An adaptive energy reduction approach for semilinear diffusion-reaction models

Centre INRIA de Paris
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Motivation

Semilinear elliptic PDE:

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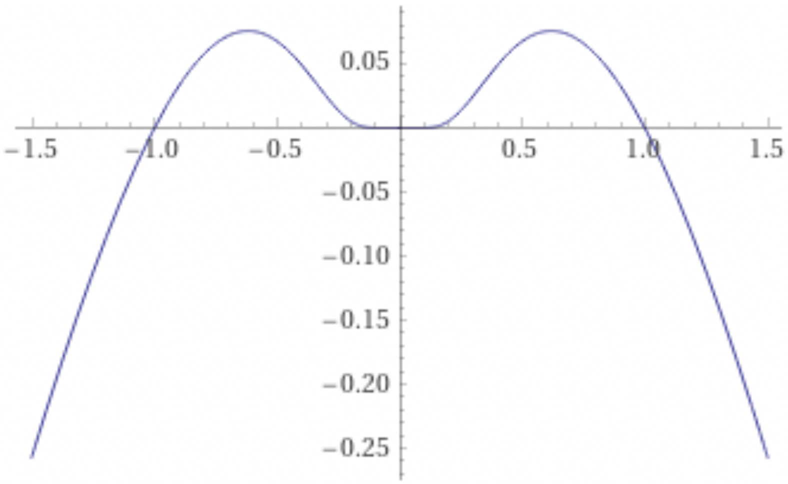
Example: Arrhenius production term

$$f(u) \sim (1 - |u|)\exp(-c|u|^{-1})$$



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Method of sub- and supersolutions[1]

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> Given (weak) sub- and supersolutions $\underline{u} \leq \overline{u}$ in $H^1(\Omega)$:

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for all $v \in H_0^1(\Omega), v \geq 0.$

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for all $v \in H^1_0(\Omega), v \geq 0.$

> Suppose that $\underline{u} \leq 0 \leq \overline{u}$ on $\partial\Omega$

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Method of sub- and supersolutions

Fix $\Delta t > 0$ *small enough* so that $z \mapsto f(z) + (\Delta t)^{-1} z$ is non-decreasing

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$|f'| \leq C$ too rough for sharp estimates on Δt

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New variational framework

Semilinear diffusion-reaction model:

$$u \in H_0^1(\Omega): \qquad -\Delta u + f(\,\cdot\,, u) = 0$$

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Semilinear diffusion-reaction model:

ASSUMPTION (Nonlinearity)

- $f(\,\cdot\,, s) \in L^2(\Omega)$ for all $s \in \mathbb{R}$
- f differentiable in u
- $\exists \rho > 0 : \Lambda_f(\rho) := \{\lambda > 0 : \; \sigma_f(\lambda) < \rho + \lambda^{-1}\} \neq \varnothing$

where

$$\sigma_f(\lambda) := \operatorname*{ess\,sup}_{x\in\Omega} \sup_{u\in\mathbb{R}} \left| \frac{\partial f}{\partial u}(x, u) + \frac{1}{\lambda} \right|$$

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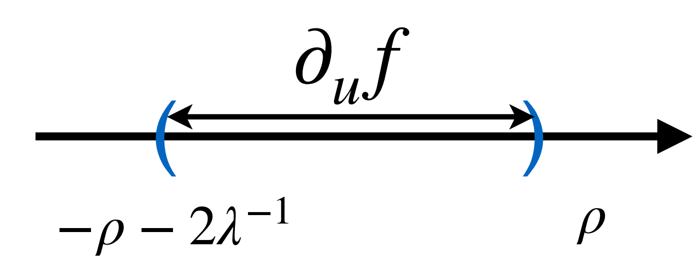

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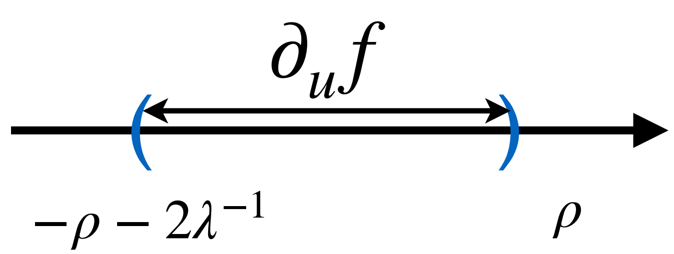

(uniform) Lipschitz constant of $g_\lambda(x,u) := f(x,u) + \lambda^{-1} u$

Define the "undershooting" coefficient: $\mu_f := \begin{cases} 2\left(\sup \Lambda(\rho)\right)^{-1} & \text{if } \sup \Lambda(\rho) < \infty \\ 0 & \text{otherwise} \end{cases}$

Convergence — small ρ

THEOREM (Steady state iteration for $\rho \leq C_P^{-1}$)

Let $\Delta t \in \Lambda_f(\rho)$. Then, for *any* $u_0 \in L^2(\Omega)$ the SSI

$$\begin{aligned} -\Delta u_{k+1} + \frac{1}{\Delta t} u_{k+1} &= f(u_k) + \frac{1}{\Delta t} u_k && \text{in } \Omega \\ u_{k+1} &= 0 && \text{on } \partial\Omega \end{aligned} \qquad (k \geq 0)$$

converges strongly to the unique weak solution $u_\infty \in H_0^1(\Omega)$ of the semilinear PDE.

Proof: Operator $u_k \mapsto u_{k+1}$ is a contraction.

Convergence — general case

Energy: $\mathsf{E}(u) := \frac{1}{2}\int_\Omega |\nabla u|^2 - \int_\Omega \mathfrak{F}(\,\cdot\,, u)$ $\left(\mathfrak{F}(x,t) = \int_0^t f(x,s)\,\mathrm{d}s\right)$

Critical points of E vs. weak solutions:

$$\langle \mathsf{E}'(u), v\rangle := \int_\Omega \{\nabla u \cdot \nabla v - f(\,\cdot\,, u)v\} \overset{!}{=} 0 \qquad \forall v \in H_0^1(\Omega)$$

We are interested in **local minima**:

$$u \in H_0^1(\Omega): \qquad \mathsf{E}(u) = \min_{v \in H_0^1(\Omega)} \mathsf{E}(v)$$

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ENERGY DECAY

Let

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for a constant $\gamma > 0$ (depending on Δt).

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CONVERGENCE OF RESIDUAL

$\{\mathsf{E}(u_k)\}_k$ bounded from below $\Longrightarrow \lim_{k\to\infty} \|\mathsf{E}'(u_k)\|_\star \to 0$.

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Involving Palais-Smale compactness (mountain pass theory[2]):

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CONVERGENCE OF SUBSEQUENCE

- f continuous
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$$u_{k'} \to u_\infty \quad \text{strongly to a weak solution in } H_0^1(\Omega)$$

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✓ Weak convergence and strong L^2-convergence in closed subspaces

✓ Strong H^1-convergence in discrete spaces!

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FEM discretization

Shape-regular partitions:

- $\{\mathcal{T}_N\}_{N\in\mathbb{N}}$ of domain Ω into simplex elements
- Fixed polynomial degree $p \in \mathbb{N}$

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On subsets $\omega \subset \mathcal{T}_N$, introduce the finite element space

$$\mathbb{V}(\omega) = \left\{ v \in H_0^1(\Omega) : \, v|_\kappa \in \mathbb{P}_p(\kappa), \kappa \in \omega, v|_{\Omega\setminus\omega} = 0 \right\}$$

$\mathbb{V}_N := \mathbb{V}(\mathcal{T}_N)$ finite element space based on mesh $\mathcal{T}_N$.

Adaptive mesh refinements – Estimate

For given $u_N^n \in \mathbb{V}_N$ and each element $\kappa \in \mathscr{T}_N$:

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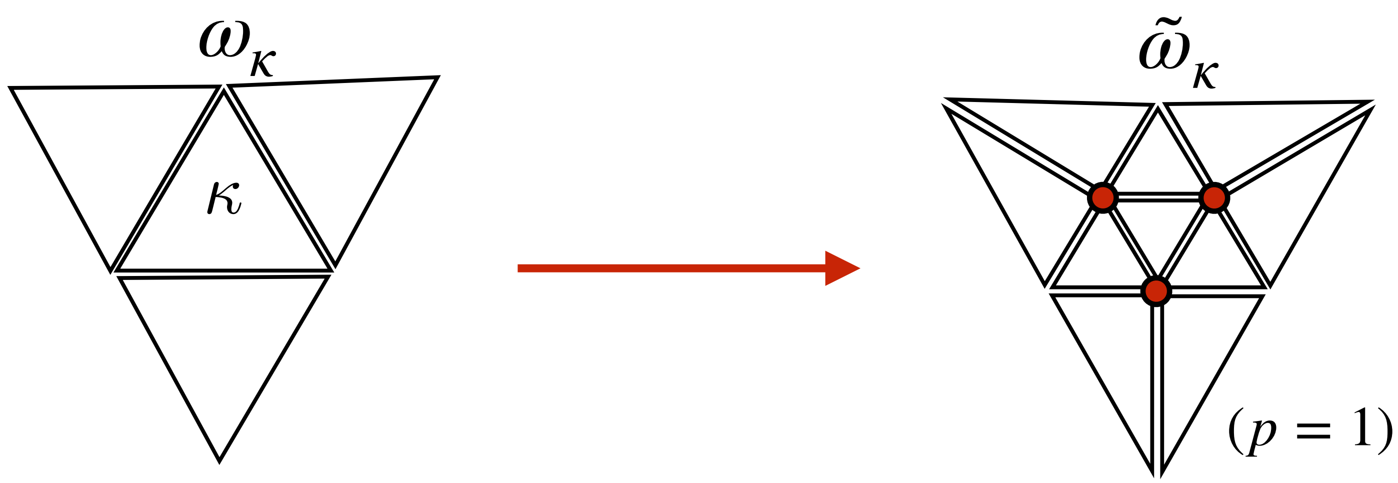
For given $u_N^n \in \mathbb{V}_N$ and each element $\kappa \in \mathscr{T}_N$:

1. Uniformly refine the patch ω_κ around κ:



Introduce new basis functions of locally supported space $\left\{\xi_\kappa^1, \ldots, \xi_\kappa^{m_\kappa}\right\} \in \mathbb{V}(\tilde{\omega}_\kappa)$

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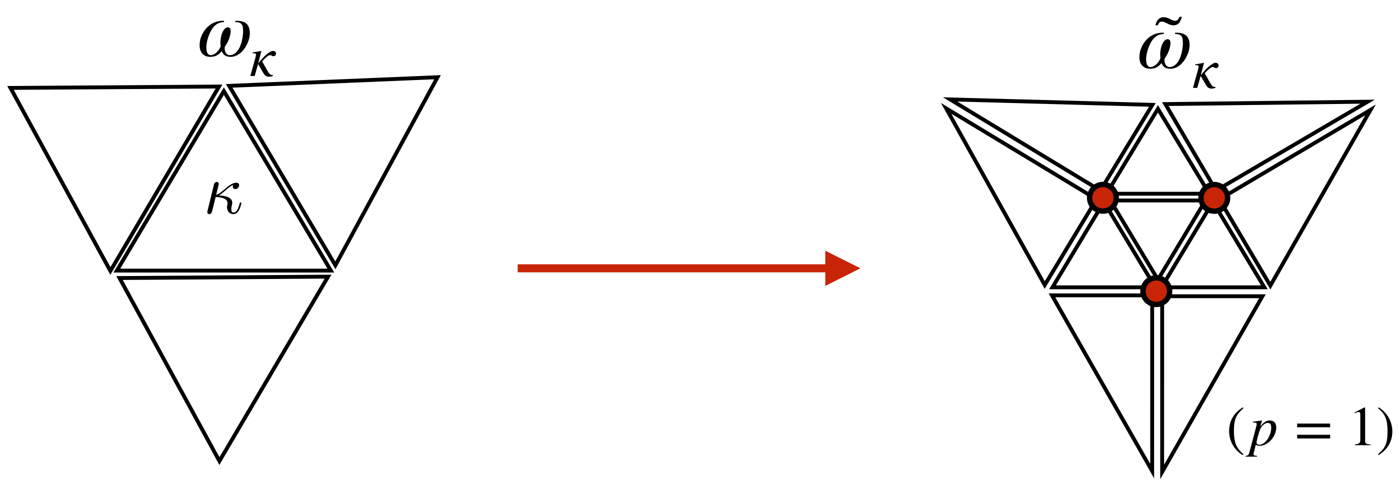

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2. Extended space:

$$\mathbb{V}(\tilde{\omega}_\kappa; u_N^n) := \text{span}\{\xi_\kappa^1, \ldots, \xi_\kappa^{m_\kappa}, u_N^n\}$$

global support

local support

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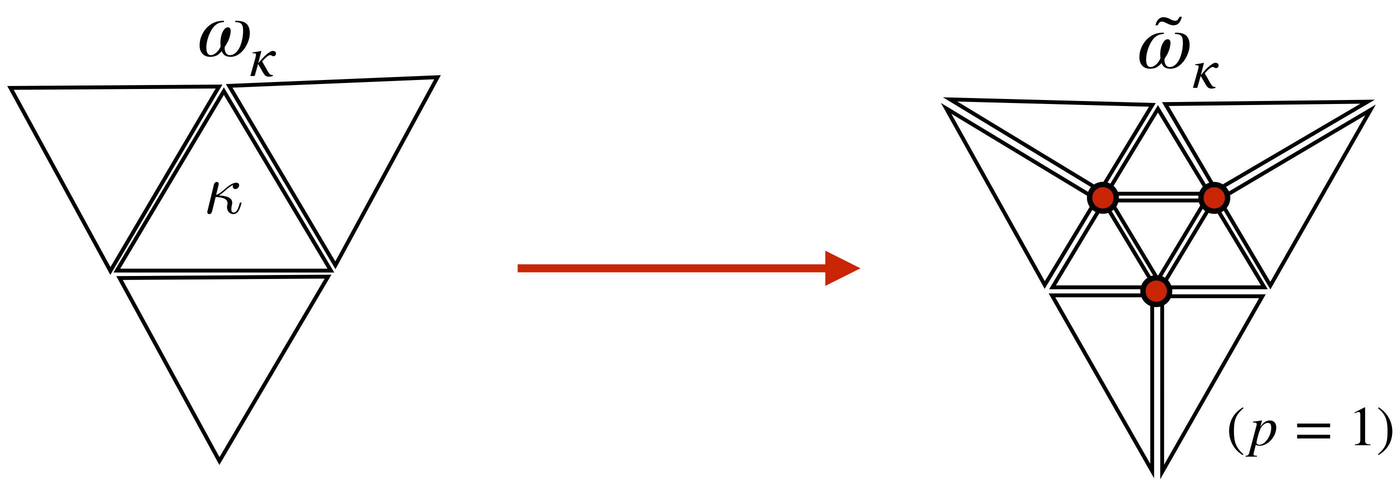

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3. Perform one SSI step in $\mathbb{V}(\tilde{\omega}_\kappa; u_N^n)$ in order to obtain approximation $\tilde{u}_{N,\kappa}^n$

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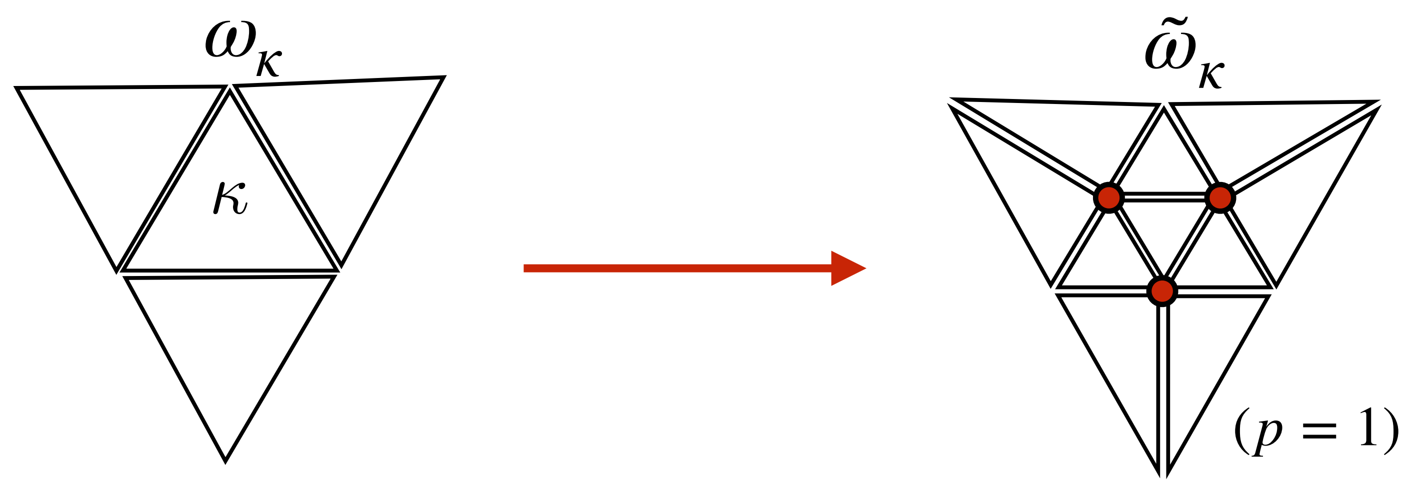

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4. Local error decay (based on local computations):

$$-\Delta \mathrm{E}_N^n(\kappa) := \mathrm{E}(\tilde{u}_{N,\kappa}^n) - \mathrm{E}(u_N^n) \leq 0$$

How to refine the mesh ?

`Mark` a subset $\mathscr{K} \subset \mathscr{T}_N$ of minimal cardinality that satisfies the Dörfler marking criterion:

$$\sum_{\kappa \in \mathscr{K}} \Delta \mathsf{E}_N^n(\kappa) \geq \theta \sum_{\kappa \in \mathscr{T}_N} \Delta \mathsf{E}_N^n(\kappa)$$

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After mesh-refinement: Continue with SSI iterations.

When to refine the mesh?

Two indicators **($n \geq 1$):**

1. $\mathrm{inc}_N^n := \mathsf{E}(u_N^{n-1}) - \mathsf{E}(u_N^n)$
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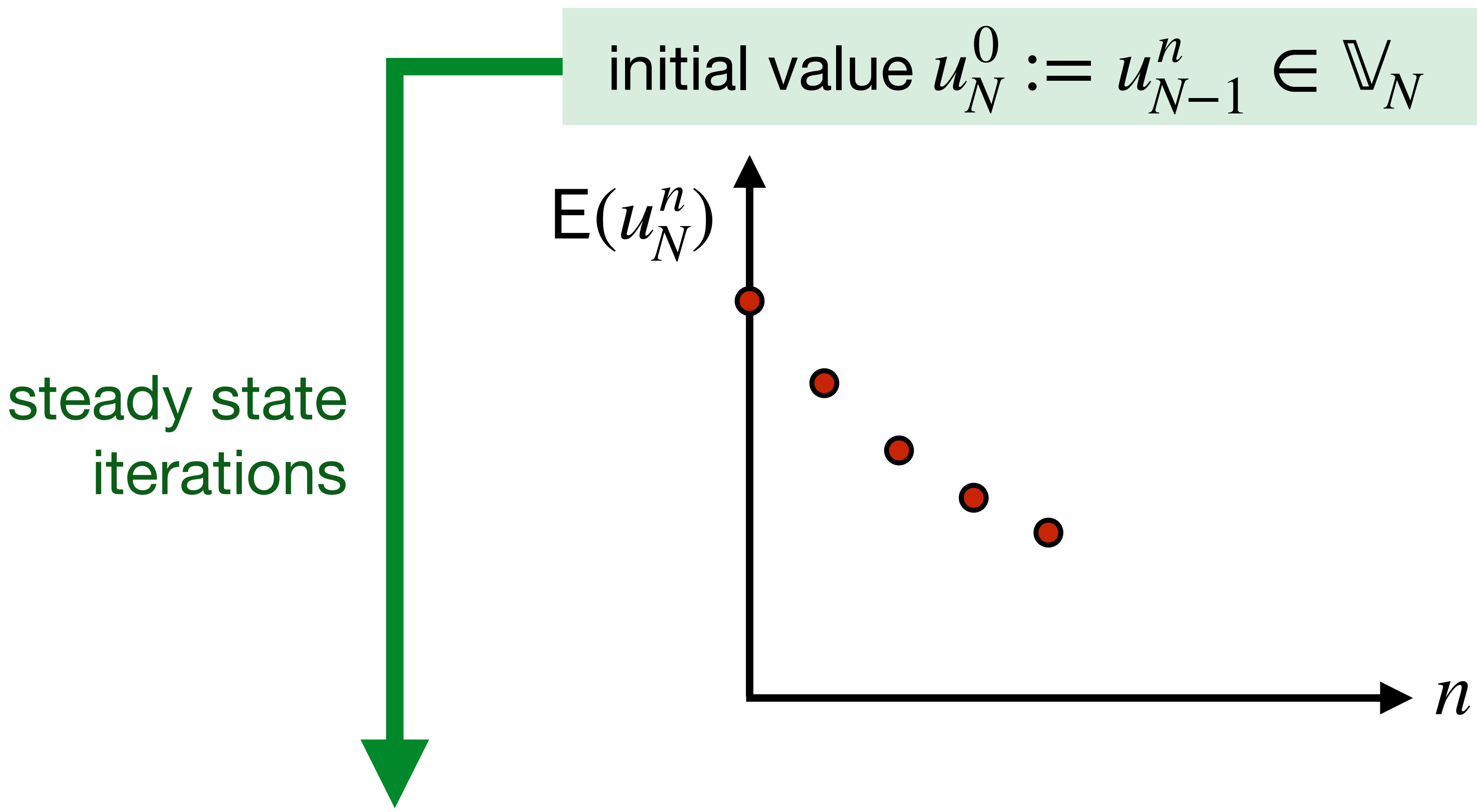

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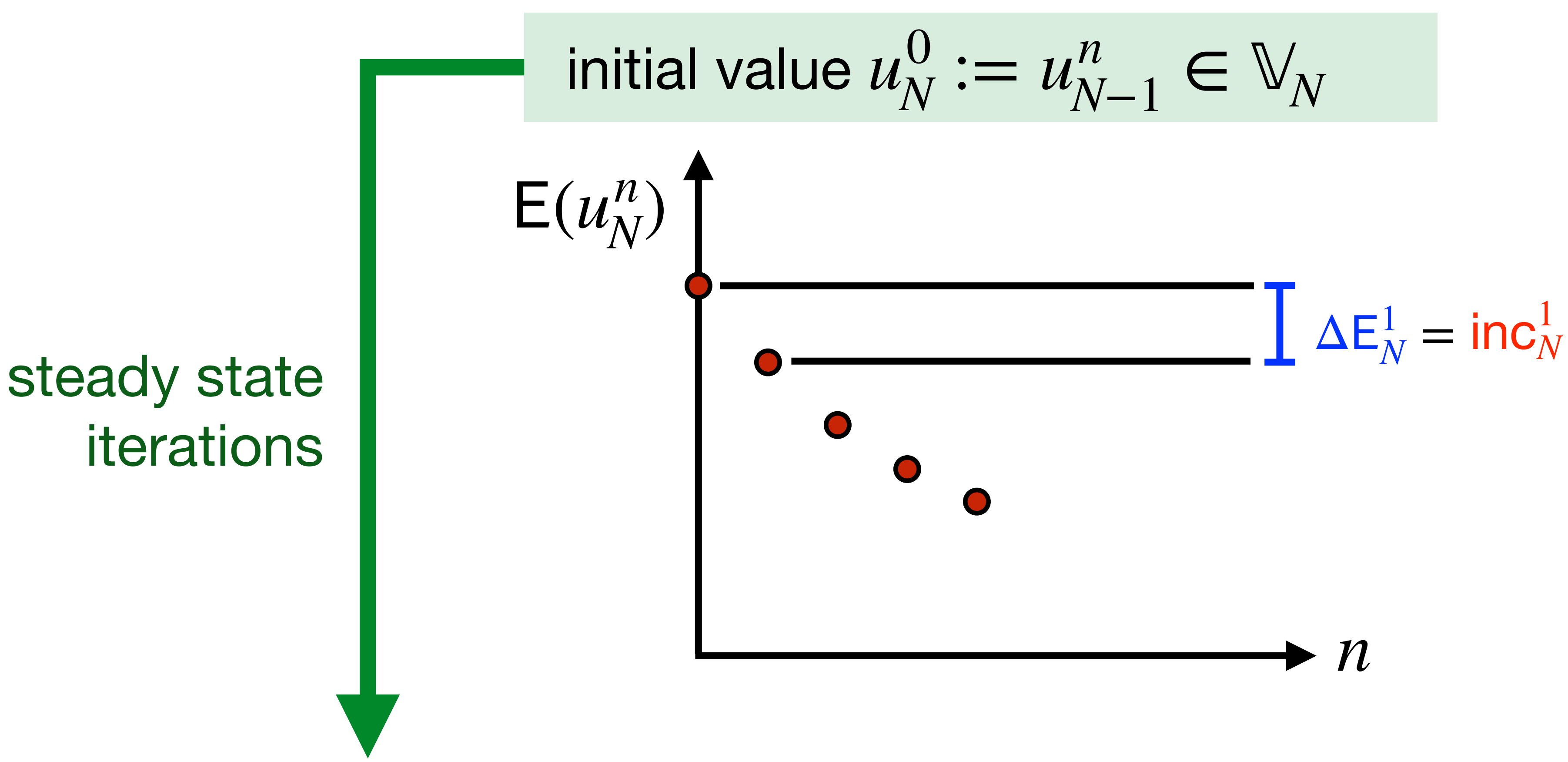

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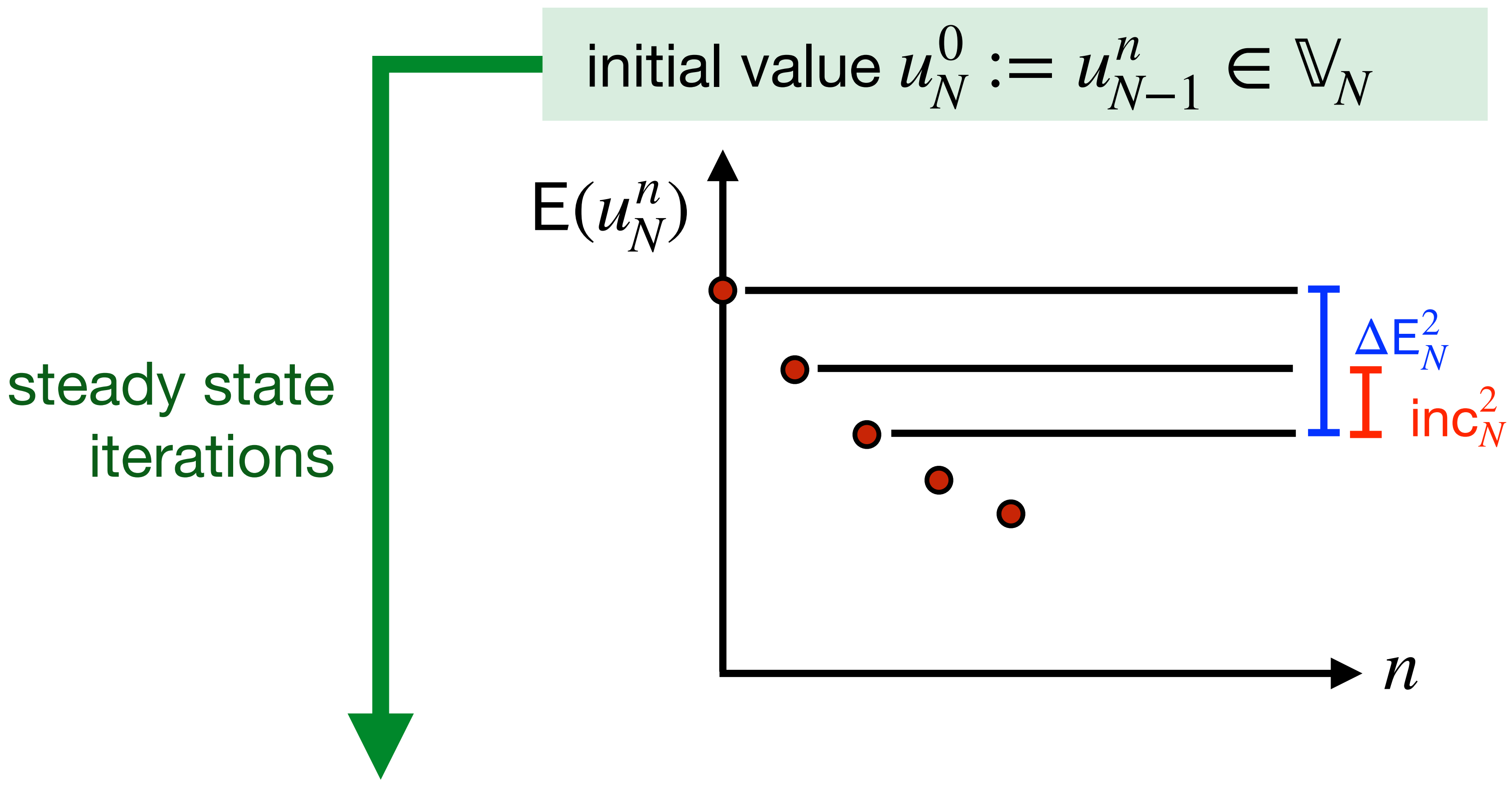

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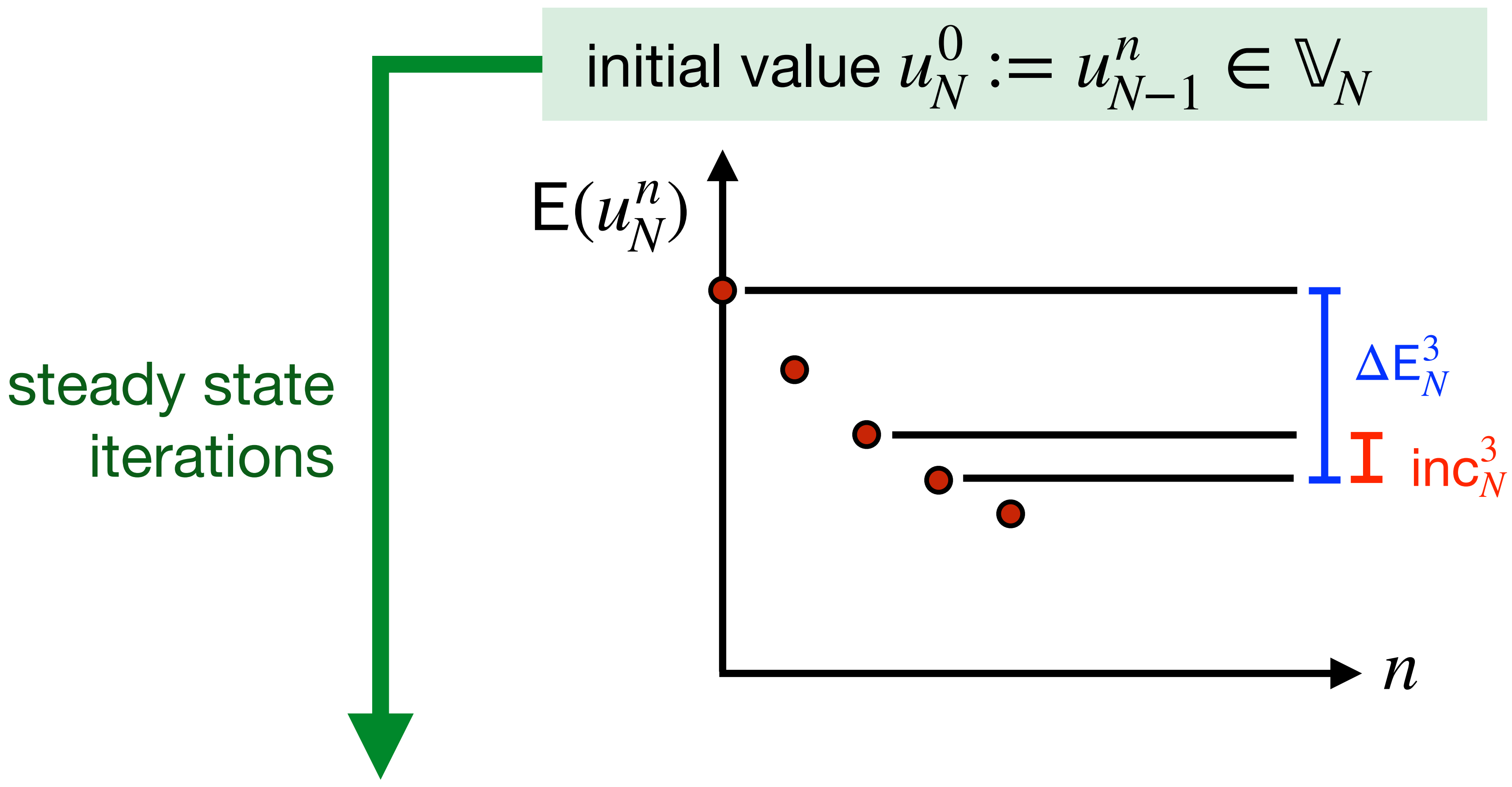

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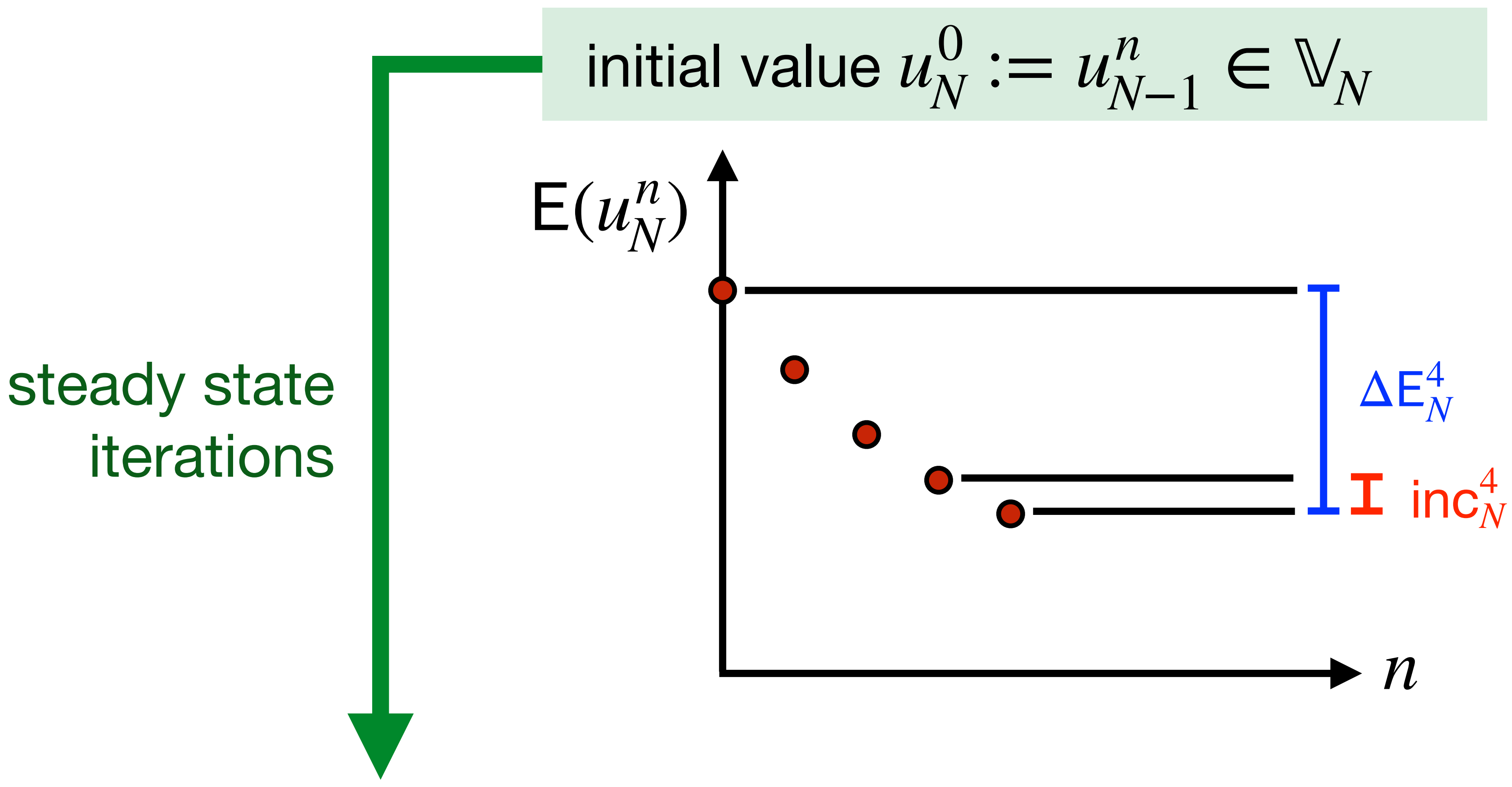

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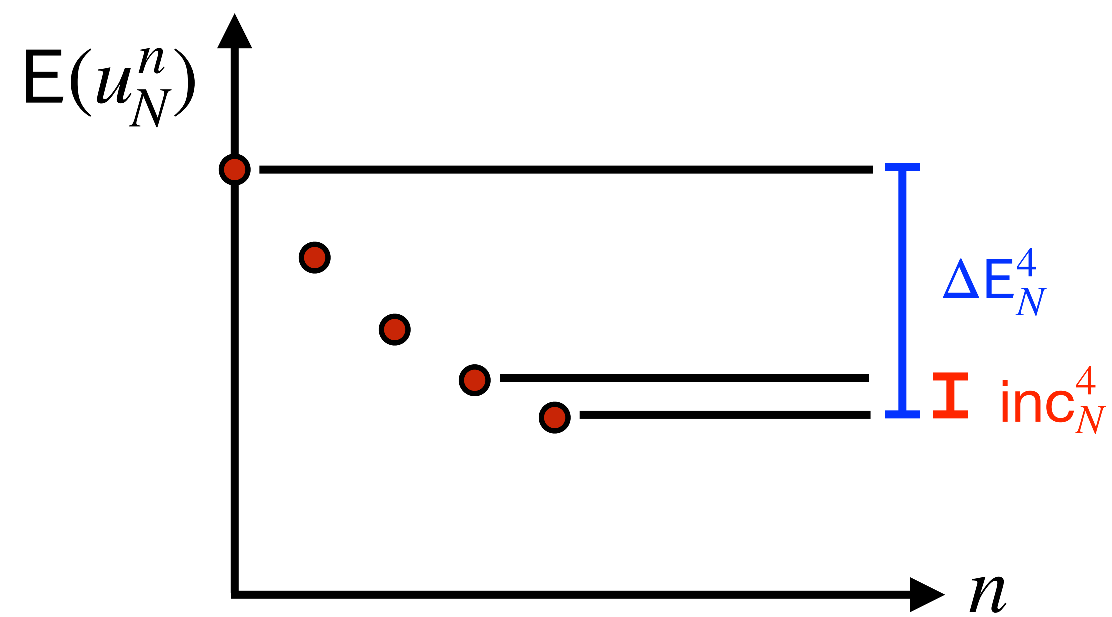
steady state iterations



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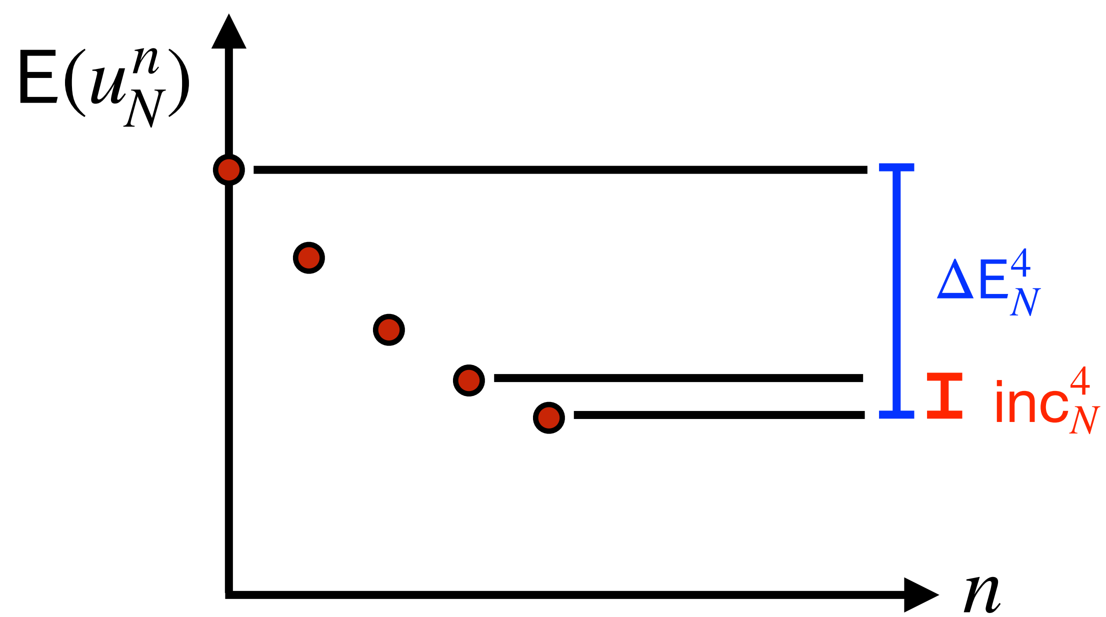

refine mesh

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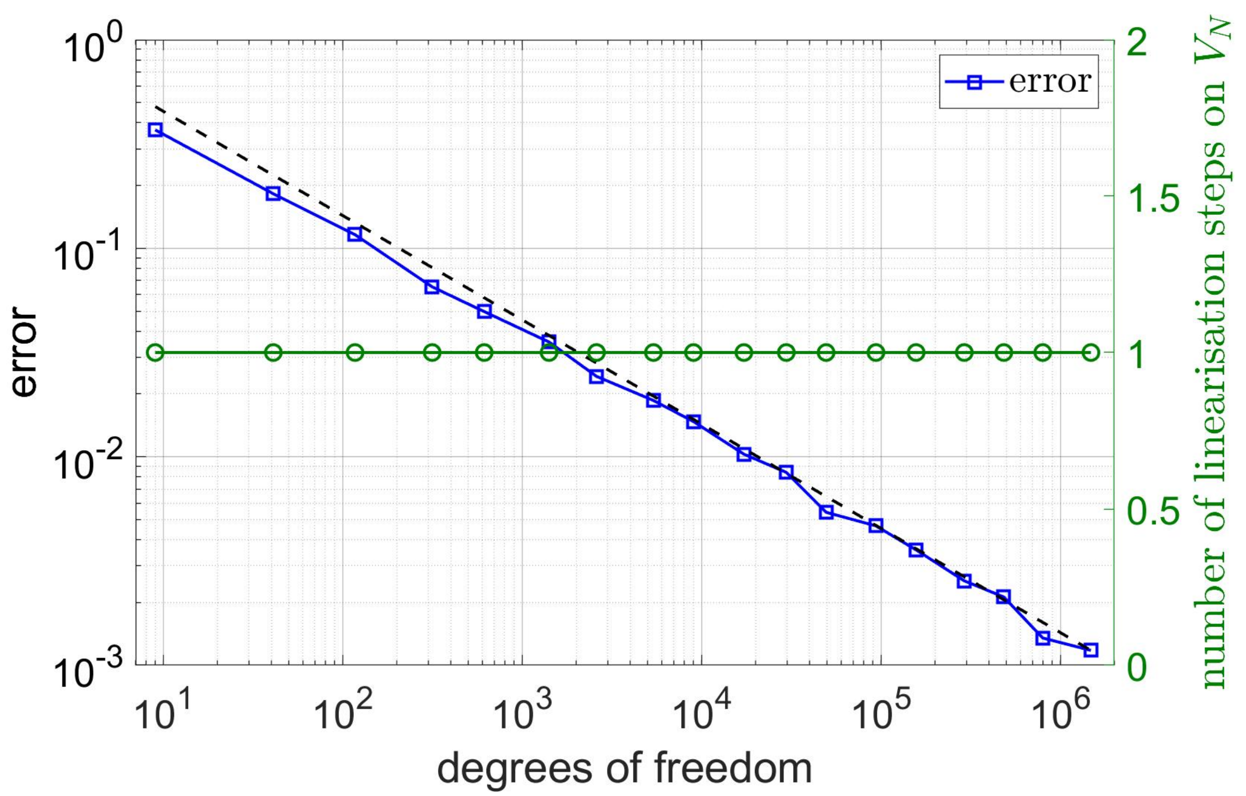
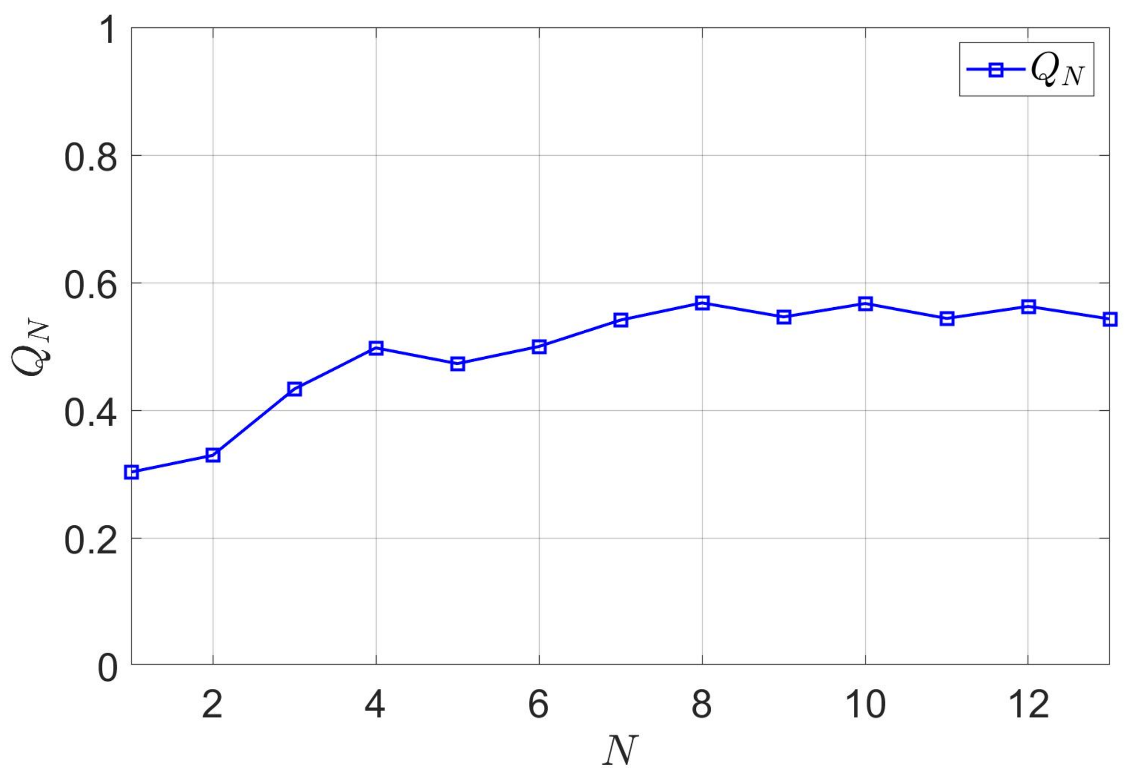
Sanity check

Sine-Gordon model:

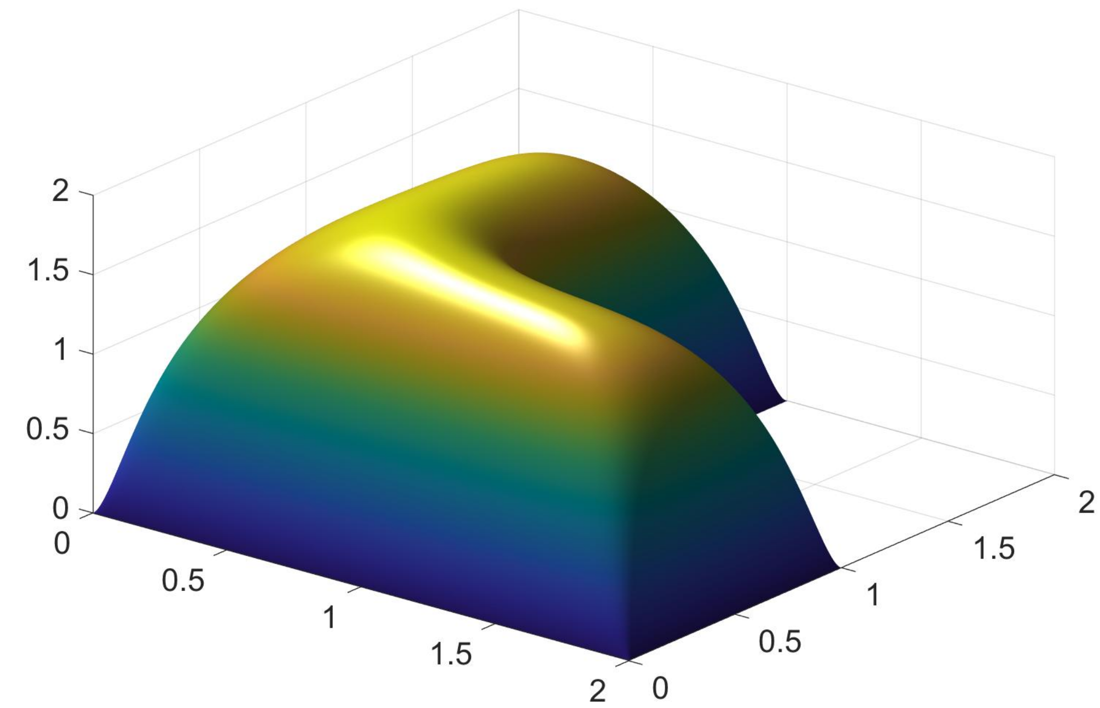
$$\begin{aligned} -\Delta u + \sin(u) + u &= g \qquad \text{in } \Omega \\ u &= 0 \qquad \text{on } \partial\Omega \end{aligned}$$

$(\Delta t = 1/2)$





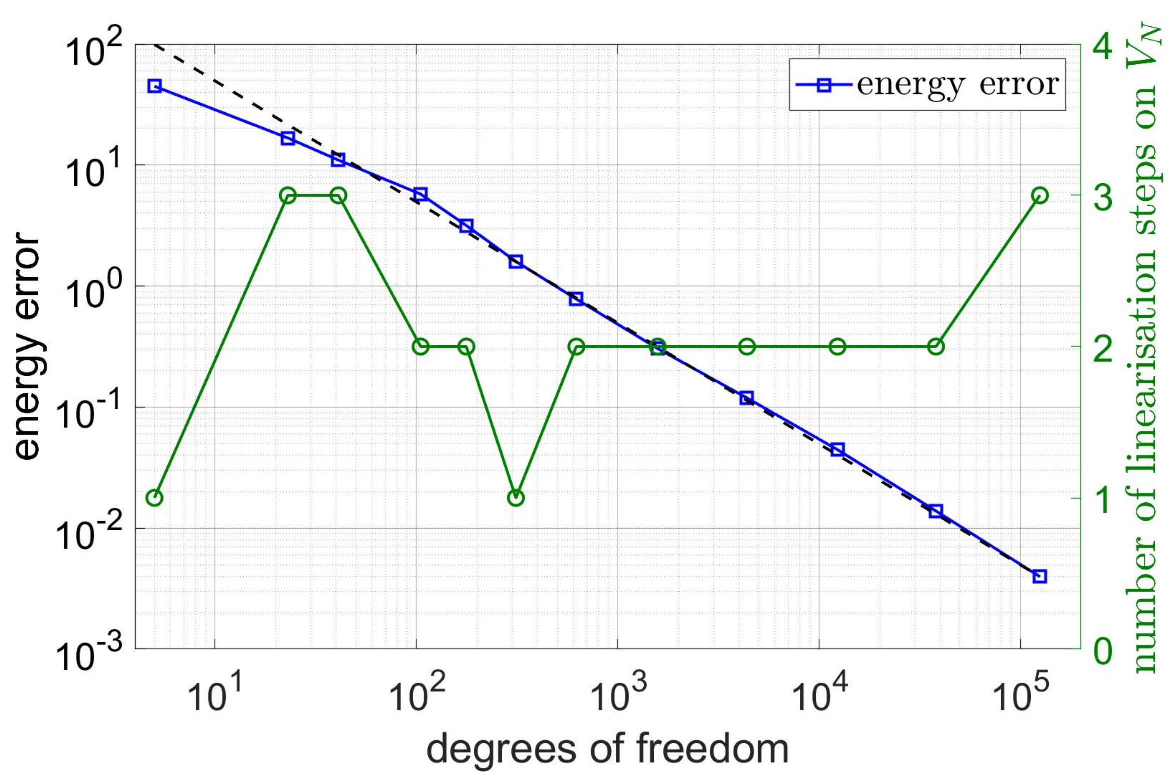
L–shaped domain

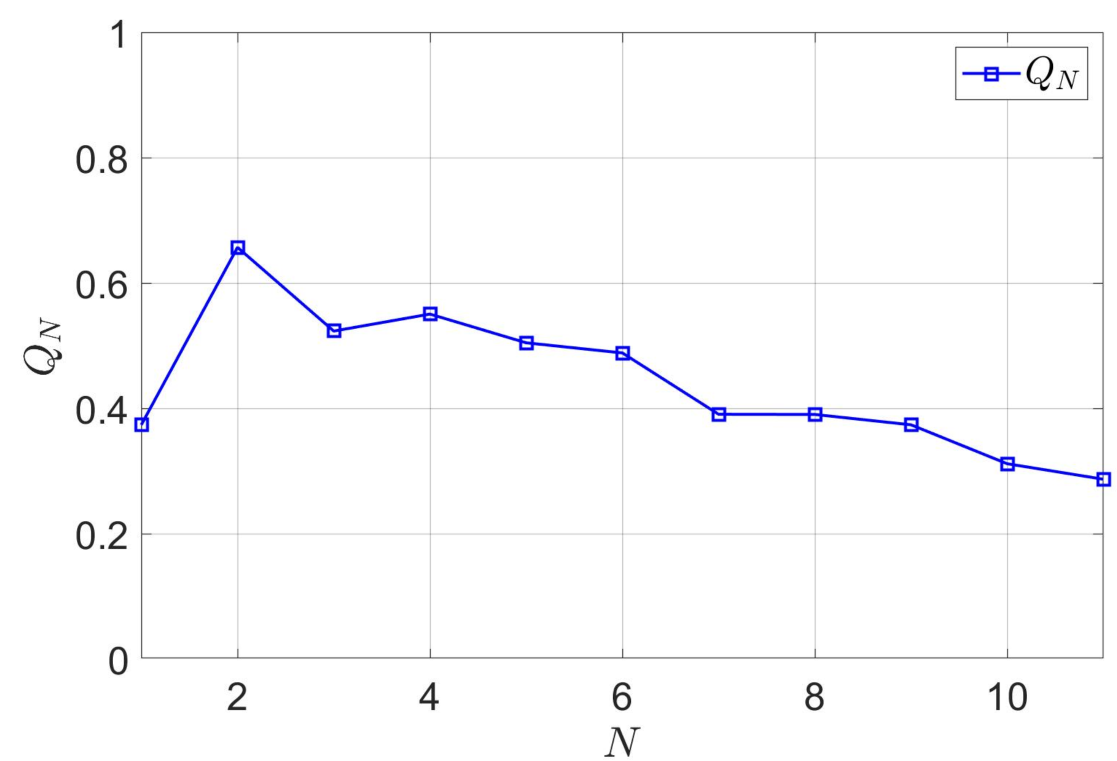


Singular perturbation model:

$$
\begin{aligned}
-\epsilon \Delta u &= e^{-u^2} && \text{in } \Omega \\
u &= 0 && \text{on } \partial\Omega
\end{aligned}
$$

$(\Delta t = \epsilon = 10^{-2})$

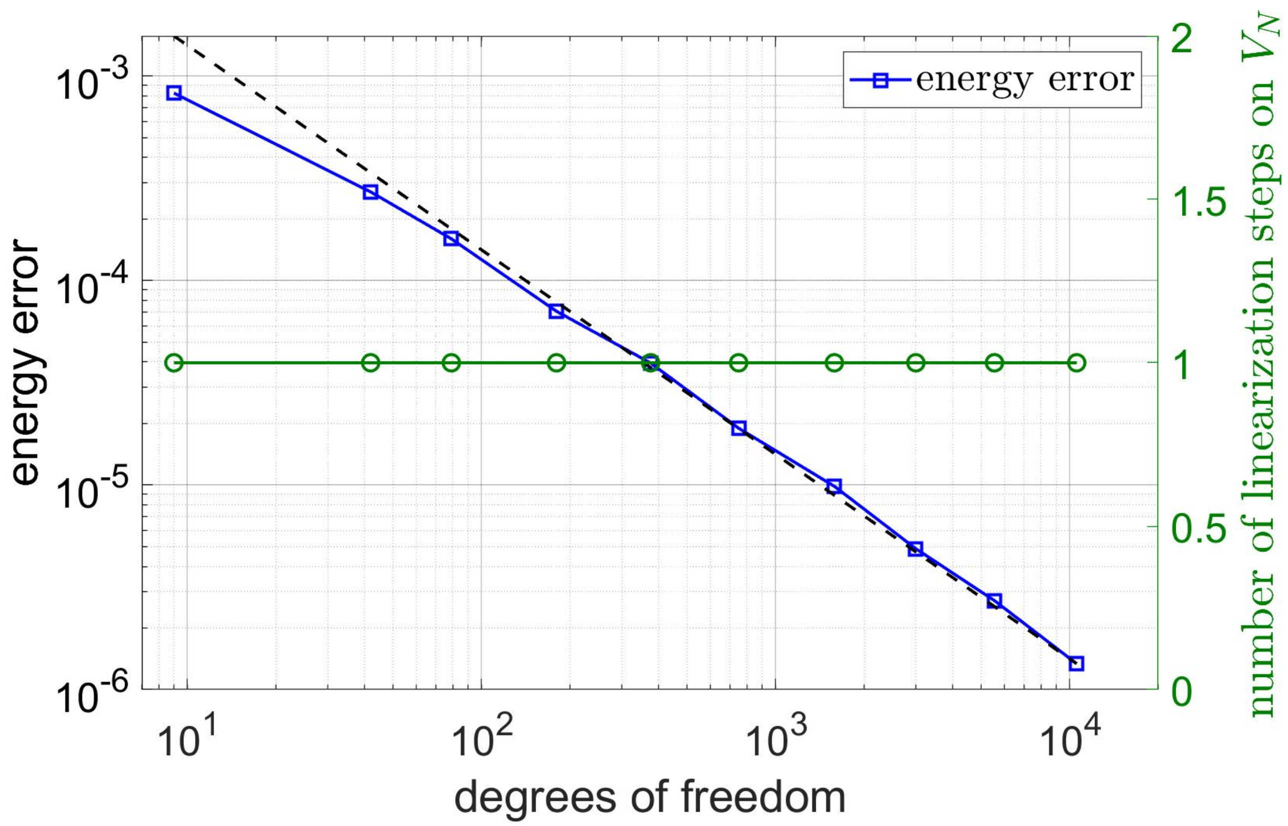


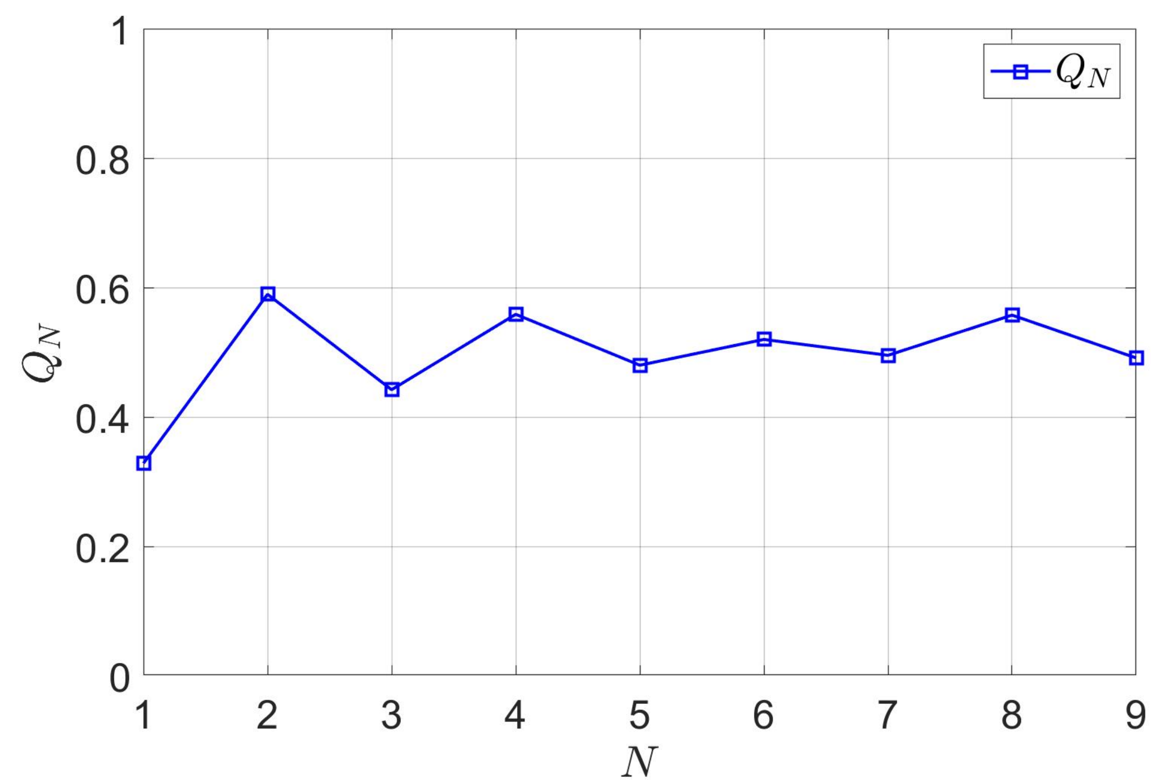


Arrhenius reaction

$$
\begin{aligned}
-\Delta u &= (1 - |u|)\exp(-1/|u|) && \text{in } \Omega \\
u &= 2 && \text{on } \partial\Omega
\end{aligned}
$$

$(\Delta t = 1)$





Current state

Define the discretization indicator on $\mathbb{V}_N$:

$$\mathscr{E}_N(\mathfrak{u}_N^n) := \|\mathsf{E}'(u_N^n)\|_{H^{-1}(\Omega)} - \|\mathsf{E}'(u_N^n)\|_{\mathbb{V}_N^\star}$$

THEOREM (ADAPTIVITY)

- $\{\mathbb{V}_N\}_N$ satisfies

$$\boxed{\mathscr{E}_{N+1}(\mathfrak{u}_N^n) \leq q\mathscr{E}_N(\mathfrak{u}_N^n), \qquad 0 < q < 1}$$

- $\{\mathfrak{u}_N\}_N$ bounded in $H_0^1(\Omega)$
- f continuous

Then there is a subsequence $\{u_{N'}\}_{N'}$ such that

$u_{N'} \to u_\infty$ strongly to a weak solution in $H_0^1(\Omega)$

Some papers

- [Amrein, Heid & TW]
  A numerical energy minimisation approach for semilinear diffusion-reaction boundary value problems based on steady state iterations
  arXiv Report 2202.07398 (2022)

- [Heid, Stamm & TW]
  Gradient Flow Finite Element Discretizations with Energy-Based Adaptivity for the Gross-Pitaevskii Equation
  J. Comp. Phys. (2021)

- [Heid, Praetorius & TW]
  Energy contraction and optimal convergence of adaptive iterative linearized finite element methods
  Comput. Meth. Appl. Math. (2021)