A reduced order model for optimisation-based domain decomposition (DD) algorithms for PDEs

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DD for Poisson's problem. Monolithic formulation

Let $\Omega \subset \mathbb{R}^2$ be open and let Γ be the boundary of Ω. Given $f : \Omega \to \mathbb{R}$, find $u : \Omega \to \mathbb{R}$ s.t.

$$-\Delta u = f \quad \text{in} \quad \Omega, \tag{1}$$

$$u = 0 \quad \text{on} \quad \Gamma. \tag{2}$$

DD for Poisson's problem. DD formulation

Let $\Omega_i,\ i = 1, 2$ be open subsets of Ω, s.t. $\overline{\Omega} = \overline{\Omega_1 \cup \Omega_2}$, $\Omega_1 \cap \Omega_2 = \emptyset$. Denote $\Gamma_i = \partial\Omega_i \cap \Gamma,\ i = 1, 2$ and $\Gamma_0 := \overline{\Omega_1} \cap \overline{\Omega_2}$. Then the DD formulation reads as follows: for $i = 1, 2$, given $f_i : \Omega_i \to \mathbb{R}$, find $u_i : \Omega_i \to \mathbb{R}$ s.t.

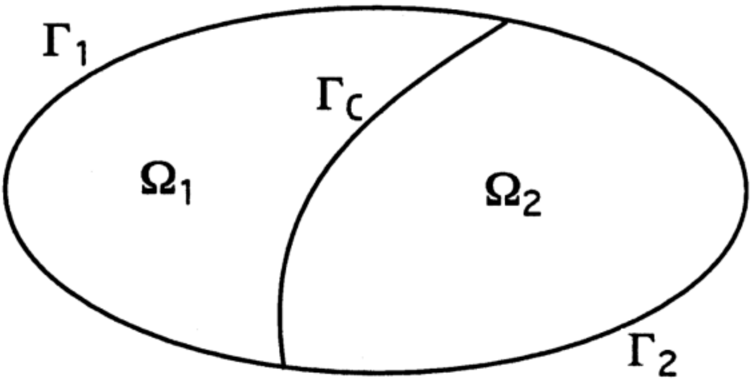
$$-\Delta u_i = f_i \quad \text{in} \quad \Omega_i, \tag{3}$$

$$u = 0 \quad \text{on} \quad \Gamma_i, \tag{4}$$

$$\frac{\partial u}{\partial n_i} = (-1)^{i+1} g \quad \text{on} \quad \Gamma_0, \tag{5}$$

for some $g : \Gamma_0 \to \mathbb{R}$.

DD for Poisson's problem. Domain Decomposition



DD for Poisson's problem. DD formulation

- For any g the solution to the DD problem is not the same as the solution to the monolithic problem, i.e. $u_1 \neq u|_{\Omega_1}$ and $u_2 \neq \Omega|_2$.
- There exists a choice for g, i.e $g = \frac{\partial u_1}{\partial n_1}|_{\Gamma_0} = -\frac{\partial u_2}{\partial n_2}|_{\Gamma_0}$, such that the solutions coincide on the corresponding subdomains.
- So we must find such a g so that u_1 is as close as possible to u_2 on the interface Γ_0.

DD for Poisson's problem. DD formulation

One way to accomplish is to minimise the functional

$$\mathcal{J}(u_1, u_2) =: \frac{1}{2} \int_{\Gamma_0} (u_1 - u_2)^2 \, d\Gamma. \qquad (6)$$

Instead of (6) we can also consider the penalised or regularised functional

$$\mathcal{J}_\gamma(u_1, u_2; g) =: \frac{1}{2} \int_{\Gamma_0} (u_1 - u_2)^2 \, d\Gamma + \frac{\gamma}{2} \int_{\Gamma_0} g^2 d\Gamma, \qquad (7)$$

where γ is a constant that can be chosen to change the relative importance of the terms in (7).
Thus we face an optimisation problem under PDE constraints: minimise the functional (6)(or (7)) over suitable function g subject to the PDE constraints.

DD for Poisson's problem. DD variational formulation

- $V_i := \left\{ u \in H^1(\Omega_i) : \ u|_{\Gamma_i} = 0 \right\}, i = 1, 2$
- Find $u_i \in V_i$ s.t.

$$(\nabla u_i, \nabla v_i)_{\Omega_i} = (f_i, v_i)_{\Omega_i} + ((-1)^{i+1} g, v_i)_{\Gamma_0}, \quad \forall v_i \in V_i. \quad (8)$$

DD for Poisson's problem. Lagrangian

We define Lagrangian functional as follows:

$$\mathcal{L}(u_1, u_2, \xi_1, \xi_2; g) := \mathcal{J}_\gamma(u_1, u_2; g) - \sum_{i=1}^{2} (\nabla u_i, \nabla \xi_i)_{\Omega_i} - \sum_{i=1}^{2} (f_i, v_i)_{\Omega_i} - \sum_{i=1}^{2} ((-1)^{i+1} g, \xi_i)_{\Gamma_0}. \quad (9)$$

- $\mathcal{L} : V_1 \times V_2 \times V_1 \times V_2 \times L^2(\Gamma_0) \to \mathbb{R}$

DD for Poisson's problem. Optimality conditions

- constrains

$$(\nabla u_1, \nabla v_1)_{\Omega_1} = (f_1, v_1)_{\Omega_1} + (g, v_1)_{\Gamma_0}, \quad \forall v_1 \in V_1, \tag{10}$$
$$(\nabla u_2, \nabla v_2)_{\Omega_2} = (f_2, v_2)_{\Omega_2} - (g, v_2)_{\Gamma_0}, \quad \forall v_2 \in V_2. \tag{11}$$

- adjoint equations

$$(\nabla \eta_1, \nabla \xi_1)_{\Omega_1} = (\eta_1, u_1 - u_2)_{\Gamma_0}, \quad \forall \eta_1 \in V_1, \tag{12}$$
$$(\nabla \eta_2, \nabla \xi_2)_{\Omega_2} = -(\eta_2, u_1 - u_2)_{\Gamma_0}, \quad \forall \eta_2 \in V_2. \tag{13}$$

- optimality condition

$$(g, h)_{\Gamma_0} = -\frac{1}{\gamma}(\xi_1 - \xi_2, h)_{\Gamma_0}, \quad \forall h \in L^2(\Gamma_0). \tag{14}$$

- Gradient (based on the sensitivity derivatives)

$$\frac{d\mathcal{J}_\gamma}{dg}(u_1, u_2; g) = \gamma g + (\xi_1 - \xi_2)|_{\Gamma_0}, \tag{15}$$

DD for Poisson's problem. Gradient method

The following simple gradient method can be considered: given a starting guess $g^{(0)}$, let

$$g^{(n+1)} = g^{(n)} - \alpha \frac{d\mathcal{J}_\gamma}{dg} \left(u_1^{(n)}, u_2^{(n)}; g^{(n)} \right) . \tag{16}$$

Combining with (24) we obtain

$$g^{(n+1)} = g^{(n)} - \alpha \left(\gamma g^{(n)} + (\xi_1^{(n)} - \xi_2^{(n)})|_{\Gamma_0} \right) , \tag{17}$$

or

$$g^{(n+1)} = (1 - \alpha\gamma)\, g^{(n)} - \alpha(\xi_1^{(n)} - \xi_2^{(n)})|_{\Gamma_0}, \tag{18}$$

where $\xi_1^{(n)}$ and $\xi_2^{(n)}$ are determined as the solutions to the adjoint equations with g replaced by $g^{(n)}$.

DD for Poisson's problem. Gradient method

Algorithm 1.

1. Choose $g^{(0)}$, α.
2. For n=0,1,2,... until convergence

   2.1 Determine $u_1^{(n)}$, $u_2^{(n)}$ s.t.

   $$(\nabla u_i^{(n)}, \nabla v_i)_{\Omega_i} = (f_i, v_i)_{\Omega_i} + ((-1)^{i+1} g^{(n)}, v_i)_{\Gamma_0}, \quad \forall v_i \in V_i, \quad i = 1, 2.$$

   2.2 Determine $\xi_1^{(n)}$, $\xi_2^{(n)}$ s.t.

   $$(\nabla \eta_i^{(n)}, \nabla \xi_i)_{\Omega_i} = ((-1)^{i+1} \eta_i, u_1^{(n)} - u_2^{(n)})_{\Gamma_0}, \quad \forall \eta_i \in V_i, \quad i = 1, 2.$$

   2.3 Determine $g^{(n+1)}$ by

   $$g^{(n+1)} := (1 - \alpha\gamma)\, g^{(n)} - \alpha \left(\xi_1^{(n)} - \xi_2^{(n)} \right) |_{\Gamma_0}.$$

DD for Poisson's problem. Numerical results

Tolerance - 10^{-5}. Zero initial approximation for g.

Step α	**Iterations**
1	22
3	8
5	18
6	diverges

Quantity	**Value**
J	$4 \cdot 10^{-10}$
$\|\|\nabla J\|\|$	10^{-5}
$\|\|u_1 - u_2\|\|_{\Gamma_0}$	$5 \cdot 10^{-5}$
Abs. error on subdomains	$7 \cdot 10^{-6}$
Rel. error on subdomains	10^{-4}

CFD. Monolithic formulation

Let $\Omega \subset \mathbb{R}^2$ be open and let Γ be the boundary of Ω. Given $f : \Omega \to \mathbb{R}^2$ - forcing term ν - kinematic viscosity, u_{in} - fluid inflow profile, find $u : \Omega \to \mathbb{R}^2$ - the velocity filed and $p : \Omega \to \mathbb{R}$ - the pressure s.t.

$$
\begin{aligned}
-\nu \Delta u + (u \cdot \nabla) u + \nabla p = f \quad & \text{in} \quad \Omega, & (19)\\
-\mathrm{div} u = 0 \quad & \text{in} \quad \Omega, & (20)\\
u = u_{in} \quad & \text{on} \quad \Gamma_{in}, & (21)\\
u = 0 \quad & \text{on} \quad \Gamma_{wall}, & (22)\\
\nu \frac{\partial u}{\partial n} - pn = 0 \quad & \text{on} \quad \Gamma_{out}, & (23)
\end{aligned}
$$

where n - is an outward normal vector to Γ.

CFD. DD formulation

- Ω_i, $i = 1, 2$ - open subsets of Ω, s.t. $\overline{\Omega} = \overline{\Omega_1 \cup \Omega_2}$, $\Omega_1 \cap \Omega_2 = \emptyset$
- $\Gamma_i = \partial\Omega_i \cap \Gamma$, $i = 1, 2$ and $\Gamma_0 := \overline{\Omega_1} \cap \overline{\Omega_2}$
- $\Gamma_{i,in}$, $\Gamma_{i,out}$ and $\Gamma_{i,wall}$, $i = 1, 2$
- For $i = 1, 2$, given $f_i : \Omega_i \to \mathbb{R}^2$, find $u_i : \Omega_i \to \mathbb{R}^2$, $p_i : \Omega_i \to \mathbb{R}$ s.t.

$$
\begin{aligned}
-\nu\Delta u_i + (u_i \cdot \nabla)\, u_i + \nabla p_i = f_i \quad &\text{in} \quad \Omega_i, && (24)\\
-\mathrm{div} u_i = 0 \quad &\text{in} \quad \Omega_i, && (25)\\
u_i = u_{in} \quad &\text{on} \quad \Gamma_{i,in}, && (26)\\
u_i = 0 \quad &\text{on} \quad \Gamma_{i,wall}, && (27)\\
\nu\frac{\partial u_i}{\partial n_i} - p_i n_i = 0 \quad &\text{on} \quad \Gamma_{i,out}, && (28)\\
\nu\frac{\partial u_i}{\partial n_i} - p_i n_i = (-1)^{i+1} g \quad &\text{on} \quad \Gamma_0, && (29)
\end{aligned}
$$

for some $g : \Gamma_0 \to \mathbb{R}^2$.

CFD. DD formulation

- For any g the solution to the DD problem is not the same as the solution to the monolithic problem, i.e. $u_1 \neq u|_{\Omega_1}$, $p_1 \neq p|_{\Omega_1}$, $u_2 \neq u|_{\Omega_2}$ and $p_2 \neq p|_{\Omega_2}$.
- On the other hand, there exists a choice for g, i.e $g = \left(\nu \frac{\partial u_1}{\partial n_1} - p_1 n_1\right)|_{\Gamma_0} = -\left(\nu \frac{\partial u_2}{\partial n_2} - p_2 n_2\right)|_{\Gamma_0}$, s.t. the solutions on the corresponding subdomains coincide.
- So we must find such a g so that u_1 is as close as possible to u_2 on the interface Γ_0. One way to accomplish is to minimise the functional

$$\mathcal{J}(u_1, u_2) =: \frac{1}{2} \int_{\Gamma_0} |u_1 - u_2|^2 \, d\Gamma. \tag{30}$$

CFD. DD formulation

Instead of (12) we can also consider the penalised or regularised functional

$$\mathcal{J}_\gamma(u_1, u_2; g) =: \frac{1}{2}\int_{\Gamma_0} |u_1 - u_2|^2 \, d\Gamma + \frac{\gamma}{2}\int_{\Gamma_0} |g|^2 \, d\Gamma, \tag{31}$$

where γ is a constant that can be chosen to change the relative importance of the terms.

CFD. Variational formulation of state equations

- $V_i := \left\{u \in H^1(\Omega_i; \mathbb{R}^2) : \; u|_{\Gamma_{i,wall}} = 0\right\}$
- $V_{i,0} := \left\{u \in H^1(\Omega_i; \mathbb{R}^2) : \; u|_{\Gamma_{i,wall} \bigcup \Gamma_{i,in}} = 0\right\}$
- $Q_i := \left\{p \in L^2(\Omega_i; \mathbb{R})\right\}, \; i = 1, 2.$
- Find $u \in V_i, \; p_i \in Q_i$ s.t

$$
\begin{aligned}
\nu(\nabla u_i, \nabla v_i)_{\Omega_i} + ((u_i \cdot \nabla)\, u_i, v_i)_{\Omega_i} - (\mathrm{div} v_i, p_i)_{\Omega_i} & \\
= (f_i, v_i)_{\Omega_i} + ((-1)^{i+1} g, v_i)_{\Gamma_0} & \qquad \forall v_i \in V_{i,0}, \\
-(\mathrm{div} u_i, q_i)_{\Omega_i} = 0 & \qquad \forall q_i \in Q_i, \\
u_i = u_{in} & \qquad \text{on } \Gamma_{i,in}.
\end{aligned}
$$

CFD. Lagrangian

$$
\begin{aligned}
\mathcal{L}(u_1, p_1, u_2, p_2, \xi_1, \xi_2, \lambda_1 \lambda_2; g) := \mathcal{J}_\gamma(u_1, u_2; g) \\
- \sum_{i=1}^{2} \Big[\nu(\nabla u_i, \nabla \xi_i)_{\Omega_i} + ((u_i \cdot \nabla)\, u_i, \xi_i)_{\Omega_i} \\
-(\mathrm{div} \xi_i, p_i)_{\Omega_i} - (\mathrm{div} u_i, \lambda_i)_{\Omega_i} \Big] \\
+ \sum_{i=1}^{2} (f_i, \xi_i)_{\Omega_i} + \sum_{i=1}^{2} ((-1)^{i+1} g, \xi_i)_{\Gamma_0}.
\end{aligned}
$$

CFD. Optimality conditions

- state equations

$$\nu(\nabla u_i, \nabla v_i)_{\Omega_i} + ((u_i \cdot \nabla)\, u_i, v_i)_{\Omega_i} - (\mathrm{div} v_i, p_i)_{\Omega_i}$$
$$= (f_i, v_i)_{\Omega_i} + ((-1)^{i+1} g, v_i)_{\Gamma_0} \quad \forall v_i \in V_{i,0},$$
$$-(\mathrm{div} u_i, q_i)_{\Omega_i} = 0 \quad \forall q_i \in Q_i.$$

- adjoint equations

$$\nu(\nabla \eta_i, \nabla \xi_i)_{\Omega_i} + ((\eta_i \cdot \nabla)\, u_i, \xi_i)_{\Omega_i}$$
$$+ ((u_i \cdot \nabla)\, \eta_i, \xi_i)_{\Omega_i} - (\mathrm{div} \eta_i, \lambda_i)_{\Omega_i}$$
$$= ((-1)^{i+1} \eta_i, u_1 - u_2)_{\Gamma_0}, \quad \forall \eta_i \in V_{i,0},$$
$$-(\mathrm{div} \xi_i, \mu_i)_{\Omega_i} = 0, \quad \forall \mu_i \in Q_i.$$

CFD. Optimality conditions

- optimality condition

$$\gamma(h, g)_{\Gamma_0} + (h, \xi_1 - \xi_2)_{\Gamma_0} = 0, \quad \forall h \in L^2(\Gamma_0). \tag{32}$$

- Gradient (through sensitivity derivatives)

$$\frac{d\mathcal{J}_\gamma}{dg}(u_1, u_2; g) = \gamma g + (\xi_1 - \xi_2)|_{\Gamma_0}, \tag{33}$$

CFD. ROM - Offline stage

- **Objective:** parametrised PDEs
- **Idea:** to create a basis (based on snaphots) to solve the problem for any problem parameters as effective as possibile
- Proper Orthogonal Decomposition (POD) for the reduced basis formation
  1. Choose a partition for the parameter space
  2. For each value of the chosen parameters solve the optimisation problem and store the value of the state, adjoint and control
  3. Additionaly solve for the pressure supremiser (to satisfy the inf-sup condition in the reduced problem, stability)
  4. Perform POD for the state (with supremiser enrichment), adjoint and control variables separately
  5. Form the reduced basis matrices $Z_s,\ Z_a,\ Z_c$

CFD. ROM - Online stage

- Z_s, Z_a, Z_c - reduced basis matrices
- ROM approximation

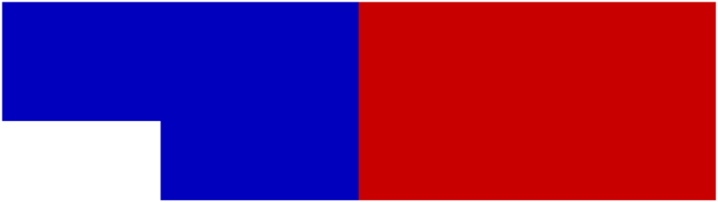
$$u_h^s = Z_s u_N^s, \quad u_h^a = Z_a u_N^a, \quad g_h = Z_c g_N$$

  where $u^s = \{u_1, p_1, u_2, p_2\}$ - state variables,
  $u^a = \{\xi_1, \eta_1, \xi_2, \eta_2\}$ - adjoint variables, g - control
- Reduced optimisation problem: minimise

$$\mathcal{J}_\gamma(u_{1,N}, u_{2,N}; g_N) = \frac{1}{2}\int_{\Gamma_0} \left|u_{1,N} - u_{2,N}\right|^2 d\Gamma + \frac{\gamma}{2}\int_{\Gamma_0} \left|g_N\right|^2 d\Gamma$$

  under the reduced PDE constraints.

CFD. Numerical results



- Left vertical boundary - inlet, parabolic velocity profile BCS
- Right vertical boundary - outlet, free outflow (homogeneous Neumann BCs)
- Lateral boundary - walls, zero velocity field

CFD. Numerical results

Physical parameters	2 : ν, u_{in}
Range ν	[0.5, 2]
Range u_{in}	[0.5, 6.5]

CFD. Numerical results

ν	u_{in}	FOM			ROM		
		Its	Dim	J	Its	Dim	J
2	0.5	25	122	$9 \cdot 10^{-5}$	10	10	$2 \cdot 10^{-4}$
		40	122	$4 \cdot 10^{-5}$	15	15	$1 \cdot 10^{-5}$
2	2.5	25	122	$2 \cdot 10^{-3}$	10	10	$8 \cdot 10^{-3}$
		40	122	$1 \cdot 10^{-3}$	15	15	$7 \cdot 10^{-4}$
1	5	25	122	$3 \cdot 10^{-2}$	10	10	$3 \cdot 10^{-2}$
		40	122	$7 \cdot 10^{-3}$	15	15	$7 \cdot 10^{-3}$
0.75	4.5	25	122	$1 \cdot 10^{-2}$	10	10	$3 \cdot 10^{-2}$
		40	122	$6 \cdot 10^{-3}$	15	15	$2 \cdot 10^{-2}$

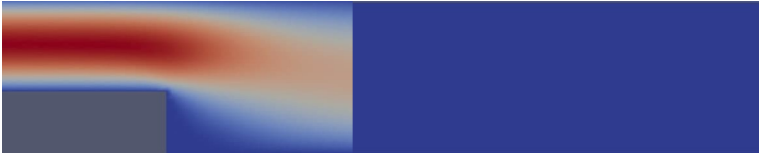
CFD. Numerical results

- Typical example of errors ($\nu = 2,\ u_{in} = 0.5$)

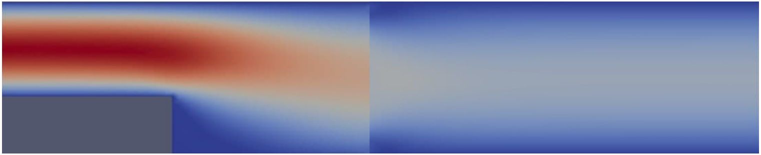
J	$7 \cdot 10^{-5}$
$\|\|\nabla J\|\|$	$4 \cdot 10^{-3}$
u_1 rel. error	1%
p_1 rel. error	1%
u_2 rel. error	2%
p_2 rel. error	3%

CFD. Numerical simulations (FOM)

- Iteration 0

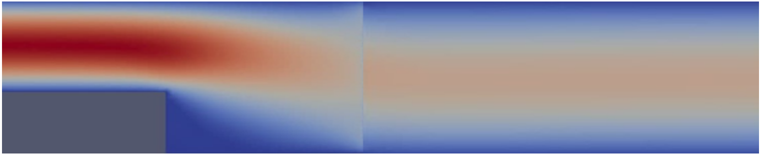


- Iteration 5

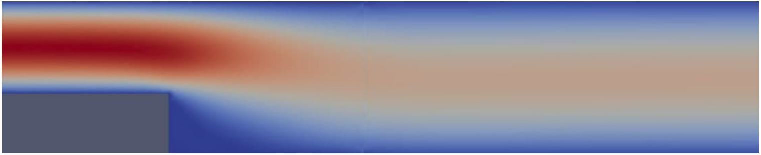


CFD. Numerical simulations (FOM)

- Iteration 25

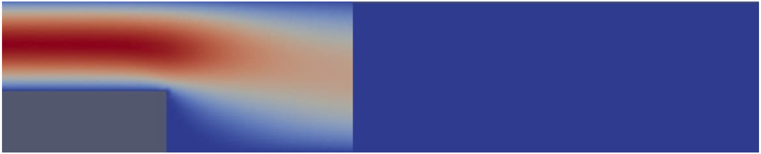


- Iteration 40

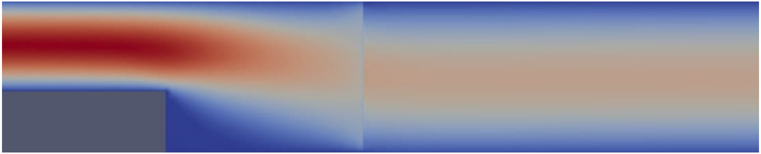


CFD. Numerical simulations (ROM)

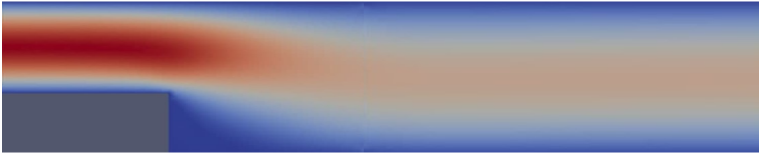
- Iteration 0



- Iteration 5



- Iteration 10



Fluid-Structure Interaction problem. Introduction

- Core elements: fluid equations + structure equations + coupling conditions
- Coupling conditions: continuity of the velocities and the stresses on the fluid-structure interface
- Two main approaches: partitioned (segregated) or monolithic
- Partitioned schemes for FSI might be unstable due to so-called "added mass effect"
- Idea: use optimisation-based DD algorithm to provide a stable partitioned scheme for FSI
- Preliminary work done so far: ROM for monolithic scheme for stationary FSI problem (coupling conditions satisfied by the use of Lagrange multipliers)

Summary

- Optimisation-based Domain Decomposition algortithms for PDS
- Reduced-order models for PDE constraint optimisation problems
- Numerical experiments: Poisson's equation, incompressible Navier-Stokes
- Preliminary steps for the case of fluid-structure interaction problems

Perspectives and future steps

- Optimisation-based DD for nonstationary Navier-Stokes equations, including ROMs
- Fluid-Structure interaction problems: ROMs for nonstationary optimisation-based domain decomposition algortihm