC for extreme scales?

Iterative Krylov-subspace BDDC preconditioned solvers can be very scalable at extreme scales:

- Mathematically supported extremely aggressive coarsening
- Coarse/local components can be computed in parallel (additive preconditioner)
- The coarse matrix has a similar sparsity as the original matrix
- A multilevel extension is possible (avoid bottlenecks due to coarse problem)

All this features are already exploited in our BDDC implementation. Till this work, excellent weak scalability results have been achieved for spatial parallelization.
Weak scaling 3-lev BDDC(ce) solver

3D Laplacian problem on IBM BG/Q (JUQUEEN@JSC)
16 MPI tasks/compute node, 1 OpenMP thread/MPI task

#PCG iterations  Total time (secs.)

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<th>Lev.</th>
<th># MPI tasks</th>
<th>FEs/core</th>
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<td>42.8K 74.1K</td>
<td>125 216 343 512 729 1000 1331</td>
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<tr>
<td>2nd</td>
<td>117.6K 175.6K 250K 343K 456.5K</td>
<td>20^3/25^3/30^3/40^3</td>
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<tr>
<td>3rd</td>
<td>1 1 1 1 1 1</td>
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Experiment set-up
Weak scaling 4-lev BDDC(ce)

3D Laplacian problem on IBM BG/Q (JUQUEEN@JSC)
64 MPI tasks/compute node, 1 OpenMP thread/MPI task

Weak scaling for 4-level BDDC(ce) solver with H2/h2=4, H3/h3=3

Total time (secs.)

<table>
<thead>
<tr>
<th>Lev.</th>
<th># MPI tasks</th>
<th>FEs/core</th>
</tr>
</thead>
<tbody>
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<td>$10^3/20^3/25^3$</td>
</tr>
<tr>
<td>2nd</td>
<td>729 1.73K 3.38K 5.83K 9.26K 13.8K 19.7K</td>
<td>$4^3$</td>
</tr>
<tr>
<td>3rd</td>
<td>27 64 125 216 343 512 729</td>
<td>$3^3$</td>
</tr>
<tr>
<td>4th</td>
<td>1 1 1 1 1 1 1</td>
<td>n/a</td>
</tr>
</tbody>
</table>
Iterative Krylov-subspace BDDC preconditioned solvers show excellent scalability properties in **spatial** parallelism for extreme scales:

- **Space-only** Domain Decomposition method formulated as a preconditioner
- Unsteady problems can apply the approach at every time step of the time integration
- Many key computational engineering problems may involve millions of time steps e.g. additive manufacturing, turbulent flow simulations ...
- At some point, **spatial** parallelism may saturate
- Consider full **space-time** parallelism

Development of space-time solvers, dealing with all time steps at once. Present work considers the BDDC method extension to full space-time parallel solvers.
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A direct ODE solver

Time parallel BDDC approach applied to ODEs:

- Using object definition, all communication objects are corners on the interface
- $\tilde{A}$-orthogonality between fine and coarse grid time propagations
- Additive combination of fine and coarse solution
- Presentation consider a DG time discretization (other also possible, i.e. Runge-Kutta)
A direct ODE solver

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A direct ODE solver

(a) Coarse shape function: \( \phi_{\pi/3} (s) = \delta_{\pi/3} (s) \) for \( s = \{ \pi/3, 2\pi/3 \} \), \( \phi_{\pi/3} \perp \tilde{A} \nabla_f \)

(b) Fine coarse solutions with 10 subintervals \( u_c \perp \tilde{A} u_f \)

A coarse shape function \( \phi_\alpha \) and solution for the simple ODE \( \frac{du}{dt} = \cos (t) \)
Nonlinear ODEs

Consider a linearization method, e.g. Newton’s Method. At every nonlinear iteration we must solve a linear ODE, where we can exploit the parallel direct method presented above.

(a) Nonlinear iterations
(b) First iteration
(c) Additive solution

Iterations for the solution of the nonlinear equation \( \partial_t u - u^2 = \cos(t) - \sin^2(t) \) on \( t = [0, 2\pi] \). Fine and coarse solutions for the first nonlinear solution update \( \delta u^1 \). The time interval is discretized with 500 time steps divided into 15 subdomains.
Space-Time BDDC methods

Space-Time BDDC Key ingredients:

- **Subassembled (local) operators** $\tilde{A}_\omega$
- Space-Time subassembled space $\tilde{V}_0$
- Global positiveness of the problem is lost locally: perturbation of the time derivative operator $\tilde{M}_\omega^*$ to end up with a well-posed local problem
- Upwinded injection operator from subassembled space to global space, i.e. $\mathcal{W} : \tilde{V}_0 \longrightarrow V_0$
- Define continuity to be imposed among subdomains, i.e. $\bar{V}_0$
  - *Fine* and *Coarse* STBDDC spaces $\bar{V}_0 = \tilde{V}_0^b \oplus V_c$
  - Particular STBDDC space $V_0 \subset \bar{V}_0 \subset \tilde{V}_0$
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*Fine* and *Coarse* STBDDC spaces $V_0 = \tilde{V}_0^b \oplus V_c$

Particular STBDDC space $V_0 \subset \tilde{V}_0 \subset \tilde{V}_0$
Find $u \in V_0$: $A(u, v) = M(u, v) + K(u, v) = f(v)$ $\forall v \in V_0$

$K_e(u, v) := \int_{e_t} \left[ \int_{e_x} \nabla u \cdot \nabla v \, dx \right] \, ds$

$f_e(v) := \int_{e_t} \left[ \int_{e_x} fv \, dx \right] \, ds$

$M_e(u, v) := \int_{e_x} \left[ -\int_{e_t} \frac{\partial u(s)}{\partial t} u(s) \, ds + u^-(\partial e^+)^2 - u^- (\partial e^-) u^+ (\partial e^-) \right] \, dx$

• Global problem assembly

$A(u, v) = \sum_{e \in \Omega} A_e(u, v)$ $f(v) = \sum_{e \in \Omega} f_e(v)$ for $u, v \in V_{0\omega}$
Space-Time subassembled spaces & operators

Find $u \in V_0$: $\mathcal{A}(u, v) = \mathcal{M}(u, v) + \mathcal{K}(u, v) = f(v) \quad \forall v \in V_0$

$$\mathcal{K}_e(u, v) := \int_{e_t} \left[ \int_{e_x} \nabla u \cdot \nabla v \, dx \right] \, ds$$
$$f_e(v) := \int_{e_t} \left[ \int_{e_x} fv \, dx \right] \, ds$$

$$\mathcal{M}_e(u, v) := \int_{e_x} \left[ - \int_{e_t} \frac{\partial u(s)}{\partial t} u(s) \, ds + u^- (\partial e^+)^2 - u^- (\partial e^-) u^+ (\partial e^-) \right] \, dx$$

- Global problem assembly

$$\mathcal{A}(u, v) = \sum_{e \in \theta} \mathcal{A}_e(u, v) \quad f(v) = \sum_{e \in \theta} f_e(v) \quad \text{for } u, v \in V_{0\omega}$$
Space-Time subassembled spaces & operators

Find $u \in V_0$: $A(u, v) = M(u, v) + K(u, v) = f(v)$ $\forall v \in V_0$

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K_e(u, v) := \int_{e_t} \left[ \int_{e_x} \nabla u \cdot \nabla v \, dx \right] \, ds
$$

$$
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$$

$$
M_e(u, v) := \int_{e_x} \left[ -\int_{e_t} \frac{\partial u(s)}{\partial t} u(s) \, ds + u^{-}(\partial e^{+})^{2} - u^{-}(\partial e^{-}) u^{+}(\partial e^{-}) \right] \, dx
$$

- Local problem

$$
A_\omega(u, v) = \sum_{e \in \theta_\omega} A_e(u, v) \quad f_\omega(v) = \sum_{e \in \theta_\omega} f_e(v) \quad \text{for } u, v \in V_{0\omega}
$$
Space-Time subassembled spaces & operators

Find $u \in V_0$: $\mathcal{A}(u, v) = \mathcal{M}(u, v) + \mathcal{K}(u, v) = f(v) \quad \forall v \in V_0$

\[
\mathcal{K}_e(u, v) := \int_{e_t} \left[ \int_{e_x} \nabla u \cdot \nabla v \, d\mathbf{x} \right] \, ds
\]

\[
f_e(v) := \int_{e_t} \left[ \int_{e_x} f \, d\mathbf{x} \right] \, ds
\]

\[
\mathcal{M}_e(u, v) := \int_{e_x} \left[ -\int_{e_t} \frac{\partial u(s)}{\partial t} u(s) \, ds + u^-(\partial e^+)^2 - u^-(\partial e^-)u^+(\partial e^-) \right] \, d\mathbf{x}
\]

- Local problem

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\mathcal{A}_\omega(u, v) = \sum_{e \in \theta_\omega} \mathcal{A}_e(u, v) \quad f_\omega(v) = \sum_{e \in \theta_\omega} f_e(v) \quad \text{for } u, v \in V_{0\omega}
\]
Space-Time subassembled spaces & operators

- Local spaces $\tilde{V}_0\omega$.
- Sub-assembled space $\tilde{V}_0 := \prod_{\omega \in \Theta} \tilde{V}_0\omega$.
- Sub-assembled operator $\tilde{A} := \prod_{\omega \in \Theta} \tilde{A}_\omega(u, v)$.

Since $V_0 \subset \tilde{V}_0$, $A$ can be interpreted as the restriction of $\tilde{A}$ onto $V_0$.
The operator $\tilde{\mathcal{M}}$ is the discretization of the time derivative. We have:

$$\tilde{\mathcal{M}}_e(u, u) = \int_{e_x} \left[ - \int_{e_t} \frac{\partial u(s)}{\partial t} u(s) ds + \{\hat{u}u\} \frac{\partial e^+}{\partial e^-} \right] dx$$

$$= \int_{e_x} \left[ - \frac{1}{2} \int_{e_t} \frac{\partial u^2(s)}{\partial t} ds + u^- (\partial e^+)^2 - u^- (\partial e^-) u^+ (\partial e^-) \right] dx$$

$$= \frac{1}{2} \int_{e_x} \left[ u^- (\partial e^+)^2 - u^- (\partial e^-)^2 + (u^+ (\partial e^-) - u^- (\partial e^-))^2 \right] dx$$
Perturbed time local boundary conditions

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$$= \frac{1}{2} \int_{e_x} \left[ u^- (\partial e^+)^2 - u^- (\partial e^-)^2 + (u^+ (\partial e^-) - u^- (\partial e^-))^2 \right] \, dx$$
Perturbed time local boundary conditions

The local problems are indefinite since \( u^-(\partial \omega^-) \) is not enforced to be equal to zero. Consider a perturbed subdomain operator \( \tilde{M}_\omega^* \):

\[
\tilde{M}_\omega^* (u, v) = \tilde{M}_\omega (u, v) - \sum_{\alpha \in \{\partial \omega^-, \partial \omega^+\}} \frac{1}{2} \int_{\omega_x} \text{sgn}(\alpha, \omega) u^-(\alpha) v^-(\alpha) dx,
\]

where \( \text{sgn}(\alpha, \omega) = 1 \) (resp. \(-1\)) when \( \alpha = \partial \omega^+ \) (resp. \( \partial \omega^- \)) and \( \text{sgn}(\alpha, \omega) = 0 \) when \( \alpha = 0 \) or \( \alpha = T \). Using this definition of \( \tilde{M}_\omega^* \), we end up with the following properties:

- \( \tilde{M}_\omega^* (u, u) \geq 0 \)
- \( \tilde{M}_\omega^* (u, v) = \tilde{M} (u, v) \) for \( u, v \in V_0 \).
- \( \tilde{M}_\omega^* (u, u) = \frac{1}{2} \| u^- (T) \|^2_{\Omega_x} \)
Time causality aware injection operator

The upwinded projection $\mathcal{W} : \tilde{V}_0 \rightarrow V_0$, given a function $u \in \tilde{V}_0$,

$$\mathcal{W}u(\xi) := \sum_{\omega \in \omega(\xi)} \frac{u_{\omega}(x_\xi, t_\xi)}{|\omega_x(x_\xi)|}, \quad \xi = x_\xi \times t_\xi \in \Xi.$$ 

Next, the harmonic correction is computed such that

$$A(\delta u_0, v_0) = -A(\mathcal{W}u, v_0), \quad \forall v_0 \in V_0^b.$$ 

$\mathcal{E} : \tilde{V}_0 \rightarrow V_0$ as some weighted average of interface values together with an harmonic extension to subdomain interiors.
Objects choice 1: 4D objects

Extension of vef’s to 4D:

- **Corners**: Edges and faces with cardinality 1, 0D objects
- **Edges**: objects that belong to more than 2 subdomains in space
- **Faces**: objects that belong to 2 subdomains in space, extended in time
- **Volumes**: Objects that belong to 2 space-time subdomains (only in 4D)
Objects choice 2: space-time continuity objects

- **Time coarse DOF** $F_\alpha^\omega := \frac{\int_{w_x} u^-(x,t=\alpha)}{|\omega_x|}$

- **Spatial coarse DOF** $F_\lambda^\omega := \frac{\int_{\omega_t} \int_{\partial \omega_x} \theta_{\lambda x}^\omega (u(s)) \sigma \, ds}{\int_{\omega_t} \int_{\partial \omega_x} \theta_{\lambda x}^\omega (1) \sigma \, ds}$ (i.e. time average)
Objects choice 2: space-time continuity objects

- **Time coarse DOF** $F^\omega_{\alpha} := \frac{\int_{\omega_x} u^- (x, t=\alpha) \omega_x}{|\omega_x|}$

- **Spatial coarse DOF** $F^\omega_\lambda := \frac{\int_{\omega_t} \int_{\partial \omega_x} \theta^\omega_{\lambda x} (u(s)) d\sigma ds}{\int_{\omega_t} \int_{\partial \omega_x} \theta^\omega_{\lambda x} (1) d\sigma ds}$ (i.e. time average)
The space-time preconditioner can be compactly written as

\[ \mathcal{P}_{STBDDC} = \mathcal{E} \bar{A}^{-1} \mathcal{E}^T \]

- \( \bar{x}_f = \bar{A}_f^{-1} \mathcal{E}^T r \) where \( \bar{A}_f \) is the Galerkin projection of \( \bar{A} \) onto \( \bar{V}_0^b \) (embarrassingly parallel!)
- \( \bar{x}_c = \Phi \bar{A}_c^{-1} \varphi^T \mathcal{E}^T r \) where \( \bar{A}_c = \varphi^T \bar{A} \Phi \), i.e. the Galerkin projection of \( \bar{A} \) onto the coarse space \( V_c \)

With objects choices 1 & 2 the preconditioner has been proved to be well posed. (S. Badia & MO article)
Outline

1 The BDDC Preconditioner
2 Space-Time BDDC
3 Numerical results
4 Conclusions and future work
Weak scalability in PDE space-time solvers

Relative weights of all the discrete differential operators is kept through the weak scalability analysis:

- Keep fixed the physical problem to be solved. BC’s, physical properties...
- Keep fixed the mesh and subdomain sizes \( h, H \)
- Scale the physical domain \( \Omega \rightarrow \alpha \Omega \) with the number of subdomains

Therefore, weak scalability proposed herein fixes local Reynolds, Péclet or CFL number through the analysis.

Gottfried complex of the HLRN-III Cray system (Hannover)
(b) Iteration counter and computing time with $\beta = 10\overrightarrow{e_x}$.

(b) Iteration counter and computing time with $\beta = \overrightarrow{e_x}$.

2D CDR Equation on $\Omega_x = [0, 1]^2$, $\Omega_t = [0, 0.1]$, Homogeneous Dirichlet BCs, Analytical sol’on: $u(x, t) = \sin(\pi x) \sin(\pi y) \sin(\pi t)$, $\nu = 10^{-3}$, $\sigma = 10^{-4}$. 
2D Heat equation on $\Omega_x = [0, 1]^2$, $\Omega_t = [0, 0.1]$, $\nu = 1$, Homogeneous Dirichlet BCs, $f = 1$
Space-time weak scalability II

(a) Comparison between different diffusion parameters, $M_x = M_t$.

2D Heat Equation on $\Omega_x = [0, 1]^2$, $\Omega_t = [0, 0.1]$, Homogeneous Dirichlet BCs, $f = 1$
Outline

1. The BDDC Preconditioner
2. Space-Time BDDC
3. Numerical results
4. Conclusions and future work
Conclusions and future work

- Highly scalable implementation of MLBDDC in FEMPAR
  - Only spatial preconditioner
  - Largest scaling/problem sizes reported so far with DD preconditioners

- Space-Time BDDC
  - Direct method for time-parallelism in ODEs
  - Iterative solver based on DD techniques
  - Exploit time direction nature
  - Excellent weak scalability results for moderate CFL numbers

- Future work includes:
  - Multilevel space-time BDDC
  - Application to nonlinear PDEs
  - Solve more complex problems (solid mechanics, incompressible fluid mechanics ...)
Farewell

Thank you!


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Coarse shape functions

DG(0)  DG(1)  DG(2)

(a) $\phi_{\frac{\pi}{3}}(s) = \delta_{\frac{\pi}{3}}(s)$ for $s = \{\frac{\pi}{3}, \frac{2\pi}{3}\}$, $\phi_{\frac{\pi}{3}} \perp A \nabla f$

(b) $\phi_{\frac{\pi}{3}}^+(s) = \delta_{\frac{\pi}{3}}(s)$ for $s = \{\frac{\pi}{3}, \frac{2\pi}{3}\}$, $\phi_{\frac{\pi}{3}} \perp A \nabla f$

A coarse shape function $\phi_\alpha$ for the simple transport operator $\frac{du}{dt}$ at $\alpha = \frac{\pi}{3}$
Fine-Coarse grid solutions

DG(0)  DG(1)  DG(2)

(a) Values \( \{ v^-(\alpha) \}_{\alpha \in \Gamma^\Theta} \) define coarse DOFs

(b) Values \( \{ v^+(\alpha) \}_{\alpha \in \Gamma^\Theta} \) define coarse DOFs