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CENTRE EUROPÉEN DE RECHERCHE ET DE FORMATION AVANCÉE EN CALCUL SCIENTIFIQUE

Resilience enhancement using discrete a priori bounds for the detection of faulty PDE solutions

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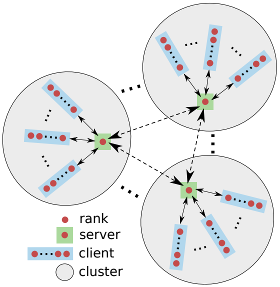
Overview — general ideas of the approach

Context: resilient solving of PDEs for problems in engineering.

- Algorithm based approach.

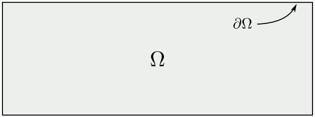
General overview [Sargsyan *et al.*, 2015, SISC]

- Server-client architecture:
  - Clusters of MPI ranks (*e.g.* node).
  - Few servers (protected against faults).
  - Many clients (subject to faults): computing units.
  - Task-based approach: servers send *tasks* to clients.
- Domain decomposition for PDEs:
  - Global domain divided into many small subdomains.
  - Local problems (on subdomains) very cheap to solve.
- Sampling approach:
  - Sample local problems on the clients (unprotected).
  - Robust regression to overcome faulty or missing data.
  - Global reconstruction on the servers (protected).



[Rizzi *et al.*, 2015]

Second-order elliptic PDE: $\begin{cases} \mathcal{L}u = f & \text{in } \Omega \\ u = g & \text{on } \partial\Omega \quad \text{(Dirichlet BCs)} \end{cases}$



Overview — overlapping subdomains

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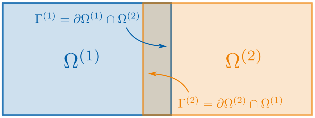

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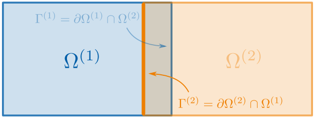

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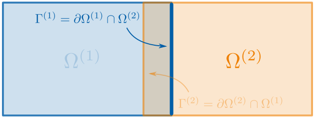

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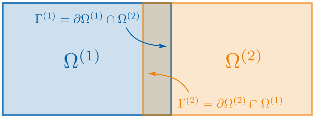

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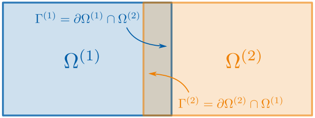

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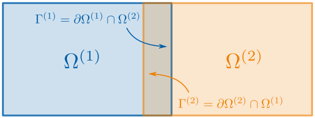

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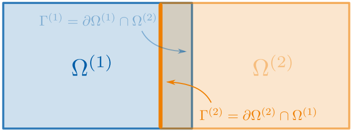
$$\Rightarrow \boxed{\boldsymbol{\mathcal{F}}(\mathbf{u}_\Gamma) = \mathbf{u}_\Gamma} \quad \text{(for linear } \mathcal{L}\text{, } \mathbf{M}\mathbf{u}_\Gamma = \mathbf{c}\text{)}$$

Focusing on $\Omega^{(1)}$:



Sampling approach:

$$\underbrace{\left\{ u_i^{(1)}\Big|_{\Gamma^{(1)}} \right\}_{i=1,\dots,M}}_{\text{inputs: } \mathbf{x}} \stackrel{\text{PDE}}{\longmapsto} \underbrace{\left\{ u_i^{(1)}\Big|_{\Gamma^{(2)}} \right\}_{i=1,\dots,M}}_{\text{obs.: } \mathbf{y}}$$

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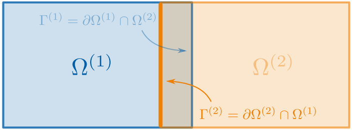

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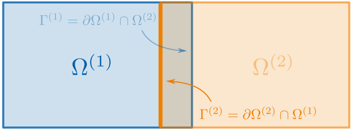

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Minimization problem: $\hat{\mathcal{F}}^{(1)} = \arg\min_{\tilde{\mathcal{F}}^{(1)}} \left\| \mathbf{y} - \tilde{\mathcal{F}}^{(1)}(\mathbf{x}) \right\|$, for some norm $\| \cdot \|$.

Outline

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Problem description:

we want to solve the following (1d) problem

$$\begin{cases} \mathcal{L}u = g, & \text{in } \Omega = (0,1) \\ u(0) = u^-, \\ u(1) = u^+, \end{cases}$$

where $\mathcal{L}$ is a **linear**, elliptic operator.

Affine mapping

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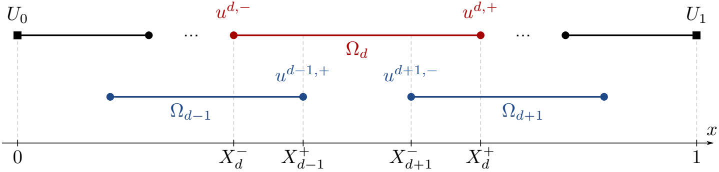
The solution at point x_0 is an **affine function** of the boundary conditions:

$$u(x_0) = f(u^-, u^+) = a + bu^- + cu^+.$$

Domain decomposition overview



■ Known boundary value ● Unknown boundary value

× Subdomain solution at inner point of interest

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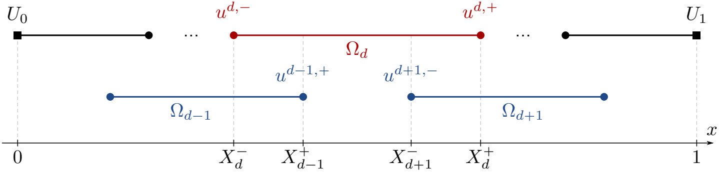

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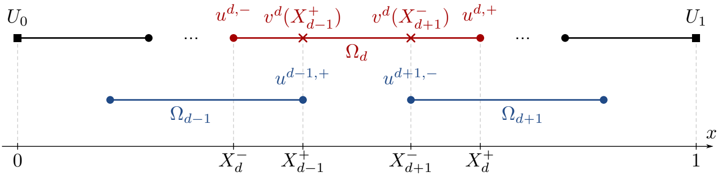
The **subproblem** is solved on each subdomain:

$$\begin{cases} \mathcal{L} v^d = g, & \text{in } \Omega_d = (X_d^-, X_d^+) \\ v^d(X_d^-) = u^{d,-}, \\ v^d(X_d^+) = u^{d,+}, \end{cases}$$



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Enforcing **compatibility conditions** ensures that v^d agrees with u:

$$\begin{cases} v^d(X^+_{d-1}) = u^{d-1,+}, \\ v^d(X^-_{d+1}) = u^{d+1,-}. \end{cases}$$

Using the affine maps yields a linear system

The compatibility conditions read:

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$$v^d(X_{d-1}^+) = f^{d,-}(u^{d,-}, u^{d,+}) = a^{d,-} + b^{d,-}u^{d,-} + c^{d,-}u^{d,+}$$
$$v^d(X_{d+1}^-) = f^{d,+}(u^{d,-}, u^{d,+}) = a^{d,+} + b^{d,+}u^{d,-} + c^{d,+}u^{d,+}$$

Using these maps, the compatibility conditions become:

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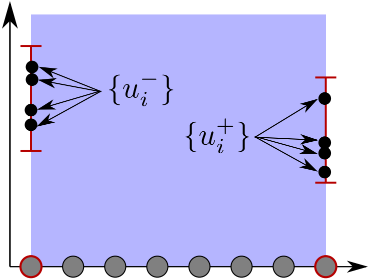
$$f(u^-, u^+) = a + bu^- + cu^+,$$

Sampling approach:

- Sample the BCs $\Rightarrow (u_i^-, u_i^+)$



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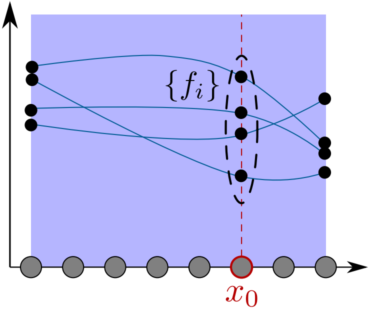

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- Distance between the **observed** and **modeled** map values:

$$r_i = f_i - \left(a + bu_i^- + cu_i^+\right).$$

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- Minimize this distance in some sense $\Rightarrow$ **regression**.

Using (robust) regression to achieve resilience

The regression problem amounts to minimizing the residuals:

$$\mathbf{r} = \mathbf{y} - \mathbf{X}\boldsymbol{\beta}, \quad \text{with } \boldsymbol{\beta} = (a, b, c)\,.$$

- **Goal**: determine a, b and c from limited number of observations y_i.
- Each y_i may be corrupted by a bit-flip (with small probability):

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- *Least squares* (LS) regression is not adapted:

$$J(\boldsymbol{\beta}) = \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 = \sum (y_i - \mathbf{X}_{i\cdot}\boldsymbol{\beta})^2\,.$$

- Solve *least absolute deviations* (LAD) regression instead:

$$J(\boldsymbol{\beta}) = \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_1 = \sum |y_i - \mathbf{X}_{i\cdot}\boldsymbol{\beta}|\,.$$

Least squares (LS) vs. Least absolute deviations (LAD):

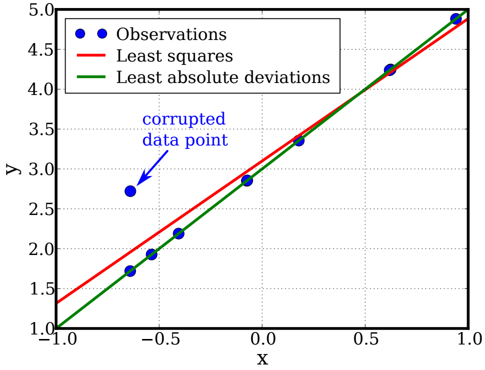

Figure: Regression with single corrupted point

ℓ_0-"norm" of a vector = number of non-zero entries.

Partial conclusion

Algorithm overview:

1. Resilient map construction (on each subdomain):
   - Sample boundary conditions.
   - Solve PDE for each sample.
   - Build the left and right maps using resilient regression.
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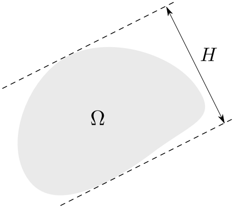
References:

- Validated in 1D [Sargsyan, 2015].
- Validated in 2D with scalability measurements [Rizzi, 2015].
  - On **110,000 cores** with a **90%** parallel efficiency;
  - Small overhead caused by faults.

Continuous a priori bounds

Theorem (see, *e.g.* [Gilbarg & Trudinger])



- *Let* $\Omega \subset \mathbb{R}^D$ *be an open bounded domain with boundary* $\partial\Omega$ *and closure* $\bar{\Omega}$.
- *Assume that* Ω *lies between two parallel planes separated by a distance* H.
- *Let* $\mathcal{L}$ *be a second-order, elliptic operator of the form:*

$$\mathcal{L}u = a^{ij}_{\mathcal{L}}(\mathbf{x})\frac{\partial^2 u}{\partial x^i \partial x^j} + b^i_{\mathcal{L}}(\mathbf{x})\frac{\partial u}{\partial x^i} + c_{\mathcal{L}}(\mathbf{x})u, \quad c_{\mathcal{L}} \leqslant 0, \quad \forall u \in C^0(\bar{\Omega}) \cap C^2(\Omega).$$

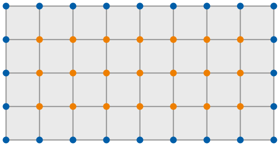
- *Let* $u \in C^0(\bar{\Omega}) \cap C^2(\Omega)$ *be such that* $\mathcal{L}u = f$ *in* Ω.
- ***Then***:

$$\sup_{\Omega}|u| \leqslant \sup_{\partial\Omega}|u| + C\sup_{\Omega}\frac{|f|}{\lambda}, \quad C \equiv e^{\gamma H} - 1, \quad \gamma \equiv 1 + \sup_{\Omega}\frac{\|\mathbf{b}_{\mathcal{L}}\|}{\lambda},$$

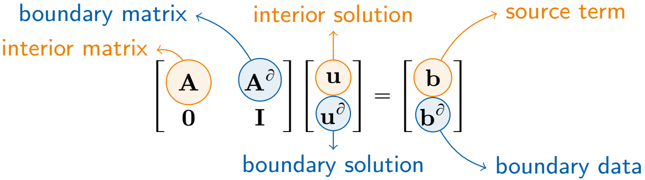
where $\lambda(\mathbf{x})$ *is the minumum eigenvalue of the matrix* $[a^{ij}_{\mathcal{L}}(\mathbf{x})]$.

Grid definition ($\mathbf{x}_k \equiv (x_k^1, \ldots, x_k^D) \in \mathbb{R}^D$):

- $\bar{\Omega}_h \equiv \{\mathbf{x}_k\}_{k=1}^{n_\mathrm{t}}, \quad n_\mathrm{t} \equiv n_\mathrm{i} + n_\mathrm{b};$
- $\Omega_h \equiv \{\mathbf{x}_k\}_{k=1}^{n_\mathrm{i}}$: interior points;
- $\partial\Omega_h \equiv \{\mathbf{x}_{n_\mathrm{i}+k}\}_{k=1}^{n_\mathrm{b}}$: boundary points.



Discrete elliptic Dirichlet problem of the augmented form $\bar{\mathbf{A}}\bar{\mathbf{u}} = \bar{\mathbf{b}}$:

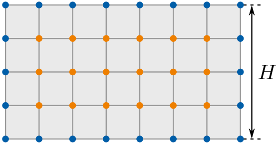


$$\begin{bmatrix} \mathbf{A} & \mathbf{A}^\partial \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{u}^\partial \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{b}^\partial \end{bmatrix}$$

with the conditions (sufficient to ensure the *discrete maximum principle* [Ciarlet, 1970]):

- $\bar{\mathbf{A}}$ is monotone, *i.e.* $\bar{\mathbf{A}}^{-1} \geqslant 0$;
- The row sums of $\bar{\mathbf{L}} \equiv \begin{bmatrix} \mathbf{A} & \mathbf{A}^\partial \end{bmatrix}$ are all zero: $\sum_{j=1}^{n_\mathrm{t}} \bar{l}_{ij} = 0 \quad \forall i = 1, \ldots, n_\mathrm{i}$.

Theorem

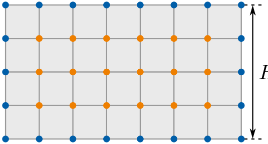


- *Let Ω_h lie between two parallel planes (say, $\perp \mathbf{e}^{\hat{d}}$) separated by a distance H.*
- *Let $\bar{\mathbf{u}} \in \mathbb{R}^{n_\mathrm{t}}$ be such that $\bar{\mathbf{L}}\bar{\mathbf{u}} = \mathbf{b}$, with $\mathbf{b} \in \mathbb{R}^{n_\mathrm{i}}$ and $\bar{\mathbf{L}}$ as defined previously.*
- *Let $\bar{\mathbf{w}} \equiv (w_1, \ldots, w_{n_\mathrm{t}}) \colon \mathbb{R} \to \mathbb{R}^{n_\mathrm{t}}$ be defined by $w_k(\alpha) = \exp(\alpha x_k^{\hat{d}})$, $\forall \alpha \in \mathbb{R}$.*
- *Assume there exists $\alpha \geqslant 0$ and $\boldsymbol{\lambda} > \mathbf{0} \in \mathbb{R}^{n_\mathrm{i}}$ such that $\bar{\mathbf{L}}\bar{\mathbf{w}}(\alpha) \geqslant \boldsymbol{\lambda}$.*
- ***Then**:*

$$\begin{cases} \min\limits_{1\leqslant k\leqslant n_\mathrm{i}} u_k \geqslant \min\limits_{1\leqslant k\leqslant n_\mathrm{b}} u_{n_\mathrm{i}+k} - C \max\limits_{1\leqslant k\leqslant n_\mathrm{i}} (|b_k^+|/\lambda_k), \\ \max\limits_{1\leqslant k\leqslant n_\mathrm{i}} u_k \leqslant \max\limits_{1\leqslant k\leqslant n_\mathrm{b}} u_{n_\mathrm{i}+k} + C \max\limits_{1\leqslant k\leqslant n_\mathrm{i}} (|b_k^-|/\lambda_k), \end{cases} \qquad C \equiv e^{\alpha H} - 1.$$

Notation: for any scalar $a \in \mathbb{R}$, $a^- \equiv \min\{0, a\}$ and $a^+ \equiv \max\{0, a\}$.

Theorem



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Diffusion equation with variable diffusion coefficient κ (assumed differentiable):

$$\mathcal{L}u \equiv \nabla \cdot [\kappa \nabla u] = \sum_{d=1}^{D} \mathcal{L}^d u.$$

Second-order finite difference (FD) operator defined by:

$$(\bar{\mathbf{L}}\bar{\mathbf{u}})_k \equiv \sum_{d=1}^{D} \left[\kappa_{k-}^{d}\, u_{k-}^{d} - 2\tilde{\kappa}_k^d\, u_k + \kappa_{k+}^{d}\, u_{k+}^{d}\right] / \left[h^d\right]^2 .$$

In the $\hat{d}$-th direction:

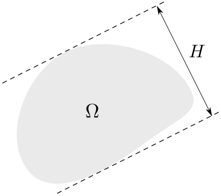
$$\alpha = \frac{1}{h} \log \left[\frac{h\sqrt{h^2 + \beta^2 + 4} + h^2 + 2}{2 - \beta h} \right] \implies [\bar{\mathbf{L}}\bar{\mathbf{w}}(\alpha)]_k \geqslant \tilde{\kappa}_k^{\hat{d}} \quad \forall k = 1, \ldots, n_{\mathrm{i}},$$

where $\beta \equiv \max_{1 \leqslant k \leqslant n_{\mathrm{i}}} \left(\left| \tilde{\nabla}_k^{\hat{d}} \kappa \right| \Big/ \tilde{\kappa}_k^{\hat{d}} \right)$ and $h \equiv h^{\hat{d}}$.

[**Reminder**: $C = e^{\alpha H} - 1$].

Continuous problem:

$$\begin{cases} \boldsymbol{\nabla} \cdot [\kappa(\mathbf{x}) \boldsymbol{\nabla} u(\mathbf{x})] = f(\mathbf{x}), \quad \forall \mathbf{x} \in \Omega, \\ u|_{\partial\Omega} = u_\Gamma. \end{cases}$$



Continuous bounds [Gilbarg & Trudinger]

$$\sup_\Omega |u| \leqslant \sup_{\partial\Omega} |u| + C \sup_\Omega (|f|/\kappa) \quad \text{where } C = e^{\gamma H} - 1.$$

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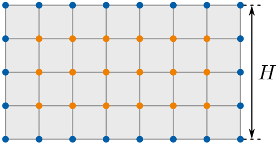


Continuous bounds [Gilbarg & Trudinger]

$$\sup_{\Omega} |u| \leqslant \sup_{\partial\Omega} |u| + C \sup_{\Omega} (|f|/\kappa) \quad \text{where } C = e^{\gamma H} - 1.$$

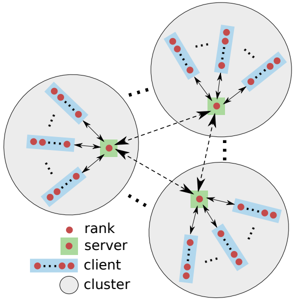
Discrete problem: 2nd-order centered finite differences (conservative form)

$$\mathbf{A}\mathbf{u} = \mathbf{b} - \mathbf{A}^{\partial}\mathbf{u}^{\partial}, \quad \underbrace{\mathbf{u} = (u_1, \ldots, u_{n_\mathrm{i}})}_{\substack{n_\mathrm{i} \text{ unknowns} \\ \text{(interior nodes)}}}, \quad \underbrace{\mathbf{u}^{\partial} = (u_{n_\mathrm{i}+1}, \ldots, u_{n_\mathrm{i}+n_\mathrm{b}})}_{\substack{n_\mathrm{b} \text{ Dirichlet BCs} \\ \text{(boundary nodes)}}},$$

Discrete bounds [Mycek *et al.*, 2017]

$$\begin{cases} \min\limits_{1 \leqslant k \leqslant n_\mathrm{i}} u_k \geqslant \min\limits_{1 \leqslant k \leqslant n_\mathrm{b}} u_{n_\mathrm{i}+k} - C \max\limits_{1 \leqslant k \leqslant n_\mathrm{i}} (|b_k^+|/\tilde{\kappa}_k) \\ \max\limits_{1 \leqslant k \leqslant n_\mathrm{i}} u_k \leqslant \max\limits_{1 \leqslant k \leqslant n_\mathrm{b}} u_{n_\mathrm{i}+k} + C \max\limits_{1 \leqslant k \leqslant n_\mathrm{i}} (|b_k^-|/\tilde{\kappa}_k) \end{cases} \quad \text{where } C = e^{\alpha H} - 1.$$

Server-client-based implementation



- Cluster: 1 server + n clients.
- Servers:

  Communicate between each other.
  Safe data/state storage (sandboxed).
- Clients:

  One or several MPI ranks (●).
  Independent from one another.
  Only serve as computing units.
  No assumption on their reliability.

- Separates state from computation: reduces the overall vulnerability.
- Fault-tolerance supported via ULFM-MPI: support for crashing MPI processes.
- Resilient to clients crashing: even if tasks are lost, state is safe.
- Aligns with the vision of exascale architectures: heterogeneous/hierarchical hardware.

$\Rightarrow$ Resilience to hard faults (SC + ULFM-MPI) and soft faults (ℓ_1-min. + bounds)

Server-client sampling mechanism

foreach *subdomain* Ω_i **do**

// [SERVER] Pre-processing stage
Compute the invariant parts of the bounds for Ω_i ;

// [SERVER] Sample boundary conditions
Sample s_i^* boundary conditions for Ω_i ;
$s_i \leftarrow s_i^*$;

foreach *sample* **do**

// [SERVER]
Add contribution of the boundary conditions to the bounds ;
Send task to a client ;

// [CLIENT]
Receive task from server ;
Solve the local PDE in Ω_i using the received sample of boundary conditions ;
Send task (with the solution) back to server ; /* Corruption may occur */

// [SERVER]
Receive returning task from client ; /* Task is potentially corrupted */
if *received solution does not lie between the bounds* then
Discard current sample ;
$s_i \leftarrow s_i - 1$;

Server-client sampling mechanism

foreach *subdomain* Ω_i **do**

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// [SERVER] Pre-processing stage
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// [CLIENT]
```

Receive task from server ;

Solve the local PDE in Ω_i using the received sample of boundary conditions ;

Send task (with the solution) back to server ; `/* Corruption may occur */`

```
// [SERVER]
```

Receive returning task from client ; `/* Task is potentially corrupted */`

if *received solution does not lie between the bounds* **then**

Discard current sample ;

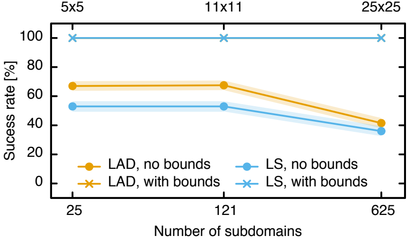
$s_i \leftarrow s_i - 1$;

Application to our (2d) solver

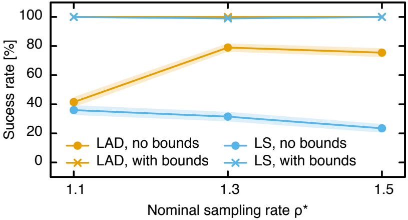
Problem:

$$\begin{cases} \nabla \cdot [\kappa(\mathbf{x}) \nabla u(\mathbf{x})] = f(\mathbf{x}), & \forall \mathbf{x} \in \Omega = (0,1)^2, \\ u|_{\partial\Omega} = 1. \end{cases} \quad \text{with} \quad \begin{cases} \kappa(\mathbf{x}) = 1, \\ f(\mathbf{x}) = \tanh[d(\mathbf{x})/0.05] \end{cases}$$

Resilience enhancement:



$\rho^* = 1.1$



$625 = 25 \times 25$ subdomains

Summary:

- Resilient algorithm for elliptic PDEs.
- Sampling approach + robust (resilient) minimization.
- Discrete a priori bounds to enhance overall resilience.

Outlook:

- Higher-order FD schemes $\rightarrow$ new expression for α.
- Other elliptic problems: tensor diffusion, reaction-diffusion, ...
- Non-uniform meshes (refinement).
- Apply to stochastic elliptic PDEs.
- Neumann boundary conditions?

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Thank you for your attention.