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Adaptive Trust Region Reduced Basis Methods for Parameter Identification Problems

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Outline

1 The parameter identification problem

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Identify $q^{\mathrm{e}} \in \mathscr{Q}_{\mathrm{ad}} \subset \mathscr{Q}$ from

$$\mathcal{F}(q^{\mathrm{e}}) = y^{\mathrm{e}}, \qquad \textbf{(IP)}$$

where instead of the exact data y^{e} only noisy data $y^{\delta} \in \mathscr{H}$ is given with

$$\|y^{\mathrm{e}} - y^{\delta}\|_{\mathscr{H}} \leq \delta.$$

Forward operator $\mathcal{F} = \mathcal{C} \circ \mathcal{S}$

1. solution map $\mathcal{S} : \mathscr{Q}_{\mathrm{ad}} \to V$ with $\mathcal{S}(q) = u(q)$ and

$$a(u(q), v; q) = \ell(v) \quad \forall v \in V$$

2. observation map $\mathcal{C} : V \to \mathscr{H}$

$$y = \mathcal{C}u$$

- $\mathscr{Q}$ parameter space
- $\mathscr{Q}_{\mathrm{ad}} \subset \mathscr{Q}$ admissible parameters
- $\mathscr{H}$ observation space
- V state space

Goal: construct certified reduced forward operator $\mathcal{F}_r$.

1 The parameter identification problem - Assumptions

$$\mathcal{F}(q^{\mathrm{e}}) = y^{\mathrm{e}}, \quad \|y^{\mathrm{e}} - y^{\delta}\|_{\mathscr{H}} \leq \delta \tag{IP}$$

Assumptions

(i) Let $\mathscr{Q}, V, \mathscr{H}$ be real Hilbert spaces and $\mathscr{Q}_{\mathrm{ad}} \subset \mathscr{Q}$ be closed and convex.

(ii) For $q \in \mathscr{Q}_{\mathrm{ad}}$, $a(\cdot\,,\cdot\,;q)$ is a coercive and continuous, bilinear form and for $u, v \in V$ the map $q \mapsto a(u,v;q)$ is linear and $l \in V'$.

(iii) The solution map $\mathcal{S} : \mathscr{Q}_{\mathrm{ad}} \to V$ is non-linear and the observation map $\mathcal{C} : V \to \mathscr{H}$ is linear and bounded.

(iv) We assume $y^{\mathrm{e}} \in \mathrm{range}(\mathcal{F})$, $q^{\mathrm{e}} \in \mathring{\mathscr{Q}}_{\mathrm{ad}}$ and $\mathcal{F} : \mathscr{Q}_{\mathrm{ad}} \to \mathscr{H}$ to be injective, continuously Fréchet-differentiable and that (**IP**) is ill-posed in the sense that $\mathcal{F}$ is not continuously invertible.

- Simple inversion fails since $\mathcal{F}^{-1}(y^{\delta}) \not\to \mathcal{F}^{-1}(y^{\mathrm{e}}) = q^{\mathrm{e}}$ as $\delta \to 0$

$\Longrightarrow$ iterative regularization methods e.g. [Kaltenbacher, Neubauer, Scherzer 2008]

1 The parameter identification problem - Examples

$$\mathcal{F}(q^{\mathrm{e}}) = y^{\mathrm{e}}, \quad \|y^{\mathrm{e}} - y^{\delta}\|_{\mathscr{H}} \leq \delta \tag{IP}$$

Examples

Let Ω be a convex, bounded domain, $\mathscr{H} = L^2(\Omega)$, $V = H_0^1(\Omega)$, $\mathcal{C} = id_{V,\mathscr{H}}$, $f \in L^2(\Omega)$ and for $q_{\mathrm{a}} \in L^\infty(\Omega)$

$$\mathscr{Q}_{\mathrm{ad}} := \left\{ q \in \mathscr{Q} \,\middle|\, 0 < q_{\mathrm{a}} \leq q \text{ in } \Omega \text{ a.e.} \right\}.$$

1. Reconstruction of the reaction coefficient $\mathscr{Q} = L^2(\Omega)$:
$$-\Delta u + qu = f \quad \text{in } H^{-1}(\Omega),$$
2. Reconstruction of the diffusion coefficient $\mathscr{Q} = H^2(\Omega)$:
$$-\nabla \cdot \left(q \nabla u\right) = f \quad \text{in } H^{-1}(\Omega).$$

Goal: fast and stable reconstruction of q^{e} from (**IP**) by regularization methods.

Iteratively regularized Gauß-Newton method (IRGNM)

- the discrepancy: $\hat{J}(q) = \frac{1}{2}\|\mathcal{F}(q) - y^\delta\|^2_{\mathscr{H}}$.

Alg. 1: FOM IRGNM [Kaltenbacher, Kirchner, Veljovic 2014]

1. Iterative linearization of (**IP**) and Tikhonov regularization:

$$q(\alpha_k) = \arg\min_{q \in \mathscr{Q}} \frac{1}{2}\|\mathcal{F}(q^k) + \mathcal{F}'(q^k)(q - q^k) - y^\delta\|^2_{\mathscr{H}} + \frac{\alpha_k}{2}\|q - q_\circ\|^2_{\mathscr{Q}}, \qquad (\mathbf{IP}^k_\alpha)$$

2. Choice of regularization parameter: accept $q^{k+1} := q(\alpha_k)$ if

$$\theta \hat{J}(q^k) \leq \|\mathcal{F}'(q^k)(q(\alpha_k) - q^k) + \mathcal{F}(q^k) - y^\delta\|^2_{\mathscr{H}} \leq \Theta \hat{J}(q^k),$$

3. Early stopping according to the discrepancy principle: for $\tau > 1$

$$\|\mathcal{F}(q^k) - y^\delta\|_{\mathscr{H}} \leq \tau\delta \leq \|\mathcal{F}(q^{k-1}) - y^\delta\|_{\mathscr{H}}, \qquad k = 0, \dots, k_*(\delta, y^\delta).$$

- Local convergence: $k_*(\delta, y^\delta)$ is finite and $q^{k_*(\delta, y^\delta)} \to q^{\mathsf{e}}$ as $\delta \to 0$.

$\Rightarrow$ FOM IRGNM is a many-query context for the forward operator $\mathcal{F}$.

2 Adaptive reduced basis approximation

The reduced basis (RB) method - Challenges

- Discretization: $\mathscr{Q}_h = \text{span}\{\phi_1, \dots, \phi_{N_\mathscr{Q}}\}$, $q = \sum_{i=1}^{N_\mathscr{Q}} \mathrm{q}_i \phi_i \in \mathscr{Q}_h$ and

$$a(u, v; q) = \sum_{i=1}^{N_\mathscr{Q}} \mathrm{q}_i \, a(u, v; \phi_i) \quad \text{for all } u, v \in V.$$

1. Greedy RB state space reduction [Hesthaven et al. 2016,...]

- offline/online phase
- construct global RB V_r
- restricted to bounded, low-dim. $\mathscr{Q}_h$ ($N_\mathscr{Q} \leq 100$)

2. Adaptive RB state space reduction [Garmatter et al. 2016]

- construct local RB V_r along the optimization path
- online enrichment
- can handle larger $\mathscr{Q}_h$ ($N_\mathscr{Q} \approx 900$)

3. Adaptive parameter- and state space reduction

- Step 1: reduce affine components ($\mathscr{Q}_h \to \mathscr{Q}_r$).
- Step 2: reduce the state space ($V_h \to V_r$)

But here the parameter space dimension $N_\mathscr{Q}$ can be arbitrary large.

(i) No projection: An arbitrary number $N_\mathscr{Q}$ of affine components needs to be projected onto the reduced state space V_r.

(ii) No certification: The assembly of residual-based error estimates is infeasible because it involves the computation of about $\mathcal{O}(N_\mathscr{Q})$ Riesz representatives.

Step 1: Reduction of the parameter space

- $\mathscr{Q}_r = \text{span}\{\phi_1, \ldots, \phi_{n_\mathscr{Q}}\} \subset \mathscr{Q}$ with dimension $n_\mathscr{Q} \ll N_\mathscr{Q}$, $q = \sum_{i=1}^{n_\mathscr{Q}} \mathsf{q}_i \phi_i \in \mathscr{Q}_r$

$$a(u, v; q) = \sum_{i=1}^{n_\mathscr{Q}} \mathsf{q}_i a_i(u, v; \phi_i) \quad \text{for all } u, v \in V.$$

How to choose the snapshots ϕ_i?

Suppose $\bar{q} \in \mathscr{Q}_{\text{ad}}$ is an unconstrained local minimizer of the regularized discrepancy

$$\hat{J}_\alpha(q) = \hat{J}(q) + \frac{\alpha}{2} \|q - q_\circ\|^2_\mathscr{Q}, \qquad q, q_\circ \in \mathscr{Q}_{\text{ad}}, \alpha > 0,$$

then there exist $\bar{u}, \bar{p} \in V$ with

$$\begin{aligned} a(\bar{u}, v; \bar{q}) &= l(v) && \text{for all } v \in V, \\ a(v, \bar{p}; \bar{q}) &= -\langle \mathcal{C}\bar{u} - y^\delta, \mathcal{C}v \rangle_\mathscr{H} && \text{for all } v \in V, \\ \alpha(\bar{q} - q_\circ) + \mathcal{J}_\mathscr{Q}^{-1} \partial_q a(\bar{u}, \bar{p}; \cdot) &= 0, \end{aligned}$$

where $\mathcal{J}_\mathscr{Q} : \mathscr{Q} \to \mathscr{Q}'$ is the Riesz map. In particular, this implies

$$\bar{q} = q_\circ - \frac{1}{\alpha} \mathcal{J}_\mathscr{Q}^{-1} \partial_q a(\bar{u}, \bar{p}; \cdot).$$

$\Rightarrow$ Iterative parameter reduction $\mathscr{Q}_r^k = \text{span}\{q_\circ, q^0, \nabla\hat{J}(q^0), \ldots, \nabla\hat{J}(q^k)\}$.

$\Rightarrow$ Iterative state reduction $V_r^k = \text{span}\{u(q^0), p(q^0), \ldots, u(q^k), p(q^k)\}$.

Step 2: Reduction of the state space

- Given reduced spaces V_r, $\mathscr{Q}_r$ and $q = \sum_{i=1}^{n_{\mathscr{Q}}} \mathsf{q}_i \phi_i \in \mathscr{Q}_r$
- Reduced solution operator: $\mathcal{S}_r : \mathscr{Q}_r \cap \mathscr{Q}_{\mathrm{ad}} \to V_r$, $q \mapsto u_r$ with

$$\sum_{i=1}^{n_{\mathscr{Q}}} \mathsf{q}_i a_i(u_r, v; \phi_i) = \ell(v) \quad \text{for all } v \in V_r \tag{2.2}$$

- Reduced forward operator: $\mathcal{F}_r = \mathcal{C} \circ \mathcal{S}_r$
- Reduced discrepancy: $\hat{J}_r(q) := \frac{1}{2} \|\mathcal{F}_r(q) - y^\delta\|_{\mathscr{H}}^2$

Lemma (A-posteriori error estimate for $\hat{J}$)

Let $q \in \mathscr{Q}_r \cap \mathscr{Q}_{\mathrm{ad}}$ and $\underline{a}_q > 0$ be the coercivity constant for $a(\cdot, \cdot; q)$. Then:

$$|\hat{J}(q) - \hat{J}_r(q)| \leq \Delta_{\hat{J}}(q),$$

with

$$\Delta_{\hat{J}}(q) := \frac{\|\mathcal{C}\|_{\mathscr{L}(V,\mathscr{H})}^2}{2} \Delta_{pr}(q)^2 + \|r_{du}(u_r, p_r; q)\|_{V'} \Delta_{pr}(q),$$

$$\Delta_{pr}(q) := \frac{1}{\underline{a}_q} \|r_{pr}(u_r; q)\|_{V'},$$

where $r_{pr}(u_r; q)$, $r_{du}(u_r, p_r; q) \in V'$ are the primal and dual residual.

Trust Region Reduced Basis IRGNM ($\mathcal{Q}_r$-V_r-IRGNM)

Error-aware trust region framework [Qian et al. 17, Banholzer et al. 22]

1. Use $\hat{J}_r$ as a model function.
2. The trust region is defined by the relative error estimator

$$\mathcal{R}^k_{\hat{J}}(q) := \frac{\Delta_{\hat{J}}(q)}{\hat{J}_r(q)} \leq \eta^{(k)} \quad \text{for } q \in \mathcal{Q}_r^k \cap \mathcal{Q}_{\mathrm{ad}},$$

where $\eta^{(k)} > 0$ is the trust region radius at iteration k.

Alg. 2: Trust Region Reduced Basis IRGNM ($\mathcal{Q}_r$-V_r-IRGNM)

1. Initialize $V_r^0 = \mathrm{span}\{u(q^0), p(q^0)\}$, $\mathcal{Q}_r^0 = \mathrm{span}\{q_\circ, q^0, \nabla \hat{J}(q^0)\}$ by orthonormalization.
2. **while** $\|\mathcal{F}(q^k) - y^\delta\|_{\mathscr{H}} > \tau\delta$**:**
3. Compute AGC point $q^k_{\mathrm{AGC}} = q^k - t_k \nabla \hat{J}_r(q^k)$.
4. Solve reduced subproblem (**IP**$_r^k$) for q_{trial}

$$\min_{q \in \mathcal{Q}_r^k} \hat{J}_r(q) \quad \text{s.t.} \quad \mathcal{R}^k_{\hat{J}}(q) \leq \eta^{(k)}. \qquad (\mathbf{IP}_r^k)$$

5. Acceptance or rejection of q_{trial}?
6. **end while**
7. **Output:** reconstruction q^{k_*}, reduced spaces $\mathcal{Q}_r^{k_*}, V_r^{k_*}$.

$\mathscr{Q}_r$-V_r-IRGNM - Acceptance or rejection?

- sufficient for acceptance:

$$\hat{J}(q_{\text{trial}}) \leq \hat{J}_r(q_{\text{trial}}) + \Delta_{\hat{J}}(q_{\text{trial}}) < \hat{J}_r(q^k_{\text{AGC}}).$$

Accept $q^{k+1} = q_{\text{trial}}$, compute $u(q^{k+1})$, $p(q^{k+1})$ and $\nabla \hat{J}((q^{k+1})$ and enrich the spaces $\mathscr{Q}_r^{k+1}$, V_r^{k+1} by orthonormalization, modify radius $\eta^{(k+1)}$ and set $k = k + 1$.

- sufficient for rejection:

$$\hat{J}_r(q_{\text{trial}}) - \Delta_{\hat{J}}(q_{\text{trial}}) > \hat{J}_r(q^k_{\text{AGC}}).$$

Reject q_{trial} and diminish the radius $\eta^{(k)}$.

Alg. 2: Trust Region Reduced Basis IRGNM ($\mathscr{Q}_r$-V_r-IRGNM)

1. Initialize $V_r^0 = \text{span}\{u(q^0), p(q^0)\}$, $\mathscr{Q}_r^0 = \text{span}\{q_\circ, q^0, \nabla \hat{J}(q^0)\}$ by orthonormalization.
2. **while** $\|\mathcal{F}(q^k) - y^\delta\|_{\mathscr{H}} > \tau\delta$**:**
3. Compute AGC point $q^k_{\text{AGC}} = q^k - t_k \nabla \hat{J}_r(q^k)$.
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6. **end while**
7. **Output:** reconstruction q^{k_*}, reduced spaces $\mathscr{Q}_r^{k_*}, V_r^{k_*}$.

3 Numerical results

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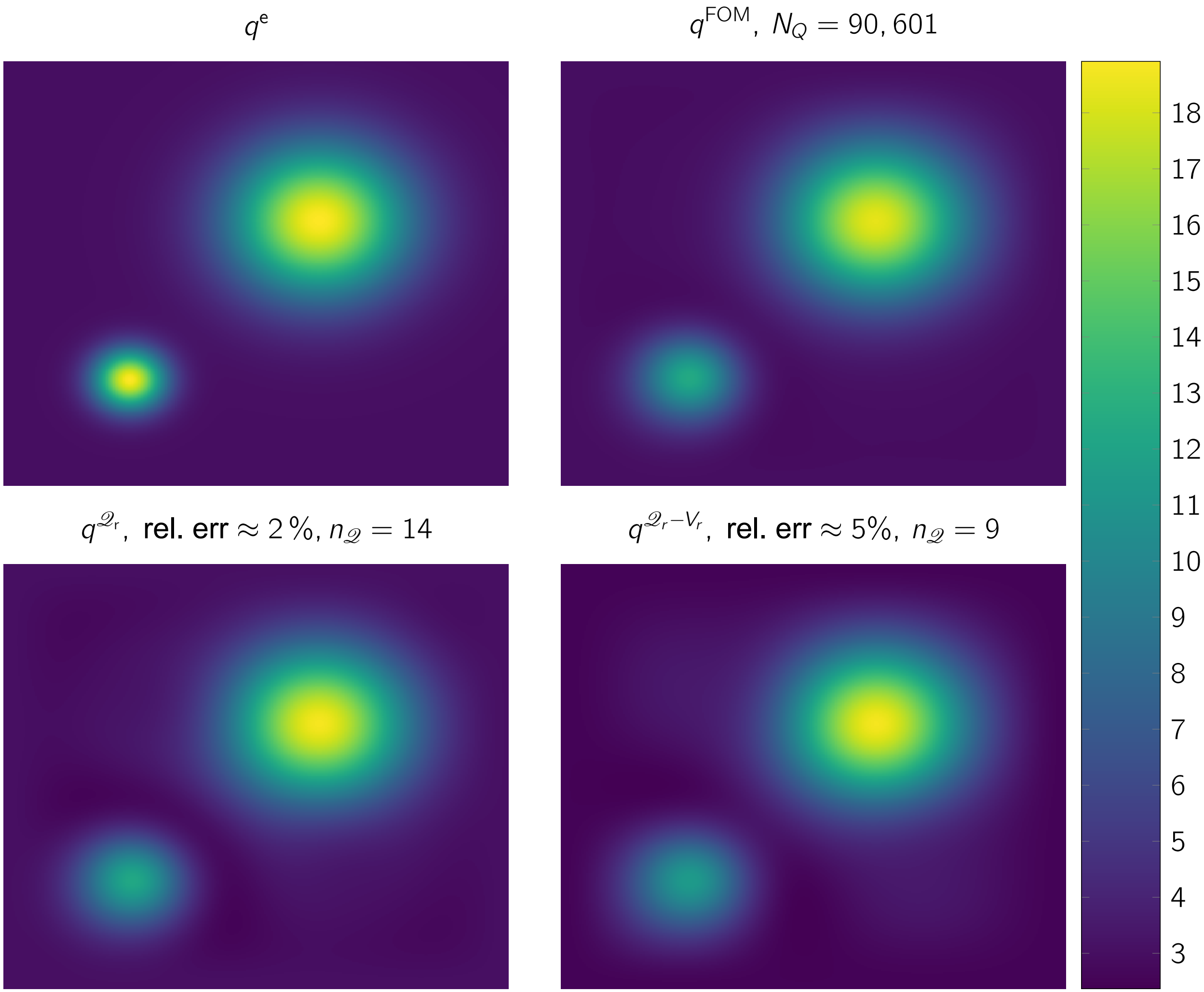
- Comparison of three algorithms:
  1. FOM-IRGNM: full-order model IRGNM (Alg. 1)
  2. $\mathscr{Q}_r$-V_r-IRGNM: parameter and state-reduced Trust Region IRGNM (Alg. 2)
  3. $\mathscr{Q}_r$-IRGNM: parameter-reduced IRGNM

- Problem setup:
  - Reaction ($\mathscr{Q} = L^2(\Omega)$) or diffusion case ($\mathscr{Q} = H^1(\Omega)$)
  - $\mathscr{H} = L^2(\Omega)$, $V = H_0^1(\Omega)$
  - $\Omega = (0, 1)^2$
  - FE discretization using $N_Q = 90,601$ dofs
  - background $q^0 = q_\circ \equiv 3 \in \mathscr{Q}_{\text{ad}}$
  - noise level $\delta = 10^{-5}$

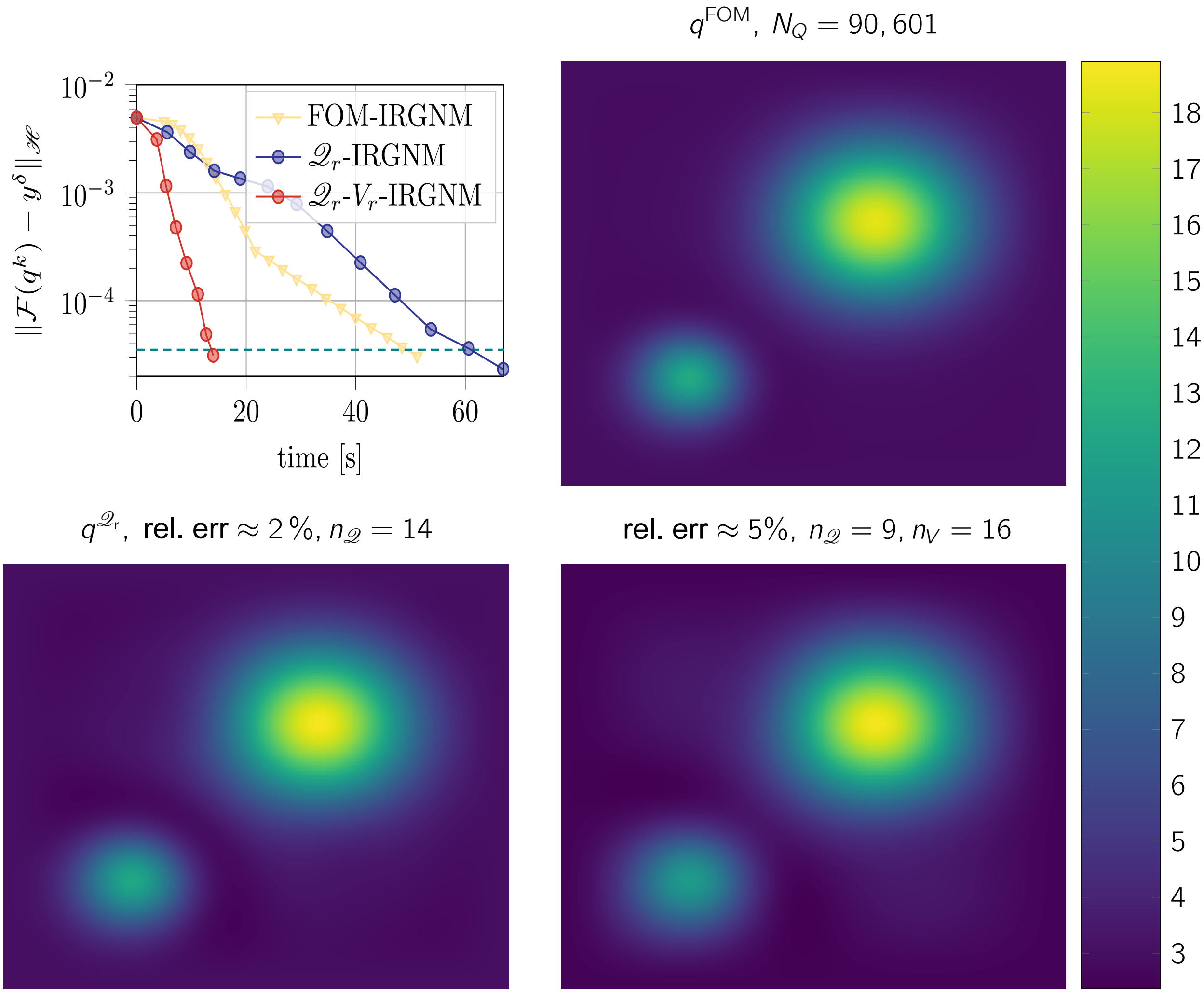
Reaction case

q^{e} from [Kirchner 2014]: $-\Delta u + qu = 1$ in $H^{-1}(\Omega)$



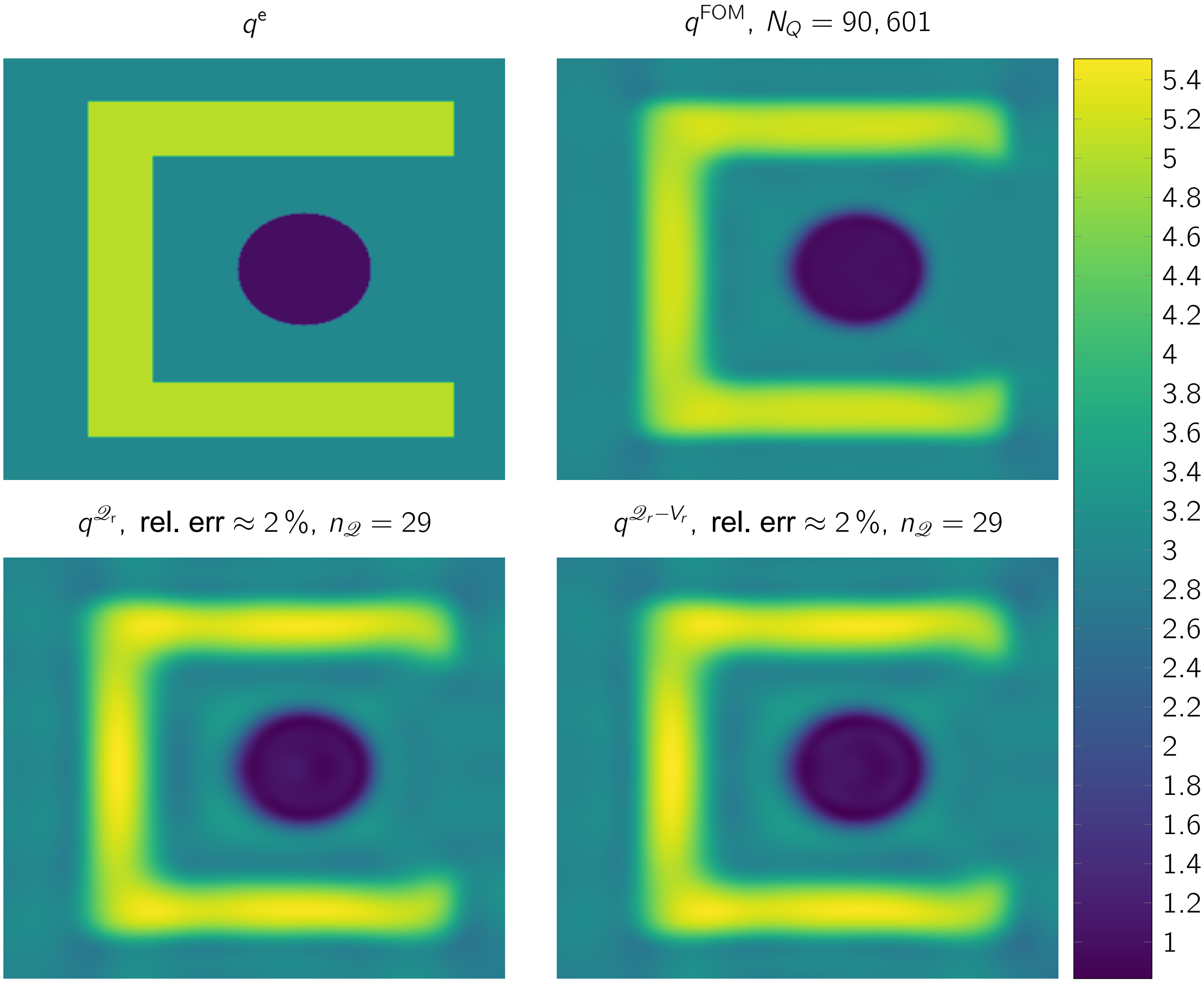
Reaction case

q^{e} from [Kirchner 2014]: $\quad -\Delta u + qu = 1$ in $H^{-1}(\Omega)$



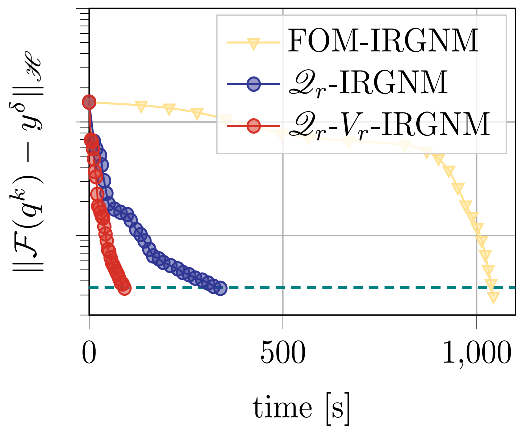
Diffusion case

q^{e} from [Garmatter et al. 16]: $-\nabla \cdot (q \nabla u) = 1$ in $H^{-1}(\Omega)$.

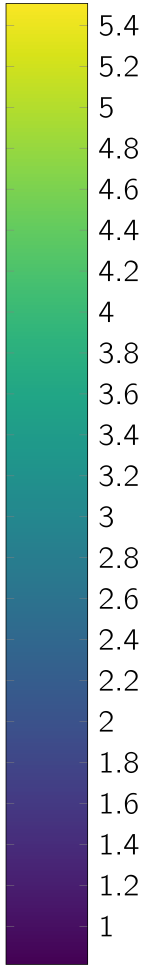


Diffusion case

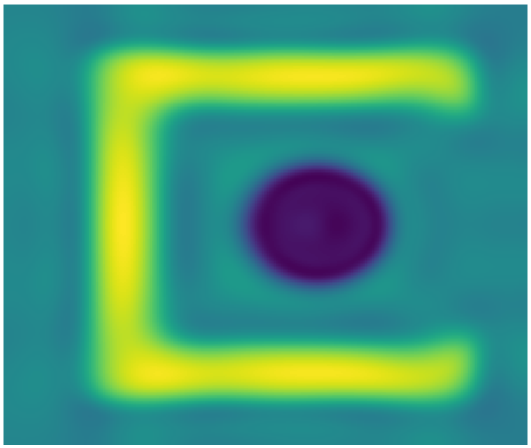
q^e from [Garmatter et al. 16]: $-\nabla \cdot (q \nabla u) = 1$ in $H^{-1}(\Omega)$.



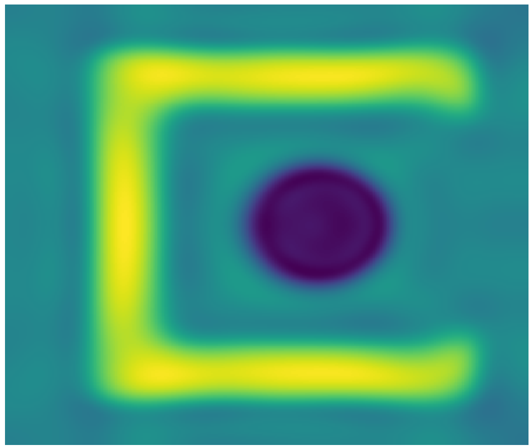
q^{FOM}, $N_Q = 90,601$



$q^{\mathscr{Q}_r}$, rel. err $\approx 2\,\%$, $n_{\mathscr{Q}} = 29$



rel. err $\approx 2\,\%$, $n_{\mathscr{Q}} = 29$, $n_V = 56$



4 Conclusion

- We introduced a new adaptive parameter and state space reduced regularization method based on RB model reduction.

- The enrichment of the reduced parameter space is motivated by the optimality condition of the regularized discrepancy, that transfers the low-rank structure of the (adjoint) state to the optimal parameter.

- The construction of the reduced parameter space allows us to apply the RB method to arbitrary dimension parameter spaces and to obtain fast low-dimensional reconstructions of the unknown parameter.

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